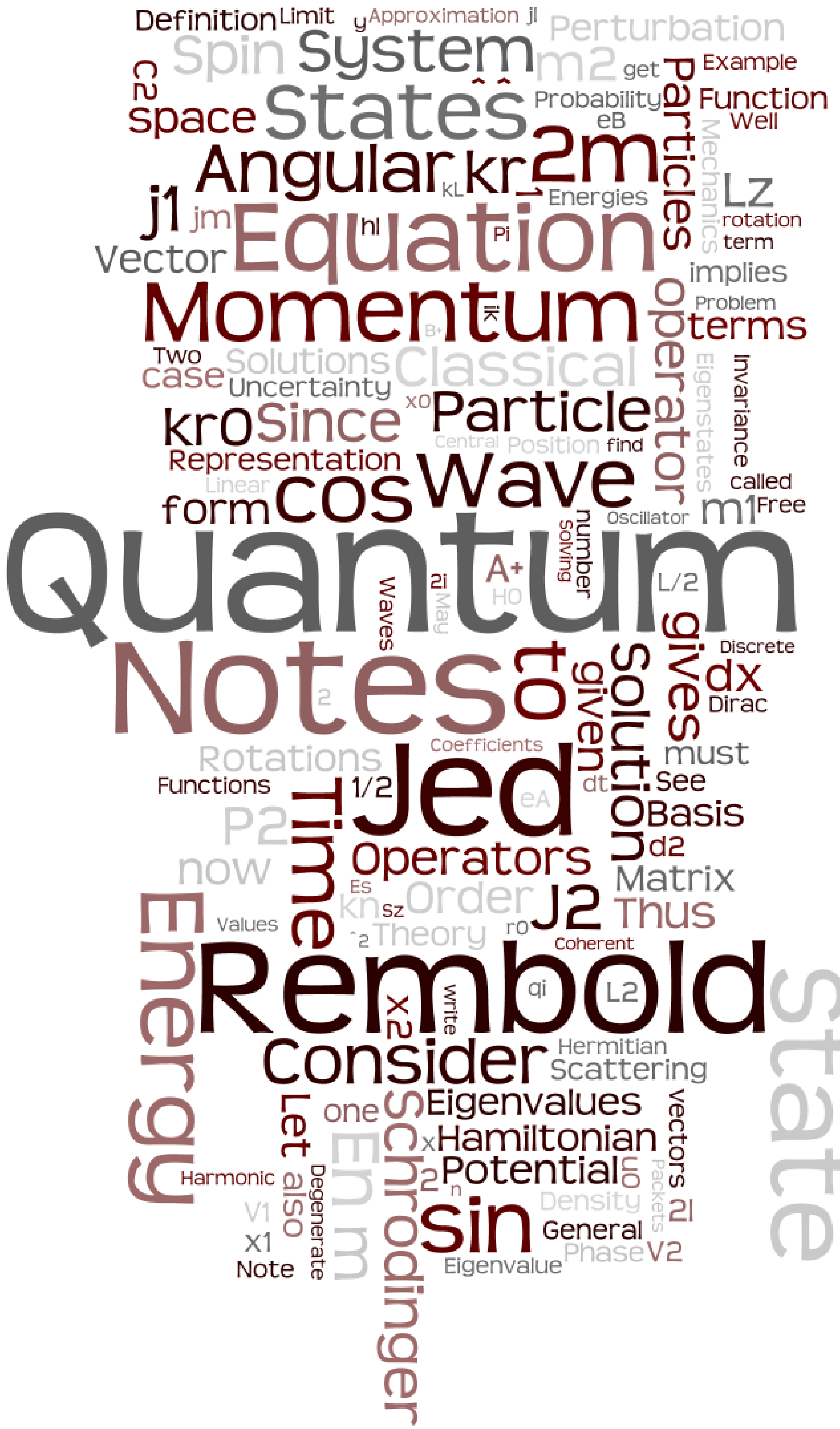
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Contents

Chapter 1

Preliminaries

Mathematical Preliminaries
A fundamental principle of QM is the superposition principle of dynamic states: The possible dynamical states of a given quantized system may be superposed linearly and therefore may be represented by vectors of a certain linear space (to be defined). In this space, dynamic variable's are associated with linear operators.

1.1 Vector Spaces, Deal Spaces, and Scalar Products

1.1.1 Vector Spaces and "kets"

Definition 1: A vector space, or linear space:

$$V = \{|1\rangle, |2\rangle, \ldots, |a\rangle, |b\rangle, \ldots\}$$

has the following properties:

1. Is a group under addition
   - closure ($|a\rangle + |b\rangle \in V$)
   - exists identity: ($|a\rangle + |0\rangle = |a\rangle \quad \forall |a\rangle$)
   - $\exists$ inverse: ($|a\rangle + |-a\rangle = |0\rangle$)
   - associative: ($|a\rangle + (|b\rangle + |c\rangle) = (|a\rangle + |b\rangle) + |c\rangle$)
2. Commutative under addition
3. We can also define a multiplication of elements of V with numbers "$\alpha, \beta, \gamma, \ldots$" so that $\forall |a\rangle, |b\rangle \in V$:
   - $\alpha |a\rangle \in V$
   - $\alpha(\beta |a\rangle) = (\alpha\beta) |a\rangle$
   - $(\alpha + \beta) |a\rangle = \alpha |a\rangle + \beta |a\rangle$
   - $\alpha(|a\rangle + |b\rangle) = \alpha |a\rangle + \alpha |b\rangle$
   - $1 \cdot |a\rangle = |a\rangle \quad \forall |a\rangle$

Remark 1: $|a\rangle, |b\rangle, \ldots$ are vectors
$\alpha, \beta, \ldots$ are scalars that define a field over which the vector space is defined
If $\alpha, \beta, \ldots \in \mathbb{R}$, then we have a real vector space
If $\alpha, \beta, \ldots \in \mathbb{C}$, then we have a complex vector space

Remark 2: $|a\rangle$ is a "ket" in Dirac notation
It is an abstraction of the more familiar column vector

Definition 2: The vectors $|i\rangle$ for $i = 1 \ldots n$ are linearly independent if:

$$\sum_{i=1}^{n} a_i |i\rangle = 0 \quad \Rightarrow \quad a_i = 0 \quad \forall i$$

Definition 3: Let n be the number of linearly independent vectors in V. Then n = the dimension of the vector space, denoted V^n, and the linearly independent vectors form a basis.

1.1.2 Dual Spaces and "Bras"

Definition 1: The adjoint of a vector $|a\rangle$ in the vector space defines a "bra" $\langle a|$, which is a member of the dual space. The dual space is antilinear.

$$\text{If } |c\rangle = \alpha = |a\rangle + \beta |b\rangle, \text{ then } \langle c| = \alpha^* \langle a| + \beta^* \langle b|$$

Remark 1: "bras" are abstractions of row vectors

Remark 2: The adjoint operator takes the "ket" from the vector space to the corresponding "bra" in dual-space and vice versa

$$|a\rangle^\dagger = \langle a| \text{ and } \langle a|^\dagger = |a\rangle$$

Remark 3: If there $\exists$ any type of scalar multipliers, they are replaced by complex conjugates. Adjoints of complicated expressions are written in reverse order.

$$\text{Ex: } [\alpha |a\rangle \langle b| \gamma\delta |c\rangle]^\dagger = \langle c| \delta^*\gamma^* |b\rangle \langle a| \alpha^*$$

1.1.3 Scalar Products

Definition 1: For any vectors $|a\rangle, |b\rangle \in V^n$, we denote $\langle a|b\rangle$ to be the inner product, or scalar product. $\langle a|b\rangle \in \mathbb{C}$, and has the properties:

- $\overline{\langle a|b\rangle} = \langle b|a\rangle^*$

- $\langle a|a\rangle \geq 0, = 0 \Leftrightarrow |a\rangle = |0\rangle$
- Linear in ket and antilinear in bra

Remark 1: The properties of the scalar product imply the Schwartz inequality:

$$|\langle a|b\rangle|^2 < \langle a|a\rangle \langle b|b\rangle$$

Postulate: The space of ket vectors (and the dual space of bra vectors) form a Hilbert Space. It is complete and separable. Here, complete refers to the existence of a basis in which any vector can be expressed as a superposition of the basis vectors.

Definition 2: $|a\rangle, |b\rangle \in V^n$ are orthogonal iff $\langle a|b\rangle = 0$

Definition 3: $\sqrt{\langle a|a\rangle} = |a|$ is the norm of the vector $|a\rangle$

Definition 4: The set of basis vectors, $|1\rangle, \ldots, |n\rangle$, that have $\langle i|j\rangle = \delta_{ij}, \forall i, j$, is an orthonormal basis.

Theorem (Gram-Schmidt): An orthonormal basis may be formed from a linear combination of basis vectors.

Remark 2: We will write vectors as expansions of orthonormal basis so that

$$|a\rangle = \sum_{i=1}^{n} a_i |i\rangle \quad \text{and} \quad |b\rangle = \sum_{j=1}^{n} b_j |j\rangle$$

$$\Rightarrow \langle a|b\rangle = \sum_{i,j=1}^{n} a_i^* b_j \underbrace{\langle i|j\rangle}_{\delta_{ij}} = \sum_{i}^{n} a_i^* b_i$$

Definition 5: A subspace is a subset of the vector space V that is also a vector space.

Definition 6: ξ_1 and ξ_2 are orthogonal subspaces if every vector in ξ_1 is orthogonal to every vector in ξ_2.

Definition 7: The vectors orthogonal to ξ_1 form a subspace ξ_1^x which is the complementary subspace to ξ_1.

Theorem: Any vector $|a\rangle \in V$ may be written

$$|a\rangle = |a_1\rangle + |a_1^x\rangle$$

where $|a_1\rangle \in \xi_1$ and $|a_1^x\rangle \in \xi_1^x$ and $\xi_1, \xi_1^x \subset V$.

Definition 8: $|a_1\rangle$ is the projection of $|a\rangle$ on the subspace of ξ_1.

1.1.4 Tensor Products of 2 Vector Spaces

To represent a system described by products of wave functions in the bra-ket notation, we use Tensor Products.

Example: Let $\left|a^1\right\rangle$ represent the state of particle 1. Let $\left|a^2\right\rangle$ represent the state of particle 2. Then the 2 particle system is represented by the tensor product:

$$\left|a^1\right\rangle \otimes \left|a^2\right\rangle \equiv \left|a^1\right\rangle \left|a^2\right\rangle \equiv \left|a^1 a^2\right\rangle$$

Remark 1: An operator $\hat{\Omega}^1(\hat{\Omega}^2)$ only operates on $\left|a^1\right\rangle$ ($\left|a^2\right\rangle$), so that, if:

$$\hat{\Omega}^1 \left|a^1\right\rangle = \left|b^1\right\rangle$$

$$\hat{\Omega}^2 \left|a^2\right\rangle = \left|b^2\right\rangle$$

Then

$$\hat{\Omega}^1 \left|a^1 a^2\right\rangle = \left|b^1 a^2\right\rangle$$

$$\hat{\Omega}^2 \left|a^1 a^2\right\rangle = \left|a^1 b^2\right\rangle$$

Furthermore, every operator $\hat{\Omega}^1$ commutes with $\hat{\Omega}^2$.

$$\text{Ex: } \hat{\Omega}^1 \hat{\Omega}^2 \left|a^1 a^2\right\rangle = \hat{\Omega}^2 \hat{\Omega}^1 \left|a^1 a^2\right\rangle$$

1.2 Linear Operators

1.2.1 Products of Operators

Consider an operator $\hat{\Omega}$ that transforms one vector $|a\rangle$ into another $|a'\rangle$:

$$\hat{\Omega} |a\rangle = \left|a'\right\rangle$$

Definition 1: a linear operator obeys the following:

- $\hat{\Omega}\alpha |a\rangle = \alpha \hat{\Omega} |a\rangle$

- $\hat{\Omega}\left[\alpha\left|a\right\rangle + \beta\left|b\right\rangle\right] = \alpha\hat{\Omega}\left|a\right\rangle + \beta\hat{\Omega}\left|b\right\rangle$
- $\left\langle a\right| \alpha\hat{\Omega} = \left\langle a\right| \hat{\Omega}\alpha$
- $\left[\left\langle a\right| \alpha + \left\langle b\right| \beta\right] \hat{\Omega} = \alpha\left\langle a\right| \hat{\Omega} + \beta\left\langle b\right| \hat{\Omega}$

Remark 1: the products of 2 operators are just 2 operations carried out in sequence:

$$(\hat{\Omega}\hat{\Lambda})\left|a\right\rangle = \hat{\Omega}(\hat{\Lambda}\left|a\right\rangle)$$

In general, the product does *not* commute. Define the commutator:

$$\hat{\Omega}\hat{\Lambda} - \hat{\Lambda}\hat{\Omega} \equiv [\hat{\Omega}, \hat{\Lambda}]$$

Definition 2: The inverse of a operator $\hat{\Omega}$ is denoted $\hat{\Omega}^{-1}$, and $\hat{\Omega}^{-1}\hat{\Omega} = \hat{\Omega}\hat{\Omega}^{-1} = I =$ identity operator.

Remark 2: The inverse of a product of operators is:

$$(\hat{\Omega}\hat{\Lambda})^{-1} = \hat{\Lambda}^{-1}\hat{\Omega}^{-1}$$

1.2.2 Matrix Representation of Operators

Consider a vector $\left|a\right\rangle$ and operator $\hat{\Omega}$ such that

$$\hat{\Omega}\left|a\right\rangle = \left|b\right\rangle$$

The matrix form of $\hat{\Omega}$ has elements $\Omega_{ij} = \left\langle i\right| \hat{\Omega}\left|j\right\rangle$, so that for:

$$\left|a\right\rangle = \sum_i a_i \left|i\right\rangle$$

$$\left|b\right\rangle = \sum_j b_j \left|j\right\rangle$$

Then

$$\begin{aligned} b_j = \langle j|b\rangle &= \left\langle j\right| \hat{\Omega}\left|a\right\rangle \\ &= \left\langle j\right| \hat{\Omega} \sum_i a_i \left|i\right\rangle \\ &= \sum_i a_i \left\langle j\right| \hat{\Omega}\left|i\right\rangle \\ &= \sum_i \Omega_{ij} a_i \end{aligned}$$

And, in matrix and vector representation:

$$\begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} \langle 1|\hat{\Omega}|1\rangle & \langle 1|\hat{\Omega}|2\rangle & \cdots & \langle 1|\hat{\Omega}|n\rangle \\ \langle 2|\hat{\Omega}|1\rangle & & & \vdots \\ \vdots & & & \vdots \\ \langle n|\hat{\Omega}|1\rangle & \cdots & \cdots & \langle n|\hat{\Omega}|n\rangle \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}$$

Examples:

- The identity operator $\hat{I}$

$$I_{ij} = \langle i|\hat{I}|j\rangle = \langle i|j\rangle = \delta_{ij}$$

- The Projection operator $\hat{P}$: Consider a set of basis vectors $|1\rangle, |2\rangle, \ldots, |n\rangle$. The projection of any vector onto the i^{th} basis vector is obtained by:

$$\hat{P}_j|a\rangle = |i\rangle\langle i|a\rangle = \langle i|a\rangle|i\rangle$$

So:

$$\hat{P}_i = |i\rangle\langle i| \equiv \text{ projector}$$

Remark 1: Because the basis vectors form a complete set (in Hilbert Space), we have

$$\begin{aligned} |a\rangle = \sum_i a_i|i\rangle &= \sum_i \underbrace{\langle i|a\rangle}_{a_i}|i\rangle \\ &= \sum_i |i\rangle\langle i|a\rangle \\ &= (\sum_i \underbrace{|i\rangle\langle i|}_{\hat{P}_i})|a\rangle \end{aligned}$$

Since this is true for all $|a\rangle$:

$$\boxed{\hat{I} = \sum_i |i\rangle\langle i|} \Rightarrow \text{ a completeness relation}$$

Remark 2: Projectors have the property that:

$$\hat{P}^2 = \hat{P}$$

$$P_iP_j = |i\rangle\langle i|j\rangle\langle j| = \delta_{ji}|i\rangle\langle j| = \delta_{ij}\hat{P}_i$$

In fact, any Hermitian operator (defined below) that satisfies the above is a projector.

Remark 3: The projector is the first example of an operator expressed as an outer product of vectors: $|i\rangle\langle i|$. The jk element of this operator in matrix form is:

$$\langle j|i\rangle\langle i|k\rangle = \delta_{ij}\delta_{ik}$$

In matrix representation it is:

$$|i\rangle\langle i| = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1(i^{th}) \\ \vdots \\ 0 \end{bmatrix} \begin{bmatrix} 0,0,0,\cdots,1(i^{th}),\cdots,0 \end{bmatrix} = \begin{bmatrix} 0 & \cdots & \cdots & i^{th} & \cdots & 0 \\ \vdots & & & \vdots & & \vdots \\ i^{th} & \cdots & \cdots & 1 & \cdots & \vdots \\ \vdots & & & \vdots & & \vdots \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 \end{bmatrix}$$

This concept can be generalized to other operators.

1.2.3 Hermitian and Unitary Operators

Definition 1: Consider an operator $\hat{\Omega}$.

- $\hat{\Omega} = \hat{\Omega}^\dagger \Rightarrow$ Hermitian
- $\hat{\Omega} = -\hat{\Omega}^\dagger \Rightarrow$ Antihermitian

Remark 1: Any operator $\hat{\Omega}$ may be decomposed into it's Hermitian and Antihermitian parts:

$$\hat{\Omega} = \hat{\Omega}_H + \hat{\Omega}_A$$

Where

$$\hat{\Omega}_H = \frac{1}{2}(\hat{\Omega} + \hat{\Omega}^\dagger)$$

$$\hat{\Omega}_A = \frac{1}{2}(\hat{\Omega} - \hat{\Omega}^\dagger)$$

Remark 2: A hermitian operator is positive-definite:

$$\langle a|\hat{\Omega}|a\rangle \geq 0 \quad \forall\, |a\rangle$$

Definition 2: An operator $\hat{U}$ is unitary if:

$$\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{I} \qquad (\hat{U}^\dagger = \hat{U}^{-1})$$

Remark 3: If $\hat{U}_1$ and $\hat{U}_2$ are unitary, then so is the product of $\hat{U}_1\hat{U}_2$.

Theorem: The inner product of vectors $|a\rangle, |b\rangle$ is invariant under a unitary transformation.

$$\hat{U}|a\rangle = |a'\rangle$$
$$\hat{U}|b\rangle = |b'\rangle$$

Then:

$$\langle a'|b'\rangle = \langle a|\hat{U}^\dagger\hat{U}|b\rangle = \langle a|b\rangle$$

1.2.4 Transformations (Unitary)

Consider a transformation $\hat{T}$.

Definition 1: An active transformation transforms all vectors in a subspace:

$$|a\rangle \to |a'\rangle = \hat{T}|a\rangle$$

Definition 2: A passive transformation transforms all operators on that space, leaving the vectors unchanged.

$$\hat{\Omega} \to \hat{\Omega}' = \hat{T}\hat{\Omega}\hat{T}^{-1}$$

Remark 1: In general, $\hat{T}$ does not conseve Hermitian conjugation. For this, we require that if:

$$\hat{\Omega}' = \hat{T}\hat{\Omega}\hat{T}^{-1} \quad \text{and} \quad (\hat{\Omega}^\dagger)' = \hat{T}\hat{\Omega}^\dagger\hat{T}^{-1}$$

Then:

$$(\hat{\Omega}')^\dagger = (\hat{T}\hat{\Omega}\hat{T}^{-1})^\dagger = (\hat{T}^{-1})^\dagger\hat{\Omega}^\dagger\hat{T}^\dagger \text{ must} = (\hat{T}\hat{\Omega}^\dagger\hat{T}^{-1})$$
$$\Rightarrow \hat{T}^\dagger = \hat{T}^{-1} \quad \text{or} \quad \hat{T}\hat{T}^{-1} = \hat{T}^{-1}\hat{T} = \hat{I}$$
$$\Rightarrow \hat{T} \text{ is unitary}$$

Remark 2: If we have unitary transformations, active and passive transformations are equivalent:

$$\langle a|\hat{\Omega}|b\rangle \to \langle a'|\hat{\Omega}|b'\rangle = \langle a|\hat{U}^\dagger\hat{\Omega}\hat{U}|b\rangle \quad \text{where } |a'\rangle = \hat{U}|a\rangle$$

Remark 3: In addition of Hermitian conjugation, unitary transformations conserve:

- Trace
- Determinant
- Algebraic equations between matrices and vectors

Remark 4: Any Hermitian matrix may be diagonalized by a unitary transformation.

$$\hat{U}\hat{\Omega}\hat{U}^\dagger = \hat{\Omega}_D \quad \text{where } \hat{\Omega}_D \text{ is diagonal.}$$

The diagonal elements are called eigenvalues of $\hat{\Omega}$. They are real, and they are solutions of the secular or characteristic equation.

$$\det(\hat{\Omega} - \lambda\hat{I}) = 0 \qquad \text{(See below)}$$

Remark 5: A single unitary matrix may diagonalize 2 (or more) Hermitian matrices $\hat{\Omega}, \hat{\Lambda}$ if: $[\hat{\Omega}, \hat{\Lambda}] = 0$.

Remark 6: If the vector space is real, then

$$\hat{U}^{-1} = \hat{U}^\dagger \rightarrow \hat{U}^{-1} = \hat{U}^\top \Rightarrow \text{orthogonal transformation}$$

which is a rotation.

1.2.5 The Eigenvalue Problem

Definition 1: Consider a linear operator $\hat{A}$ and $|u\rangle$. Then $\alpha \in \mathbb{C}$ is an eigenvalue of $\hat{A}$ if:

$$\hat{A}\,|u\rangle = \alpha\,|u\rangle$$

and $|u\rangle$ is an eigenvector or eigenket.

Remark 1: If $|u\rangle$ is an eigenket of $\hat{A}$, then any multiple of $|u\rangle$ is also an eigenket belonging to the eigenvalue α. These eigenkets form a subspace of the eigenvalue α. If n equals the dimension of the subspace, then:

- $n = 1 \Rightarrow$ single or non-degenerate eigenvalues
- $n > 1 \Rightarrow$ degenerate eigenvalues, where n equals the order of degeneracy

Remark 2: If $\langle v|\,\hat{A} = \alpha'\,\langle v|$, then $\langle v|$ is an eigenbra of $\hat{A}$. If $\hat{A}$ is Hermitian, then:

- The eigenvalues for bras and kets are the same
- The eigenvalues are real

- The subspace of eigenbra's is dual to the subspace of eigenkets for the same eigenvalue.

Remark 3: Eigenkets make up the columns of the unitary matrix that diagonalizes a Hermitian matrix.

Remark 4: In some cases, the unitary matrix is time dependent, and gives the time evolution of a vector in some initial state.

$$|x(t)\rangle = \hat{U}(t)\,|x(0)\rangle$$

In these cases, it is called the time-evolution operator, or propagator.

1.2.6 Functions of Operators, Generalizations to Infinite Dimensions, and More

In some cases, we will encounter functions of operators. (In fact, the propagator can be expressed as $e^{i\hat{H}t/\hbar}$ with $\hat{H}$ the Hamiltonian, see Section 2)

In order to evaluate the action of these on vectors, we expand functions in a Taylor Series.

$$f(\hat{\Omega}) = \sum_{n=0}^{\infty} a_n \hat{\Omega}^n$$

Remark 1: Expressing $f(\hat{\Omega})$ as a Taylor Series in fine so long as the series converges.

Remark 2: It is often helpful to transform into an eigenbasis. For example, if

$$f(\hat{\Omega}) = e^{\hat{\Omega}}$$

Then

$$
\begin{aligned}
e^{\hat{\Omega}} &= \sum_{n=0}^{\infty} \frac{\hat{\Omega}^n}{n!} = \sum_{n=0}^{\infty} \frac{1}{n!} \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{pmatrix}^n \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} \begin{pmatrix} \lambda_1^n & & & \\ & \lambda_2^n & & \\ & & \ddots & \\ & & & \lambda_n^n \end{pmatrix} \\
&= \begin{pmatrix} e^{\lambda_1} & & & \\ & e^{\lambda_2} & & \\ & & \ddots & \\ & & & e^{\lambda_n} \end{pmatrix}
\end{aligned}
$$

Remark 3: A power series expansion is also useful for taking derivatives with respect to a parameter. For instance, consider:

$$f(\hat{\Omega}) = e^{\alpha\hat{\Omega}}$$

Then

$$
\begin{aligned}
\frac{d}{d\alpha} e^{\alpha\hat{\Omega}} &= \frac{d}{d\alpha} \sum_{n=0}^{\infty} \frac{\alpha^n \hat{\Omega}^n}{n!} \\
&= \sum_{n=0}^{\infty} \frac{n\alpha^{n-1}\hat{\Omega}^n}{n!} \\
&= \sum_{n=1}^{\infty} \frac{\alpha^{n-1}\hat{\Omega}^n}{(n-1)!} \\
&= \sum_{n=0}^{\infty} \frac{\alpha^n \hat{\Omega}^{n+1}}{n!} \\
&= \hat{\Omega} e^{\alpha\hat{\Omega}}
\end{aligned}
$$

Remark 4: Here $\hat{\Omega}$ behaves as if it was a complex number. The important distinction is that multiple operators in general *do not* commute.

Generalization to Infinite Vector Space

Most of the the formalism we've encountered deals with finite vector spaces.

Sometimes we will need to consider infinite vector spaces which contain vectors having infinite norm. The eigenvalues in this case are part of a continuous spectrum, and most of the formalism still holds. (For instance, Section 1.2.5, remark 2 remains valid.) Other generalizations are:

$$\langle x|y\rangle = \delta(x-y) \rightarrow \text{ Delta Dirac Function}$$
$$\text{where } \delta(x-y) = 0 \quad x \neq y$$
$$\int_a^b \delta(x-y)\,dy = 1 \qquad \forall a \leq x \leq b$$

Also,

$$\hat{I} = \int_a^b |x\rangle \langle x|\ dx$$

expresses completeness for a continuous spectrum.

Remark 5: One caveat concerning operators in a continuous vector space:

$$\hat{\Omega}^\dagger = \hat{\Omega}$$

is *not* sufficient to be Hermitian.

Example: Consider the operator:

$$\hat{p} = -i\hbar\frac{d}{dx}$$

acting in real space representation. The matrix elements in this representation:

$$\langle x|\,\hat{p}\,|y\rangle = -i\hbar\delta(x-y)\frac{d}{dy}$$

where x, y are eigenvectors. Checking to see if $\hat{p}$ is Hermitian:

$$\text{Is } \langle\theta|\,\hat{p}\,|\psi\rangle = \langle\psi|\,\hat{p}\,|\theta\rangle^*$$

$$\begin{aligned}
\langle\theta|\,\hat{p}\,|\psi\rangle &= \int_a^b\int_a^b \langle\theta|x\rangle\,\langle k|\,\hat{p}\,|y\rangle\,\langle y|\psi\rangle\ dx\,dy \\
&= \int_a^b\int_a^b \langle\theta|x\rangle\,(-i\hbar)\delta(x-y)\frac{d}{dy}\,\langle y|\psi\rangle\ dx\,dy \\
&= \int_a^b \langle\theta|x\rangle\,(-i\hbar)\frac{d}{dx}\,\langle x|\psi\rangle\ dx \\
&= \int_a^b \langle x|\theta\rangle^*\,(-i\hbar)\frac{d}{dx}\,\langle x|\psi\rangle\ dx \\
&= (-i\hbar)\,\langle x|\theta\rangle^*\,\langle x|\psi\rangle\,|_a^b - \int_a^b (-i\hbar)\,\langle x|\psi\rangle\,\frac{d}{dx}\,\langle x|\theta\rangle^*\ dx \\
&= (-i\hbar)\,\langle x|\theta\rangle^*\,\langle x|\psi\rangle\,|_a^b - \int_a^b \left(\langle\psi|x\rangle\,(-i\hbar\frac{d}{dx})\,\langle x|\theta\rangle\right)^*\ dx
\end{aligned}$$

which will equal what we want *if*:

$$(-i\hbar)\,\langle x|\theta\rangle^*\,\langle x|\psi\rangle\,|_a^b = 0$$

So we require surface terms to vanish for continuous Hermitian operators.

Remark 6: Restricting surface terms to vanish is equivalent to considering the Physical Hilbert Space.

Remark 7: If $(a,b) = (-\infty,\infty)$, then the typical functions

$$\langle x|\psi\rangle \equiv \psi(x) \to_{x\to a,b} 0 \text{ or } e^{ikx}$$

End of Chapter Asides:

$$e^{ikx}e^{-ik'x}\Big|_{-\infty}^{\infty} = 0 \qquad \text{if } k = k'$$

If $k \neq k'$, then:

$$\lim_{k\to\infty} e^{ikx}e^{-ik'x} = \lim_{\substack{L\to\infty\\ \Delta\to\infty}} \frac{1}{\Delta}\int_0^{L+\Delta} e^{i(k-k')x}\,dx = 0$$

Some other properties:

$$\hat{p} = \hbar\hat{k}$$

$$\hat{x}\,|x\rangle = x\,|x\rangle \quad \text{or} \quad k'\,|k\rangle = k\,|k\rangle$$

$$\Rightarrow \hat{k} = -i\frac{d}{dx} \qquad \text{in position}$$

$$\Rightarrow \hat{k} = i\frac{d}{dx} \qquad \text{in momentum}$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik(x-y)}\,dk = \delta(x-y)$$

Chapter 2

Classical Mechanics Review

2.1 Lagrange's and Hamilton's Formulations of Classical Theory

2.1.1 Lagrangian

Consider a system with N degrees of freedom. In classical theory, the dynamical state of the system is completely specified by the generalized coordinates $q_1, q_2, \ldots, q_N$ and generalized velocities $\dot{q_1}, \dot{q_2}, \ldots, \dot{q_N}$.

Remark 1: The description gives the evolution of the system in configuration space.

Definition 1: The Lagrangian of the system:

$$\mathcal{L} \equiv \mathcal{L}(q_1, q_2, \ldots, q_N, \dot{q_1}, \dot{q_2}, \ldots, \dot{q_N})$$

is a characteristic function from which the equations of motion can be derived:

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q_i}}\right) - \frac{\partial \mathcal{L}}{\partial q_i} = 0 \quad \text{for } i = 1, \ldots, N$$

These are called Lagrange's Equations of Motion.

Remark 2:

$$p_i = \frac{\partial \mathcal{L}}{\partial q_i}$$

These are called Lagrange conjugate momentum.

Remark 3: If all forces in the system are derivable from a static potential (the situation we usually encounter), then the Lagrangian takes the form:

$$\mathcal{L} = \underbrace{T}_{Kinetic} - \underbrace{V}_{Potential}$$

Remark 4: The Lagrange Equations of Motion may be derived by minimizing the action of the system:

$$\text{Action } = S = \int_{t_1}^{t_2} \mathcal{L}\, dt$$

$$\delta S = \delta \int_{t_1}^{t_2} \mathcal{L}\, dt \longrightarrow \text{Principle of Least Action}$$

2.1.2 Hamiltonian

An alternative but equivalent formulation of mechanics is in terms of the Hamiltonian. Here, the dynamical state of the system is represented by a point in 2n dimensional phase space, whose coordinates are the N position coordinates, $q_1, q_2, \ldots, q_N$, and the N corresponding conjugate momenta $p_1, p_2, \ldots, p_N$.

Definition 1: The Hamiltonian is defined as the function H:

$$H \equiv H(q_1, q_2, \ldots, q_N, p_1, p_2, \ldots, p_N) = \sum_{i=}^{N} \dot{q}_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \mathcal{L}$$

The equations of motion are:

$$\dot{q}_i = \frac{\partial H}{\partial p_i},\ i = 1 \ldots N$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i},\ i = 1 \ldots N$$

Remark 1: If $\mathcal{L} = T - V$, then $H = T + V =$ the total energy. In more general situations, we still consider the Hamiltonian to be the total energy of the system.

Remark 2:

$$\dot{H} \equiv \frac{dH}{dt} = \frac{\partial H}{\partial t}$$

This can be seen by using the chain rule and the Hamiltonian Equations of Motion. This implies that if the Hamiltonian is *not* an explicit function of time, then energy is conserved and we say that the system is conservative.

Remark 3: The Hamiltonian formulation is particularly important for QM since the generalized coordinates and the conjugate momenta become operators in the Hilbert Space.

2.1.3 Cyclic Coordinates, Poisson Brackets, and Canonical Transformations

Definition 1: A coordinate q_i is cyclic if:

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} = 0$$

which is a statement of conservation of conjugate momentum.

Definition 2: The Poisson Bracket between two variable $\omega(p,q)$,$\lambda(p,q)$ is given by

$$\{\omega, \lambda\} \equiv \sum_i \left(\frac{\partial \omega}{\partial q_i}\frac{\partial \lambda}{\partial p_i} - \frac{\partial \omega}{\partial p_i}\frac{\partial \lambda}{\partial p_i} \right)$$

Remark 1: Consider $\omega(p,q)$. Then

$$\begin{aligned} \frac{d\omega}{dt} &= \sum_i^N \left(\frac{\partial \omega}{\partial p_i}\dot{p}_i + \frac{\partial \omega}{\partial q_i}\dot{q}_i \right) \\ &= \sum_i^N \left(\frac{\partial \omega}{\partial p_i}\frac{\partial H}{\partial p_i} - \frac{\partial \omega}{\partial q_i}\frac{\partial H}{\partial q_i} \right) \\ &= \{\omega, H\} \end{aligned}$$

So, if a variable's Poisson Bracket with the Hamiltonian vanishes, then that variable is conserved.

Remark 2: Note the similarity between the Poisson bracket and the commutator.

Remark 3:

$$\{q_i, q_j\} = \{p_i, p_j\} = 0$$
$$\{q_i, p_j\} = \delta_{ij}$$

Definition 3: A transformation of coordinates and momenta

$$q \to q'(q,p)$$
$$p \to p'(q,p)$$

that preserves Hamilton's equations of motion is canonical.

$$\dot{q}'_i = \frac{\partial H}{\partial p'_i} \qquad \text{and} \qquad \dot{p}'_i = -\frac{\partial H}{\partial q'_i}$$

Remark 4: Poisson brackets are invariant under canonical transformations.

2.1.4 Symmetries

Theorem (Nother's Theorem): Symmetry properties in the Hamiltonian imply the existence of conserved quantities (conservation laws).
Proof: See Goldstein (p587, Section 13.7)

Remark 1: In classical mechanics, this is equivalent to finding a variable whose Poisson bracket with the Hamiltonian vanishes. In QM, we'll see that an operator whose commutator with the Hamiltonian vanishes, then this implies that there exists a conserved quantity.

Examples:

- Translational Invariance ⇒ Conservation of Linear Momentum
- Rotational Invariance ⇒ Conservation of Angular Momentum
- Time Translational Invariance ⇒ Conservation of Energy

Some examples closely related to QM:

- Reflection Invariance ⇒ Conservation of Parity
- Invariance under Permutation ⇒ Conservation of Symmetry (symmetric, anti-symmetric)

Remark 2: Symmetries imply degeneracy in the eigenspectrum. Breaking the symmetry often lifts the degeneracy of the system. (Eg: Zeeman Effect)

Chapter 3

Postulates of QM

3.1 Postulates

I. The state of a particle is represented by a vector $|\psi(t)\rangle$ in Hilbert Space.

II. Every observable in classical mechanics corresponds to a linear Hermitian operator in QM. In particular:

$$x \to \hat{X}$$
$$p \to \hat{P}$$
$$\omega(x,p) \to \hat{\Omega}(\hat{X},\hat{P}) \begin{cases} \hat{T}=\hat{P}^2/2m \\ \hat{V}=\hat{V}(\hat{X}) \end{cases}$$

The particular action of the operators depends on the choice of basis.

III. Any measurement of the observable associated with the operator $\hat{\Omega}$ will result only in values, ω, which satisfy

$$\hat{\Omega}\,|\psi\rangle = \omega\,|\psi\rangle$$

IV. For a system described by the normalized wave function $|\psi\rangle$, the average value of the observable corresponding to $\hat{\Omega}$ is

$$\langle\hat{\Omega}\rangle \equiv \langle\psi|\,\hat{\Omega}\,|\psi\rangle$$

This is called the expectation of $\hat{\Omega}$. Note: if $|\psi\rangle$ is not normalized, one need only divide the above equation by $\langle\psi|\psi\rangle$.

V. The time evolution of the state vector is governed by the Schrodinger Equation:

$$i\hbar\frac{d}{dt}\,|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle$$

where $\hat{H}$ is the Hamiltonian.

Remark 1: In measurements, $|\psi\rangle$ may not initially be an eigenstate of $\hat{\Omega}$ (Postulate III). But one can expand $|\psi\rangle$ in an eigenbasis:

$$|\psi\rangle = \sum_i |\omega_i\rangle \langle\omega_i|\psi\rangle$$

The coefficients in the expansion $\langle\omega_i|\psi\rangle$ give the probability of finding the system in eigenstate $|\omega_i\rangle$ according to:

$$P(\omega) = |\langle\omega|\psi\rangle|^2$$

Remark 2: Once an eigenvalue is measured, the system has probability of 1 of being in the corresponding eigenstate. The measurement (even if "idea") has changed the state of the system; this is known as the collapse of the wave function.

Example:

$$|\psi\rangle = \frac{1}{2}|\omega_1\rangle + \frac{1}{2}|\omega_2\rangle + \frac{1}{\sqrt{2}}|\omega_3\rangle$$

$$\text{The system has probability } \begin{cases} 1/4 \text{ of being in state } \omega_1 \\ 1/4 \text{ of being in state } \omega_2 \\ 1/2 \text{ of being in state } \omega_3 \end{cases}$$

Say that a measurement gives the eigenvalues of ω_3, then the state after the measurement is

$$|\psi\rangle = |\omega_3\rangle$$

Remark 3: Because coefficients correspond to probabilities, expansions of normalized wave functions must have

$$\sum_i |\langle\omega_i|\psi\rangle|^2 = 1$$

Remark 4: We must be careful with the consequences of Postulate II! Operators, unlike observables, must obey commutation relations. In general, we will take the symmetrized form (though this is *not* a universal prescription).

$$\text{Eg:} \quad xp \rightarrow \underbrace{\frac{\hat{X}\hat{P} + \hat{P}\hat{X}}{2}}_{\text{This also makes a Hermitian operator!}}$$

Remark 5: For degenerate eigenvalues, probabilities represent projection onto the corresponding "eigenspace". Probability is for measuring a certain eigenvalue.

Remark 6: For continuous eigenspectra, we require that

$$\begin{aligned}\int P(\omega)\, d\omega &= \int |\, \langle \omega|\psi\rangle \,|^2\, d\omega \\ &= \int \langle\psi|\omega\rangle\, \langle\omega|\psi\rangle\ d\omega \\ &= \langle\psi|\psi\rangle = 1\end{aligned}$$

And $P(\omega)$ is called the probability density. $P(\omega)\, d\omega$ is the probability that the measurement will give a value in the range ω to $\omega + d\omega$.

Remark 7: Not all QM observables have classical counterparts. (Eg. Spin)

Remark 8: The probabilistic nature of QM is a fundamental aspect of the theory. It is *not* the same as the classical probabilistic description of a many-particle system where the probabilistic approach is for practical purposes and where, in principle, know the exact $q(0), p(0)$ and the nature of the interaction would give exact time evolution solutions.

3.2 Compatability, Incompatibility and Uncertainty

3.2.1 Compatible Variables

Definition 1: Two variables are compatible if their corresponding operators commute:

$$[\hat{\Omega}, \hat{\Lambda}] = 0$$

Remark 1: If two (Hermitian) operators commute, one can find a unitary transformation which simultaneously diagonalizes them. Also, they will have a simultaneous eigenbasis. (See, for example, HW 2, Problem 2c, Shankar 1.8.10)

Definition 2: Two variables are incompatible if their corresponding operators do *not* commute.

$$[\hat{\Omega}, \hat{\Lambda}] \neq 0$$

Remark 2: Incompatible variables do have have *any* simultaneous eigenkets.

Remark 3: Two variables do not have to be either compatible or incompatible; they may have some simultaneous eigenkets, but still do not commute. Thus they fall into neither classification.

Definition 3: For any number of variables that mutually commute, one can find a simultaneous eigenbasis which simultaneously diagonalizes each observable. The set of these commuting variables is called a complete set of commuting observables or a complete set of compatible variables if the eigenbasis is unique (up to an overall phase); ie: is degenerate.

Remark 4: Consider an observable $\hat{\Omega}$ and state vector $|\psi\rangle$. One can expand $|\psi\rangle$ in an eigenbasis of $\hat{\Omega}$. The basis of $\hat{\Omega}$ is unique (up to an overall phase) if none of it's eigenvalues are degenerate. If there is a degenerate eigenvalue, and if there is an observable $\hat{\Lambda}$ that is compatible with $\hat{\Omega}$, then the simultaneous eigenbasis will be unique (up to an overall phase). If there are no longer any degenerate eigenvalues, then $\hat{\Omega}$ and $\hat{\Lambda}$ form a complete set of commuting observables.

Remark 5: Compatible variables may be measured simultaneously and precisely. A simultaneous measurement of all compatible variables will completely define the state vector of the physical system (and furthermore, that state will be unique). Also, the dynamical state of the system is completely specified by the quantum numbers associated with the eigenbasis.

Remark 6: A simultaneous measurement of a complete set of compatible variables is akin to preparing the system at the time t_0, after which the system evolves according to the Schrodinger Equation (See 3.1, Postulate V)

Definition 4: A pure state is one that has been prepared by measuring *all* values of compatible variables so that the state vector is know exactly.

Remark 7: In practice, a complete preparation is rare, and the dynamical state is *not* specified exactly. In this case, the system is in a mixed state, and is described by a statistical measure of states.

Remark 8: Mixed states include the statistical description in a classical sense, as well as the inherent probabilistic nature of QM. We will visit this shortly in Section 3.3 below).

3.2.2 Incompatible Variables and Uncertainty Relationships

Recall Section 3.1, Postulate IV ($\langle\hat{\Omega}\rangle = \langle\psi|\,\hat{\Omega}\,|\psi\rangle$).

Definition 1: The uncertainty in $\hat{\Omega}$ is given by:

$$\Delta\hat{\Omega} \equiv \left\langle (\hat{\Omega} - \left\langle\hat{\Omega}\right\rangle)^2 \right\rangle^{1/2} = \sqrt{\langle\psi|\,(\hat{\Omega} - \left\langle\hat{\Omega}\right\rangle)^2\,|\psi\rangle}$$

In a statistical description, this is also called the standard deviation or root-mean-square, and is a measure of the uncertainty due to fluctuations.

Note:

$$\begin{aligned}\Delta\hat{\Omega} &= \left\langle (\hat{\Omega} - \left\langle \hat{\Omega} \right\rangle)^2 \right\rangle^{1/2} \\ &= \left\langle \hat{\Omega}^2 - 2\hat{\Omega}\left\langle \hat{\Omega} \right\rangle + \left\langle \hat{\Omega} \right\rangle^2 \right\rangle^{1/2} \\ &= \left(\left\langle \hat{\Omega}^2 \right\rangle - \left\langle \hat{\Omega} \right\rangle^2 \right)^{1/2}\end{aligned}$$

Remark 1: If the state $|\psi\rangle$ is an eigenstate of $\hat{\Omega}$, then there is no uncertainty. ($\Delta\hat{\Omega} = 0$)

Uncertainty Derivation: Consider two *incompatible* Hermitian operators $\hat{\Omega}$ and $\hat{\Lambda}$ that have

$$[\hat{\Omega}, \hat{\Lambda}] = i\hat{\Gamma}$$

where $\hat{\Gamma}$ is also Hermitian. Let $[\hat{\Omega}, \hat{\Lambda}]_+ = \hat{\Omega}\hat{\Lambda} + \hat{\Lambda}\hat{\Omega}$ denote the *anticommutator*, and let $|\psi\rangle$ be a normalized state so that:

$$\left\langle \hat{\Omega} \right\rangle = \langle\psi| \hat{\Omega} |\psi\rangle$$

$$\left\langle \hat{\Lambda} \right\rangle = \langle\psi| \hat{\Lambda} |\psi\rangle$$

Then

$$(\Delta\hat{\Omega})^2(\Delta\hat{\Lambda})^2 = \langle\psi| (\hat{\Omega} - \left\langle \hat{\Omega} \right\rangle)^2 |\psi\rangle \langle\psi| (\hat{\Lambda} - \left\langle \hat{\Lambda} \right\rangle)^2 |\psi\rangle$$

If we let $\delta\hat{\Omega} = \hat{\Omega} - \left\langle \hat{\Omega} \right\rangle$ and $\delta\hat{\Lambda} = \hat{\Lambda} - \left\langle \hat{\Lambda} \right\rangle$, then we have:

$$\begin{aligned}(\Delta\hat{\Omega})^2(\Delta\hat{\Lambda})^2 &= \langle\psi| (\delta\hat{\Omega})^2 |\psi\rangle \langle\psi| (\delta\hat{\Lambda})^2 |\psi\rangle \\ &= \langle\psi| (\delta\hat{\Omega})(\delta\hat{\Omega}) |\psi\rangle \langle\psi| (\delta\hat{\Lambda})(\delta\hat{\Lambda}) |\psi\rangle \\ &= \langle\psi| (\delta\hat{\Omega})^\dagger(\delta\hat{\Omega}) |\psi\rangle \langle\psi| (\delta\hat{\Lambda})^\dagger(\delta\hat{\Lambda}) |\psi\rangle \qquad \text{since Hermitian.} \\ &\geq \left| \langle\psi| \delta\hat{\Omega}^\dagger \delta\hat{\Lambda} |\psi\rangle \right|^2 \qquad \text{by Schwartz Inequality} \\ &= \left| \langle\psi| \delta\hat{\Omega}\delta\hat{\Lambda} |\psi\rangle \right|^2\end{aligned}$$

But now, we also have that

$$\begin{aligned}(\delta\hat{\Omega})(\delta\hat{\Lambda}) &= \frac{\delta\hat{\Omega}\delta\hat{\Lambda} + \delta\hat{\Lambda}\delta\hat{\Omega}}{2} + \frac{\delta\hat{\Omega}\delta\hat{\Lambda} - \delta\hat{\Lambda}\delta\hat{\Omega}}{2} \\ &= \frac{1}{2}[\delta\hat{\Omega}, \delta\hat{\Lambda}]_+ + \frac{1}{2}[\delta\hat{\Omega}, \delta\hat{\Lambda}]\end{aligned}$$

And so we get that:

$$\begin{aligned}(\Delta\hat{\Omega})^2(\Delta\hat{\Lambda})^2 &\geq \left|\langle\psi|\, \delta\hat{\Omega}\delta\hat{\Lambda}\, |\psi\rangle\right|^2 \\ &= \left|\langle\psi|\, \frac{1}{2}[\delta\hat{\Omega}, \delta\hat{\Lambda}]_+\, |\psi\rangle + \frac{1}{2}\,\langle\psi|\, \hat{\Gamma}\, |\psi\rangle\right|^2 \\ &\geq \frac{1}{4}\,\langle\psi|\, [\delta\hat{\Omega}, \delta\hat{\Lambda}]_+\, |\psi\rangle^2 + \frac{1}{4}\,\langle\psi|\, \hat{\Gamma}\, |\psi\rangle^2\end{aligned}$$

This is the most general uncertainty relation between any two Hermitian operators.

Remark 2: If $\hat{\Omega}$ and $\hat{\Lambda}$ are canonically conjugate, then

$$\hat{\Gamma} = \hbar\hat{I}$$

And thus

$$\begin{aligned}(\Delta\hat{\Omega})^2(\Delta\hat{\Lambda})^2 &\geq \frac{1}{4}\,\langle\psi|\, [\delta\hat{\Omega}, \delta\hat{\Lambda}]_+\, |\psi\rangle^2 + \frac{\hbar^2}{4} \\ &\geq \frac{\hbar^2}{4}\end{aligned}$$

$$\Rightarrow \Delta\hat{\Omega}\Delta\hat{\Lambda} \geq \frac{\hbar}{2} \qquad \leftarrow \text{THE uncertainty relation}$$

Remark 3: The equality holds for

- $\delta\hat{\Omega}\,|\psi\rangle = (\text{constant}) \cdot \delta\hat{\Lambda}\,|\psi\rangle$
- $\langle\psi|\, [\delta\hat{\Omega}, \delta\hat{\Lambda}]_+\, |\psi\rangle = 0$

Remark 4: The most popular statements are

- $\Delta\hat{x}\Delta\hat{p} \geq \frac{\hbar}{2}$ $\qquad \leftarrow$ holds for each component
- $\Delta E\Delta t \geq \frac{\hbar}{2}$

3.3 Pure States and Mixtures: Density Matrices

Recall from Section 3.2.1 that:

- A pure state is one where we know the dynamical state of the system exactly
- A mixed state is one where the exact state of the system is unknown.

Suppose that we want to measure the quantity $\hat{\Omega}$ in a mixed system. Then there is a probability P_m of obtaining the average $\left\langle \hat{\Omega} \right\rangle_m = \langle m| \hat{\Omega} |m\rangle$, and

$$\left\langle \bar{\hat{\Omega}} \right\rangle = \sum_m P_m \langle m| \hat{\Omega} |m\rangle$$

where $\bar{\hat{\Omega}}$ indicates an average in the classical sense.

Remark 1: In the above equation, the $|m\rangle$'s are normalized but not necessarily orthogonal, and

$$P_m \geq 0 \qquad \text{and} \qquad \sum_m P_m = 1$$

Remark 2: There are two kinds of averaging in the equation above:

- Quantum average $\langle m| \hat{\Omega} |m\rangle$ for each system in $|m\rangle$
- Classical average over systems with different $|m\rangle$

3.3.1 Density Matrix

Definition 1: A density matrix (or operator) is a convenient way to describe a mixed state:

$$\hat{\rho} \equiv \sum_m P_m |m\rangle \langle m|$$

This is called the density operator.

Remark 1: The average value of $\hat{\Omega}$ in a mixed state is given by

$$\left\langle \bar{\hat{\Omega}} \right\rangle = \text{Tr } (\hat{\rho}\hat{\Omega})$$

To see this:

$$\begin{aligned}
\text{Tr } (\hat{\rho}\hat{\Omega}) &= \sum_n \langle n| \hat{\rho}\hat{\Omega} |n\rangle \\
&= \sum_{n,m} P_m \underbrace{\langle n|m\rangle}_{\delta_{nm}} \langle m| \hat{\Omega} |n\rangle \\
&= \sum_m P_m \langle m| \hat{\Omega} |m\rangle \\
&= \left\langle \bar{\hat{\Omega}} \right\rangle
\end{aligned}$$

Remark 2: It is sufficient to know $\hat{\rho}$ in order to calculate all measurable physical quantities, and thus every quantized, statistical mixture is exactly and completely defined by it's density operator.

Remark 3: $\hat{\rho} = |\psi\rangle\langle\psi|$ is a special case: it is the density matrix formulation of a pure state (all $P_m = 0$ except 1). In this case:

$$\begin{aligned}\left\langle\hat{\Omega}\right\rangle &= \langle\psi|\,\hat{\Omega}\,|\psi\rangle \\ &= \mathrm{Tr}\,\langle\psi|\,\hat{\Omega}\,|\psi\rangle \\ &= \mathrm{Tr}\,(|\psi\rangle\langle\psi|\,\hat{\Omega}) \\ &= \mathrm{Tr}\,(\hat{\rho}\hat{\Omega})\end{aligned}$$

which is the usual quantum average.

Properties of the Density Matrix:

1. $\hat{\rho}$ is positive definite: $\langle\psi|\,\hat{\rho}\,|\psi\rangle \geq 0 \quad \forall\psi \in \mathbb{H}$.

$$\langle\psi|\,\hat{\rho}\,|\psi\rangle = \sum_m P_m\,\langle\psi|m\rangle\,\langle m|\psi\rangle = \sum_m P_m|\,\langle\psi|m\rangle\,|^2 \geq 0$$

2. $\hat{\rho}$ is Hermitian

$$\hat{\rho}^\dagger = \left(\sum_m P_m\,|m\rangle\,\langle m|\right)^\dagger = \sum_m P_m\,|m\rangle\,\langle m| = \hat{\rho}$$

3. $\hat{\rho}$ has unit trace

$$\mathrm{Tr}\,(\hat{\rho}) = \mathrm{Tr}\,\left(\sum_m P_m\,|m\rangle\,\langle m|\right) = \sum_m P_m \underbrace{\mathrm{Tr}\,(|m\rangle\,\langle m|)}_{1} = \sum_m P_m = 1$$

4. $\mathrm{Tr}\,(\hat{\rho}^2) \leq 1$

$$\mathrm{Tr}\,(\hat{\rho}^2) = \sum_m\sum_n P_m P_n\,|m\rangle\,\underbrace{\langle m|n\rangle}_{\delta_{nm}}\,\langle m| = \sum_m P_m^2 \leq 1$$

3.3.2 Density Matrix of a Pure State

If the density operator represents a pure state, ie. $\hat{\rho} = |m\rangle\langle m|$, then we also have

- $\hat{\rho}^2 = \hat{\rho}$ $\quad\rightarrow$ (projector)
- $\mathrm{Tr}\,(\hat{\rho}^2) = 1$ $\quad\rightarrow$ (see properties above)

Suppose the density operator is expressed in its matrix form in a particular representation:

$$\begin{pmatrix} \rho_{11} & \rho_{12} & \cdots & \rho_{1n} \\ \rho_{21} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \rho_{n1} & \cdots & \cdots & \rho_{nn} \end{pmatrix}$$

with $\rho_{nm} = \langle n| \hat{\rho} |m\rangle$.

Question: Given the explicit matrix form, how do we determine whether it represents a pure state or a mixed state?

Answer: Since the pure state can be written $\hat{\rho} = |\psi\rangle \langle\psi|$, and

$$|\psi\rangle = \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{bmatrix}$$

Then we have that:

$$|\psi\rangle \langle\psi| = \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{bmatrix} [\alpha_1^*, \cdots, \alpha_n^*] = \begin{bmatrix} |\alpha_1|^2 & \alpha_1\alpha_2^* & \cdots & \alpha_1\alpha_n^* \\ \alpha_2\alpha_1^* & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \alpha_n\alpha_1^* & \cdots & \cdots & |\alpha_n|^2 \end{bmatrix}$$

Now, if $\hat{\rho}$ satisfies a pure state, then its elements must satisfy:

$$\rho_{ij}\rho_{ji} = \rho_{ij}\rho_{ij}^* = |\rho_{ij}|^2 = \rho_{ii}\rho_{jj}$$

If this holds for all i, j, then the density matrix is a pure state; otherwise it is a mixed state. This can be seen by doing the matrix multiplication.

3.3.3 Density Matrix of Mixed States

Given that $\hat{\rho} = \sum_j P_j |\psi_j\rangle \langle\psi_j|$ $\longleftarrow$ it is not required that the ψ_j's be orthogonal.

Example: Consider a two state system where $|1\rangle$ and $|2\rangle$ form the orthogonal basis for the 2D Hilbert space. One possible density operator is:

$$\hat{\rho} = \frac{1}{2} |1\rangle \langle 1| + \frac{1}{2} \left\{ \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) \frac{1}{\sqrt{2}}(\langle 1| + \langle 2|) \right\}$$

$\Rightarrow$ 50% mixture of state $|1\rangle$ and $\frac{1}{2}(|1\rangle + |2\rangle)$ which are *not* orthogonal.

Remark 1: The density operator in the above is a non-unique representation of non-orthogonal mixtures.

Remark 2: It is always possible to write $\hat{\rho}$ as a mixture of orthogonal states. For example, consider the general density operator $\hat{\rho} = \sum_j P_j \left|\psi_j\right\rangle \left\langle\psi_j\right|$. Let $\mathbb{R}$ be the matrix representation of $\hat{\rho}$ in the orthonormal basis defined by $\left|1\right\rangle, \left|2\right\rangle, \ldots, \left|N\right\rangle$. Then:

$$\mathbb{R} = \begin{bmatrix} \rho_{11} & \rho_{12} & \cdots & \rho_{1N} \\ \rho_{21} & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \rho_{N1} & \cdots & \cdots & \rho_{NN} \end{bmatrix} \Rightarrow \rho_{mn} = \left\langle m\right| \hat{\rho} \left|n\right\rangle = \sum_j P_j \left\langle m|\psi_j\right\rangle \left\langle\psi_j|n\right\rangle$$

Then we write:

$$\hat{\rho} = \left[\left|1\right\rangle, \left|2\right\rangle, \ldots, \left|N\right\rangle\right] \mathbb{R} \begin{bmatrix} \left\langle 1\right| \\ \left\langle 2\right| \\ \vdots \\ \left\langle N\right| \end{bmatrix}$$

$$\Rightarrow \hat{\rho} = \underbrace{\left[\left|1\right\rangle, \left|2\right\rangle, \ldots, \left|N\right\rangle\right]\hat{U}^\dagger}_{\left[\left|\phi_1\right\rangle, \left|\phi_2\right\rangle, \ldots, \left|\phi_N\right\rangle\right]} \cdot \underbrace{\hat{U}\mathbb{R}\hat{U}^\dagger}_{\begin{bmatrix} p_1 & & \\ & \ddots & \\ & & p_N \end{bmatrix}} \cdot \hat{U} \underbrace{\begin{bmatrix} \left\langle 1\right| \\ \left\langle 2\right| \\ \vdots \\ \left\langle N\right| \end{bmatrix}}_{\begin{bmatrix} \left\langle \phi_1\right| \\ \vdots \\ \left\langle \phi_N\right| \end{bmatrix}}$$

$$\Rightarrow \hat{\rho} = \sum_j P_j \left|\phi_j\right\rangle \left\langle\phi_j\right|$$

Remark 3: If $\left|1\right\rangle, \left|2\right\rangle, \ldots, \left|N\right\rangle$ form a orthonormal basis, then so does $\left|\phi_1\right\rangle, \left|\phi_2\right\rangle, \ldots, \left|\phi_N\right\rangle$ because $\hat{U}$ is unitary.

Recall Example:

$$\begin{aligned}\hat{\rho} &= \frac{1}{2}|1\rangle\langle 1| + \frac{1}{2}\left\{\frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)\frac{1}{\sqrt{2}}(\langle 1| + \langle 2|)\right\} \\ &= \frac{3}{4}|1\rangle\langle 1| + \frac{1}{4}|1\rangle\langle 2| + \frac{1}{4}|2\rangle\langle 1| + \frac{1}{4}|2\rangle\langle 2| \\ &= [|1\rangle, |2\rangle]\begin{bmatrix}3/4 & 1/4\\ 1/4 & 1/4\end{bmatrix}\begin{bmatrix}\langle 1|\\ \langle 2|\end{bmatrix} \\ &= [|1\rangle, |2\rangle]\mathbb{R}\begin{bmatrix}\langle 1|\\ \langle 2|\end{bmatrix}\end{aligned}$$

Now we would just diagonalize $\mathbb{R}$ to create a diagonalized $\hat{\rho}$ in some basis.

Remark 4: In some cases, the non-uniqueness of $\hat{\rho}$ goes even further.

$$\begin{aligned}\hat{\rho} &= [|1\rangle, |2\rangle]\begin{bmatrix}1/2 & 0\\ 0 & 1/2\end{bmatrix}\begin{bmatrix}\langle 1|\\ \langle 2|\end{bmatrix} \\ &= [|1\rangle, |2\rangle]\hat{U}\underbrace{\hat{U}^\dagger\begin{bmatrix}1/2 & 0\\ 0 & 1/2\end{bmatrix}\hat{U}}_{\frac{1}{2}\hat{I}\quad\forall\hat{U}}\hat{U}^\dagger\begin{bmatrix}\langle 1|\\ \langle 2|\end{bmatrix} \\ &= \underbrace{[|1\rangle, |2\rangle]\hat{U}}\begin{bmatrix}1/2 & 0\\ 0 & 1/2\end{bmatrix}\underbrace{\hat{U}^\dagger\begin{bmatrix}\langle 1|\\ \langle 2|\end{bmatrix}} \\ &= [|\phi_1\rangle, |\phi_2\rangle]\begin{bmatrix}1/2 & 0\\ 0 & 1/2\end{bmatrix}\begin{bmatrix}\langle \phi_1|\\ \langle \phi_2|\end{bmatrix}\end{aligned}$$

In this case, $\hat{\rho}$ can be expressed in an infinite number of forms depending on the unitary transformation $\hat{U}$ used.

3.3.4 Time Evolution of the Density Matrix

Regression: QM can be expressed in equivalent "pictures" depending on whether the transformations which govern time evolution are passive or active. (Recall §1.2.4)

- The Schrodinger picture (active) has state vectors evolve with time while operators remain constant.
- The Heisenberg picture (passive) has states remain constant while operators evolve.

In addition, there is

- Interaction Picture: Here, the non-interacting part of the Hamiltonian is in the Schrodinger picture while the interacting piece has time-dependent operators.

Time Evolution of $\hat{\rho}$: Recall §3.1 - Postulate V $\rightarrow i\hbar\,|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle$. What then is the time evolution of $\hat{\rho}$?

$$\begin{aligned}
\dot{\hat{\rho}} &= \sum_j P_j \left[|\psi_j\rangle \left(\frac{d}{dt} \langle\psi_j| \right) + \left(\frac{d}{dt} |\psi_j\rangle \right) \langle\psi_j| \right] \\
&= \sum_j P_j \left[\langle\psi_j| \left(\frac{1}{i\hbar} \hat{H} |\psi_j\rangle \right)^\dagger + \frac{1}{i\hbar} |\psi_j\rangle \langle\psi_j| \right] \\
&= \frac{1}{i\hbar} \sum_j P_j \left[\hat{H} |\psi_j\rangle \langle\psi_j| - |\psi_j\rangle \langle\psi_j| \hat{H} \right] \\
&= \frac{1}{i\hbar} [\hat{H}, \hat{\rho}]
\end{aligned}$$

Remark 1: This is the quantum version of the Liouville Equation from classical statistical mechanics. (see §2.1.3, remark 1 with $\hat{\rho}$ = the density of phase space.)

Remark 2: We'll see later that the Heisenberg equation of motion for an operator, $\hat{A}_H$, is given by:

$$\dot{\hat{A}}_H = \frac{1}{i\hbar} [\hat{A}_H, \hat{H}]$$

Witness that the equation of motion for $\hat{\rho}$ has the commutator in reverse order.

Remark 3: The density matrix is a special operator since it changes in time in the Schrodinger picture.

3.4 Schrodinger Equation

Recall §3.1, Postulate V, which said that the Schrodinger equation is:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

where $\hat{H}$ is the Hamiltonian of the system.

Remark 1: In general, one may use Postulate II to construct the Hamiltonian $\hat{H}$ from the classical Hamiltonian. Modifications to this are required if there is no classical analog (eg spin).

Remark 2: Though we can only postulate about the form of the time evolution of a vector in Hilbert space, we do know that it must be *linear* and *homogeneous* (so that we can have linear superposition). We also know that it must be a DE of the 1st order with respect to time (so that the evolution is uniquely determined by the state at some initial time).

Remark 3: Predictions of Quantum Theory must coincide with classical mechanics in the regime where classical mechanics is valid (so there is some formal analogy with classical mechanics). This is called the correspondence principle.

3.4.1 Solving the Schrodinger Equation

For now, we will consider $\hat{H} = \hat{H}(\hat{x}, \hat{p})$, where the Hamiltonian is a function of position and momentum, but *not* explicitly time. In general, the time dependence (if present) is treated perturbatively, so we will discuss Hamiltonians with explicit time dependence later.

Solving the equation formally gives a solution of the form:

$$|\psi\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle \tag{$\star$}$$

Remark 1: One can write this as:

$$|\psi(t)\rangle = \hat{U}(t) |\psi(0)\rangle$$

where $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$ is called the propagator or time evolution operator.

Remark 2: Since $\hat{H}$ is Hermitian, $\hat{U}$ is unitary.

Remark 3: Time evolution may be thought of as a rotation of a state in Hilbert space.

To evaluate $(\star)$, it is useful to expand $|\psi(0)\rangle$ in an energy eigenbasis. This will diagonalize the Hamiltonian and allows one to write:

$$\begin{aligned} e^{-i\hat{H}t/\hbar} |E\rangle &= \sum_{n}^{\infty} \frac{1}{n!} \left(\frac{-it}{\hbar}\right)^n \begin{pmatrix} E_1 & & \\ & \ddots & \\ & & E_n \end{pmatrix} |E\rangle \\ &= \begin{pmatrix} e^{-iE_1 t/\hbar} & & \\ & \ddots & \\ & & e^{-iE_n t/\hbar} \end{pmatrix} |E\rangle \end{aligned}$$

To determine the energy eigenbasis:

1. First solve the time-independent Schrodinger equation:

$$\hat{H} |E\rangle = E |E\rangle$$

2. The expand the wavefunction in terms of the energy eigenbasis:

$$|\psi(t)\rangle = \sum_E |E\rangle \underbrace{\langle E|\psi(t)\rangle}_{a_E(t)} = \sum_E a_E(t) |E\rangle$$

3. Now substitute this into $i\hbar|\dot{\psi}\rangle = \hat{H}\,|\psi\rangle$ to obtain:

$$i\hbar\frac{d}{dt}a_E(t) = Ea_E$$

$$\Rightarrow a_E(t) = a_E(0)e^{-iEt/\hbar} = \langle E|\psi(0)\rangle\, e^{-iEt/\hbar}$$

$$\Rightarrow |\psi(t)\rangle = \sum_E |E\rangle\,\langle E|\psi(0)\rangle\, e^{-iEt/\hbar} = \hat{U}(t)\,|\psi(0)\rangle$$

This, by comparison, gives a propagator of the form:

$$\hat{U}(t) = \sum_E |E\rangle\,\langle E|\, e^{-iEt/\hbar}$$

Remark 4: If the eigenspectrum is degenerate, an additional index is required to specify the state:

$$\hat{U}(t) = \sum_\alpha \sum_E |E,\alpha\rangle\,\langle E,\alpha|\, e^{-iEt/\hbar}$$

If the eigenspace is continuous, then $\sum_E \to \int dE$

Remark 5: $|E(t)\rangle = |E\rangle\, e^{iEt/\hbar}$ are the normal modes called stationary states since the probability distribution for any variable is time independent in these states.

Chapter 4

Simple Problems in 1 Dimension

In general, we will need to chose a basis to solve Schrodinger's equation. Though one can choose any basis, some choices are better than others depending on the form of the Hamiltonian. The following are some examples of 1 dimensional problems.

Remark 1: The x basis (position basis) is the basis for the alternative form for QM based on the wave equation. In this basis, $\hat{x} \to x$, $\hat{P} \to -i\hbar\frac{d}{dx}$, and $\hat{H} \to i\hbar\frac{\partial}{\partial t}$.

4.1 Free Particle

4.1.1 Solving the Schrodinger Equation

In the free particle case, we have

$$\hat{H} = \frac{1}{2m}\hat{P}^2$$

Solving the time dependent Schrodinger equation:

$$i\hbar\frac{d}{dt}\left|\psi(t)\right\rangle = \frac{\hat{P}^2}{2m}\left|\psi\right\rangle \qquad (\star)$$

which gives us general solutions of

$$\left|\psi(t)\right\rangle = \left|E\right\rangle e^{-iEt/\hbar}$$

Substituting this back into $(\star)$ gets us the time independent Schrodinger equation

$$\frac{\hat{P}^2}{2m}\left|E\right\rangle = E\left|E\right\rangle$$

Remark 1: Here, we may choose the momentum basis since $|P\rangle$ is also an eigenstate of $\hat{P}^2$

$$\frac{\hat{P}^2}{2m}|P\rangle = E|P\rangle$$
$$\left(\frac{p^2}{2m} - E\right)|P\rangle = 0$$
$$\Rightarrow p = \pm\sqrt{2mE}$$

Thus the two orthogonal eigenstates are:

$$|E_+\rangle = \left|p = \sqrt{2mE}\right\rangle$$
$$|E_-\rangle = \left|p = -\sqrt{2mE}\right\rangle$$

Remark 2: The energy eigenstate is degenerate since a particle can be moving to the right or the left with the same energy. Using the compatible operator $\hat{P}$, we can determine the possible outcomes so that a measurement of p, and thus E, will give us a complete description of the dynamical state of the system.

Remark 3: The most general state is given by

$$|\psi\rangle = \alpha|E_+\rangle + \beta|E_-\rangle$$

which is a superposition of the particle moving to the left *and* right.

Remark 4: Note that measuring the momentum gives us *no* information about the position of the particle since $\Delta p = 0 \Rightarrow \Delta x = \infty$ by Heisenberg's uncertainty principle.

4.1.2 Propagator for a Free Particle in the Position Basis

The matrix elements for the propagator in the x-basis are

$$U(x,t;\underbrace{y}_{(x_0)}) \equiv \langle x|\hat{U}(t)|y\rangle = \int_{-\infty}^{\infty} dp\,\langle x|\,e^{-ip^2t/2m\hbar}\,|P\rangle\,\langle P|y\rangle$$

Now consider:

$$\begin{aligned}\langle x|y\rangle = \delta(x-y) &= \frac{1}{2\pi}\int_{\infty}^{\infty} dk e^{ik(x-y)} \\ &= \int_{-\infty}^{\infty} dp\,\langle x|P\rangle\,\langle P|y\rangle \qquad \text{inserting a complete set} \\ &= \hbar\int_{-\infty}^{\infty} dk\,\langle x|k = p/\hbar\rangle\,\langle k = p/\hbar|y\rangle\end{aligned}$$

where the last step follows since we know $p = \hbar k$. Now, by comparison, we can see that

$$\langle x|k\rangle \langle k|y\rangle = \frac{1}{2\pi\hbar} e^{ik(x-y)}$$

or

$$\langle x|k = p/\hbar\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} = \langle x|P\rangle$$

Now, using this to evaluate $U(x,t;y)$, we get

$$\begin{aligned} U(x,t;y) &= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ip(x-y)/\hbar} e^{-ip^2 t/2m\hbar}\, dp \\ &= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp\left(\frac{-it}{2m\hbar}\left(p - \frac{m(x-y)}{t}\right)^2\right) \underbrace{\exp\left(im(x-y)^2/2\hbar t\right)}_{\text{from completing the square}} \\ &= \frac{1}{2\pi\hbar}\sqrt{\frac{2m\hbar\pi}{it}} e^{im(x-y)^2/2\hbar t} \\ &= \sqrt{\frac{m}{2i\pi\hbar t}} e^{im(x-y)^2/2\hbar t} \end{aligned}$$

Remark 1: For a free particle whose state is known at some time t_0, the state at some $t > t_0$ is given by

$$\psi(x,t) = \int U(x,t;y,t_0)\psi(y,t_0)\, dy$$

where

$$U(x,t;y,t_0) = \langle x|\, U(t-t_0)\, |y\rangle$$

Note that this depends *only* on $t - t_0$. This is because there is no explicit time dependence in the Hamiltonian.

Remark 2: If we consider a free particle whose position is known at time t_0:

$$\psi(t_0) = \delta(x - x_0)$$

Then

$$\psi(x,t) = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{im(x-x_0)^2/2\hbar t}$$

Physically, this corresponds to the delta function broadening as a function of time.

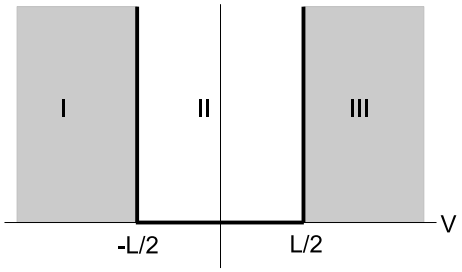


Figure 4.1: Diagram of the "Box" Potential

4.2 Particle in a Box

Consider a particle under the influence of a potential $V(x)$ where:

$$V(x) = \begin{cases} 0 & |x| \leq L/2 \\ \infty & \text{otherwise} \end{cases}$$

We will choose the position basis for the time-independent Schrodinger equation:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V} \qquad \hat{H}\,|\psi\rangle = E\,|\psi\rangle$$

$$\langle x|\,\hat{H}\,|\psi\rangle = E\,\langle x|\psi\rangle = E\psi(x)$$

$$\langle x|\,\frac{1}{2m}\left(-i\hbar\frac{d}{dx}\right)^2 + \hat{V}\,|\psi\rangle = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \hat{V}\psi(x)$$

Combining the last two, we have

$$\frac{d^2}{dx^2}\psi + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

Now in Regions I and III, $\psi_I = \psi_{III} = 0$ (we'll see why in §4.4)

In Region II:

$$V = 0 \Rightarrow \frac{d^2}{dx^2}\psi = -\frac{2mE}{\hbar^2}\psi$$

$$\Rightarrow \psi_{II} = A\exp\left[i\sqrt{2mE/\hbar^2}x\right] + B\exp\left[-i\sqrt{2mE/\hbar^2}x\right]$$

$$= Ae^{ikx} + Be^{-ikx} \qquad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

Remark 1: We require that the wavefunction must be continuous

$$\psi_I(-L/2) = \psi_{II}(-L/2) \quad \text{and} \quad \psi_{II}(L/2) = \psi_{III}(L/2)$$

So then, applying the boundary conditions, we have that

$$\begin{aligned} 0 &= Ae^{-ikL/2} + Be^{ikL/2} \\ 0 &= Ae^{ikL/2} + Be^{-ikL/2} \end{aligned} \qquad (\star)$$

Which implies

$$\begin{pmatrix} e^{-ikL/2} & e^{ikL/2} \\ e^{ikL/2} & e^{-ikL/2} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = |0\rangle$$

The non-trivial solutions to this problem are found by finding the zeroes of the determinant.

$$\Rightarrow e^{-ikL} - e^{ikL} = 0 = -2i\sin(kL) \quad \Rightarrow k = \frac{n\pi}{L} \quad n = 0, \pm 1, \pm 2, \cdots$$

Now we substitute k back into $(\star)$ to get the allowed values of A and B:

$$Ae^{-in\pi/2} + Be^{in\pi/2} = 0$$

$$\Rightarrow A = -Be^{in\pi} = -B \cdot \begin{cases} 1 & \text{if n is even} \\ -1 & \text{if n is odd} \end{cases}$$

Thus we have that

$$\psi(x) = \begin{cases} A\left(e^{ikx} + e^{-ikx}\right) & \text{n odd} \\ A\left(e^{ikx} - e^{-ikx}\right) & \text{n even} \end{cases}$$

Remark 2: Choose A so that $\int \psi^* \psi \, dx = 1$ (normalize):

$$\psi(x) = \begin{cases} \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right) & \text{n is odd} \\ \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & \text{n is even} \end{cases}$$

Remark 3: If $n = 0$, then $\psi = 0$ everywhere, which is not very exciting. Also, $\pm$ values of n are physically equivalent, so we only deal with positive n to make life simpler.

Remark 4: Comparing our expressions for k:

$$\sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{L}$$

We find that the energy in the box in quantized

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad n = 1, 2, 3, \cdots$$

Remark 5: As L goes to infinity, the energy spectrum becomes continuous.

Remark 6: The ground state, $n = 1$, has $E = \pi^2\hbar^2/2mL^2 > 0$ which in a necessary consequence of the uncertainty principle.

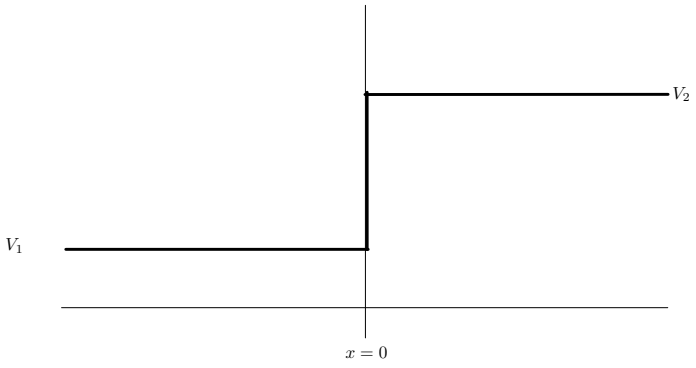
$$\Delta x = L/2 \Rightarrow \Delta p \geq \hbar/2$$

since

$$\begin{aligned} \Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \quad \text{and} \quad \langle p \rangle = 0 \\ \geq (2m \langle E_1 \rangle)^{1/2} = \frac{\pi \hbar}{L} \\ \Rightarrow \Delta x \Delta p = \frac{L}{2} \frac{\pi \hbar}{L} > \frac{\hbar}{2} \end{aligned}$$

4.3 Step Potentials: Reflection and Transmission

Consider the potential:



Here, the time-independent Schrodinger equation is

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi = (E - V_1)\psi \quad , \quad x < 0 \\ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi = (E - V_2)\psi \quad , \quad x > 0 \end{aligned} \tag{4.1}$$

Remark 1: We must consider two different energy regions: $V_1 < E < V_2$ and $E > V_2$

$\mathbf{V_1 < E < V_2}$:

We expect the wavefunctions to have the following form:

$$\psi(x) = \begin{cases} e^{\pm i\sqrt{2m(E-V_1)}}, & x<0 \\ e^{\pm\sqrt{2m(V_2-E)}}, & x>0 \end{cases} \tag{4.2}$$

Remark 2: The actual solution is constructed as linear combinations of the forms in (4.2)

Remark 3: The solution oscillates in the region where $E < V_2$, and decays (or grows) exponentially when $E > V_2$.

Remark 4: To satisfy the boundary conditions, we impose the following conditions:

1. $\psi(x)$ must remain finite as $x \to \infty$ to be physically realizable
2. $\psi(x)$ and $\psi'(x)$ must be continuous at the discontinuity at $x = 0$. This gives a continuous probability in space (no source or sink of particles).

Taking these considerations into account, the general solution will have the following form:

$$\psi(x) = \begin{cases} A_+ e^{ikx} + A_- e^{-ikx}, & x < 0 \\ B_+ e^{\kappa x} + B_- e^{-\kappa x}, & x > 0 \end{cases} \tag{4.3}$$

where

$$\hbar k = \sqrt{2m(E - V_1)} \qquad ; \qquad \hbar\kappa = \sqrt{2m(V_2 - E)} \tag{4.4}$$

Now, from Remark 4, we know that:

- $B_+ = 0$ (from condition 1)
- $A_+ - A_- = B_-$ (from condition 2, continuity of ψ)
- $ik(A_+ - A_-) = -\kappa B_-$ (from condition 2, continuity of ψ')

Combining these and solving:

$$\begin{aligned} ik(A_+ - A_-) &= -\kappa(A_+ + A_-) \\ (ik + \kappa)A_+ &= (ik - \kappa)A_- \end{aligned}$$

$$(\kappa^2 + k^2)e^{-i\phi} = -(\kappa^2 + k^2)e^{i\phi}A_- \tag{4.5}$$

where

$$\begin{aligned} \tan(\phi) &= -\frac{k}{\kappa} \\ \Rightarrow A_- &= -e^{-2i\phi}A_+ \end{aligned}$$

Remark 5: A_+ and A_- are not necessarily complex conjugates of one another, but we can introduce an overall phase. We multiply (4.5) by i so that

$$A_+ = \frac{A}{2i}e^{i\phi} \qquad \text{and} \qquad A_- = -\frac{A}{2i}e^{-i\phi}$$

where A is some real constant.

Then, we have

$$\psi(x) = \begin{cases} A\sin(ki + \phi), & x < 0 \\ A\sin(\phi)e^{-\kappa x}, & x > 0 \end{cases} \tag{4.6}$$

Remark 6: In the region $x < 0$, we have a wave traveling toward the step potential and a reflected component of equal magnitude traveling away. We see this by the time-dependent Schrodinger equation:

$$\begin{aligned}\psi(x,t) &= e^{iEt/\hbar} A \sin(kx+\phi) \\ &= \underbrace{\frac{A}{2i} e^{-i(Et/\hbar - kx - \phi)}}_{\text{Wave going right}} \quad \underbrace{-\frac{A}{2i} e^{-i(Et/\hbar + kx - \phi)}}_{\text{Wave going left phase shifted by } \pi}\end{aligned}$$

Remark 7: Note that the wavefunction doesn't vanish for $x > 0$; there is some barrier penetration that decays more rapidly for larger step sizes. If $V_2 \to \infty$, there is no barrier penetration. This is the justification for setting $\psi(x) = 0$ outside of the infinite square well in the previous section.

Remark 8: In wave phenomena, this penetration is a familiar part of reflection and transmission. In E&M, the penetrating part of light at an interface is called an evanescent wave.

$\mathbf{E > V_2}$:

In this case, the solution of the Schrodinger equation is:

$$\psi(x) = \begin{cases} A_+ e^{ikx} + A_- e^{-ikx}, & x < 0 \\ B_+ e^{ik'x} + B_- e^{-ik'x}, & x > 0 \end{cases} \tag{4.7}$$

with

$$\hbar k' = \sqrt{2m(E - V_2)} \tag{4.8}$$

Imposing boundary conditions, we have

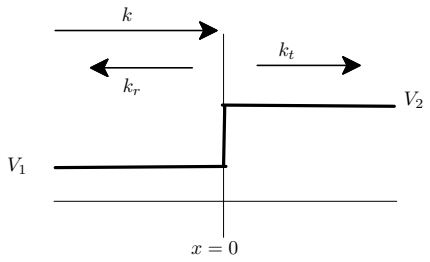
$$A_+ + A_- = B_+ + B_- \tag{4.9}$$

$$ik(A_+ - A_-) = ik'(B_+ - B_-) \tag{4.10}$$

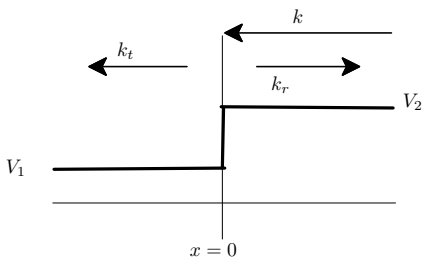
Remark 9: Note that we only have 2 equations to specify 4 unknowns. This is because there are 2 linearly independent solutions for each energy (energy is 2-fold degenerate, or doubly degenerate, or has a degeneracy of order 2.

The 2 possible scenarios corresponding to this degeneracy are:

So we see that the wave is "launched" from either the right or the left and is partially reflected (or transmitted) at the step boundary.



Case A



Case B

Consider now scenario A above, where the wave is launched from the left. In this case, we have $B_- = 0$, which, from Eq (4.9) above implies that

$$B_+ = A_+ + A_-$$

Using Eq (4.10) above, we also have that

$$ik(A_+ + A_-) = ik'(A_+ + A_-)$$
$$A_+(k - k') = A_-(k + k') \tag{4.11}$$

Thus we get that the solution for a wave originating from the left is

$$\psi(x) = \begin{cases} A(e^{ikx} + \dfrac{k-k'}{k+k'}e^{-ikx}), & x < 0 \\ A\dfrac{2k}{k+k'}e^{ik'x}, & x > 0 \end{cases} \tag{4.12}$$

where $A_+ = A$ for convenience. Now, including the time dependence for $x < 0$:

$$\psi(x,t) = Ae^{-i(Et/\hbar - kx)} + A\frac{k-k'}{k+k'}e^{-i(Et/\hbar + kx)} \tag{4.13}$$

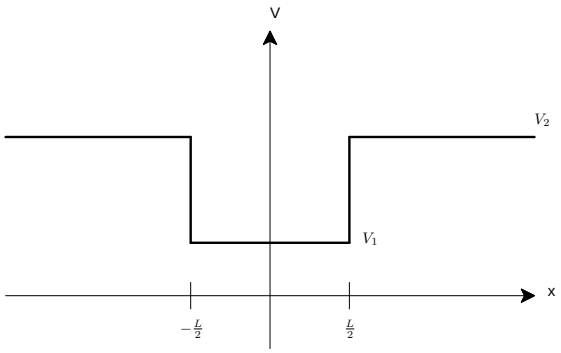
Remark 10: As $E \to \infty$, the amplitude $\frac{A(k-k')}{k+k'}$ of the reflected wave $\to 0$ while the amplitude $\frac{A(2k)}{k+k'}$ of the transmitted wave goes to the amplitude of the incident wave (eg, the step became negligible). As the energy $E \to V_2$, then $k' \to 0$ and the amplitude of the reflected wave goes to the amplitude of the incident wave and the transmitted wave amplitude $\to 0$ since it is preparing to become exponentially damped barrier penetration.

4.4 Finite Square Well: Discrete Energies and Resonances

Consider the potential
So we have

$$V(x) = \begin{cases} V_1, & |x| \le L/2 \\ V_2, & |x| > L/2 \end{cases}$$

From our previous two examples, we expect the following:



- Discrete energies for $V_1 < E < V_2$
- Barrier penetration for $V_1 < E < V_2$ where $|x| > L/2$
- For $E > V_2$, transmission and reflection at discontinuities in potential. We also expect 2-fold degeneracy since we can have waves coming from the left or the right.
- Resonances as a function of energy in the transmission and reflection of waves.

To actually solve the problem, we will again consider each energy range separately:

$\mathbf{V_1 < E < V_2}$:

The time independent Schrodinger equation is:

$$\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi = \begin{cases} (E-V_1), & |x|<L/2 \\ -(V_2-E), & |x|>L/2 \end{cases} \tag{1}$$

Then the solutions are

$$\psi(x) = \begin{cases} A_+e^{ikx} + A_-e^{-ikx}, & |x| \le L/2 \\ B_+e^{\kappa x} + B_-e^{-\kappa x}, & |x| > L/2 \end{cases} \tag{2}$$

where

$$\hbar k = \sqrt{2m(E-V_1)} \qquad \text{and} \qquad \hbar\kappa = \sqrt{2m(V_2-E)} \tag{3}$$

Applying boundary conditions, we have

- $\psi(x \to \pm\infty) < \infty$

$$\Rightarrow B_+ = 0 \quad \text{for } x > L/2$$
$$B_- = 0 \quad \text{for } x < -L/2$$

$$\Rightarrow \psi(x) = \begin{cases} A_+e^{ikx} + A_-e^{-ikx}, & |x| < L/2 \\ B_+e^{\kappa x}, & x < -L/2 \\ B_-e^{-\kappa x}, & x > L/2 \end{cases} \tag{4}$$

- Continuity of ψ at $x = \pm L/2$

$$\Rightarrow A_+e^{-ikL/2} + A_-e^{ikL/2} = B_+e^{-\kappa L/2} \tag{5}$$
$$A_+e^{ikL/2} + A_-e^{-ikL/2} = B_-e^{-\kappa L/2} \tag{6}$$

- Continuity of ψ' at $x = \pm L/2$

$$\Rightarrow ik\left(A_+ e^{-ikL/2} - A_- e^{ikL/2}\right) = \kappa B_+ e^{-\kappa L/2} \tag{7}$$

$$ik\left(A_+ e^{ikL/2} - A_- e^{-ikL/2}\right) = -\kappa B_- e^{-\kappa L/2} \tag{8}$$

Now we solve the system:

1. take $\kappa \cdot (5) \pm (7)$

$$(\kappa + ik)A_+ e^{-ikL/2} + (\kappa - ik)A_- e^{ikL/2} = 2\kappa B_+ e^{-\kappa L/2} \tag{9}$$

$$(\kappa - ik)A_+ e^{-ikL/2} + (\kappa + ik)A_- e^{ikL/2} = 0 \tag{10}$$

2. Similarly, take $\kappa \cdot (6) \pm (8)$

$$(\kappa + ik)A_+ e^{ikL/2} + (\kappa - ki)A_- e^{-ikL/2} = 0 \tag{11}$$

$$(\kappa - ik)A_+ e^{ikL/2} + (\kappa + ki)A_- e^{-ikL/2} = 2\kappa B_- e^{-\kappa L/2} \tag{12}$$

3. From (10) and (11), we have

$$A_+^2 = A_-^2 \Rightarrow A_+ = \pm A_- \tag{13}$$

Remark 1: The "plus" in (13) corresponds to an even parity solution (cosines in box)' the negative sign corresponds to an odd parity solution (sines in box).

Even Parity Solutions: Let

$$A_+ = A_- = \frac{A}{2} \tag{14}$$

Then from (10) or (11):

$$\sqrt{\kappa^2 + k^2}\cos\left(\frac{kL}{2} + \phi\right) = 0 \tag{15}$$

where $\phi = \arctan(k/\kappa)$.

$$\Rightarrow \frac{kL}{2} + \arctan\left(\frac{k}{\kappa}\right) = \frac{n\pi}{2} \quad \text{where } n = \text{odd} \tag{16}$$

Also, from (9) and (12), we get:

$$\begin{aligned} \sqrt{\kappa^2 + k^2}A\cos(kL/2 - \phi) &= 2\kappa B_+ e^{-\kappa L/2} \\ \sqrt{\kappa^2 + k^2}A\cos(kL/2 - \phi) &= 2\kappa B_- e^{-\kappa L/2} \end{aligned} \tag{17}$$

$$\Rightarrow B_+ = B_- = \frac{A\sqrt{\kappa^2 + k^2}}{2\kappa}\cos\left(\frac{kL}{2} - \phi\right)e^{\kappa L/2} \tag{18}$$

So the wave function for the even parity solutions is

$$\psi(x) = \begin{cases} A\cos(kx), & |x| < L/2 \\ \dfrac{A\sqrt{\kappa^2+k^2}}{2\kappa}\cos\left(\dfrac{kL}{2}-\phi\right)e^{\kappa L/2}e^{\kappa x}, & x < -L/2 \\ \dfrac{A\sqrt{\kappa^2+k^2}}{2\kappa}\cos\left(\dfrac{kL}{2}-\phi\right)e^{\kappa L/2}e^{-\kappa x}, & x > L/2 \end{cases} \tag{19}$$

Odd Parity Solutions: Let

$$A_+ = -A_- \equiv \frac{A}{2i} \tag{20}$$

Then, following the same procedure as in the even case, we get the energy constraints:

$$\frac{kL}{2} + \arctan\left(\frac{k}{\kappa}\right) = \frac{n\pi}{2} \tag{21}$$

And the coefficients B_+ and B_- are:

$$B_+ = -B_- = -A\frac{\sqrt{\kappa^2+k^2}}{2\kappa}\sin\left(\frac{kL}{2}-\phi\right)e^{\kappa L/2} \tag{22}$$

This gives us odd parity solutions of:

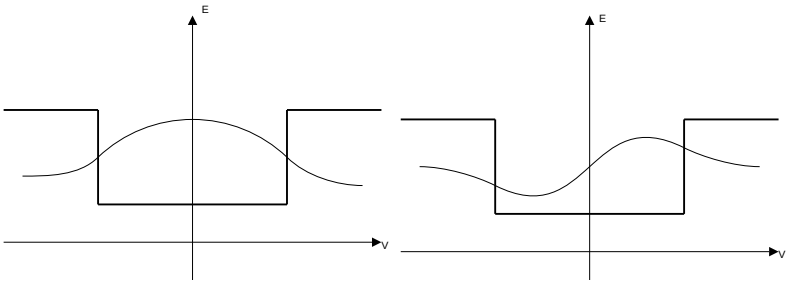
$$\psi(x) = \begin{cases} A\sin(kx), & |x| < L/2 \\ \dfrac{A\sqrt{\kappa^2+k^2}}{2\kappa}\sin\left(\dfrac{kL}{2}+\phi\right)e^{\kappa L/2}(-e^{\kappa x}), & x < -L/2 \\ \dfrac{A\sqrt{\kappa^2+k^2}}{2\kappa}\sin\left(\dfrac{kL}{2}+\phi\right)e^{\kappa L/2}(e^{-\kappa x}), & x > L/2 \end{cases} \tag{23}$$

Remark 2: The general form of the solutions looks like:

Remark 3: The allowed energies are obtained from Eq (16) and (21) for the even and odd parities (respectively). Consider the even parity energy values. It is helpful to eliminate the κ so that all energy dependence is in k. As a reminder, Eq (16) was:

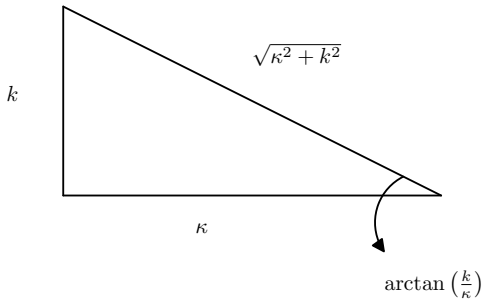
$$\frac{n\pi}{2} = \frac{kL}{2} + \arctan\left(\frac{k}{\kappa}\right)$$

Looking at just the trig. component, we have the triangle:



(a) Even case: Note that the exponential decay parts have the same sign

(b) Odd case: Note that the exponential decay parts have opposite signs



Which means that we have:

$$\begin{aligned}\arctan\left(\frac{k}{\kappa}\right) &= \arcsin\left(\frac{k}{\sqrt{k^2+\kappa^2}}\right)\\ &= \arcsin\left(\frac{\hbar k}{2m(E-V_1)+2m(V_2-E)}\right) \qquad \text{by Eq (3)}\\ &= \arcsin\left(\frac{\hbar k}{\sqrt{2m(V_2-V_1)}}\right) \qquad (24)\end{aligned}$$

Thus, Eq (16) becomes:

$$\frac{n\pi}{2}-\frac{kL}{2}=\arcsin\left(\frac{\hbar k}{\sqrt{2m(V_2-V_1)}}\right) \qquad (25)$$

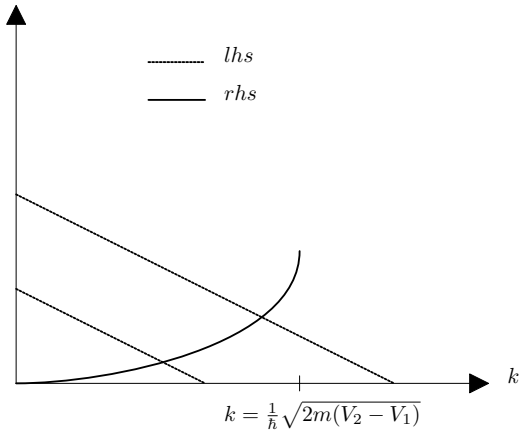
To find the actual energy levels is very difficult, as the above is a transcendental equation and thus must be solved either graphically or numerically. We can look at it graphically by plotting the left and right hand sides of the equation and looking for their intersections.

So solutions for $n > 1$ require:

$$\frac{n\pi}{2}-\frac{1}{\hbar}\sqrt{2m(V_2-V-1)}\frac{L}{2}\leq\frac{\pi}{2}$$

where

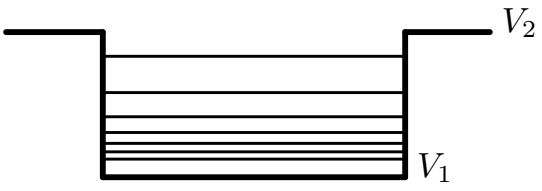
$$\frac{1}{\hbar}\sqrt{2m(V_2-V-1)}\frac{L}{2}$$



is the largest k allowed by the rhs of Eq (25).

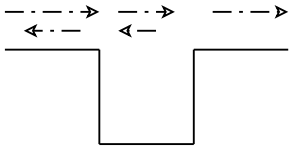
$$\Rightarrow \frac{L\sqrt{2m(V_2 - V_1)}}{\hbar} \geq (n-1)\pi$$

And thus there are a finite number of intersection points since the maximum value allowed for k is $\frac{\sqrt{2m(V_2-V_1)}}{\hbar}$ (which corresponds to the kinetic energy being equal to the depth of the well). Eg: in the figure below there are 7 allowed values (energies/intersection points).



$\underline{\mathbf{E} > \mathbf{V_2}}$:

Remark 4: In this range, there is 2-fold degeneracy. We will construct solutions for the wave originating form $-\infty$.



Thus, we will have a solution of the form:

$$\psi(x) = \begin{cases} A_+ e^{ik'x} + A_- e^{-ik'x}, & x < -L/2 \\ B_+ e^{ikx} + B_- e^{-ikx}, & |x| < L/2 \\ Ce^{ik'x}, & x > L/2 \end{cases} \tag{1}$$

where

$$\hbar k = \sqrt{2m(E - V_1)} \qquad \text{and} \qquad \hbar k' = \sqrt{2m(E - V_2)} \tag{2}$$

Solving the boundary conditions, we have continuity of ψ at $x = \pm L/2$:

$$A_+ e^{-ik'L/2} + A_- e^{ik'L/2} = B_+ e^{-ikL/2} + B_- e^{ikL/2} \tag{3}$$

$$B_+ e^{ikL/2} + B_- e^{-ikL/2} = Ce^{ik'L/2} \tag{4}$$

And by the continuity of ψ' at $x = \pm L/2$:

$$ik' \left(A_+ e^{-ik'L/2} - A_- e^{ik'L/2} \right) = ik \left(B_+ e^{-ikL/2} - B_- e^{ikL/2} \right) \tag{5}$$

$$ik \left(B_+ e^{ikL/2} - B_- e^{-ikL/2} \right) = ik' C e^{ik'L/2} \tag{6}$$

Solving these, if we go $k' \cdot (4) \pm (6)$, we get:

$$(k' + k) B_+ e^{ikL/2} + (k' - k) B_- e^{ikL/2} = 2k' C e^{ik'L/2} \tag{7}$$

$$(k' - k) B_+ e^{ikL/2} + (k' + k) B_- e^{-ikL/2} = 0 \tag{8}$$

From (8), we have

$$B_- = B_+ \frac{k - k'}{k + k'} e^{ikL} \tag{9}$$

Putting (9) $\rightarrow$ (6), gives C in terms of B_+

$$k \left(B_+ e^{ikL/2} - B_+ \frac{k - k'}{k + k'} e^{ikL/2} \right) = k' C e^{ik'L/2} \tag{10}$$

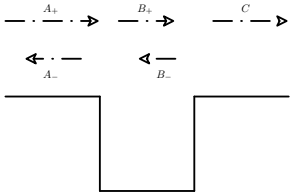
$$\Rightarrow C = \frac{-2k B_+ e^{i(k-k')L/2}}{k + k'} \tag{11}$$

Now, relate these to A_+ and A_-. Take $k' \cdot (3) + (5)$:

$$\begin{aligned} 2k' A_+ e^{-ik'L/2} &= (k' + k) B_+ e^{-ikL/2} + (k' - k) B_- e^{ikL/2} \\ &= B_+ e^{ikL/2} \left[(k + k') e^{-ikL} - \frac{(k - k')^2}{(k + k')} e^{ikL} \right] \quad \text{by (9)} \\ &= \frac{B_+ e^{ikL/2}}{(k + k')} \left[4kk' \cos(kL) - 2i(k^2 + (k')^2) \sin(kL) \right] \end{aligned}$$

$$\Rightarrow B_+ = \frac{A_+ e^{i(k+k')L/2}}{\frac{2k}{k+k'}\cos(kL) - \frac{i(k^2+(k')^2)}{k'(k+k')}\sin(kL)} \tag{12}$$

Remark 5: Note that



where $A_\pm, B_\pm, C$ are the amplitudes of the waves.

Remark 6: We may choose A_+ to be the overall scale factor of the wave, and thus we get the other constants in terms of A_+. The most important coefficients are C and A_-.

Now from (11) and (12):

$$\frac{C}{A_+} = \frac{e^{-ik'L}}{\cos(kL) - \frac{i(k^2+(k')^2)}{2kk'}\sin(kL)} \tag{13}$$

And we also have:

$$\frac{A_-}{A_+} = e^{-ik'L} \cdot \frac{(k^2-(k')^2)}{2kk'} \cdot \frac{\sin(kL)}{\cos(kL) - \frac{i(k^2+(k')^2)}{2kk'}\sin(kL)} \tag{14}$$

Remark 7: One can show that

$$\left|\frac{C}{A_+}\right|^2 + \left|\frac{A_-}{A_+}\right|^2 = 1 \tag{15}$$

Physically, A_+, as illustrated in Remark 5, represents an incoming beam of particles which scatter off the square potential. Transmitted particles are represented by the beam with amplitude C, and the reflected particles are represented by the beam with amplitude A_-. So, by (15), the incident particle flux ($\propto |A_+|^2$) = the transmitted flux flux ($\propto |C|^2$) + the reflected flux ($\propto |A_-|^2$).

Remark 8: From (13) and (14), we know that if:

$$k_n L = n\pi \tag{16}$$

then the transmission coefficient $\left|\frac{C}{A_+}\right|^2 = 1$ and the reflection coefficient $\left|\frac{A_-}{A_+}\right|^2 = 0$. This gives a series of transmission resonances with resonance energies:

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 \tag{17}$$

At these energies, the entire wave is transmitted.

Remark 9: The energies in (17) are not discrete in the sense of the energies confined in the well. All the energies in the neighborhood of the resonance energies are allowed, but the transmitted wave amplitude is diminished if not at resonance.

Remark 10: The sharpness of resonances is determined by the ratio between k and k'. Consider the case where

$$(\frac{k'}{k})^2 = \frac{E - V_2}{E - V_1} \ll 1 \qquad \Rightarrow V_1 \ll V_2 \text{ (a deep well)} \tag{18}$$

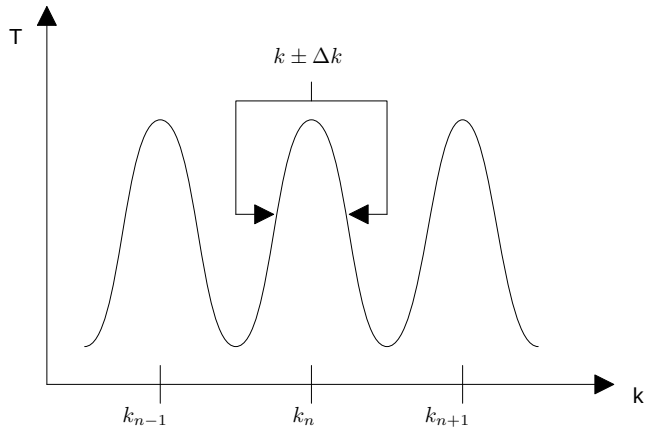
Then

$$\left|\frac{C}{A_+}\right|^2 \approx \frac{1}{\cos^2(kL) + \left(\frac{k}{2k'}\right)^2 \sin^2(kL)} \tag{19}$$

In between resonances, where $\sin^2(kL) \approx 1$, we have

$$\left|\frac{C}{A_+}\right|^2 \approx 4\left(\frac{k'}{k}\right)^2 \ll 1 \tag{20}$$

This implies that transmission nearly vanishes between resonances (but not completely!).



To approximate resonance widths, let's expand the $\cos(kL)$ and $\sin(kL)$ in the vicinity of the resonance.

$$\begin{aligned}
\cos(kL) = \cos(k_nL + \Delta k_nL) &= \cos(k_nL)\cos(\Delta k_nL) - \sin(k_nL)\sin(\Delta k_nL) \\
&\approx (\pm 1)\cos(\Delta k_nL) + (0)\sin(\Delta k_nL) \\
&\approx \pm 1 \qquad \text{for small } \Delta k_n \\
\sin(kL) = \sin(k_nL + \Delta k_nL) &= \cos(k_nL)\sin(\Delta k_nL) + \cos(\Delta k_nL)\sin(k_nL) \\
&\approx (\pm 1)\sin(\Delta k_nL) + \cos(\Delta k_nL)(0) \\
&\approx \pm \Delta k_nL \qquad \text{for small } \Delta k_n
\end{aligned}$$

With this in mind, in the vicinity of the resonance, (19) becomes:

$$\left|\frac{C}{A_+}\right|^2 \approx \frac{1}{1+\left(\frac{k_n}{2k_n'}\right)^2(\Delta k_n)^2L^2} \tag{21}$$

In order to get the width at the half-max point of the peak, we set the above to 1/2. This implies that:

$$\begin{aligned}\Delta k_n L &= \frac{2k_n'}{k_n} \\ &\ll 1 \qquad \text{for deep wells}\end{aligned}$$

And so we can define a half-width in k by

$$\underbrace{\Delta k_n}_{k-k_n} = \frac{2k_n'}{k_n L} \tag{22}$$

Remark 11: We can convert to the half-width in energy by substituting (3) into (22):

$$\begin{aligned}\sqrt{2m(E-V_1)} - \hbar k_n &= \frac{2\hbar k_n'}{k_n L} \\ \sqrt{2m(E-V_1)+2m(E_n-V_1)} - \hbar k_n &= \frac{2\hbar k_n'}{k_n L} \\ \underbrace{\sqrt{2m(E_n-V_1)}}_{\hbar k_n}\cdot\left(1+\frac{1}{2}\frac{E-E_n}{E_n-V_1}\right) - \hbar k_n &\approx \frac{2\hbar k_n'}{k_n L}\end{aligned}$$

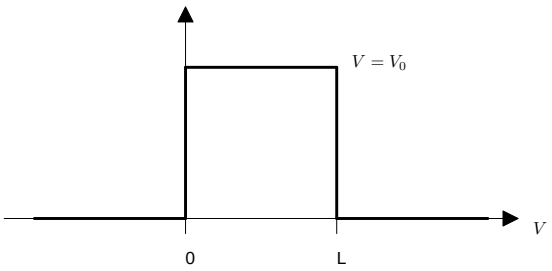
where the term in parenthesis is the first terms of the Taylor expansion, which we can use since we are in a deep well and the ratio is very small. Now, if we let $\Delta E_n = E - E_n$, we have:

$$\begin{aligned}\Delta E_n &\approx \frac{4\hbar k_n'}{k_n L}\frac{(E_n-V_1)}{\hbar k_n} \\ &\approx \frac{4\sqrt{2m(E_n-V_2)}(E_n-V_1)\hbar}{L\cdot 2m(E_n-V_1)} \\ &\approx \sqrt{\frac{8\hbar^2(E_n-V_2)}{mL^2}}\end{aligned} \tag{23}$$

Remark 12: Eq (23) is valid *only* for *deep* potentials.

4.5 Square Potential Barrier and Tunneling

Consider the following potential



The methods from §2.2-2.4 can be applied here, though we don't do them explicitly here.
The new feature here is the tunneling effect, which can occur when $0 < E < V_0$. Classically, an incoming particle will be reflected at the barrier. Quantum Mechanicaly, a wave function can experience barrier penetration. In some cases, this penetration is far enough that the wave can emerge from the other side, as seen in Fig. 4.2.

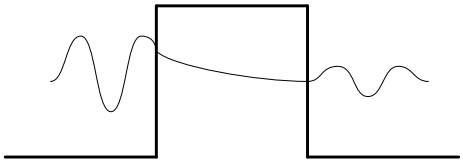


Figure 4.2: An incident wave tunneling through a step barrier.

Thus, the quantum particle can tunnel through the potential.

Remark 1: The size of the transmitted wave is determined by the height of the potential (which sets the decay rate for the exponential solution), and the width of the potential.

4.6 General Properties of 1-D Schrodinger Equation

Here, we summarize some of the results of §2.1-2.5.

Remark 1: Here we are considering the time independent Schrodinger equation in 1-D with one restriction on the potential, $V(x)$:

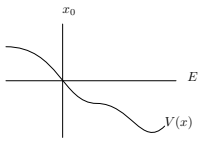
- $V(x)$ is a real function, bounded from below and piece-wise continuous over the real line.

Remark 2: The following properties can be shown mathematically in Messiah. Here, we just state the results. These should be *MEMORIZED*!

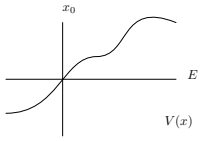
4.6.1 Asymptotic Behavior of Solutions

Here, let's state the results for $x \to \infty$; similar results hold for $x \to -\infty$. Choose x_0 so that either

1. $E - V(x) > 0 \qquad \forall x > x_0$



2. $E - V(x) < 0 \qquad \forall x > x_0$



Case 1: Solutions to the Schrodinger equation oscillate and are bounded as $x \to \infty$. If $\lim_{x\to\infty} V(x) = V^+ < \infty$, (or $V(x) < \infty$), and if it does so faster than $\frac{1}{x}$, then the asymptotic solution of the equation is:

$$\psi \sim_{x\to\infty} A_+ \sin(kx + \phi_+), \qquad \text{where } \hbar k = \sqrt{2m(E - V^+)}$$

Case 2: For $E < V_{min} < V(x)$, and for $x > x_0$, one solution decays faster than

$$\psi \sim e^{-\kappa x}, \qquad \text{where } \hbar\kappa = \sqrt{2m(V_{min} - E)}$$

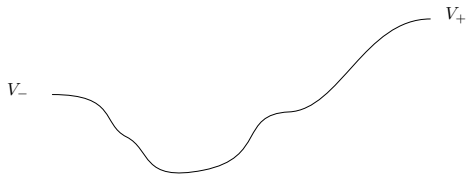
All other solutions diverge at least as fast as $e^{\kappa x}$, and are eliminated on the basis of physical realizability. (§2.3 - Remark 4)

4.6.2 Nature of Energy Eigenvalues

Assume that

$$V(x) \xrightarrow{x\to\infty} V_+, \qquad V(x) \xrightarrow{x\to-\infty} V_-, \qquad V_+ > V_-$$

which will look something like:



Then there are 3 energy ranges for which the following properties hold:

1. $E > V_+$: Energy spectrum is *continuous* and *degenerate* (there can be left or right travelling waves). The states themselves are *unbounded*.
2. $V_- < E < V_+$: Spectrum is continuous, but *non-degenerate* (waves can only come in from the left and reflect back to the left). States are unbounded.
3. $E < V_-$: If solutions exist, they have discrete energies and are bounded ($\psi \to 0$ as $x \to \pm\infty$). Spectrum is non-degenerate.

Remark 1: Non-degeneracy is *not* a general property of bound states. In multi-dimensions, we can have bound, degenerate states.

Chapter 5

Wave Packets

In the previous chapter, we looked at a variety of 1-D problems, and particularly at solutions with waves extended from $-\infty$ to ∞. Physically, such waves don't exist(though reflection, transmission, barrier penetration and tunneling *do* occur). Instead, we have wave packets.

5.1 Plane Waves

The simplest wave with frequency ν and wavelength λ is a plane wave:

$$\psi(\mathbf{r}, t) \sim e^{-i(\omega t - \mathbf{k}\cdot\mathbf{r})}$$

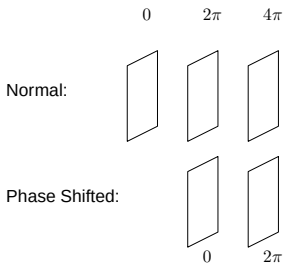
where $\omega = 2\pi\nu$ and $k = \frac{2\pi}{\lambda}$.

Remark 1: The wave propagates in the direction of $\hat{k}$.

Definition 1: The phase velocity of this wave is:

$$v_{phase} = \frac{\omega}{k}\hat{k} = \nu\lambda\hat{k}$$

This gives the speed at which planes of equal phase move in the direction $\hat{k}$. As a visual confirmation, consider a normal set of plane waves and a phase shifted set, as shown below.



We can see that the speed of the plane will be

$$\frac{\lambda}{T} = \lambda\nu = \frac{\omega}{k}$$

in *both* cases.

Definition 2: The period, T, is $T = \frac{1}{\nu}$.

Remark 2: We can not really associate plane waves with the motion of a particle (at least, not in the classical sense). For this, we need to use wave packets.

5.2 Wave Packets

First, consider the motion of a classical particle. Here, the velocity is given by

$$v_{class} = \frac{p}{m}\hat{p} = \frac{2E}{p}; \qquad \text{Since } E = \frac{p^2}{2m} \text{ for free particles}$$

Remark 1: Quantum mechanical particles, like light, possess wave-particle duality, in which they can exhibit properties of both waves and particles, though the properties can not be simultaneously observed.

For a quantum particle with energy E, we associate a wave-frequency by

$$E = \hbar\omega$$

Remark 2: de Broglie developed the theory of matter waves based on the assumption that particles have wave properties.

For a particle with momentum $\mathbf{p}$, we assign a wave number k by

$$\mathbf{p} = \hbar\mathbf{k} = \hbar k\hat{k}$$

This is called the de Broglie relation. Since we can identify a wave with a particle, we can also identify a phase speed:

$$\mathbf{v}_{phase} = \frac{\omega}{k}\hat{k} = \frac{E}{p}\hat{k} = \frac{E}{p}\hat{p}$$

which differs from the classical case by a factor of 2.
To find a relation between de Broglie's matter waves and the speed of a classical particle, consider

$$\hbar\omega = E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

which gives

$$\omega = \frac{\hbar k^2}{2m} = \frac{\hbar}{2m}(k_x^2 + k_y^2 + k_z^2) \tag{†}$$

And

$$\begin{aligned}\nabla_{\mathbf{k}}\omega &= \frac{\partial\omega}{\partial k_x}\hat{x} + \frac{\partial\omega}{\partial k_y}\hat{y} + \frac{\partial\omega}{\partial k_z}\hat{z} \\ &= \frac{\hbar}{m}(k_x\hat{x} + k_y\hat{y} + k_z\hat{z}) \\ &= \frac{\mathbf{p}}{m} \\ \Rightarrow \nabla_{\mathbf{k}}\omega &= \mathbf{v}_{class}\end{aligned}$$

Or, in 1-D

$$\frac{\partial\omega}{\partial k} = \frac{\hbar k}{m} = \frac{p}{m} = v_{class}$$

Remark 3: A dispersion relation is given by the frequency as a function of k: $\omega(k)$.

Remark 4: Here, we can obtain the classical velocity from the dispersion relation. To associate a wave with a particle, we need waves of limited extent (not plane waves, but wave packets). Wave packets can be constructed as a superposition of plane waves and can be expressed as

$$\psi(\mathbf{r}, t) = \int_{-\infty}^{\infty} d^3k'\, f(k')e^{-i(\omega' t - \mathbf{k}'\cdot\mathbf{r})} \tag{‡}$$

Remark 5: $f(k)$ gives the "weighting" of the superimposed plane waves. It is generally complex, so it defines the amplitudes *and* the phases of the waves that are added together.

Remark 6: Wave packets that are localized in space(like (‡)), move as a whole at the group velocity.

$$\mathbf{v}_{group} = \nabla_{\mathbf{k}'}\omega'\big|_{k'=k}$$

where k is the value of k' where $f(k')$ is peaked. The group velocity corresponds to the classical velocity of a particle.

5.2.1 Spacial Extent of Wave Packets

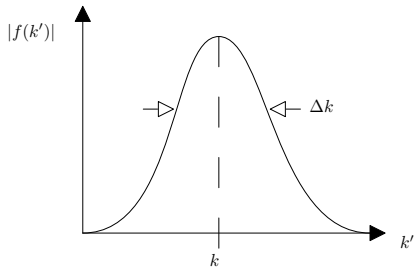
For now, let us consider a 1-D wave packet.

$$\psi(x, t) = \int_{-\infty}^{\infty} dk'\, f(k')e^{-i(\omega t - k'x)} \tag{1}$$

At time t=0:

$$\psi(x,0) = \int_{-\infty}^{\infty} dk'\, f(k') e^{ik'x} \tag{2}$$

A generic form of $|f(k')|$ is:



If we let $k' = k + \Delta k'$,

$$\psi(x,0) = e^{ikx} \int_{-\infty}^{\infty} d\Delta k'\, f(k + \Delta k') e^{i\Delta k' x} \tag{3}$$

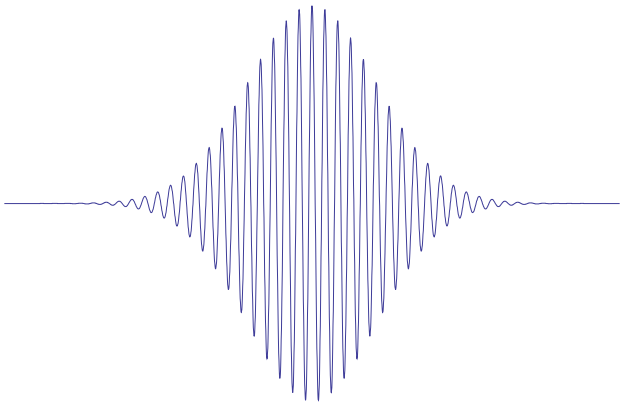
The above is akin to shifting the peak to the origin in the $\Delta k'$ integration.
Now, consider (3) for different values of x:

- x=0:

  $$\psi(0,0) = \int_{-\infty}^{\infty} d\Delta k'\, f(k + \Delta k') \neq 0$$

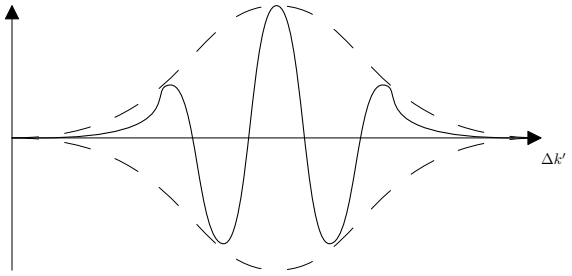
  If $f(k')$ is real, this is just the area under the curve, and thus $\neq 0$.

- $x = \frac{100}{\Delta k}$: $f(k')$ is only significantly different from 0 for the range of $\Delta k'$ given by $-\Delta k < \Delta k' < \Delta k$. This implies that the phase of the oscillary term inside (3) varies over the range $-100 < \Delta k' x < 100$. This range covers about 30 cycles of 2π, so that the real part of $f(k+\Delta k')e^{i\Delta k' x}$ looks like:

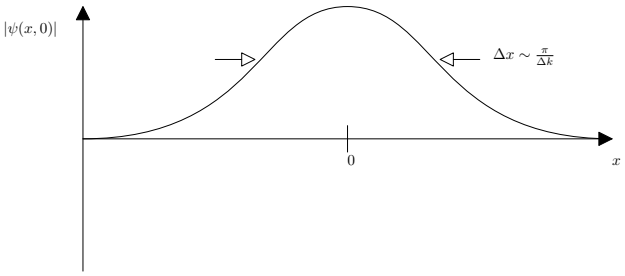
  

  The imaginary part looks similar with oscillating phase shifted by π. When the integral (3) is done over this function, it is very close to zero, which results in a limited spacial extent of the packet.

Remark 1: $x = 0$ gives the largest contribution to the wave function ($\psi(x, 0)$), and, for $x \gg \frac{1}{\Delta k}$, we get almost no contribution. For ranges $\frac{-\pi}{\Delta k} \lesssim x \lesssim \frac{\pi}{\Delta k}$, there is a small, but negligible contribution to $\psi(x, 0)$. Take $x = \frac{\pi}{\Delta k}$:



And integral (3) doesn't quite vanish because small values of x imply slower oscillations which give bigger contributions, while large values of x imply faster oscillations, which contribute nearly zero. This behavior gives a modulus wavefunction that looks like:



Remark 2: This acts as an envelope function for e^{ikx}, multiplying the integral in (3). So the wave function is a rapidly oscillating function with peaks at $x = 0$ and is only significantly different from zero in the region $\frac{-\pi}{\Delta k} \sim -\Delta x < x < \Delta x \sim \frac{\pi}{\Delta k}$.

Remark 3: For instance, a classical particle:

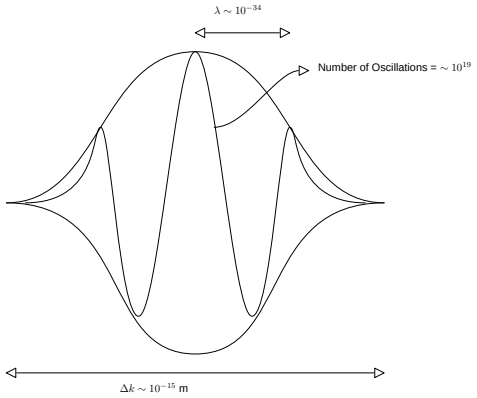
$$m = 1 \text{ kg}, \qquad v = 10 \text{ m/s}, \qquad \Delta x \sim 10^{-15} \text{ m}$$

where the value of Δx is approximately the size of an atomic nucleus. Now,

$$\begin{aligned} mv = \hbar k &= 10 \text{ kg m /s} \\ \Rightarrow k &= 10^{35} \text{ m}^{-1} \\ \Rightarrow \lambda &= \frac{2\pi}{k} \sim 10^{-24} \text{ m} \end{aligned}$$

The range, Δk of k needed to achieve this localization (Δx) is

$$\Delta k \sim \frac{\pi}{\Delta x} \sim 10^{15} \text{m}^{-1}$$



$$\Rightarrow \frac{\Delta k}{k} \sim 10^{-20}$$

This implies that we need an accuracy to 21 decimal places if we want more than a single wave number to contribute to the wave packet. And thus a classical particle has a well defined position and momentum.

Remark 4: Now, for an electron:

$$m = 9 \times 10^{-31} \text{ kg}, \qquad E = 1 \text{ eV } = 1.6 \times 10^{-19} \text{ J}$$

Consider $\Delta k \sim 10^{-10}$ m, which is about the size of an atom.

$$\hbar k = \sqrt{2mE} \Rightarrow k \sim 2 \times 10^{11} \text{ m}^{-1}$$
$$= \lambda = \frac{2\pi}{k} = 3 \times 10^{-11} \text{ m}$$

Here, the range needed to achieve localization is $\Delta k \sim \frac{\pi}{\Delta x} \sim 3 \times 10^{10} \text{m}^{-1}$.

$$\Rightarrow \frac{\Delta k}{k} \sim 0.1$$

And so a wave packet living in $\Delta x \sim 10^{-10}$ is made up of many wave numbers and does not have a well defined momentum.

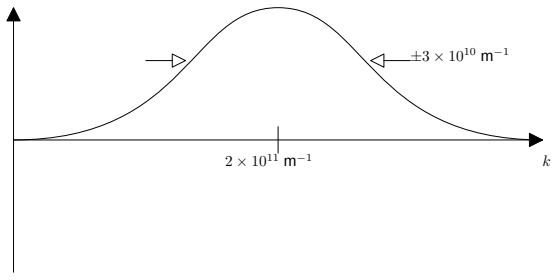


Figure 5.1: K Space representation of the wave packet.

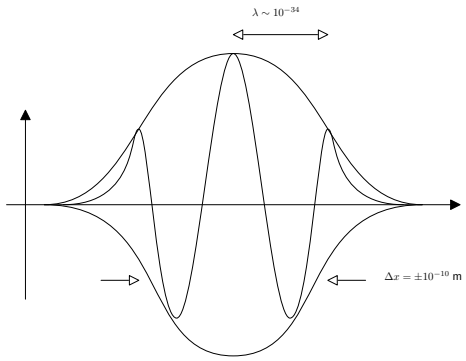


Figure 5.2: Real Space representation of the wave packet.

5.2.2 Motion of the Wave Packet

For a wave packet that represents a particle in the classical limit, the group velocity (as defined in §5.2, Remark 6) corresponds to the classical velocity of a particle.
Consider (1) of the previous section.

$$\psi(x,t) = \int_{-\infty}^{\infty} dk'\, f(k') e^{-i(\omega' t - k' x)}$$

with $k' \to k + \Delta k'$ and $\omega' \to \omega + \Delta\omega'$

$$\Rightarrow \psi(x,t) = e^{-i(\omega t - kx)} \int_{-\infty}^{\infty} d\Delta k' f(k + \Delta k') e^{-i(\Delta\omega' t - \Delta k' x)}$$

Following the same arguments, we can demonstrate that there is a localized wave packet, but, if $t \neq 0$, the wave packet has moved.
Consider the phase $\phi = \Delta\omega' t - \Delta k' x$. The position x is given as the position that causes ϕ to change the slowest as $\Delta k'$ varies over the relevant range.

$$\left.\frac{d\phi}{d\Delta k'}\right|_{\Delta k'=0} = 0$$

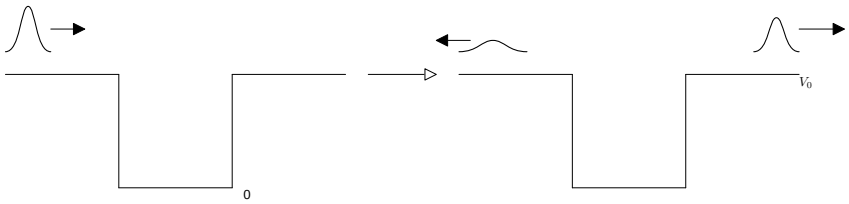
$$\Rightarrow 0 = \left.\frac{d\Delta\omega'}{d\Delta k'}\right|_{\Delta k'=0} \cdot t - x$$

And this gives exactly the group velocity of the wave:

$$v_{group} = \frac{x}{t} = \left.\frac{d\Delta\omega'}{d\Delta k'}\right|_{\Delta k'=0} = \left.\frac{d\omega'}{dk'}\right|_{k'=0}$$

5.2.3 Delay of Wave Packets at Resonance

Consider reflection and transmission of a wave packet at a square potential for energies $E > V_0$:



What is the delay in the appearance of the transmitted pulse?
The incident wave packet is:

$$\psi_i(x,t) = \int dk' A_+(k') e^{-i(\omega' t - k' x)} \tag{†}$$

where $A_+(k')$ is centered at k'_n resonance.
The transmitted wave packet is:

$$\psi_T(x,t) = \int dk' A_+(k') \frac{C(k')}{A_+(k')} e^{-i(\omega' t - k' x)}$$

From Ch 4, Section 2, Eqn (13):

$$\frac{C}{A_+} = \frac{e^{ik'L}}{\cos(kL) - \frac{i(k^2+(k')^2)}{2kk'}\sin(kL)}$$

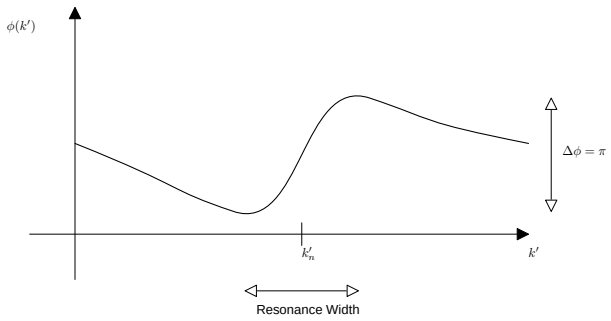
$$\Rightarrow \psi_T(x,t) = \int dk' \frac{A_+(k') e^{-i(\omega' t - k' x - \phi)}}{\cos^2(kL) + \frac{(k^2+(k')^2)^2}{(2kk')^2}\sin^2(kL)} \tag{‡}$$

where

$$\phi(k') = -k'L + \arctan\left(\frac{k^2+(k')^2}{2kk'}\tan(kL)\right)$$

(Here we just have written the complex number C/A_+ in its polar form). For sharp resonances, $k'/k \ll 1$, and in the vicinity of the resonance we have

$$\phi(k') \approx -k'_n L + \arctan\left(\frac{k_n}{2k'_n}\tan\left((k-k_n)L\right)\right)$$



To figure out the time delay, we note that the phase in the integrals (†) and (‡) must be minimized for the maximum contribution to the incident and transmitted waves. The incident wave simply comes in at the group velocity (§5.2.2), while the transmitted wave has a delay.

$$\begin{aligned}\Rightarrow \frac{d}{dk'}(\omega' t - k' x - \phi)\Big|_{k'=k'_n} &= \frac{d\omega'}{dk'}\Big|_{k'=k'_n} t - x - \frac{d\phi}{dk'}\Big|_{k'=k'_n} = 0 \\ &= v_{group} t - x - \frac{d\phi}{dk'}\Big|_{k'=k'_n} = 0\end{aligned}$$

where

$$\frac{d\phi}{dk'} \approx \frac{\pi}{\text{Res. Width}}$$

by a rise over run argument. Then

$$x = \frac{\hbar k}{m} t + \frac{d\phi}{dk'}\Big|_{k'=k'_n} = \frac{\hbar k}{m}(t+\tau)$$

where τ is the time delay at resonance.

$$\tau = \frac{m}{\hbar k}\,\frac{d\phi}{dk'}\Big|_{k'=k'_n} \approx \frac{m}{\hbar k'_n}\frac{\pi}{\text{Res. Width}}$$

Remark 1: In order for this picture to hold, we assume that the envelope function of the wave packet hold together so that there is a well defined peak across the barrier. To ensure this, the wave must be broad enough (in x), so that the delay is small compared to the motion of the packet:

$$\tau \ll \left(\frac{\hbar k}{m}\right)^{-1} \Delta k$$

Chapter 6

Harmonic Oscillator and Second Quantization

The harmonic oscillator (H.O.) is an important example in QM. A major application of H.O. is QED, where elementary excitations (modes) of the electromagnetic field are formally harmonic oscillations. This also leads to the generalization of QED, which is quantum field theory. Another major application covers all areas where there are harmonic oscillations about some equilibrium (like vibrations of molecules in crystals).

6.1 Harmonic Oscillator in Position Representation

The Hamiltonian for a single oscillator is

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \tag{1}$$

where $\omega = \sqrt{k/m}$ is the classical frequency.

Remark 1: A particle that is experiencing small oscillations about a stable equilibrium of potential V(x) may be approximated by (1). If x_0 is a stable equilibrium about V(x), then

$$V(x) \approx V(x_0) + \underbrace{\left.\frac{dV}{dx}\right|_{x_0}}_{0}(x - x_0) + \frac{1}{2}\left.\frac{d^2V}{dx^2}\right|_{x_0}(x - x_0)^2 + \cdots$$

For small oscillators,

$$V(x) \approx \frac{1}{2}\left.\frac{d^2V}{dx^2}\right|_{x=x_0}(x - x_0)^2 \to \frac{1}{2}\left.\frac{d^2V}{dx^2}\right|_0 x^2 = \frac{1}{2}m\omega^2x^2$$

with $m\omega^2 = \frac{d^2V}{dx^2}|_0$.

Remark 2: For an n-oscillator system, the Hamiltonian may be diagonalized to a system of n decoupled oscillators, as was done in Problem 1.8.10 for 2 oscillators. In such a system, the Hamiltonian may be written as:

$$\hat{H} = \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{P_i P_j \delta_{ij}}{2m} + \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} x_i V_{ij} x_j$$

with

$$V_{ij} = \left.\frac{\partial^2 V}{\partial x_i \partial x_j}\right|_0 = \left.\frac{\partial^2 V}{\partial x_j \partial x_i}\right|_0 = V_{ji}$$

The time dependent solution of the quantized HO can be captured by acting the propagator (§3.4.1) on the time-independent solution. So our goal here is to solve the time-independent Schrodinger equation in the coordinate basis:

$$\hat{H}\left|E_n\right\rangle = E_n \left|E_n\right\rangle$$

where $\hat{H}$ is given in (1). In position representation:

$$\begin{aligned}\left\langle x\right|\hat{H}\left|E_n\right\rangle &\to \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right)\psi_E(x)\\ \left\langle x\right|E_n\left|E_n\right\rangle &\to E\psi_E(x)\end{aligned}$$

So the time independent eigenvalue equation is:

$$\frac{d^2}{dx^2}\psi_E + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega^2 x^2\right)\psi_E = 0 \tag{2}$$

Following the procedure is Shankar:

1. Non-dimensionalize (2). Let

$$y = \sqrt{\frac{m\omega}{\hbar}}x \qquad \text{and} \qquad \xi = \frac{E}{\hbar\omega} \tag{3}$$

Then

$$\frac{d}{dx} \to \sqrt{\frac{m\omega}{\hbar}}\frac{d}{dy}$$

And thus, under the change of coordinates, (2) becomes

$$\frac{d^2}{dy^2}\psi_E + (2\xi - y^2)\psi_E = 0 \tag{4}$$

Remark 3: The scaling defines a natural length scale in the problem $\sim \frac{\hbar}{m\omega}$

2. Investigate the asymptotic behavior.
   Consider $\lim_{y\to 0}$ and $\lim_{y\to\infty}$.

$$\lim_{y\to\infty}(4) \Rightarrow \frac{d^2\psi}{dy^2} - y^2 = 0 \tag{5}$$

The solution as $y \to \infty$ then is:

$$\psi = Ay^m e^{\pm y^2/2} \tag{6}$$

$$\lim_{y\to 0}(4) \Rightarrow \frac{d^2\psi}{dy^2} + 2\xi\psi = 0 \tag{7}$$

This has a solution of the form:

$$\psi = A\cos(\sqrt{2\xi}y) + B\sin(\sqrt{2\xi}y) \tag{8}$$

Remark 4: In Eq (7), we have already neglected terms of order y^2, so we should only keep terms with order $< y^2$ in (8).

$$\Rightarrow \psi \sim A + B\sqrt{2\xi}y + \mathcal{O}(y^2) \tag{9}$$

3. Make an ansatz of a solution that satisfies the asymptotic behavior. Note that an ansatz is like an educated guess as to the solution.

$$\psi(y) = u(y)e^{-y^2/2} \tag{10}$$

Now, substitute (10) into (4) to derive a DE for $u(y)$:

$$\begin{aligned}\frac{d^2\psi}{dy^2} &= \frac{d}{dy}\left(\frac{du}{dy}e^{-y^2/2} - uye^{-y^2/2}\right)\\ &= \frac{d^2u}{dy^2}e^{-y^2/2} - 2\frac{du}{dy}ye^{-y^2/2} + uy^2e^{-y^2/2} - ue^{-y^2/2}\\ &= -(2\xi - y^2)ue^{-y^2/2} \qquad \text{by (4)}\end{aligned}$$

$$\Rightarrow \frac{d^2u}{dy^2} - 2y\frac{du}{dy} + (2\xi - 1)u = 0 \tag{11}$$

4. Solve (11); Try a power series solution. Let's try:

$$u(y) = \sum_{n=1}^{\infty} C_n y^2 \tag{12}$$

Substituting (12) into (11) yields:

$$\begin{aligned}
0 &= \sum_{n=0}^{\infty} C_n \left[n(n-1)y^{n-2} - 2ny^n + (2\xi - 1)y^n \right] \\
&= \sum_{n=0}^{\infty} C_n \left[n(n-1)y^{n-2} + (-2n + 2\xi - 1)y^n \right] \\
&= \sum_{n=2}^{\infty} C_n n(n-1)y^{n-2} + \sum_{n=0}^{\infty} C_n(2\xi - 1 - 2n)y^n \\
&= \sum_{n=0}^{\infty} C_{n+2}(n+2)(n+1)y^n + \sum_{n=0}^{\infty} C_n(2\xi - 1 - 2n)y^n \\
&= \sum_{n=0}^{\infty} \left[C_{n+2}(n+2)(n+1) + C_n(2\xi - 1 - 2n) \right] y^n
\end{aligned}$$

Since the y's are linearly independent, the coefficients must vanish and this results in a recursion relation for the coefficients:

$$C_{n+2} = \frac{-C_n(2\xi - 1 - 2n)}{(n+2)(n+1)} \tag{13}$$

So given C_0 and C_1, (13) gives all the rest of the coefficients in (12), and thus the solution to (10)...and thus the solution to our non-dimensionalized Schrodinger equation (4).

Remark 5: The solution given by (3),(10),(12),and (13) doesn't seem to constrain the energy eigenvalues as expected. However, recall the asymptotic solution as $y \to \infty$ (See (6)). For a finite wavefunction, we take the negative in the exponential, and thus $u(y) \xrightarrow{y \to \infty} y^m$. But the solution (12) does not terminate at finite n unless $C_n = 0$ for some n. The recursion relation (13) has C_{n+2} vanish for arbitrary C_n when

$$\xi = n + \frac{1}{2} \tag{14}$$

So physically realizable solutions only occur at discretized energy eigenvalues. From (3) and (14):

$$E = \hbar\omega(n + \frac{1}{2}), \qquad n = 0, 1, 2, \ldots \tag{15}$$

Remark 6: Here we have only positive (or 0) values of n since we can easily show that the energy eigenvalues can not be negative.

$$\left\langle \hat{H} \right\rangle = \frac{1}{2m} \underbrace{\langle \psi | P^2 | \psi \rangle}_{\text{positive}} + \frac{1}{2} m\omega^2 \underbrace{\langle \psi | x^2 | \psi \rangle}_{\text{positive}} \geq 0$$

Remark 7: For n odd, let $C_0 = 0$, and for n even, let $C_1 = 0$. Then the solution to (4) is

$$\begin{aligned}\psi(y) &= u(y)e^{-y^2/2} \\ &= e^{-y^2/2} \underbrace{\begin{cases} C_0 + C_2 y^2 + C_4 y^4 + \cdots + C_n y^n, & n = \text{even} \\ C_1 y + C_3 y^3 + \cdots + C_n y^n, & n = \text{odd} \end{cases}}_{\text{These are Hermite Polynomials, } H_n(y)}\end{aligned}$$

Remark 8: Normalizing (15) to get C_0 or C_1 gives the final solution

$$\begin{aligned}\psi_E(x) &\equiv \psi_{(n+1/2)\hbar\omega}(x) \equiv \psi_n(x) \\ &= \left(\frac{m\omega}{\pi\hbar 2^{2n}(n!)^2}\right)^{1/2} \exp\left(\frac{-m\omega x^2}{2\hbar}\right) H_n\left[\left(\frac{m\omega}{\hbar}\right)^{1/2} x\right] \end{aligned} \tag{17}$$

6.2 Second Quantization: Creation and Annihilation Operators

6.2.1 Harmonic Oscillator in Energy Eigenbasis

Remark 1: Here we solve the HO using an entirely different approach using creation and annihilation operators. This method is due to Dirac and is central to QED. One advantage is that we do not have to solve any differential equations–we can extract the energy eigenvalues from the underlying operator algebra. In this approach, we can also extract the physical content from the Hilbert space and the operators that act on it, rather than from the wave functions obtained from the solution of the Schrodinger equation.

Definition 1: The Creation and Annihilation operators are given by the following:

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} - \frac{i}{m\omega}\hat{p}\right)$$

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} + \frac{i}{m\omega}\hat{p}\right)$$

respectively, where $\hat{q}$ is the position operator. The reason for the names will become obvious shortly.

Remark 2: The commutation relation for $\hat{a}$ and $\hat{a}^\dagger$ are:

$$[\hat{a}, \hat{a}] = 0 = [\hat{a}^\dagger, \hat{a}^\dagger]$$

$$\begin{aligned}
[\hat{a}, \hat{a}^\dagger] &= \frac{m\omega}{2\hbar}\left[\hat{q} + \frac{i}{m\omega}\hat{p}, \hat{q} - \frac{i}{m\omega}\hat{p}\right] \\
&= \frac{m\omega}{2\hbar}\left([\hat{q},\hat{q}] + \frac{1}{m^2\omega^2}[\hat{p},\hat{p}] + \frac{i}{m\omega}[\hat{p},\hat{q}] - \frac{i}{m\omega}[\hat{q},\hat{p}]\right) \\
&= \frac{m\omega}{2\hbar}\left(-\frac{2i}{m\omega}\underbrace{[\hat{q},\hat{p}]}_{i\hbar}\right) \\
&= 1
\end{aligned}$$

Remark 3: we can obtain the operators $\hat{p}$ and $\hat{q}$ in terms of $\hat{a}$ and $\hat{a}^\dagger$:

$$\hat{q} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger)$$

$$\hat{p} = -i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a} - \hat{a}^\dagger)$$

Therefore, we can write the Hamiltonian as:

$$\begin{aligned}
\hat{H} &= \frac{1}{2m}\left(-\frac{\hbar m\omega}{2}\right)(\hat{a}\hat{a} - \hat{a}\hat{a}^\dagger - \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}^\dagger) + \\
&\quad + \frac{1}{2}m\omega^2\left(\frac{\hbar}{2m\omega}\right)(\hat{a}\hat{a} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}^\dagger) \\
&= \frac{1}{2}\hbar\omega(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) \\
&= \hbar\omega\left(\hat{N} + \frac{1}{2}\right) \qquad (\dagger)
\end{aligned}$$

Where we define the number operator $\hat{N} \equiv \hat{a}^\dagger\hat{a}$.

Remark 4: With the Hamiltonian given in the form (†), the problem is reduced to finding eigenvalues of $\hat{N}$.

To determine the eigenvalues of $\hat{N}$, we can denote the eigenstates of $\hat{N}$:

$$\hat{N}\,|\nu\rangle = \nu\,|\nu\rangle$$

and establish a relationship between the eigenstates.

Remark 5: If $|\nu\rangle$ is an eigenstate of $\hat{N}$, so is $\hat{a}\,|\nu\rangle$ (an eigenstate).

$$\begin{aligned}\hat{N}\hat{a}\,|\nu\rangle &= \hat{a}^\dagger\hat{a}\hat{a}\,|\nu\rangle \\ &= (\hat{a}\hat{a}^\dagger - 1)\hat{a}\,|\nu\rangle \\ &= \hat{a}(\underbrace{\hat{a}^\dagger\hat{a}}_{\hat{N}})\,|\nu\rangle - \hat{a}\,|\nu\rangle \\ &= \hat{a}\nu\,|\nu\rangle - \hat{a}\,|\nu\rangle \\ &= (\nu-1)\hat{a}\,|\nu\rangle\end{aligned}$$

with eigenvalue $(\nu - 1)$. Similarly, $\hat{a}^\dagger$ is an eigenstate of $\hat{N}$ with eigenvalue $(\nu + 1)$.

$$\hat{N}\hat{a}^\dagger\,|\nu\rangle = (\nu+1)\hat{a}^\dagger\,|\nu\rangle$$

Remark 6: The eigenstates $|\nu\rangle, \hat{a}\,|\nu\rangle, \hat{a}^\dagger\,|\nu\rangle$ of $\hat{N}$ are also eigenstates of $\hat{H}$ with energy eigenvalues:

$$\left(\nu + \frac{1}{2}\right)\hbar\omega \qquad \text{for } |\nu\rangle$$

$$\left(\nu - \frac{1}{2}\right)\hbar\omega \qquad \text{for } \hat{a}\,|\nu\rangle$$

$$\left(\nu + \frac{3}{2}\right)\hbar\omega \qquad \text{for } \hat{a}^\dagger\,|\nu\rangle$$

Repeated application of $\hat{a}$ or $\hat{a}^\dagger$ generates a whole series of energy eigenstates. Eg:

E-States	E-Values
$\vdots$	$\vdots$
$\hat{a}^2\,\|\nu\rangle$	$\left(\nu - \frac{3}{2}\right)\hbar\omega$
$\hat{a}\,\|\nu\rangle$	$\left(\nu - \frac{1}{2}\right)\hbar\omega$
$\|\nu\rangle$	$\left(\nu + \frac{1}{2}\right)\hbar\omega$
$\hat{a}^\dagger\,\|\nu\rangle$	$\left(\nu + \frac{3}{2}\right)\hbar\omega$
$\hat{a}^\dagger\,\|\nu\rangle$	$\left(\nu + \frac{5}{2}\right)\hbar\omega$
$\vdots$	$\vdots$

Remark 7: Eigenstates $\hat{a}^n\,|\nu\rangle$ will have negative energies if $n \geq \nu$. This would correspond to energies below the minimum HO potential, which is physically not allowed. To fix this, we require ν to be an integer, say n. Then

$$\hat{N}(\hat{a}^n\,|\nu\rangle) = (\nu - n)(\hat{a}^n\,|\nu\rangle) = 0 \qquad \text{for } \nu = n$$

and thus

$$\hat{H}(\hat{a}^n |\nu\rangle) = \frac{1}{2}\hbar\omega(\hat{a}^n |\nu\rangle)$$

where $\frac{1}{2}\hbar\omega$ is the energy for the $\hat{a}^n |\nu\rangle$ state. But that means that

$$\hat{H}(\hat{a}^{n+1} |\nu\rangle) = -\frac{1}{2}\hbar\omega(\hat{a}^{n+1} |\nu\rangle)$$

where we have negative energy–which we just argued was physically impossible. How is this possible? Let us calculate the norm of $\hat{a}^{n+1} |\nu\rangle$. To see how this works, we'll go back to the wavefunction language. Thus, we have $\hat{a} |\psi\rangle \to \hat{a}\psi$.

$$\begin{aligned}
\langle \hat{a}\psi|\hat{a}\psi\rangle &= \frac{m\omega}{2\hbar}\left\langle (q+\frac{\hbar}{m\omega}\frac{\partial}{\partial q})\psi \middle| (q+\frac{\hbar}{m\omega}\frac{\partial}{\partial q})\psi \right\rangle \\
&= \frac{m\omega}{2\hbar}\int dq \left(\left(q+\frac{\hbar}{m\omega}\frac{\partial}{\partial q}\right)\psi^*\right)\left(\left(q+\frac{\hbar}{m\omega}\frac{\partial}{\partial q}\right)\psi\right) \\
&= \frac{m\omega}{2\hbar}\int dq\, \psi^* \left(q-\frac{\hbar}{m\omega}\frac{\partial}{\partial q}\right)\left(q+\frac{\hbar}{m\omega}\frac{\partial}{\partial q}\right)\psi \qquad \text{by int. by parts} \\
&= \left\langle \psi \middle| \hat{a}^\dagger\hat{a}\psi \right\rangle \\
&= \left\langle \psi \middle| \hat{N}\psi \right\rangle \\
&= \left\langle \hat{N} \right\rangle
\end{aligned}$$

Hence, the norm of the state $\hat{a}\psi$ is the expectation of $\hat{N}$ in the state ψ.

Therefore, the norm of $\hat{a}(\hat{a}^n |\nu = n\rangle$ equals the expectation value of $\hat{N}$ in the state $\hat{a}^n |\nu = n\rangle$. But this equals zero, since $\hat{a}^n |\nu = n\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue equal to 0 (as shown above). Thus we conclude that the state $\hat{a}^{n+1} |\nu = n\rangle$ is identically 0. Therefore, as long as ν is an integer, the states with negative energy eigenvalues are *not* generated (So our ν's must by integer to be physical).

Remark 8: To summarize: The eigenstates of $\hat{N}$ are represented by $|0\rangle, |1\rangle, |2\rangle, \ldots, |n\rangle, \ldots$ with eigenvalues $0, 1, 2, \ldots, n, \ldots$. These states are also energy eigenstates with energy eigenvalues $\frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \ldots, (n+\frac{1}{2})\hbar\omega, \ldots$.

Remark 9: We can see why $\hat{N}$ is the *number operator*: It's eigenvalue "counts" the number of $\hbar\omega$ energy quanta in a given eigenstate. Similarly, we can see why $\hat{a}$ and $\hat{a}^\dagger$ are the annihilation and creation operators. From Remark 7:

$$\hat{a} |n\rangle \text{ has norm } = \langle n| \hat{a}^\dagger\hat{a} |n\rangle = \langle n| \hat{N} |n\rangle$$

and

$$\begin{aligned}\hat{a}^2 |n\rangle \text{ has norm } &= \langle n| (\hat{a}^\dagger)^2 \hat{a}^2 |n\rangle = \langle n| \hat{a}^\dagger \hat{N} \underbrace{\hat{a} |n\rangle}_{\substack{\text{E-state w/} \\ \text{E-value } n-1}} \\ &= (n-1) \langle n| \hat{a}^\dagger \hat{a} |n\rangle \\ &= n \langle n-1| \hat{N} |n-1\rangle\end{aligned}$$

Thus we deduce that

$$\begin{aligned}\hat{a} |n\rangle &= C_- |n-1\rangle \\ \hat{a}^\dagger |n\rangle &= C_+ |n+1\rangle\end{aligned}$$

with C_- and C_+ constants. We can see that the $\hat{a}$ removes (annihilates) one quanta of energy while $\hat{a}^\dagger$ adds (creates) one quanta of energy-and hence their respective names. To find C_+ and C_-, we take $\langle n|n\rangle = 1$ and use:

$$\begin{aligned}\langle n| \hat{a}^\dagger \hat{a} |n\rangle &= \langle n| \hat{N} |n\rangle = n \langle n|n\rangle = n \\ &= \langle n-1| C_-^* C_- |n-1\rangle \\ &= |C_-|^2 \langle n-1|n-1\rangle = |C_-|^2 \\ \Rightarrow C_n &= \sqrt{n}\end{aligned}$$

So that

$$\hat{a} |n\rangle = \sqrt{n} |n-1\rangle$$

To find C_+:

$$\begin{aligned}\hat{a}^\dagger |n\rangle &= C_+ |n+1\rangle \\ \hat{a}\hat{a}^\dagger |n\rangle &= \hat{a} C_+ |n+1\rangle \\ \hat{a}\hat{a}^\dagger |n\rangle &= C_+ \sqrt{n+1} |n\rangle \\ (\hat{a}^\dagger \hat{a} + 1) |n\rangle &= C_+ \sqrt{n+1} |n\rangle \\ (n+1) |n\rangle &= C_+ \sqrt{n+1} |n\rangle \\ \Rightarrow C_+ &= \sqrt{n+1}\end{aligned}$$

So that

$$\hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$

Remark 10: we can construct any eigenstate of $|n\rangle$ from the ground state.

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle$$

6.2.2 Eigenfunctions in the Position Representation

We can apply the above method to obtain the eigenfunctions in the position representation without solving the Schrodinger equation. We have

$$\hat{a}\,|0\rangle = 0$$

which, in position representation, corresponds to

$$\hat{a}\psi_0 \Rightarrow \left(q + \frac{\hbar}{m\omega}\frac{d}{dq}\right)\psi_0 = 0$$

$$\begin{aligned}
\Rightarrow \frac{d\psi_0}{dq} &= -\frac{m\omega}{\hbar}q\psi_0 \\
\int \frac{d\psi_0}{\psi_0} &= \int -\frac{m\omega}{\hbar}q\,dq \\
\ln(\psi_0) &= -\frac{m\omega}{2\hbar}q^2 + C \\
\psi_0 &= Ae^{-\frac{m\omega}{2\hbar}q^2}
\end{aligned}$$

where A is a normalization constant.

$$1 = \int \psi_0^*\psi_0 = A^2\int e^{-\frac{m\omega}{\hbar}q^2}\,dq = A^2\sqrt{\frac{2\pi\hbar}{2m\omega}} \Rightarrow A = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

Giving the ground state wave-function:

$$\psi_0(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}q^2}$$

The excited states can be obtained by repeatedly applying the creation operator:

$$|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\,|0\rangle$$

which, in the position representation, corresponds to:

$$\psi_n(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{n!}}\left(\frac{m\omega}{2\hbar}\right)^{n/2}\left(q - \frac{\hbar}{m\omega}\frac{d}{dq}\right)^n e^{-\frac{m\omega}{2\hbar}q^2}$$

This is equivalent to:

$$\psi_n(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{n!}}\frac{1}{2^{n/2}}e^{-\frac{m\omega}{2\hbar}q^2}H_n\left(\sqrt{\frac{m\omega}{\hbar}}q\right)$$

where H_n is a Hermite polynomial.

6.3 Coherent States: Minimum Uncertainty Wave Packets

6.3.1 Uncertainty Relations in Energy Eigenstates

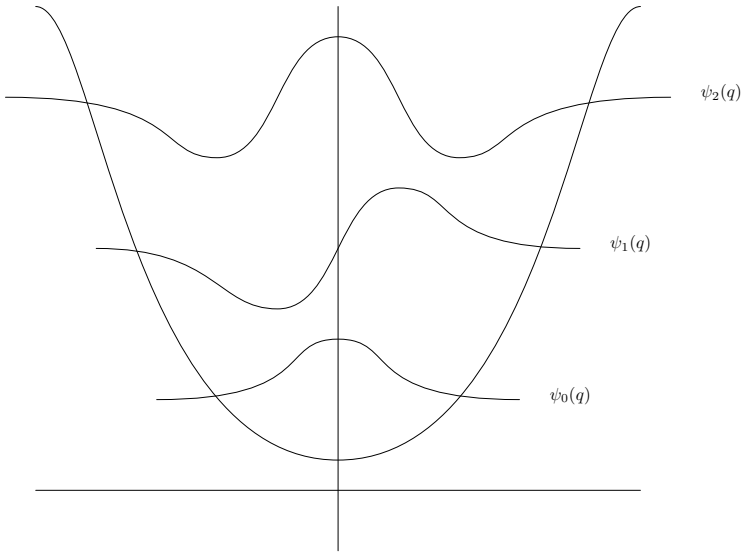
Let's calculate the Heisenberg uncertainty relations in the energy representation. From §6.2, Remark 3:

$$\begin{aligned}\langle n|\,\hat{q}\,|n\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\,\langle n|\,(\hat{a}+\hat{a}^\dagger)\,|n\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}}\,\langle n|\,(\sqrt{n}\,|n-1\rangle + \sqrt{n+1}\,|n+1\rangle) \\ &= 0\end{aligned}$$

Similarly,

$$\langle n|\,\hat{p}\,|n\rangle = 0$$

Remark 1: This result is expected from the symmetry of the stationary HO wavefunction $\psi_n(q)$:



The uncertainty in position is given by:

$$\begin{aligned}\langle n|\,\hat{q}^2\,|n\rangle &= \frac{\hbar}{2m\omega}\,\langle n|\,(\hat{a}^2+\hat{a}\hat{a}^\dagger+\hat{a}^\dagger\hat{a}+(\hat{a}^\dagger)^2)\,|n\rangle \\ &= \frac{\hbar}{2m\omega}\,\langle n|\,\left(\sqrt{n(n-1)}\,|n-1\rangle + (n+1)\,|n\rangle + n\,|n\rangle + \sqrt{(n+1)(n+2)}\,|n+2\rangle\right) \\ &= \frac{\hbar}{2m\omega}(2n+1)\end{aligned}$$

The uncertainty in momentum is given by:

$$\langle n|\,\hat{p}^2\,|n\rangle = \frac{\hbar m\omega}{2}(2n+1)$$

Remark 2: We can rewrite these as

$$\langle n|\,\hat{q}^2\,|n\rangle = \frac{E_n}{m\omega^2}, \qquad \langle n|\,\hat{p}^2\,|n\rangle = mE_n$$

$$\Rightarrow \Delta x\Delta p = \sqrt{\langle n|\,\hat{q}^2\,|n\rangle}\sqrt{\langle n|\,\hat{p}^2\,|n\rangle} = \sqrt{\frac{E_n^2}{\omega^2}} = \frac{\hbar}{2}(2n+1)$$

So the minimum in uncertainty according to the Heisenberg relations is $\hbar/2$. This is satisfied by the ground state–all other states are not minimum uncertainty states.

6.3.2 Minimum Uncertainty States

It is possible to construct non-stationary minimum uncertainty states. It turns out that these states are eigenstates of the annihilation operator.

$$\hat{a}\,|\alpha\rangle = \alpha\,|\alpha\rangle$$

where α is a complex number.

Remark 1: We must make sure these states exist. Expand the state $|\alpha\rangle$ in terms of the stationary states $|n\rangle$.

$$|\alpha\rangle = \sum_{n=0}^{\infty} C_n\,|n\rangle$$

$$\hat{a}\,|\alpha\rangle = \sum_{n=1}^{\infty} C_n\sqrt{n}\,|n-1\rangle = \sum_{n=0}^{\infty} C_{n+1}\sqrt{n+1}\,|n\rangle = \alpha\sum_{n=0}^{\infty} C_n\,|n\rangle$$

$$\Rightarrow C_{n+1}\sqrt{n+1} = \alpha C_n$$

$$\Rightarrow C_n = \frac{\alpha^n}{\sqrt{n!}}C_0$$

which gives

$$|\alpha\rangle = C_0\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\,|n\rangle$$

and C_0 is obtained by normalizing:

$$1 = \langle\alpha|\alpha\rangle = \sum_n |C_n|^2 = |C_0|^2\sum_{n=0}^{\infty}\frac{|\alpha|^{2n}}{n!} = |C_0|^2 e^{|\alpha|^2}$$

$$\Rightarrow |C_0|^2 = e^{-|\alpha|^2}$$
$$\Rightarrow C_0 = e^{-|\alpha|^2/2}$$

which has an arbitrary phase chosen to be 0. Thus we have

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$

which is known as the coherent state with complex amplitude α.

Remark 2: These states were first constructed by Schrodinger as minimum uncertainty wavepackets. They are now used extensively in quantum optics– coherent states are important in describing optical coherence.

Remark 3: We can show that $|\alpha\rangle$ is indeed a minimum uncertainty state (See HW!)

6.3.3 Physical Meaning of the Coherent State

Let us relate the coherent state $|\alpha\rangle$ to the ground state:

$$\begin{aligned} |\alpha\rangle &= e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \\ &= e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle \\ &= e^{-|\alpha|^2/2} e^{\alpha \hat{a}^\dagger} |0\rangle \end{aligned}$$

Consider now $|0\rangle = e^{-\alpha^* \hat{a}} |0\rangle$ where $|0\rangle$ is the only constant term in the exponential expansion that is not zero. Then

$$|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha \hat{a}^\dagger} e^{-\alpha^* \hat{a}} |0\rangle \qquad (\dagger)$$

Now we want to make use of the following relationship. Let $\hat{A}$ and $\hat{B}$ be operators. Then $[\hat{A}, \hat{B}]$ is their commutation relation. If $\hat{A}$ and $\hat{B}$ commute *with* $[\hat{A}, \hat{B}]$, eg

$$[\hat{A}, [\hat{A}, \hat{B}]] = [\hat{B}, [\hat{A}, \hat{B}]] = 0$$

Then

$$\Rightarrow e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{[\hat{A},\hat{B}]/2}$$

So let $\hat{A} = \alpha \hat{a}^\dagger$ and $\hat{B} = -\alpha^* \hat{a}$. Thus we have:

$$\alpha \hat{a}^\dagger, -\alpha^* \hat{a}] = |\alpha|^2 [\hat{a}, \hat{a}^\dagger] = |\alpha|^2$$
$$\Rightarrow e^{\alpha \hat{a}^\dagger} e^{-\alpha^* \hat{a}} = e^{\alpha \hat{a}^\dagger - \alpha^* \hat{a}} e^{|\alpha|^2/2}$$

and thus

$$|\alpha\rangle = e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}\,|0\rangle = \hat{\mathcal{D}}(\alpha)\,|0\rangle$$

where $\hat{\mathcal{D}}(\alpha) = e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}$ is called the displacement operator.
To see what this means, assume $\alpha = x$ (a real number) for simplicity. Then

$$\begin{aligned}\hat{D}(x) = e^{x(\hat{a}^\dagger - \hat{a})} &= e^{x\sqrt{\frac{2}{\hbar m\omega}}(-\hat{p}i)} \\ &= e^{-x\sqrt{\frac{2\hbar}{m\omega}}\frac{d}{dq}} \\ &= e^{-Q\frac{d}{dq}}\end{aligned}$$

where $Q = x\sqrt{\frac{2\hbar}{m\omega}}$ is a number with dimensions of length. (Which implies α and x are dimensionless. The displacement operator acting on an arbitrary function of q is:

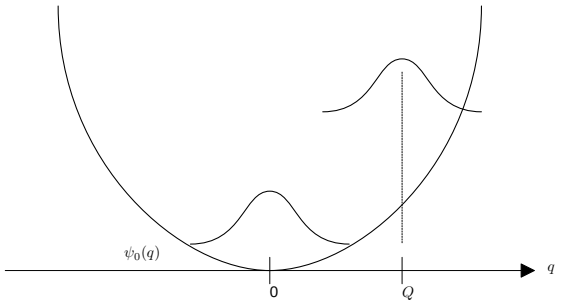
$$\begin{aligned}\hat{D}F(q) = e^{-Q\frac{d}{dq}}F(q) &= \left(1 - Q\frac{d}{dq} + \frac{1}{2}Q^2\frac{d^2}{dq^2} + \cdots\right)F(q) \\ &= F(q-Q) \qquad \text{for small Q}\end{aligned}$$

Remark 1: So the action of $\hat{D}$ on an arbitrary function is to displace the function by an amount Q (and hence the name).

Remark 2: Expressing $|\alpha\rangle = \hat{D}(\alpha)\,|0\rangle$ in the coordinate representation:

$$\begin{aligned}\underbrace{\psi_{\alpha=x}(q)}_{\substack{\text{Wavefunction of}\\ \text{coherent state}\\ \text{where } |\alpha\rangle=|x\rangle}} &= \underbrace{e^{-Q\frac{d}{dq}}}_{\substack{\hat{D}(\alpha) \text{ in coord.}\\ \text{representation}\\ \text{with } \alpha=x}} \cdot \underbrace{\phi_{n=0}(q)}_{\substack{\text{Wavefunction of}\\ \text{HO in state } |0\rangle}} \\ &= e^{-Q\frac{d}{dq}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}q^2} \\ &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}(q-Q)^2}\end{aligned}$$

So the coherent state has the same gaussian wavefunction as the HO ground state, it is just displaced a distance $Q = x\sqrt{\frac{2\hbar}{m\omega}}$.



Remark 3: The coherent state is *not* stationary (it evolves with time according to the Schrodinger equation). The formal solution is given by

$$\begin{aligned}
|\alpha(t)\rangle &= e^{-\frac{i}{\hbar}\hat{H}t} \underbrace{|\alpha\rangle}_{\text{Init. State}} \\
&= \exp\left(-\frac{i}{\hbar}\hbar\omega\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)t\right)|\alpha\rangle \\
&= \exp\left(-i\omega\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)t\right)\exp\left(-\frac{1}{2}|\alpha|^2\right)\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle \\
&= \exp\left(-\frac{|\alpha|^2}{2}\right)\sum_{n=0}^{\infty}\exp\left(-i\omega\left(n+\frac{1}{2}\right)t\right)\frac{\alpha^n}{\sqrt{n!}}|n\rangle \\
&= e^{-\frac{1}{2}(i\omega t+|\alpha|^2)}\sum_{n=0}^{\infty}\frac{\left(\alpha e^{-i\omega t}\right)^n}{\sqrt{n!}}|n\rangle \\
&= \underbrace{e^{-i\omega t/2}}_{\substack{\text{overall arbitrary}\\ \text{phase can be}\\ \text{dropped}}}\left|e^{-i\omega t}\alpha\right\rangle
\end{aligned}$$

Which gives the evolution of $\langle\hat{q}(t)\rangle$ and $\langle\hat{p}(t)\rangle$:

$$\begin{aligned}
\langle\hat{q}(t)\rangle &= \left\langle e^{-i\omega t}\alpha\right|\hat{q}\left|e^{-i\omega t}\alpha\right\rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\left\langle e^{-i\omega t}\alpha\right|\hat{a}\left|e^{-i\omega t}\alpha\right\rangle + \left\langle e^{-i\omega t}\alpha\right|\hat{a}^\dagger\left|e^{-i\omega t}\alpha\right\rangle\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(e^{-i\omega t}\alpha + e^{i\omega t}\alpha^*\right) \\
&= \sqrt{\frac{\hbar}{2m\omega}}\left(\cos(\omega t)(\alpha+\alpha^*) - i\sin(\omega t)(\alpha-\alpha^*)\right)
\end{aligned}$$

And so at $t=0$

$$\langle\hat{q}(0)\rangle = \sqrt{\frac{\hbar}{2m\omega}}(\alpha+\alpha^*)$$

And we can show that

$$\langle \hat{p}(0) \rangle = -i\sqrt{\frac{\hbar m\omega}{2}}(\alpha - \alpha^*)$$

Thus we have that

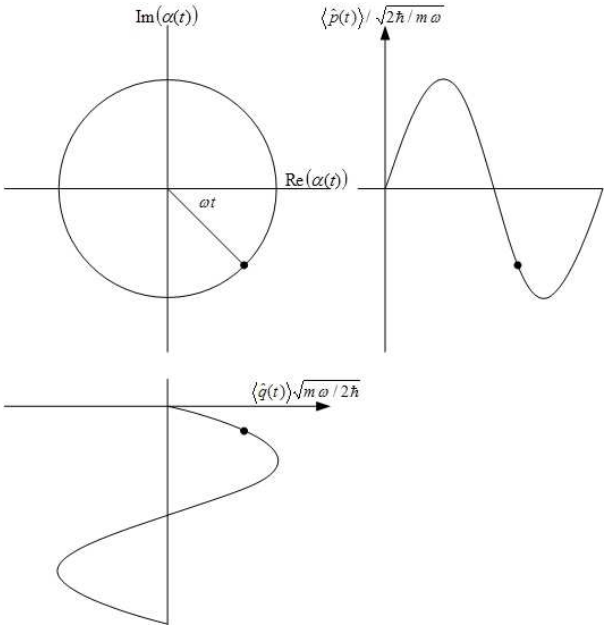
$$\langle \hat{q}(t) \rangle = \langle \hat{q}(0) \rangle \cos(\omega t) + \frac{1}{m\omega} \langle \hat{p}(0) \rangle \sin(\omega t)$$

And similarly

$$\langle \hat{p}(t) \rangle = \langle \hat{p}(0) \rangle \cos(\omega t) - m\omega \langle \hat{q}(0) \rangle \sin(\omega t)$$

which are the solutions to the Heisenberg equations of motion for the operators $\hat{q}$ and $\hat{p}$.

Remark 4: The time dependence of the coherent state can be represented as a trajectory in the complex plane.



And we see that the circular trajectory in the complex plane is related to the phase space trajectory of classical Hamiltonian mechanics.

Remark 5: Consider the coherent state wave packet in coordinate representation. From Remark 2, we can see $\langle \hat{q} \rangle = Q$ (the mean position), while all coherent states have $\Delta q = \sqrt{\frac{\hbar}{2m\omega}}$ (Remark 3 - HW). And the wave packet moves in a harmonic potential without changing it's width. The coherent state of the HO

is a non-dispersing wavepacket. This is significant since we can recall that free particle wave-packets *always* disperse (Ch. 4, §4.1).

Remark 6: We can calculate the explicit time dependence of the wave packet. Remark 3 implies:

$$\begin{aligned}|\alpha(t)\rangle &= e^{\frac{-i}{\hbar}\hat{H}t}|\alpha\rangle = \left|e^{-i\omega t}\alpha\right\rangle \\ &= \hat{D}(e^{-i\omega t}\alpha)|0\rangle\end{aligned}$$

where

$$\hat{D}(e^{-i\omega t}\alpha) = \exp\left[e^{-i\omega t}\alpha\hat{a}^\dagger - e^{i\omega t}\alpha^*\hat{a}\right]$$

In the coordinate representation, the time dependent coherent state is represented by the wave function:

$$\psi_{e^{-i\omega t}\alpha}(q) = \underbrace{\hat{D}(e^{-i\omega t}\alpha)}_{\substack{\text{Displacement}\\ \text{Operator}}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}q^2}$$

To find what the Displacement operator actually is:

$$\begin{aligned}\hat{D} &= e^{-i\omega t}\alpha\hat{a}^\dagger - e^{i\omega t}\alpha^*\hat{a}^\dagger \\ &= e^{-i\omega t}\alpha\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} - \frac{i}{m\omega}\hat{p}\right) - e^{i\omega t}\alpha^*\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} + \frac{i}{m\omega}\hat{p}\right) \\ &= \hat{q}\sqrt{\frac{m\omega}{2\hbar}}\left(e^{-i\omega t}\alpha - e^{i\omega t}\alpha^*\right) + \hat{p}\left(\frac{-i}{\sqrt{2\hbar m\omega}}\right)\left(\alpha e^{-i\omega t} + \alpha^* e^{i\omega t}\right) \\ &= \exp\left[\frac{i}{\hbar}\left(\hat{q}\,\langle\hat{p}(t)\rangle - \hat{p}\,\langle\hat{q}(t)\rangle\right)\right]\end{aligned}$$

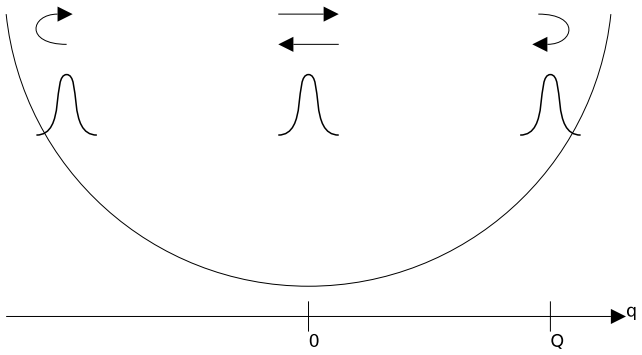
$$\Rightarrow \hat{D}(e^{-i\omega t}\alpha) = e^{\frac{i}{\hbar}(\hat{q}\langle\hat{p}(t)\rangle - \hat{p}\langle\hat{q}(t)\rangle)}$$

$$\begin{aligned}&= e^{\frac{i}{\hbar}\hat{q}\langle\hat{p}(t)\rangle}e^{-\frac{i}{\hbar}\hat{p}\langle\hat{q}(t)\rangle}e^{-\frac{1}{2\hbar^2}\langle\hat{p}(t)\rangle\langle\hat{q}(t)\rangle\overbrace{[\hat{q},\hat{p}]}^{i\hbar}} \\ &= e^{-\frac{i}{2\hbar}\langle\hat{p}(t)\rangle\langle\hat{q}(t)\rangle}e^{\frac{i}{\hbar}\hat{q}\langle\hat{p}(t)\rangle}e^{-\frac{i}{\hbar}\hat{p}\langle\hat{q}(t)\rangle} \\ &= e^{\frac{i}{2\hbar}\langle\hat{q}(t)\rangle\langle\hat{p}(t)\rangle}e^{\frac{i}{\hbar}q\langle\hat{p}(t)\rangle}e^{-\langle\hat{q}(t)\rangle\frac{\partial}{\partial q}}\end{aligned}$$

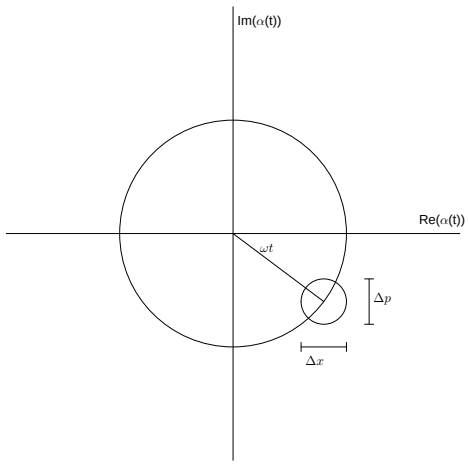
The last term is the displacement operator that we had when we let $\alpha = \alpha^*$. If we have an arbitrary α, then the displacement operator generalizes and acquires time dependent phase factors.
The coordinate representation of the time dependent coherent state becomes:

$$\psi_{e^{-i\omega t}\alpha}(q) = \underbrace{e^{\frac{-i}{2\hbar}\langle\hat{q}(t)\rangle\langle\hat{p}(t)\rangle}}_{\substack{\text{overall phase}\\ \text{changes with time}\\ \text{and is indep of q}}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\underbrace{e^{\frac{i}{\hbar}q\langle\hat{p}(t)\rangle}}_{\substack{\text{this phase carries}\\ \text{info about mean}\\ \text{momentum}}}\underbrace{e^{-\frac{m\omega}{2\hbar}(\hat{q}-\langle\hat{q}(t)\rangle)^2}}_{\substack{\text{Gaussian envelope}\\ \text{carries info about}\\ \text{mean position and}\\ \Delta\hat{q},\Delta\hat{p}}}$$

In the last comment, we can find $\Delta\hat{p}$ by knowing that $|\alpha\rangle$ is a minimum uncertainty and knowing $\Delta\hat{q}$. The related picture is a gaussian wavepacket that oscillates back and forth along the classical HO trajectory with a fixed width.



If we want to represent this by the coherent state trajectory in the complex plane, the width of the gaussian can be related to the radius of a small circle.



Remark 7: There is another class of minimum uncertainty states which are closely related to coherent states. These are known as Squeeze States.

As minimum uncertainty states, the squeeze states satisfy $\Delta q \Delta p = \hbar/2$, but they differ from coherent states since they have either:

$$\Delta q < \sqrt{\frac{\hbar}{2m\omega}} \qquad \text{and} \qquad \Delta p > \sqrt{\frac{\hbar m\omega}{2}}$$

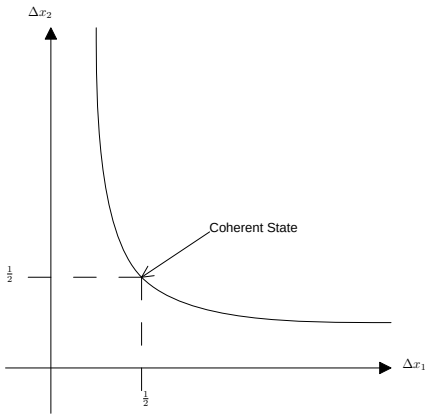
or

$$\Delta p < \sqrt{\frac{\hbar m\omega}{2}} \qquad \text{and} \qquad \Delta q > \sqrt{\frac{\hbar}{2m\omega}}$$

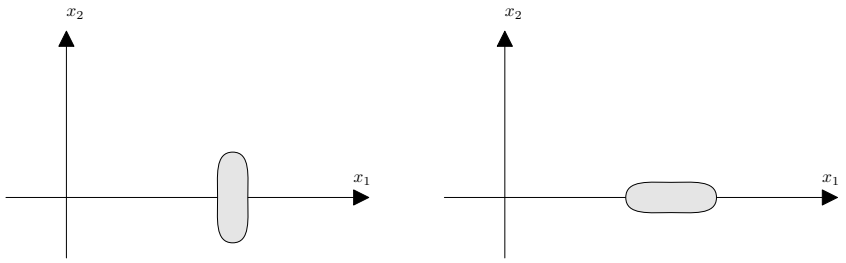
while preserving the minimum uncertainty. In this case, the uncertainty in $\hat{p}$ or the uncertainty in $\hat{q}$ is less than it is for a coherent state.
To visualize the squeezed states, define quadrature phase operators:

$$\hat{x}_1 = \frac{1}{2}(\hat{a} + \hat{a}^\dagger) = \sqrt{\frac{m\omega}{2\hbar}}\hat{q}$$
$$\hat{x}_2 = \frac{-i}{2}(\hat{a} - \hat{a}^\dagger) = \sqrt{\frac{1}{2\hbar m\omega}}\hat{p}$$

In a coherent state, these operators have uncertainties $\Delta x_1 = \Delta x_2 = \frac{1}{2}$. In a squeeze state, $\Delta x_1 < \frac{1}{2}$ or $\Delta x_2 < \frac{1}{2}$ such that $\Delta x_1 \Delta x_2 = \frac{1}{4}$. Graphically, the minimum uncertainty states lie along the line $\Delta x_1 \Delta x_2 = \frac{1}{4}$.



All other states along the line are squeeze states.
A complex plot, in this case, can be represented by a plot on the $x_1 - x_2$ plane. In this picture, the squeeze states are represented as:



The time evolution of a squeeze state is analogous to a rotation of frequency ω in the complex plane (in this case, the $x_1 - x_2$ plane). This is seen in Fig. 6.1.
The wave packet in coordinate representation has a gaussian envelope whose width changes as it oscillates in the harmonic potential, as can be seen in Fig. 6.2
More generally, the coordinate representation is squeezed twice during the cycle, though not necessarily at the end or middle of an oscillation. Eg: See Fig. 6.3

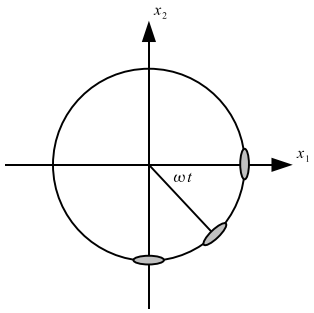


Figure 6.1: The initial squeezing is in x_1, which evolves in time to a squeezing in x_2.

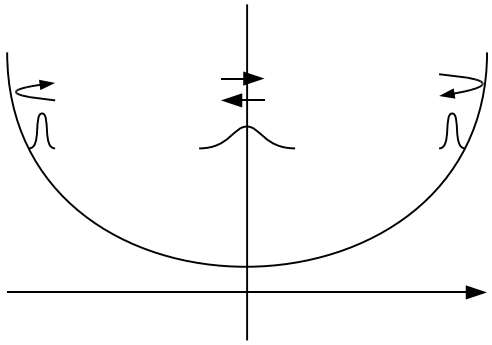


Figure 6.2: The outer gaussians are squeezed in position, while the center gaussian is squeezed in momentum.

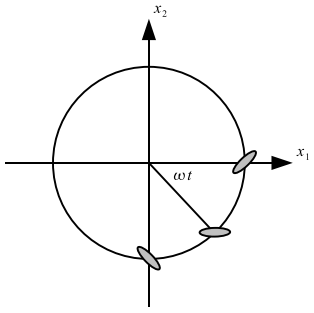


Figure 6.3: Example of squeeze cycles not fully squeezed on the main axes.

Chapter 7

Systems with N Degrees of Freedom

7.1 Tensor Products (Direct Products)

Definition 1: Let $|\omega_1\rangle$ be a basis vector of the Hilbert space V_1 so that the set of all $|\omega_1\rangle$ spans V_1. Similarly, let the set of all $|\omega_2\rangle$ be basis vectors that span V_2. Then $|\omega_1\rangle \otimes |\omega_2\rangle$ forms a basis vector in the combined Hilbert space $V_1 \otimes V_2$.

Remark 1: Physically, V_1 and V_2 may correspond to Hilbert spaces for 2 individual particles (1 and 2), while $V_1 \otimes V_2$ represents the Hilbert space for the *combined* 2 particle system. Alternatively, this may represent single particle system that spans 2 (or more) dimensions.

Remark 2: Consider an operator $\hat{\Omega}_1$ that operates on the space V_1 with eigenstates $|\omega_1\rangle$ and eigenvalues ω_1. Eg:

$$\hat{\Omega}_1 |\omega_1\rangle = \omega_1 |\omega_1\rangle$$

In the combined system, we write:

$$\begin{aligned}
\hat{\Omega}_1 |\omega_1\rangle \otimes |\omega_2\rangle &\equiv \hat{\Omega}_1^{(1)\otimes(2)} |\omega_1\rangle \otimes |\omega_2\rangle \\
&\equiv \hat{\Omega}_1^{(1)} \otimes \hat{I}^{(2)} |\omega_1\rangle \otimes |\omega_2\rangle \\
&\equiv \hat{\Omega}_1^{(1)} |\omega_1\rangle \otimes \hat{I}^{(2)} |\omega_2\rangle \\
&\equiv \left|\hat{\Omega}_1^{(1)}\omega_1\right\rangle \otimes |\omega_2\rangle
\end{aligned}$$

where the superscripts denote the target Hilbert space (either V_1 or V_2) on which the operator acts, and where $\left|\hat{\Omega}_1^{(1)}\omega_1\right\rangle = \hat{\Omega}_1^{(1)} |\omega_1\rangle$. Similarly, we can write

$$\hat{\Omega}_2^{(2)} \equiv \hat{\Omega}_2^{(1)\otimes(2)} \equiv \hat{I}^{(1)} \otimes \hat{\Omega}_2^{(2)}$$

So that

$$\hat{\Omega}_2^{(2)} |\omega_1\rangle \otimes |\omega_2\rangle = |\omega_1\rangle \otimes \left|\hat{\Omega}_2^{(2)}\omega_2\right\rangle$$

The bottom line is that $\hat{\Omega}_i^{(i)}$ only acts on the basis vectors $|\omega_i\rangle$ which span V_i.

Remark 3: It is common to use a compact representation of the vectors which span the combined space.

$$|\omega_1\rangle \otimes |\omega_2\rangle \equiv |\omega_1\rangle\,|\omega_2\rangle \equiv |\omega_1\omega_2\rangle$$

Since this also represents the simultaneous eigenkets of operators $\hat{\Omega}_1^{(1)}$ and $\hat{\Omega}_2^{(2)}$.

Remark 4: The inner product of the direct products

$$\left(\langle\omega_1'| \otimes \langle\omega_2'|\right)\left(|\omega_1\rangle \otimes |\omega_2\rangle\right) = \langle\omega_1'|\omega_1\rangle\,\langle\omega_2'|\omega_2\rangle$$

Similarly,

$$\left(\langle\omega_1'| \otimes \langle\omega_2'|\right)\left(\hat{\Omega}_1^{(1)} \otimes \hat{\Lambda}_2^{(2)}\right)\left(|\omega_1\rangle \otimes |\omega_2\rangle\right) = \langle\omega_1'|\,\hat{\Omega}_1^{(1)}\,|\omega_1\rangle\,\langle\omega_2'|\,\hat{\Lambda}_2^{(2)}\,|\omega_2\rangle$$

Remark 5: Properties of the Tensor Product of Operators:
Denote

$$\hat{\Omega}_1^{(1)} \otimes \hat{I}^{(2)} \equiv \hat{\Omega}_1 \rightarrow \text{ acts only on } |\omega_1\rangle$$
$$\hat{I}^{(2)} \otimes \hat{\Lambda}_2^{(2)} \equiv \hat{\Lambda}_2 \rightarrow \text{ acts only on } |\omega_2\rangle$$

- $\left[\hat{\Omega}_1, \hat{\Lambda}_2\right] = 0$
- $\left(\hat{\Omega}_1^{(1)} \otimes \hat{\Gamma}_2^{(2)}\right)\left(\hat{\Theta}_1^{(1)} \otimes \hat{\Lambda}_2^{(2)}\right) = \left(\hat{\Omega}\hat{\Theta}\right)_1^{(1)} \otimes \left(\hat{\Gamma}\hat{\Lambda}\right)_2^{(2)}$
- Squares of sums:

$$\begin{aligned}\left(\hat{\Omega}_1 + \hat{\Omega}_2\right)^2 &= \left(\hat{\Omega}_1^{(1)\otimes(2)} + \hat{\Omega}_2^{(1)\otimes(2)}\right)^2 \\ &= \left(\hat{\Omega}_1^2\right)^{(1)} \otimes \hat{I}^{(2)} + \hat{I}^{(1)} \otimes \left(\hat{\Omega}_2^2\right)^{(2)} + 2\hat{\Omega}_1^{(1)} \otimes \hat{\Omega}_2^{(2)}\end{aligned}$$

Remark 6: The time evolution of the state vectors that are composed of direct products is still governed by the Hamiltonian:

$$\hat{H} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} + \hat{V}(\hat{x}_1, \hat{x}_2)$$

for a two particle system in 1 dimension. If the Hamiltonian is *separable*:

$$\hat{H} = \hat{H}_1 + \hat{H}_2 \Rightarrow \hat{V}(\hat{x}_1, \hat{x}_2) = \hat{V}_1(\hat{x}_1) + \hat{V}_2(\hat{x}_2)$$

then the two particles will evolve independently of one another, giving the time evolution as

$$|\psi(t)\rangle = |E_1\rangle\, e^{-iE_1 t/\hbar} \otimes |E_2\rangle\, e^{-iE_2 t/\hbar}$$

which is obtained by solving the individual Schrodinger equations (with $E = E_1 + E_2$). Separation of variables is often employed in solving the Schrodinger equations in position representation. If the Hamiltonian is *not* separable (ie. $\hat{V}(\hat{x}_1, \hat{x}_2) \neq \hat{V}_1(\hat{x}_1) + \hat{V}_2(\hat{x}_2)$), then there is not a general method for solving the Schrodinger equations unless $\hat{V}(\hat{x}_1, \hat{x}_2) = \hat{V}(|\hat{x}_1 - \hat{x}_2|)$, in which case the problem can be separated into center of mass plus the motion about the center of mass (see Central Potential, coming soon!)

7.2 Identical Particles

Classically, two identical particles can be distinguished by fallowing their trajectories (ie. by looking at their non-identical histories), which can be done without disturbing the system. Quantum mechanically, no such trajectory exists for particles, and thus there is no physical basis for distinguishing 2 or more particles. This implies that the same state vector must describe two configurations which differ only in particle exchange.

7.2.1 Symmetric and Anti-symmetric States: Bosons and Fermions

Consider the following state vector:

$$|\psi\rangle = |x_1 = a,\, x_2 = b\rangle \equiv |ab\rangle \qquad (\dagger)$$

which represents the result of a measurement that finds a particle at a, and one at b. If the particles are distinguishable, then the state (†) is distinct from the state $|\psi\rangle = |x_1 = b,\, x_2 = a\rangle \equiv |ba\rangle$. However, if the particles are indistinguishable, then we can not differentiate one state from another. Instead, we write the state vector as a superposition of these possible states. (These will define a 2-D degenerate eigenspace.)

$$|\psi(a,b)\rangle = \alpha\,|ab\rangle + \beta\,|ba\rangle$$

These two states are physically equivalent, so we can also write

$$|\psi(a,b)\rangle = \gamma\,|\psi(b,a)\rangle$$

where γ is an arbitrary phase (complex number).

$$\Rightarrow \alpha\,|ab\rangle + \beta\,|ba\rangle = \gamma\,(\alpha\,|ba\rangle + \beta\,|ab\rangle)$$

$$\Rightarrow \alpha = \gamma\beta, \qquad \beta = \gamma\alpha$$

$$\Rightarrow \alpha = \alpha\gamma^2 \Rightarrow \gamma = \pm 1$$

Taking the "+", we define the symmetric wavefunction:

$$|\psi(a,b)\rangle_S = |ab\rangle + |ba\rangle$$

and the "-" gives the anti-symmetric wavefunction:

$$|\psi(a,b)\rangle_A = |ab\rangle - |ba\rangle$$

Definition 1: Particles whose wavefunctions are symmetric are called Bosons, and those with anti-symmetric wavefunctions are called Fermions.

Remark 1: One of the primary consequences of the anti-symmetric wavefunction is the Pauli Exclusion Principle:
Suppose we have a 2 fermion system with the following state vector:

$$|\psi(\omega_1,\omega_2)\rangle_A = |\omega_1\omega_2\rangle - |\omega_2\omega_1\rangle$$

so that one fermion is in state ω_1, and the other is in state ω_2. If $\omega_1 = \omega_2 \Rightarrow |\psi(\omega_1,\omega_2)\rangle_A = 0$, which implies that no two fermions can be in the same quantum state.

Consider the 2 particle Hilbert space $V_{1\otimes 2}$ made up of all vectors of the form $|\omega_1\rangle \otimes |\omega_2\rangle$. Since each pair of vectors $|\omega_1 = a, \omega_2 = b\rangle$ and $|\omega_1 = b, \omega_2 = a\rangle$ can form one symmetric and one anti-symmetric state, if follows that $V_{1\otimes 2}$ can be decomposed into symmetric and anti-symmetric parts:

$$V_{1\otimes 2} = \underbrace{V_S}_{\substack{\text{Bosonic}\\ \text{Hilbert}\\ \text{Space}}} \otimes \underbrace{V_A}_{\substack{\text{Fermionic}\\ \text{Hilbert}\\ \text{Space}}}$$

This leads to an ambiguity in determing whether the state of the system is a member of the symmetric Hilbert space (V_S) or the anti-symmetric Hilbert space (V_A). (We will see in §2.2 that the measurement made depends on which case applies.) To remove the ambiguity, we introduce the Symmetrization Postulate, which states:

The state of a system containing N identical particles is either all symmetric or all anti-symmetric with respect to permutation (particle exchange) of the N particles

The *Corollary* to this is that the symmetry (or anti-symmetry) will be independent of the number of particles.

Remark 2: The normalized states for a system of n identical bosons is given by:

$$|1,2,\ldots,n\rangle_S = \frac{1}{\sqrt{n!}}\left(|1,2,\ldots,n\rangle + |2,1,3,\ldots,n\rangle + \cdots + n! \text{ permutations}\right)$$

where $1,2,\ldots,n$ are generic state labels.

Remark 3: The normalized states for a system of n identical fermions is given by the Slate Determinant:

$$\psi_{1,2,\ldots,n}(x_1, x_2, \ldots, x_n) = \frac{1}{\sqrt{n!}} \begin{vmatrix} \psi_1(x_1) & \psi_2(x_1) & \cdots & \psi_n(x_1) \\ \psi_1(x_2) & & & \vdots \\ \vdots & & & \vdots \\ \psi_1(x_n) & \cdots & \cdots & \psi_n(x_n) \end{vmatrix}$$

The determinant gives all the correct minus signs in the anti-symmetric wave-function, *and* vanishes if any two j's or x_j's are the same.

7.2.2 Distinguishing Fermions and Bosons

The are two ways to identify whether a particle is a fermion or a boson:

1. Spin (intrinsic angular momentum)
2. Experiments

We will discuss spin in much more detail later, though we note here that bosons have integral spin $(0, \hbar, 2\hbar, \ldots)$, and fermions have half-integral spin $(\frac{\hbar}{2}, \frac{3\hbar}{2}, \ldots)$.
To determine the nature of the particle experimentally, place two identical particles in a 1-D (for simplicity) box. Let

$$\left.\begin{matrix} \psi_S(x_1, x_2) \\ \psi_A(x_1, x_2) \end{matrix}\right\} \text{The 2 particle wave function for bosons and fermions}$$

In general, each particle could have different energy levels, so

$$\psi_{S,A} = \frac{1}{\sqrt{2}} \{\psi_n(x_1)\psi_m(x_2) \pm \psi_n(x_2)\psi_m(x_1)\}$$

where n,m are energy levels and the "+" is for the symmetric cases and the "-" for the anti-symmetric cases. Also, $n \neq m$ (they don't have the same energy).
The probability distribution in x-space is determined by

$$P_{S,A}(x_1, x_2) = 2\,|\psi_{S,A}(x_1, x_2)|^2 \qquad (\dagger)$$

Remark 1: The factor of 2 in (†) is a consequence of the normalization condition. We require:

$$1 = \iint dx_1\, dx_2\ |\psi_{S,A}(x_1, x_2)|^2$$

and accounting for the double counting in the $x_1 - x_2$ integral:

$$1 = \iint \frac{1}{2} P_{S,A}(x_1, x_2)\, dx_1\, dx_2$$

where

$$\begin{aligned} P_{S,A}(x_1, x_2) &= \left| \langle x_1 x_2 | \psi_{S,A} \rangle_{S,A} \right|^2 \\ &= \sqrt{2} \psi_{S,A}(x_1, x_2) \end{aligned}$$

where the $\sqrt{2}$ in for convenience.

Taking (†):

$$\begin{aligned} P_{S,A}(x_1, x_2) &= 2 \left| \frac{1}{\sqrt{2}} (\psi_n(x_1)\psi_m(x_2) \pm \psi_n(x_2)\psi_m(x_1) \right|^2 \\ &= |\psi_n(x_1)\psi_m(x_2)|^2 + |\psi_m(x_1)\psi_n(x_2)|^2 \pm \\ &\quad \pm |\psi_n(x_1)\psi_m^*(x_1)\psi_m(x_2)\psi_n^*(x_2) + \psi_n^*(x_1)\psi_m(x_1)\psi_m^*(x_2)\psi_n(x_2)| \end{aligned}$$

Remark 2: So the differenence between fermiens and bosons is detectable in the interferecence in the probability distribution. In the extreme cases, lets consider the limit that these particle have as $x_1 \to x_2 \to x$. Then

$$\begin{aligned} &P_S(x_1 \to x, x_2 \to x) \to 2 \left\{ |\psi_n(x)|^2 |\psi_m(x)|^2 + |\psi_n(x)|^2 |\psi_m(x)|^2 \right\} \\ &P_A(x_1 \to x, x_2 \to x) \to 0 \end{aligned}$$

Where the antisymmetric case is consistant with the Pauli exclusion principle. Thus, two fermions will show probability 0 of being in the same state, while two bosons double the probability density for two distinct particles to be in the same state.

Chapter 8

Classical Limit and WKB Approximation

Correspondence Principle: In the limit that $\hbar \to 0$, laws of quantum mechanics *must* reduce to the laws of classical mechanics.

Remark 1: $\hbar$ gives a measure of the energy spacing between discrete energy levels. Thus, in order to justisfy the limit as $\hbar \to 0$, the system must have *large quantum numbers*.

Remark 2: The limit as $\hbar \to 0$ is called the classical approximation, and the conditions of validity are the same as those of geometrical optics.

Remark 3: Note that in the classical limit, we have:

- $[q_i, p_i] = i\hbar\delta_{ij} \to 0$
- $\Delta q_i \Delta p_i \geq \frac{\hbar}{2} \to 0$. This implies

$$\Delta q_i = \sqrt{\langle q_i^2 \rangle - \langle q_i \rangle^2}$$

which is the same as ignoring fluxuations about the mean.

In order to ignore the effects of fluxuations, we require that:

- The mean values approximately follow classic laws of motion,
- Dimensions of the wave packets are small (and remain small as the system evolves) compared to the characteristic dimensions of the problem.

Remark 4: Since wavepackets disperse with time, the classical approximation is, in general, only valid over a finite time interval.

Remark 5: The correspondence principle, as stated above, is most useful when applied to commutators, uncertainty, and *differences* is energy levels, angular momentum, etc... A second

formulation of the classical approximation basically amounts to:

$$\lim_{\text{Geo. Optics}} \text{Schrodinger Eqn.} \rightarrow \text{Eqns. of Classical Mechanics}$$

In this view, the wavefunction represents a statistical mixture of *classical* systems. The density of this mixture, at some point in configuration space, equals the probability density of a quantum system at that point.

8.1 Ehrenfest's Theorem

Consider a system which evolves according to the Schrodinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi \Rightarrow i\hbar\frac{\partial\psi^*}{\partial t} = -(\hat{H}\psi)^*$$

And the mean value of an observable $\hat{A}$ is:

$$\left\langle \hat{A} \right\rangle = \langle\psi|\,\hat{A}\,|\psi\rangle$$

Since ψ in general evolves in time, $\left\langle \hat{A} \right\rangle$ will also evolve in time:

$$\begin{aligned}
\frac{d}{dt}\left\langle \hat{A} \right\rangle &= \frac{d}{dt}\langle\psi|\,\hat{A}\,|\psi\rangle \\
&= \frac{d}{dt}\int dq_1 \ldots dq_n\, \psi^*\hat{A}\psi \\
&= \int dq_1 \ldots dq_n \left(\frac{\partial\psi^*}{\partial t}\hat{A}\psi + \psi^*\hat{A}\frac{\partial\psi}{\partial t} + \psi^*\frac{\partial\hat{A}}{\partial t}\psi\right) \\
&= \int dq_1 \ldots dq_n \left(-\frac{1}{i\hbar}(\hat{H}\psi)^*\hat{A}\psi + \psi^*\hat{A}\left(\frac{1}{i\hbar}\hat{H}\psi\right) + \psi^*\frac{\partial\hat{A}}{\partial t}\psi\right) \\
&= \int dq_1 \ldots dq_n \left(-\frac{1}{i\hbar}\psi^*(\hat{H}\hat{A})\psi + \frac{1}{i\hbar}\psi^*(\hat{A}\hat{H})\psi + \psi^*\frac{\partial\hat{A}}{\partial t}\psi\right) \\
&= \frac{1}{i\hbar}\left(\left\langle[\hat{A},\hat{H}]\right\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle\right)
\end{aligned}$$

Thus, if $\hat{A}$ has no explicit time dependence, then

$$\frac{d}{dt}\left\langle \hat{A} \right\rangle = \frac{1}{i\hbar}\left\langle[\hat{A},\hat{H}]\right\rangle \qquad (\dagger)$$

Remark 1: An immediate consequence of (†) is that if $[\hat{A},\hat{H}] = 0$, then $\hat{A}$ does not change with time and is a constant of motion (a conserved quantity). This is analogous to classical mechanics where we have $\{\hat{A},\hat{H}\} = 0$ (The Poisson bracket from §2.1.3).

To connect with classical mechanics, apply (†) to $\hat{q}_i$ and $\hat{p}_i$:

$$\begin{aligned} \frac{d}{dt}\langle \hat{q}_i \rangle &= \frac{1}{i\hbar}\left\langle [\hat{q}_i, \hat{H}] \right\rangle \\ \frac{d}{dt}\langle \hat{p}_i \rangle &= \frac{1}{i\hbar}\left\langle [\hat{p}_i, \hat{H}] \right\rangle \end{aligned} \tag{††}$$

Now consider the $\hat{q}_i$ and $\hat{p}_i$ commutator with

$$\hat{A}(\hat{q}_1, \hat{q}_2, \ldots, \hat{q}_n, \hat{p}_1, \hat{p}_2, \ldots, \hat{p}_n)$$

where $\hat{A}$ is only well defined when the order in each term is specified. We note that:

$$\begin{aligned} \left[\hat{q}_i, \hat{F}(\hat{q}_1, \hat{q}_2, \ldots, \hat{q}_n)\right] &= 0 \\ \left[\hat{p}_i, \hat{F}(\hat{p}_1, \hat{p}_2, \ldots, \hat{p}_n)\right] &= 0 \\ \left[\hat{q}_i, \hat{G}(\hat{p}_1, \hat{p}_2, \ldots, \hat{p}_n)\right] &= i\hbar \frac{\partial \hat{G}}{\partial \hat{p}_i} \\ \left[\hat{p}_i, \hat{F}(\hat{q}_1, \hat{q}_2, \ldots, \hat{q}_n)\right] &= -i\hbar \frac{\partial \hat{F}}{\partial \hat{q}_i} \end{aligned}$$

Generalizing the above, one can show that

$$\begin{aligned} \left[\hat{q}_i, \hat{A}\right] &= i\hbar \frac{\partial \hat{A}}{\partial \hat{p}_i} \\ \left[\hat{p}_i, \hat{A}\right] &= -i\hbar \frac{\partial \hat{A}}{\partial \hat{q}_i} \end{aligned}$$

Using this result in (††) gives:

$$\begin{aligned} \frac{d}{dt}\langle \hat{q}_i \rangle &= \left\langle \frac{\partial \hat{H}}{\partial \hat{p}_i} \right\rangle \\ \frac{d}{dt}\langle \hat{p}_i \rangle &= -\left\langle \frac{\partial \hat{H}}{\partial \hat{q}_i} \right\rangle \end{aligned} \tag{☺}$$

which are the quantum averages of Hamilton's equations of motion.

Remark 2: Equation (☺) represents Ehrenfest's Theorem, which states that equations of motion for the quantum mean values coordinates and momenta are equivalent to those of classical mechanics.

Remark 3:

WARNING! ¡CUIDADO! ACHTUNG!

This is not exactly equivalent to saying that mean values of $\hat{p}$ and $\hat{q}$ follow classic trajectories in phase space. For this, we require that $\frac{\partial \hat{H}}{\partial \hat{p}_i}$ and $\frac{\partial \hat{H}}{\partial \hat{q}_i}$ to be at *most* linear functions of $\hat{q}$ and $\hat{p}$ since:

$$\langle \hat{q}_i \hat{p}_i \rangle \neq \langle \hat{q}_i \rangle \langle \hat{p}_i \rangle$$
$$\left\langle \frac{1}{\hat{q}_i^2} \right\rangle \neq \frac{1}{\langle \hat{q}_i \rangle^2}, \text{ etc}$$

unless fluctuations about the averages can be neglected.

8.2 Classical Limit and Wavepacket Spreading

Though Ehrenfest's theorem provides a formal connection between quantum mechanics and classical mechanics, it doesn't allow us to think of the motion of a quantum wave function as we do the trajectory of a classical particle.
To a good approximation, we can do this if

1. Quantum means follow the classical trajectories
2. Δq and Δp are small on a scale of dimensions of the trajectory.

Using point 2 above to justify the approximate validity of point 1 (they are related), let

$$\hat{q} = \langle \hat{q} \rangle + \delta \hat{q}$$
$$\hat{p} = \langle \hat{p} \rangle + \delta \hat{p}$$

Then

$$\begin{aligned} \langle \hat{q}\hat{p} \rangle &= \langle (\langle \hat{q} \rangle + \delta \hat{q}) (\langle \hat{p} \rangle + \delta \hat{p}) \rangle \\ &= \langle \hat{q} \rangle \langle \hat{p} \rangle + \langle \delta \hat{q} \delta \hat{p} \rangle \end{aligned}$$

Where the second term is approximately $\Delta q \Delta p$. If this term is small compared to $\hat{q}$ and $\hat{p}$, we can approximately absorb it into $\langle \hat{q} \rangle \langle \hat{p} \rangle$. For example, consider:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{q})$$
$$\Rightarrow \frac{d}{dt} \langle \hat{q} \rangle = \frac{\langle \hat{p} \rangle}{m} \qquad \text{and} \qquad \frac{d}{dt} \langle \hat{p} \rangle = - \left\langle \frac{\partial \hat{V}(\hat{q})}{\partial \hat{q}} \right\rangle$$

Then

$$\begin{aligned} \hat{V}(\hat{q}) &= \hat{V}(\langle \hat{q} \rangle + \delta \hat{q}) \\ &\approx \hat{V}(\langle \hat{q} \rangle) + \hat{V}'(\langle \hat{q} \rangle) \delta \hat{q} + \frac{1}{2} \hat{V}''(\langle \hat{q} \rangle) \delta \hat{q}^2 \\ \Rightarrow \hat{V}(\hat{q}) &\approx \hat{V}(\langle \hat{q} \rangle) + \frac{1}{2} \hat{V}''(\langle \hat{q} \rangle) \langle \delta \hat{q}^2 \rangle \end{aligned}$$

$$\Rightarrow \left\langle \frac{d}{d\hat{q}}\hat{V}(\hat{q}) \right\rangle \approx \hat{V}'(\langle\hat{q}\rangle) + \frac{1}{2}\hat{V}'''(\langle\hat{q}\rangle)\left\langle \delta\hat{q}^2 \right\rangle$$

If the $\left\langle \delta\hat{q}^2 \right\rangle$ is small enough to neglect, then

$$\frac{d}{dt}\langle\hat{p}\rangle \approx -\frac{d}{dq}\hat{V}(\langle\hat{q}\rangle)$$

Remark 4: If $\left\langle \delta\hat{q}^2 \right\rangle$ starts out small, does it remain small? To answer this, we use equation (†) from §8.1:

$$\begin{aligned}
\frac{d}{dt}\left\langle \delta\hat{q}^2 \right\rangle &= \frac{1}{i\hbar}\left\langle \left[\delta\hat{q}^2, \hat{H}\right] \right\rangle \\
&= \frac{1}{i\hbar}\left\langle \left[\delta\hat{q}^2, \frac{\hat{p}^2}{2m}\right] \right\rangle \\
&= \frac{1}{i\hbar}\left\langle \left[(\hat{q}-\langle\hat{q}\rangle)^2, \frac{\hat{p}^2}{2m}\right] \right\rangle \\
&\vdots \\
&= \frac{1}{m}\left(\langle\hat{q}\hat{p}+\hat{p}\hat{q}\rangle - 2\langle\hat{q}\rangle\langle\hat{p}\rangle\right)
\end{aligned}$$

Similarly,

$$\frac{d}{dt}\left\langle \delta\hat{q}^2 \right\rangle = \left\langle \frac{1}{m}(\hat{q}\hat{p}+\hat{p}\hat{q} - 2\langle\hat{q}\rangle\hat{p} \right\rangle$$

$$\begin{aligned}
\Rightarrow \frac{d^2}{dt^2}\left\langle \delta\hat{q}^2 \right\rangle &= \frac{1}{i\hbar m}\left\langle \left[\hat{q}\hat{p}+\hat{p}\hat{q} - 2\langle\hat{q}\rangle\hat{p}, \hat{H}\right] \right\rangle \\
&\vdots \\
&= \frac{4}{m}\left(\left\langle \hat{H} \right\rangle - \frac{\langle\hat{p}\rangle^2}{2m} - \hat{V}(\langle\hat{q}\rangle) - \hat{V}''(\langle\hat{q}\rangle)\left\langle \delta\hat{q}^2 \right\rangle \right)
\end{aligned}$$

Let's let

$$\varepsilon = \left\langle \hat{H} \right\rangle - \underbrace{\frac{\langle\hat{p}\rangle^2}{2m} - \hat{V}(\langle\hat{q}\rangle)}_{\text{Classical Energy}}$$

$$\Rightarrow \frac{d^2}{dt^2}\left\langle \delta\hat{q}^2 \right\rangle \approx \frac{4}{m}\left(\varepsilon - \hat{V}''(\langle\hat{q}\rangle)\left\langle \delta\hat{q}^2 \right\rangle \right) \qquad (\dagger\dagger\dagger)$$

One can use the above to determine the error introduced by replacing

$$\left\langle \frac{d\hat{V}}{d\hat{q}} \right\rangle \quad \text{by} \quad \frac{d}{d\hat{q}}\hat{V}(\langle\hat{q}\rangle) \quad \text{in Ehrenfest's Equation}$$

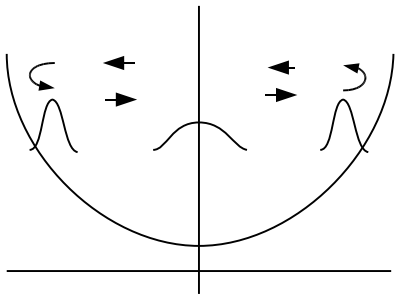
Remark 5: For a harmonic oscillator with potential $\hat{V}(\hat{q}) = \frac{1}{2}m\omega^2\hat{q}^2$,

$$(\dagger\dagger\dagger) \Rightarrow \qquad \frac{d^2}{dt^2}\left\langle \delta\hat{q}^2 \right\rangle = \frac{4\varepsilon}{m} - 4\omega^2\left\langle \delta\hat{q}^2 \right\rangle$$

while the equation for the mean is:

$$\frac{d^2}{dt^2}\left\langle \hat{q} \right\rangle = -\omega^2\left\langle \hat{q} \right\rangle$$

which we get from solving Ehrenfest's equations for the harmonic oscillator potential. The two above equations imply that $\langle\hat{q}\rangle$ oscillates at frequency ω, while $\left\langle \delta\hat{q}^2 \right\rangle$ oscillates at a frequency of 2ω.



But this looks just like our squeeze states!

Remark 6: For a free particle, $\hat{V}(\hat{q}) = 0$:

$$\begin{aligned} \Rightarrow \frac{d^2}{dt^2}\left\langle \delta\hat{q}^2 \right\rangle &= \frac{4}{m}\varepsilon \\ &= \frac{4}{m}\left(\frac{\left\langle \hat{p}^2 \right\rangle}{2m} - \frac{\left\langle \hat{p} \right\rangle^2}{2m} \right) \\ &= \frac{2}{m^2}\underbrace{\left\langle \delta\hat{p}^2 \right\rangle}_{\text{const.}} \end{aligned}$$

$$\left\langle \delta\hat{q}^2 \right\rangle(t) = \left\langle \delta\hat{p}^2 \right\rangle t^2 + \left.\frac{d}{dt}\left\langle \delta\hat{q}^2 \right\rangle\right|_{t=0} + \left\langle \delta\hat{q}^2 \right\rangle(0)$$

This implies that the wavepacket disperses in time, and thus the classical approximation remains valid only for a limited time.

8.3 Classical Limit of Schrodinger Equation and the WKB Approximation

The alternative formulation of the classical limit is to make a connection between the flow of probability density by the Schrodinger equation and the flow of probability density in classical statistical mechanics.

8.3.1 Quantum Mechanical Probability Current

The quantum mechanical probability density in quantum mechanics is given by

$$P(\vec{r},t) = \psi^*(\vec{r},t)\psi(\vec{r},t)$$

$$\rightarrow \int P(\vec{r},t)\, d\vec{r} = 1$$

Now imagine that the probability density represents a particle or fluid density. Then, the evolution of the probability density (according to the Schrodinger equation) may be thought of as a result of fluid flow:

$$\frac{dP}{dt} = \frac{\partial P}{\partial t} + \nabla \cdot \vec{J} = 0$$

where $\vec{J}$ is the probability current and the whole expression equals 0 so that normalization is conserved.

$$\Rightarrow \frac{\partial P}{\partial t} = -\nabla \cdot \vec{J}$$

But

$$\begin{aligned}
\frac{\partial P}{\partial t} &= \frac{\partial}{\partial t}\left(\psi^*\psi\right) \\
&= \frac{\partial \psi^*}{\partial t}\psi + \psi^*\frac{\partial \psi}{\partial t} \\
&= -\frac{1}{i\hbar}(\hat{H}\psi)^* + \frac{1}{i\hbar}\psi^*(\hat{H}\psi) \\
&= \frac{i}{\hbar}\left((\hat{H}\psi)^*\psi - \psi^*(\hat{H}\psi)\right) \qquad (\dagger)
\end{aligned}$$

And so $\vec{J}$ must be defined to agree with the right hand side of (†).

Remark 1: There is some ambiguity in the definition of the probability current since satisfying (†) does not uniquely determine $\vec{J}$. We choose a symmetrized definition:

$$\begin{aligned}
\vec{J}(\vec{r}) &= \frac{1}{2}\left(\psi^*\frac{\vec{p}}{m}\psi + \left(\frac{\vec{p}}{m}\psi\right)^*\psi\right) \\
&= \frac{1}{2}\left(\frac{-i\hbar}{m}\psi^*\nabla\psi + \frac{i\hbar}{m}\psi\nabla\psi^*\right) \\
&= -\frac{i\hbar}{2m}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) \qquad (\ddagger)
\end{aligned}$$

Remark 2: $\frac{\hat{p}}{2m}$ is chosen so that (‡) looks like velocity times density as in classical current density.

So $-\nabla \cdot \vec{J}$, with definition (‡), gives:

$$\begin{aligned}
-\nabla \cdot \vec{J} &= \frac{i\hbar}{2m}\left(\nabla\psi^* \cdot \nabla\psi + \psi^*\nabla^2\psi - \nabla\psi \cdot \nabla\psi^* - \psi\nabla^2\psi^*\right) \\
&= \frac{-i}{\hbar}\left(\psi^*\frac{\hat{p}^2}{2m}\psi - \psi\frac{\hat{p}^2}{2m}\psi^*\right) \\
&= \frac{-i}{\hbar}\left(\psi^*\left(\frac{\hat{p}^2}{2m} + V(\vec{r})\right)\psi - \psi\left(\frac{\hat{p}^2}{2m} + V(\vec{r})\right)\psi^*\right) \\
&= \frac{-i}{\hbar}\left(\psi^*(\hat{H}\psi) - \psi(\hat{H}\psi)^*\right) \\
&= \frac{\partial P}{\partial t} \leftarrow \text{probability flow}
\end{aligned}$$

8.3.2 Connect Probability Current in Classical Mechanics to Quantum Mechanics

To formally connect the flow of probability in QM to that in CM, write the wave function in terms of amplitude and phase variable.

$$\psi(\vec{r},t) = \underbrace{A(\vec{r},t)}_{\text{amplitude}}\underbrace{e^{iS(\vec{r},t)/\hbar}}_{\text{phase}}$$

Substituting this into the Schrodinger equation to obtain 2-coupled equations:

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi &= \frac{-\hbar^2}{2m}\nabla^2\psi + V\psi \\
i\hbar\frac{\partial}{\partial t}\left(Ae^{-S/\hbar}\right) &= \left(\frac{-\hbar^2}{2m}\nabla^2 + V\right)Ae^{-iS/\hbar} \\
&\vdots \\
&\text{Equating real and imaginary parts:} \\
&\vdots
\end{aligned}$$

$$\Rightarrow \left.\begin{aligned}
\frac{\partial A}{\partial t} &= \frac{-1}{m}\nabla A \cdot \nabla S - \frac{1}{2m}A\nabla^2 S \\
\frac{\partial S}{\partial t} &= -\frac{1}{2m}\left(\nabla S\right)^2 - V + \frac{\hbar^2}{2m}\nabla^2 A
\end{aligned}\right\} \quad (\dagger)$$

From this we can obtain an expression for the equation of motion for the probability current.

$$P(\vec{r}) = \psi^*\psi = A(\vec{r})^2$$

$$\Rightarrow \frac{\partial P}{\partial t} = 2A\frac{\partial A}{\partial t} = -\frac{2A}{m}\nabla A \cdot \nabla S - \frac{A^2}{m}\nabla^2 S$$
$$\frac{\partial}{\partial t}A^2 = -\frac{1}{m}\nabla \cdot \left(A^2 \nabla S\right)$$

And we can identify the probability current density:

$$\vec{J} = \frac{1}{m}A^2 \nabla S \Rightarrow \frac{\partial P}{\partial t} = -\nabla \cdot \vec{J}$$

Remark 1: The classical limit here is taking $\hbar \to 0$ in equation (†). This implies:

$$\frac{\partial S}{\partial t} = -\frac{1}{2m}\left(\nabla S\right)^2 - V \qquad (\dagger\dagger)$$

This gives the flow of probability density in phase space. The S that satisfies (††) is the principle function of Hamilton as seen in the Hamilton-Jacobi formulation of classical mechanics. (See Phys 505!)

Remark 2: For the special case of stationary states ($\hat{H}\psi = E\psi$):

$$\frac{\partial A}{\partial t} = 0 \qquad \text{and} \qquad \frac{\partial S}{\partial t} = -E$$

and equation (†) becomes

$$\left.\begin{aligned} \nabla \cdot \left(A^2 \nabla S\right) &= 0 \\ \left(\nabla S\right)^2 + 2m(V - E) &= \frac{\hbar^2 \nabla^2 A}{A} \end{aligned}\right\}$$

8.3.3 WKB Approximation

Here, the idea is similar to the classical approximation, but less extreme, since we keep the $\hbar$ dependence to the lowest order. Taking the wavefunction:

$$\psi(\vec{r}) = A(\vec{r})e^{iS(\vec{r})/\hbar}$$

and write this as

$$\psi(\vec{r}) = \exp\left(\frac{i}{\hbar}W(\vec{r})\right)$$

with

$$W(\vec{r}) = S(\vec{r}) + \frac{\hbar}{i}\ln\left(A(\vec{r})\right)$$

Remark 1: $A(\vec{r})$ and $S(\vec{r})$ still evolve accordingly to (†) in §8.3.2, but they are no longer restricted to be real functions.

The idea now is to expand our $W(\vec{r})$ to order $\hbar^2$ and drop higher level terms. Take, for example, the case of stationary states in 1-D:

$$\frac{d}{dx}\left(A^2\frac{dS}{dx}\right) = 0 \tag{1}$$

$$\left(\frac{dS}{dx}\right)^2 + 2m(V(x) - E) = \frac{\hbar^2}{A}\frac{d^2A}{dx^2} \tag{2}$$

$$\begin{aligned}
(1) \Rightarrow 2A\frac{dA}{dx}\frac{dS}{dx} + A^2\frac{d^2S}{dx^2} &= 0 \\
2\frac{dA}{dx}\frac{dS}{dx} + A\frac{d^2S}{dx^2} &= 0 \\
\int \frac{1}{A}\frac{dA}{dx}\,dx &= -\frac{1}{2}\int \frac{\frac{d}{dx}\left(\frac{dS}{dx}\right)}{\frac{dS}{dx}}\,dx \\
\ln(A) &= -\frac{1}{2}\ln\left(\frac{dS}{dx}\right) + \text{ constant} \\
\Rightarrow A &= C\left(\frac{dS}{dx}\right)^{-1/2}
\end{aligned}$$

Substituting this into (2):

$$\begin{aligned}
\left(\frac{dS}{dx}\right)^2 &= 2m(E-V) + \hbar^2\left(\frac{dS}{dx}\right)^{1/2}\frac{d}{dx}\left[-\frac{1}{2}\left(\frac{dS}{dx}\right)^{-3/2}\frac{d^2S}{dx^2}\right] \\
&= 2m(E-V) + \hbar^2\left(\frac{dS}{dx}\right)^{1/2}\left[\frac{3}{4}\left(\frac{dS}{dx}\right)^{-5/2}\left(\frac{d^2S}{dx^2}\right)^2 - \frac{1}{2}\left(\frac{dS}{dx}\right)^{-5/2}\frac{d^3S}{dx^3}\right] \\
&= 2m(E-V) + \hbar^2\left[\frac{3}{4}\left(\frac{\frac{d^2S}{dx^2}}{\frac{dS}{dx}}\right)^2 - \frac{1}{2}\left(\frac{\frac{d^3S}{dx^3}}{\frac{dS}{dx}}\right)\right]
\end{aligned} \tag{3}$$

Remark 2: Solving (3) exactly is equivalent to solving the original Schrodinger equation. The WKB approximation enters here: we begin by expanding S in powers of $\hbar^2$. Let $S = S_0 + S_1\hbar^2 + \ldots$, and substitute into (3). Doing this will generate a system of equations for $S_0, S_1, \ldots$ by equating powers of $\hbar^2$.
To Zeroeth Order:

$$\left(\frac{dS_0}{dx}\right)^2 = 2m(E-V)$$

To order $\hbar^2$:

$$2\frac{dS_0}{dx}\frac{dS_1}{dx} = \frac{3}{4}\left(\frac{\frac{d^2S_0}{dx^2}}{\frac{dS_0}{dx}}\right)^2 - \frac{1}{2}\frac{\frac{d^3S_0}{dx^3}}{\frac{dS_0}{dx}}$$

Remark 3: In general, the expansion of S in powers of $\hbar^2$ does *not* converge–it is an asymptotic expansion (initially decrease, and then increase in error), so a good approximation is obtained *if* a series is truncated at some finite values.

The simplest approximation is truncation at zero order:

$$\psi(x) = \begin{cases} \pm \int dx \sqrt{2m(E - V(x))} + \alpha_{\pm}, & E > V(x) \\ \pm i \int dx \sqrt{2m(V(x) - E)} + \beta_{\pm}, & E < V(x) \end{cases}$$

where $\alpha_p m$ and $\beta_{\pm}$ are arbitrary constants. Then

$$A = \text{ const } \cdot \left(\frac{dS}{dx}\right)^{-1/2}$$

$$\Rightarrow A_0(x) = \begin{cases} \gamma_{\pm} \left(2m(E - V(x))\right)^{-1/4}, & E > V(x) \\ \delta_{\pm} \left(2m(V(x) - E)\right)^{-1/4}, & E < V(x) \end{cases}$$

where $\gamma_{\pm}$ and $\delta_{\pm}$ are arbitrary constants. So the solution will be a linear combination of the plus and minus solutions:

$$\psi(\vec{r}) = e^{\frac{i}{\hbar} W(\vec{r})} \qquad \text{with} \qquad W(\vec{r}) = S(\vec{r}) + \frac{\hbar}{i} \ln\left(A(\vec{r})\right)$$

gives

- For $E > V(x)$:

$$\psi(x) = \left(2m(E - V(x)\right)^{-1/4} \left(C_+ e^{\frac{i}{\hbar} \int dx \sqrt{2m(E - V(x))}} + C_- e^{\frac{i}{\hbar} \int dx \sqrt{2m(E - V(x))}}\right) \tag{4}$$

- For $E < V(x)$:

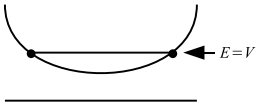
$$\psi(x) = \left(2m(V(x) - E\right)^{-1/4} \left(D_+ e^{\frac{1}{\hbar} \int dx \sqrt{2m(V(x) - E)}} + D_- e^{\frac{1}{\hbar} \int dx \sqrt{2m(V(x) - E)}}\right) \tag{5}$$

Remark 4: To determine the accuracy of the solutions (4) and (5), consider the term $\mathcal{O}(\hbar^2)$ in the expansion of S. Note that once we have S_0, we can, in principle, find S_1. In order for this to be a good approximation, we require that

$$\left|\hbar^2 S_1\right| \ll |S_0|$$

$$\Rightarrow m\hbar^2 \frac{|dV/dx|}{|2m(E - V(x))|^{3/2}} \ll 1$$

(See Messiah Eqn VI.47 for details) Thus, the potential must change slowly in space compared to the rate of change of zero approximation for the wave function. This *does not* happen when $E = V$ (turning points in the classical trajectories).



Remark 5: The solutions (4) and (5) represent oscillatory solutions in classically allowed regions and exponential decay in classically forbidden regions. These solutions must still match at the boundaries; however, the solutions are only asymptotic and not necessarily well defined near the boundaries. If the form of the wavefunction can be determined unambiguously near the boundary, then it is possible to connect the two solutions. (See Messiah Ch. 6, §11 for HO for how to do this in this case)

Chapter 9

Symmetries

In §2.1.4, we stated Nothers Theorem: symmetries in the system correspond to conservation laws. This holds for whether we are speaking of classical or quantum systems. Here we investigate from a quantum mechanical viewpoint.

9.1 Translations, Translational Invariance, and Conservation of Momentum

Classically, if the Hamiltonian is invariant with respect to $x \to x + a$, then p_x is conserved.

Remark 1: In quantum mechanics, we do not have a well defined position or momentum, so we replace these quantities by their quantum averages:

$$x \to \langle \hat{x} \rangle$$

$$p \to \langle \hat{p} \rangle$$

Remark 2: In analogy with classical mechanics, we expect translations to give:

$$\left.\begin{array}{c} \langle \hat{x} \rangle \to \langle \hat{x} \rangle + \varepsilon \\ \langle \hat{p} \rangle \to \langle \hat{p} \rangle \end{array}\right\} \text{Translation}$$

$$\left.\left\langle \hat{H} \right\rangle \to \left\langle \hat{H} \right\rangle\right\} \text{Translational Invariance}$$

$$\left.\left\langle \dot{\hat{p}} \right\rangle = 0\right\} \text{Conservation Law}$$

9.1.1 Active Translations

Recall §1.2.4: There were 2 types of transformations:

- the Active: transformed vectors in Hilbert space

- the Passive: transformed Hilbert space operators

Here, we define the (infinitesimal) translation operator $\hat{T}(\varepsilon)$ to have the following action:

$$\hat{T}(\varepsilon)|\psi\rangle \equiv |\psi_\varepsilon\rangle$$

so that

$$\langle\hat{x}\rangle \to \langle\hat{x}\rangle + \varepsilon$$

or that

$$\langle\psi_\varepsilon|\hat{x}|\psi_\varepsilon\rangle = \langle\psi|\hat{x}|\psi\rangle + \varepsilon$$

Consider the action of the translation operator on the position eigenstate:

$$\hat{T}(\varepsilon)|x\rangle = |x+\varepsilon\rangle$$

which shifts the position to the right by amount ε. Then, if $\langle x|\psi\rangle = \psi(x)$, we have

$$\begin{aligned}
\langle x|\psi_\varepsilon\rangle &= \langle x|\hat{T}(\varepsilon)|\psi\rangle \\
&= \langle x|\hat{T}(\varepsilon)\int_{-\infty}^{\infty}|y\rangle\langle y|\,dy\;|\psi\rangle \\
&= \langle x|\int_{-\infty}^{\infty}dy\;|y+\varepsilon\rangle\langle y|\psi\rangle \\
&= \langle x|\int_{-\infty}^{\infty}dy\;|y\rangle\langle y-\varepsilon|\psi\rangle \\
&= \delta_{xy}\langle y-\varepsilon|\psi\rangle \\
&= \langle x-\varepsilon|\psi\rangle \\
&= \psi(x-\varepsilon)
\end{aligned}$$

Remark 1: $\hat{T}(\varepsilon)|x\rangle = |x+\varepsilon\rangle$ is not the most general result. In fact, we could write:

$$\hat{T}(\varepsilon)|x\rangle = \underbrace{e^{i\varepsilon g(x)/\hbar}}_{\substack{\text{space dependent}\\ \text{phase factor}}}|x+\varepsilon\rangle$$

This result still gives:

$$\langle\hat{x}\rangle \to \langle\hat{x}\rangle + \varepsilon$$

but gives

$$\begin{aligned}
\langle\hat{p}\rangle &\to \langle x|\hat{T}^\dagger(\varepsilon)\hat{p}\hat{T}(\varepsilon)|x\rangle \\
&= \langle x+\varepsilon|e^{-i\varepsilon g(x)/\hbar}(-i\hbar)\frac{d}{dx}e^{i\varepsilon g(x)/\hbar}|x+\varepsilon\rangle \\
&= \langle x+\varepsilon|e^{-i\varepsilon g(x)/\hbar}\left((-i\hbar)\frac{i\varepsilon}{\hbar}g'(x)e^{i\varepsilon g(x)/\hbar}|x+\varepsilon\rangle + (-i\hbar)e^{i\varepsilon g(x)/\hbar}\frac{\partial}{\partial x}|x+\varepsilon\rangle\right) \\
&= \langle\hat{p}\rangle + \varepsilon\left\langle\frac{dg}{dx}\right\rangle
\end{aligned}$$

For translations, we require that

$$\langle \hat{p} \rangle \to \langle \hat{p} \rangle \Rightarrow g = \text{ constant}$$

and we take this constant to be zero (for simplicity).

Definition 1: Translational Invariance is defined by

$$\langle \psi | \hat{H} | \psi \rangle = \langle \psi_\varepsilon | \hat{H} | \psi_\varepsilon \rangle$$

i.e., the expectation of the Hamiltonian is invariant under infinitesimal translation.

Remark 2: According to Nother's Theorem, translational symmetry implies a conservation law. (Here, it will be conservation of momentum.)

Proposition 1: Momentum, $\hat{p}$, is the generator of infinitesimal translations.

- Proof: Since ε is small, we expand $\hat{T}(\varepsilon)$ in a Taylor series about ε to $\mathcal{O}(\varepsilon)$:

$$\hat{T}(\varepsilon) = \hat{I} + \varepsilon \hat{G}$$

where $\hat{T}(0) \Leftrightarrow$ no translations. Then:

$$\langle x | \hat{T}(\varepsilon) | x \rangle = \langle x | \psi_\varepsilon \rangle \equiv \psi(x - \varepsilon)$$

Expanding both sides to $\mathcal{O}(\varepsilon)$:

$$\begin{aligned}
\langle x | \hat{I} + \varepsilon \hat{G} | \psi \rangle &= \psi(x) - \varepsilon \frac{d\psi}{dx} \\
\psi(x) + \varepsilon \langle x | \hat{G} | \psi \rangle &= \psi(x) - \varepsilon \frac{d\psi}{dx} \\
\Rightarrow \langle x | \hat{G} | \psi \rangle &= -\frac{d\psi}{dx} = \frac{1}{i\hbar} \langle x | \hat{p} | \psi \rangle \\
\Rightarrow \hat{G} &= \frac{1}{i\hbar} \hat{p} \\
\Rightarrow \hat{T}(\varepsilon) &= \hat{I} + \frac{\varepsilon}{i\hbar} \hat{p}
\end{aligned}$$

Proposition 2: Momentum is conserved in a translationally invariant system.

- Proof: We begin with the definition of translational invariance:

$$\begin{aligned}
\langle \psi | \hat{H} | \psi \rangle &= \langle \psi_\varepsilon | \hat{H} | \psi_\varepsilon \rangle \\
&= \langle \psi | \hat{T}^\dagger(\varepsilon) \hat{H} \hat{T}(\varepsilon) | \psi \rangle \\
&= \langle \psi | \left(\hat{I} - \frac{\varepsilon}{i\hbar} \hat{p} \right) \hat{H} \left(\hat{I} + \frac{\varepsilon}{i\hbar} \hat{p} \right) | \psi \rangle \\
&= \langle \psi | \hat{H} | \psi \rangle - \frac{\varepsilon}{i\hbar} \langle \psi | \hat{p} \hat{H} - \hat{H} \hat{p} | \psi \rangle + \mathcal{O}(\varepsilon^2)
\end{aligned}$$

Since we are translationally invariant, $\mathcal{O}(\varepsilon^2) = \langle\psi|\,[\hat{p}, \hat{H}]\,|\psi\rangle = 0$. And by Ehrenfest's theorem:

$$\left\langle [\hat{p}, \hat{H}] \right\rangle = 0 \Rightarrow \left\langle \dot{\hat{p}} \right\rangle = 0 \Rightarrow \text{ momentum is conserved}$$

Remark 3: So far, we have considered only infinitesimal translations. If we need finite translations, say $\langle\hat{x}\rangle \to \langle\hat{x}\rangle + a$, where $a \gg \varepsilon$, we divide a into N intervals of a/N and let $N \to \infty$. Then we consider infinitesimal translations:

$$\hat{T}\left(\frac{a}{N}\right) = \hat{I} - \frac{ia}{\hbar N}\hat{p}$$

and define our finite translation operator as

$$\hat{T}\,(a) = \lim_{N\to\infty}\left[\hat{T}\left(\frac{a}{N}\right)\right]^N = e^{-ia\hat{p}/\hbar}$$

In coordinate basis:

$$\hat{T}\,(a) \to e^{-a\frac{d}{dx}}$$

So

$$\begin{aligned}\langle x|\,\hat{T}\,(a)\,|\psi\rangle &= \langle x|\,e^{-a\frac{d}{dx}}\,|\psi\rangle \\ &= \psi(x) - a\frac{d\psi}{dx} + \frac{1}{2}a^2\frac{d^2\psi}{dx^2} + \cdots \\ &= \psi(x-a)\end{aligned}$$

Remark 4: For consecutive translations

$$\hat{T}\,(a)\,\hat{T}\,(b) = e^{-ia\hat{p}/\hbar}e^{-ib\hat{p}/\hbar} = e^{i(a+b)\hat{p}/\hbar} = \hat{T}\,(a+b)$$

9.1.2 Passive Transformations

Passive translations leave quantum states invariant, whil shifting the coordinate system to the left by the amount ε (assuming position is shifted to the right in the active case). See Shankar for the complete derivation of the translational operator in passive version. Briefly, the requirement that the position and momentum operators must obey is:

$$\hat{T}^\dagger(\varepsilon)\hat{x}\hat{T}\,(\varepsilon) \to \hat{x} + \varepsilon\hat{I}$$
$$\hat{T}^\dagger(\varepsilon)\hat{p}\hat{T}\,(\varepsilon) \to \hat{p}$$

Expanding $\hat{T}\,(\varepsilon)$ in powers of ε results in:

$$\hat{T}\,(\varepsilon) = \hat{I} + \frac{\varepsilon}{i\hbar}\hat{p}$$

which we note is the same expression as in the active case. In the passive transformation picture, translational invariance requires

$$\hat{T}^{\dagger}(\varepsilon)\hat{H}\hat{T}(\varepsilon) = \hat{H}$$

which again requires that the Hamiltonian is invariant under translation. Now we want to show that this is equivalent to

$$\hat{H}\left(\hat{x} + \varepsilon\hat{I}, \hat{p}\right) = \hat{H}(\hat{x}, \hat{p})$$

Proposition: For any $\hat{\Omega}(\hat{x}, \hat{p})$ that can be expanded in a power series, and for and unitary operator $\hat{U}$:

$$\hat{U}^{\dagger}\hat{\Omega}\hat{U} = \hat{\Omega}\left(\hat{U}^{\dagger}\hat{x}\hat{U}, \hat{U}^{\dagger}\hat{p}\hat{U}\right)$$

- Proof: Expand $\hat{\Omega}$ in a power series and consider a typical term (i.e. $\hat{p}\hat{x}\hat{p}$). Then, for this term, we have

$$\hat{U}^{\dagger}\hat{p}\hat{x}\hat{p}\hat{U} = \hat{U}^{\dagger}\hat{p}\hat{U}\hat{U}^{\dagger}\hat{x}\hat{U}\hat{U}^{\dagger}\hat{p}\hat{U}$$

Collapsing the expansion, we get:

$$\hat{\Omega}\left(\hat{U}^{\dagger}\hat{x}\hat{U}, \hat{U}^{\dagger}\hat{p}\hat{U}\right)$$

Corollary:

$$\hat{\Omega}(\hat{x}, \hat{p}) \to \hat{T}^{\dagger}\hat{\Omega}\hat{T} = \hat{\Omega}\left(\hat{T}^{\dagger}\hat{x}\hat{T}, \hat{T}^{\dagger}\hat{p}\hat{T}\right) = \hat{\Omega}\left(\hat{x} + \varepsilon\hat{I}, \hat{p}\right)$$

- Proof: $\hat{T}$ is unitary. The rest follows from above.

Thus we see that for $\hat{\Omega} = \hat{H}$, translational invariance implies that

$$\hat{H}(\hat{x}, \hat{p}) = \hat{H}(\hat{x} + \varepsilon\hat{I}, \hat{p})$$

9.1.3 Translations For a Many Particle System

For a system of N particles, the translated many body wave-function becomes:

$$\langle x_1, \ldots, x_N | \hat{T}(\varepsilon) | \psi \rangle = \psi(x_1 - \varepsilon, x_2 - \varepsilon, \ldots, x_N - \varepsilon)$$

and, to $\mathcal{O}(\varepsilon)$,

$$\langle x_1, \ldots, x_N | \left(\hat{I} - \frac{i\varepsilon}{\hbar}\hat{p}\right) | \psi \rangle = \psi(x_1, \ldots, x_N) - \sum_{i=1}^{N} \varepsilon \frac{\partial \psi}{\partial x_i}$$

$$\Rightarrow \hat{T}(\varepsilon) = \hat{I} - \frac{i\varepsilon}{\hbar}\sum_{i=1}^{N}\hat{p}_i = \hat{I} - \frac{i\varepsilon}{\hbar}\hat{\mathcal{P}}$$

where $\hat{\mathcal{P}}$ is the total momentum operator.

Remark 1: For many particles, translations generalize to

$$\hat{T}^\dagger(\varepsilon)\hat{x}_i\hat{T}(\varepsilon) = \hat{x}_i + \varepsilon\hat{I}$$
$$\hat{T}^\dagger(\varepsilon)\hat{p}_i\hat{T}(\varepsilon) = \hat{p}_i$$

and translational invariance becomes:

$$\begin{aligned}\hat{T}^\dagger(\varepsilon)\hat{H}(\hat{x}_1,\hat{x}_2,\ldots,\hat{x}_N;\hat{p}_1,\hat{p}_2,\ldots,\hat{p}_N)\hat{T}(\varepsilon) &= \hat{H}(\hat{x}_1+\varepsilon\hat{I},\hat{x}_2+\varepsilon\hat{I},\ldots,\hat{x}_N+\varepsilon\hat{I};\hat{p}_1,\hat{p}_2,\ldots,\hat{p}_N)\\ &= \hat{H}(\hat{x}_1,\hat{x}_2,\ldots,\hat{x}_N;\hat{p}_1,\hat{p}_2,\ldots,\hat{p}_N)\end{aligned}$$

Remark 2: For a single particle system, translational invariance implies free particle which implies that $V = 0$. For a system of particles, translational invariance implies than $V = V(\hat{x}_i - \hat{x}_j)$–so that the Hamiltonian depends only on interactions between particles and not on "external" interactions.

Remark 3: In a translationally invariant system:

$$\hat{T}^\dagger(a)\hat{H}\hat{T}(a) = \hat{H} \qquad \text{and} \qquad \hat{T}^\dagger = \hat{T}$$

$$\Rightarrow \hat{H} = \hat{T}(a)\,\hat{H}\hat{T}^\dagger(a)$$
$$\Rightarrow \left[\hat{T}(a), \hat{H}\right] = 0$$
$$\Rightarrow \left[\hat{T}(a), \hat{U}(t)\right] = 0$$

This tells us that a system that starts translationally invariant remains translationally invariant.

9.2 Time Translational Invariance and Energy Conservation

We expect that homogeneity of time will give the same result if an experiment is repeated at different times.
A system is prepared in an initial state, $|\psi_0\rangle$ at time t_1. The Hamiltonian at this time is H_1, and the system evolves for a short time τ.

$$\begin{aligned}|\psi(t_1+\tau)\rangle &= \hat{U}(\tau)|\psi_0\rangle\\ &= e^{-i\hat{H}_1\tau/\hbar}|\psi_0\rangle\\ &= \left(\hat{I} - \frac{i}{\hbar}\hat{H}_1\tau\right)|\psi_0\rangle\end{aligned}$$

where $\hat{H}_1 = \hat{H}(t_1)$. The experiment is repeated, only system is prepared at time t_2:

$$|\psi(t_2+\tau)\rangle = \left(\hat{I} - \frac{i}{\hbar}\hat{H}_2\tau\right)|\psi_0\rangle$$

where $\hat{H}_2 = \hat{H}(t_2)$. Since the outcome does not depend on when the experiment is done, we require that

$$|\psi(t_1+\tau)\rangle = |\psi(t_2+\tau)\rangle$$
$$\Rightarrow \hat{H}(t_1) = \hat{H}(t_2)$$

This holds for arbitrary t_1 and t_2, so we can conclude that

$$\frac{\partial \hat{H}}{\partial t} = 0$$

which implies that $\hat{H}$ has no explicit time dependence.

Remark 1: Time translational invariance mean $\hat{H}$ is time-independent.

Remark 2: Remember Eherenfest's Theorem:

$$\frac{d}{dt}\left\langle \hat{A}\right\rangle = \frac{1}{i\hbar}\left\langle \left[\hat{A},\hat{H}\right]\right\rangle + \left\langle \frac{\partial \hat{A}}{\partial t}\right\rangle$$

Setting $\hat{A} = \hat{H}$ and using that $\left\langle \frac{\partial \hat{H}}{\partial t}\right\rangle = 0$, we have that

$$\frac{d}{dt}\left\langle \hat{H}\right\rangle = \frac{1}{i\hbar}\left\langle \left[\hat{H},\hat{H}\right]\right\rangle = 0$$

which implies that we have conservation of energy.

9.3 Discrete Symmetries: Parity and Time Reversal

9.3.1 Parity Invariance

Definition 1: The Parity operator, $\hat{\Pi}$, is defined by its action on the position eigenstate:

$$\hat{\Pi}|x\rangle = |-x\rangle$$

And it has the following properties:

1. $\hat{\Pi} = \hat{\Pi}^{-1}$

Proof:

$$\hat{\Pi}^2|x\rangle = \hat{\Pi}|-x\rangle = |x\rangle$$
$$\Rightarrow \hat{\Pi}^2 = \hat{I} \Rightarrow \hat{\Pi}^2\hat{\Pi}^{-1} = \hat{I}\hat{\Pi}^{-1} \Rightarrow \hat{\Pi} = \hat{\Pi}^{-1}$$

2. $\hat{\Pi}$ has e-values ± 1, which follows from $\hat{\Pi}^2 = \hat{I}$ and $\hat{\Pi}$ acting on an eigenstate.

$$\begin{aligned} \text{Eigenvalue } &= 1 \quad \Rightarrow \quad \text{Even parity} \\ \text{Eigenvalue } &= -1 \quad \Rightarrow \quad \text{Odd parity} \end{aligned}$$

3. $\hat{\Pi}^\dagger = \hat{\Pi}$ (Hermitian), and $\hat{\Pi}^\dagger \hat{\Pi} = \hat{I}$ (Unitary)

The action of the parity operator on an arbitrary ket is

$$\begin{aligned} \hat{\Pi} \left|\psi\right\rangle &= \hat{\Pi} \int_{-\infty}^{\infty} \left|y\right\rangle \left\langle y|\psi\right\rangle \, dy \\ &= \int_{-\infty}^{\infty} \left|-y\right\rangle \left\langle y|\psi\right\rangle \, dy \\ &= \int_{-\infty}^{\infty} \left|y\right\rangle \left\langle -y|\psi\right\rangle \, dy \end{aligned}$$

where the last line is by a simple change of variables. We know that $\langle x|\psi\rangle = \psi(x)$, and thus from the above we find that

$$\left|x\right\rangle \hat{\Pi} \left|\psi\right\rangle = \psi(-x)$$

and even or odd parity corresponds to the even or odd nature of the function $\psi(x)$.

Remark 1: $\hat{\Pi} \left|p\right\rangle = \left|p\right\rangle$ (which follows from the definition of $\hat{p}$ in position representation.)

Remark 2: The parity operator is the mirror image of a function about the origin.

Remark 3: For passive transformations

$$\begin{aligned} \hat{\Pi}\hat{x} &= -\hat{x} \\ \hat{\Pi}\hat{p} &= -\hat{p} \end{aligned}$$

and parity invariance happens when

$$\hat{\Pi}^\dagger \hat{H}(\hat{x}, \hat{p}) \hat{\Pi} = \hat{H}(-\hat{x}, -\hat{p}) = \hat{H}(\hat{x}, \hat{p})$$

which means that $\hat{\Pi}\hat{U}(t) = \hat{U}(t)\hat{\Pi}$ and thus parity is preserved over time.

Remark 4: If weak interactions are present, $\left[\hat{\Pi}, \hat{H}\right] \neq 0$ and thus parity is *not* preserved over time.

Remark 5: Parity transformations are different from space and time translations (and rotations) since this is a discrete transformation. It may be thought of as a mirror image of some process.

9.3.2 Time-Reversal

Definition 1: The time-reversed state is defined by

$$x_R(t) = x(t) \qquad \text{and} \qquad p_R(t) = -p(t)$$

(The system is moving in reverse.)

Time-Reversal Invariance (TRI): From an initial state of a system $x(0)$ and $p(0)$, the system evolves and at time T is at $x(T)$ and $p(T)$. Then we reverse the system and run for time T. We have TRI when

$$x(2T) = x(0) \qquad \text{and} \qquad p(2T) = -p(0)$$

Remark 1: TRI exists when you can time evolve the system forward or backward in time and there is no violation of physical laws.

Remark 2: Quantum mechanically, time reversal is consistent with our $\psi \to \psi^*$ since, in position representation,

$$x \to x \quad \text{and} \quad p \to -p$$

under complex conjugation. For example, if we have an initial state $\psi(x, 0)$ and we time evolve that state for time T:

$$\psi(x, T) = e^{-i\hat{H}T/\hbar}\psi(x, 0)$$

If we then time-reverse the system for time T:

$$\psi(x, T) \to \psi^*(x, T) = e^{i\hat{H}^*T/\hbar}\psi^*(x, 0)$$

We then evolve the system forward again (for time T)

$$e^{-i\hat{H}T/\hbar}e^{i\hat{H}^*T/\hbar}\psi^*(x, 0)$$

Now, for TRI, we want $\psi(x, 2T) = \psi(x, 0)$ and $\hat{H} = \hat{H}^*$, the latter of which happen automatically whenever the Hamiltonian in real (for ever powers of $\hat{p}$).

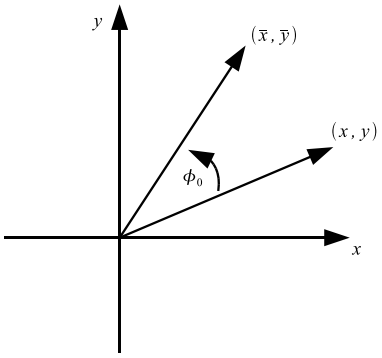
Remark 3: This is another example of discrete symmetry.

9.4 Rotations, Rotational Invariance, and Conservation of Angular Momentum

9.4.1 Rotations

9.4.1.1 Rotations in 2D

Recall in classical mechanics, we define a counterclockwise rotation of a vector about the z-axis by:



$$\bar{x} = x\cos(\phi_0) - y\sin(\phi_0)$$
$$\bar{y} = x\sin(\phi_0) + y\cos(\phi_0)$$

$$\Rightarrow \begin{pmatrix}\bar{x}\\ \bar{y}\end{pmatrix} = \begin{pmatrix}\cos(\phi_0) & -\sin(\phi_0)\\ \sin(\phi_0) & \cos(\phi_0)\end{pmatrix}\begin{pmatrix}x\\ y\end{pmatrix}$$

And we identify a rotation matrix

$$R(\phi) = \begin{pmatrix}\cos(\phi) & -\sin(\phi)\\ \sin(\phi) & \cos(\phi)\end{pmatrix}$$

which also rotates momentum vectors.
In QM, define the operator $\hat{U}[R(\phi\hat{z})]$ as the operator which rotates a vector in Hilbert space:

$$|\psi\rangle \xrightarrow{\hat{U}[R]} |\psi_R\rangle = \hat{U}[R]\,|\psi\rangle$$

Here we abbreviate $\hat{U}[R(\phi\hat{z})] \to \hat{U}[R]$ and the rotated vector $|\psi_R\rangle$ must satisfy

$$\langle\hat{x}\rangle_R = \langle\psi_R|\hat{x}|\psi_R\rangle = \langle\hat{x}\rangle\cos(\phi_0) - \langle\hat{y}\rangle\sin(\phi_0)$$
$$\langle\hat{y}\rangle_R = \langle\psi_R|\hat{y}|\psi_R\rangle = \langle\hat{x}\rangle\sin(\phi_0) + \langle\hat{y}\rangle\cos(\phi_0)$$

where

$$\langle\hat{x}\rangle = \langle\psi|\hat{x}|\psi\rangle$$
$$\langle\hat{y}\rangle = \langle\psi|\hat{y}|\psi\rangle$$

and similar expression hold for the x and y components of momentum.

Remark 1: Operating $\hat{U}[R]$ on position eigenkets:

$$\hat{U}[R]\,|x,y\rangle = |x\cos(\psi_0) - y\sin(\phi_0), x\sin(\phi_0) + y\cos(\phi_0)\rangle$$

Now consider infinitesimal rotations about the z-axis:

$$\hat{U}[R(\varepsilon\hat{z})] = \hat{I} + \frac{\varepsilon_z \hat{L}_z}{i\hbar}$$

where $\hat{L}_z$ is the generator of infinitesimal rotations. Consider now this action on a position eigenket:

$$\hat{U}[R]\,|x,y\rangle = |x - y\varepsilon_z, y + x\varepsilon_z\rangle$$

From this, we can show that

$$\left\langle x,y\middle|\hat{I} + \frac{\varepsilon_z\hat{L}_z}{i\hbar}\middle|\psi\right\rangle = \psi(x + y\varepsilon_z, y - x\varepsilon_z)$$

Expanding this to $\mathcal{O}(\varepsilon_z)$:

$$\left\langle x,y\middle|\hat{I}\middle|\psi\right\rangle + \frac{\varepsilon_z}{i\hbar}\left\langle x,y\middle|\hat{L}_z\middle|\psi\right\rangle = \psi(x,y) + \frac{\partial\psi}{\partial x}(\varepsilon_z y) + \frac{\partial\psi}{\partial y}(-\varepsilon_z x)$$

$$\Rightarrow \left\langle x,y\middle|\hat{L}_z\middle|\psi\right\rangle = \left(i\hbar y\frac{\partial}{\partial x} - i\hbar x\frac{\partial}{\partial y}\right)\psi(x,y)$$

So in position representation

$$\hat{L}_z \to x\left(-i\hbar\frac{\partial}{\partial y}\right) - y\left(-i\hbar\frac{\partial}{\partial x}\right)$$

or, more generally,

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \tag{†}$$

Remark 2: Putting (†) into momentum representation and acting on $\psi(p_x, p_y)$ rotates the momentum space wavefunctionso that momentum expectations are consistant with classical rotations.

Remark 3: The passive version of a rotational transformation has:

$$\left.\begin{aligned}
\hat{U}^\dagger[R]\hat{x}\hat{U}[R] &= \hat{x} - \hat{y}\varepsilon_z \\
\hat{U}^\dagger[R]\hat{y}\hat{U}[R] &= \hat{x}\varepsilon_z + \hat{y} \\
\hat{U}^\dagger[R]\hat{p}_x\hat{U}[R] &= \hat{p}_x - \hat{p}_y\varepsilon_z \\
\hat{U}^\dagger[R]\hat{p}_y\hat{U}[R] &= \hat{p}_y + \hat{p}_x\varepsilon_z
\end{aligned}\right\} \tag{††}$$

Remark 4: Substitute the infinitesimal version of $\hat{U}[R]$ $(\hat{I} + \frac{\varepsilon_z \hat{L}_z}{i\hbar})$ into (††) and get, to $\mathcal{O}(\varepsilon_z)$:

$$\left.\begin{aligned} \left[\hat{x}, \hat{L}_z\right] &= -i\hbar\hat{y} \\ \left[\hat{y}, \hat{L}_z\right] &= i\hbar\hat{x} \\ \left[\hat{p}_x, \hat{L}_z\right] &= -i\hbar\hat{p}_y \\ \left[\hat{p}_y, \hat{L}_z\right] &= i\hbar\hat{p}_y \end{aligned}\right\} \rightarrow \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

Remark 5: For finite rotations, take N infinitesimal rotations of size ϕ_0/N as $N \rightarrow \infty$

$$\hat{U}[R(\phi_0\hat{z})] = \lim_{N\rightarrow\infty}\left(\hat{I} - \frac{i}{\hbar}\frac{\phi_0}{N}\hat{L}_z\right)^N = e^{-i\phi_0\hat{L}_z/\hbar}$$

Writing $\hat{L}_z \rightarrow x\left(-i\hbar\frac{\partial}{\partial y}\right) - y\left(-i\hbar\frac{\partial}{\partial x}\right)$ in polar coordinates yields

$$\hat{L}_z \rightarrow -i\hbar\frac{\partial}{\partial\phi}$$

So

$$\hat{U}[R(\phi_0\hat{z})] = e^{-\phi\frac{\partial}{\partial\phi}}$$

And

$$\begin{aligned} e^{-\phi\frac{\partial}{\partial\phi}}\psi(\rho,\phi) &= \left(1 - \phi_0\frac{\partial}{\partial\phi} + \frac{1}{2!}\phi_0^2\frac{\partial^2}{\partial\phi^2} + \cdots\right)\psi(\rho,\phi) \\ &= \psi(\rho,\phi-\phi_0) \end{aligned}$$

Remark 6: Two consecutive rotations

$$\hat{U}[R(\phi_0'\hat{z})]\hat{U}[R\phi_0\hat{z})] = \hat{U}[R((\phi_0' + \phi_0)\hat{z})]$$

Remark 7: Physically, $\hat{L}_z$ is the angular momentum operator, which is analogous to the classical definition, and is the generator of infinitesimal rotations about the z axis.

Remark 8: If the system is invariant under rotations about the z axis, then

$$\hat{U}^\dagger[R]\hat{H}(\hat{x},\hat{p}_x,\hat{y},\hat{p}_y)\hat{U}[R] = \hat{H}(\hat{x},\hat{p}_x,\hat{y},\hat{p}_y)$$

Expanding this to order ε_z for infinitesimal rotations gives

$$\left[\hat{L}_z, \hat{H}\right] = 0$$

which implies

1. $\left\langle \hat{L}_z \right\rangle$ equals a constant, which then implies that angular momentum is conserved.
2. Outcomes of experiments on rotationally invariant systems will be the same for differing orientations of the system.
3. $\hat{L}_z$ and $\hat{H}$ can be simultaneously diagonalized, and therefore a common eigenbasis exists

Remark 9: A transformation which consists of a product of translations and rotations will, in general, depend on the order of individual transformations– e.g. translations and rotations do *not* commute.

9.4.1.2 Rotations in 3D

The results of the previous section may be generalized to include rotations about all 3 coordinate axes. The corresponding rotation matrices are:

$$R(\phi\hat{z}) = \begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R(\phi\hat{x}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\phi) & -\sin(\phi) \\ 0 & \sin(\phi) & \cos(\phi) \end{pmatrix}$$

$$R(\phi\hat{y}) = \begin{pmatrix} \cos(\phi) & 0 & \sin(\phi) \\ 0 & 1 & 0 \\ -\sin(\phi) & 0 & \cos(\phi) \end{pmatrix}$$

The generalization gives the components of angular momentum:

$$\left.\begin{aligned} \hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{L}_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{L}_z &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \end{aligned}\right\} \qquad (\dagger)$$

Remark 1: Equatios (†) are related by cyclic permutations of indices. i.e.

$$xyz \to yzx \to zxy$$

Remark 2: One can consider products of infinitesimal translations to derive commutation relations between components of angular momentum. We know that

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \xrightarrow{\hat{U}[R(\varepsilon_x \hat{x})]} \begin{pmatrix} x \\ y - \varepsilon_x z \\ z + \varepsilon_x y \end{pmatrix}, \quad \begin{pmatrix} x \\ y \\ z \end{pmatrix} \xrightarrow{\hat{U}[R(\varepsilon_y \hat{y})]} \begin{pmatrix} x + \varepsilon_y z \\ y \\ z - \varepsilon_y x \end{pmatrix}, \quad \begin{pmatrix} x \\ y \\ z \end{pmatrix} \xrightarrow{\hat{U}[R(\varepsilon_z \hat{z})]} \begin{pmatrix} x - \varepsilon_z y \\ y + \varepsilon_z x \\ z \end{pmatrix}$$

So now if we consider the following sequence of rotations:

$$R(\varepsilon_x \hat{x}) R(\varepsilon_y \hat{y}) R(-\varepsilon_x \hat{x}) R(-\varepsilon_y \hat{y})$$

$$\begin{aligned}
\Rightarrow \begin{pmatrix} x \\ y \\ z \end{pmatrix} &\xrightarrow{R(\varepsilon_x \hat{x})} \begin{pmatrix} x \\ y - \varepsilon_x z \\ z + \varepsilon_x y \end{pmatrix} \\
&\xrightarrow{R(\varepsilon_y \hat{y})} \begin{pmatrix} x + \varepsilon_y (z + \varepsilon_x y) \\ y - \varepsilon_x z \\ z + \varepsilon_x y - \varepsilon_y x \end{pmatrix} \\
&\xrightarrow{R(-\varepsilon_x \hat{x})} \begin{pmatrix} x + \varepsilon_y z + \varepsilon_y \varepsilon_x y \\ y - \varepsilon_x z + \varepsilon_x (z + \varepsilon_x y - \varepsilon_y x) \\ z + \varepsilon_x y - \varepsilon_y x - \varepsilon_x (y - \varepsilon_x z) \end{pmatrix} \\
&\xrightarrow{R(-\varepsilon_y \hat{y})} \begin{pmatrix} x + \varepsilon_y z + \varepsilon_y \varepsilon_x y - \varepsilon_y (z - \varepsilon_y x + \varepsilon_x^2 z) \\ y + \varepsilon_x^2 y - \varepsilon_x \varepsilon_y x \\ z - \varepsilon_y x + \varepsilon_x^2 z + \varepsilon_y (x + \varepsilon_y z + \varepsilon_y \varepsilon_x y) \end{pmatrix} \\
&= \begin{pmatrix} x + \varepsilon_y \varepsilon_x y + \varepsilon_y^2 x - \varepsilon_y \varepsilon_x z \\ y - \varepsilon_x \varepsilon_y x + \varepsilon_x^2 y \\ z + (\varepsilon_x^2 + \varepsilon_y^2) z + \varepsilon_x \varepsilon_y^2 y \end{pmatrix} \\
&\approx \begin{pmatrix} x + \varepsilon_y \varepsilon_x y \\ y - \varepsilon_x \varepsilon_y x \\ z \end{pmatrix}
\end{aligned}$$

Which is equivalent to

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \xrightarrow{R(-\varepsilon_x \varepsilon_y \hat{z})} \begin{pmatrix} x + \varepsilon_y \varepsilon_x y \\ y - \varepsilon_x \varepsilon_y x \\ z \end{pmatrix}$$

From this, we require that the quantum rotations must satisfy

$$\hat{U}[R(-\varepsilon_y \hat{y})] \hat{U}[R(-\varepsilon_x \hat{x})] \hat{U}[R(\varepsilon_y \hat{y})] \hat{U}[R(\varepsilon_x \hat{x})] = \hat{U}[R(-\varepsilon_x \varepsilon_y \hat{z})] \qquad (\dagger\dagger)$$

Writing

$$\hat{U}[R(\varepsilon_x \hat{x})] = \hat{I} + \frac{\varepsilon_x \hat{L}_x}{i\hbar}$$
$$\hat{U}[R(\varepsilon_y \hat{y})] = \hat{I} + \frac{\varepsilon_y \hat{L}_y}{i\hbar}$$
$$\hat{U}[R(\varepsilon_z \hat{z})] = \hat{I} + \frac{\varepsilon_z \hat{L}_z}{i\hbar}$$

and expanding and matching coefficients gives

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar \hat{L}_z$$

Similarly, one can find

$$\left[\hat{L}_y, \hat{L}_z\right] = i\hbar \hat{L}_x$$
$$\left[\hat{L}_z, \hat{L}_x\right] = i\hbar \hat{L}_y$$

Remark 3: The commutation relations are also related by cyclic permutations of the indices.

Remark 4: Alternative ways to express these commutation relations are

$$\hat{L} \times \hat{L} = i\hbar \hat{L}$$

which is legitimate since the components don't commute.

Remark 5: Also, introducing the Levi-Civita fully antisymmetric tensor ϵ_{ijk} where

$$\epsilon_{ijk} = \begin{cases} 0 & \text{if } i = j, j = k, k = i \\ 1 & \text{for even permutations} \\ -1 & \text{for odd permutations} \end{cases}$$

and $\epsilon_{123} = 1$, we can write

$$\left[\hat{L}_i, \hat{L}_j\right] = i\hbar \epsilon_{ijk} \hat{L}_k$$

where summation over repeated indices is implied.

Remark 6: For finite rotations in 3D–let $\hat{\theta} = \frac{\vec{\theta}}{\theta}$ be an arbitrary axis of rotation. Then $\hat{L}_\theta$ is the generator of infinitesimal rotations about that axis and

$$\begin{aligned}\hat{U}[R(\hat{\theta})] &= \lim_{N\to\infty}\left(\hat{I} + \frac{1}{i\hbar}\frac{\vec{\theta}}{\theta}\hat{\vec{L}}\right)^N \\ &= e^{-i\theta\frac{\vec{\theta}}{\theta}\hat{\vec{L}}/\hbar} \\ &= e^{-i\hat{\vec{\theta}}\cdot\hat{\vec{L}}/\hbar}\end{aligned}$$

9.4.2 Eigenvalues of Angular Momentum

9.4.2.1 Eigenvalues of $\hat{L}_z$

For a problem that is invariant with respect to rotations about the z-axis,

$\left[\hat{L}_z, \hat{H}\right] = 0 \quad \Rightarrow \quad$ there exists a common eigenbasis for $\hat{L}_z$ and $\hat{H}$

To find that basis, start with the eigenvalue problem for $\hat{L}_z$:

$$\hat{L}_z \left|l_z\right\rangle = l_z \left|l_z\right\rangle$$

In the coordinate basis, $\hat{L}_z \to -i\hbar\frac{\partial}{\partial\phi}$:

$$\begin{aligned}\Rightarrow -i\hbar\frac{\partial}{\partial\phi}\psi_{l_z}(\rho,\phi) &= l_z\psi_{l_z}(\rho,\phi) \\ \Rightarrow \psi_{l_z}(\rho,\phi) &= R(\rho)e^{il_z\phi/\hbar} \qquad (\dagger)\end{aligned}$$

where $R(\rho)$ is an arbitrary function of ρ.

Remark 1: For $\psi_{l_z}(\rho,\phi)$ to be normalized, we require:

$$\int_0^\infty \rho\, d\rho \int_0^{2\pi} d\phi\ \psi_{l_z}^*\psi_{l_z} = 1$$

Remark 2: For the normalization requirement, l_z seems arbitrary. However, it is *not* since we require our angular momentum operator to be Hermitian:

$$\left\langle\psi_1\middle|\hat{L}_z\middle|\psi_2\right\rangle = \left\langle\psi_2\middle|\hat{L}_z\middle|\psi_1\right\rangle^*$$

In the coordinate basis:

$$\begin{aligned}\int_0^\infty\int_0^{2\pi}\psi_1^*\left(-i\hbar\frac{\partial}{\partial\phi}\right)\psi_2\rho\,d\rho\,d\phi &= \left[\int_0^\infty\int_0^{2\pi}\psi_2^*\left(-i\hbar\frac{\partial}{\partial\phi}\right)\psi_1\rho\,d\rho\,d\phi\right]^* \\ &= \int_0^\infty\int_0^{2\pi}\psi_2\left(i\hbar\frac{\partial}{\partial\phi}\right)\psi_1^*\rho\,d\rho\,d\phi \\ &= i\hbar\int_0^\infty\rho\,d\rho\,\psi_2\psi_1^*\Big|_0^{2\pi} - \int_0^\infty\int_0^{2\pi}\psi_1^*\left(-i\hbar\frac{\partial}{\partial\phi}\right)\psi_2\rho\,d\rho\,d\phi\end{aligned}$$

Thus, to be Hermitian we want the first term to vanish, which happens when $\psi(\rho, 0) = \psi(\rho, 2\pi)$. Combining this with (†) implies that

$$1 = e^{il_z 2\pi/\hbar}$$

$$\Rightarrow l_z = m\hbar \qquad \text{where } m = 0, \pm 1, \pm 2, \ldots$$

Remark 3: Eigenvalues of $\hat{L}_z$ are discrete and m is called the magnetic quantum number.

Remark 4: At this point, $R(\rho)$ is arbitrary. However, if we are looking for a simultaneous eigenbasis for $\hat{L}_z$ and $\hat{H}$, then we use the eigenfunctions of $\hat{L}_z$ and (†) in the eigenvalue problem for $\hat{H}$. Thus the energy eigenvalues and eigenfunctions determine $R(\rho)$.

Remark 5: It is convenient to introduce the following functions:

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

This is the normalized angular part of (†):

$$\int_0^{2\pi} \Phi_n^*(\phi)\Phi_m(\phi)\, d\phi = \delta_{nm}$$

9.4.2.2 Solutions to Problems with Azimuthal Symmetry

Once we have determined the eigenfunctions of angular momentum, we can proceed to solve the eigenvalue equation for $\hat{H}$.

$$\left[\hat{L}_z, \hat{H}\right] = 0 \quad \Rightarrow \quad \hat{H} \text{ is not an explicit function of } \phi$$

$$\Rightarrow \hat{V}(\rho, \phi) = \hat{V}(\rho)$$

In cylindrical coordinates, the Schrodinger equation is

$$\left[\frac{-\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right) + V(\rho)\right]\psi_E(\rho, \phi) = E\psi_E(\rho, \phi)$$

Remark 1: μ here is equal to the mass, and is used so as to not be confused with the magnetic quantum number.

Trying a solution of the form:

$$\psi_{E,m}(\rho, \phi) = R_{Em}(\rho)\Phi_m(\phi)$$

which is an eigenfunction of $\hat{L}_z$ and $\Phi_m = \frac{1}{\sqrt{2\pi}} e^{im\phi}$. Substituting this into the Schrodinger equation:

$$\left[\frac{-\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} - \frac{m^2}{\rho^2}\right) + V(\rho)\right] R_{Em}(\rho) = E R_{Em}(\rho)$$

Remark 2: The azimuthally symmetric problem is reduced to solving a 1-D radial problem. The angular contribution is an effective repulsive potential that corresponds to the centrifugal force.

9.4.2.3 Eigenvalues of $\hat{L}^2$ and $\hat{L}_z$

Define $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$. One can show that

$$\left[\hat{L}^2, \hat{L}_i\right] = 0 \qquad \text{for all } i = x, y, z$$

Remark 1: We already have shown that if the Hamiltonian is invariant under rotations about the z-axis, then then $\left[\hat{H}, \hat{L}_z\right] = 0$ and $\hat{L}_z$ is thus conserved. It follows that if $\hat{H}$ is invariant under arbitrary rotations, then

$$\left[\hat{H}, \hat{L}_i\right] = 0 \quad \text{for all } i = x, y, z$$

and

$$\left[\hat{H}, \hat{L}^2\right] = 0$$

implies that $\hat{L}^2, \hat{L}_x, \hat{L}_y$, and $\hat{L}_z$ are conserved.

Remark 2: Since the components of the angular momentum vector *do not* commute, we can not construct a common eigenbasis between $\hat{H}, \hat{L}^2, \hat{L}_i$ for all $i = x, y, z$. So we pick a single component, usually $\hat{L}_z$, and form a common basis with $\hat{H}$ and $\hat{L}^2$.

Now to find a common eigenbasis between $\hat{L}_z$ and $\hat{L}^2$. Let $|\alpha\beta\rangle$ be a common eigenvector so that

$$\hat{L}^2 |\alpha\beta\rangle = \alpha |\alpha\beta\rangle$$
$$\hat{L}_z |\alpha\beta\rangle = \beta |\alpha\beta\rangle$$

Remark 3: Recall the HO problem where we defined the annihilation and creation operators in terms of $\hat{x}, \hat{p}$. Here we define $\hat{L}_+, \hat{L}_-$ in terms of $\hat{L}_x$ and $\hat{L}_y$.

Definition 1: Let

$$\hat{L}_{\pm} \equiv \hat{L}_x \pm i\hat{L}_y$$

be the raising and lowering operators. We note that

$$\left[\hat{L}_z, \hat{L}_{\pm}\right] = \pm\hbar\hat{L}_{\pm}$$

$$\left[\hat{L}^2, \hat{L}_{\pm}\right] = 0$$

Remark 4: $\hat{L}_{\pm}$ raise/lower the eigenvalue of $\hat{L}_z$ while leaving the eigenvalues of $\hat{L}^2$ fixed.

$$\begin{aligned}\hat{L}_z\left(\hat{L}_{\pm}|\alpha\beta\rangle\right) &= \left(\hat{L}_{\pm}\hat{L}_z \pm \hbar\hat{L}_{\pm}\right)|\alpha\beta\rangle \\ &= \hat{L}_{\pm}\left(\hat{L}_z \pm \hbar\right)|\alpha\beta\rangle \\ &= \hat{L}_{\pm}\left(\beta \pm \hbar\right)|\alpha\beta\rangle \\ &= \left(\beta \pm \hbar\right)\hat{L}_{\pm}|\alpha\beta\rangle\end{aligned}$$

and

$$\begin{aligned}\hat{L}^2\left(\hat{L}_{\pm}|\alpha\beta\rangle\right) &= \hat{L}_{\pm}\left(\hat{L}^2|\alpha\beta\rangle\right) \\ &= \alpha\left(\hat{L}_{\pm}|\alpha\beta\rangle\right)\end{aligned}$$

Remark 5: Since $\hat{L}_{\pm}$ raises/lowers the eigenvalue of the z-component of the angular momentum, we deduce that

$$\hat{L}_{\pm}|\alpha\beta\rangle = C_{\pm}(\alpha,\beta)|\alpha,\beta\pm\hbar\rangle$$

However, given a state $|\alpha\beta\rangle$, we can not raise or lower β an arbitrary amount as $|l_z| \leq \sqrt{l^2}$. This implies

$$\begin{aligned}\left\langle\alpha\beta\middle|\hat{L}^2 - \hat{L}_z^2\middle|\alpha\beta\right\rangle &= \alpha - \beta^2 \\ &= \left\langle\alpha\beta\middle|\hat{L}_x^2 + \hat{L}_y^2\middle|\alpha\beta\right\rangle \geq 0\end{aligned}$$

$$\Rightarrow \alpha \geq \beta^2$$

Remark 6: Since β^2 is bounded by α, there must exist a state $|\alpha\beta_{max}\rangle$ that can not be raised any further.

$$\hat{L}_{+}|\alpha\beta_{max}\rangle = 0$$

Similarly, there must be a $|\alpha\beta_{min}\rangle$ that can not be lowered.

$$\hat{L}_- |\alpha\beta_{min}\rangle = 0$$

Starting with the "top state" and considering the above, we have that

$$\begin{aligned}
\hat{L}_-\hat{L}_+ |\alpha\beta_{max}\rangle &= 0 \\
&= \left(\hat{L}_x - i\hat{L}_y\right)\left(\hat{L}_x + i\hat{L}_y\right)|\alpha\beta_{max}\rangle \\
&= \left(\hat{L}_x^2 + \hat{L}_y^2 + i\left(\hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x\right)\right)|\alpha\beta_{max}\rangle \\
&= \left(\hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z\right)|\alpha\beta_{max}\rangle \\
&= \left(\alpha - \beta_{max}^2 - \hbar\beta_{max}\right)|\alpha\beta_{max}\rangle \\
\Rightarrow \alpha &= \beta_{max}\left(\beta_{max} + \hbar\right)
\end{aligned}$$

Similarly, starting with the "bottom state":

$$\begin{aligned}
\hat{L}_+\hat{L}_- |\alpha\beta_{min}\rangle &= 0 \\
&= \left(\hat{L}^2 - \hat{L}_z^2 + \hbar\hat{L}_z\right)|\alpha\beta_{min}\rangle \\
&= \left(\alpha - \beta_{min}^2 - \hbar\beta_{min}\right)|\alpha\beta_{min}\rangle \\
\Rightarrow \alpha &= \beta_{min}\left(\beta_{min} - \hbar\right)
\end{aligned}$$

Comparing values of α implies that $\beta_{min} = -\beta_{max}$.

Remark 7: One can also start at the top state and use $\hat{L}_-$ to get to the bottom (or use $\hat{L}_+$ to go from $|\alpha\beta_{min}\rangle$ to $|\alpha\beta_{max}\rangle$). In general, this will take k steps, where $k = 0, 1, 2, \ldots$, so that

$$\beta_{max} - \beta_{min} = 2\beta_{max} = \hbar k$$

$$\Rightarrow \beta_{max} = \frac{\hbar k}{2} \quad \text{where } k = 0, 1, 2, \ldots$$

$$\Rightarrow \alpha = \hbar^2\left(\frac{k}{2}\right)\left(\frac{k}{2} + 1\right)$$

Remark 8: Let $\frac{\beta_{max}}{\hbar} = \frac{k}{2}$ denote the angular momentum of the state.

Remark 9: Note that in §9.4.2.1, we found the eigenvalues of $\hat{L}_z$ to be $m\hbar$ (where m is an integer), while here we find that the eigenvalues can be half-integers. The reason is that here we used only commutation relations and not the specific form of $\hat{L}_z$ ($\Rightarrow -i\hbar\frac{\partial}{\partial\phi}$). So, in fact, the result here is valid for any angular momentum with the same commutation relations without

specifying the type of angular momentum. We will study two types of angular momentum: orbital angular momentum (denoted by $\hat{\vec{L}}$), which has only integer eigenvalues, and spin angular momentum (denoted by $\hat{\vec{S}}$), which can have integer or half-integer eigenvalues. The total angular momentum, $\hat{\vec{J}} = \hat{\vec{L}} + \hat{\vec{S}}$, obeys the same commutation relations that were derived for $\hat{\vec{L}}$, and hence the eigenvalues derived above hold for $\hat{\vec{J}}$. For total angular momentum then:

$$\hat{J}^2 |jm\rangle = j(j+1)\hbar^2 |jm\rangle, \quad \text{where } j = \frac{1}{2}, 1, \frac{3}{2}, \ldots$$

$$\hat{J}_z |jm\rangle = m\hbar |jm\rangle, \quad \text{where } m = j, j-1, \ldots, -j+1, j$$

For $\vec{J} = \vec{L}$:

$$\hat{L}^2 |lm\rangle = l(l+1)\hbar^2 |lm\rangle, \quad \text{where } l = 0, 1, 2, \ldots$$

$$\hat{L}_z |lm\rangle = m\hbar |lm\rangle, \quad \text{where } m = l, l-1, \ldots, -l+1, -l$$

Remark 10: We will discuss rules for addition of angular momentum shortly – for now, we will just use the notion of total angular momentum and determine general eigenfunctions.

9.4.3 Matrix Representation of Angular Momentum

Finding the matirx representation of $\hat{J}^2, \hat{J}_x, \hat{J}_y, \hat{J}_z$ is sufficient for determining the eigenvectors of angular momentum. We will look at the coordinate representation of these eigenvectors when we undertake central potential problems.

9.4.3.1 Matrix Elements of $\hat{J}^2$ and $\hat{J}_z$

These are both diagonal and therefore straight forward to compute. For $\hat{J}^2$ we have:

$$\left\langle jm \middle| \hat{J}^2 \middle| jm \right\rangle = j(j+1)\hbar^2, \quad \text{where } j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$$

$$\Rightarrow \hat{J}^2 = \begin{pmatrix} 0 & & & & & & 0 \\ & \frac{3}{4}\hbar^2 & & & & & \\ & & \frac{3}{4}\hbar^2 & & & & \\ & & & 2\hbar^2 & & & \\ & & & & 2\hbar^2 & & \\ & & & & & 2\hbar^2 & \\ 0 & & & & & & \ddots \end{pmatrix}$$

And for $\hat{J}_z$ we have:

$$\left\langle jm\middle|\hat{J}_z\middle|jm\right\rangle = m\hbar$$

$$\Rightarrow \hat{J}_z = \begin{pmatrix} 0 & & & & & & 0 \\ & \frac{1}{2}\hbar & & & & & \\ & & \frac{1}{2}\hbar & & & & \\ & & & \hbar & & & \\ & & & & 0 & & \\ & & & & & -\hbar & \\ 0 & & & & & & \ddots \end{pmatrix}$$

9.4.3.2 Matrix Elements of $\hat{J}_x$ and $\hat{J}_y$

These are non-diagonal. We will use

$$\hat{J}_x = \frac{1}{2}\left(\hat{J}_+ + \hat{J}_-\right) \quad \text{and} \quad \hat{J}_y = \frac{1}{2i}\left(\hat{J}_+ - \hat{J}_-\right)$$

and find the action of $\hat{J}_\pm$ on the state $|jm\rangle$. We know:

$$\hat{J}_\pm |jm\rangle = C_\pm(j,m)\,|j, m\pm 1\rangle$$

where we need to determine $C_\pm(j,m)$. In dual space, we have

$$\langle jm|\,\hat{J}^*_\pm = \langle jm|\,\hat{J}_\mp = C^*_\pm\,\langle j, m\pm 1|$$

Consider just C_+ for now. We know that

$$\left\langle jm\middle|\hat{J}_-\hat{J}_+\middle|jm\right\rangle = |C_+|^2\,\langle j, m+1|j, m+1\rangle = |C_+|^2$$

and

$$\left\langle jm\middle|\hat{J}^2 - \hat{J}_z^2 - \hbar\hat{J}_z\middle|jm\right\rangle = |C_+|^2$$

$$\begin{aligned} \Rightarrow |C_+|^2 &= j(j+1)\hbar^2 - m^2\hbar^2 - m\hbar^2 \\ &= \hbar^2(j-m)(j+m+1) \\ \Rightarrow C_+ &= \hbar\sqrt{(j-m)(j+m+1)} \end{aligned}$$

Remark 1: In general, C_+ can have an overall phase, which we choose to be unity.

Similarly, considering C_-:

$$\left\langle jm\middle|\hat{J}_+\hat{J}_-\middle|jm\right\rangle = |C_-|^2$$

We find that

$$C_- = \hbar\sqrt{(j+m)(j-m+1)}$$
$$\Rightarrow \hat{J}_\pm |jm\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}\,|j,m\pm 1\rangle$$

Using this to determine the matrix elements of $\hat{J}_x$ and $\hat{J}_y$:

$$\begin{aligned}\left\langle j'm'\middle|\hat{J}_x\middle|jm\right\rangle &= \frac{1}{2}\left\langle j'm'\middle|\hat{J}_+ + \hat{J}_-\middle|jm\right\rangle \\ &= \frac{1}{2}\left\langle j'm'\middle|\hbar\sqrt{(j-m)(j+m+1)}\middle|j,m+1\right\rangle + \frac{1}{2}\left\langle j'm'\middle|\hbar\sqrt{(j+m)(j-m+1)}\middle|jm\right\rangle \\ &= \frac{1}{2}\hbar\left[\sqrt{(j-m)(j+m+1)}\delta_{j,j'}\delta_{m+1,m'} + \sqrt{(j+m)(j-m+1)}\delta_{j,j'}\delta_{m-1,m'}\right]\end{aligned}$$

Thus

$$\hat{J}_x = \left(\begin{array}{c:cc:ccc:c} 0 & & & & & 0 \\ \hdashline & 0 & \frac{\hbar}{2} & & & \\ & \frac{\hbar}{2} & 0 & & & \\ \hdashline & & & 0 & \frac{\hbar}{\sqrt{2}} & 0 \\ & & & \frac{\hbar}{\sqrt{2}} & 0 & \frac{\hbar}{\sqrt{2}} \\ & & & 0 & \frac{\hbar}{\sqrt{2}} & 0 \\ \hdashline 0 & & & & & \ddots \end{array}\right)$$

Similarly, for $\hat{J}_y$ we have

$$\begin{aligned}\left\langle j'm'\middle|\hat{J}_y\middle|jm\right\rangle &= \frac{1}{2i}\left\langle j'm'\middle|\hat{J}_+ - \hat{J}_-\middle|jm\right\rangle \\ &= \frac{\hbar}{2i}\left[\sqrt{(j-m)(j+m+1)}\delta_{j,j'}\delta_{m+1,m'} - \sqrt{(j+m)(j-m+1)}\delta_{j,j'}\delta_{m-1,m'}\right]\end{aligned}$$

Thus

$$\hat{J}_y = \left(\begin{array}{c:cc:ccc:c} 0 & & & & & 0 \\ \hdashline & 0 & \frac{\hbar}{2i} & & & \\ & \frac{-\hbar}{2i} & 0 & & & \\ \hdashline & & & 0 & \frac{\hbar}{i\sqrt{2}} & 0 \\ & & & \frac{-\hbar}{i\sqrt{2}} & 0 & \frac{\hbar}{i\sqrt{2}} \\ & & & 0 & \frac{-\hbar}{i\sqrt{2}} & 0 \\ \hdashline 0 & & & & & \ddots \end{array}\right)$$

Remark 2: Though $\hat{J}_x$ and $\hat{J}_y$ are not diagonal, they are block diagonal (all matrix elements have $\delta_{j,j'}$). This implies that the blocks do not mix upon multiplication, and we can conclude that:

$$\left[\hat{J}_x^{(j)}, \hat{J}_y^{(j)}\right] = i\hbar\hat{J}_z^{(j)} \quad \text{for } j = 0, \frac{1}{2}, 1, \ldots$$

9.4.4 Finite Rotations

Recall from §9.4.1.2 Remark 6 that finite rotations may be expressed as

$$\hat{U}[R(\theta)] = e^{-i\hat{\theta}\cdot\hat{J}/\hbar}$$

Remark 1: We have all components of $\hat{J}$; however, $\hat{J}$ is block diagonal with only blocks of the same j multiplying. So, schematically, we represent $\hat{U}[R]$ by the following:

$$\hat{U}[R] \xrightarrow[|jm\rangle \text{ basis}]{} \begin{pmatrix} D^{(0)} & & & 0 \\ & D^{(1/2)} & & \\ & & D^{(1)} & \\ 0 & & & \ddots \end{pmatrix}$$

where $D^{(j)}$ is the $(2j+1)$ dimensional block for a given j.

Remark 2: Since a vector $|\psi_j\rangle$ need only be spanned by $2j+1$ vectors $|jj\rangle, \ldots, |j,-j\rangle$, we only need $D^{(j)}[R]$ to rotate $|\psi_j\rangle$ (which stays within the subspace $\mathbb{V}_j$).

Consider

$$D^{(j)}[R(\theta)] = e^{-i\vec{\theta}\cdot\vec{j}^{(j)}/\hbar} = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{-i\theta}{\hbar}\right)^n \left(\vec{\theta}\cdot\vec{j}^{(j)}\right)^n \qquad (\dagger)$$

Remark 3: This series expansion can be truncated at $n = 2j$.

$$D^{(j)}[R] = \sum_{n=0}^{2j} f_n(\theta)\left(\vec{\theta}\cdot\vec{j}^{(j)}\right)^n$$

The terms $\left(\vec{\theta}\cdot\vec{j}^{(j)}\right)^n$ for $n > 2j$ can be written as linear combinations of the first $2j$ terms, and the $f_n(\theta)$ represents that combination.

Remark 4: Consider the subspace $\mathbb{V}_j$ spanned by basis vectors $|jm\rangle$ where $m = j, \ldots, -j$. The subspace is identified by the eigenvalue of $\hat{J}^2$: $j(j+1)\hbar^2$. Since

$$\left[\hat{J}^2, \hat{U}[R]\right] = 0$$

then a rotation of any state spanned in this basis will not change the eigenvalues and therefore this is called an invariant subspace (invariant under arbitrary rotations).

Remark 5: Furthermore, the invariant subspaces are irreducible, i.e., it does not contain any other invariant subspace.

Remark 6: The block diagonal matrices, $D^{(j)}$, which make up $\hat{U}[R]$ are an irreducible representation of rotation in the $|jm\rangle$ basis.

Remark 7: Also, since $\left[\hat{H}, \hat{J}_{\pm}\right] = 0$, each block represented by $D^{(j)}$ will have a single energy eigenvalue E_j. This implies that all states with a given j are degenerate in the rotationally invariant problem.

Remark 8: Classically, this degeneracy is because one state can be rotated to another without changing the energy. Quantum mechanically, a rotation combined with $\hat{J}_{\pm}$ is required to take one state to another, but these operators all commute with $\hat{H}$, so the energy is unchanged under $\hat{U}[R]$ and $\hat{J}_{\pm}$.

Chapter 10

Central Potential

10.1 Hamiltonian in Spherical Coordinates

For a particle with mass μ and momentum $\vec{p}$, the Hamiltonian in a spherically symmetric potential, $V(r)$, is

$$\hat{H} = \frac{\vec{p}^2}{2\mu} + \hat{V}(r)$$

which corresponds to a time independent Schrodinger equation:

$$\hat{H}\psi(\vec{r}) \equiv \left[-\frac{\hbar^2}{2\mu}\nabla^2 + \hat{V}(r)\right]\psi(\vec{r}) = E\psi(\vec{r}) \tag{1}$$

In spherical coordinates, this is:

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\sin(\theta)\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right) + \hat{V}(r)\right]\psi_E(r,\theta,\phi) = E\psi(r,\theta,\phi) \tag{2}$$

Remark 1: Though we can tackle (2) as is, it is useful at this point to note the spherical symmetry and thus that we have conservation of angular momentum. Consequently, we can express (1) in terms of a conserved quantity.

Remark 2: Recall that $\vec{L} = \vec{r}\times\vec{p} = i\hbar(\vec{r}\times\nabla) =$ angular momentum, and that all three components of angular momentum commute with the Hamiltonian.

Remark 3: For the radial momentum, we will *not* use $-i\hbar\frac{\partial}{\partial r} = \frac{\vec{r}}{r}\cdot\vec{p}$ since it is not Hermitian. Instead, we will use the symmetrized form:

$$\hat{p}_r = \frac{1}{2}\left(\frac{\vec{r}}{r}\cdot\vec{p} + \vec{p}\cdot\frac{\vec{r}}{r}\right)$$

Remark 4: $\hat{p}_r$ commutes with any function of θ and ϕ, and also with l_x, l_y, l_z, but

$$[\hat{r}, \hat{p}_r] = i\hbar$$

Proposition:

$$\hat{p}^2 = \hat{p}_r^2 + \frac{\hat{L}^2}{r^2} \qquad \text{for } r \neq 0$$

- Proof:

$$\begin{aligned}\hat{L}^2 &= (\vec{r} \times \vec{p}) \cdot (\vec{r} \times \vec{p}) \\ &= r^2\hat{p}^2 - r^2\hat{p}_r^2 \qquad \text{by vector identities}\end{aligned}$$

So an alternate form of the Hamiltonian for a spherically symmetric system is:

$$\hat{H} = \frac{\hat{p}_r^2}{2\mu} + \frac{\hat{L}^2}{2\mu r^2} + \hat{V}(r) \tag{3}$$

Remark 5: Comparing the Schrodinger equation obtained by (3)

$$\left[\frac{\hat{p}_r^2}{2\mu} + \frac{\hat{L}^2}{2\mu r^2} + \hat{V}(r)\right]\psi(r,\theta,\phi) = E\psi(r,\theta,\phi) \tag{4}$$

with (2) gives us

$$\hat{L}^2 = \frac{-\hbar^2}{\sin^2(\theta)}\left[\sin(\theta)\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) + \frac{\partial^2}{\partial\phi^2}\right] \tag{5}$$

10.2 Solution of Spherically Symmetric Schrodinger Equation

Recall from Chapter 9 that spherical symmetry implies

- $\hat{H}$ is invariant under transformation
- $\left[\hat{H}, \hat{L}_i\right] = 0$ for $i = x, y, z$
- $\left[\hat{H}, \hat{L}^2\right] = 0$
- There exists an eigenbasis common to $\hat{H}, \hat{L}^2$ and one $\hat{L}_i$, usually $\hat{L}_z$.

The steps to finding a common eigenbasis are:

1. Separate the angular and radial parts of the Schrodinger equation.
2. Solve the eigenvalue problem of $\hat{L}_z$ and $\hat{L}^2$ for the angular part.
3. Solve the full problem to get the radial part.

Remark 1: The particular form of $V(r)$ enters only in Step 3!

10.2.1 Solution of the Angular Part

We've actually done this using the bra-ket notation in previous chapters using:

$$\hat{H}\left|n,l,m\right\rangle = E_{lm}\left|n,l,m\right\rangle$$

and starting by solving the eigenvalue equation for $\hat{L}^2$ and $\hat{L}_z$. Again, we will solve the eigenvalue equation for $\hat{L}^2$ and $\hat{L}_z$, but this time we'll do it in coordinate representation. Following the same strategy as before, we'll start with

$$\hat{L}_+\left|l,l\right\rangle = 0$$

In coordinate representation:

$$\hat{L}_\pm = \pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot(\theta)\frac{\partial}{\partial\phi}\right)$$

We let $|l,l\rangle \to \psi_l^l(r,\theta,\phi)$ so that we have:

$$\left(\frac{\partial}{\partial\theta} + i\cot(\theta)\frac{\partial}{\partial\phi}\right)\psi_l^l(r,\theta,\phi) = 0 \qquad (\dagger)$$

Remark 1: ψ_l^l is an eigenfunction of $\hat{L}_z$ with eigenvalue $l\hbar$:

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

So let

$$\psi_l^l(r,\theta,\phi) = U_l^l(r,\theta)e^{il\phi}$$

Substituting this into (†) gives:

$$\left(\frac{\partial}{\partial\theta} + \cot(\theta)l\right)U_l^l(r,\theta) = 0 \qquad (\ddagger)$$

Remark 2: We can ignore the r dependence in (‡), and we can write

$$\frac{dU_l^l}{U_l^l} = \frac{l\cos(\theta)}{\sin(\theta)}d\theta = \frac{l}{\sin(\theta)}d\left(\sin(\theta)\right)$$

which is satisfied if

$$U_l^l(r,\theta) = R(r)\left(\sin(\theta)\right)^l$$

Remark 3: $R(r)$ is normalizable, but otherwise arbitrary–in actuality, it is determined by the radial part of the solution.

Remark 4: Requiring $R(r)$ to be normalizable with respect to r implies that the angular part must be normalizable with respect to the angles. A function that satisfies this requirement is:

$$Y_l^l(\theta,\phi) = (-1)^l \left[\frac{2l+1}{2\pi}\right]^{1/2} \frac{1}{2^l l!} \left(\sin(\theta)\right)^l e^{il\phi} \qquad (\dagger\dagger)$$

Remark 5: Applying the lowering operator to this top state

$$\begin{aligned} \hat{L}_- \left|l,l\right\rangle &= \hbar \left[(l+l)(1)\right]^{1/2} \left|l,l-1\right\rangle \\ &= \hbar\sqrt{2l}\left|l,l-1\right\rangle \end{aligned}$$

$$\Rightarrow Y_l^{l-1}(\theta,\phi) = \frac{1}{\sqrt{2l}} \underbrace{(-)\left(\frac{\partial}{\partial\theta} - i\cot(\theta)\frac{\partial}{\partial\phi}\right)}_{\hat{L}_-} Y_l^l$$

Repeating this gives the spherical harmonics. For $m \geq 0$ they are

$$Y_l^m(\theta,\phi) = (-1)^l \left[\frac{(2l+1)!}{4\pi}\right]^{1/2} \frac{1}{2^l l!} \left[\frac{(l+m)!}{(2l)!(l-m)!}\right]^{1/2} e^{im\phi} (\sin\theta)^{-m} \frac{d^{l-m}}{d(\cos\theta)^{l-m}} (\sin\theta)^{2l}$$

And for $m < 0$:

$$Y_l^{-m} = (-1)^m \left(Y_l^m\right)^*$$

These function satisfy the orthonormality condition:

$$\int Y_l^{m*}(\theta,\phi) Y_{l'}^{m'}(\theta,\phi)\, d\Omega = \delta_{l,l'}\delta_{m,m'} \qquad \text{with } d\Omega = \sin\theta\, d\theta d\phi$$

Remark 6: The Spherical-Harmonics are closely related to the Associated Legendre Polynomials. For P_l^m with $0 \leq m \leq l$, they are:

$$Y_l^m(\theta,\phi) = \left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right]^{1/2} (-1)^m e^{im\phi} P_l^m(\cos\theta)$$

10.2.2 Solution to the Radial Part

Since the solutions will be simultaneous eigenfunctions of $\hat{L}^2$ and $\hat{H}$, we assume a solution of the form

$$\psi_{nlm}(r,\theta,\phi) = R_{El}(r) Y_l^m(\theta,\phi)$$

Substituting this into the spherically symmetric Schrodinger equation:

$$\left[\frac{\hat{p}_r^2}{2\mu} + \frac{\hat{L}^2}{2\mu r^2} + \hat{V}(r)\right] Y_l^m(\theta,\phi)R(r) = E_{lm}Y_l^m(\theta,\phi)R(r)$$
$$\left[\frac{\hat{p}_r^2}{2\mu} + \frac{l(l+1)\hbar^2}{2\mu r^2} + \hat{V}(r)\right] Y_l^m(\theta,\phi)R(r) = E_{lm}Y_l^m(\theta,\phi)R(r)$$
$$\left[\frac{\hat{p}_r^2}{2\mu} + \frac{l(l+1)\hbar^2}{2\mu r^2} + \hat{V}(r) - E\right] R_{El}(r) = 0$$

Since

$$\hat{p}_r = -i\hbar\frac{1}{r}\frac{\partial}{\partial r}r = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$$

$$\Rightarrow \hat{p}_r^2 = -\hbar^2\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \underbrace{\frac{\partial}{\partial r}\frac{1}{r}}_{-\frac{1}{r^2}+\frac{1}{r}\frac{\partial}{\partial r}} + \frac{1}{r^2}\right)$$
$$= -\hbar^2\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)$$
$$= -\frac{\hbar^2}{r}\left(r\frac{\partial^2}{\partial r^2} + \frac{\partial}{\partial r} + \frac{\partial}{\partial r}\right)$$
$$= -\frac{\hbar^2}{r}\left(\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{\partial}{\partial r}\right)$$
$$= -\frac{\hbar^2}{r}\frac{\partial^2}{\partial r^2}r$$

Thus we have that

$$\left[\frac{-\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}r + \frac{l(l+1)\hbar^2}{2\mu r^2} + \hat{V}(r) - E\right] R_{El}(r) = 0$$

To solve this, let $U_{El}(r) = rR_{El}(r)$:

$$\left[-\frac{\hbar^2}{2\mu r}\frac{\partial^2}{\partial r^2} + \frac{l(l+1)\hbar^2}{2\mu r^3} + \frac{\hat{V}(r) - E}{r}\right] U(r) = 0$$
$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + \hat{V}(r) - E\right] U(r) = 0 \qquad (\dagger)$$

Remark 1: (†) is called the radial equation and closely resembles the 1-D Schrodinger equation. The differences are:

- $0 < r < \infty$ instead of $-\infty < x < \infty$

- For $l \neq 0$, there exists a repulsive centrifugal barrier $\frac{l(l+1)\hbar^2}{2\mu r^2}$. So the total effective potential is

$$V_{eff} = V(r) + \frac{l(l+1)\hbar^2}{2\mu r^2}$$

- Boundary conditions on $U(r)$ are different.

Remark 2: As in the 1-D Schrodinger equation, the asymptotic solutions (ie, the solutions as $r \to \infty$) are exponentials which decay to 0 ($E < 0$) for fixed discrete values of E (bound state solutions), or they are oscillatory solutions ($E > 0$) which are the continuum or unbound states.

Remark 3: The solutions are generally degenerate with respect to the energy eigenvalue:

- Energies with discrete spectrum are degenerate with respect to quantum number m, and may be, but not necessarily, degenerate with respect to the angular momentum quantum number l.

- Continuous energy spectrum are always infinitely degenerate, since for each $E > 0$ there are eigenfunctions for all values of $l = 0, 1, 2, \ldots$ and $m = 0, \pm 1, \pm 2, \ldots, \pm l$ (assuming that $V(r) \to 0$ monotonically as $r \to \infty$).

Remark 4: We must determine boundary conditions at $r = 0$ so that the solutions are physically acceptable. First of all, we require that

$$D_l(r) = -\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)$$

to be Hermitian with respect to functions U_{El}. Here,

$$D_l(r)U_{El} = EU_{El}$$

is the eigenvalue equation representing the radial equation, (†).

Remark 5: Requiring that $D_l(r)$ is Hermitian is equivalent to requiring that $\hat{p}_r$ be Hermitian (Convince yourself of this with Exercise 12.6.3 in Shankar).

$$\begin{aligned}
\langle\psi|\hat{p}_r|\psi\rangle &= \int d\Omega \int_0^\infty r^2\, dr\, \psi^* \left(-i\hbar\frac{1}{r}\frac{\partial}{\partial r}r\right)\psi \\
&= \int d\Omega \int_0^\infty r\, dr\, \psi^* \left(-i\hbar\frac{\partial}{\partial r}r\right)\psi \\
&= \int d\Omega \int_0^\infty dr\, rY_l^{m*}R_{El}^* \left(-i\hbar\frac{\partial}{\partial r}rY_l^m R_{El}\right) \\
&= \underbrace{\int d\Omega\, Y_l^{m*}Y_l^m}_{1} \int_0^\infty dr\, (-i\hbar)rR_{El}^*\frac{\partial}{\partial r}\left(rR_{El}\right) \\
&= -i\hbar\,|rR_{El}|^2\big|_0^\infty + i\hbar\int_0^\infty dr\, \left[\frac{\partial}{\partial r}\left(rR_{El}^*\right)\right] rR_{El} \\
&= -i\hbar\,|rR_{El}|^2\big|_0^\infty + i\hbar\int d\Omega Y_l^{m*}Y_l^m \int_0^\infty dr\, \left[\frac{\partial}{\partial r}\left(rR_{El}^*\right)\right] rR_{El} \\
&= -i\hbar\,|rR_{El}|^2\big|_0^\infty + \langle\psi|\hat{p}_r|\psi\rangle^*
\end{aligned}$$

So $\hat{p}_r$ is Hermitian if

$$-i\hbar\,|rR_{El}|^2\big|_0^\infty \equiv |U_{El}|^2\big|_0^\infty \to 0$$

Since we require ψ to be normalizable, this does vanish for sure at the upper limit. For physical solutions then, we have the requirement that

$$U_{El}(r=0) = 0$$

Our goal now is to understand how solutions to the radial equation behave at the origin. To investigate this, let's try an expansion of the form

$$U_{El}(r\to 0) \sim r^s\left(1 + a_1 r + a_2 r^2 + \ldots\right)$$

where $s, a_1, a_2, \ldots$ are constants and $s > 0$.
We will assume that if $V(r) \to \infty$ as $r \to 0$, then it does so no faster than $\frac{1}{r}$ (the Coulomb potential). Let's substitute this into the radial equation:

$$\left[\frac{-\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r) - E\right]\left(r^s + a_1 r^{s+1} + a_2 r^{s+2} + \ldots\right) = 0$$

$$-\frac{\hbar^2}{2\mu}\left[s(s-1)r^{s-2} + a_1 r^{s-1}(s+1)s\right] + \frac{l(l+1)\hbar^2}{2\mu}\left(r^{s-2} + a_1 r^{s-1}\right) + V(r)r^s - Er^s = 0$$

Keeping only the dominant terms leaves

$$-\frac{\hbar^2}{2\mu}\left[\underbrace{s(s-1)}_{\substack{\text{radial}\\ \text{KE}}} - \underbrace{l(l+1)}_{\substack{\text{Centrifugal}\\ \text{KE}}}\right] r^{s-2} = 0$$

$$\Rightarrow s(s-1) = l(l+1)$$
$$\Rightarrow s = l+1 \quad \text{or} \quad s = -l$$

So, near the origin:

$$U_{El} \xrightarrow{r\to 0} r^{l+1} \quad \text{which is the } \textit{regular} \text{ solution.}$$

or

$$U_{El} \xrightarrow{r\to 0} r^{-l} \quad \text{which is the } \textit{irregular} \text{ solution}$$

Remark 6: The irregular solution is rejected since it is not normalizable, and it does not satisfy the boundary conditions $U_{El}(0) = 0$.

Remark 7: It is clear that the irregular solution must be discarded for $l \neq 0$, but it also must be discarded for $l = 0$. If $l = 0$, then the corresponding wave function:

$$\psi_0 = Y_0^0 R_{E0} = Y_0^0 \frac{1}{r} U_{E0} \sim \frac{1}{r}$$

which doesn't satisfy the Schrodinger equation:

$$\left(\hat{H} - E\right)\psi_0 = \frac{2\pi k}{\mu}\delta(r) \neq 0$$

since $\nabla^2 \frac{1}{r} = 4\pi\delta(r)$.

10.2.3 Examples: Free Particles and Central Square Well Potentials

There are several "classic" problems that correspond to central potential problems:

- Free particle in spherical coordinates: $V(r) = V_0 = \text{constant}$
- Isotropic H.O: $V(r)/\frac{1}{2}\mu\omega^2 r^2$
- Hydrogen atom: $V(r) = -\frac{e^2}{r}$
- 3D versions of square wells and step potentials

10.2.3.1 Free Particles and Spherical Bessel Functions

Consider a free particle such that $V(r) = V_0$ for all $r > 0$. Then the solution to the spherically symmetric Schrodinger equation is:

$$\psi_{Elm}(r,\theta,\phi) = R_{El}(r)Y_l^m(\theta,\phi)$$

And the radial equation is:

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V_0 - E\right] U_{El}(r) = 0$$

with $U_{El}(r) = rR_{El}(r)$ (See §10.2.2). Consider now the case where $E > V_0$. Let $k^2 = \frac{2\mu(E-V_0)}{\hbar^2}$.

$$\Rightarrow \left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2}\right] U_{El} = 0$$

Or, in terms of R_{El}:

$$\begin{aligned}
\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2}\right] rR_{El} &= 0 \\
\vdots \qquad\qquad & \vdots \\
r\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + k^2 - \frac{l(l+1)}{r^2}\right] R_{El} &= 0 \\
\left[\frac{d^2}{d(kr)^2} + \frac{2}{(kr)}\frac{d}{d(kr)} + 1 - \frac{l(l+1)}{(kr)^2}\right] R_{El} &= 0 \qquad (\dagger)
\end{aligned}$$

Remark 1: (†) is a differential equation whose solutions are spherical Bessel functions.

$$\begin{aligned}
j_l(kr) &\rightarrow \text{ The proper spherical Bessel functions} \\
n_l(kr) &\rightarrow \text{ The Neumann functions} \\
h_r^{(+)}(kr) &\rightarrow \text{ The Hankel functions of the 1st kind} \\
h_r^{(-)}(kr) &\rightarrow \text{ The Hankel functions of the 2nd kind}
\end{aligned}$$

Remark 2: The general solution is a linear combination of $j_l(kr)$ and $n_l(kr)$ which are defined in terms of ordinary Bessel functions:

$$\begin{aligned}
j_l(kr) &= \left(\frac{\pi}{2kr}\right)^{1/2} J_{l+1/2}(kr) \\
n_l(kr) &= (-1)^l \left(\frac{\pi}{2kr}\right)^{1/2} J_{-l-1/2}(kr)
\end{aligned}$$

Remark 3: Near the origin:

$$\begin{aligned}
j_l(kr) &\xrightarrow{kr\to 0} (kr)^l \quad \Rightarrow \text{ regular} \\
n_l(kr) &\xrightarrow{kr\to 0} (kr)^{-(l+1)} \quad \Rightarrow \text{ irregular}
\end{aligned}$$

Remark 4: The Hankel functions are given by

$$h_l^{(\pm)} = n_l(kr) \pm i j_l(kr)$$

which are both irregular at the origin.

Remark 5: For physical solutions, only regular solutions are allowed in regions containing the origin. However, the other functions may be important for matching discontinuities in the potential (Eg. a central square well problem).

Remark 6: Asymptotically,

$$j_l(kr) \xrightarrow{kr\to\infty} \frac{1}{kr}\sin\left(kr - \frac{l\pi}{2}\right)$$
$$n_l(kr) \xrightarrow{kr\to\infty} -\frac{1}{kr}\cos\left(kr - \frac{l\pi}{2}\right)$$

and

$$h_l^{(\pm)}(kr) \xrightarrow{kr\to\infty} \frac{1}{kr}e^{\pm i(kr - l\pi/2)}$$

Remark 7: Asymptotically, the factor of $\frac{1}{kr}$ in $j_l(kr)$, $n_l(kr)$, and $h_l^{(\pm)}(kr)$ gives the inverse square law behavior expected in a central potential problem.

Remark 8: To lowest order, the spherical Bessel functions are:

$$j_0(kr) = \frac{\sin(kr)}{kr}, \qquad j_1(kr) = \frac{\sin(kr)}{(kr)^2} - \frac{\cos(kr)}{kr}$$
$$n_0(kr) = \frac{\cos(kr)}{kr}, \qquad n_1(kr) = \frac{\cos(kr)}{(kr)^2} + \frac{\sin(kr)}{kr}$$

Remark 9: The solution to the spherical Schrodinger equation with $V = V_0$ and $E > V_0$ is

$$\psi_{Elm}(r,\theta,\phi) = j_l(kr)Y_l^m(\theta,\phi) \qquad (\ddagger)$$

where $k^2 = \frac{2\mu(E-V_0}{\hbar^2}$ and the solutions satisfy

$$\iiint \psi^*_{Elm}\psi_{E'l'm'}r^2\,dr\,d\Omega = \frac{2}{\pi k^2}\delta(k-k')\delta_{l,l'}\delta_{m,m'}$$

where

$$\int_0^\infty j_l(kr)j_l(k'r)r^2\,dr = \frac{\pi}{2k^2}\delta(k-k')$$

Remark 10: For $V(r) = V_0$ and $E < V_0$, we simply let

$$k = \sqrt{\frac{2\mu(E - V_0)}{\hbar^2}} \rightarrow i\kappa = i\sqrt{\frac{2\mu(V_0 - E)}{\hbar^2}}$$

so that the analogs in trigonometric functions become analogs of hyperbolic functions. In this case, it turns out that $h_l^{(+)}$ is the only solution that doesn't diverge at infinity.

$$h_l^{(+)}(i\kappa r) \xrightarrow{r\rightarrow\infty} \frac{e^{-\kappa r}}{\kappa r}$$

whereas all other functions diverge as $\frac{e^{\kappa r}}{\kappa r}$.

Remark 11: In Cartesian coordinates, the solution for the free particle is given in terms of plane waves:

$$\psi_{\vec{k}} \sim e^{i\vec{k}\cdot\vec{r}}$$

which are eigenfunctions of the energy $\frac{\hat{p}^2}{2\mu}$ and the components of linear momentum $\hat{p}_x, \hat{p}_y, \hat{p}_z$. These plane waves form a complete set of functions which may be used to expand any wavepacket. The spherical standing wave (‡) in Remark 9 is an alternate complete set.

We can expand the plane waves in terms of the spherical standing waves (‡):

$$e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(kr) Y_l^{m*}\left(\frac{\vec{k}}{k}\right) Y_l^m\left(\frac{\vec{r}}{r}\right)$$

where the two terms in parenthesis denote angles θ and ϕ which define the unit vectors in the $\vec{k}$ and $\vec{r}$ directions. If $\vec{k}$ is along the z-axis, this simplifies to

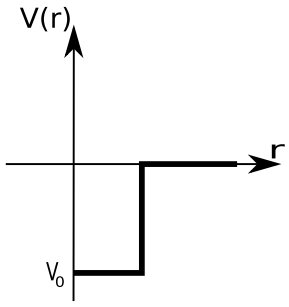
$$e^{i\vec{k}\cdot\vec{r}} = e^{ikr\cos\theta} \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta)$$

where $P_l(\cos\theta)$ are the Legendre polynomials. In this case, a particle moving along the z-axis has no angular momentum in this direction. Thus, $Y_l^m \rightarrow Y_l^0$ and the m in the sum in completed explicitly.

10.2.3.2 Central Square Well

Consider now the central potential defined by

$$V(r) = \begin{cases} V_0, & 0 < r < a \\ 0, & r > a \end{cases}$$



For $E < 0$ (Bound case)::

$$R_{El}(r) = \begin{cases} Aj_l(kr), & r < a \quad \text{regular at origin} \\ Bh_l^{(+)}(ir\kappa), & r > a \quad \text{finite at infinity} \end{cases}$$

Solutions must match at $r = a$.

$$Aj_l(ka) = Bh_l^{(+)}(ia\kappa)$$
$$Akj_l'(ka) = Bh_l^{(+)'}(ia\kappa)i\kappa$$

Recursion relations relate derivatives of spherical Bessel functions to other spherical Bessel functions. Let us consider the $l = 0$ case. Then:

$$\begin{aligned} \frac{A\sin(ka)}{ka} &= B\left(\frac{\cos(i\kappa a)}{i\kappa a} + i\frac{\sin(i\kappa a)}{i\kappa a}\right) \\ &= B\frac{e^{i(i\kappa a)}}{i\kappa a} \\ &= B\frac{e^{-\kappa a}}{\kappa a} \qquad \text{(The B absorbed the i)} \end{aligned} \tag{1}$$

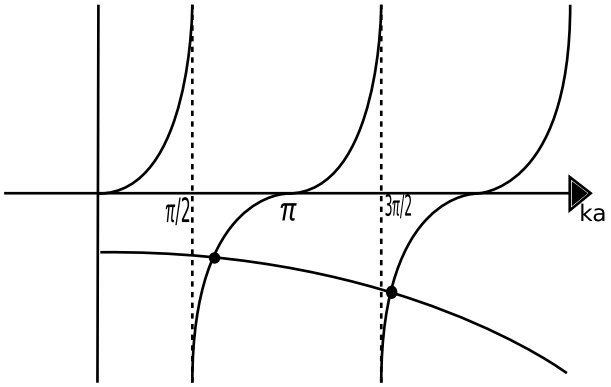
and

$$Ak\left(\frac{\cos(ka)}{ka} - \frac{\sin(ka)}{(ka)^2}\right) = Bi\kappa\left(\frac{ie^{-\kappa a}}{\kappa a} - \frac{e^{-\kappa a}}{i(\kappa a)^2}\right)$$
$$\Rightarrow A\left(\cos(ka) - \frac{\sin(ka)}{ka}\right) = B\left(-e^{-\kappa a} - \frac{e^{-\kappa a}}{\kappa a}\right) \tag{2}$$

Adding equations (1) and (2) yields:

$$\begin{aligned} A\cos(ka) &= -Be^{-\kappa a} \\ &= -A\sin(ka)\left(\frac{\kappa}{k}\right) \quad \text{by (1)} \\ \Rightarrow \tan(ka) &= \frac{-k}{\kappa} \end{aligned}$$

Solving graphically: We found the bottom line by finding κ in terms of k and plugging into $-\frac{k}{\kappa}$:



10.2.3.3 The Coulomb Potential: Hydrogen and H-like Atoms (Ions)

Consider the 2 particle coulomb interaction between an electron and a proton, as in a Hydrogen atom. In the center of mass frame, this becomes a central potential problem, with a Schrodinger equation:

$$\hat{H}\psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{z_1 z_2 e^2}{r}\right]\psi = E\psi$$

where $m = \frac{m_1 m_2}{m_1+m_2}$ is the reduced mass and $z_1 = +1(protons)$ and $z_2 = -1(electrons)$. If one neglects nuclear structure, then this equation also describes other 1 electron atoms such as He^+, Li^{2+} ($z_1 = +2, +3, \ldots$); it also approximates atoms with a single electron outside one or more complete shells.
Recall the Bohr model, in which we toake the electron to be distributed uniformly over a spherical surface of radius r_0. In this case, the mean potential energy is given by

$$\bar{V}(r) = \frac{-e^2}{r_0}$$

With this model, we can assume the particle is confined on the scale of r_0, and by the Heisenberg uncertainty principle, the uncertainty in momentum is at least

$$\Delta\hat{p} \sim \frac{\hbar}{r_0}$$

Letting this be the mean value of momentum, the total energy in the ground state is:

$$E_g = \frac{1}{2m}\left(\frac{\hbar}{r_0}\right)^2 - \frac{e^2}{r_0}$$

The stable configuration is where this is at a minimum:

$$\frac{dE_g}{dr_0} = -\frac{2\hbar^2}{2mr_0^3} + \frac{e^2}{r_0^2} = 0$$

$$\Rightarrow r_0 = \frac{\hbar^2}{me^2}$$

And plugging this into the ground state energy gives:

$$E_g = \frac{\hbar^2}{2m}\left(\frac{me^2}{\hbar^2}\right)^2 - e^2\left(\frac{me^2}{\hbar^2}\right) = -\frac{1}{2}\frac{me^4}{\hbar^2}$$

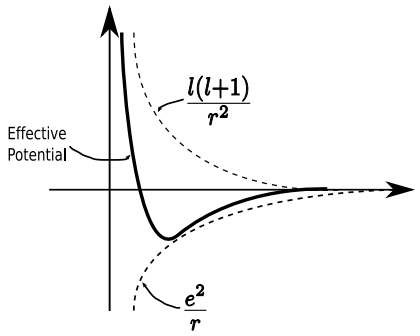
Remark 1: r_0 is called the Bohr Radius.

Remark 2: The simple arguments actually give the exact results calculated from the Schrodinger equation! However, in order to get the excited state energies, we must actually solve the Schrodinger equation.

Thus, we have a classic central potential problem, so the angular and radial parts separate and the main problem is solving the radial equation. The angular part is the same as always, for the radial we have:

$$\left[\frac{d^2}{dr^2} + \frac{2m}{\hbar^2}\left(E + \frac{e^2}{r}\right) - \frac{l(l+1)}{r^2}\right] U_{El}(r) = 0$$

We are solving for the bound states, and hence are looking in the region where



$E < 0$. We begin by making the change of variables $\rho = r\sqrt{-\frac{2mE}{\hbar^2}}$ (i.e., $\rho = kr$ from the free particle solution).

$$\Rightarrow \left[\frac{d^2}{d\rho^2} - 1 + \frac{e^2}{-E}\frac{\sqrt{-\frac{2mE}{\hbar^2}}}{\rho} - \frac{l(l+1)}{\rho^2}\right] U_{El}(r) = 0$$

Let

$$\lambda = \frac{1}{-E}\sqrt{-\frac{2mE}{\hbar^2}} = \sqrt{\frac{-2m}{\hbar^2 E}}$$

Now, we know that

$$U_{El} \sim \rho^{l+1} \qquad \text{as } \rho \to 0$$
$$U_{El} \sim e^{-\rho} \qquad \text{as } \rho \to \infty$$

Hence, we will let

$$U_{El} = \rho^{l+1} e^{-\rho} v_{El}(\rho)$$

to explicitly capture the asymptotic behavior. Substituting this into the radial equation:

$$\begin{aligned}
\Rightarrow \frac{d^2}{d\rho^2}\left(\rho^{l+1}e^{-\rho}v_{El}(\rho)\right) &= \frac{d}{d\rho}\left[(l+1)\rho^l e^{-\rho}v_{El} - \rho^{l+1}e^{-\rho}V_{El} + \rho^{l+1}e^{-\rho}v'_{El}\right] \\
&= (l+1)l\rho^{l-1}e^{-\rho}v_{El} - (l+1)\rho^l e^{-\rho}v_{El} + \rho^l(l+1)e^{-\rho}v'_{El} \\
&\quad - \rho^l(l+1)e^{-\rho}v_{El} + \rho^{l+1}e^{-\rho}v_{El} - \rho^{l+1}e^{-\rho}v'_{El} \\
&\quad + \rho^l(l+1)e^{-\rho}v'_{El} - \rho^{l+1}e^{-\rho}v'_{El} + \rho^{l+1}e^{-\rho}v''_{El} \\
&\quad \vdots \\
&= \left[\left(l(l+1)\rho^{l-1} - 2(l+1)\rho^l + \rho^{l+1}\right)v_{El} + \left((l+1)\rho^l - \rho^{l+1}\right)2v'_{El} + \rho^{l+1}v''_{El}\right]e^{-\rho}
\end{aligned}$$

And the radial equation becomes:

$$\left\{\rho^{l+1}\frac{d^2}{d\rho^2} + \left((l+1)\rho^l - \rho^{l+1}\right)2\frac{d}{d\rho} + \left(\rho^{l+1} - 2(l+1) + l(l+1)\rho^{l-}\right) + \left(-1 + \frac{\lambda e^2}{\rho} - \frac{l(l+1)}{\rho^2}\right)\rho^{l+1}\right\}v_{El} = 0$$

$$\Rightarrow \left\{\rho\frac{d^2}{d\rho^2} + 2\left(l+1-\rho\right)\frac{d}{d\rho} + \left(-2(l+1) + \lambda e^2\right)\right\}v_{El} = 0 \qquad (\dagger)$$

We will try solutions of the form:

$$v_{El}(\rho) = \sum_{k=0}^{\infty} C_k \rho^k \qquad (\ddagger)$$

Substituting this into (†):

$$\begin{aligned}
\sum_{k=0}^{\infty}\left\{k(k-1)C_k\rho k - 1 + 2\left(l+1-\rho\right)kC_k\rho^{k-1} + \left(-2(l+1)+\lambda e^2\right)C_k\rho^k\right\} &= 0 \\
\sum_{k=0}^{\infty}\left\{[-2(l+1)+\lambda e^2 - 2k]C_k\rho^k + [(k(k-1)+2k(l+1)]C_k\rho^{k-1}\right\} &= 0 \\
\sum_{k=0}^{\infty}[-2(l+1)+\lambda e^2 - 2k]C_k\rho^k + \sum_{k=1}^{\infty}[k(k-1)+2k(l+1)]C_k\rho^{k-1} &= 0 \\
\sum_{k=0}^{\infty}[-2(l+1)+\lambda e^2 - 2k]C_k\rho^k + \sum_{k=0}^{\infty}[(k+1)k+2(k+1)(l+1)]C_{k+1}\rho^k &= 0 \\
\sum_{k=0}^{\infty}\left\{[-2(l+1)+\lambda e^2 - 2k]C_k + [(k+1)k+2(k+1)(l+1)]C_{k+1}\right\}\rho^k &= 0
\end{aligned}$$

$$\Rightarrow \frac{C_{k+1}}{C_k} = \frac{-2(l+1)+\lambda e^2-2k}{(k+1)k+2(k+1)(l+1)} = \frac{-\lambda e^2+2(l+1+k)}{(k+1)(2(l+1)+k)}$$

And hence we see that we get a recursion relation between the successive coefficients in the polynomial expansion (so long as we are assuming a power series solution for $R(r)$). Consider now again the series solution (‡). To see how this behaves for large ρ, consider the form of the radial equation given earlier in this section:

$$\left[\frac{d^2}{d\rho^2} - 1 + \frac{\lambda e^2}{\rho} - \frac{l(l+1)}{\rho^2}\right] U_{El} = 0 \qquad (\dagger\dagger)$$

For large ρ, try a solution of the form:

$$U_{El} \sim \rho^a e^{b\rho}$$

$$\begin{aligned}\Rightarrow \frac{d^2}{d\rho^2}U_{El} &\sim \frac{d}{d\rho}\left(a\rho^{a-1}e^{b\rho} + b\rho^a e^{b\rho}\right) \\ &\sim a(a-1)\rho^{a-2}e^{b\rho} + 2ab\rho^{a-1}e^{b\rho} + b^2\rho^a e^{b\rho} \\ &\sim \left[a(a-1)\rho^{a-2} + 2ab\rho^{a-1} + b^2\rho^a\right]e^{b\rho}\end{aligned}$$

Keeping the terms up to order ρ^{a-1} in (††):

$$\Rightarrow 2ab\rho^{a-1} + b^2\rho^a - \rho^a + \lambda e^2\rho^{a-1} = 0$$

$$b = \pm 1 \qquad a = \mp\frac{\lambda e^2}{2}$$

So, $U_{El} \sim \rho^{-\lambda e^2/2}e^{\rho}$ dominates in the $\rho \to \infty$ limit. Now,

$$U_{El} = \rho^{l+1}e^{-\rho}v_{El}(\rho)$$

with

$$v_{El}(\rho) = \sum_{k=0}^{\infty} C_k \rho^k.$$

But, we also have:

$$U_{El} = \rho^{l+1}e^{-\rho}\sum_{k=0}^{\infty} C_k\rho^k \xrightarrow{\rho\to\infty} \rho^{-\lambda e^2/2}e^{\rho}$$

$$\Rightarrow \sum_{k=0}^{\infty} C_k\rho^k \xrightarrow{\rho\to\infty} \rho^{-l-1-\lambda e^2/2}e^{2\rho}$$

In order to avoid a divergent solution, we can force the series to terminate at finite k by requiring the coefficient to vanish at some k. This can happen if we set the numerator in the recursion relation for successive coefficients to 0.

$$\Rightarrow e^2\lambda + 2(k+l+1) = 0$$

Since we have that $\lambda = \sqrt{\frac{-2m}{\hbar^2 E}}$ (where m = mass), then we can conclude:

$$\Rightarrow E = -\frac{2m}{\hbar^2 \lambda^2} = -\frac{me^4}{2\hbar^2(k+l+1)^2} \qquad \text{for } k, l = 0, 1, 2, \ldots$$

Remark 3: We define $n = k + l + 1$ to be the principle quantum number, and

$$E = \frac{-me^4}{2\hbar^2 n^2}, \qquad \text{for } n = 1, 2, 3, \ldots$$

the allowed energies.

Remark 4: Given $n = 1, 2, 3, \ldots$:

$$l = n - k - 1 = n - 1, n - 2, \ldots, 1, 0 \qquad \text{(The ang. mom. Q \#'s)}$$

are allowed values for l, and there in degeneracy for different l at each n:

$$\sum l = 0^{n-1}(2l+1) = 2 \cdot \frac{1}{2}(n-1)(n) + n = n^2 \qquad (\#\text{ degeneracy})$$

Remark 5: A Rydberg (R_y) is a unit of energy that measures the energy levels of Hydrogen:

$$R_y = \frac{me^4}{2\hbar^2} \Rightarrow E_n = -\frac{1}{n^2} R_y$$

Remark 6: Equation (†),

$$\Rightarrow \left\{ \rho \frac{d^2}{d\rho^2} + 2\left(l + 1 - \rho\right) \frac{d}{d\rho} + \left(-2(l+1) + \lambda e^2\right) \right\} v_{El} = 0$$

is the Laplace Equation, which has *one* solution that is regular at the origin. That solution can be expressed as a confluent hypergeometric series:

$$F_1(2l + 2 - \lambda e^2; 2l + 2; \rho) = \sum_{k=0}^{\infty} \frac{\Gamma(2l + 2 + k - \lambda e^2)}{\Gamma(2l + 2 - \lambda e^2)} \frac{(2l+1)!}{(2l+1+k)!} \frac{\rho^k}{k!}$$

where

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t}\, dt$$

$$\Gamma(n+1) = n! \qquad \text{for integer, positive n}$$

Remark 7: The final wave functions are obtained from the recursion relation for the coefficients. Note that the series:

$$v_{El}(\rho) = \sum_{k=0}^{n-l-1} C_k \rho^k$$

terminates at $n-l-1$. The recursion relation can be solved:

$$\frac{C_{k+1}}{C_k} = \frac{2(l+1+\lambda) - \lambda e^2}{(k+1)(2l+2+k)}$$
$$C_{k+1} = \frac{2(l+1+k-n)C_k}{(k+1)(2l+2+k)}$$

where we used that fact that $\lambda e^2 = 2n$ since $n = l+1+k$. Letting $C_0 = 1$ implies:

$$\begin{aligned} & C_1 \frac{2(l+1-n}{2l+2} \\ & C_2 = \frac{2(l+2-n)}{2(2l+3)} C_1 \\ \Rightarrow C_k &= \frac{2^k}{k!} \frac{(l+1-n)(l+2-n)\cdots(l+k-n)}{(2l+2)(2l+3)\cdots(2l+k+1)} \\ &= \frac{2^k}{k!}(-1)^k \frac{(n-l-k)!}{(n-1)!} \frac{(2l+1)!}{(2l+k+1)!} \end{aligned}$$

Thus,

$$v_{El}(\rho) = \sum_{k=0}^{n-l-1} \frac{(-1)^k}{k!} \frac{(n-l-k)!}{(n-1)!} \frac{(2l+1)!}{(2l+k+1)!} (2\rho)^k$$

which in the Laguerre Polynomial: $L_{n-l-1}^{2l+1}(2\rho)$.

Remark 8: Finally, we write the normalized wavefunction for the Hydrogen atom:

$$\psi_{nlm} = \frac{2}{n^2} \sqrt{\frac{(n-l-1)!}{3(n+1)!}} r_0^{-3/2} \left(\frac{2r}{nr_0}\right) (2\rho)^l e^{-\rho} L_{n-l-1}^{2l+1}(2\rho) Y_l^m(\theta, \phi)$$

with

$$\rho = \sqrt{\frac{-2mE}{\hbar^2}} r = \frac{r}{\hbar} \sqrt{\frac{2m^2e^4}{2\hbar^2 n^2}} = \frac{rme^2}{n\hbar^2} = \frac{1}{n} \frac{r}{r_0}$$

where

$$r_0 = \frac{\hbar^2}{me^2}$$

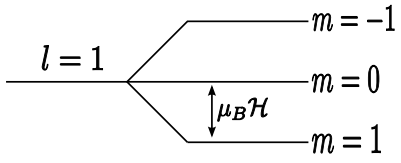
is the Bohr radius.

Chapter 11

Angular Momentum: Spin

Spin in another concept that completes the angular momentum picture. Loosely, spin is imagined as angular momentum associated with a particle rotating about its axis (like Earth). However, there really is no such mechanical analogy. Nevertheless, spin represents an intrinsic angular momentum of a particle that is not associated with the angular momentum operator $\hat{L}$.

Principle Evidence of Spin: The principle evidence of spin is in the behavior of electrons in a magnetic field, where the degeneracy is lifted (Zeemann effect). For example, for $l = 1$: where $\mathcal{H}$ is the external magnetic field. Spin is an angular momentum quantity and thus



it's corresponding operator behaves much the same as $\hat{L}$ (See §9.4).

11.1 Brief Review of Properties of Angular Momentum Operators

From §9.4.2.3, we know that eigenvalues of angular momentum as determined strictly by commutator algebra are integer or $\frac{1}{2}$ integer quantum numbers:

$$\hat{J}^2 |jm\rangle = j(j+1)\hbar^2 |jm\rangle$$
$$\hat{J}_z |jm\rangle = m\hbar |jm\rangle$$

where $j = 0, 1, 2, \ldots$ or $j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$ and $m = \pm j, \ldots, 0$ and $\hat{J}$ is the total angular momentum. The commutation relations hold for all types of angular momentum:

$$\begin{aligned}
\left[\hat{J}_i, \hat{J}^2\right] &= 0 \\
\left[\hat{J}_i, \hat{J}_i\right] &= i\epsilon_{ijk}\hat{J}_k\hbar \\
\left[\hat{J}_\pm, \hat{J}_z\right] &= \mp\hat{J}_\pm\hbar \\
\left[\hat{J}_+, \hat{J}_-\right] &= 2\hbar\hat{J}_z
\end{aligned}$$

where $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$ are the raising and lowering operators.

$$\hat{J}_\pm |jm\rangle = \hbar\sqrt{(j \mp m)(j \pm m + 1)}\, |j, m \pm 1\rangle$$

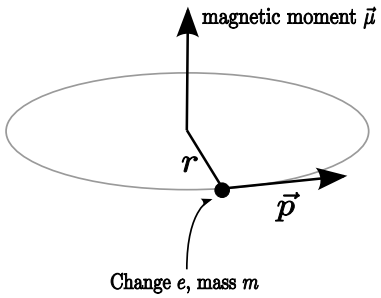
11.2 Spin: Evidence in Atomic Spectroscopy

Let us briefly review the physical context in which electron spin was proposed. Consider a multi-electron atom in a magnetic field. If we did *not* know about spin, we would write the Hamiltonian as:

$$\hat{H} = \hat{H}_0 - \vec{\mathcal{H}} \cdot \vec{M}$$

where $\vec{\mathcal{H}}$ is the externally applied field and $\vec{M} = \frac{e}{2\mu c}\hat{L} = \frac{e}{2\mu c}\sum_{j=1}^{z}(\hat{r_j} \times \hat{p_j})$ is the magnetic moment obtained by summing over the z magnetic moments of the individual electrons.

Remark 1: Let's recall that the concept of electron magnetic moment comes from the classical definition for the magnetic moment in a current loop.



$$\begin{aligned}\mu_l &= \frac{1}{c}\frac{e}{2\pi r/v}\pi r^2\left(\frac{\vec{r}\times\vec{p}}{|\vec{r}\times\vec{p}|}\right)\\ &= \frac{1}{c}\frac{e}{2\pi r}\quad \underbrace{\frac{1}{m}\left|\frac{\vec{r}}{|r|}\times\vec{p}\right|}_{\left|\frac{\vec{r}}{|r|}\times\vec{v}\right|=v\sin(90)=v}\quad \pi r^2\left(\frac{\vec{r}\times\vec{p}}{|\vec{r}\times\vec{p}|}\right)\\ &= \frac{e}{2mc}\vec{r}\times\vec{p}\\ &= \frac{e}{2mc}\hat{L}\end{aligned}$$

Remark 2: $\hat{H}_0$ is invariant under rotations about the nucleus (coulomb interaction depends only on distance between particles), and therefore commutes with all components of angular momentum $\Rightarrow \hat{H}_0, \hat{L}^2, \hat{L}_z$ form a mutually commuting set of operators. We choose $\mathcal{H}$ to be in the z-direction and form a representation in terms of $|nlm\rangle$ where:

$$\begin{aligned}\hat{H}_0\,|nlm\rangle &= E_0^{nl}\,|nlm\rangle\\ \hat{L}^2\,|nlm\rangle &= \hbar^2 l(l+1)\,|nlm\rangle\\ \hat{L}_z\,|nlm\rangle &= \hbar m\,|nlm\rangle\end{aligned}$$

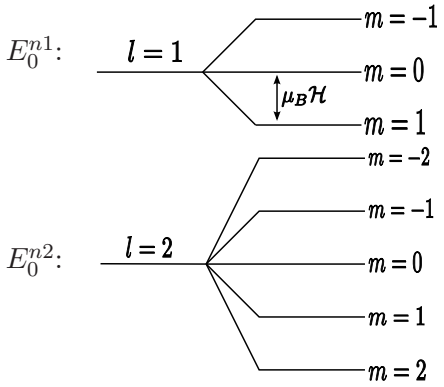
and E_0^{nl} energies are $2l+1$ -fold degenerate since they are independent of m. The Hamiltonian is written

$$\hat{H} = \hat{H}_0 - \frac{e}{2\mu c}\mathcal{H}\hat{L}_z$$

Since $\hat{H}$ commutes with $\hat{H}_0$,$\hat{L}^2$, and $\hat{L}_z$, the $|nlm\rangle$ states are also eigenstates of $\hat{H}$, with eigenvalues:

$$E_0^{nl} - \underbrace{\frac{e}{2\mu c}}_{\mu_B}\hbar\mathcal{H}m$$

where μ_B is the Bohr magneton. Thus, in the presence of a magnetic field, the degeneracy is lifted:



Remark 3: The above energy splitting was not always observed in atomic spectroscopic experiments. If the number of electrons was odd, the number of splitting was even. Also, the spacing in energy levels was not always given by $\mu_B \mathcal{H}$. Given the even number of levels, it seems there must be $\frac{1}{2}$ integer spin values of angular momentum $(2j+1)$. Since orbital momentum can not give $\frac{1}{2}$ integer angular momentum quantum numbers, it was hypothesized that electrons contain some intrinsic angular momentum that is independent of orbital angular momentum. This implies electron spin.

Remark 4: The magnetic moment associated with spin is:

$$\hat{\boldsymbol{\mu}}_{\boldsymbol{s}} = g_s \frac{e}{2\mu c} \hat{\boldsymbol{S}}$$

where

$$\begin{aligned} \hat{\boldsymbol{\mu}}_{\boldsymbol{s}} &= \text{ spin magnetic moment} \\ \hat{\boldsymbol{S}} &= \text{ spin angular momentum} \end{aligned}$$

and g_s is the factor that produces the correct energy level splitting in spectroscopic experiments; $g_s \approx 2$.

Remark 5: Since $\hat{\boldsymbol{S}}$ is an angular momentum operator, we assume $\S^2$ has eigenvalues $\hbar^2 \left(\frac{1}{2}\right)\left(\frac{1}{2}+1\right)$ for $S = \frac{1}{2}$, and that the $\hat{S}_z$ eigenvalues are $\pm\frac{1}{2}\hbar$.

Remark 6: Spectroscopy gave physical evidence of spin. Dirac demonstrated mathematically that electron spin was required to make the wave function covariant.

11.3 Spin Kinematics

11.3.1 Spin Operators, Spinors, and Eigenvalues

Consider an infinitesimal rotation of an n-component wave function about the z-axis:

$$\begin{bmatrix} \psi_1' \\ \psi_2' \\ \vdots \\ \psi_n' \end{bmatrix} = \left(\hat{I}_{(n)} - \underbrace{\frac{i\varepsilon}{\hbar} \begin{bmatrix} -i\hbar\frac{\partial}{\partial\phi} & & \\ & \ddots & \\ & & -i\hbar\frac{\partial}{\partial\phi} \end{bmatrix}}_{(1)} - \underbrace{\frac{i\varepsilon}{\hbar}\hat{S}_z}_{(2)} \right) \begin{bmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{bmatrix}$$

where

1. Corresponds to a physical rotation which assigns points in space to rotated points

2. Corresponds to taking components of wave functions and transforming them into linear combinations of other components

Equivalently:

$$\left|\psi'\right\rangle = \left[\hat{I} - \frac{i\varepsilon}{\hbar}\left(\hat{L}_z + \hat{S}_z\right)\right]|\psi\rangle = \left[\hat{I} - \frac{i\varepsilon}{\hbar}\hat{J}_z\right]|\psi\rangle$$

where $\hat{J}_z = \hat{L}_z + \hat{S}_z$ is the generator of rotations about the z-axis. More generally,

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$$

is the total angular momentum.

Remark 1: $\hat{\boldsymbol{J}}$ and $\hat{\boldsymbol{L}}$ obey angular momentum commutation relations (§1). Since $\left[\hat{\boldsymbol{L}}, \hat{\boldsymbol{J}}\right] = 0$ ($\hat{\boldsymbol{L}}$ acts on the spacial part of wave functions x,y,z, and $\hat{\boldsymbol{S}}$ acts on components $1, \ldots, n$), it follows that $\hat{\boldsymbol{S}}$ also obeys angular momentum commutation relations.

$$\left[\hat{S}_i, \hat{S}_j\right] = i\hbar\epsilon_{ijk}\hat{S}_k$$

Remark 2: In Chapter 9, we found that rotation operators are block diagonal matrices and each block represents a rotation matrix for a specific value of angular momentum. Since we are assuming that the electron has spin eigenvalues $\pm\frac{1}{2}$, the relevant block in $D^{(1/2)}$, which implies that the electron spin operators are given by:

$$\hat{S}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \hat{S}_y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \qquad \hat{S}_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Remark 3: Given the spin operators, the electron can be described as a 2-component wave function:

$$\psi = \begin{bmatrix} \psi_+(x,y,z) \\ \psi_-(x,y,z) \end{bmatrix} = \psi_+ \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \psi_- \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

where ψ is called a spinor.

Remark 4: This can be represented as

$$|+\rangle \equiv \left|\frac{1}{2}, \frac{1}{2}\right\rangle$$
$$|-\rangle \equiv \left|\frac{1}{2}, -\frac{1}{2}\right\rangle$$

In an $\hat{S}_z$ basis, $|+\rangle$ points up the z-axis and $|-\rangle$ points down. Here, $\hat{S}_z$ in matrix form is:

$$\begin{pmatrix}\langle+|\\ \langle-|\end{pmatrix}\hat{S}_z\left(|+\rangle\ \ |-\rangle\right) = \begin{pmatrix}\langle+|\\ \langle-|\end{pmatrix}\left(\frac{\hbar}{2}|+\rangle - \frac{\hbar}{2}|-\rangle\right)$$
$$= \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

which is what we said above.

In the spirit of raising and lowering operators:

$$\hat{S}_x = \frac{1}{2}\left(\hat{S}_+ + \hat{S}_-\right)$$
$$\hat{S}_y = \frac{1}{2i}\left(\hat{S}_+ - \hat{S}_-\right)$$

where

$$\hat{S}_+|+\rangle = 0$$
$$\hat{S}_+|-\rangle = \hbar|+\rangle$$
$$\hat{S}_-|+\rangle = \hbar|-\rangle$$
$$\hat{S}_-|-\rangle = 0$$

These give $\hat{S}_x$ and $\hat{S}_y$ matrices that are consistant with Remark 2.

Remark 5: Note that

$$\hat{S}^2|\pm\rangle = \frac{\hbar^2}{2}\left(1+\frac{1}{2}\right)|\pm\rangle = \frac{3}{4}\hbar^2|\pm\rangle$$
$$\hat{S}_z|\pm\rangle = \pm\frac{\hbar}{2}|\pm\rangle$$

Remark 6: One important difference between spin and orbital angular momentum is that the magnitude of spin is fixed whereas the magnitude of orbital angular momentum can change (as in an external field).

Remark 7: So far, we are only considering the case where $\left[\hat{\boldsymbol{L}}, \hat{\boldsymbol{S}}\right] = 0$. In some instances, this is spin-orbit coupling, where $\left[\hat{\boldsymbol{L}}, \hat{\boldsymbol{S}}\right] \neq 0$, but we'll worry about that later (perturbation theory). For now, we assume:

$$\hat{H} = \hat{H}_o + \hat{H}_s$$

Since we are taking the spin to evolve separately, the wavefunction separates:

$$|\psi(t)\rangle = |\psi_o(t)\rangle \otimes |\chi_s(t)\rangle$$

Remark 8: Generalizing the spin components to an arbitrary direction $\boldsymbol{n}$, rather than in the z-direction:

$$\langle \boldsymbol{n}, \pm | \, \hat{\boldsymbol{S}} \, | \boldsymbol{n}, \pm \rangle$$

are the spin states that point up or down the $\boldsymbol{n}$ axis. So if $\boldsymbol{n}$ points in the direction of (θ, ϕ):

$$\begin{aligned} n_x &= \sin\theta\cos\phi \\ n_y &= \sin\theta\sin\phi \\ n_z &= \cos\theta \end{aligned}$$

And

$$\begin{aligned} \boldsymbol{n}\cdot\hat{\boldsymbol{S}} &= n_x\hat{S}_x + n_y\hat{S}_y + n_z\hat{S}_z \\ &= \frac{\hbar}{2}\begin{bmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{bmatrix} \quad \text{using Remark 2} \\ &= \frac{\hbar}{2}\begin{bmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{bmatrix} \end{aligned}$$

Solving the eigenvalue problem gives the following eigenvectors:

$$|\boldsymbol{n}_+\rangle = \begin{bmatrix} \cos\left(\frac{\theta}{2}\right) e^{-i\phi/2} \\ \sin\left(\frac{\theta}{2}\right) e^{i\phi/2} \end{bmatrix}, \qquad |\boldsymbol{n}_-\rangle = \begin{bmatrix} -\sin\left(\frac{\theta}{2}\right) e^{-i\phi/2} \\ \cos\left(\frac{\theta}{2}\right) e^{i\phi/2} \end{bmatrix}$$

11.3.2 Pauli Spin Matrices

It is conventional to drop the $\frac{\hbar}{2}$ factor in the spin matrices $\hat{S}_x, \hat{S}_y, \hat{S}_z$ to get the Pauli Spin Matrices:

$$\hat{\boldsymbol{S}} = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}}$$

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 - 1 & \end{pmatrix}$$

Remark 1: The Pauli matrices anti-commute:

$$[\hat{\sigma}_i, \hat{\sigma}_j]_+ = \hat{\sigma}_i\hat{\sigma}_j + \hat{\sigma}_j\hat{\sigma}_i = 0 \qquad (i \neq j)$$

Remark 2: $\hat{\sigma}_x\hat{\sigma}_y = i\hat{\sigma}_z$ and other cyclic permutations (by the anti-commuting nature).

Remark 3: $\mathrm{Tr}(\hat{\sigma}_i = 0$

Remark 4: $\hat{\sigma}_i^2 = \hat{I}$. Moreover, $(\boldsymbol{n} \cdot \hat{\boldsymbol{\sigma}}) = \hat{I}$.

Remark 5: $[\hat{\sigma}_i, \hat{\sigma}_j]_+ = 2\delta_{ij}\hat{I}$

Remark 6: $[\hat{\sigma}_x, \hat{\sigma}_y] = 2i\hat{\sigma}_z$ and cyclic permutations

Remark 7: $\mathrm{Tr}(\hat{\sigma}_i\hat{\sigma}_j) = 2\delta_{ij}$. If we choose $\hat{\sigma}_0 \equiv \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$, then

$$\mathrm{Tr}\left(\hat{\sigma}_\alpha\hat{\sigma}_\beta\right) = 2\delta_{\alpha,\beta}; \qquad \alpha, \beta = 0, x, y, z$$

This implies that the $\hat{\sigma}_\alpha$'s are linearly independent, and thus any matrix M can be written

$$M = \sum_\alpha m_\alpha \hat{\sigma}_\alpha \qquad \text{where} \qquad m_\alpha = \frac{1}{2}\mathrm{Tr}\left(M\hat{\sigma}_\alpha\right)$$

11.3.3 Rotations

The rotation operator for spin $\frac{1}{2}$ is in a simple form. Consider rotations about the z-axis:

$$\begin{aligned}
\hat{U}[R(\hat{z})] &= e^{i\hat{S}_z\phi/\hbar} \\
&= e^{-i\hat{\sigma}_z\phi/2} \\
&= \sum_{k=0}^{\infty} \underbrace{\frac{(-i\phi)^{2k}}{(2k!)}\left(\frac{\hat{\sigma}_z^2}{2^2}\right)^k}_{\text{Even terms}} + \sum_{k=0}^{\infty} \underbrace{\frac{(-i\phi)^{2k+1}}{(2k+1)!}\left(\frac{\hat{\sigma}_z^2}{2^2}\right)^k \frac{\hat{\sigma}_z}{2}}_{\text{Odd terms}}
\end{aligned}$$

Since $\hat{\sigma}_z^2 = \hat{I}$:

$$= \cos\left(\frac{\phi}{2}\right)\hat{I} - i\sin\left(\frac{\phi}{2}\right)\hat{\sigma}_z$$

For rotations about a general axis, this becomes:

$$\hat{U}[R(\hat{\theta})] = \cos\left(\frac{\theta}{2}\right) - i\sin\left(\frac{\theta}{2}\right)\boldsymbol{\theta} \cdot \hat{\boldsymbol{\sigma}}$$

11.4 Spin Dynamics

Consider a stationary electron in a magnetic field $\boldsymbol{B}$. The Hamiltonian is given by

$$\hat{H} = -\boldsymbol{\mu} \cdot \boldsymbol{B} = -g_s\frac{e}{2mc}\hat{\boldsymbol{S}} \cdot \boldsymbol{B} \approx -\frac{e}{mc}\hat{\boldsymbol{S}} \cdot \boldsymbol{B}$$

The time evolution for a state is given by

$$|\psi(t)\rangle = \hat{U}(t)\,|\psi(0)\rangle$$

where the propagator

$$\hat{U}(t) = e^{i\hat{H}t/\hbar} = \exp\left(-\frac{ie}{mc\hbar}\hat{\boldsymbol{S}}\cdot\boldsymbol{B}t\right)$$

Remark 1: We see that the propagator closely resembles the rotation operator $e^{-i\boldsymbol{\theta}\cdot\hat{\boldsymbol{S}}}$. This implies that the propagator rotates the state by an angle $\boldsymbol{\theta} = -\frac{e}{mc}\boldsymbol{B}t$.

Consider now the case where $\boldsymbol{B} = B\hat{z}$. Then

$$\hat{U}(t) = \exp\left(\tfrac{i}{\hbar}\tfrac{eB}{mc}\hat{S}_z t\right) = e^{i\omega_0\hat{\sigma}_z t/2} = \begin{pmatrix} e^{i\omega_0 t/2} & 0 \\ 0 & e^{-i\omega_0 t/2}\end{pmatrix}$$

where $\omega_0 = \frac{mB}{mc}$. Let's let

$$\begin{aligned}|\psi(0)\rangle &= |\boldsymbol{n}+\rangle \\ &= \begin{pmatrix}\cos\left(\frac{\theta}{2}\right)e^{-i\phi/2} \\ \sin\left(\frac{\theta}{2}\right)e^{i\phi/2}\end{pmatrix}\end{aligned}$$

where $|\boldsymbol{n}+\rangle$ indicates a spin up along an arbitrary axis. Then:

$$\begin{aligned}|\psi(t)\rangle &= \hat{U}(t)\,|\psi(0)\rangle \\ &= \begin{pmatrix} e^{i\omega_0 t/2} & 0 \\ 0 & e^{-i\omega_0 t/2}\end{pmatrix}\begin{pmatrix}\cos\left(\frac{\theta}{2}\right)e^{-i\phi/2} \\ \sin\left(\frac{\theta}{2}\right)e^{i\phi/2}\end{pmatrix} \\ &= \begin{pmatrix}\cos\left(\frac{\theta}{2}\right)e^{-i(\phi-\omega_0 t)/2} \\ \sin\left(\frac{\theta}{2}\right)e^{i(\phi-\omega_0 t)/2}\end{pmatrix}\end{aligned}$$

implying that the rotation angle ϕ changes at a rate ω_0.

11.4.1 Spin $\frac{1}{2}$ and the Bloch Sphere

Let us consider a geometrical representation for the state of a spin-$\frac{1}{2}$ system. This representation is the work of Felix Bloch and is used extensively in optical physics (a spin-$\frac{1}{2}$ system is isomorphic to a 2-state system and this makes a nice way to study transitions in atoms and molecules). The most general state of a spin-$\frac{1}{2}$ system is a superposition of up and down states:

$$|\psi\rangle = C_1\,|+\rangle + C_2\,|-\rangle$$

where C_1 and C_2 are complex numbers.

Remark 1: C_1 and C_2 are complex, and thus there exist 4 parameters that specify the state. We can reduce this to 2 by noting:

- $\langle\psi|\psi\rangle = 1 \quad \Rightarrow \quad |C_1|^2 + |C_2|^2 = 1$
- Overall phase of a state does not matter, we only need the relative phase of C_1 and C_2.

Remark 2: Let the 2 parameters be the angles θ, ϕ so that we can write

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right) e^{-i\phi/2} |+\rangle + \sin\left(\frac{\theta}{2}\right) e^{i\phi/2} |-\rangle$$

Let the state $|\psi\rangle$ be represented by a point of the surface of the unit sphere. This is called the Bloch sphere.

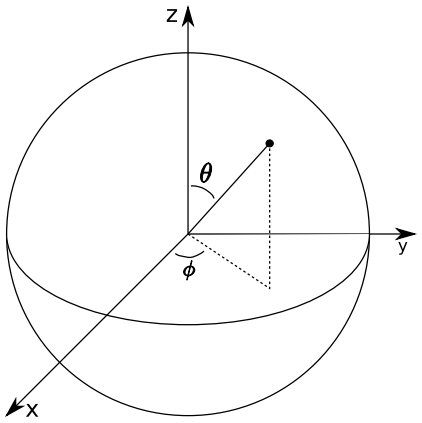


Figure 11.1: The Bloch Sphere

Remark 3: The axes on the Bloch sphere have physical significance. Consider:

$$\theta = 0 \Rightarrow |\psi\rangle = |+\rangle = \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle$$
$$\theta = \pi \Rightarrow |\psi\rangle = |-\rangle = \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle$$

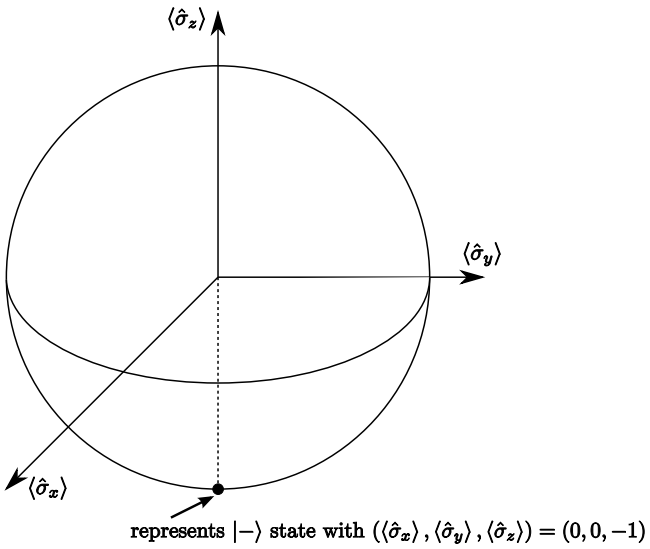
Thus the points represent eigenstates of $\hat{S}_z$ with eigenvalues $\pm\frac{1}{2}\hbar$. Expressing these in terms of Pauli matrices, the north and south pole of the Bloch sphere represent:

$$\langle\hat{\sigma}_z\rangle = 1 \quad (\theta = 0)$$
$$\langle\hat{\sigma}_z\rangle = -1 \quad (\theta = \pi)$$

Remark 4: The expectation values for $\hat{\sigma}_x, \hat{\sigma}_y$ at these locations are:

$$\theta = 0:$$
$$\langle \hat{\sigma}_x \rangle = \frac{1}{\hbar} \left\langle + \middle| (\hat{S}_+ + \hat{S}_-) \middle| + \right\rangle = 0$$
$$\langle \hat{\sigma}_y \rangle = \frac{1}{\hbar} \left\langle + \middle| (-i)(\hat{S}_+ - \hat{S}_-) \middle| + \right\rangle = 0$$
$$\theta = \pi:$$
$$\langle \hat{\sigma}_x \rangle = \frac{1}{\hbar} \left\langle - \middle| (\hat{S}_+ + \hat{S}_-) \middle| - \right\rangle = 0$$
$$\langle \hat{\sigma}_y \rangle = \frac{1}{\hbar} \left\langle - \middle| (-i)(\hat{S}_+ - \hat{S}_-) \middle| - \right\rangle = 0$$

which suggests that the projection of the state onto each of the Cartesian axes of the Bloch sphere corresponds to $\langle \hat{\sigma}_x \rangle, \langle \hat{\sigma}_y \rangle$ and $\langle \hat{\sigma}_z \rangle$:



Remark 5: Consider the general case

$$|\psi\rangle = \cos\left(\tfrac{\theta}{2}\right) e^{-i\phi/2} |+\rangle + \sin\left(\tfrac{\theta}{2}\right) e^{i\phi/2} |-\rangle$$

$$\begin{aligned}
\Rightarrow \langle\hat{\sigma}_x\rangle &= \left[\cos\left(\tfrac{\theta}{2}\right) e^{i\phi/2}\langle+| + \sin\left(\tfrac{\theta}{2}\right) e^{-i\phi/2}\langle-|\right]\left(\hat{S}_x + \hat{S}_-\right)\left[\cos\left(\tfrac{\theta}{2}\right) e^{-i\phi/2}|+\rangle + \sin\left(\tfrac{\theta}{2}\right) e^{i\phi/2}|-\rangle\right] \\
&= \cos\left(\tfrac{\theta}{2}\right) e^{-i\phi} + \sin\left(\tfrac{\theta}{2}\right) e^{i\phi} \\
&= \sin(\theta)\cos(\phi) \\
\langle\hat{\sigma}_y\rangle &= \sin(\theta)\sin(\phi) \\
\langle\hat{\sigma}_z\rangle &= \left[\cos\left(\tfrac{\theta}{2}\right) e^{i\phi/2}\langle+| + \sin\left(\tfrac{\theta}{2}\right) e^{-i\phi/2}\langle-|\right]\hat{\sigma}_z\left[\cos\left(\tfrac{\theta}{2}\right) e^{-i\phi/2}|+\rangle + \sin\left(\tfrac{\theta}{2}\right) e^{i\phi/2}|-\rangle\right] \\
&= \cos^2\left(\tfrac{\theta}{2}\right) - \sin^2\left(\tfrac{\theta}{2}\right) \\
&= \cos(\theta)
\end{aligned}$$

These correspond to the Cartesian coordinates for a point located at θ, ϕ on the unit sphere.

11.4.2 Rotations on the Bloch Sphere

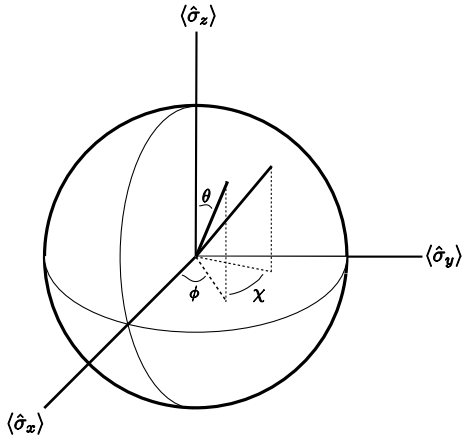
Consider a rotation about the z-axis. From §11.3.3:

$$\hat{U}[R(\hat{z})] = \cos\left(\tfrac{\chi}{2}\right)\hat{I} - i\sin\left(\tfrac{\chi}{2}\right)\hat{\sigma}_z$$

where χ is the angle we have rotated through. Applying this to the general state:

$$\begin{aligned}
\hat{U}[R(\hat{z})]|\psi\rangle &= \left[\cos\left(\tfrac{\chi}{2}\right)\hat{I} - i\sin\left(\tfrac{\chi}{2}\right)\hat{\sigma}_z\right]\left[\cos\left(\tfrac{\theta}{2}\right) e^{-i\phi/2}|+\rangle + \sin\left(\tfrac{\theta}{2}\right) e^{i\phi/2}|-\rangle\right] \\
&= \left[\cos\left(\tfrac{\chi}{2}\right) - i\sin\left(\tfrac{\chi}{2}\right)\right]\cos\left(\tfrac{\theta}{2}\right) e^{-i\phi/2}|+\rangle + \left[\cos\left(\tfrac{\chi}{2}\right) + i\sin\left(\tfrac{\chi}{2}\right)\right]\sin\left(\tfrac{\theta}{2}\right) e^{i\phi/2}|-\rangle \\
&= \cos\left(\tfrac{\theta}{2}\right) e^{-i(\phi+\chi)/2}|+\rangle + \sin\left(\tfrac{\theta}{2}\right) e^{i(\phi+\chi)/2}|-\rangle
\end{aligned}$$

Which shows that a point on the Bloch sphere represented by state θ, ϕ gets rotated about the z-axis by an angle χ.

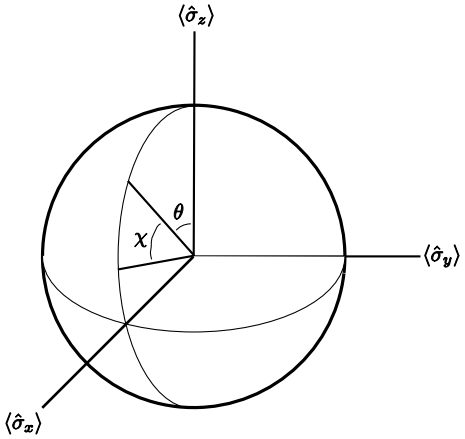


Now, consider a rotation about the y-axis:

$$\begin{aligned}
\hat{U}[R(\hat{y})]|\psi\rangle &= \left[\cos\left(\tfrac{\chi}{2}\right)\hat{I} - i\hat{\sigma}_y\sin\left(\tfrac{\chi}{2}\right)\right]\left[\cos\left(\tfrac{\theta}{2}\right) e^{-i\phi/2}|+\rangle + \sin\left(\tfrac{\theta}{2}\right) e^{i\phi/2}|-\rangle\right] \\
&= \left[\cos\left(\tfrac{\chi}{2}\right)\cos\left(\tfrac{\theta}{2}\right) e^{-i\phi/2} - \sin\left(\tfrac{\chi}{2}\right)\sin\left(\tfrac{\theta}{2}\right) e^{i\phi/2}\right]|+\rangle + \left[\cos\left(\tfrac{\chi}{2}\right)\sin\left(\tfrac{\theta}{2}\right) e^{i\phi/2} + \sin\left(\tfrac{\chi}{2}\right)\cos\left(\tfrac{\theta}{2}\right) e^{-i\phi/2}\right]|-
\end{aligned}$$

This is more complicated, but looking at the case where $\phi = 0$, (in the $\langle\hat{\sigma}_x\rangle - \langle\hat{\sigma}_z\rangle$ plane), we have:

$$\hat{U}[R(\hat{y})]\,|\psi(\phi=0)\rangle = \cos\left(\tfrac{\theta+\chi}{2}\right)|+\rangle + \sin\left(\tfrac{\theta+\chi}{2}\right)|-\rangle$$



Remark 1: Since the evolution of a state can be considered a rotation (§11.4), the evolution can be described as a point moving with time on the surface of the Bloch sphere.

11.5 Particles with Spin 1

Electrons gave the first clues to the existence of an intrinsic angular momentum. However, this properly applies to a wide assortment of particles.

Remark 1: Recall that particles with $\frac{1}{2}$ integer spin are called *fermions*. Particles with integer spin are *bosons*.

Consider the rotated state of §11.3.1:

$$|\psi'\rangle = \left[\hat{I} - \frac{i\varepsilon}{\hbar}\left(\hat{L}_z + \hat{S}_z\right)\right]|\psi\rangle$$

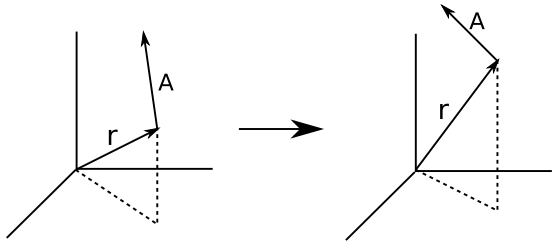
The rotation matrix for this rotation is:

$$R_z(\varepsilon) = \begin{pmatrix} \cos\varepsilon & -\sin\varepsilon & 0 \\ \sin\varepsilon & \cos\varepsilon & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

11.5.1 Rotations of a Vector Field

(*Disclaimer: Sometimes* $\hbar = 1$ *in this section*)

Now, if we consider an arbitrary vector field $\boldsymbol{A}(\boldsymbol{r})$, we can imagine this as having a vector associated with every point in space.



When we rotate the vector field, we are rotating the vectors $\boldsymbol{A}$ as well as the positions $\boldsymbol{r}$. we want to relate this rotation to angular momentum.

$$\boldsymbol{A} \to \boldsymbol{A'}, \qquad \boldsymbol{r} \to R\boldsymbol{r}$$

So the transformation:

$$\boldsymbol{A'}(R\boldsymbol{r}) = R\boldsymbol{A}(\boldsymbol{r})$$

-or-

$$\boldsymbol{A'}(\boldsymbol{r}) = R\boldsymbol{A}(R^{-1}\boldsymbol{r}) \tag{$\dagger$}$$

where the two different forms correspond to active or passive transformations. The rotation matrix given for rotations about the z-axis has

$$R_z^{-1}(\varepsilon) = R_z(\varepsilon)$$

Thus, the vector field $\boldsymbol{A'}(\boldsymbol{r})$, according to ($\dagger$), is given by

$$\boldsymbol{A'}(\boldsymbol{r}) = \begin{pmatrix} \cos\varepsilon & -\sin\varepsilon & 0 \\ \sin\varepsilon & \cos\varepsilon & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} A_x(R^{-1}\boldsymbol{r}) \\ A_y(R^{-1}\boldsymbol{r}) \\ A_z(R^{-1}\boldsymbol{r}) \end{pmatrix}$$

$$\begin{aligned} \Rightarrow A'_x &= A_x(R^{-1}\boldsymbol{r})\cos\varepsilon - A_y(R^{-1}\boldsymbol{r})\sin\varepsilon \\ A'_y &= A_x(R^{-1}\boldsymbol{r})\sin\varepsilon + A_y(R^{-1}\boldsymbol{r})\cos\varepsilon \\ A'_z &= A_z(R^{-1}\boldsymbol{r}) \end{aligned}$$

where

$$R^{-1}\boldsymbol{r} = \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} x\cos\varepsilon + y\sin\varepsilon \\ y\cos\varepsilon - x\sin\varepsilon \\ z \end{pmatrix}$$

Since ε is *small*, we can write this as:

$$\begin{aligned}
A'_x &= A_x\left(\underbrace{x\cos\varepsilon + y\sin\varepsilon}_{x+\varepsilon y}, \underbrace{y\cos\varepsilon - x\sin\varepsilon}_{y-\varepsilon x}, z\right) - \varepsilon A_y\left(x+\varepsilon y, y-\varepsilon x, z\right) \\
&= A_x\left(x+\varepsilon y, y-\varepsilon x, z\right) - \varepsilon A_y\left(x,y,z\right) \qquad \text{to } \mathcal{O}(\varepsilon) \\
&= A_x(x,y,z) + \varepsilon\left(\left.\frac{\partial A_x}{\partial x'}\right|_{x=x'}\frac{\partial x'}{\partial \varepsilon} + \left.\frac{\partial A_x}{\partial y'}\right|_{y=y'}\frac{\partial y'}{\partial \varepsilon}\right) - \varepsilon A_y(\boldsymbol{r}) \\
&= A_x(x,y,z) + \varepsilon \underbrace{\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right)}_{-\frac{i}{\hbar}\hat{L}_z} A_x(\boldsymbol{r}) - \varepsilon A_y(\boldsymbol{r}) \\
&= \left(\hat{I} - \frac{i\varepsilon}{\hbar}\hat{L}_z\right) A_x(\boldsymbol{r}) - \varepsilon A_y(\boldsymbol{r})
\end{aligned}$$

Similarly,

$$\begin{aligned}
A'_y(\boldsymbol{r}) &= \varepsilon A_x(\boldsymbol{r}) + \left(\hat{I} - \frac{i\varepsilon}{\hbar}\hat{L}_z\right) A_y(\boldsymbol{r}) \\
A'_z(\boldsymbol{r}) &= \left(\hat{I} - \frac{i\varepsilon}{\hbar}\hat{L}_z\right) A_x(\boldsymbol{r}) \\
\Rightarrow \boldsymbol{A'}(\boldsymbol{r}) &= \underbrace{\left(\hat{I} - \frac{i\varepsilon}{\hbar}\hat{L}_z\right)\boldsymbol{A}(\boldsymbol{r})}_{\text{Usual Rotation}} - \underbrace{\frac{i\varepsilon}{\hbar}\left(-iA_y(\boldsymbol{r})\hat{\boldsymbol{x}} + iA_x(\boldsymbol{r})\hat{\boldsymbol{y}}\right)}_{\text{Spin part}}
\end{aligned}$$

Thus we have

$$\boldsymbol{A'}(\boldsymbol{r}) = \left[\hat{I} - \frac{i\varepsilon}{\hbar}\left(\hat{L}_z + \hat{S}_z\right)\right]\boldsymbol{A}(\boldsymbol{r})$$

where we define

$$\hat{S}_z\boldsymbol{A}(\boldsymbol{r}) = \frac{-i}{\hbar}A_y(\boldsymbol{r})\hat{\boldsymbol{x}} + \frac{i}{\hbar}A_x(\boldsymbol{r})\hat{\boldsymbol{y}}$$

since

$$\hat{S}_z\begin{pmatrix}A_x(\boldsymbol{r})\\A_y(\boldsymbol{r})\\A_z(\boldsymbol{r})\end{pmatrix} = \begin{pmatrix}-iA_y(\boldsymbol{r})\\iA_x(\boldsymbol{r})\\0\end{pmatrix}$$

Therefore, we can represent $\hat{S}_z$ as the matrix

$$\hat{S}_z = \begin{pmatrix}0 & -i & 0\\ i & 0 & 0\\ 0 & 0 & 0\end{pmatrix}\hbar$$

Similarly, rotations about the x and y axis give

$$\hat{S}_x = \hbar \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \qquad \hat{S}_y = \hbar \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$$

Remark 1: $\hat{S}_x, \hat{S}_y, \hat{S}_z$ are related by row-column interchanges.

Remark 2: if $\hat{S}_x, \hat{S}_y, \hat{S}_z$ are components of angular momentum, they must obey commutation relations. This can be checked directly. For example:

$$\begin{aligned}
\hat{S}_x\hat{S}_y - \hat{S}_y\hat{S}_x &= \hbar^2 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} - \hbar^2 \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \\
&= \hbar^2 \begin{pmatrix} 0 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \hbar^2 \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
&= \hbar^2 \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} i \\
&= i\hbar\hat{S}_z
\end{aligned}$$

Remark 3: The magnitude of angular momentum is given by

$$\begin{aligned}
\hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{S}} &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}^2 + \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}^2 + \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}^2 \\
&= 2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
&= s(s+1)\hat{I} \\
\Rightarrow s(s+1) = 2 \quad &\Rightarrow s = 1 \quad \Rightarrow \text{ Spin 1}
\end{aligned}$$

Remark 4: Working in the standard representation for a $s = 1$ system, $|1, m\rangle$, with

$$\hat{S}_z |1, m\rangle = m\hbar |1, m\rangle ; \quad m = 0, \pm 1$$

We find that, in this representation,

$$\begin{aligned}\hat{S}_z &= \begin{pmatrix}\langle 1,1| \\ \langle 1,0| \\ \langle 1,-1|\end{pmatrix} \hat{S}_z \begin{pmatrix}|1,1\rangle & |1,0\rangle & |1,-1\rangle\end{pmatrix} \\ &= \begin{pmatrix}1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1\end{pmatrix}\end{aligned}$$

To find the other components, we'll use the relations from §11.1:

$$\begin{aligned}\hat{S}_+ |1,0\rangle &= \hbar\sqrt{(1-0)(1+0+1)}\,|1,1\rangle = \hbar\sqrt{2}\,|1,1\rangle \\ \hat{S}_+ |1,-1\rangle &= \hbar\sqrt{(1+1)(1-1+1)}\,|1,0\rangle = \hbar\sqrt{2}\,|1,0\rangle \\ \hat{S}_- |1,1\rangle &= \hbar\sqrt{(1+1)(1-1+1)}\,|1,0\rangle = \hbar\sqrt{2}\,|1,0\rangle \\ \hat{S}_+ |1,0\rangle &= \hbar\sqrt{(1-0)(1+0+1)}\,|1,-1\rangle = \hbar\sqrt{2}\,|1,-1\rangle\end{aligned}$$

So that

$$\hat{S}_x \to \begin{pmatrix}\langle 1,1| \\ \langle 1,0| \\ \langle 1,-1|\end{pmatrix} \hat{S}_x \begin{pmatrix}|1,1\rangle & |1,0\rangle & |1,-1\rangle\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0\end{pmatrix}$$

$$Sp_y \to \begin{pmatrix}\langle 1,1| \\ \langle 1,0| \\ \langle 1,-1|\end{pmatrix} \hat{S}_y \begin{pmatrix}|1,1\rangle & |1,0\rangle & |1,-1\rangle\end{pmatrix} = \frac{i}{\sqrt{2}}\begin{pmatrix}0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0\end{pmatrix}$$

Remark 5: Notice that the matrices in Remark 4 are different than those given at the beginning of this section. This is because the first set are identified with vector cartesian components, and the matrices in Remark 4 form a basis that is not identified as such. To understand, recall that we defined the "spin" part of the rotation by

$$\hat{S}_z \boldsymbol{A}(\boldsymbol{r}) = -iA_y(\boldsymbol{r})\hat{\boldsymbol{x}} + iA_x(\boldsymbol{r})\hat{\boldsymbol{y}}$$

Let

$$\boldsymbol{u}_\pm = \frac{1}{\sqrt{2}}\left(\hat{\boldsymbol{x}} \pm i\hat{\boldsymbol{y}}\right)$$

with $\boldsymbol{u_0} = \hat{\boldsymbol{z}}$. Then any vector can be expressed in terms of these as

$$\begin{aligned}\boldsymbol{A} &= A_x\hat{\boldsymbol{x}} + A_y\hat{\boldsymbol{y}} + A_z\hat{\boldsymbol{z}} \\ &= \frac{1}{\sqrt{2}}A_x\left(\boldsymbol{u}_+ + \boldsymbol{u}_-\right) + \frac{1}{i\sqrt{2}}A_y\left(\boldsymbol{u}_+ - \boldsymbol{u}_-\right) + \boldsymbol{u_0}A_z \\ &= A_+\boldsymbol{u}_+ + A_-\boldsymbol{u}_- + A_0\boldsymbol{u_0}\end{aligned}$$

with

$$A_\pm = \frac{1}{\sqrt{2}}\left(A_x \mp iA_y\right), \quad A_0 = A_z$$

So

$$\begin{aligned}\hat{S}_z\boldsymbol{A}(\boldsymbol{r}) &= \frac{-i}{\sqrt{2}}\left(\boldsymbol{u}_+ + \boldsymbol{u}_-\right)\frac{i}{\sqrt{2}}\left(A_+(\boldsymbol{r}) - A_-(\boldsymbol{r})\right) + \frac{1}{\sqrt{2}}\left(\boldsymbol{u}_+ - \boldsymbol{u}_-\right)\frac{1}{\sqrt{2}}\left(A_+(\boldsymbol{r}) + A_-(\boldsymbol{r})\right) \\ &= \boldsymbol{u}_+A_+(\boldsymbol{r}) - \boldsymbol{u}_-A_-(\boldsymbol{r})\end{aligned}$$

And thus

$$\hat{S}_z\begin{pmatrix}A_+\\0\\A_-\end{pmatrix} = \begin{pmatrix}A_+\\0\\-A_-\end{pmatrix} \quad \Rightarrow \hat{S}_z = \underbrace{\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}}_{\text{Matrix from Remark 4}}$$

Similar arguments work for $\hat{S}_x, \hat{S}_y$. Physically, this change of basis can be related to the polarization of a photon, which is a spin 1 particle. These spin states of a photon are associated with circular polarization in the x-y plane where $m = \pm 1$, and linear polarization in the z direction ($m = 0$). Hence, it is *not* associated with the 3 linear polarization directions. Therefore, $\boldsymbol{u}_+, \boldsymbol{u}_-$ and A_+, A_- describe circular polarization of an EM field.

Chapter 12

Addition of Angular Momentum

Consider the situation in which we have many particles that make up a system, and this system has rotational invariance, and therefore angular momentum commutes with the Hamiltonian. The total angular momentum of the system is the sum of the spin and orbital angular momentum for *all* the particles. Given that we know the eigenstates for the individual pieces, we want to find the eigenstates of the total angular momentum.

12.1 Addition of 2 Angular Momenta

Consider 2 angular momenta, $\hat{\boldsymbol{j}}_{\mathbf{1}}, \hat{\boldsymbol{j}}_{\mathbf{2}}$, and let

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{j}}_{\mathbf{1}} + \hat{\boldsymbol{j}}_{\mathbf{2}}$$

be the total angular momentum. The eigenstates for the individual pieces we already know:

$$\hat{j}_1^2 \left|j_1, m_1\right\rangle = \hbar j_1(j_1+1) \left|j_1, m_1\right\rangle$$
$$\hat{j}_{1z} \left|j_1, m_1\right\rangle = m_1 \hbar \left|j_1, m_1\right\rangle$$

We have similar results for $\hat{\boldsymbol{j}}_{\mathbf{2}}$. Let

$$\left|j_1, j_2, m_1, m_2\right\rangle \equiv \left|j_1, m_1\right\rangle \otimes \left|j_2, m_2\right\rangle \equiv \left|j_1, m_1\right\rangle \left|j_2, m_2\right\rangle$$

be a representation based on the common eigenstates of $\hat{j}_1^2, \hat{j}_2^2, \hat{j}_{1z}, \hat{j}_{2z}$.

Remark 1: Since $\hat{J}_z = \hat{j}_{1z} + \hat{j}_{2z}$,

$$\hat{J}_z \left|j_1, j_2, m_1, m_2\right\rangle = \hbar(m_1+m_2) \left|j_1, j_2, m_1, m_2\right\rangle$$

So the state $\left|j_1, j_2, m_1, m_2\right\rangle$ is also an eigenstate of $\hat{J}_z$.

Remark 2: $\left|j_1, j_2, m_1, m_2\right\rangle$ is *not* an eigenstate of $\hat{J}^2$, so we need to find the eigenstates of $\hat{J}^2$.

Remark 3: Since $\hat{j}_1^2$ commutes with every component of $\hat{j}_1$ and $\hat{j}_2$ (and similarly for $\hat{j}_2^2$), we have that

$$\left[\hat{\boldsymbol{j}}_{\boldsymbol{1}}^{\boldsymbol{2}}, \hat{\boldsymbol{J}}\right] = \left[\hat{\boldsymbol{j}}_{\boldsymbol{2}}^{\boldsymbol{2}}, \hat{\boldsymbol{J}}\right] = 0$$

So we take $\hat{j}_1^2, \hat{j}_2^2, \hat{J}^2, \hat{J}_z$ as our complete set of commuting observables, and instead of $|j_1, j_2, m_1, m_2\rangle$, we use $|j_1, j_2, J, M\rangle$ (so $\hat{j}_{1z}$ and $\hat{j}_{2z}$ are replaced by J and M). In this representation, we have:

$$\begin{aligned}
\hat{j}_1^2 |j_1, j_2, J, M\rangle &= \hbar^2 j_1(j_1+1) |j_1, j_2, J, M\rangle \\
\hat{j}_2^2 |j_1, j_2, J, M\rangle &= \hbar^2 j_2(j_2+1) |j_1, j_2, J, M\rangle \\
\hat{J}^2 |j_1, j_2, J, M\rangle &= \hbar J(J+1) |j_1, j_2, J, M\rangle \\
\hat{J}_z |j_1, j_2, J, M\rangle &= \hbar M |j_1, j_2, J, M\rangle
\end{aligned}$$

With this representation, we need to find

1. The allowed values of J and M for a given j_1, j_2, and
2. How to express $|j_1, j_2, J, M\rangle$ as a linear combination of $|j_1, j_2, m_1, m_2\rangle$.

12.1.1 Finding Allowed Values of J and M

For individual particles, we have allowed m values given by

$$\begin{aligned}
m_1 &= -j_1, -j_1+1, \ldots, +j_1 \\
m_2 &= -j_2, -j_2+1, \ldots, +2_1
\end{aligned}$$

and

$$\begin{aligned}
\hat{j}_{1z} |j_1, j_2, m_1, m_2\rangle &= \hbar m_1 |j_1, j_2, m_1, m_2\rangle \\
\hat{j}_{2z} |j_1, j_2, m_1, m_2\rangle &= \hbar m_2 |j_1, j_2, m_1, m_2\rangle
\end{aligned}$$

and

$$\hat{J}_z |j_1, j_2, m_1, m_2\rangle = \hbar(m_1+m_2) |j_1, j_2, m_1, m_2\rangle$$

So we expect the M eigenvalue to be given by

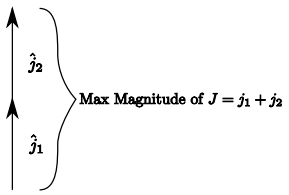
$$M = -(j_1+j_2), -(j_1+j_2)+1, \ldots, +(j_1+j_2)$$

Remark 1: In general, there will be more than 1 state with the same M eigenvalue, but these states will have different J eigenvalues.

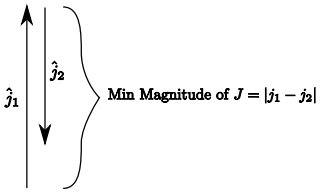
Remark 2: In order for us to get the allowed M values as $|M| \leq j_1 + j_2$, we need a $J = j_1 + j_2$ eigenvalue. This would give:

$$\begin{aligned} J: \quad & j_1 + j_2 \to M = -(j_1 + j_2), \ldots, +(j_1 + j_2) \\ & j_1 + j_2 - 1 \to M = -(j_1 + j_2) + 1, \ldots, (j_1 + j_2) - 1 \\ & j_1 + j_2 - 2 \to M = -(j_1 + j_2) + 2, \ldots, (j_1 + j_2) - 2 \\ & \vdots \end{aligned}$$

But where does the sequence terminate? We can determine this with vectors. If $\hat{\boldsymbol{j}}_{\mathbf{1}}$ and $\hat{\boldsymbol{j}}_{\mathbf{2}}$ can be represented as vectors (and they can), then the maximum angular momentum should be obtained when they are parallel:



The minimum occurs when they are anti-parallel:



Remark 3: We can now find the total number of $|j_1, j_2, J, M\rangle$ states. Without loss of generality, let $j_1 > j_2$. Then

$$\#\text{ states } = \underbrace{[2(j_1 + j_2) + 1]}_{\substack{\text{Allowed M if} \\ J = j_1 + j_2}} + [2(j_1 + j_2 - 1) + 1] + \ldots + [2(j_1 - j_2 + 1) + 1] + [2(j_1 - j_2) + 1]$$

Many of these terms cancel, leaving only $(2j_1 + 1)$ in each term. Since there are $(2j_2 + 1)$ terms, the number of states is

$$\#\text{ states } = (2j_1 + 1)(2j_2 + 1)$$

which is the same number of states as we had in the $|j_1, j_2, m_1, m_2\rangle$ basis. So we have the correct number of J and M eigenvalues.

Remark 4: To summarize: for a fixed j_1 and j_2, the $(2j_1 + 1)(2j_2 + 1)$-dimensional space spanned by $|j_1, j_2, m_1, m_2\rangle$ has possible values of J given by $j_1 + j_2, j_1 + j_2 - 1, \ldots, |j_1 - j_2|$, and for each J, there are $(2J + 1)$ states $|J, M\rangle$ with different M values.

12.1.2 Example of Addition of Two S=$\frac{1}{2}$ States

Consider 2 particles with spin $\frac{1}{2}$. The individual eigenstates are:

$$\hat{\boldsymbol{S}}_{\mathbf{1}} = \left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle_1 \text{ and } \left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle_1 \Rightarrow |+\rangle_1 \text{ and } |-\rangle_1$$
$$\hat{\boldsymbol{S}}_{\mathbf{2}} = \left|\tfrac{1}{2},\tfrac{1}{2}\right\rangle_2 \text{ and } \left|\tfrac{1}{2},-\tfrac{1}{2}\right\rangle_2 \Rightarrow |+\rangle_2 \text{ and } |-\rangle_2$$

We define

$$\hat{\boldsymbol{S}} = \hat{\boldsymbol{S}}_{\mathbf{1}} + \hat{\boldsymbol{S}}_{\mathbf{2}}$$

and we denote the eigenstates of $\hat{S}^2$ and $\hat{S}_z$ by $|SM\rangle$.

Remark 1: For the 4 $|s_1, s_2, m_1, m_2\rangle$ states: $|+\rangle_1 |-\rangle_2 ; |+\rangle_1 |-\rangle_2 ; |-\rangle_1 |+\rangle_2 ; |-\rangle_1 |-\rangle_2$, there are 4 $|SM\rangle$ states:

$$S = 1 \Rightarrow |1,-1\rangle, |1,0\rangle, |1,1\rangle$$
$$S = 0 \Rightarrow |0,0\rangle$$

The state with $S = 1$ is called a triplet and the state with $S = 0$ is called the singlet.

We now want to express the $|SM\rangle$ states in terms of the $|s_1, s_2, m_1, m_2\rangle$ states. Note that there is only 1 state in each set with $M = m_1 + m_2 = 1$ and one state with $M = m_1 + m_2 = -1$. So we can write:

$$|1,1\rangle = |+\rangle_1 |+\rangle_2$$
$$|1,-1\rangle = |-\rangle_1 |-\rangle_2$$

We can find the other $S = 1$ states by using the lowering operator:

$$\begin{aligned} |1,0\rangle &= \frac{1}{\sqrt{2}} \hat{S}_- |1,1\rangle \\ &= \frac{1}{\sqrt{2}} \left(\hat{S}_{1-} + \hat{S}_{2-}\right) |+\rangle_1 |+\rangle_2 \\ &= \frac{1}{\sqrt{2}} \left(|-\rangle_1 |+\rangle_2 + |+\rangle_1 |-\rangle_2\right) \end{aligned}$$

For the state corresponding to $S = 0$, we must have a linear combination of $|+\rangle_1 |-\rangle_2, |-\rangle_1 |+\rangle_2$ which is orthogonal to the other states:

$$\Rightarrow |0,0\rangle = \frac{1}{\sqrt{2}} \left(|+\rangle_1 |-\rangle_2 - |-\rangle_1 |+\rangle_2\right)$$

Remark 2: In the $|s_1, s_2, m_1, m_2\rangle$ basis, we have a tensor product of $\frac{1}{2} \otimes \frac{1}{2}$, which is equivalent to $1 \oplus 0$ in the $|SM\rangle$ basis. In other words,

$$\frac{1}{2} \otimes \frac{1}{2} \Rightarrow (2s_1 + 1)(2s_2 + 1) = (\tfrac{2}{2} + 1)(\tfrac{2}{2} + 1) = 4$$
$$1 \oplus 0 \Rightarrow \sum_{S=0}^{1} (2S + 1) = 1 + 3 = 4$$

which must be equal.

12.2 Two Nucleon System

Let's consider a system of 2 nucleons each with spin $\frac{1}{2}$, but with the addition of orbital angular momentum. Only the angular momentum of the relative motion is relevant, so the total angular momentum is given by:

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}_{\boldsymbol{1}} + \hat{\boldsymbol{S}}_{\boldsymbol{2}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}$$

where $\hat{\boldsymbol{S}} = \hat{\boldsymbol{S}}_{\boldsymbol{1}} + \hat{\boldsymbol{S}}_{\boldsymbol{2}}$ is the total spin of the system and $\hat{\boldsymbol{L}}$ is the total angular momentum of relative motion. We then have

$$|L, S, M_L, M_S\rangle = |L, M_L\rangle \otimes |S, M_S\rangle = |L, M_L\rangle\,|S, M_S\rangle$$

with

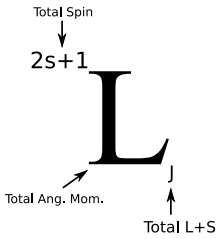
$$\begin{array}{ll} L = 0, 1, 2, \ldots & M_L = -L, \ldots, L \\ S = 1 & M_S = -1, 0, 1 \\ S = 0 & M_S = 0 \end{array}$$

Giving the allowed $\hat{\boldsymbol{J}}$ values of

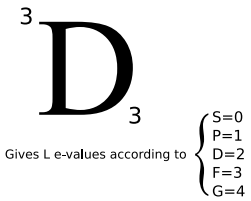
$$\text{For } S = 1 \Rightarrow \hat{J} = \begin{cases} L + 1, L, L - 1 & L \geq 1 \\ 1 & L = 0 \end{cases}$$
$$S = 0 \Rightarrow \hat{J} = L$$

The states of total angular momentum are given by $|L, S, J, M\rangle$.

Remark 1: The quantum numbers L, S, J are related to spectroscopic language:



(a) General Form



(b) Specific Instance

12.3 Clebsch-Gordan Coefficients

In §12.1, we noted that for a given j_1, j_2 we needed to find the allowed values of J, M (done in §12.1.1) and an expression for $|j_1, j_2, J, M\rangle$ in terms of $|j_1, j_2, m_1, m_2\rangle$ (done as an example of 2 spin $\frac{1}{2}$ particles). We now wish to come up with a general scheme for expressing the eigenstates of j_1, j_2, J, M. Formally, we can write:

$$|j_1, j_2, J, M\rangle = \sum_{m_1, m_2} \underbrace{\langle j_1, j_2, m_1, m_2 | j_1, j_2, J, M\rangle}_{\text{Clebsch-Gordan Coefficients}} |j_1, j_2, m_1, m_2\rangle$$

Remark 1: The Clebsch-Gordan coefficients depend only on the angular momentum quantum numbers, *not* on the specific details of a physical system. Thus they can be calculated from the addition of angular momentum in general (without repeating for each physical application).

Remark 2: In practive, extensive tables of these coefficients are available.

Remark 3: To simplify notation, let

$$\langle j_1, j_2, m_1, m_2 | j_1, j_2, J, M\rangle = \langle j_1, j_2, m_1, m_2 | J, M\rangle$$

Remark 4: We already have some of the Clebsch-Gordan coefficients from previous examples:

$$\text{From §1.2 } \Rightarrow |0,0\rangle = \frac{1}{\sqrt{2}} |+\rangle_1 |-\rangle_2 - \frac{1}{\sqrt{2}} |-\rangle_1 |+\rangle_2$$

$$\Rightarrow \left\langle \tfrac{1}{2}\tfrac{1}{2} m_1 m_2 \middle| 00 \right\rangle = \begin{cases} \frac{1}{\sqrt{2}} & m_1 = \frac{1}{2}, m_2 = -\frac{1}{2} \\ -\frac{1}{\sqrt{2}} & m_1 = -\frac{1}{2}, m_2 = \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$

Similarly,

$$\left\langle \tfrac{1}{2}\tfrac{1}{2} m_1 m_2 \middle| 11 \right\rangle = \begin{cases} 1 & m_1 = m_2 = \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$

$$\left\langle \tfrac{1}{2}\tfrac{1}{2} m_1 m_2 \middle| 1,-1 \right\rangle = \begin{cases} 1 & m_1 = m_2 = -\frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$

$$\left\langle \tfrac{1}{2}\tfrac{1}{2} m_1 m_2 \middle| 10 \right\rangle = \begin{cases} \frac{1}{\sqrt{2}} & m_1 = \frac{1}{2}, m_2 = -\frac{1}{2} \\ \frac{1}{\sqrt{2}} & m_1 = -\frac{1}{2}, m_2 = \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$

Remark 5: Note that there can be an ambiguity in the overall phase (minus sign) of the states $|JM\rangle$. This is fixed by convention.

Remark 6: General properties of Clebsch-Gordan coefficients:

1. $\langle j_1 j_2 m_1 m_2 | JM\rangle = 0$ *unless* $M = m_1 + m_2$ and $j_1 + j_2 \leq J \leq |j_1 - j_2|$.
2. They are real.
3. The convention for sign is that
$$\langle j_1 j_2 j_1, J - j_1 | JM\rangle > 0$$
where $m_1 = j_1$ and $m_2 = J - j_1$.
4. The equation
$$\langle j_1 j_2 m_1 m_2 | JM\rangle = (-1)^{j_1 + j_2 - J} \langle j_1 j_2, -m_1, m_2 | J, -M\rangle$$
gives the coefficients of $-M$ in terms of M.
5. Starting at the bottom (top) state and applying $\hat{J}_+$ ($\hat{J}_-$) gives recurrence relations between successive coefficients:
$$\begin{aligned}\sqrt{J(J+1) - M(M+1)}\, \langle j_1 j_2 m_1 m_2 | J, M+1\rangle = \\ \sqrt{j_1(j_1+1) - m_1(m_1-1)}\, \langle j_1 j_2, m_1 - 1, m_2 | JM\rangle \\ + \sqrt{j_2(j_2+1) - m_2(m_2-1)}\, \langle j_1 j_2 m_1, m_2 - 1 | JM\rangle\end{aligned}$$
and
$$\begin{aligned}\sqrt{J(J+1) - M(M-1)}\, \langle j_1 j_2 m_1 m_2 | J, M-1\rangle = \\ \sqrt{j_1(j_1+1) - m_1(m_1+1)}\, \langle j_1 j_2, m_1 + 1, m_2 | JM\rangle \\ + \sqrt{j_2(j_2+1) - m_2(m_2+1)}\, \langle j_1 j_2 m_1, m_2 + 1 | JM\rangle\end{aligned}$$

Remark 7: The transformation from the $|j_1 j_2 m_1 m_2\rangle$ basis to the $|j_1 j_2 JM\rangle$ basis is an example of a unitary transformation between 2 orthonormal basis. Thus, for $j_1 j_2$:
$$\underbrace{U}_{\text{matrix elem.}} \equiv \left\langle j_1 j_2 \ \underbrace{m_1 m_2}_{\text{col. index}} \middle| \underbrace{JM}_{\text{row index}} \right\rangle$$
such that
$$UU^\dagger = U^\dagger U = I$$
$$\Rightarrow \sum_{JM} \langle j_1 j_2 m_1 m_2 | JM\rangle \left\langle JM \middle| j_1' j_2' m_1' m_2' \right\rangle = \delta_{m_1, m_1'} \delta_{m_2, m_2'}$$
and
$$\sum_{m_1 m_2} \langle JM | j_1 j_2 m_1 m_2\rangle \left\langle j_1 j_2 m_1 m_2 \middle| J'M' \right\rangle = \delta_{J,J'} \delta_{M,M'}$$

12.4 Irreducable Tensor Operators

12.4.1 Irreducable Invariant Subspaces

Consider a state $|\lambda, j, m\rangle$ such that

$$\hat{J}^2 |\lambda, j, j\rangle = \hbar j(j+1) |\lambda, j, j\rangle$$
$$\hat{J}_z |\lambda, j, j\rangle = \hbar j |\lambda, j, j\rangle$$

and the $(2j+1)$ orthonormal states obtained by §11.1:

$$|\lambda, j, m\rangle = \sqrt{\frac{(j+m)!}{(2j)!(j-m)!}} \hat{J}_-^{j-m} |\lambda, j, j\rangle$$

which span the subspace of Hilbert space having eigenvalues of $\hat{J}^2$ and degeneracy index λ. Let $\xi^{(J)}$ denote this subspace. Rotations involve only operators $\hat{J}_x, \hat{J}_y, \hat{J}_z$ (or, alternatively, $\hat{J}_+, \hat{J}_-, \hat{J}_z$), so that a state that is initially in $\xi^{(J)}$ is rotated into another state in $\xi^{(J)}$. We say that $\xi^{(J)}$ is invariant under rotations.

Remark 1: Consider a state $|\psi\rangle$ in $\xi^{(J)}$. All possible rotations of $|\psi\rangle$ will span the entire $\xi^{(J)}$. Because of this property, we say that $\xi^{(J)}$ is irreducible under rotations.

Remark 2: These rotations can be represented in standard representation by a matrix:

$$\underbrace{\mathbb{R}^{(J)}_{MM'}(\alpha, \beta, \gamma)}_{\substack{(2J+1)\times(2J+1) \\ \text{matrix}}} = \left\langle \lambda, J, M \middle| \hat{R}(\alpha, \beta, \gamma) \middle| \lambda, J, M' \right\rangle$$

The $\mathbb{R}^{(J)}_{MM'}$ are called rotation matrices and represent rotations in Hilbert space. The rotated basis vectors $\hat{R} |\lambda, J, M\rangle$ can be expressed in terms of the non-rotated basis using these rotation matrices:

$$\begin{aligned} \hat{R} |\lambda, J, M\rangle &= \sum_{M'} |\lambda, J, M'\rangle \left\langle \lambda, J, M' \middle| \hat{R} \middle| \lambda, J, M \right\rangle \\ &= \sum_{M'} \mathbb{R}^{(J)}_{MM'} |\lambda, J, M'\rangle \end{aligned}$$

12.4.2 Irreducable Tensors

Scalars, vectors, and tensors are distinguished by their transformation properties. For instance, consider transformations under rotations:

Scalar: $S \to S' = U^\dagger S U = s U^\dagger U = S$

So scalars are invariant under rotations

Vector: $v_i \to v_i' = U^\dagger v_i U = R_{ij} v^j$

and, equivalently,

$v_i \to v_i' = U v_i U^\dagger = R_{ij} v^j$

since $\hat{U}[R] \to \hat{U}[R^{-1}] = \hat{U}^\dagger[R]$

Definition 1: A rank k tensor operator is a collection of (2k+1) operators denoted $T_q^{(k)}, q = -k, -k+1, \ldots, k$ that transform according to:

$$\hat{T}_q^{(k)} \to \hat{U} \hat{T}_q^{(k)} \hat{U}^\dagger = \hat{T}_{q'} R^{q'q} \qquad (\dagger)$$

Remark 1: These tensor operators are irreducible under rotations.

Remark 2: Equation (†) represents a transformation of a group ("basis") of operators. The equivalent and more familiar case is a transformation of states:

$$\hat{R} \left| k, q \right\rangle = \sum_{q'} \left| k, q' \right\rangle \underbrace{R^{(k)}_{q'q}}_{\left\langle kq' \middle| \hat{R} \middle| kq \right\rangle}$$

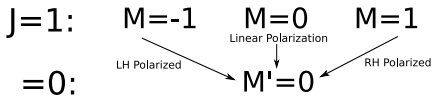
12.4.3 Wigner-Eckart Theorem

This theorem is widely used in atomi and nuclear physics and is used to calculate matrix elements for evaluating transition rates between states. It says that the matrix elements in a standard representation of the q^{th} component in a k^{th} order irreducible tensor operator is given by:

$$\left\langle \lambda J M \middle| T_q^{(k)} \middle| \lambda' j' M' \right\rangle = \underbrace{\frac{1}{\sqrt{2J+1}}}_{\substack{\text{unimportant} \\ \text{conversion} \\ \text{factor}}} \underbrace{\left\langle \lambda J \middle| \middle| T^{(k)} \middle| \middle| \lambda' J' \right\rangle}_{\text{reduced matrix element}} \underbrace{\left\langle J' k M_q \middle| J M \right\rangle}_{\text{CG-coefficient}}$$

Remark 1: The Wigner-Eckart Theorem does not tell us what the reduced matrix element is – this depends on the particular tensor operator under consideration.

The value lies in the way the q, M, M' quantum numbers are extracted in the Clebsch-Gordan coefficients. For example, in atomic physics, the M, M' quantum numbers for the initial and final states in a radiative transition are connected with the polarization of the emitted photon. In this example, the



Wigner-Eckart theorem tells us the ratios of radiative decay rates for different polarizations. These ratios are given by ratios of the squares of the Clebsch-Gordan coefficients.

Remark 2: The Clebsch-Gordan coefficients $\langle J'kM'q|JM\rangle$ give the angular momentum selection rules:

$$q = M - M'$$

$$\left|J - J'\right| \leq k \leq J + J'$$

Chapter 13

Perturbation Theory

Most QM problem can not be solved exactly, thus approximations are an important part of the actual applications. Perturbation theory is one of the main approximation techniques used. The idea is to approximate eigenvalues and eigenstates of a Hamiltonian which differs slightly from a Hamiltonian whose eigenvalues and eigenstates are known exactly.

13.1 Perturbation Theory for a Non-Degenerate, Discrete, Energy Level

Consider the Hamiltonian:

$$\hat{H} = \hat{H}_0 + \lambda \hat{V}$$

where $\hat{H}_0$ is a Hamiltonian whose eigenvalues and eigenstates $E_n^{(0)}, \left|n^{(0)}\right\rangle$ are known. So

$$\hat{H}_0 \left|n^{(0)}\right\rangle = E_n^{(0)} \left|n^{(0)}\right\rangle$$

For now we consider *only* the case where the states are discrete and non-degenerate. $\lambda\hat{V}$ is a perturbation with λ the size of the perturbation and $\hat{V}$ has the same "size" as $\hat{H}_0$. The eigenvalues and eigenstates of the full Hamiltonian are given by:

$$\hat{H}_n \left|n\right\rangle = E_n \left|n\right\rangle \tag{†}$$

where we write

$$\left.\begin{aligned} E_n &= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots \\ |n\rangle &= |n\rangle + \lambda \left|n^{(1)}\right\rangle + \lambda^2 \left|n^{(2)}\right\rangle + \cdots \end{aligned}\right\} \tag{‡}$$

So that

$$\lim_{\lambda\to 0} E_n = E_n^{(0)} \qquad \text{and} \qquad \lim_{\lambda\to 0} |n\rangle = \left|n^{(0)}\right\rangle$$

Substituting (‡) into (†) gives:

$$\begin{aligned} &\left(\hat{H}_0 + \lambda\hat{V}\right)\left(\left|n^{(0)}\right\rangle + \lambda\left|n^{(1)}\right\rangle \lambda^2 \left|n^{(2)}\right\rangle + \cdots\right) = \\ &\quad = \left(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots\right)\left(\left|n^{(0)}\right\rangle + \lambda\left|n^{(1)}\right\rangle \lambda^2 \left|n^{(2)}\right\rangle + \cdots\right) \end{aligned}$$

Now, equating power of λ on both sides:

$$\hat{H}_0 \left|n^{(k)}\right\rangle + \hat{V}\left|n^{(k-1)}\right\rangle = E_n^{(0)}\left|n^{(k)}\right\rangle + E_n^{(1)}\left|n^{(k-1)}\right\rangle + \cdots + E_n^{(k)}\left|n^{(0)}\right\rangle$$

or

$$\begin{cases} \left(\hat{H}_0 - E_n^{(0)}\right)\left|n^{(1)}\right\rangle = -\left(\hat{V} - E_n^{(1)}\right)\left|n^{(0)}\right\rangle, & k = 1 \\ \left(\hat{H}_0 - E_n^{(0)}\right)\left|n^{(k)}\right\rangle = -\left(\hat{V} - E_n^{(1)}\right)\left|n^{(k-1)}\right\rangle + \sum_{j=2}^{k} E_n^{(j)}\left|n^{(k-j)}\right\rangle, & k \geq 2 \end{cases}$$

where terms with superscripts (k) refer to the kth order term in the perturbative expansion.

13.1.1 First Order Approximation

Consider $k = 1$. Then we can apply $\left\langle n^{(0)}\right|$ to

$$\left(\hat{H}_0 - E_n^{(0)}\right)\left|n^{(1)}\right\rangle = -\left(\hat{V} - E_n^{(1)}\right)\left|n^{(0)}\right\rangle \tag{††}$$

$$\Rightarrow \underbrace{\left\langle n^{(0)}\right|\left(\hat{H}_0\right.}_{E_n^{(0)}} \left. - E_n^{(0)}\right)\left|n^{(1)}\right\rangle = -\left\langle n^{(0)}\right|\left(\hat{V} - E_n^{(1)}\right)\left|n^{(0)}\right\rangle$$

$$0 = -\left\langle n^{(0)}\right|\hat{V}\left|n^{(0)}\right\rangle + E_n^{(1)}$$

$$\Rightarrow E_n^{(1)} = \left\langle n^{(0)}\right|\hat{V}\left|n^{(0)}\right\rangle$$

Thus the first order correction to the energy is just the expectation of the perturbation taken with respect to the unperturbed state. To get the 1st order correction to the eigenstate, we must expand $\left|n^{(1)}\right\rangle$ in the basis of the unperturbed state:

$$n^{(1)} = \sum_m \left\langle m^{(0)}\right|\left.n^{(1)}\right\rangle\left|m^{(0)}\right\rangle$$

where m is the unperturbed state. To find the coefficients, we will apply $\left\langle m^{(0)}\right|$ to (††):

$$\underbrace{\left\langle m^{(0)}\right|\left(\hat{H}_0\right.}_{E_m^{(0)}} \left. - E_n^{(0)}\right)\left\langle n^{(1)}\right| = -\left\langle m^{(0)}\right|\left(\hat{V} - \underbrace{E_n^{(1)}}_{0}\right)\left|n^{(0)}\right\rangle$$

$$\Rightarrow \left\langle m^{(0)}\right|\left.n^{(1)}\right\rangle = -\frac{\left\langle m^{(0)}\right|\hat{V}\left|n^{(0)}\right\rangle}{E_m^{(0)} - E_n^{(0)}}$$

where the $E_n^{(1)}$ term goes to zero since we are considering when $m \neq n$ and thus $\left\langle m^{(0)}\right|\left.n^{(0)}\right\rangle = 0$.

Remark 1: At this point, it becomes important that we are considering a non-degenerate state since this trick will not work if $E_m^{(0)} = E_n^{(0)}$ for $m \neq n$.

Remark 2: In the expansion of $\left|n^{(1)}\right\rangle$ in terms of $\left|m^{(0)}\right\rangle$, there will be a coefficient corresponding to $n = m$ which appears to yield a diverging coefficient. To fix this, we set

$$\left\langle n^{(1)} \middle| n^{(0)} \right\rangle = 0$$

We can justify this by considering

$$|n\rangle = \left|n^{(0)}\right\rangle + \lambda \left|n^{(1)}\right\rangle + \lambda^2 \left|n^{(2)}\right\rangle + \cdots$$

If $\left|n^{(k)}\right\rangle$ has an $\left|n^{(0)}\right\rangle$ term in its expansion, then

$$\left|n^{(k)}\right\rangle = \left\langle n^{(0)} \middle| n^{(k)} \right\rangle \left|n^{(0)}\right\rangle + \left|n^{(k)}\right\rangle'$$

where the last term is an expansion of $\left|n^{(k)}\right\rangle$ in terms of $\left|m^{(0)}\right\rangle$ with $m \neq n$. Thus we have

$$\begin{aligned} |n\rangle &= \left|n^{(0)}\right\rangle \underbrace{\left(1 + \sum_{k=1}^{\infty} \lambda^k \left\langle n^{(0)} \middle| n^{(k)} \right\rangle\right)}_{\text{all n=m terms here}} + \underbrace{\lambda \left|n^{(1)}\right\rangle' + \lambda^2 \left|n^{(2)}\right\rangle' + \cdots}_{\text{expansions with } n \neq m} \\ &= \alpha \left|n^{(0)}\right\rangle + \lambda \left|n^{(1)}\right\rangle' + \lambda^2 \left|n^{(2)}\right\rangle' + \cdots \end{aligned}$$

where

$$\alpha = 1 + \sum_{k=1}^{\infty} \lambda^k \left\langle n^{(0)} \middle| n^{(k)} \right\rangle$$

is a scaling factor that can be absorbed into the length of $|n\rangle$. Dividing by α and letting $\frac{1}{\alpha}|n\rangle \to |n\rangle$ and $\left|n^{(k)}\right\rangle'' = \frac{1}{\alpha}\left|n^{(k)}\right\rangle'$ gives:

$$|n\rangle = \left|n^{(0)}\right\rangle + \lambda \left|n^{(1)}\right\rangle'' + \lambda^2 \left|n^{(2)}\right\rangle'' + \cdots$$

which is the expansion of $|n\rangle$ with states $\left|n^{(k)}\right\rangle''$ having no projection onto the state $\left|n^{(0)}\right\rangle$. This is equivalent to writing

$$|n\rangle = \left|n^{(0)}\right\rangle + \lambda \left|n^{(1)}\right\rangle + \lambda^2 \left|n^{(2)}\right\rangle + \cdots$$

and setting

$$\left\langle n^{(0)} \middle| n^{(k)} \right\rangle = 0, \qquad \forall k = 1, 2, 3, \ldots$$

Remark 3: The procedure used to obtain the first order correction in eigenvalues and eigenstates can be applied successively to get higher order corrections in terms of previous determined corrections of lower orders. Taking terms λ^k with $k \geq 2$ implies:

$$\left(\hat{H}_0 - E_n^{(0)}\right)\left|n^{(k)}\right\rangle = -\left(\hat{V} - E_n^{(1)}\right)\left|n^{(k-1)}\right\rangle + \sum_{j=2}^{k} E_n^{(j)}\left|n^{(k-j)}\right\rangle$$

on which we apply $\left\langle n^{(0)}\right|$ to get

$$\begin{aligned} 0 &= -\left\langle n^{(0)}\right|\left(\hat{V} - \underbrace{E_n^{(1)}}_{0}\right)\left|n^{(k-1)}\right\rangle + \sum_{j=2}^{k} E_n^{(j)}\left\langle n^{(0)}\middle|n^{(k-j)}\right\rangle \\ &= -\left\langle n^{(0)}\middle|\hat{V}\middle|n^{(k-1)}\right\rangle + \left(E_n^{(k)} + \sum_{i=1}^{k-2} E_n^{(k-i)}\underbrace{\left\langle n^{(0)}\middle|n^{(1)}\right\rangle}_{0}\right) \\ \Rightarrow E_n^{(k)} &= \left\langle n^{(0)}\middle|\hat{V}\middle|n^{(k-1)}\right\rangle \end{aligned}$$

Now, applying $\left\langle m^{(0)}\right|$ to terms $\mathcal{O}(\lambda^k)$ implies

$$\left\langle m^{(0)}\middle|\left(\hat{H}_0 - E_n^{(0)}\right)\middle|n^{(k)}\right\rangle = -\left\langle m^{(0)}\middle|\left(\hat{V} - E_n^{(1)}\right)\middle|n^{(k-1)}\right\rangle + \sum_{j=2}^{k} E_n^{(j)}\left\langle m^{(0)}\middle|n^{(k-j)}\right\rangle$$

$$\left\langle m^{(0)}\middle|n^{(k)}\right\rangle = \frac{1}{\left(E_m^{(0)} - E_n^{(0)}\right)}\left(-\left\langle m^{(0)}\middle|\left(\hat{V} - E_n^{(1)}\right)\middle|n^{(k-1)}\right\rangle + \underbrace{\sum_{j=2}^{k-1} E_n^{(j)}\left\langle m^{(0)}\middle|n^{(k-j)}\right\rangle}_{\text{to } k-1 \text{ since } \left\langle m^{(0)}|n^{(0)}\right\rangle = 0}\right)$$

which are coefficients for the expansion

$$\left|n^{(k)}\right\rangle = \sum_m \left\langle m^{(0)}\middle|n^{(k)}\right\rangle\left|m^{(0)}\right\rangle$$

13.1.2 Example: Harmonic Oscillator in an Electric Field

Consider a particle of charge q and mass m in a harmonic oscillator potential and corresponding to an unperturbed Hamiltonian:

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

Applying an electric field with magnitude f along the $+x$ direction corresponds to an electrostatic potential $\Phi = -fx$ and potential energy

$$\hat{V} = -qf\hat{x}$$

The full Hamiltonian then is

$$\hat{H} = \hat{H}_0 + \lambda\hat{V}$$

where λ is the strength of the perturbation. The first order correction to the energy is given by

$$\begin{aligned} E_n^{(1)} &= \left\langle n^{(0)} \middle| \hat{V} \middle| n^{(0)} \right\rangle \\ &= -qf \left\langle n^{(0)} \middle| \hat{x} \middle| n^{(0)} \right\rangle \\ &= -qf \left(\frac{\hbar}{2m\omega}\right)^{1/2} \left\langle n^{(0)} \middle| \hat{a}^\dagger + \hat{a} \middle| n^{(0)} \right\rangle \end{aligned}$$

Remark 1: Physically, the average interaction of the particle in the electric field is 0 since the particle's unperturbed wavefunction is a H.O.

$$\rightarrow E_n^{(1)} = -qf \int \left(\psi_n^{(0)}\right)^* x \left(\psi_n^{(0)}\right) dx = -qf \int_{-\infty}^{\infty} \underbrace{\left|\psi_n^{(0)}\right|^2}_{\text{even}} \underbrace{x}_{\text{odd}} dx = 0$$

The first order correction to the eigenstate is:

$$\begin{aligned} \left\langle m^{(0)} \middle| n^{(1)} \right\rangle &= -\frac{\left\langle m^{(0)} \middle| (-qf\hat{x}) \middle| n^{(0)} \right\rangle}{E_m^{(0)} - E_n^{(0)}} \\ &= qf \left(\frac{\hbar}{2m\omega}\right)^{1/2} \frac{\left\langle m^{(0)} \middle| \hat{a} + \hat{a}^\dagger \middle| n^{(0)} \right\rangle}{E_m^{(0)} - E_n^{(0)}} \\ &= \frac{qf\sqrt{\frac{\hbar}{2m\omega}}}{E_m^{(0)} - E_n^{(0)}} \left(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right) \end{aligned}$$

$$\begin{aligned} \Rightarrow \left|n^{(1)}\right\rangle &= qf\sqrt{\frac{\hbar}{2m\omega}} \sum_m \frac{1}{E_m^{(0)} - E_n^{(0)}} \left(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}\right) \left|m^{(0)}\right\rangle \\ &= qf\sqrt{\frac{\hbar}{2m\omega}} \left(\frac{\sqrt{n}\left|(n-1)^{(0)}\right\rangle}{\underbrace{E_{n-1}^{(0)} - E_n^{(0)}}_{-h\omega}} + \frac{\sqrt{n+}\left|(n+1)^{(0)}\right\rangle}{\underbrace{E_{n+1}^{(0)} - E_n^{(0)}}_{h\omega}} \right) \\ &= qf\sqrt{\frac{1}{2m\hbar\omega^3}} \left(\sqrt{n+1}\left|(n+1)^{(0)}\right\rangle - \sqrt{n}\left|(n-1)^{(0)}\right\rangle\right) \end{aligned}$$

So, to first order, our eigenstate is:

$$\begin{aligned}|n\rangle &= \left|n^{(0)}\right\rangle + \lambda\left|n^{(1)}\right\rangle \\ &= \left|n^{(0)}\right\rangle + \lambda qf\sqrt{\frac{1}{2m\hbar\omega^3}}\left(\sqrt{n+1}\left|(n+1)^{(0)}\right\rangle - \sqrt{n}\left|(n-1)^{(0)}\right\rangle\right)\end{aligned}$$

Since the first order energy correction was 0, let's calculate the 2nd order correction:

$$\begin{aligned}E_n^{(2)} &= \left\langle n^{(0)}\middle|\hat{V}\middle|n^{(1)}\right\rangle \\ &= -qf\left\langle n^{(0)}\middle|\hat{x}\middle|n^{(1)}\right\rangle \\ &= -qf\sqrt{\frac{\hbar}{2m\omega}}\left\langle n^{(0)}\middle|\hat{a}+\hat{a}^\dagger\middle|n^{(1)}\right\rangle \\ &= -(qf)^2\frac{1}{2m\omega^2}\left\langle n^{(0)}\middle|\hat{a}+\hat{a}^\dagger\middle|\left(\sqrt{n+1}\left|(n+1)^{(0)}\right\rangle - \sqrt{n}\left|(n-1)^{(0)}\right\rangle\right)\right\rangle \\ &= -\frac{(qf)^2}{2m\omega^2}\left\langle n^{(0)}\right|\left[(n+1)\left|n^{(0)}\right\rangle - \sqrt{n}\sqrt{n-1}\left|(n-2)^{(0)}\right\rangle + \sqrt{n+1}\sqrt{n+1}\left|(n+2)^{(0)}\right\rangle - n\left|n^{(0)}\right\rangle\right] \\ &= -\frac{(qf)^2}{2m\omega^2}(n+1-n) \\ &= -\frac{(qf)^2}{2m\omega^2}\end{aligned}$$

Remark 2: This is a problem that can be solved exactly, which makes it a nice test for perturbation theory. Consider:

$$\begin{aligned}\hat{H} &= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - \lambda qf\hat{x} \\ &= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\underbrace{\left(\hat{x} - \frac{\lambda qf}{m\omega^2}\right)^2}_{\text{shifted H.O.}} - \underbrace{\frac{1}{2}\frac{q^2f^2\lambda^2}{m\omega^2}}_{\substack{\text{const. potential that} \\ \text{we don't care about}}}\end{aligned}$$

resulting in energy eigenvalues given by

$$E_n = E_n^{(0)} - \underbrace{\frac{q^2f^2\lambda^2}{2m\omega^2}}_{\text{energy shift}} = E_n^{(0)} + \underbrace{\lambda E_n^{(1)}}_{0} + \lambda^2 E_n^{(2)}$$

and eigenstates of the H.O. with oscillator displaced by:

$$Q = \frac{\lambda qf}{m\omega^2} = \lambda x\sqrt{\frac{2\hbar}{m\omega}} \Rightarrow x = \frac{qf}{m\omega^2}\sqrt{\frac{m\omega}{2\hbar}} = \frac{qf}{\sqrt{2m\hbar m\omega^2}}$$

$$|n\rangle + D(\lambda x)\left|n^{(0)}\right\rangle$$

where $D(\lambda x)$ is the displacement operator of §6.3.3.

$$D(\lambda x) = e^{\lambda x(\hat{a}^\dagger + \hat{a})} \approx 1 + \underbrace{\lambda x \left(\hat{a}^\dagger + \hat{a}\right)}_{\text{to 1st order}}$$

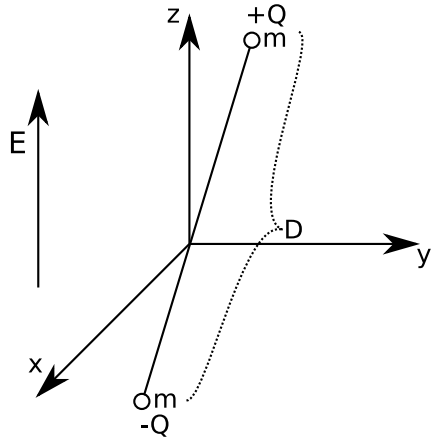
$$\Rightarrow |n\rangle = \left|n^{(0)}\right\rangle + \frac{\lambda q f}{\sqrt{2m\hbar\omega^3}} \left(\sqrt{n+1}\left|(n+1)^{(0)}\right\rangle - \sqrt{n}\left|(n-1)^{(0)}\right\rangle\right)$$

Here we note that computing higher order terms in the perturbation expansion is equivalent to taking higher order terms in the $D(\lambda x)$ expansion. Also, note that the energy eigenvalue is exact at 2nd order–computing higher order terms in E_n will give 0 contribution.

13.1.3 Example: Stark Effect

See Homework!

The picture is: Here we have that $\boldsymbol{L} \parallel \boldsymbol{\omega}$ and the rotation occurs in the plane defined



by the angles θ and ϕ relative to the Cartesian axis.

$$E = \frac{1}{2} I\omega^2 = \frac{1}{2}\frac{\hat{L}^2}{I} = \frac{1}{2}\frac{\left(\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2\right)}{I}$$

with

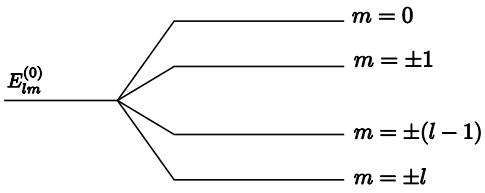
$$I = \frac{1}{2} m D^2$$

Hint:

$$\cos\theta Y_l^m = \left[\frac{(l+1+m)(l+1-m)}{(2l+1)(2l+3)}\right]^{1/2} Y_{l+1}^m + \left[\frac{(l+m)(l-m)}{(2l+1)(2l-1)}\right]^{1/2} Y_{l-1}^m$$

We will see that 2nd order perturbation removes the degeneracy in the unperturbed eigenvalue.

Note: a degeneracy remains with respect to the sign of m which physically corresponds to the configuration of a rigid rotor by invariance with respect to $\theta \to \pi - \theta$.



13.2 Degenerate Perturbation Theory

Now, consider the case where the unperturbed eigenstates are degenerate. Start with the simplest case of 2-fold degeneracy (higher order degeneracy is straight forward).

$$\left.\begin{aligned} \hat{H}_0 \left|n^{(0)}, 1\right\rangle &= E_n^{(0)} \left|n^{(0)}, 1\right\rangle \\ \hat{H}_0 \left|n^{(0)}, 2\right\rangle &= E_n^{(0)} \left|n^{(0)}, 2\right\rangle \end{aligned}\right\} \tag{1}$$

where the 1's and 2's and the degeneracy index. So eigenstates $\left|n^{(0)}, 1\right\rangle$ and $\left|n^{(0)}, 2\right\rangle$ (which are assumed to be orthonormal), give the same eigenvalue $E_n^{(0)}$. We expect the full solution to look like:

$$\left.\begin{aligned} \hat{H} \left|n, 1\right\rangle &= E_{n_1} \left|n, 1\right\rangle \\ \hat{H} \left|n, 2\right\rangle &= E_{n_2} \left|n, 2\right\rangle \end{aligned}\right\} \tag{2}$$

to give $E_n \to E_n^{(0)}$ as $\lambda \to 0$. Also, for now, assume that one eigenstate approaches $\left|n^{(0)}, 1\right\rangle$ and the other approaches $\left|n^{(0)}\right\rangle$. To simplify notation, lets let:

$$\left|n^{(k)}, j\right\rangle \equiv \left|k\right\rangle_j$$

with $j = 1, 2$ and $k =$ the order of perturbation. Then,

$$\left.\begin{aligned} E_{n_1} &= E_n^{(0)} + \lambda E_{n_1}^{(1)} + \cdots + \lambda^k E_{n_1}^{(k)} + \cdots \\ E_{n_2} &= E_n^{(0)} + \lambda E_{n_2}^{(1)} + \cdots + \lambda^k E_{n_2}^{(k)} + \cdots \end{aligned}\right\} \tag{3}$$

and

$$\left.\begin{aligned} \left|n, 1\right\rangle &= \left|0\right\rangle_1 + \lambda \left|1\right\rangle_1 + \cdots + \lambda^k \left|k\right\rangle_1 + \cdots \\ \left|n, 2\right\rangle &= \left|0\right\rangle_2 + \lambda \left|1\right\rangle_2 + \cdots + \lambda^k \left|k\right\rangle_2 + \cdots \end{aligned}\right\} \tag{4}$$

Now, substitute (3) and (4) into (2) to get the expansion in terms of powers of λ. As outlined in §13.1, the terms to 1st order in λ give:

$$\left.\begin{aligned} \left(\hat{H}_0 - E_n^{(0)}\right) \left|1\right\rangle_1 &= -\left(\hat{V} - E_{n_1}^{(0)}\right) \left|0\right\rangle_1 \\ \left(\hat{H}_0 - E_n^{(0)}\right) \left|1\right\rangle_2 &= -\left(\hat{V} - E_{n_2}^{(0)}\right) \left|0\right\rangle_2 \end{aligned}\right\} \tag{5}$$

Multiplying on the left by $\left\langle 0\right|_1$ gives:

$$0 = -{}_1\left\langle 0 \middle| \hat{V} \middle| 0 \right\rangle_1 + E_{n_1}^{(1)} \tag{6}$$

$$0 = -{}_1\left\langle 0 \middle| \hat{V} \middle| 0 \right\rangle_2 \tag{7}$$

While multiplying on the left by ${}_2\langle 0|$ gives:

$$0 = -\,{}_2\left\langle 0\middle|\hat{V}\middle|0\right\rangle_1 \tag{8}$$

$$0 = -\,{}_2\left\langle 0\middle|\hat{V}\middle|0\right\rangle_2 + E^{(1)}_{n_2} \tag{9}$$

Remark 1: This analysis is sufficient if equations (7) and (8) hold. In reality, however, they may not. In fact, if they do hold, this situation is identical to the non-degenerate results (as in the rigid rotor problem) and we've gained nothing. If (7) and (8) do not hold, then we have to do something new. In this case, what we've done must be incorrect since (7) and (8) would be contradictory. What went wrong above was the assumption that $|E_n, 1\rangle$ and $|E_n, 2\rangle$ approached specific $|0\rangle_1$ and $|0\rangle_2$ respectively as $\lambda \to 0$. In fact, the full eigenstates can hypothetically approach any mutually orthogonal linear combination of those states (since any linear combination of these states is also an eigenstate of $\hat{H}_0$). We must determine the linear combinations for the degenerate perturbed states.

Let us proceed without making any assumptions on the actual form of the unperturbed degenerate eigenstates, (let those be mutually orthogonal, normalized, linear combinations of the degenerate states), such that the expansions given by (4) still hold.

$$\left.\begin{aligned} |n,1\rangle &= |0\rangle_1 + \lambda\,|1\rangle_1 + \cdots + \lambda^k\,|k\rangle_1 + \cdots \\ |n,2\rangle &= |0\rangle_2 + \lambda\,|1\rangle_2 + \cdots + \lambda^k\,|k\rangle_2 + \cdots \end{aligned}\right\} \tag{4}$$

where $|0\rangle_1$ and $|0\rangle_2$ are now unknown states. Then the 1st order in the perturbation expansion still gives

$$\left.\begin{aligned} \left(\hat{H}_0 - E^{(0)}_n\right)|1\rangle_1 &= -\left(\hat{V} - E^{(0)}_{n_1}\right)|0\rangle_1 \\ \left(\hat{H}_0 - E^{(0)}_n\right)|1\rangle_2 &= -\left(\hat{V} - E^{(0)}_{n_2}\right)|0\rangle_2 \end{aligned}\right\} \tag{5}$$

where we multiply (5) by *any* $\left\langle n^{(0)}\right|$ for which (1) holds to get 0 on the left hand side. Formally, we can express this as:

$$\hat{P}\left(\hat{V} - E^{(1)}_{n_1}\right)|0\rangle_1 = 0 \tag{6'}$$

$$\hat{P}\left(\hat{V} - E^{(1)}_{n_2}\right)|0\rangle_2 = 0 \tag{7'}$$

where $\hat{P} = \left|n^{(0)},1\right\rangle\left\langle n^{(0)},1\right| + \left|n^{(0)},2\right\rangle\left\langle n^{(0)},2\right|$ is the projection onto the subspace of degenerate states. $\left|n^{(0)},1\right\rangle$ and $\left|n^{(0)},2\right\rangle$ form an orthonormal basis over this subspace. In practice, this calculation reduces to the diagonalization of a 2×2 matrix. To see this, let's let

$$|0\rangle_1 = \alpha\left|n^{(0)},1\right\rangle + \beta\left|n^{(0)},2\right\rangle \tag{8'}$$

where α, β are unknown. Then (6') gives

$$\left(\left|n^{(0)},1\right\rangle\left\langle n^{(0)},1\right| + \left|n^{(0)},2\right\rangle\left\langle n^{(0)},2\right|\right)\left(\hat{V} - E^{(1)}_{n_1}\right)\left(\alpha\left|n^{(0)},1\right\rangle + \beta\left|n^{(0)},2\right\rangle\right) = 0$$

$$\Rightarrow 0 = \left|n^{(0)},1\right\rangle \left[\left(\left\langle n^{(0)},1\right|\hat{V}\left|n^{(0)},1\right\rangle - E_{n_1}^{(1)}\right)\alpha + \left\langle n^{(0)},1\right|\hat{V}\left|n^{(0)},2\right\rangle \beta\right] + \\ + \left|n^{(0)},2\right\rangle \left[\left(\left\langle n^{(0)},2\right|\hat{V}\left|n^{(0)},2\right\rangle - E_{n_1}^{(1)}\right)\beta + \left\langle n^{(0)},2\right|\hat{V}\left|n^{(0)},1\right\rangle \alpha\right]$$

$$\Rightarrow \left(\left\langle n^{(0)},1\right|\hat{V}\left|n^{(0)},1\right\rangle - E_{n_1}^{(1)}\right)\alpha + \left\langle n^{(0)},1\right|\hat{V}\left|n^{(0)},2\right\rangle \beta = 0$$
$$\left(\left\langle n^{(0)},2\right|\hat{V}\left|n^{(0)},2\right\rangle - E_{n_1}^{(1)}\right)\beta + \left\langle n^{(0)},2\right|\hat{V}\left|n^{(0)},1\right\rangle \alpha = 0$$

$$\left[\begin{pmatrix} \left\langle n^{(0)},1\right|\hat{V}\left|n^{(0)},1\right\rangle & \left\langle n^{(0)},1\right|\hat{V}\left|n^{(0)},2\right\rangle \\ \left\langle n^{(0)},2\right|\hat{V}\left|n^{(0)},1\right\rangle & \left\langle n^{(0)},2\right|\hat{V}\left|n^{(0)},2\right\rangle \end{pmatrix} - E_n^{(1)}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\right]\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \begin{pmatrix}0\\ 0\end{pmatrix} \tag{9'}$$

which is the standard 2×2 matrix eigenvalue equation. Solving the eigenvalues, eigenvectors, and normalizing gives first order energy corrections, and the right linear combinations of the unperturbed degenerate ground states.

Remark 2: Solving the characteristic equation given by (9') can result in 1st order energy corrections ($E_{n_{1,2}}^{(1)}$) that are the same or distinct, depending on the roots of the quadratic equation. So, to first order, the degeneracy may or may not be lifted.

13.2.1 Example: Coupled Harmonic Oscillator

Consider 2 identical H.O.'s with frequency ω that are coupled by an interaction energy proportional to the product of oscillator displacements from equilibrium. The Hamiltonian is:

$$\hat{H} = \hat{H}_0 + \hat{V}$$

where

$$\hat{H}_0 = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \hat{b}^\dagger\hat{b}\right)$$

$$\hat{V} = \hbar g\left(\hat{a} + \hat{a}^\dagger\right)\left(\hat{b} + \hat{b}^\dagger\right)$$

and where $\hat{a}, \hat{a}^\dagger$ and $\hat{b}, \hat{b}^\dagger$ are annihilation and creation operators, and we drop 2 factors $\frac{1}{2}\hbar\omega$ in $\hat{H}_0$.
The unperturbed energy is

$$E_N = E_n + E_m = N\hbar\omega = (n+m)\hbar\omega$$

And the degeneracy arises because there is more than 1 way to break up the energy. All we require is that $N = n+m$ and the degeneracy increases with increasing energy. n and m are numbers of quanta in independent, uncoupled oscillators.

States	Degeneracy
$\|0,0\rangle$	none
$\|1,0\rangle, \|0,1\rangle$	2-fold
$\|0,2\rangle, \|1,1\rangle, \|2,0\rangle$	3-fold

Consider 1st order perturbation theory for the 1st excited state (2-fold degeneracy). In the limit $g \to 0$, the exact eigenstate goes to

$$\left|E^{(0)}_{N_{1,2}}\right\rangle = \alpha\,|0,1\rangle + \beta\,|1,0\rangle$$

The matrix elements required in (9') of the previous section are

$$\begin{aligned}
\left\langle 0,1\middle|\hbar g\left(\hat{a}+\hat{a}^\dagger\right)\left(\hat{b}+\hat{b}^\dagger\right)\middle|0,1\right\rangle &= 0\\
\left\langle 1,0\middle|\hbar g\left(\hat{a}+\hat{a}^\dagger\right)\left(\hat{b}+\hat{b}^\dagger\right)\middle|1,0\right\rangle &= 0\\
\left\langle 0,1\middle|\hbar g\left(\hat{a}+\hat{a}^\dagger\right)\left(\hat{b}+\hat{b}^\dagger\right)\middle|1,0\right\rangle &= \hbar g\\
\left\langle 1,0\middle|\hbar g\left(\hat{a}+\hat{a}^\dagger\right)\left(\hat{b}+\hat{b}^\dagger\right)\middle|0,1\right\rangle &= \hbar g
\end{aligned}$$

And (9') becomes

$$\begin{pmatrix} -E^{(1)}_{N_1} & \hbar g \\ \hbar g & -E^{(1)}_{N_2} \end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix}$$

Solving the characteristic equation gives

$$\left.\begin{aligned} E^{(1)}_{N_1} &= \hbar g\\ E^{(1)}_{N_2} &= -\hbar g\end{aligned}\right\} \tag{10}$$

And the ground state, unperturbed eigenstates follow:

$$\left.\begin{aligned} \left|E^{(1)}_{N_1}\right\rangle &= \frac{1}{\sqrt{2}}\left(|0,1\rangle + |1,0\rangle\right)\\ \left|E^{(1)}_{N_2}\right\rangle &= \frac{1}{\sqrt{2}}\left(|0,1\rangle - |1,0\rangle\right)\end{aligned}\right\} \tag{11}$$

Now we need 1st order corrections to the eigenstates

$$\begin{aligned}
\left|E^{(1)}_N,1\right\rangle &= \sum_{M\neq N}\left\langle E^{(0)}_M\middle|E^{(0)}_N,1\right\rangle\left|E^{(0)}_m\right\rangle\\
&= -\sum_{M\neq N}\frac{\left\langle E^{(0)}_M\middle|\hat{V}\middle|E^{(0)}_N,1\right\rangle}{E^{(0)}_M - E^{(0)}_{N_1}}\left|E^{(0)}_M\right\rangle
\end{aligned} \tag{12}$$

Remark 1: This is the same procedure used in non-degenerate perturbation theory, but the summation is more restrictive since $E^{(0)}_{N_1}$ and $E^{(0)}_{N_2}$ have no projection on the degenerate subspace.

Remark 2: An expression similar to (12) gives $\left|E^{(0)}_N,2\right\rangle$.

To get the 1st order correction to the eigenstates, calculate the matrix elements

$$\left\langle E_M^{(0)} \middle| \hat{V} \middle| E_N^{(0)}, (1 \text{ or } 2 \right\rangle$$

and specifically for the H.O.:

$$\underbrace{|n,m\rangle}_{\substack{\text{all unperturbed} \\ \text{states other than} \\ |1,0\rangle \text{ \& } |0,1\rangle}} \hbar g \left(\hat{a} + \hat{a}^\dagger\right)\left(\hat{b} + \hat{b}^\dagger\right)(|0,1\rangle \pm |1,0\rangle) = \langle n,m| \frac{\hbar g}{\sqrt{2}}\left[\sqrt{2}\,|1,2\rangle \pm \sqrt{2}\,|2,1\rangle\right]$$

$$\Rightarrow \quad \left.\begin{aligned} \langle 1,2| \frac{\hat{V}}{\sqrt{2}}(|0,1\rangle \pm |1,0\rangle) &= \hbar g \\ \langle 2,1| \frac{\hat{V}}{\sqrt{2}}(|0,1\rangle \pm |1,0\rangle) &= -\hbar g \end{aligned}\right\} \tag{13}$$

Remark 3: The states $|1,2\rangle$ and $|2,1\rangle$ both have energy $E_M^{(0)} = 3\hbar\omega$.

Plugging (13) into (12) gives:

$$\left|E_{N_1}^{(1)}\right\rangle = -\frac{\hbar g}{3\hbar\omega - \hbar\omega}|1,2\rangle - \frac{\hbar g}{3\hbar\omega - \hbar\omega} = -\frac{g}{2\omega}(|1,2\rangle + |2,1\rangle) \tag{14}$$

$$\left|E_{N_2}^{(1)}\right\rangle = -\frac{g}{2\omega}(|1,2\rangle - |2,1\rangle) \tag{15}$$

Remark 4: The interacting Hamiltonian in this example is often approximated by

$$\hat{V}_{RWA} = \hbar g\left(\hat{a}^\dagger\hat{b} + \hat{a}\hat{b}^\dagger\right)$$

This gives the 1st order corrections that are exact (no higher order approximations from $\hat{a}^\dagger\hat{b}, \hat{a}\hat{b}^\dagger$). This interaction is referred to as the rotating wave approximation.

Remark 5: In this case, the 1st order corrections lifted the degeneracy, and higher order corrections may proceed with non-degenerate perturbation theory. If degeneracy was *not* lifted at first order, we must diagonalize another matrix (use non-degenerate perturbation theory) again.

The second order corrections in energy for coupled H.O. are given by

$$\begin{aligned} E_{N_1}^{(2)} &= \left\langle E_N^{(0)}, 1 \middle| \hat{V} \middle| E_N^{(1)}, 1 \right\rangle \\ &= \frac{1}{\sqrt{2}}(|0,1\rangle + \langle 1,0|)\,\hbar g\left(\hat{a} + \hat{a}^\dagger\right)\left(\hat{b} + \hat{b}^\dagger\right)\left(\frac{-g}{2\omega}\right)(|1,2\rangle + |2,1\rangle) \\ &= -\frac{\hbar g^2}{\omega} \end{aligned}$$

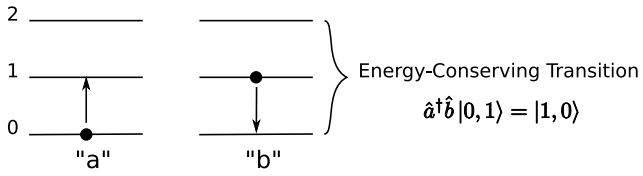
and

$$E_{N_2}^{(2)} = \left\langle E_N^{(0)}, 2 \middle| \hat{V} \middle| E_n^{(1)}, 2 \right\rangle$$
$$= -\frac{\hbar g^2}{\omega}$$

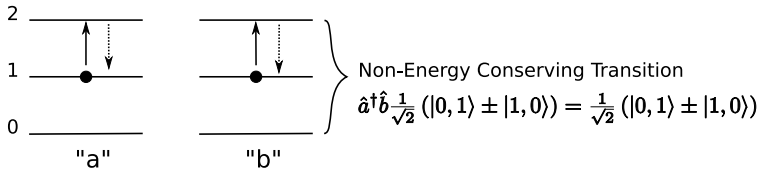
So, to second order, we have

$$E_{N_1} = \hbar\left(\omega + g - \frac{g^2}{\omega}\right)$$
$$E_{N_2} = \hbar\left(\omega - g - \frac{g^2}{\omega}\right)$$

Remark 6: Note that it was the non-rotating wave approximation part of the interaction that gives the second order corrections ($\hat{a}\hat{b}$ term). This is an example of a non-energy conserving, or virtual transition.



or



Only the intermediate step is non-conserving, overall, energy *is* conserved.

13.3 Time Dependent Perturbation Theory

For this analysis, we are going to consider the unitary propagator (aka time-evolution operator):

$$\hat{U}(t, t_0) = e^{-i\hat{H}(t-t_0)/\hbar} \tag{1}$$

which gives the solution to the Schrodinger equation:

$$|\psi(t)\rangle = \hat{U}(t, t_0)\,|\psi(t_0)\rangle \tag{2}$$

The propagator itself obeys the equation of motion.

$$\frac{\partial}{\partial t}\hat{U}(t, t_0) = \frac{1}{i\hbar}\hat{H}\hat{U}(t, t_0) \tag{3}$$

with the initial condition that $\hat{U}(t_0, t_0) = 1$. Formally integrating (3) gives

$$\hat{U}(t, t_0) = 1 + \frac{1}{i\hbar} \int_{t_0}^{t} \hat{H}\hat{U}(\tau, t_0)\, d\tau \tag{4}$$

Time dependent perturbation theory is based on (4). Our 1st goal is to rewrite (4) so that the dynamics generated by the unperturbed interacting part of the Hamiltonian are separate.

$$\hat{H}(t) = \hat{H}_0(t) + \hat{V}(t) \tag{5}$$

Here we are allowing $\hat{H}_0$ and $\hat{V}$ to explicitly depend on time.

Remark 1: We will use the interaction picture to separate the perturbed and unperturbed dynamics. Let $\hat{U}_0(t, t_0)$ represent the propagator which governs the unperturbed motion such that $\hat{U}_0(t, t_0)$ satisfies

$$\hat{U}(t, t_0) = \frac{1}{i\hbar}\hat{H}_0(t)\hat{U}_0(t, t_0) \tag{6}$$

with initial condition $\hat{U}_0(t_0, t_0) = 1$. Now, $\hat{U}_0(t, t_0)$ can be thought of as a "rotation" in Hilbert space. If we go into a reference frame that rotates at a rate determined by $\hat{U}_0(t, t_0)$, then the state only evolves in that frame if $\hat{V}(t) \neq 0$. In the case that $\hat{V}(t) \neq 0$, we are in the interaction picture.

Remark 2: Alternatively, a non-rotating frame in which the state evolves according to both $\hat{H}_0$ and $\hat{V}_0$ gives the usual Schrodinger picture, while a frame that rotates at a rote determined by *both* $\hat{H}_0$ and $\hat{V}_0$ (the state is stationary in this frame) gives the Heisenberg picture.

Remark 3: The states in the Schrodinger and interaction pictures are related by

$$\underbrace{|\psi_S(t)\rangle}_{\substack{\text{Schrodinger}\\ \text{picture}}} = \hat{U}_0(t, t_0) \underbrace{|\psi_I(t)\rangle}_{\substack{\text{Interaction}\\ \text{picture}}} \tag{7}$$

so that if $\hat{V}(t) = 0$, $|\psi_I(t)\rangle$ is stationary, and $|\psi_I(t)\rangle = |\psi_I(t_0)\rangle = |\psi_S(t_0)\rangle$. If $\hat{V}(t) \neq 0$, then the state in the interaction picture evolves according to

$$|\psi_I(t)\rangle = \hat{U}_I(t, t_0)\, |\psi_I(t_0)\rangle \tag{8}$$

where $\hat{U}_I(t, t_0)$ is the interaction picture evolution operator.

Remark 4: The evolution equation for $\hat{U}_I(t, t_0)$ can be obtained via (7) and (8):

$$\begin{aligned} |\psi_S(t)\rangle &= \hat{U}_0(t, t_0)\hat{U}_I(t, t_0)\, |\psi_I(t_0)\rangle \\ &= \hat{U}_0(t, t_0)\hat{U}_I(t, t_0)\, |\psi_S(t_0)\rangle \end{aligned} \tag{9}$$

Comparing to (2):

$$\Rightarrow \hat{U}_S(t, t_0) = \hat{U}_0(t, t_0)\hat{U}_I(t, t_0) \tag{10}$$

Substituting(10) and (5) into (3):

$$\frac{\partial}{\partial t}\left(\hat{U}_0\hat{U}_I\right) = \frac{1}{i\hbar}\left(\hat{H}_0+\hat{V}\right)\hat{U}_0\hat{U}_I$$
$$\left(\frac{\partial\hat{U}_0}{\partial t}\right)\hat{U}_I + \hat{U}_0\left(\frac{\partial\hat{U}_I}{\partial t}\right) = \left(\frac{1}{i\hbar}\hat{H}_0\hat{U}_0\right)\hat{U}_I + \frac{1}{i\hbar}\hat{V}\hat{U}_0\hat{U}_I$$
$$\Rightarrow \frac{\partial\hat{U}_I}{\partial t} = \frac{1}{i\hbar}\left(\hat{U}_0\hat{V}\hat{U}_0\right)\hat{U}_I \tag{11}$$

since $\hat{U}_0$ is unitary (and thus $\hat{U}_0^\dagger\hat{U}_0 = I$).

Defining

$$\hat{V}_I(t) = \hat{U}_0^\dagger(t,t_0)\hat{V}(t)\hat{U}_0(t,t_0) \tag{12}$$

we have that

$$\frac{\partial}{\partial t}\hat{U}_I(t,t_0) = \frac{1}{i\hbar}\hat{V}_I\hat{U}_I(t,t_0) \tag{13}$$

Formally integrating gives

$$\hat{U}_I(t,t_0) = 1 + \frac{1}{i\hbar}\int_{t_0}^{t}\hat{V}_I\hat{U}_I(\tau,t_0)\,d\tau \tag{14}$$

Time dependent perturbation corrections are obtained by iterating (14):

$$\begin{aligned}\hat{U}_I(t,t_0) &= 1 + \frac{1}{i\hbar}\int_{t_0}^{t}\hat{V}_I(\tau)\,d\tau\left[1+\frac{1}{i\hbar}\int_{t_0}^{\tau}\hat{V}_I(\tau')\hat{U}_I(\tau',t_0)\,d\tau'\right]\\ &= 1 + \frac{1}{i\hbar}\int_{t_0}^{t}\hat{V}_I(\tau)\,d\tau - \frac{1}{\hbar^2}\int_{t_0}^{t}d\tau\int_{t_0}^{\tau}d\tau'\,\hat{V}_I(\tau)\hat{V}(\tau')\hat{U}_I(\tau',t_0)\end{aligned} \tag{15}$$

Higher order corrections can be obtained via an infinite number of iterations. In powers of $\hat{V}(t)$, this becomes:

$$\hat{U}_I(t,t_0) = 1 + \sum_{n=1}^{\infty}\left(\frac{1}{i\hbar}\right)^n\int_{t_0}^{t}d\tau_n\int_{t_0}^{\tau_n}d\tau_{n-1}\cdots\int_{t_0}^{\tau_2}d\tau_1\hat{V}_I(\tau_n)\hat{V}_I(\tau_{n-1})\cdots\hat{V}_I(\tau_1) \tag{16}$$

where the order of integration is such that

$$t_0 < \tau_1 < \tau_2 < \cdots < \tau_{n-1} < \tau_n < t$$

Remark 5: We now transform (16) back into the Schrodinger picture using

$$\hat{U}_S(t,t_0) = \hat{U}_0(t,t_0)\hat{U}_I(t,t_0)$$

and

$$\hat{V}_I(\tau_j) = \hat{U}_0^\dagger(\tau_j,t_0)\hat{V}(\tau_j)\hat{U}_0(\tau_j,t_0)$$

Also, note that

$$\hat{U}_0(\tau_j,t_0)\hat{U}_0^\dagger(\tau_{j-1},t_0) = \hat{U}_0(\tau_j,\tau_{j-1})$$

Thus we have that

$$\hat{U}_S(t,t_0) = \hat{U}_0(t,t_0) + \sum_{n=1}^{\infty}\left(\frac{1}{i\hbar}\right)^n \int_{t_0}^{t} d\tau_n \int_{t_0}^{\tau_n} d\tau_{n-1}\cdots\int_{t_0}^{\tau_2} d\tau_1 \cdot$$
$$\cdot \quad \underbrace{\hat{U}_0(t,\tau_n)\hat{V}(\tau_n)\hat{U}_0(\tau_n,\tau_{n-1})}_{\hat{U}_0(t,t_0)\underbrace{\hat{U}_0^\dagger(\tau_n,t_0)\hat{V}(\tau_n)\hat{U}_0(\tau_n,t_0)}_{\hat{V}_I}\hat{U}_0^\dagger(\tau_{n-1},t_0)} \hat{V}(\tau_{n-1})\cdots\hat{U}_0(\tau_2,\tau_1)\hat{V}(\tau_1)\hat{U}_0(\tau_1,t_0) \tag{17}$$

Remark 6: Starting at the earliest times (right) and moving to interacting (left) in the integrand represents

1. Free evolution from t_0 to τ_1
2. Interaction at τ_1
3. Free evolution from τ_1 to τ_2

   $\vdots$
4. Interaction at τ_n
5. Free evolution from τ_n to t

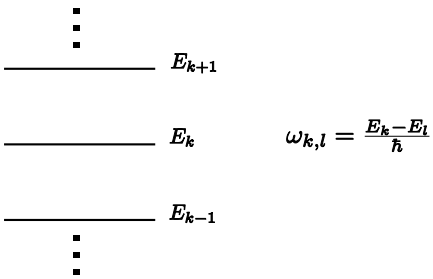
So that the full evolution represents a sum over all elementary time evolutions, taking into account all possible numbers of interactions between t_0 and t.

13.3.1 Transition Properties Between Energy States

For this analysis, consider the case where the free Hamiltonian $\hat{H}_0$ is time independent. Then

$$\hat{U}_0(\tau_j,\tau_{j-1}) = e^{-i\hat{H}_0(\tau_j-\tau_{j-1})/\hbar} \tag{18}$$

and we consider a system with discrete energies $E_1, E_2, \ldots$. We develop the perturbation theory in terms of jumps between the levels.



The transition probability between some initial state $|E_a\rangle$ and some final state $|E_b\rangle$ is defined as

$$W_{a\to b} = \left|\left\langle E_b\middle|\hat{U}_S(t,t_0)\middle|E_a\right\rangle\right|^2 \tag{19}$$

Remark 1: The transition probability depends on the interval $t_0 \to t$ during which the transition takes place. We expect non-zero transition probabilities if there is an interaction $\hat{V}(\tau)$ which couples the initial and final states $|E_a\rangle, |E_b\rangle$. The interaction is specified in terms of matrix elements in the unperturbed energy basis:

$$\hat{V}(\tau) = \sum_{k,l} V_{kl}(\tau) |E_k\rangle \langle E_l| \tag{20}$$

where $V_{kl}(\tau)$ is:

$$V_{kl}(\tau) = \left\langle E_a \middle| \hat{V}(\tau) \middle| E_l \right\rangle \tag{21}$$

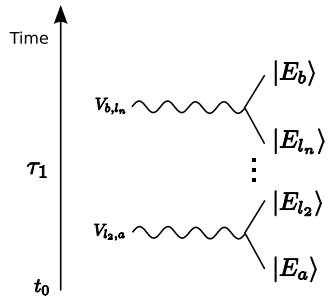
Substituting (17), (18) and (20) into (19) gives:

$$\begin{aligned} W_{a\to b} = \Bigg| & \sum_{n=1}^{\infty} \left(\frac{1}{i\hbar}\right) \int_{t_0}^{t} d\tau_n \int_{t_0}^{\tau_n} d\tau_{n-1} \cdots \int_{t_0}^{\tau_2} d\tau_1 \sum_{k_n,l_n} \cdot \sum_{k_{n-1},l_{n-1}} \cdot \sum_{k_1,l_1} \left\langle E_b \middle| e^{-i\hat{H}_0(t-\tau_n)/\hbar} \middle| E_{k_n} \right\rangle \cdot \\ & \cdot V_{k_n,l_n}(\tau_n) \left\langle E_{l_n} \middle| e^{-i\hat{H}_0(\tau_n-\tau_{n-1})/\hbar} \middle| E_{k_{n-1}} \right\rangle \cdot \\ & \cdot V_{k_{n-1},l_{n-1}}(\tau_{n-1}) \left\langle E_{l_{n-1}} \right| \cdots e^{-i\hat{H}_0(\tau_2-\tau_1)/\hbar} |E_{k_1}\rangle V_{k_1,l_1}(\tau_1) \left\langle E_{l_n} \middle| e^{-i\hat{H}_0(\tau_1-t_0)/\hbar} \middle| E_a \right\rangle \Bigg|^2 \\ = \Bigg| & \sum_{n=1}^{\infty} \left(\frac{1}{i\hbar}\right)^n \int_{t_0}^{t} d\tau_n \int_{t_0}^{\tau_n} d\tau_{n-1} \cdots \int_{t_0}^{\tau_2} d\tau_1 \cdot \sum_{l_n} \sum_{l_{n-1}} \cdots \sum_{l_2} e^{-iE_b(t-\tau_n)/\hbar} V_{b,l_n}(\tau_n) \cdot \\ & \cdot e^{-iE_{l_n}(\tau_n-\tau_{n-1})/\hbar} V_{l_n,l_{n-1}}(\tau_{n-1}) \cdots e^{-iE_{l_2}(\tau_2-\tau_1)/\hbar} V_{l_2,a} e^{-iE_a(\tau_1-t_0)/\hbar} \Bigg|^2 \end{aligned} \tag{22}$$

Remark 2:

- $\sum_{n=1}^{\infty} \to$ sum over the number of intermediate state interactions between t_0 and t
- $\int_{t_0}^{\tau_j} \to$ integration over all possible times for intermediate state interactions
- $V_{l_j,l_{j-1}} \to$ strength of interaction connecting intermediate states $\left|E_{l_{j-1}}\right\rangle$ and $\left|E_{l_j}\right\rangle$
- $(\cdots) \to$ transition amplitude is sum over amplitudes for transitions taking place via a set of intermediate or <u>virtual states</u> $|E_{l_2}\rangle, |E_{l_3}\rangle, \ldots, |E_{l_n}\rangle$. There are $n-1$ intermediate states (stepping stones) so that there are n steps between $|E_a\rangle$ and $|E_b\rangle$.

Remark 3: Diagrammatically, the transitions can be represented as:
where the vertices are where the state of the system changes.



Remark 4: To first order in perturbation theory, (22) looks like

$$\begin{aligned} W_{a\to b} &= \frac{1}{\hbar^2}\left|\int_{t_0}^{t} e^{-iE_b(t-\tau)/\hbar} V_{ba}(\tau) e^{-iE_a(\tau-t_0)/\hbar}\, d\tau\right|^2 \\ &= \frac{1}{\hbar^2}\left|\int_{t_0}^{t} e^{i\omega_{ba}\tau} V_{ba}(\tau)\, d\tau\right|^2 \end{aligned} \tag{23}$$

where $\omega_{ba} = \frac{E_b - E_a}{\hbar}$.

13.3.2 Time-Independent Interactions

The time integral in (23) is easy if the interaction is independent of time:

$$\begin{aligned} W_{a\to b} &= \frac{1}{\hbar^2}\left|V_{ba}\right|^2 \left|\frac{e^{i\omega_{ba}t} - e^{i\omega_{ba}t_0}}{i\omega_{ba}}\right|^2 \\ &= \frac{1}{\hbar^2}\left|V_{ba}\right|^2 \frac{1}{\omega_{ba}^2}\left(1 + 1 - e^{-i\omega_{ba}(t-t_0)} - e^{-i\omega_{ba}(t-t_0)}\right) \\ &= \frac{2}{\hbar^2}\left|V_{ba}\right|^2 \frac{1}{\omega_{ba}^2}\left(1 - \cos\left(\omega_{ba}(t-t_0)\right)\right) \end{aligned} \tag{24}$$

Let $\Delta t = t - t_0$ and define

$$f(\omega, \Delta t) \equiv \frac{2(1-\cos(\omega\Delta t))}{\omega^2} \tag{25}$$

Remark 1: $f(\omega, \Delta t)$ contains information about energy conservation during the transition. It is peaked at $\omega = 0$, with a maximum $f(0, \Delta t) = (\Delta t)^2$. This is seen in Fig 13.1.

In the final limit $\Delta t \to$ big, this function becomes highly peaked about $\omega = 0$ with half-width $\Delta\omega \approx \frac{\pi}{\Delta t}$ and

$$f(\omega, \Delta t) \xrightarrow[\Delta t\to\infty]{} A\delta(\omega) \tag{26}$$

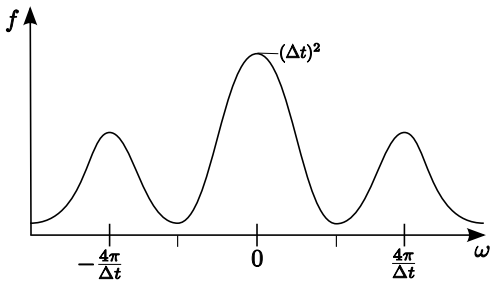


Figure 13.1: Plot of $f(\omega, \Delta t)$.

where A is found by integrating (25) over ω.

$$\begin{aligned} A &= 2\int_{-\infty}^{\infty} \frac{1-\cos(\omega\Delta t)}{\omega^2}\, d\omega \\ &= 2\pi\Delta t \end{aligned} \tag{27}$$

where the integral is done by contour integration. (Let $f(z) = \frac{1-e^{-iz\Delta t}}{z^2}$ and the integral is the real part of this along the x-axis.) So, in the limit of infinite interaction time, the transition probability is 0 unless

$$\omega_{ba} = \frac{E_b - E_a}{\hbar} = 0 \tag{28}$$

This is a statement of conservation of energy: A mismatch of energies is tolerated for finite time intervals as long as

$$\Delta E \Delta t \approx \pi\hbar, \qquad \text{with } \Delta E = \hbar\omega \approx \frac{\hbar\pi}{\Delta t} \tag{29}$$

Transitions occurring in a finite time Δt involve an uncertainty about the energies. These transitions can occur if E_a and E_b are close enough together so that the *total system* energy uncertainty can bring them together during a finite interaction. Note that ΔE in (29) is the difference in unperturbed energies, not the energy shift due to the perturbation.

Remark 2: For transitions between states of same energy:

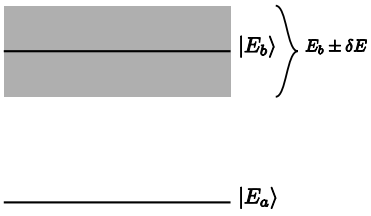
$$W_{a\to b} = \frac{1}{\hbar^2} |V_{ba}|^2 (\Delta t)^2 \tag{30}$$

which has limited validity since $W_{a\to b}$ must not exceed 1, even as $\Delta t \to \infty$. Hence (30) is valid only if

$$\Delta t \ll \frac{\hbar}{|V_{ba}|}$$

13.3.3 Transition to a Continuum of States

Often, $|E_b\rangle$ is not a discrete state, but is part of a continuous spectrum:



In these cases, we must find the transition probability to the state whose energy falls in the range of energies centered at E_b. Let B denote the subspace of final states with energies in the range $E_b - \delta E$ to $E_b + \delta E$ and define

$$W_{a\to B} = \sum_{\substack{\text{all states} \\ \text{in B}}} W_{a\to b} \tag{31}$$

where $W_{a\to b}$ is given by (24). For a continuum of states, we replace the sum in (31) with an integral which includes the density of states:

$$\rho E_b \cdot dE_b = \text{Number of states with energy in the range } E_b \text{ to } E_b \pm \delta E \tag{32}$$

So (31) becomes

$$W_{a\to B} = \int_{E_0-\delta E}^{E_0+\delta E} dE\, \rho(E) \frac{2}{\hbar^2} \left|\left\langle E\middle|\hat{V}\middle|E_a\right\rangle\right|^2 \left[\frac{1-\cos\left(\frac{E-E_a}{\hbar}\Delta t\right)}{\left(\frac{E-E_a}{\hbar}\right)^2}\right] \tag{33}$$

Remark 1: If the range of final energies is sufficiently small, then

$$\rho(E) \approx \rho(E_b)$$

$$\Rightarrow \left|\left\langle E\middle|\hat{V}\middle|E_a\right\rangle\right|^2 \approx \left|\left\langle E_b\middle|\hat{V}\middle|E_a\right\rangle\right|^2 = |V_{ba}|^2$$

in which case

$$W_{a\to B} = 2\rho(E)\,|V_{ba}|^2 \int_{E_0-\delta E}^{E_0+\delta E} dE \left[\frac{1-\cos\left(\frac{E-E_a}{\hbar}\Delta t\right)}{(E-E_a)^2}\right] \tag{34}$$

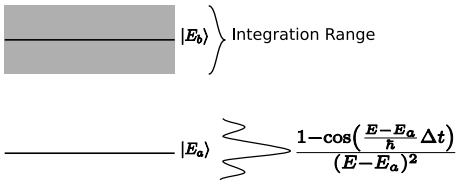
Remark 2: From §13.3.2.R1, we know that the function in (34) has a max value of $\left(\frac{\Delta t}{\hbar}\right)^2$ at $E = E_a$, then secondary maxima get smaller as deviations from the resonant energies ($E = E_a$) decrease. The width of the central maximum

is $\approx \frac{\hbar\pi}{\Delta t}$, and we assume that the integration range is much larger than this width.

$$\delta E \gg \frac{\hbar\pi}{\Delta t} \tag{35}$$

With this approximation, we consider (34) for 2 distinct cases:

1. $|E_b - E_a| > \delta E$ implies that the final states are non-conserving by an amount larger than the width of the transition probability maximum



In this case,

$$\frac{1}{(E-E_a)^2} \approx \frac{1}{E_b - E_a)^2}$$

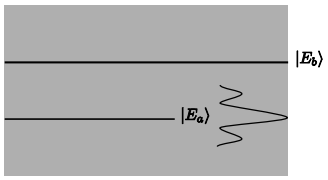
So that

$$\int_{E_0-\delta E}^{E_0+\delta E} dE \underbrace{\left[1 - \cos\left(\frac{E-E_a}{\hbar}\Delta t\right)\right]}_{2\delta E \gg -\hbar\Delta t}$$

And so

$$W_{a\to B} = \frac{4\rho(E_b)\delta E\,|V_{ba}|^2}{(E_b - E_a)^2} \tag{36}$$

2. $|E_b - E_a| < \delta E$ implies that the transition probability peak falls within the range of final energies. This means that the transition is energy conserving. Now,



$$\int_{E_0-\delta E}^{E_0+\delta E} \text{ in (34)} \;\to \int_{-\infty}^{\infty}$$

and (34) in given by (27). Thus

$$W_{a\to B} = \frac{2\pi\Delta t}{\hbar}\rho(E_b)\,|V_{ba}|^2 \tag{37}$$

Remark 3: Eqn (37) is an important result since it represents the dynamical behavior in many quantum systems. I.e., imagine N_a systems in state $|E_a\rangle$ at time t. A short time Δt later, the number of systems in state $|E_a\rangle$ is

$$N_a(t+\Delta t) = N_a(t)\left[1 - \frac{2\pi}{\hbar}\rho(E_b)\,|V_{ba}|^2\,\Delta t\right]$$

So

$$\frac{N_a(t+\Delta t) - N_a(t)}{\Delta t} = -\frac{2\pi}{\hbar}\rho(E_b)\,|V_{ba}|^2\,N_a(t)$$

$$\Rightarrow \dot{N}_a = -\Gamma N_a \tag{38}$$

where

$$\Gamma = \frac{W_{a\to B}}{\Delta t} = \frac{2\pi}{\hbar}\rho(E_b)\,|V_{ba}|^2 \tag{39}$$

and thus Γ is a transition rate (transition probability per unit time), and (38) describes an exponential decay at this rate.

$$N_a(t) = N_a(0)e^{-\Gamma t} \tag{40}$$

Examples of where this holds: β-decay, spontaneous emission from an excited state of an atom or molecule.

13.3.4 Periodic Perturbations

Consider a harmonic interaction of the form:

$$\hat{V}(t) = \hat{A}^\dagger e^{-i\omega t} + \hat{A}e^{i\omega t}$$

with $\hat{A}$ an unspecified time-independent operator. Then (23) becomes

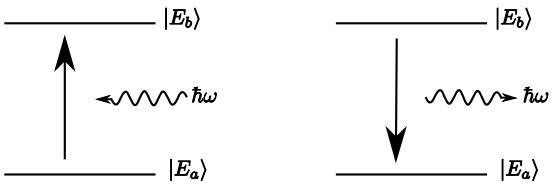
$$W_{a\to b} = \frac{1}{\hbar^2}\left|\int_{t_0}^{t_0+\Delta t} d\tau\left[\left\langle E_b\middle|\hat{A}^\dagger\middle|E_a\right\rangle e^{i(\omega_{ba}-\omega)\tau} + \left\langle E_b\middle|\hat{A}\middle|E_a\right\rangle e^{i(\omega_{ba}+\omega)\tau}\right]\right|^2 \tag{41}$$

And the integral is largest when $\omega_{ba} - \omega = 0$ or $\omega_{ba} + \omega = 0$. These are *resonance conditions* corresponding to energy conservation.

$$\left.\begin{aligned} E_b &= E_a + \hbar\omega \\ E_b &= E_a - \hbar\omega \end{aligned}\right\} \tag{42}$$

Physically, these represent an energy quanta absorbed or emitted (respectively) from the system providing the periodic potential, as seen in Fig. 13.2.

Remark 1: We require that $\omega \gg \frac{\pi}{\Delta t}$ so that the frequency is much greater than the width of the transition resonance peak. This establishes that the system has enough time to "feel" the periodicity of the perturbation.



(a) Resonance and energy conservation with absorption of a quanta

(b) Resonance and energy conservation with emission of a quanta

Figure 13.2: Resonances of Periodic Perturbations

Following through with the integration in (41) gives us:

$$W_{a\to b} = \frac{2}{\hbar^2}\left|\left\langle E_b\middle|\hat{A}^\dagger\middle|E_a\right\rangle\right|^2 \frac{1-\cos\left((\omega_{ba}-\omega)\Delta t\right)}{(\omega_{ba}-\omega)^2} + \frac{2}{\hbar^2}\left|\left\langle E_b\middle|\hat{A}\middle|E_a\right\rangle\right|^2 \frac{1-\cos\left((\omega_{ba}-\omega)\Delta t\right)}{(\omega_{ba}-\omega)^2}$$

Considering transitions to a continuous band of final states gives energy conserving transition rates:

1. For the case where $E_b + \delta E > E_a + \hbar\omega > E_b - \delta E$:

$$\frac{W_{a\to b}}{\Delta t} = \frac{2\pi}{\hbar}\rho(E_a+\hbar\omega)\left|\left\langle E_a+\hbar\omega\middle|\hat{A}^\dagger\middle|E_a\right\rangle\right|^2 \tag{43}$$

2. For the case where $E_b + \delta E > E_a - \hbar\omega > E_b - \delta E$:

$$\frac{W_{a\to b}}{\Delta t} = \frac{2\pi}{\hbar}\rho(E_a-\hbar\omega)\left|\left\langle E_a-\hbar\omega\middle|\hat{A}^\dagger\middle|E_a\right\rangle\right|^2 \tag{44}$$

Remark 2: Equations (43) and (44) give transition rates that are often referred to as Fermi's Golden Rules. The $\hbar\omega$ supplied by the perturbation provides the energy to make the transition energy conserving.

13.3.5 Sudden and Adiabatic Perturbations

Two situations in which the response of the quantum systems changes is easy to calculate is:

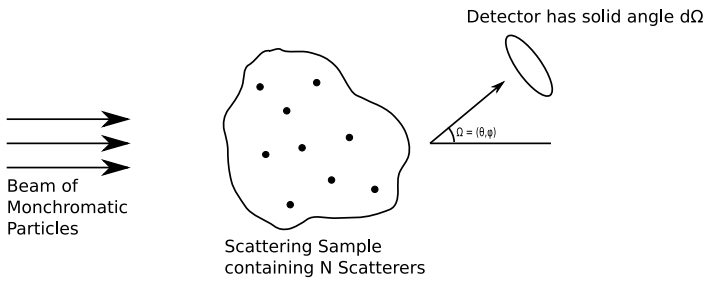
1. Sudden Approximation: Here we assume the system can not change it's state arbitrarily fast, so a sudden change in external field will not change the state of the quantum system during the field change.
2. Adiabatic Perturbation: When perturbation is slow enough that the state of the system changes adiabatically with applied perturbations.

Chapter 14

Scattering

14.1 Scattering Cross Sections

Consider a general scattering experiment:



Where the particle flux J is the number of particles crossing unit area per unit time. Also, the beam is weak enough so that the particles scatter independently (no coherence).

Remark 1: We neglect coherence of scattered waves between scatterers–each scatterer acts as if it were alone. This assumption fails for x-ray diffraction.

We define:

$$\mathcal{N} = \text{ \# of particles recorded at the detector per unit time}$$

$$\Rightarrow \mathcal{N} = JN\sigma(\Omega)d\Omega \tag{1}$$

where $\sigma(\Omega)$ is the differential scattering cross section, and is a parameter that characterizes the collision between the incident particles and scatterers. The "differential" refers to the detector only monitoring a small solid angle $d\Omega$.

Remark 2: The total scattering cross section is

$$\sigma_{tot} = \int \sigma(\Omega)\, d\Omega \tag{2}$$

Remark 3: Though the target can be quite complicated (an atom made up of electrons and protons, etc...), it is often sufficient to describe the scatterer by a central potential $\hat{V}(r)$. (if we consider elastic collions only!) This is what we will do in this section.

Remark 4: The goal is to relate what is measured in experiments (the differential cross section), to a solution to the Schrodinger equation.

Assume incoming particles have energy E, and momentum $\hbar\boldsymbol{k}$. Then the stationary solution must satisfy

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(r)\right]\psi_{\boldsymbol{k}} = E\psi_{\boldsymbol{k}} \tag{3}$$

where $\hat{V}(r)$ defines the interaction between particles and scatterers, and E is the energy of the incident and outgoing particles. We want a solution that describes the scattering process, so we look for a solution of the form:

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}, t) = e^{-iEt/\hbar}\psi_{\boldsymbol{k}}(\boldsymbol{r}) \tag{4}$$

with asymptotic form

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) \sim \underbrace{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}_{\substack{\text{incoming}\\ \text{particles}}} + \underbrace{f(\Omega)\frac{e^{ikr}}{r}}_{\substack{\text{outgoing spherical}\\ \text{wave of scattered}\\ \text{particles}}} \tag{5}$$

as $r \to \infty$. This means that $\psi_{\boldsymbol{k}}(\boldsymbol{r}, t)$ gives an expanding spherical wave.

Remark 5: The $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ represents a beam of particles with speed $\frac{\hbar k}{m}$ and a density of 1 particle per unit volume. The corresponding particle flux is

$$J = 1 \cdot \frac{\hbar k}{m}$$

The flux of particles entering the detector at angle $\Omega(\theta, \phi)$ is:

$$\mathcal{N} = \left(\begin{smallmatrix}\text{number of outgoing}\\ \text{particles per unit}\\ \text{volume}\end{smallmatrix}\right) \cdot \frac{\hbar k}{m} \cdot \left(\begin{smallmatrix}\text{Detector}\\ \text{area}\end{smallmatrix}\right)$$

For large distances r, the first term is $\frac{|f(\Omega)|^2}{r^2}$ and the detector area is $r^2\, d\Omega$.

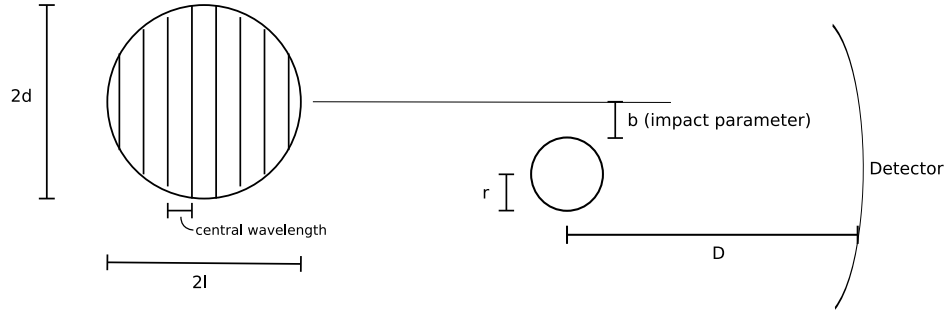
$$\mathcal{N} = |f(\Omega)|^2 \frac{\hbar k}{m}\, d\Omega \tag{6}$$

Comparing (6) with (1) gives:

$$\underbrace{\sigma(\Omega)}_{\text{measured}} = \underbrace{|f(\Omega)|^2}_{\text{calculated}}$$

Remark 6: Now the main task is to calculate what is called the scattering amplitude $f(\Omega)$.

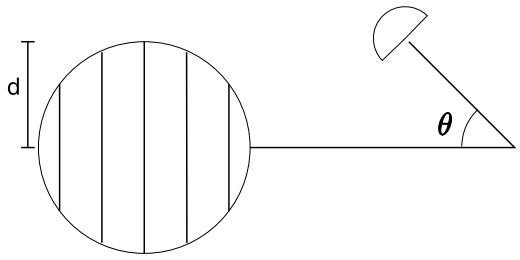
Remark 7: Often we are considering the scattering of individual particles off one another. In this case, an incoming singe particle would be described by a time independent wave-packet rather than a plane wave, and the picture would look like: where the big particle is being



scattered by the smaller. The incident particle (wavepacket) has velocity $v = \frac{\hbar k}{m} = \frac{2\pi\hbar}{\lambda m}$. The longitudial and transverse dimensions of the wavepacket are determined by the spread in momentum.

In the above picture we've made the approximations that:

- $l, d \gg a$ - otherwise the scattering depends on the details of the shape of the incoming wavepacket.
- $l, d \gg \lambda$ - otherwise the wavepacket description of the incoming particle will not give well defined energy and momentum to be small compared to the scale on which the scattering properties change with energy and momentum.
- $d \geq b$ - for non-trivial results (if $d \ll b$, then there is no significant perturbation, assuming short range potentials that fall off faster than $\frac{1}{r}$).
- $D \gg a, \lambda$ - so that the influence of the potential on the detector has dropped to 0 (detector is asymptotic regime).
- $D \sin\theta \gg d$ - so as to separate the transmitted and scattered parts of the incident wave packet:



Mathematically, for the description we would multiply the incoming plane wave by a real envelope function which depends on the distance from the scatterer (more precisely, on the *impact parameter*). We would eventually derive a description of the scattered wave packet that depends on the solution to the Schrodinger equation in a central potential. Given this description and the above

constraints, we can show that the differential cross section (which depends on the probability for a wavepacket to scatter within $d\Omega$ of Ω (location of the detector)) is still given by

$$\sigma(\omega) = |f_{\boldsymbol{k}}(\Omega)|^2 \tag{7}$$

where the asymptotic solution to the Schrodinger equation is:

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) \sim e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + f_{\boldsymbol{k}}(\Omega)\frac{e^{ikr}}{r} \tag{5}$$

14.2 Waves and Phase Shifts

Our goal now is to find $f(\Omega)$ for a given central potential. Recall that in §10.2.2 and §8.2.3 we found that the solution to the spherically symmetric Schrodinger equation could be written

$$\psi(r,\theta,\phi) = \sum_{l,m} A_{lm}\frac{U_{El}(r)}{r}Y_{lm}(\theta,\phi)$$

where U_{El} is a solution to the radial equation (§10.2.2.E2) and $Y_{lm}(\theta,\phi)$ are the spherical harmonics.

Remark 1: The scattering problem has azimuthal symmetry. For initial propagation direction, aligned with the z-axis, the solution is $\phi-$independent, and only $m = 0$ terms are involved. Thus we have

$$\psi(r,\theta) = \sum_{l=0}^{\infty} a_l\frac{U_{El}}{r}P_l(\cos\theta) \tag{8}$$

where $P_l(\cos\theta)$ is the Legendre polynomial and $a_l = \sqrt{\frac{2l+1}{4\pi}}A_{l,0}$.

Remark 2: The goal is to match (8) to the asymptotic form (5)

$$\psi(r,\theta) \xrightarrow[r\to\infty]{} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + f(\theta)\frac{e^{ikr}}{r}$$

where we are using arrows to represent asymptotically similar.

If we take $\boldsymbol{k}$ in the z-direction, the incident plane wave can also be expressed as:

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \sum_{l=0}^{\infty}(2l+1)(i)^l\cdot j_l(kr)P_l(\cos\theta) \tag{9}$$

(See §10.2.3.R11). Expanding $f(\theta)$ in Legendre polynomials:

$$f(\theta) = \sum_{l=0}^{\infty} f_l P_l(\cos\theta) \tag{10}$$

We require $U_{El}(r)$ to be a regular solution to the radial equation, and asymptotically, we can write it as

$$U_{El}(r) \xrightarrow[r\to\infty]{} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right) \tag{11}$$

where δ_l is called a *phase shift*. The asymptotic form of (8) is:

$$\psi(r,\theta) \xrightarrow[r\to\infty]{} \sum_{l=0}^{\infty} a_l \left(\frac{(-i)^l}{2i} e^{i\delta_l}\frac{e^{ikr}}{r} - \frac{(i)^l}{2i} e^{-i\delta_l}\frac{e^{-ikr}}{r}\right) P_l(\cos\theta) \tag{12}$$

In order to match this to the asymptotic form (5), we write the asymptotic form of $j_l(kr)$ in (9):

$$\psi(r,\theta) \xrightarrow[r\to\infty]{} \sum_{l=0}^{\infty} \left[(2l+1)\frac{(i)^l}{kr}\left(\frac{(-i)^l}{2i}e^{ikr} - \frac{(i)^l}{2i}e^{-ikr}\right) + f_l\frac{e^{ikr}}{r}\right] P_l(\cos\theta) \tag{13}$$

Now, (12) and (13) *must match* as there are 2 different forms of the same incoming and outgoing spherical waves. This requirement gives an expression for a_l:

- Incoming Waves:

$$a_l\left(\frac{(-i)^l}{2i}e^{-i\delta_l}\right) = (2l+1)\frac{i^l}{k}\left(\frac{-i^l}{2i}\right)$$

$$\Rightarrow a_l = \frac{(2l+1)}{k} i^l e^{i\delta_l} \tag{14}$$

- Outgoing Waves: (matching coefficients)

$$a_l\left(\frac{(-i)^l}{2i}e^{i\delta_l}\right) = \frac{(2l+1)i^l}{k}\frac{(-i)^l}{2i} + f_l$$

$$\Rightarrow \frac{(2l+1)e^{i\delta_l}}{k}\frac{e^{i\delta_l}}{2i} = \frac{(2l+1)}{2ik} + f_l$$

$$f_l = \frac{(2l+1)}{2ik}\left(e^{2i\delta_l} - 1\right) \tag{15}$$

And the expression for the scattering amplitude in terms of the phase shifts is:

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin(\delta_l)P_l(\cos\theta) \tag{16}$$

Remark 3: Solving the differential scattering cross-section is reduced to finding the phase shift for the different angular momentum components of the scattered wave.

Remark 4: Note that we can write the asymptotic solution (13) with a_l from (14).

$$\psi(r,\theta) \xrightarrow[r\to\infty]{} \sum_{l=0}^{\infty} \frac{(2l+1)}{2i}\left[-\frac{(-1)^l e^{-ikr}}{kr} + e^{2i\delta_l}\frac{e^{ikr}}{kr}\right] P_l(\cos\theta)$$

where this phase factor shifts the phase of the outgoing partial wave relative to the incident plane wave–this is where the entire scattering process is captured. (Partial waves refer to individual terms in the spherical wave expansion.)

Remark 5: The differential scattering cross-section is terms of phase shifts is:

$$\sigma(\theta) = |f(\theta)|^2 = \frac{1}{k^2}\sum_{l,l'}(2l+1)(2l'+1)e^{i(\delta_l - \delta_{l'})}\sin(\delta_l)\sin(\delta_{l'})P_{l'}(\cos\theta)P_l(\cos\theta) \tag{17}$$

Integrating this over a unit sphere gives the total scattering cross-section. Noting the orthogonality of the Legendre polynomials:

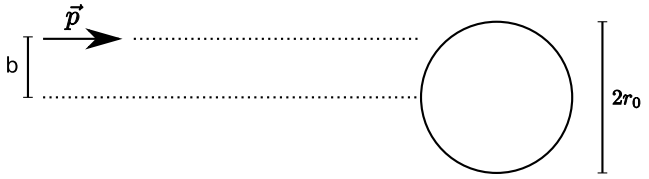
$$\sigma_{tot} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2(\delta_l) \tag{18}$$

We can write

$$\left.\begin{aligned} \sigma_{tot} &= \sum_{l=0}^{\infty}\sigma_l \\ \text{with} & \\ \sigma_l &= \frac{4\pi}{k^2}(2l+1)\sin^2(\delta_l) \end{aligned}\right\} \tag{19}$$

and σ_l gives the contribution to scattering cross-section from partial waves with angular momentum l.

Remark 6: The partial wave expansion is most useful when only a few terms in (18) contribute. To get an idea of which terms dominate, consider a scattering (classical) problem. Here



$V(r) = 0$ for $r > r_0$. Now the angular momentum of the incoming particle is $L = bp$ and is a constant of motion. If $b > r_0$ ($L > r_0 p$), then there is no scattering. Quantum mechanically, $L \to \hbar l$ (more precisely, $L \to \hbar^2 l(l+1)$) and $p = \hbar k$. Thus, we expect the *strongest* scattering when

$$l < kr_0 \tag{20}$$

and the *weakest* scattering when

$$l > kr_0 \tag{21}$$

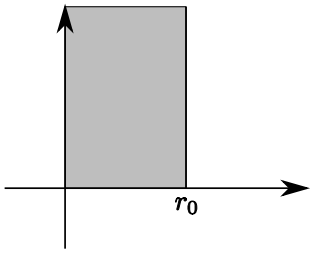
Generally speaking, we expect σ_l to become unimportant for $l \geq kr_0$. This holds if $V(r) = 0$ for $r > r_0$, but turns out to be true also if $V(r)$ is very small (though not strictly 0) at some range r_0.

Remark 7: Equation (8) (weak scattering) holds when there is either low energy ($k \to 0$), or high angular momentum ($l \to \infty$). Recall that high angular momentum particles will "miss" the target if $L > r_0 p$. Physically, lower energy corresponds to large wavelength. In the limit $\frac{r_0}{\lambda} = \frac{kr}{2\pi} \ll 1$, a small scatterer will have little effect on a large incident wave. (Imagine a small obstacle in sound and water waves.) Any scattering that does occur will be isotropic since large wavelength waves cannot probe the spacial structure of the scatterer.

14.3 Example: Scattering from a Hard Sphere

Consider the potential:

$$V(r) = \begin{cases} \infty, & 0 < r < r_0 \\ 0, & r_0 < r < \infty \end{cases}$$



The general solution to the radial equation (§10.2.3) is

$$R_l(r) = A_l j_l(kr) + B_l \eta_l(kr)$$

where A_l, B_l are constants and the BC's are

$$A_l j_l(r_0 k) + B_l \eta_l(kr_0) = 0$$

$$\Rightarrow B_l = -A_l \frac{j_l(kr_0}{\eta_l(kr_0)}$$

$$\Rightarrow R_l(r) = A_l' \left(\eta_l(kr_0) j_l(kr) - j_l(kr_0)\eta_l(kr)\right)$$

where $A_l' = \frac{A_l}{\eta_l(kr_0)}$. The asymptotic form of the solution (§10.3.1.R6) is

$$R_l(r) \xrightarrow[r\to\infty]{} \frac{\eta_l(kr_0)}{kr} \sin\left(kr - \tfrac{l\pi}{2}\right) + \frac{j_l(kr_0)}{kr} \cos\left(kr - \tfrac{l\pi}{2}\right)$$

Comparing this with the general form (§14.2.E11):

$$R_l(r) \xrightarrow[r\to\infty]{} \frac{1}{kr} \sin\left(kr - \tfrac{l\pi}{2} + \delta_l\right)$$
$$\xrightarrow[r\to\infty]{} \frac{1}{kr} \sin\left(kr - \tfrac{l\pi}{2}\right) \cos\delta_l + \frac{1}{kr} \cos\left(kr - \tfrac{l\pi}{2}\right) \sin\delta_l$$

$$\Rightarrow \eta_l(kr_0) = \cos\delta_l \qquad \text{and} \qquad j_l(kr_0) = \sin\delta_l$$

$$\Rightarrow \tan\delta_l = \frac{j_l(kr_0)}{\eta_l(kr_0)}$$

$$\Rightarrow \delta_l = \arctan\left(\frac{j_l(kr_0)}{\eta_l(kr_0)}\right)$$

$$\Rightarrow \sin^2(\delta_l) = \frac{j_l^2(kr_0)}{\eta_l^2(kr_0) + j_l^2(kr_0)}$$

Remark 1: At *low energies*, the spherical Bessel functions become

$$j_l(kr) \xrightarrow[r\to 0]{} \frac{(kr)^l}{(2l+1)!!}$$

$$\eta_l(kr) \xrightarrow[r\to 0]{} \frac{(2l-1)!!}{(kr)^{l+1}}$$

So that the partial cross section for scattering off a hard sphere is

$$\sigma_l \xrightarrow[k\to 0]{} \frac{4\pi}{k^2}\frac{(2l+1)(kr_0)^{4l+2}}{[(2l+1)!!(2l-1)!!]^2}$$

The dominant cross section is s-wave scattering (l=0):

$$\sigma_l \xrightarrow[k\to 0]{} \frac{4\pi}{k^2}(kr_0)^2 = 4\pi r_0^2$$

where r_0 is the length scale characterizing the range of the scatterer, and is sometime called the scattering length.

Remark 2: At high energies, we'll use the asymptotic forms of the Bessel functions (see Messiah) to get:

$$\sigma(\Omega) \xrightarrow[k\to\infty]{} \frac{1}{4}r_0^2\left(1 + \cot^2(\tfrac{\theta}{2})J_1^2\left(kr_0\sin\theta\right)\right) \qquad (\dagger)$$

and

$$\sigma_{tot} \xrightarrow[k\to\infty]{} 2\pi r_0^2$$

This limit corresponds to very short wavelengths, from which we might expect the classical results:

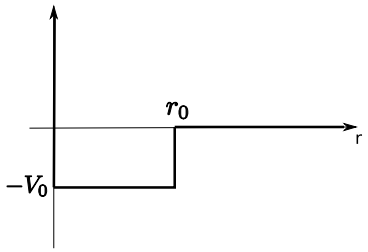
$$\left.\begin{aligned}\sigma(\Omega) &= \frac{1}{4}r_0^2\\ \sigma_{tot} &= \pi r_0^2\end{aligned}\right\} \text{ Classical results}$$

We do not get these results since the wave nature of the scattering process does not completely vanish. This is because the hard sphere has "sharp" edges, so that any wavelength, no matter how short, is affected by the discontinuity and there are diffraction effects. The Bessel function in (†) is the diffraction term.

14.4 Scattering from a Square Well – Resonances

Consider the potential

$$V(r) = \begin{cases} -V_0, & r < r_0 \\ 0, & r > r_0 \end{cases}$$



Remark 1: From before we know that a 1D square well exhibits resonances which are very sharp when the well is very deep and incident particles have low energies. Similar resonances occur when scattering from a 3D well.

Remark 2: Recall from §10.3.2 that regular solutions inside the square well are

$$R_l(r) = j_l(\kappa r) \qquad (r < r_0)$$

with

$$\kappa = \sqrt{\frac{2m}{\hbar^2}(E + V_0)}$$

and we have chosen to normalize $R_l(r)$ for convenience. Outside of the well, the solution is a superposition of the Hankel functions.

$$R_l(r) = A_l h_l^{(+)}(kr) + B_l h_l^{(-)}(kr) \qquad (r > r_0)$$

with

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

These solutions correspond to $E > 0$ since we are interested in the unbound states outside the well for scattering phenomena. The boundary conditions require continuity at $r = r_0$:

$$j_l(\kappa r_0) = A_l h_l^{(+)}(kr_0) + B_l h_l^{(-)}(kr_0) \tag{1}$$

and continuity of the derivatives at $r = r_0$:

$$\kappa j_l'(\kappa r_0) = k \left[A_l h_l^{(+)\prime}(kr_0) + B_l h_l^{(-)\prime}(kr_0) \right] \tag{2}$$

Remark 3: We also want to match the asymptotic form of the solution outside the well to the scattering solution:

$$\begin{aligned} R_l(r) &\xrightarrow[r\to\infty]{} \frac{1}{kr}\sin\left(kr - \tfrac{l\pi}{2} + \delta_l\right) \\ &\xrightarrow[r\to\infty]{} \frac{1}{kr}\frac{1}{2i}\left[e^{i(kr-l\pi/2)}e^{i\delta_l} - e^{-i(kr-l\pi/2)}e^{i\delta_l}\right] \end{aligned}$$

Inserting the asymptotic form of the Hankel functions:

$$R_l(r) \xrightarrow[r\to\infty]{} \frac{1}{kr}\left[A_l e^{i(kr-l\pi/2)} + B_l e^{-i(kr-l\pi/2)}\right]$$

Comparing the forms gives

$$\begin{aligned} A_l = e^{i\delta_l}, \qquad B_l &= e^{-i\delta_l} \\ \Rightarrow e^{2i\delta_l} &= -\frac{A_l}{B_l} \end{aligned}$$

So we need *only* the ratio of the unknown coefficients. From (1) then,

$$\frac{A_l}{B_l} = \frac{1}{B_l}\frac{j_l(\kappa r_0}{h_l^{(+)}(kr_0)} - \frac{h_l^{(-)}(kr_0)}{h_l^{(+)}(kr_0)}$$

Now, taking $(1)\cdot kh_l^{(+)\prime}(kr_0) - (2)\cdot h_l^{(+)}(kr_0)$:

$$\begin{aligned} kj_l(\kappa r_0)h_l^{(+)\prime}(kr_0) - \kappa j_l'(\kappa r_0)h_l^{(+)}(kr_0) &= A_l k \overbrace{\left[h_l^{(+)}(kr_0)h_l^{(+)\prime}(kr_0) - h_l^{(+)\prime}(kr_0)h_l^{(+)}(kr_0)\right]}^{0} + \\ &\quad + B_l k\left[h_l^{(-)}(kr_0)h_l^{(+)\prime}(kr_0) - h_l^{(-)\prime}(kr_0)h_l^{(+)}(kr_0)\right] \\ &= B_l k\left(\frac{2i}{kr_0^2}\right) \end{aligned}$$

where the last term is from the Wronskian relation of Hankel functions (Messiah X.38).

$$\begin{aligned} \Rightarrow e^{2i\delta_l} &= \frac{h_l^{(-)}(kr_0)}{h_l^{(+)}(kr_0)} - \frac{j_l(\kappa r_0)}{h_l^{(+)}(kr_0)}\cdot\frac{k2i}{(kr_0)^2}\frac{1}{kj_l(\kappa r_0)h_l^{(+)}(kr_0) - \kappa j_l'(\kappa r_0)h_l^{(+)}(kr_0)} \\ &= \frac{h_l^{(-)}(kr_0)}{h_l^{(+)}(kr_0)}\left[1 - 2i\frac{k}{\kappa}\frac{1}{(kr_0)^2}\frac{\frac{1}{h_l^{(-)}(kr_0)}}{\left[\frac{k}{\kappa}h_l^{(+)\prime}(kr_0) - \frac{j_l'(\kappa r_0)}{j_l(\kappa r_0)}h_l^{(+)}(kr_0)\right]}\right] \end{aligned}$$

Remark 4: For a deep potential and moderately low energies:

$$\kappa r_0 \gg l \qquad \text{and} \qquad \kappa \gg k$$

So

$$\begin{aligned} e^{2i\delta_l} \approx \frac{h_l^{(-)}(kr_0)}{h_l^{(+)}(kr_0)} &= \frac{1 - ij_l(kr_0)/\eta_l(kr_0)}{1 + ij_l(kr_0)/\eta_l(kr_0)} \\ &= \frac{1 - \left(\frac{j_l(kr_0)}{n_l(kr_0)}\right)^2 - \frac{2ij_l(kr_0)}{\eta_l(kr_0)}}{1 + \left(\frac{j_l(kr_0)}{\eta_l(kr_0)}\right)^2} \\ &= \cos(2\delta_l) + i\sin(2\delta_l) \end{aligned} \tag{3}$$

$$\Rightarrow \tan\delta_l \approx -\frac{j_l(kr_0)}{\eta_l(kr_0)}$$

which is the same result as for the hard sphere.

Remark 5: For certain energies, the denominator in the second term of (3) vanishes. In this case, note that

$$\frac{j_l'(\kappa r_0)}{j_l(\kappa r_0)} \xrightarrow[\kappa r_0 \gg l]{} \cot\left(\kappa r_0 - l\pi/2\right)$$

For simplicities sake, let $kr_0 \gg l$ so that

$$\frac{h_l^{(-)}(kr_0)}{h_l^{(+)}(kr_0)} \xrightarrow[kr_0 \gg l]{} e^{-2i(kr_0 - l\pi/2)}$$

$$\Rightarrow (kr_0)^2 h_l^{(-)}(kr_0) h_l^{(+)}(kr_0) \xrightarrow[kr_0 \gg l]{} 1$$

$$\Rightarrow (kr_0)^2 h_l^{(-)}(kr_0) h_l^{(+)\prime}(kr_0) \xrightarrow[kr_0 \gg l]{} i$$

Thus (3) becomes

$$\begin{aligned} e^{2i\delta_l} &\approx e^{-2i(kr_0 - l\pi/2)} \left[1 - \frac{2i\frac{k}{\kappa}}{i\frac{k}{\kappa} - \cot\left(\kappa r_0 - \frac{l\pi}{2}\right)}\right] \\ &\approx e^{-2i(kr_0 - l\pi/2)} \frac{\cot(\kappa r_0 - l\pi/2) + i\frac{k}{\kappa}}{\cot(\kappa r_0 - l\pi/2) - i\frac{k}{\kappa}} \end{aligned}$$

$$\Rightarrow \delta_l = -(kr_0 - l\pi/2) + \phi$$

where

$$\tan\phi = \frac{\frac{k}{\kappa}}{\cot(\kappa r_0 - l\pi/2)}$$

Now ϕ is generally negligible when $\frac{k}{\kappa} \ll 1$, unless $\kappa r_0 - l\pi/2 = (2m+1)\pi/2$, where m is an integer. When we have this secondary case, we have resonances.

The distance between resonances is $\Delta\kappa r_0 = \pi$.

$$\Rightarrow \left[\sqrt{\frac{2m}{\hbar^2}(E + \Delta E + V_0)} - \sqrt{\frac{2m}{\hbar^2}(E + V_0)}\right] r_0 = \pi$$

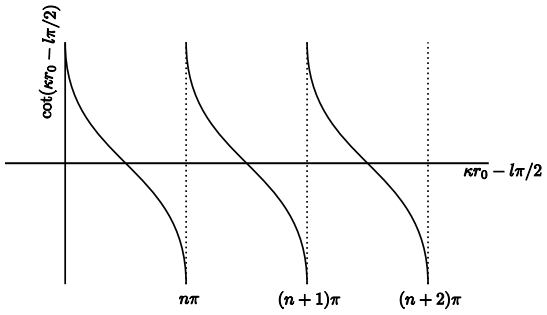
$$\Rightarrow \kappa \left[1 + \frac{m}{\hbar^2}\frac{\Delta E}{\kappa^2} - 1\right] r_0 = \pi$$

$$\Rightarrow \Delta E = \frac{\pi^2\hbar^2\kappa}{mr_0}$$

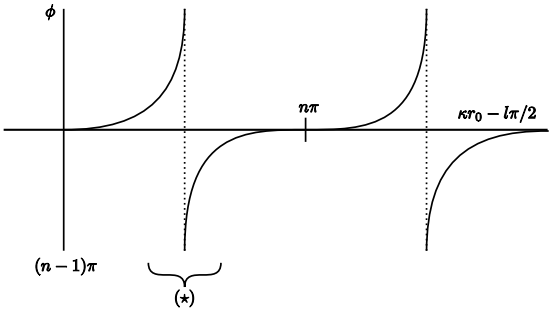
Assuming $\kappa \gg k \Rightarrow V_0 \gg E \Rightarrow \kappa^2 \approx \frac{2m}{\hbar^2}V_0 \equiv \kappa_0^2$:

$$\Rightarrow \Delta E \approx \frac{2\pi V_0}{mr_0}$$

Since



Which implies



where in the range $(\star)$, $\tan\phi$ goes to $0 \to \infty$ and $-\infty \to 0$ which corresponds to a change of π in ϕ. So $\delta_l = -(kr_0 - l\pi/2) + \phi$ increases by π each resonance. In between resonances, background scattering is determined by $\delta_l = -(kr_0 - l\pi/2) + \phi$.

Chapter 15

Relativistic Quantum Mechanics: The Dirac Equation

The Dirac equation is a relativistic description of a quantum system that includes the relativistic nature of some systems (like high-Z atoms) as well as spin and spin-orbit coupling.

15.1 Spinless Free Particles - The Klein-Gordan Equation

Recall that in deriving the Schrodinger equation, we started with the kinetic energy:

$$H = \frac{p^2}{2m}$$

and let

$$\left.\begin{array}{l} p \to \hat{p} \\ H \to i\hbar\dfrac{\partial}{\partial t} \end{array}\right\} \Rightarrow i\hbar\frac{\partial}{\partial t}\left|\psi\right\rangle = \frac{\hat{p}^2}{2m}\left|\psi\right\rangle$$

In deriving a relativistic description, let

$$H^2 = c^2p^2 + m^2c^4$$

So that the substitution of operators gives

$$\frac{\partial^2}{\partial t^2}\left|\psi\right\rangle = -\frac{1}{\hbar^2}\left(c^2\hat{p}^2 + m^2c^4\right)\left|\psi\right\rangle \qquad (\dagger)$$

This is the Klein-Gordan equation.

Remark 1: Note that we considered H^2 rather than $H = \sqrt{c^2p^2 + m^2c^4}$. This is because the former gives a symmetric description of space and time as desired by relativity. Otherwise, expanding H in a momentum basis:

$$H = mc^2\left(1 + \frac{1}{2}\frac{p^2}{m^2c^2} - \frac{1}{8}\frac{p^4}{m^4c^4} + \cdots\right)$$

gives even and odd derivatives not on an "equal footing".

Remark 2: (†) is a good description for spinless particles, but is insufficient for particles with $S \neq 0$.

15.2 Dirac Equation for Free Particle

The Dirac equation for a free particle is given by

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \left(c\hat{\boldsymbol{\alpha}}\cdot\hat{\boldsymbol{p}} + \hat{\beta}mc^2\right)|\psi\rangle \tag{1}$$

where

$$\hat{\boldsymbol{\alpha}} = \begin{pmatrix} 0 & \hat{\boldsymbol{\sigma}} \\ \hat{\boldsymbol{\sigma}} & 0 \end{pmatrix}, \qquad \hat{\beta} = \begin{pmatrix} \hat{I} & 0 \\ 0 & -\hat{I} \end{pmatrix} \tag{2}$$

where

- $\hat{\boldsymbol{\sigma}}$ is the Pauli spin matrices
- $\hat{I}$ is the 2x2 identity
- c is the speed of light

Remark 1: In the derivation of the Klein-Gordan equation, we took $H \to H^2$ to get the space-time symmetry. Here, Dirac assumed that $\sqrt{c^2p^2 + m^2c^4} \propto p+$ something without momentum to get space-time symmetry in an equation of 1st order in space and time.

$$c^2p^2 + m^2c^4 = c\hat{\boldsymbol{\alpha}}\cdot\hat{\boldsymbol{p}} + \hat{\beta}mc^2$$

where $\hat{\boldsymbol{\alpha}}, \hat{\beta}$ are determined by matching coefficients:

$$c^2\left(p_x^2 + p_y^2 + p_z^2\right) + m^2c^4 = c^2\left(\hat{\boldsymbol{\alpha}}\cdot\hat{\boldsymbol{p}}\right)^2 + mc^3\left(\hat{\boldsymbol{\alpha}}\cdot\hat{\boldsymbol{p}}\hat{\beta} + \hat{\beta}\hat{\boldsymbol{\alpha}}\cdot\hat{\boldsymbol{p}}\right) + \hat{\beta}^2m^2c^4$$

Matching coefficients gives the following relations:

1. $\hat{\alpha}_i^2 = \hat{\beta}^2 = I$ where $i = x, y, z$
2. $\hat{\alpha}_i\hat{\alpha}_j + \hat{\alpha}_j\hat{\alpha}_i = [\hat{\alpha}_i, \hat{\alpha}_j]_+ = 0$ for $i \neq j$
3. $\hat{\beta}\hat{\alpha}_i + \hat{\alpha}_i\hat{\beta} = \left[\hat{\beta}, \hat{\alpha}_i\right]_+ = 0$

Remark 2: From these relationships, we conclude that $\hat{\boldsymbol{\alpha}}, \hat{\beta}$ are traceless Hermitian matrices with eigenvalues $= \pm 1$.

Remark 3: Traceless with eigenvalues$=\pm 1 \Rightarrow$ even dimensional. But they cannot be the 2x2 Pauli matrices (since there are 4 matrices here, and there are only 3 Pauli matrices with these properties) $\Rightarrow$ try 4x4 matrices

Remark 4: The choice of $\hat{\boldsymbol{\alpha}}$ and $\hat{\beta}$ given in (2) satisfy these requirements, though it is not unique (since the properties of Remark 2 are preserved under a unitary transformation).

Remark 5: $|\psi\rangle$ in (1) is called the Lorentz Spinor and has 4 components (to be compatible with 4x4 $\hat{\boldsymbol{\alpha}}$'s and $\hat{\beta}$'s).

Remark 6: $\langle\psi|\psi\rangle$ = a constant since the Hamiltonian is Hermitian.

15.3 Electromagnetic Interactions

The classical Hamiltonian for a particle with charge q is:

$$H = \left[\left(\boldsymbol{p} - \tfrac{q}{c}\boldsymbol{A}\right)c^2 + m^2c^4\right]^{1/2} + q\Phi$$

where Φ and $\boldsymbol{A}$ are the electrodynamic scalar and vector potentials. Generalizing the Dirac equation so that $\hat{\boldsymbol{p}} \to \hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}$ and adding the electromagnetic potential energy:

$$i\hbar\frac{\partial\psi}{\partial t} = \left[c\hat{\boldsymbol{\alpha}}\cdot\left(\hat{\boldsymbol{p}} - \tfrac{q}{c}\boldsymbol{A}\right) + \hat{\beta}mc^2 + q\Phi\right]\psi \tag{1}$$

15.3.1 Electron Spin and Magnetic Moment

To see how spin and magnetic moment drop out of the Dirac equation, it is sufficient to let $\Phi = 0$ and keep only $\mathcal{O}(\frac{v}{c})^2$ terms. Let $\psi(t) = \psi e^{-iEt/\hbar}$ to find energy eigenstates. Plugging this into (1):

$$i\hbar\left(-\frac{iE}{\hbar}\right)e^{-iEt/\hbar}\psi = \left[c\hat{\boldsymbol{\alpha}}\cdot\left(\hat{\boldsymbol{p}} - \tfrac{q}{c}\boldsymbol{A}\right) + \hat{\beta}mc^2\right]e^{-iEt/\hbar}\psi$$

$$\Rightarrow E\psi = \left(c\hat{\boldsymbol{\alpha}}\cdot\hat{\boldsymbol{\Pi}} + \hat{\beta}mc^2\right)\psi \tag{2}$$

where

$$\hat{\boldsymbol{\Pi}} = \hat{\boldsymbol{p}} - \tfrac{q}{c}\boldsymbol{A} \tag{3}$$

Remark 1: $\hat{\boldsymbol{\Pi}}$ is called the kinetic momentum operator.

Remark 2: Recall that ψ is a 4 component spinor and that $\hat{\boldsymbol{\alpha}}, \hat{\beta}$ are given by

$$\hat{\boldsymbol{\alpha}} = \hat{\sigma}_x \otimes \hat{\sigma} \qquad \text{and} \qquad \hat{\beta} = \hat{\sigma}_z \otimes \hat{I}$$

which suggests that we can write

$$\psi = \begin{bmatrix}\chi\\ \varphi\end{bmatrix} \tag{4}$$

where χ and φ are 2 component spinors.

Plugging (4) into (2):

$$E\begin{bmatrix}\chi\\ \varphi\end{bmatrix} = \begin{bmatrix} mc^2\hat{I} & c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\Pi}} \\ c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\Pi}} & -mc^2\hat{I}\end{bmatrix}\begin{bmatrix}\chi\\ \varphi\end{bmatrix}$$

$$\begin{bmatrix}(E-mc^2)\hat{I} & -c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\Pi}} \\ -c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\Pi}} & (E+mc^2)\hat{I}\end{bmatrix}\begin{bmatrix}\chi\\ \varphi\end{bmatrix} = \begin{bmatrix}0\\0\end{bmatrix}$$

which gives a set of coupled equations for χ and φ:

$$(E-mc^2)\chi = c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\Pi}}\varphi \tag{5}$$

$$(E+mc^2)\varphi = c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\Pi}}\chi \tag{6}$$

From (6):

$$\Rightarrow \varphi = \frac{c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\Pi}}}{E+mc^2}\chi \tag{7}$$

Remark 3: In the non-relativistic limit,

$$\left|\frac{\varphi}{\chi}\right| = \left|\frac{c\hat{\boldsymbol{\sigma}}\cdot\left(\hat{\boldsymbol{p}}-\frac{q}{c}\boldsymbol{A}\right)}{E_s+mc^2+mc^2}\right| \approx \frac{c(mv)}{2mc^2} \sim \frac{1}{2}\frac{v}{c} \ll 1$$

where

- E_s is the Schrodinger energy $\ll mc^2$
- mv is the typical momentum

So in the non-relativistic limit, φ is the small component and χ is the big component.

$$\Rightarrow \varphi \approx \frac{\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\Pi}}\chi}{2mc} \tag{8}$$

In the non-relativistic limit, (5) becomes:

$$\begin{aligned} E_s\chi = c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\Pi}}\varphi &= \frac{1}{2m}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\Pi}}\right)\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\Pi}}\right)\chi \\ &= \frac{1}{2m}\left(\hat{\boldsymbol{\Pi}}\cdot\hat{\boldsymbol{\Pi}} + i\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{\Pi}}\times\hat{\boldsymbol{\Pi}}\right)\chi \end{aligned} \tag{9}$$

and $\hat{\boldsymbol{\Pi}}\times\hat{\boldsymbol{\Pi}} = \frac{i\hbar q}{c}\boldsymbol{B}$. So now (9) becomes

$$\left[\frac{1}{2m}\left(\hat{\boldsymbol{p}}-\tfrac{q}{c}\boldsymbol{A}\right)^2 - \frac{\hbar q}{2mc}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}\right]\chi = E_s\chi \tag{10}$$

which describes a spin $\frac{1}{2}$ particle in a magnetic field. The energy splitting (Zeemann effect) gives

$$\delta E = \pm\frac{eB}{mc}\left(\frac{\hbar}{2}\right)$$

and the picture in Fig. 15.1:

Here $2\mu_B B = 2\delta E = g\mu_B B \Rightarrow g = 2s+1$, and we see that electron spin and magnetic moment are accounted for in the Dirac equation.

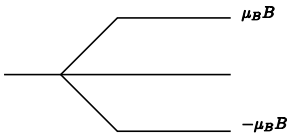


Figure 15.1: Zeemann splitting

15.4 The Dirac Equation for the Hydrogen Atom

For the hydrogen atom:

$$V = e\Phi = -\frac{e^2}{r}$$

and the Dirac equation is

$$i\hbar\frac{\partial\psi}{\partial t} = \left[c\hat{\boldsymbol{\alpha}}\cdot\left(\hat{\boldsymbol{p}} - \tfrac{q}{c}\boldsymbol{A}\right) + \hat{\beta}mc^2 - \frac{e^2}{r}\right]\psi$$

We still decompose ψ into the 2 component spinors and obtain equations for χ and φ (§15.3 (5) and (6) with $E \to E - V$).

$$(E - V - mc^2)\chi = c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\varphi \tag{1}$$

$$(E - V + mc^2)\varphi = c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\chi \tag{2}$$

Remark 1: In absence of a $\boldsymbol{B}$ field, we can let $\boldsymbol{A} = 0$ so $\hat{\boldsymbol{\Pi}} \to \hat{\boldsymbol{p}}$, and hence the above results in (1) and (2).

From (2), we have

$$\varphi = (E - V + mc^2)^{-1}c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\chi \tag{3}$$

which is substituted into (1), giving:

$$(E - \hat{V} + mc^2)\chi = c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}(E - \hat{V} + mc^2)^{-1}c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\chi \tag{4}$$

Remark 2: Note that we were careful to keep the order correct, as $\hat{\boldsymbol{p}}$ can operate of $\hat{V}$, so order *does* matter.

Remark 3: Solving (4) and plugging into (3) gives the solution to the full Lorentz spinor φ.

Remark 4: Keep $\mathcal{O}(\frac{v}{c})^2$, (4) becomes:

$$\begin{aligned}(E_s - \hat{V})\chi &= c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}(E_- - \hat{V} + 2mc^2)^{-1}c\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\chi \\ &\approx \frac{c^2}{2mc^2}\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\right)\left(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\right)\chi \\ &= \frac{1}{2m}\hat{\boldsymbol{p}}^2\chi\end{aligned}$$

which is just the non-relativistic Schrodinger equation.

15.4.1 Fine Structure

Recall that in solving the Schrodinger equation for the hydrogen atom, we resorted to perturbation theory to get the fine structure of the energy eigenspectrum (previous HW). The time structure was due to relativistic effec8ts which emerge naturally from the Dirac equation. Expanding (4) to $\mathcal{O}(\frac{v}{c})^4$ (one order higher than that required to recover the Schrodinger equation), and letting $E = E_s + mc^2$ in (4) with E_s the solution for the Schrodinger equation gives:

$$(E_s - V + 2mc^2)^{-1} = \frac{1}{2mc^2}\left(1 + \frac{E_s - V}{2mc^2}\right)^{-1} \tag{15.1}$$

$$\approx \frac{1}{2mc^2}\left(1 - \frac{E_s - V}{2mc^2}\right) \tag{15.2}$$

$$= \frac{1}{2mc^2} - \frac{E_s - V}{4m^2c^4} \tag{15.3}$$

And (4) becomes

$$(E_s - V)\chi = c\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}}\left[\frac{1}{2mc^2} - \frac{E_s - V}{4m^2c^4}\right] c\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}}\chi$$

$$\Rightarrow E_s\chi = \left[\frac{1}{2m}\underbrace{(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}})^2}_{\hat{\boldsymbol{p}}^2} + V - \frac{\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}}(E_s - V)(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}})}{4m^2c^4}\right]\chi$$

$$\Rightarrow E_s\chi = \left[\frac{\hat{\boldsymbol{p}}^2}{2m} + V - \underbrace{\frac{\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}}(E_s - V)(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}})}{4m^2c^4}}_{\text{extra piece giving fine structure}}\right]\chi \tag{5}$$

Remark 1: Note that (5) is not simply a more complicated Schrodinger equation as E_s is on both sides of the equation.

Remark 2: From §15.4.R4, the Schrodinger equation is recovered from $\mathcal{O}(\frac{v}{c})^2$, so:

$$E_s\chi = \left(\frac{\hat{p}^2}{2m} + V\right)\chi \quad \text{are} \quad \mathcal{O}(\tfrac{v}{c})^2$$

$$\Rightarrow (E_s - V)\chi = \frac{\hat{p}^2}{2m}\chi + \mathcal{O}(\tfrac{v}{c})^4$$

since

$$\frac{\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}}(E_s - V)(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}})}{4m^2c^4} \sim \frac{v^2}{c^2}(E_s - V)\chi$$

$$\sim \frac{v^2}{c^2}\left[\frac{\hat{p}^2}{2m}\chi + \mathcal{O}(\tfrac{v}{c})^4\right]$$

So in the third term of the rhs of (5), it will be sufficient to let $(E_s - V)\chi \to \frac{\hat{p}^2}{2m}\chi$. But we have

$$(E_s - V) \underbrace{\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}}}_{\text{awkward}} \chi$$

So

$$\begin{aligned}(E_s - V)\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}}\chi &= \hat{\boldsymbol{\sigma}} \cdot [(E_s - V)\hat{\boldsymbol{p}}\chi] \\ &= \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} E_s\chi + \hat{\boldsymbol{\sigma}} \cdot \left[-\hat{V}\hat{\boldsymbol{p}} + \hat{\boldsymbol{p}}\hat{V} - \hat{\boldsymbol{p}}\hat{V}\right] \\ &= \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}}(E_s - V)\chi + \hat{\boldsymbol{\sigma}} \cdot \left[\hat{p}, \hat{V}\right]\chi\end{aligned}$$

which we substitute into (5):

$$\begin{aligned}E_s\chi &= \left[\frac{\hat{p}^2}{2m} + \hat{V} - \frac{(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}})^2 \frac{\hat{p}^2}{2m} + (\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}})\left(\hat{\boldsymbol{\sigma}} \cdot \left[\hat{\boldsymbol{p}}, \hat{V}\right]\right)}{4m^2c^4}\right]\chi \\ &= \left[\frac{\hat{p}^2}{2m} + \hat{V} - \frac{\hat{p}^4}{8m^3c^2} - \frac{\hat{\boldsymbol{p}}\left[\hat{\boldsymbol{p}}, \hat{V}\right]}{4m^2c^2} - \frac{i\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} \times \left[\hat{\boldsymbol{p}}, \hat{V}\right]}{4m^2c^2}\right]\chi \\ &= \hat{H}\chi \qquad (6)\end{aligned}$$

Remark 3: (6) now looks like the Schrodinger equation!

Remark 4: On the rhs of (6), the 3rd term is the relativistic correction to the kinetic energy.

Remark 5: The 5th term can be manipulated:

$$\begin{aligned}[\hat{\boldsymbol{p}}, f(x)] &= -i\hbar\frac{\partial}{\partial x}f + i\hbar f\frac{\partial}{\partial x} \\ &= -i\hbar\left(\frac{\partial f}{\partial x}\right) - i\hbar f\frac{\partial}{\partial x} + i\hbar f\frac{\partial}{\partial x} \\ &= -i\hbar\left(\frac{\partial f}{\partial x}\right)\end{aligned}$$

$$\Rightarrow \frac{i\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\times\left[\hat{\boldsymbol{p}},\hat{V}\right]}{4m^2c^2} = \frac{-i}{4m^2c^2}\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\times\left[-i\hbar\underbrace{\nabla\left(-\frac{e^2}{r}\right)}_{+e^2\frac{\boldsymbol{r}}{r^3}}\right]$$

$$= -\frac{\hbar e^2}{4m^2c^2}\frac{1}{r^3}\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{p}}\times\boldsymbol{r}$$

$$= \frac{\hbar e^2}{4m^2c^2}\frac{1}{r^3}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{r}\times\hat{\boldsymbol{p}}$$

where it is ok to switch $\boldsymbol{r}$ and $\hat{\boldsymbol{p}}$ since the $\hat{\boldsymbol{p}}$ operator never operates on the conjugate coordinate.

$$= \frac{e^2}{2m^2c^2}\frac{1}{r^3}\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{L}}$$

$$= \hat{H}_{S.O.} \quad \rightarrow \quad \text{the spin-orbit interaction}$$

where it is ok to switch $\boldsymbol{r}$ and $\hat{\boldsymbol{p}}$ since the $\hat{\boldsymbol{p}}$ operator never operates on the conjugate coordinate.

Remark 6: The 4rth term in (6) is *not* Hermitian.

$$\Rightarrow \int |\chi|^2\, d^3r \neq \text{ constant}$$

$$\Rightarrow \chi \text{ is not a good Schrodinger wave function}$$

But what *is* required is

$$\begin{aligned}
\int \psi^\dagger \psi \, d^3r &= \int \left[|\chi|^2 + |\varphi|^2 \right] d^3r = \text{ constant} \\
&= \int \left[|\chi|^2 + \frac{(\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} \chi)^\dagger (\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} \chi)}{4m^2c^2} \right] d^3r \\
&= \int \left[|\chi|^2 + \frac{\chi^\dagger (\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}})^\dagger (\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}}) \chi}{4m^2c^2} \right] d^3r \\
&= \int \left[|\chi|^2 + \frac{\chi^\dagger \hat{\boldsymbol{p}}^2 \chi}{4m^2c^2} \right] d^3r \\
&= \int \chi^\dagger \left[1 + \frac{\hat{\boldsymbol{p}}^2}{2m^2c^2} \right] \chi \, d^3r \\
&= \int \chi^\dagger \left[\left(1 + \frac{\hat{\boldsymbol{p}}^2}{8m^2c^2} \right) \left(1 + \frac{\hat{\boldsymbol{p}}^2}{8m^2c^2} \right) \right] \chi \, d^3r \\
&= \int \chi^\dagger \left[\left(1 + \frac{\hat{\boldsymbol{p}}^2}{8m^2c^2} \right)^\dagger \left(1 + \frac{\hat{\boldsymbol{p}}^2}{8m^2c^2} \right) \right] \chi \, d^3r \\
&= \int \left[1 + \frac{\hat{\boldsymbol{p}}^2}{8m^2c^2} \chi \right]^\dagger \left[1 + \frac{\hat{\boldsymbol{p}}^2}{8m^2c^2} \chi \right] d^3r \\
&= \int |\chi_s|^2 \, d^3r
\end{aligned}$$

So to $\mathcal{O}(\frac{v}{c})^4$, χ_s has a constant norm. But now we must write (6) in terms of χ_s.

$$\chi_s = \left(1 + \frac{\hat{p}^2}{8m^2c^2} \right) \chi \tag{7}$$

Since $E_s \chi = \hat{H} \chi$ by (6), we have that

$$E_s \left(1 + \frac{\hat{p}^2}{8m^2c^2} \right)^{-1} \chi_s = \hat{H} \left(1 + \frac{\hat{p}^2}{8m^2c^2} \right)^{-1} \chi_s$$

$$\begin{aligned}
\Rightarrow E_s \chi_s &= \left(1 + \frac{\hat{p}^2}{8m^2c^2} \right) \hat{H} \left(1 + \frac{\hat{p}^2}{8m^2c^2} \right)^{-1} \chi_s \\
&\approx \left(1 + \frac{\hat{p}^2}{8m^2c^2} \right) \hat{H} \left(1 - \frac{\hat{p}^2}{8m^2c^2} \right) \chi_s \\
&= \left[\hat{H} + \frac{1}{8m^2c^2} \left(\hat{\boldsymbol{p}}^2 \hat{H} - \hat{H} \hat{\boldsymbol{p}}^2 \right) \right] \chi_s + \mathcal{O}(\tfrac{v}{c})^6 \\
&\approx \left[\hat{H} + \frac{1}{8m^2c^2} \left[\hat{\boldsymbol{p}}^2, \hat{H} \right] \right] \chi_s \\
&= \hat{H}_s \chi_s
\end{aligned} \tag{8}$$

$$\begin{aligned}
\Rightarrow \hat{H}_s &= \hat{H} + \frac{1}{8m^2c^2}\left[\hat{\boldsymbol{p}}^2, \hat{H}\right] \\
&\approx \hat{H} + \frac{1}{8m^2c^2}\left[\hat{\boldsymbol{p}}^2, \hat{V}\right] + \mathcal{O}(\tfrac{v}{c})^6 \\
\Rightarrow \hat{H}_s &= \hat{H} + \frac{1}{8m^2c^2}\left[\hat{\boldsymbol{p}}^2, \hat{V}\right] \qquad (9)
\end{aligned}$$

Remark 7: Equation (9) gives an extra term that comes from creating a suitable wavefunction with constant norm, so that (8) is a suitable Schrodinger equation that includes relativistic effects in the Dirac equation. Combining this extra term in (9) with the non-Hermitian 4rth term in (6) gives:

$$\frac{1}{8m^2c^2}\left[\hat{\boldsymbol{p}}\cdot\hat{\boldsymbol{p}}, \hat{V}\right] - \frac{1}{4m^2c^2}\hat{\boldsymbol{p}}\cdot\left[\hat{\boldsymbol{p}}, \hat{V}\right] = \frac{1}{8m^2c^2}\left[\hat{\boldsymbol{p}}\cdot\left[\hat{\boldsymbol{p}}, \hat{V}\right] + \left[\hat{\boldsymbol{p}}, \hat{V}\right]\cdot\hat{\boldsymbol{p}} - 2\hat{\boldsymbol{p}}\cdot\left[\hat{\boldsymbol{p}}, \hat{V}\right]\right]$$

where we used $[AB, C] = A[B, C] + [A, C]B$.

$$\begin{aligned}
&= \frac{1}{8m^2c^2}\left[-\hat{\boldsymbol{p}}\cdot\left[\hat{\boldsymbol{p}}, \hat{V}\right] + \left[\hat{\boldsymbol{p}}, \hat{V}\right]\cdot\hat{\boldsymbol{p}}\right] \\
&= \frac{\hbar^2}{8m^2c^2}\nabla^2\hat{V} \\
&= \frac{-e^2\hbar^2}{8m^2c^2}\nabla^2\left(\frac{1}{r}\right) \\
&= -\frac{e^2\hbar^2}{2m^2c^2}\pi\delta^3(\boldsymbol{r}) \\
&= \hat{H}_D
\end{aligned}$$

which is the Darwin term!

Remark 8: Putting these together (Relativistic Kinetic Energy, Spin-Orbit Interaction, and Darwin) gives the potentials that, in perturbation theory, resulted in the fine structure for the Hydrogen atom.

Remark 9: Recall that the Darwin term contributed when $l = 0$ and the S.O. coupling contributed only when $l \neq 0$ such that the contribution gave the same result independent of l. This is in spite of the fact that $\hat{H}_D$ has nothing to do with angular momentum. Physically, this term comes because a particle can not be localized more that $\frac{\hbar}{mc}$ (the compton wavelength).

$$V(r) \to \bar{V(r)} = \text{ some smeared average about } \vec{r}$$

Remark 10: Solving the full Dirac equation (rather than just to $\mathcal{O}(\frac{v}{c})^4$), gives the

energy spectrum:

$$E_{nj} = mc^2 \left[1 + \left(\frac{\alpha}{n - (j+\frac{1}{2}) + \left[(j+\frac{1}{2})^2 - \alpha^2 \right]^{1/2}} \right)^2 \right]^{1/2} \tag{11}$$

Expanding in powers of α:

- $\mathcal{O}(\alpha^0) \rightarrow$ rest energy
- $\mathcal{O}(\alpha) \rightarrow$ Schrodinger energy
- $\mathcal{O}(\alpha^2) \rightarrow$ fine structure (compare with perturbation results)

Remark 11: Equation (11) is still not 100% correct when compared to experiment (One can not account for Lamb shift for example). To get this correct, the $E + M$ field itself must also be quantized (i.e. the field must be treated as a bunch of harmonic oscillators).

15.5 Negative Energy Solutions

In general

$$\underbrace{\text{Relativity}}_{\substack{\text{particle production} \\ \text{with enough energy}}} + \underbrace{\text{Quantum Mechanics}}_{\substack{\text{arbitrarily enough} \\ \text{energy for short time}}} = \begin{array}{c}\text{the possible outcome of a system} \\ \text{of 1 or several particles}\end{array}$$

Question: How does Dirac theory account for this?

Answer: With Negative Energy Solutions!

For simplicity, let $\hbar = c = 1$, then the free particle Dirac equation is:

$$i\frac{\partial \psi}{\partial t} = \left(\hat{\boldsymbol{\alpha}} \cdot \hat{\boldsymbol{p}} + \hat{\beta} m \right) \psi$$

$$\psi = \begin{bmatrix} \chi \\ \varphi \end{bmatrix} \Rightarrow \begin{bmatrix} E - m & -\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} \\ -\hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} & E + m \end{bmatrix} \begin{bmatrix} \chi \\ \varphi \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

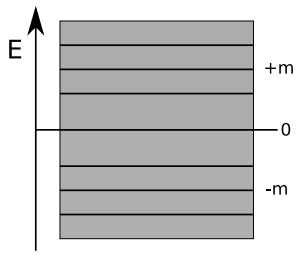
or

$$(E - m)\chi = \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} \varphi$$
$$(E + m)\varphi = \hat{\boldsymbol{\sigma}} \cdot \hat{\boldsymbol{p}} \chi$$

$$\Rightarrow \chi = \frac{\hat{\boldsymbol{p}}^2}{E^2 - m^2}\chi \Rightarrow \frac{\hat{p}^2}{E^2 - m^2} = 1$$
$$\Rightarrow E^2 = \hat{p}^2 + m^2$$
$$\Rightarrow E = \pm\sqrt{\hat{p}^2 + m^2} \tag{$\dagger$}$$

Remark 1: We can not neglect the negative energy solutions, though note that if $p = 0 \Rightarrow E = \pm mc^2$.

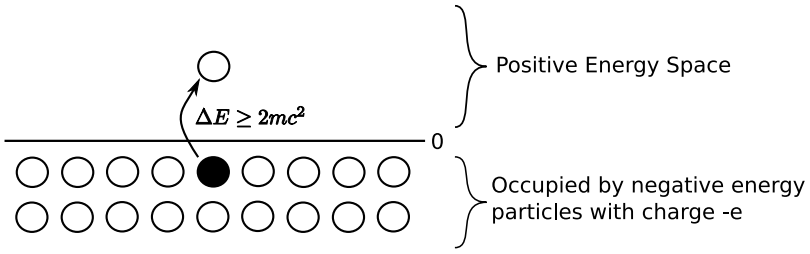
But what do we do with the negative energy solutions?



Even if $+mc^2$ states are stable, quantum fluctuations should be enough to allow transitions to negative energy states. The problem is that this is not observed.

15.5.1 Dirac Solution

The vaccuum is really occupied by fermions, which don't allow positive energy particles to occupy negative energy states (Pauli-exclusion principle). Consider



Remark 1: The filled Dirac sea is unobservable, but the hole *is* observable–it has change $+e$ and $|E| \geq mc^2$, and is called a positron.

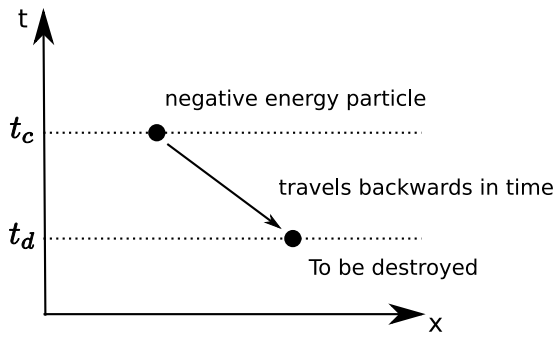
Remark 2: When an electron jumps back into the hole left in the Dirac sea, 2 particles are destroyed (an electron and a positron), but an energy $\geq 2mc^2$ is liberated in the form of a photon.

Remark 3: Note that this explanation only works if the particles are fermions. But bosons can have negative energy solutions (and the negative energy solutions of the spinless Klein-Gordan equation are what motivated Dirac to look for a first order theory in the first place).

15.5.2 Feynmann's Solution

Negative energy solutions *only* travel *backwards* in time.

Remark 1: We still have the notion of an anti-particle (positron in this case). This is how things progress:



What we *observe* is the positron (particles with positive energy) created at t_d and destroyed at t_c. This implies that the creation of the positive energy positron coincides with the destruction of the negative energy electron (and vice-versa).

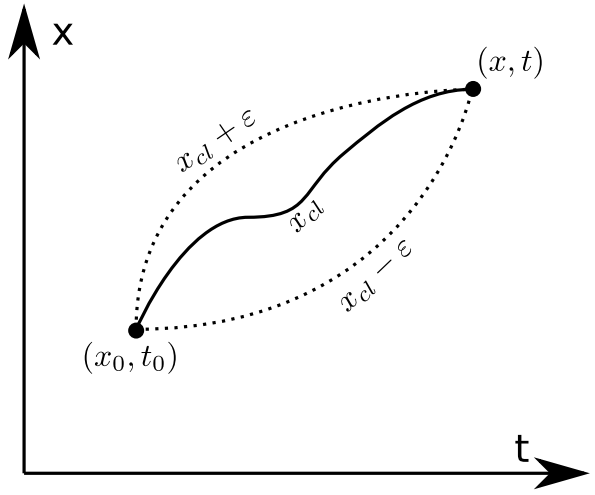
Chapter 16

Feynmann Path Integral Formulation of Quantum Mechanics

In the Schrodinger approach, we first find eigenvalues and eigenvectors of the Hamiltonian, then determine the propagator, $\hat{U}(t)$ (the full solution). In the path integral approach, $\hat{U}(t)$ is found directly.

16.1 Path Integrals - Concepts and the Classical Action

Here we consider only a single particle in 1-D (the generalization to higher dimensions is straight forward).



where the initial and final points are fixed.

Recipe:

1. Draw all the paths between (x_0, t_0) and (x, t).
2. Calculate the action $S[x, t]$ for each path.

3. $U(x,t;x_0,t_0) = A\sum_{\text{all paths}} e^{iS[x,t]/\hbar}$, where A is a normalization factor.

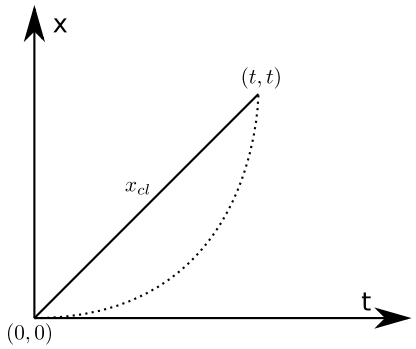
Remark 1: Recall that the action is a functional defined by

$$S = \int_{t_0}^{t} \mathcal{L}(t')\,dt' \tag{1}$$

where $\mathcal{L}(t)$ is the Lagrangian (usually $\mathcal{L} = T - U$). Also, a functional eats a function and excretes a number.

Remark 2: Note that the propagator is *not* a weighted sum, thus, the classical action does not seem to be more likely (as it should in the classical limit). However, the paths are all treated as phases, which add together constructively near the path that corresponds to the classical action, and destructively for paths away from the classical action path by more than $\frac{\pi}{\hbar}$.

Example: For a free particle with $x = t$:



Here the alternate path is $x = t^2$. Letting $(x_0,t_0) = (0,0)$ and $(x,t) = (1\text{ cm}, 1\text{ s})$:

$$S_{cl} = \int_0^1 \left[\tfrac{1}{2}m\dot{x}^2\right]\,dt \underbrace{=}_{x=t\Rightarrow\dot{x}=1} \tfrac{1}{2}m\int_0^1 dt = \tfrac{1}{2}m$$

$$S_{alt} = \int_0^1 \left[\tfrac{1}{2}m\dot{x}^2\right]\,dt = 2m\int_0^1 t^2\,dt = \tfrac{2}{3}m$$

For a classical particle, $m \sim 1$ gram, which implies that the phase changes by

$$\frac{S_{alt} - S_{cl}}{\hbar} = \left(\tfrac{2}{3} - \tfrac{1}{2}\right)\frac{m}{\hbar} = \frac{m}{6\hbar} \approx 1.6 \times 10^{26} \gg \pi$$

So we can ignore non-classical paths. For an electron, $m \sim 10^{-27}$ grams, implying that

$$\frac{S_{alt} - S_{cl}}{\hbar} = \frac{m}{6\hbar} \approx .16 \leq \pi$$

and so we can not ignore non-classical paths.

16.2 $\hat{U}(t)$ for a free particle

Recall that propagating $\hat{U}(t)$ as the solution to the time-dependent Schrodinger equation gave

$$U(x,t;x_0,t_0) \equiv U(x,t;x_0) = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{im(x-x_0)^2/2\hbar t} \tag{1}$$

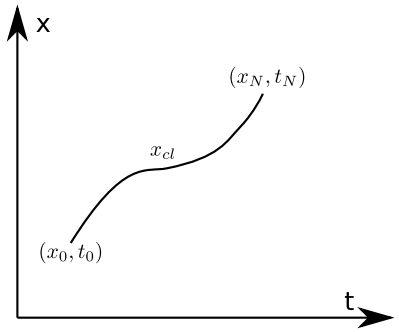
It turns out that for potentials of the form

$$V = a + bx + cx^2 + d\dot{x} + ex\dot{x}$$

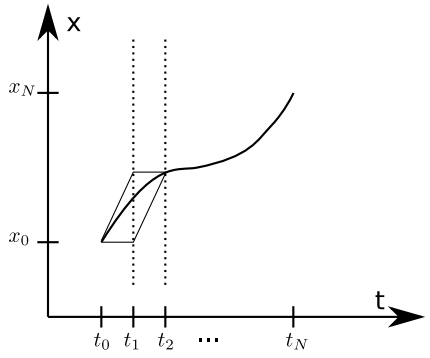
$$\Rightarrow U(t) = A(t)e^{iS_{cl}/\hbar} \tag{2}$$

with $A(t)$ a normalization (HW). A free particle is of this form, so show that (2) is sufficient to obtain the exact answer (1). For a free particle: $a = b = c = d = e = 0$. So,

$$S = \int_{t_0}^{t_N} \mathcal{L}(t)\,dt = \int_{t_0}^{t_N} \tfrac{1}{2}m\dot{x}^2\,dt \tag{3}$$



Imagine that the path is broken up into n-discrete steps so that as $N \to \infty$, the path is continuous:



Remark 1: In this picture, "draw all the paths" from (x_0, t_0) to (x_N, t_N) corresponds to using all possible values of x at a given t (like moving the "beads" up and down on an abacus).

Remark 2: "Calculate the action for all possible paths" is represented in the discretized form by

$$S = \sum_{t=0}^{N-1} \frac{m}{2} \left(\frac{x_{i+1} - x_i}{\varepsilon} \right)^2 \varepsilon \qquad \text{with} \varepsilon = \delta t \tag{4}$$

Remark 3: Finally, calculate the propagator as a "sum of all paths". Symbolically, this is written as

$$\int_{x_0}^{x_N} e^{iS[x(t)]/\hbar} \mathcal{D}[x,t] \tag{5}$$

where

$$\int_{x_0}^{x_N} \mathcal{D}[x,t] \Rightarrow \text{Integrate between all paths between } x_0, x_N$$

In this case, we write

$$\begin{aligned} U(x_N, t_N; x_0, t_0) &= \int_{x_0}^{x_N} e^{iS[x,t]/\hbar} \mathcal{D}[x(t)] \\ &= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} A \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_{N-1} \exp\left(\frac{im}{2\hbar} \sum_{i=0}^{N-1} \frac{(x_{i+1} - x_i)^2}{\varepsilon} \right) \end{aligned}$$

Scaling x by $\sqrt{\frac{m}{2\hbar\varepsilon}}$:

$$y_i = \left(\frac{m}{2\hbar\varepsilon} \right)^{1/2} x_i = \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \left(\frac{2\hbar\varepsilon}{m} \right)^{\frac{1}{2}(N-1)} \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dy_2 \cdots \int_{-\infty}^{\infty} dy_{N-1} e^{-\sum_{i=0}^{N-1} \frac{(y_{i+1} - y_i)^2}{i}}$$

Taking terms with y_1 implies

$$\int_{-\infty}^{\infty} dy_1 e^{\frac{-(y_1 - y_0)^2}{i}} e^{\frac{-(y_2 - y_1)^2}{i}} = \sqrt{\frac{i\pi}{2}} e^{\frac{-(y_2 - y_0)^2}{2i}}$$

Inserting this result into the next integral...

$$\sqrt{\frac{i\pi}{2}} \int_{-\infty}^{\infty} dy_2 e^{-(y_3 - y_2)^2/i} e^{-(y_2 - y_0)^2/2i} = \left(\frac{(i\pi)^2}{3} \right)^{1/2} e^{-(y_3 - y_0)^2/3i}$$

Doing all the $N-1$ integrations gives:

$$\begin{aligned} U(x_N, t_N; x_0, t_0) &= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} A \left(\frac{2\hbar\varepsilon}{m} \right)^{\frac{1}{2}(N-1)} \frac{(i\pi)^{\frac{1}{2}(N-1)}}{N^{1/2}} e^{-(y_N - y_0)^2/Ni} \\ &= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} A \left(\frac{2i\pi\hbar\varepsilon}{m} \right)^{(N-1)/2} N^{-1/2} e^{-(x_N - x_0)^2 m/2iN\hbar\varepsilon} \\ &= \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} A \left(\frac{2i\pi\hbar\varepsilon}{m} \right)^{N/2} \left(\frac{m}{2i\pi\hbar N\varepsilon} \right)^{1/2} e^{-(x_N - x_0)^2 m/2i\hbar N\varepsilon} \end{aligned}$$

Remark 4: Taking the limit $N \to \infty$ and $\varepsilon \to 0$ gives $N\varepsilon = t$, which is the exact answer in (1) *if*

$$A = \left(\frac{2i\pi\hbar\varepsilon}{m}\right)^{-N/2}$$

This means we can write

$$\int \mathcal{D}[x,t] \equiv \lim_{\substack{N\to\infty \\ \varepsilon\to 0}} \left(\frac{m}{2i\pi\hbar\varepsilon}\right)^{1/2} \int_{-\infty}^{\infty} \frac{dx_1}{\left(\frac{m}{2i\pi\hbar\varepsilon}\right)^{1/2}} \int \cdots \int_{-\infty}^{\infty} \frac{dx_{N-1}}{\left(\frac{m}{2i\pi\hbar\varepsilon}\right)^{1/2}} \tag{6}$$

Remark 5: The propagator, $U(x_f, t_f; x_i, t_i)$ is sometimes called the Feynmann amplitude.