Proceedings of the International School of Physics "Enrico Fermi" Course CXXI, eds. R. A. Broglia and J. R. Schrieffer (North Holland, Amsterdam, 1994) p. 31

Strong-Coupling Approaches to Correlated Fermions.

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1. – Strongly correlated lattice electrons.

1·1. *Introduction.* – Condensed-matter physics involves the study of interacting many-particle systems. Due to the structure of matter it is, therefore, to a large extent the physics of many-*electron* systems. Their theoretical investigations are notoriously difficult—particularly in the dimensions most interesting to us, *i.e.* $d = 2$ and 3. Hence many fundamental questions are still open. These difficulties are well known from a long time already, and exactly five years ago, in the introduction of his lectures here in Varenna, ANDERSON [1] presented an authoritative and fascinating account of the development of the theory of strongly correlated electron systems during 1937-87.

Due to the discovery of high-T_c superconductivity and the unprecedented activity triggered by it, the entire community suddenly realized that, in spite of many years of research, some of the most basic problems in condensed-matter physics were not yet understood. In particular, it soon became clear that high-T_c superconductivity had to be the result of an interplay between various different phenomena which were not yet sufficiently understood even by themselves. These phenomena include i) the generation of magnetic correlations as a consequence of strong interactions between electrons and the influence of mobile vacancies on such magnetic states, ii) the particular behaviour of electrons in the vicinity of a Mott-Hubbard metal-insulator transition, iii) the effect of (static) disorder on the correlated behaviour of electrons, iv) the peculiarities of two-dimensional Fermi systems, and, of course, v) the preconditions for superconductivity in a strongly correlated system. In this respect the discovery of high-T_c superconductivity had a sobering effect. Suddenly the new motto was «back to the roots», and there was general consensus about the need for *controlled* ap-

proximations, etc. The ensuing concerted research efforts during the last five years have provided significant new insight into some of these fundamental questions, although we are still far away from a satisfactory situation.

Most of the questions listed above involve the presence of intermediate or strong interactions between the electrons. Consequently, a large part of recent theoretical investigations of correlated electron systems—perhaps the largest part—dealt with strong-coupling approaches. In view of the plethora of available material the title of my lectures is bound to lead to false expectations. It is clearly impossible to present in four lectures a half-way adequate account of all the concepts, ideas, techniques and physical results developed in the course of even the most recent investigations—in particular since these lectures are supposed to have pedagogical value. I am, therefore, bound to limit myself to a presentation of only a few strong-coupling approaches. By this selection I do not wish to imply that these approaches are necessarily the most important, reliable, potent or promising ones—it is simply a limitation by necessity. The two recent books on correlated electron systems by FRADKIN [2] and FULDE [3] provide extensive discussions of several strong-coupling approaches from quite different perspectives, and I refer the reader to these books for some approaches not discussed by me, *e.g.* effective field-theoretical models and gauge field theories [2], or Liouville projection techniques [3].

To elucidate the typical problem involved in strong-coupling approaches I will concentrate on the Hubbard model and its generalization, since it is the generic model for correlated lattice fermions. I will try to point out and clarify, using different perspectives and methods, why it is precisely the Hubbard interaction which makes the strong-coupling approach so difficult. For pedagogical reasons I will first discuss the problem of a single vacancy in a quantum-mechanical spin background and will then present a discussion of variational wave functions, especially Gutzwiller-type wave functions, because they are explicit, conceptually simple and physically intuitive and provide immediate insight into almost all fundamental questions of the strong-coupling problem, without demanding a solid background of rather complicated techniques. These two topics have been addressed already five years ago by RICE [4]; however, since then considerable new insight has been gained which I wish to present, too. I will then discuss a projection method which employs auxiliary («slave») particles to enforce the local constraints in the strong-coupling limit. We will find intimate connections between the mean-field results for slave bosons and Gutzwiller-type wave functions. Finally, I will discuss the concept of a dynamical mean-field theory for strongly correlated electrons, *i.e.* a nonperturbative approach, as obtained by an exact solution in the limit of high spatial dimensions ($d \to \infty$). This will lead us to an effective, dynamical single-site problem of considerable complexity. Although the topics of the four lectures are all different, the emerging *physics* is closely related. It is my intention to stress these connections, *i.e.* the common features, as much as possible.

1·2. *Weak vs. strong.* – I will begin with some very elementary points which are none the less important enough to warrant recapitulation. For the notion of «strong» *vs.* «weak» coupling to be meaningful one needs a model consisting of at least two parts, *e.g.*

$$\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{I}} \tag{1.1}$$

(a hat always refers to an operator). Here $\hat{H}_{\text{kin}}$ is a kinetic part, which is of purely quantum-mechanical origin, and $\hat{H}_{\text{I}} = \lambda \hat{V}$ is the interaction part, with λ as a dimensionless coupling parameter; $\lambda = 0$ is supposed to correspond to the non-interacting case. In the ground state we refer to $|\lambda| \ll 1$ as the «weak-coupling limit» and to $|\lambda| \gg 1$ as the «strong-coupling limit». Note that in the case of a model with only one term, *e.g.* the Heisenberg model

$$\hat{H} = -J \sum_{\langle \boldsymbol{R}_i, \boldsymbol{R}_j \rangle} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j \tag{1.2}$$

which describes a nearest-neighbour (nn) interaction between *localized* spins, the coupling constant J can always be set ± 1, depending on the sign of J. Here a distinction between weak and strong coupling makes no sense. While the kinetic energy of noninteracting particles is only simple in momentum space, the physical origin of the interaction usually implies that the interaction term is only simple in position space. Hence the generic case is $[\hat{H}_{\text{kin}}, \hat{H}_{\text{I}}] \neq 0$, *i.e.* there is a nontrivial competition between the two terms. It is then clear that in the weak-coupling limit the $\boldsymbol{k}$ (*i.e.* «band») aspects dominate, while for strong coupling the *positional order of itinerant quantum-mechanical particles* is stressed. This is the origin of the main difficulties arising in any strong-coupling approach.

1·3. *The Hubbard model.* – The generic model for interacting lattice fermions of the type (1.1) is the one-band, spin-1/2 Hubbard model [5-7] (for historical remarks, see [1]), where

$$\hat{H}_{\text{kin}} = -t \sum_{\langle \boldsymbol{R}_i, \boldsymbol{R}_j \rangle} \sum_{\sigma} \hat{c}_{i\sigma}^{+} \hat{c}_{j\sigma} = \sum_{\boldsymbol{k}, \sigma} \varepsilon_{\boldsymbol{k}} \hat{n}_{\boldsymbol{k}\sigma} , \tag{1.3a}$$

$$\hat{H}_{\text{I}} = U \sum_{\boldsymbol{R}_i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} = U \sum_{\boldsymbol{k}, \sigma} \hat{\rho}_{\boldsymbol{k}\uparrow} \hat{\rho}_{-\boldsymbol{k}\downarrow} . \tag{1.3b}$$

Here $\hat{c}_{i\sigma}^{+}$ ($\hat{c}_{i\sigma}$) are creation (annihilation) operators of electrons with spin σ at site $\boldsymbol{R}_i$, and $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^{+} \hat{c}_{i\sigma}$. The corresponding quantities in $\boldsymbol{k}$-space are $\hat{a}_{\boldsymbol{k}\sigma}^{+}$ ($\hat{a}_{\boldsymbol{k}\sigma}$) and $\hat{n}_{\boldsymbol{k}\sigma}$. The Fourier transform of the kinetic energy in (1.3*a*) involves the dispersion $\varepsilon_{\boldsymbol{k}}$, and $\hat{\rho}_{\boldsymbol{k}\sigma} = L^{-1/2} \sum_{\boldsymbol{q}} \hat{a}_{\boldsymbol{q}+\boldsymbol{k},\sigma}^{+} \hat{a}_{\boldsymbol{q},\sigma}$ is the Fourier transform of $\hat{n}_{i\sigma}$, with L as the number of lattice sites. As mentioned above, $\hat{H}_{\text{kin}}$ is simple in $\boldsymbol{k}$-space, while $\hat{H}_{\text{I}}$ is only simple in position space. With

$$\hat{D}_i = \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \tag{1.4a}$$

as the number operator for double occupancy of a lattice site, the Hubbard model takes the form

$$\hat{H} = \sum_{k,\sigma} \varepsilon_k \hat{n}_{k\sigma} + U \sum_i \hat{D}_i \,. \tag{1.4b}$$

Here the kinetic energy is diagonal in k-space ($\hat{n}_{k\sigma}^2 = \hat{n}_{k\sigma}$) and the interaction energy is diagonal in position space ($\hat{D}_i^2 = \hat{D}_i$). Considering the ground state, it would be energetically favourable to introduce constraints in real space (*i.e.* $\langle \hat{D}_i \rangle = 0$) to minimize the interaction energy. However, the kinetic energy prefers maximal mobility of the particles, *i.e.* the absence of constraints. This clearly expresses the fact that $[\hat{n}_{k\sigma}, \hat{D}_i] \neq 0$.

In the weak-coupling limit ($U \ll t$) the starting point is the Fermi gas in k-representation. In principle, a perturbation expansion in U/t can be performed, using standard techniques, since $\hat{H}_{\text{kin}}$ is a one-particle operator and Wick's theorem is applicable. (The range of validity of such an expansion is a different matter [8].) On the other hand, in the strong-coupling limit, where double occupancy of lattice sites is suppressed, a real-space picture is more helpful. Indeed, in position space the Hilbert space for the Hubbard model may be simply written as a tensor product over the four possible states at a lattice site R_i

$$\mathcal{H} = \bigotimes_{R_i} \text{span}\{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}_i \,. \tag{1.5}$$

A strong-coupling approach should, therefore, take the $U = \infty$ limit, where $\hat{D}_i = 0$, as a starting point, or else the «atomic limit», *i.e.* $t = 0$. (Note that these limits are in general very different, since $t = 0$ is not *a priori* related to strong coupling.) However, there exist some well-known difficulties, caused precisely by the structure of the Hubbard interaction, which make a straightforward application of these approaches impossible: namely, at $U = \infty$ the ground state has an infinite degeneracy (2^L in the case of a half-filled band, *i.e.* $N = L$). Hence the ground state cannot simply be obtained by degenerate perturbation theory in t/U, since this requires first the exact solution of an effective Hamiltonian for $U \gg t$ (the «t-J model»; see below) which, however, is not much simpler than the Hubbard model itself. It is, therefore, necessary to work with a *restricted* Hilbert space $\mathcal{H}^{\text{restr}}$, where doubly occupied sites are excluded. This is very difficult to incorporate if one starts from the noninteracting case (where particles obey simple commutation rules). One must, therefore, *project* onto $\mathcal{H}^{\text{restr}}$, the allowed part of $\mathcal{H}$. However, projected operators usually do not obey canonical commutation rules; besides that Wick's theorem is generally not applicable.

The requirement of projection and the ensuing problems are the central theme of any strong-coupling approach.

1·4. *The t-J model.* – We now want to derive an «effective» model which is equivalent to the Hubbard model in the limit $U \gg t$; naturally we expect this

model to be simpler than the full Hubbard model and thus easier to investigate. The corresponding transformation can be obtained in several ways. Perhaps the most intuitive method is to use a straightforward projection onto the Hilbert space without doubly occupied sites («*d*-sites») as first discussed by BULAEVSKII, NAGAEV and KHOMSKII [9]; for details see ref. [3] and [10]. In the extreme limit $U = \infty$ the effective Hamiltonian is simply given by

$$\hat{H}_{\text{eff}}^{U=\infty} \equiv \hat{H}_t = \hat{P}\hat{H}_{\text{kin}}\hat{P}\,, \tag{1.6a}$$

where

$$\hat{P} = \prod_{\boldsymbol{R}_i} \hat{P}_i\,, \qquad \hat{P}_i = 1 - \hat{D}_i\,, \tag{1.6b}$$

is the projection operator ($\hat{P}^2 = \hat{P}$) eliminating all states with *d*-sites, *i.e.* $\hat{D}_i\hat{P} = \hat{P}\hat{D}_i = 0$. Equation (1.6*a*) says that we first project with $\hat{P}$, then apply $\hat{H}$ (*i.e.* $\hat{H}_{\text{kin}}$) and then project again with $\hat{P}$ to eliminate those new states with a *d*-site which were generated by the action of the kinetic-energy operator. Due to $\hat{P}_i\hat{c}_{i\sigma}^{+} = (1 - \hat{n}_{i,-\sigma})\hat{c}_{i\sigma}^{+} \equiv \hat{X}_{i\sigma}^{+}$ one obtains

$$\hat{H}_t = -t \sum_{\langle \boldsymbol{R}_i, \boldsymbol{R}_j \rangle} \sum_{\sigma} (1 - \hat{n}_{i,-\sigma})\hat{c}_{i\sigma}^{+}\hat{c}_{j\sigma}(1 - \hat{n}_{j,-\sigma})\,, \tag{1.7a}$$

$$= -t \sum_{\langle \boldsymbol{R}_i, \boldsymbol{R}_j \rangle} \sum_{\sigma} \hat{X}_{i\sigma}^{+}\hat{X}_{j\sigma}\,, \tag{1.7b}$$

where the remaining projection operators $\hat{P}_m$, $m \neq i, j$, are omitted for clarity; so we have to keep in mind that $\hat{H}_t$ acts only on the subspace of states without *d*-sites. $\hat{H}_t$ describes the hopping of a σ-electron to an empty site as shown in fig. 1.1*a*); equivalently, this may be viewed as the hopping of an *e*mpty site («*e*-site») or «hole» in opposite direction. This requires that the number of electrons $N = N_{\uparrow} + N_{\downarrow} < L$, *i.e.* $\delta \equiv 1 - n > 0$, with $n = N/L$. It is a remarkable fact that in the limit of $U = \infty$ a *single* hole can move at all. This is a consequence of the purely local nature of the Hubbard interaction!

The representation of $\hat{H}_t$ in (1.7*b*) in terms of the composite operator $\hat{X}_{i\sigma}$ is particularly concise. However, $\hat{X}_{i\sigma}$ does not have canonical commutation rules and hence the apparent simplicity has no immediate advantage. We will come back to such a representation in sect. 3.

In the limit of large, but finite U ($U \gg t$) *d*-sites will exist, too. Since «real» *d*-sites carry an energy U, they are strongly suppressed and hence can be neglected. Double occupancies may, therefore, only exist as *virtual* (*i.e.* intermediate) states: creation and consecutive destruction of a *d*-site must occur in the same process. The effective Hamiltonian is then given by

$$\hat{H}_{\text{eff}}^{U \gg t} \equiv \hat{P}\left[\hat{H}_{\text{kin}} - \hat{H}_{\text{kin}}\,\frac{1-\hat{P}}{U}\,\hat{H}_{\text{kin}}\right]\hat{P} + \mathcal{O}\left(\frac{t^3}{U^2}\right). \tag{1.8}$$

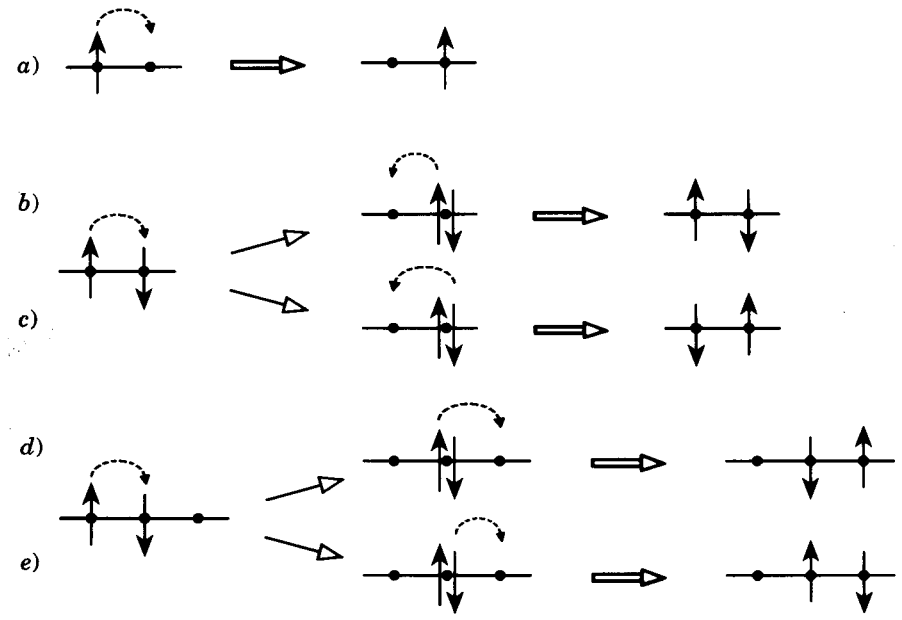

Fig. 1.1. – Hopping processes of a spin in the Hubbard model at $U \gg t$; *a*) hopping at $U = \infty$; *b*) and *c*) spin exchange process; *d*) and *e*) three-site contributions.

The second term in the parenthesis describes precisely the virtual process discussed above (the minus sign indicates that thereby energy is gained): first we project onto states without any d-sites, then we apply $\hat{H}$ (*i.e.* $\hat{H}_{\text{kin}}$) which leads to states with exactly one d-site. We now project onto these latter states (the ones without d-sites are already included in the first term in (1.8)) by applying $1 - \hat{P}$, and then use $\hat{H}_{\text{kin}}$ once more to annihilate the d-site again; the intermediate energy of this process is U and appears in the denominator. Finally, $\hat{P}$ is applied to make sure that we are again in the subspace without double occupancy. The second term in (1.8) is then clearly of order t^2/U small and describes the hopping processes shown in fig. 1.1*b*)-*e*). The ones in *b*), *c*) are possible even for $\delta = 0$ and describe *spin exchange* (including a spin flip in *c*)), while those in *d*), *e*) require the presence of an e-site for the d-site to relax («three-site contribution»); for $\delta \ll 1$ the energy gain due to the latter process is, therefore, a factor δ smaller than that due to the exchange process. The figures clearly express the fact that for $U \gg t$ we deal with the creation of a virtual pair of d-e-sites («vacuum polarization»). They also elucidate the procedure of degenerate perturbation theory required to calculate the t^2/U contribution. For $\delta = 0$ the spin exchange contributions correspond to a nearest-neighbour antiferromagnetic coupling of $S = 1/2$ Heisenberg spins. An explicit evaluation of (1.8) in the limit

$\delta \ll 1$, therefore, leads to the effective Hamiltonian [9-12]

$$\hat{H}_{\text{eff}}^{U \gg t} \equiv \hat{H}_{tJ} = \hat{H}_t + J \sum_{\langle R_i, R_j \rangle} \left[\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - \frac{1}{4} \hat{n}_i \hat{n}_j \right] + O\left(\frac{\delta t^2}{U}, \frac{t^3}{U^2} \right). \tag{1.9}$$

This is the so-called «t-J model», where $J = 4t^2/U$ (the summation is supposed to extend over nearest-neighbour bonds) and $\hat{\mathbf{S}}_i = (1/2) \sum_{\sigma\sigma'} \hat{c}_{i\sigma}^{+} (\hat{\boldsymbol{\sigma}})_{\sigma\sigma'} \hat{c}_{i\sigma'}$ is the spin operator, with $\hat{\boldsymbol{\sigma}}$ as the vector of Pauli matrices. The term $\hat{n}_i \hat{n}_j$, where $\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$, is usually discarded, since $\langle \hat{n}_i \rangle = 1$ for $\delta = 0$. In (1.9) we did not include the three-site contributions (see, for example, [13]); indeed they are almost always neglected—purely for reasons of convenience. However, the mere fact that they are an order δ smaller than the J-term in (1.9) does not guarantee that they are actually unimportant. This point is still open.

An equivalent derivation of the t-J model makes use of a unitary transformation as in the Schrieffer-Wolff transformation [14] for the single-impurity Anderson model, namely [10-12]

$$\hat{H}_{\text{eff}} = \exp[i\hat{S}] \hat{H} \exp[-i\hat{S}] = \hat{H} + i[\hat{S}, \hat{H}] + \dots . \tag{1.10}$$

Here $\hat{S}$ is determined by the requirement that the application of $\hat{H}_{\text{kin}}$ on states without d-sites only leads to virtual d-sites and not to a real mixing of Hubbard bands with different numbers of d-sites.

The derivation of the t-J model may lead to the following question: how can the t-J model, which works in the subspace without d-sites, be equivalent to the large-U Hubbard model for which the number of doubly occupied sites $\langle \hat{D} \rangle$ is clearly finite for all $U < \infty$? The answer can be deduced by considering the ground-state energy expressions

$$E_0 = \langle \Psi_{\text{HM}} | \hat{H} | \Psi_{\text{HM}} \rangle \stackrel{!}{=} \langle \Psi_{\text{eff}} | \hat{H}_{\text{eff}} | \Psi_{\text{eff}} \rangle . \tag{1.11}$$

Here $|\Psi_{\text{HM}}\rangle$ and $|\Psi_{\text{eff}}\rangle$ are supposed to represent the exact ground-state wave functions for the Hubbard model at $U \gg t$ (which contains states with d-sites) and for the t-J model (without d-sites), respectively. These are *different* wave functions, but they are related by $|\Psi_{\text{eff}}\rangle = \exp[i\hat{S}] \, |\Psi_{\text{HM}}\rangle$, where the factor $\exp[i\hat{S}]$ removes the contributions with d-sites from $|\Psi_{\text{HM}}\rangle$. Hamiltonian and wave function are hence closely linked. Working with $\hat{H}$ implies that E_0 is always determined by spin and density correlations in $|\Psi_{\text{HM}}\rangle$, while working with $\hat{H}_{\text{eff}}$ means that, at least for $\delta = 0$, E_0 is determined only by the *spin* correlations in $|\Psi_{\text{eff}}\rangle$. Although for $\delta > 0$ density correlations become important even in $|\Psi_{\text{eff}}\rangle$, they still do not involve d-sites. This stresses again the advantage of an effective model.

Unfortunately the t-J model is not really significantly simpler than the Hubbard model itself. Its *structure* is simple, reflecting the local character of the underlying Hubbard interaction. But it is precisely the *absence* of a more restrictive interaction that leads to complications. In particular, it implies that i)

there is a macroscopic spin degeneracy, ii) even at $U = \infty$ a single hole can move, iii) virtual states involve only 2 particles. It is instructive to compare this with the situation for a considerably simpler model, namely spinless fermions with nearest-neighbour interaction [15-17]

$$\hat{H}_{\mathrm{SF}} = \sum_{\langle R_i, R_j \rangle} (-t\hat{c}_i^{+}\hat{c}_j + V\hat{n}_i\hat{n}_j). \tag{1.12}$$

Such a model may be used to describe ferro (or ferri)-magnetic electronic systems where, for example, the down-spin bands are filled and only an up-spin band needs to be considered, as is the case of magnetite (Fe_3O_4) [18]. The effective model for $V = \infty$ is again given by (1.6*a*) where now the operator $\hat{P}$ projects onto the subspace of states without particles at nearest-neighbour positions. Hence $\hat{P}$ tests the entire neighbourhood of every site which is obviously much more restrictive than (1.6*b*). For the ground state on a hypercubic lattice in d dimensions it is then easy to see that i) for $n = 1/2$ the particles assume a checkerboard structure, *i.e.* there is only a *twofold* degeneracy; ii) for $n < 1/2$ it takes at least $2d - 1$ vacancies for motion to be possible at all; iii) for $V \gg t$ intermediate states involve $2d$ particles, and the form of the exchange term corresponding to the spin-spin interaction in (1.9) is quite complicated. *Although* the effective large-V model has a much more complicated form than $\hat{H}_{tJ}$, we will later see that the physics involved is considerably simpler, since for $d \to \infty$ the Hartree approximation becomes exact. This is a direct consequence of the non-Hubbard interaction.

The t-J model, (1.9), has been derived from the Hubbard model in the limit $J \ll t$. It may, however, also be viewed as an interesting *new* model with arbitrary J. For $t = 0$ it corresponds to the Heisenberg model, which is quite well understood. For $J = 0$ it describes hopping of holes and can be solved exactly in $d = 1$, since in this case the holes correspond to *noninteracting*, spinless fermions [19, 20]. For other dimensions, or even on a Bethe lattice, no exact solutions of $\hat{H}_t$ for thermodynamically relevant situations exist. The full t-J model is then even more difficult and analytic investigations have to resort to limiting cases, *e.g.* to $d = 1$ (see Haldane's lectures during this school) or to the dynamics of a single hole (see below), etc. In general, approximations have to be employed. One possiblity is to make use of the simplifications that occur when some parameter (*e.g.*, the length of a spin S, the spin degeneracy N, the spatial dimension d, etc.) is taken to be large (in fact, infinite). Investigations in such limits may provide valuable insight into the fundamental properties of a system even when this parameter is *not* large. Another possibility is to introduce new constituents or composites of the original electrons. By «lumping» the (hopefully) essential physics into new entities, decoupling approximations are hoped to be accurate enough to describe important aspects of the problem correctly. The usual strategy is, therefore, to perform some approximation, compare with experiment and, if consistent, go on (and only ask later why the approximation

was good), and otherwise work out a new approximation scheme. This is a purely pragmatic approach, enforced by the complexity of quantum-mechanical many-body systems.

1·5. *Hole motion in the t-J model.* – The spin exchange term in (1.9) may be written as

$$\hat{H}_J = J \sum_{\langle R_i, R_j \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \,, \tag{1.13a}$$

$$= \sum_{\langle R_i, R_j \rangle} \left[J_z \hat{S}_i^z \hat{S}_j^z + \frac{1}{2} J_\perp (\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+) \right]. \tag{1.13b}$$

The first term in (1.13*b*) describes Ising spins, while the second contains the spin-flip terms. In the *t-J* model one has $J_z = J_\perp$. However, in the limit of large spin S or large dimensions d (see below) the spin-flip terms disappear, which effectively corresponds to $J_\perp = 0$ (indeed, for the Heisenberg model both limits lead to the classical case[21]). Neglecting quantum spin fluctuations, there are three basic types of spin configurations possible for the *t-J* model:

1) *antiferromagnetic, i.e. Néel* (N), for $T, \delta \cdot t \ll J$ and $\delta \ll 1$ in $d \geq 3$;

2) *random* (R), for $T \gg \delta \cdot t, J$ such that all spin configurations appear with the same probability;

3) *ferromagnetic* (F), for $T = 0$, $J = 0$ and a single hole; this is the Nagaoka state[22], *i.e.* the saturated ferromagnet. For a finite concentration of holes, $\delta > 0$, the stability of the ferromagnetic state is far from clear (see below).

The effects of spin fluctuations have, for example, been considered by KANE, LEE and READ[23] and DAGOTTO *et al.*[24].

To leading order in δ hole-hole correlations may be expected to be negligibly small. In this case the simplest, nontrivial problem is to study the behaviour of a *single* hole in a given spin background and calculate quantities such as the density of states (DOS) $N(E)$, the spectral function $\rho_k(E)$, the conductivity $\sigma(\omega)$, etc. (For concise summaries of the results obtained so far see, for example, the introductory sections of the articles by ELSER, HUSE, SHRAIMAN and SIGGIA[25] and LIU and MANOUSAKIS[26].) This restricted problem is still physically relevant, since single-particle excitations in magnetic insulators can actually be studied by photoemission and inverse-photoemission spectroscopy. It should be noted, however, that, with the exception of the ferromagnetic background, *none* of the above quantities can be calculated exactly in $1 < d < \infty$. One of the problems is that the dynamics of a hole and the structure of the spin background are not independent aspects, but are self-consistently linked: the spin background determines the motion of the vacancy, which in turn affects this background. The latter effect is rather subtle. For example, on the basis of a semiclassical analysis SHRAIMAN and SIGGIA[27] found that the motion of a vacancy

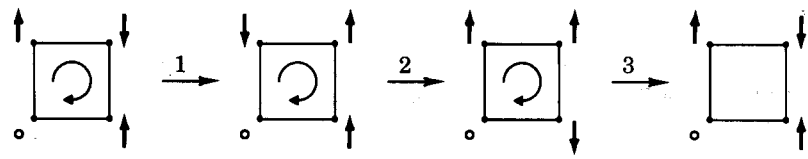

Fig. 1.2. – Three circulations are necessary for a hole to restore the Néel configuration on a square.

in a quantum antiferromagnet generates a transverse *distortion* of the background spins with dipolar symmetry. This long-range distortion may be viewed as a «twist» in the direction of the staggered order parameter of the spin background. It leads to a dipolar backflow of magnetization in close analogy to the roton excitation in superfluid ^{4}He.

On an approximate level the self-consistency between the vacancy motion and the structure of the spin background may be decoupled. In the following the hole dynamics will, therefore, be investigated for a *given* background (*e.g.*, a Néel state). We first consider the hole dynamics in the extreme limit $U = \infty$, *i.e.* $J = 0$. Even this restricted problem cannot be solved exactly. The reason for the difficulty is that the motion of the hole scrambles up the spins! Indeed, a hole is not a simple Bloch state, and thus its motion leads to a complicated many-body problem. This is illustrated in fig. 1.2 for a hole in a Néel background on a square lattice. The hole has to circulate around a square *three* times, *i.e.* has to hop 12 times, to restore the spin background. Any motion of a hole, therefore, produces a «string» of flipped spins along its path. By contrast, in the ferromagnetic background the hole is effectively free.

To calculate the DOS of a hole for a fixed spin configuration we need to know its single-particle Green function

$$G_{ij}^{X}(z) = \sum_{\sigma} \langle X | \hat{c}_{i\sigma}^{+} \frac{1}{z - \hat{H}_{tJ}} \hat{c}_{j\sigma} | X \rangle , \tag{1.14}$$

which is the probability amplitude for the hopping from $\boldsymbol{R}_j$ to $\boldsymbol{R}_i$. Here z is the complex frequency and $|X\rangle$ describes the spin configuration (here $X = \mathrm{N}, \mathrm{F}, \mathrm{R}$). The spectral function and the DOS are then given by

$$\rho_{ij}^{X}(\omega) = -\frac{1}{\pi} \operatorname{Im} G_{ij}^{X}(\omega + i0^{+}) , \tag{1.15a}$$

$$N^{X}(\omega) = \rho_{ii}^{X}(\omega) . \tag{1.15b}$$

As shown by NAGAOKA [22], this Green function may be written as

$$G_{ij}^{X}(z) = \frac{1}{z} \left[\delta_{ij} + \sum_{n=1}^{\infty} A_{ij,n}^{X} \left(\frac{-t}{z} \right)^{n} \right], \tag{1.16}$$

where $A_{ij,n}^{X}$ is the number of distinct paths of a hole from $\boldsymbol{R}_j$ to $\boldsymbol{R}_i$, consisting of n

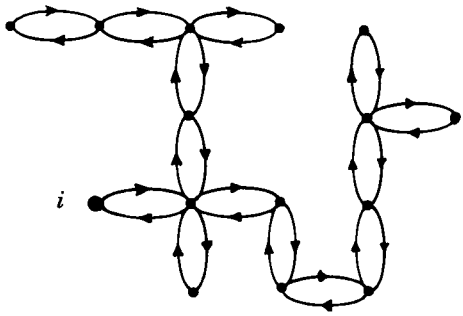

Fig. 1.3. – Self-retracing path.

steps, which leave $|X\rangle$ *unchanged* (except for $\boldsymbol{R}_i$ and $\boldsymbol{R}_j$ themselves, of course). The calculation of (1.16) hence requires the investigation of «background-restoring paths». We first consider the case $i = j$, *i.e.* when the hole returns to its starting point.

In a ferromagnetic background *every* path is background restoring. Up to a phase factor in the case of odd n, a hole, therefore, shows *free*-particle behaviour and the DOS is given by

$$N^{\mathrm{F}}(\omega) = N(\omega), \tag{1.17}$$

where $N(\omega)$ is the free DOS. By contrast, for the Néel and random background and general n the calculation of $A^X_{ii,n}$ is not possible, because the contribution of *loops* is too complicated. Consequently, BRINKMAN and RICE [28] introduced an approximation in which loops are neglected altogether. In this «retraceable-path approximation» (rpa) a hole moves into the spin background and returns to its starting point by exactly *retracing* its path as shown in fig. 1.3. These paths are naturally background restoring for *all* spin configurations. Hence the rpa becomes exact in $d = 1$ and on a Bethe lattice where loops do not exist by construction. Within the rpa the local Green function is found to be given by

$$G^{\mathrm{rpa}}_{ii}(\omega) = \frac{1}{2}\,\frac{\omega(Z-2) - Z[\omega^2 - 4(Z-1)t^2]^{1/2}}{Z^2t^2 - \omega^2}, \tag{1.18}$$

where Z is the number of nearest neighbours (coordination number); this immediately yields $N^{\mathrm{rpa}}(\omega)$. A comparison with a moment expansion [28] of the DOS shows that the rpa is particularly accurate for a Néel background. In fact, in this case the contribution of loops is strongly suppressed by the requirement of background conservation. The leading correction to the rpa enters only at order $(t/\omega)^{12}$ since on the smallest loop (a square as shown in fig. 1.2) the hole must circulate three times to restore the configuration (see below). For the conductivity of a hole in the Néel background and, in particular, other backgrounds where loops *are* important, the rpa is less satisfactory. The main disadvantages

of the rpa are that i) the results do not depend on the spin background at all, ii) there is no Hall effect or magnetoresistance, iii) the conducticity $\sigma(\omega)$ does not fulfil the f-sum rule

$$\int_{-\infty}^{\infty} d\omega \, \mathrm{Re}\,\sigma(\omega) = -\frac{\pi e^2 a^2}{Vd} \langle \hat{H}_\alpha \rangle, \tag{1.19}$$

where $\langle \hat{H}_\alpha \rangle \equiv \langle \hat{H} \rangle / d$ is the average kinetic energy in one direction $\boldsymbol{a}$, with a and V as the lattice constant and total volume, respectively.

The conductivity $\sigma(\omega)$ in (1.19) is given by the Kubo formula

$$\sigma(\omega) = \frac{1}{V} \int_0^\infty dt \int_0^\beta d\tau \langle \hat{j}_\alpha(0) \hat{j}_\alpha(t + i\tau) \rangle_h \exp[i\omega t], \tag{1.20}$$

where $\hat{j}_\alpha$ is the current operator in a specific direction $\boldsymbol{a}$ ($|\boldsymbol{a}| = 1$)

$$\hat{j}_\alpha(0) = -ieat \sum_{\boldsymbol{R}_i, \sigma} (\hat{c}^+_{i+\alpha,\sigma} \hat{c}_{i,\sigma} - \hat{c}^+_{i-\alpha,\sigma} \hat{c}_{i,\sigma}) \tag{1.21}$$

and $\langle \ldots \rangle_h$ is the thermal average over all single hole states. The latter can again be expressed as a sum over closed paths. RICE and ZHANG [29] showed that, for a Néel (N) background, at $T = 0$ the rpa yields

$$\mathrm{Re}\,\sigma^{\mathrm{N}}(\omega) = \frac{2\pi e^2 a^2 t^2}{V} \frac{N^{\mathrm{N}}(\omega - \omega_0)}{\omega}, \tag{1.22}$$

where ω_0 corresponds to the lower band edge of $N^{\mathrm{N}}(\omega)$. So far we only considered the case $J = 0$, where spins are completely decoupled. We now include the antiferromagnetic spin exchange between nearest-neighbour spins. As a first step we take $J_z > 0$, $J_\perp = 0$ in (1.13) («Ising limit») [23, 30]; spin flips, *i.e.* quantum fluctuations, are, therefore, still neglected. As already mentioned, the motion of a vacancy in an otherwise perfect Néel background leads to a «string» of overturned spins. (In fact, it is more appropriate to speak of a d-dimensional «tube» of diameter twice the lattice spacing a.) This obstructs the hole motion since it produces intermediate states of higher energy. Let us assume the motion of the hole to be such that the corresponding tube never intersects with itself (this rules out any loops, *i.e.* the hole moves only on self-retracing paths; furthermore, no segment of this path is allowed to run parallel to itself at a distance less than $2a$). As pointed out by BULAEVSKII *et al.* [9] the motion is then a strictly one-dimensional problem. In particular, the energy of the tube is proportional to its length, and the hole moves in a *linear* potential. It is well known that in this case the bound states are described by Airy functions and hence the discrete energy levels are proportional to $t(J_z/t)^{2/3}$ [9]. This implies «confinement», *i.e.* localization of a vacancy at its individual origin, and the corresponding energy band $E_{\mathrm{hole}}(\boldsymbol{k})$ is dispersionless. However, TRUGMAN [31] showed that

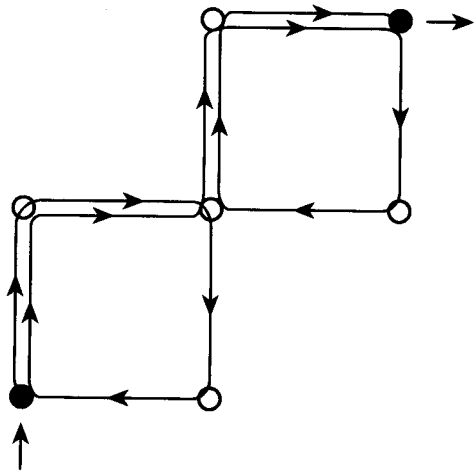

Fig. 1.4. – Trugman path [31] for a hole in an antiferromagnet.

even in the Ising limit there exist possibilities for a hole to move such that its energy is *not* proportional to the length of its path. Namely, when a hole moves around a closed path twice except for the last two steps, it will find itself translated by two lattice spacings, with the background completely restored. In particular, for the motion around a square (see fig. 1.2) this means that after $1 + 1/2$ circulations the hole has effectively moved across the diagonal, this state having the same energy as the initial one. The hole can, therefore, propagate by performing a spiraling motion as shown in fig. 1.4. This leads to a finite (but small) band width of the hole eigenstates and hence to a finite mobility of the holes.

In the realistic case $J_z = J_\perp > 0$ the quantum spin fluctuations will spontaneously flip, *i.e.* «heal», the unfavourable string states (or at least parts of a string), and hence vacancies are naturally expected to be mobile. Coherent excitations of the vacancy are then possible which show up in the hole Green function. Indeed, sharp peaks in the spectral function $\varrho_{\boldsymbol{k}}(\omega)$ at certain momenta $\boldsymbol{k}$ were found in several approaches [23, 24, 26, 31, 32]. Their positions as a function of ω determine the hole band, from which one obtains the effective mass of the quasi-particles.

We saw that analytic investigations of the hole motion in terms of the t-J model are only possible under certain approximations, *e.g.* the retraceable-path approximation, the neglect of quantum spin fluctuations (Ising limit, $J_\perp = 0$) and the assumption of a string with a linear potential. An assessment of the validity and reliability of these approximations is not *a priori* possible, and hence it is not clear how one should go on to improve them systematically. Now, in the most ideal situation it is possible to identify a small, external parameter which *controls* an approximation systematically. Fortunately this is the case in our

problem: the small parameter turns out to be $1/d$, where d is the number of spatial dimensions. We will see that all three approximations mentioned above become exact for $d \to \infty$, *i.e.* $1/d \to 0$, and hence can be derived and improved systematically by an expansion in a *single* small parameter.

1·6. *The limit $d \to \infty$ for itinerant quantum-mechanical lattice models.* – In a perfectly crystalline system every lattice site has the same number of nearest neighbours Z. In three dimensions ($d = 3$) one has $Z = 6$ for a simple cubic lattice ($Z = 2d$ for a hypercubic lattice in general dimensions d), $Z = 8$ for a b.c.c. lattice and $Z = 12$ for an f.c.c. lattice. The dimensionality of a lattice system is directly described by the number Z, rather than by the somewhat more abstract «number of dimensions d». Since $Z \sim \mathcal{O}(10)$ is already quite large in $d = 3$, such that $1/Z$ is rather small, it is only natural and in the general spirit of theoretical physics to consider the extreme limit $Z \to \infty$ first, and then use $1/Z$ as a small expansion parameter to reach finite Z.

In the case of classical spin models (*e.g.*, Ising, Heisenberg) the $Z \to \infty$ limit is very well known (see, for example, ref. [33]). It leads to the results of the Weiss molecular-field theory and may be viewed as the prototypical method for constructing a mean-field theory (MFT). In the limit $Z \to \infty$ the coupling parameter J in (1.13) has to be rescaled as

$$J \to \frac{J^*}{Z}, \qquad J^* = \text{const}, \tag{1.23}$$

for the energy density to remain finite.

It is natural to ask whether the limit $Z \to \infty$ can also be employed in the case of lattice models with *itinerant*, quantum-mechanical degrees of freedom, such as the Hubbard model, (1.13), and whether this is again a useful limit. This question was recently addressed by METZNER and VOLLHARDT [34]. The main question is whether the energy parameters in the Hubbard model can be scaled in such a way that the model remains nontrivial in the limit $Z \to \infty$. By «nontrivial» we mean that both $\hat{H}_{\text{kin}}$ and $\hat{H}_{\text{I}}$ stay finite, such that the competition between these terms, expressed by $[\hat{H}_{\text{kin}}, \hat{H}_{\text{I}}] \neq 0$, remains. (Note: it is not guaranteed that such a scaling exists at all; for example, in the well-known approach where the spin degree of freedom in the Hubbard model, (1.4*b*), is allowed to take arbitrary values ($\sigma = 1, \ldots, N$), the strict $N \to \infty$ limit always leads to the

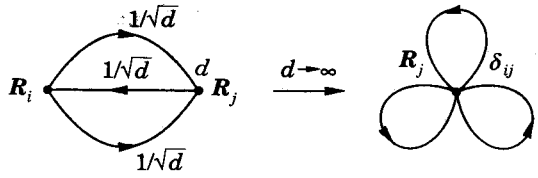

Fig. 1.5. – Contribution to the irreducible self-energy for the Hubbard model in second order in U, and its collapse in the limit $d \to \infty$.

trivial atomic limit—hence there exists no scaling in this case for which $\hat{H}_{\text{kin}}$ *and* $\hat{H}_{\text{I}}$ remain finite [35].) For the Hubbard model a nontrivial $Z \to \infty$ limit can indeed be found [34]. The Hubbard interaction, (1.3*b*), is purely local and independent of its surrounding; hence it is independent of the spatial dimension and U need not scale with Z at all. On the other hand, for a hypercubic lattice with unit lattice spacing, the kinetic energy has a dispersion

$$\varepsilon_{\boldsymbol{k}} = -2t \sum_{i=1}^{d} \cos k_i \overset{d \to \infty}{\sim} \mathcal{O}(t\sqrt{d}), \tag{1.24}$$

which in the limit $d \to \infty$, and for randomly chosen momentum $\boldsymbol{k}$, is of order $t\sqrt{d}$ (since $\cos k_i \in [-1, 1]$) according to the law of large numbers. Hence for the kinetic energy $E_{\text{kin}} = \sum_{\boldsymbol{k}, \sigma} \varepsilon_{\boldsymbol{k}} n_{\boldsymbol{k}\sigma}$ to remain finite in $d = \infty$ the only possible scaling of t is [34]

$$t \to \frac{t^*}{\sqrt{2d}}, \qquad t^* = \text{const}. \tag{1.25}$$

The central-limit theorem tells us furthermore that the DOS, which is the probability distribution of the quantity $E = \varepsilon_{\boldsymbol{k}}$ for a random choice of $\boldsymbol{k}$, is given by a Gaussian

$$N_\infty(E) = \frac{1}{\sqrt{2\pi}t^*} \exp\left[-\frac{1}{2}\left(\frac{E}{t^*}\right)^2\right]. \tag{1.26}$$

The scaling of the nearest-neighbour hopping matrix element t in (1.25) implies that the corresponding one-particle Green function («propagator») of the noninteracting system has the same d-dependence, *i. e.* for $\boldsymbol{R}_i, \boldsymbol{R}_j$ at nearest-neighbour positions we have [36, 37]

$$G^0_{ij,\sigma} \sim \frac{1}{\sqrt{d}}. \tag{1.27}$$

It is the property (1.27) which is the origin of all simplifications arising in the limit $d \to \infty$. In particular, it implies the *collapse of all connected, irreducible perturbation-theoretical diagrams in position space* [34, 36, 37]. This is illustrated in fig. 1.5, where a contribution in 2nd-order perturbation theory to the irreducible self-energy, $\Sigma^{(2)}_{ij}$, is shown. Usually $\Sigma^{(2)}_{ij}$ will only enter in a sum over $\boldsymbol{R}_i$ and $\boldsymbol{R}_j$. Then it becomes apparent that $\Sigma^{(2)}_{ij}$ is only of order $1/\sqrt{d}$ small, unless $i = j$. Namely, for nearest-neighbour sites $\boldsymbol{R}_i, \boldsymbol{R}_j$ the three lines, corresponding to $G^0_{ij,\sigma}$, contribute a factor $1/d^{3/2}$, while the sum over $\boldsymbol{R}_j$ relative to $\boldsymbol{R}_i$ contributes a factor d. Only for $i = j$ is the value of $\Sigma^{(2)}_{ij}$ independent of d. Hence in the limit $d \to \infty$ the diagram on the l.h.s. of fig. 1.5 is equivalent to the «collapsed», petal-shaped diagram on the r.h.s. provided $i = j$; otherwise it is zero. More generally, *any two vertices which are connected by more than two separate paths will collapse onto the same site.* (Here a «path» is any sequence of

lines in a diagram; they are «separate» when they have no lines in common.) In particular, the external vertices of any irreducible self-energy diagram are always connected by three separate paths and hence always collapse. As shown by METZNER and VOLLHARDT [34] and MÜLLER-HARTMANN [36], the full, irreducible self-energy then becomes a purely local quantity:

$$\Sigma_{ij,\sigma}(\omega) \overset{d\to\infty}{=} \Sigma_{ii,\sigma}(\omega)\delta_{ij} . \tag{1.28a}$$

The Fourier transform of $\Sigma_{ij,\sigma}$ is hence seen to become *momentum-independent*:

$$\Sigma_{\sigma}(\boldsymbol{k},\omega) \overset{d\to\infty}{\equiv} \Sigma_{\sigma}(\omega) . \tag{1.28b}$$

This leads to tremendous simplifications in all many-body calculations for the Hubbard model and related models. Indeed, in the limit $d\to\infty$ the Hubbard model reduces to a nontrivial (and yet unsolved) effective single-site problem in a fermionic bath [38-41], which will be addressed in the last section.

It is interesting to note that in many respects our real, three-dimensional world seems to be already a *high*-dimensional world. In particular, a large number of standard approximations, which are routinely used to make contact with experiments, are *only* correct in $d=\infty$. For a more comprehensive presentation I refer to short reviews by MÜLLER-HARTMANN [41] and myself [42] and, in particular, to my recent lecture notes [43] on the large-d limit, of which parts are also used here.

1·7. *Hole motion in the t-J model: exact results in the $d=\infty$ limit.* – In the limit $d\to\infty$ the problem of a single vacancy in a quantum antiferromagnet, as described by the t-J model, can be solved exactly, and I will only summarize the results (for details, see [44] and [45], and ref. [43]).

1) In $d=\infty$ quantum spin fluctuations, *i.e.* the spin-flip contributions in (1.13*b*), vanish ($J_{\perp}\equiv 0$) and the quantum antiferromagnet becomes a Néel state.

2) As explained in subsect. **1·4**, it takes three circulations, *i.e.* 12 hopping processes, for a hole moving around a square to restore the Néel order (see fig. 1.2). For $d\to\infty$, using (1.25), this process is of order $(1/\sqrt{d})^{12}\times d^2 = 1/d^4$ small (the factor d^2 comes from the number of possibilities to embed a square in d dimensions). Loops are, therefore, suppressed and the hole can only move on self-retracing paths: in $d=\infty$ the retraceable-path approximation (rpa) [28] becomes exact for the Néel state [44], and the Green function is given by

$$G_{ij}^{\mathrm{N}}(z) = \frac{1}{2t^{*2}}\left[z-\sqrt{z^2-4t^{*2}}\right]\delta_{ij} . \tag{1.29}$$

The DOS has the shape of a half-ellipse. Since G_{ij}^{N} is purely local, its Fourier

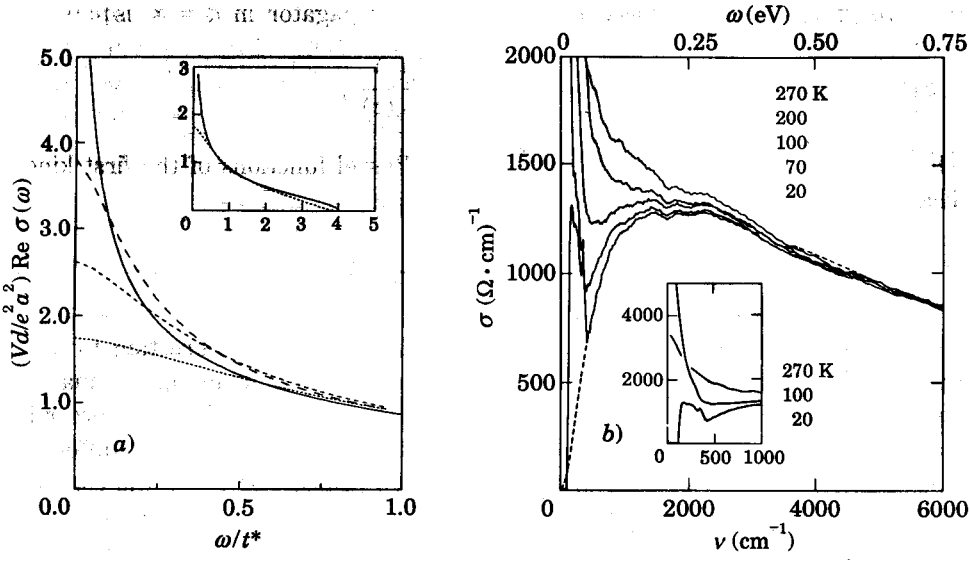

Fig. 1.6. – *a*) Re $\sigma(\omega)$ *vs.* ω/t^* for a Néel background in $d < \infty$ at various temperatures $T = 1/k_B\beta$: ····· $\beta = 3$, ----- $\beta = 6$, – – – $\beta = 12$, —— $\beta = \infty$; *b*) frequency-dependent conductivity as measured by THOMAS *et al.* [46] on $YBa_2Cu_3O_{7-\delta}$.

transform, and hence the spectral function $\rho_{\boldsymbol{k}}(\omega)$, is $\boldsymbol{k}$-independent—there exist no quasi-particle peaks.

3) The full rpa expression for G_{ij}^{N}, (1.18), can be derived systematically by a self-consistent $1/d$ expansion around $d = \infty$ [45].

4) By using the DOS obtained from (1.29) even in finite dimensions, the $d = \infty$ limit may be employed to derive a self-consistent approximation for $\sigma(\omega)$ in $d < \infty$, which—in contrast to the rpa—fulfills the f-sum rule (1.19) [44]. In particular, for $U = \infty$ and $T = 0$ one finds from (1.22)

$$\text{Re}\,\sigma^{N}(\omega) = \frac{e^2a^2}{Vd}\sqrt{\frac{t^*}{\omega} - \frac{1}{4}}\,. \tag{1.30}$$

This result is shown in fig. 1.6*a*) together with numerical results for $T > 0$. A qualitatively rather similar frequency dependence of $\sigma(\omega)$, shown in fig. 1.6*b*), has been observed in some high-T_c materials, *e.g.* $YBa_2Cu_3O_{7-\delta}$, by THOMAS *et al.* [46] using reflectivity measurements (for a very readable introduction see [47]). The structure at low ω that emerges as T_c is approached from above, cannot, of course, be described within the theory presented above.

5) For $J > 0$ the assumption of a *linear* potential, generated by the string of overturned spins [9,23], is exact up to order $1/d^2$, since in $d = \infty$ loops do not contribute and a string does not interact with itself (both effects come in at or-

der $1/d^2$). The exact expression for the local propagator in $d = \infty$ is [45]

$$G_{ii}^{N}(\omega) = -\frac{1}{t^*}\frac{J_\nu(z)}{J_{\nu-1}(z)}, \tag{1.31}$$

where $\nu = -2\omega J^*$, $z = 4t^*/J^*$ and $J_\nu(z)$ are Bessel functions of the first kind. The poles of (1.31) are found at discrete energies

$$E_n = -a_n t^* \left(\frac{J^*}{2t^*}\right)^{2/3} + \text{const}, \tag{1.32}$$

where the a_n are the zeros of the Airy function $\mathrm{Ai}(z)$. It is interesting to note that (1.32) agrees exactly with the result from a continuum approximation based on a Schrödinger equation with a linear potential $V = rJ^*/2$, where r is the length of the string [9]. The DOS corresponding to (1.31) is very different from that for $J^* = 0$, *i.e.* is given by a series of δ-peaks. For $T = 0$ the conductivity $\sigma(\omega)$ is again given by (1.22), with ω_0 replaced by $\omega_0 - J^*/2$, and hence is also given by a series of δ-peaks. The d.c. conductivity is then always zero for finite J^*, since Trugman paths [31] (fig. 1.4) contribute only at higher orders in $1/d$.

6) The inclusion of local disorder to the model, which still allows an exact solution in $d = \infty$, gives rise to new effects, too [45]. As expected, the δ-peaks are broadened by the disorder. For $T \to 0$, very small J^* and weak disorder and for not too small ω, $\sigma(\omega)$ reduces to the result shown in fig. 1.6*a*), but has more or less pronounced «wiggles». Interestingly enough, one finds that the inclusion of weak disorder *favours* the d.c. conductivity since it acts like an additional kinetic energy (fig. 1.7).

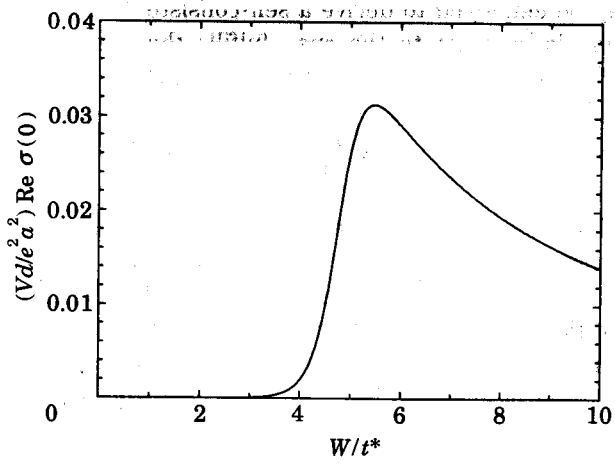

Fig. 1.7. – D.c. conductvity *vs.* disorder strength of a hole in the t-J model with local disorder in $d = \infty$ [45], $J^*/t^* = 1$, $k_B T/t^* = 0.1$.

One of the main advantages of the $d \to \infty$ limit is that it allows one to include important physical effects (*e.g.*, disorder, next-nearest-neighbour hopping, etc.), which are absent in the original t-J model, in a systematic and consistent way.

2. – Projected wave functions.

Variational wave functions are among the very few theoretical tools that allow straightforward, conceptually simple investigations of interacting many-body systems. They are used to describe correlations among quantum-mechanical objects in an approximate, but explicit and physically intuitive, manner. They are particularly valuable in situations where standard perturbation theory fails or is not tractable. The problems in which variational wave functions have been employed include such diverse examples as rotons in superfluid ^{4}He, the plasma state of electrons in metals, the quantum liquids ^{3}He and ^{4}He, nuclear physics, superconductivity and the (fractional) quantum Hall effect. Of these the BCS wave function is certainly the most famous. Variational wave functions have also been used to study possible magnetic order of lattice electrons, *i.e.* ferromagnetism and antiferromagnetism. They have recently received a particular attention in the study of heavy fermions and high-T_c superconductivity [48].

The general strategy in this approach is to construct an explicit wave function of the form

$$|\Psi_{\text{var}}\rangle = \hat{C}|\Psi_0\rangle, \tag{2.1}$$

where $|\Psi_0\rangle$ is a simple one-particle starting wave function on which a projection, or «correlation» operator $\hat{C}(\lambda_1, \ldots, \lambda_n)$ acts. The latter depends on variational parameters λ_i and has to describe the microscopic interaction between the particles in a more or less detailed way. This wave function is then used to calculate the expectation value of some operator $\hat{\mathcal{O}}$

$$\langle\hat{\mathcal{O}}\rangle = \frac{\langle\Psi_{\text{var}}|\hat{\mathcal{O}}|\Psi_{\text{var}}\rangle}{\langle\Psi_{\text{var}}|\Psi_{\text{var}}\rangle}. \tag{2.2}$$

In particular, by calculating and minimizing the ground-state energy $E_{\text{var}} = \langle\hat{H}\rangle$, where $\hat{H}$ is the Hamiltonian, the variational parameters λ_i contained in $\hat{C}$ (and perhaps also in $|\Psi_0\rangle$) can be determined. These parameters are used to suppress those configurations in $|\Psi_0\rangle$ which for a given interaction strength are energetically unfavourable. The variational principle guarantees that E_{var} provides a rigorous upper bound for the exact ground-state energy.

2·1. *The Gutzwiller wave function.* – For the Hubbard model, (1.4), the simplest variational wave function of the form (2.1) is the so-called Gutzwiller wave

function (GWF) [6, 49], with $\hat{C} = \exp[\lambda \hat{H}_I]$,

$$|\Psi_G\rangle = g^{\hat{D}} |FS\rangle, \tag{2.3a}$$

$$= \prod_{R_i} [1 - (1-g)\hat{D}_i] |FS\rangle. \tag{2.3b}$$

Here $\hat{D} = \hat{H}_I/U = \sum_i \hat{D}_i$ is the number operator for doubly occupied sites, $\lambda = \ln g/U$ and $|\Psi_0\rangle$ is the Fermi sea ($\equiv |FS\rangle$). Hence $\hat{C}$ *globally* reduces the amplitude of those spin configurations in $|\Psi_0\rangle$ with too many doubly occupied sites. The limit $g = 1$ corresponds to the noninteracting case, while $g \to 0$, implying $\langle \hat{D} \rangle \to 0$, corresponds to the limit $U \to \infty$. Indeed, for $g \to 0$, $g^{\hat{D}}$ reduces exactly to the projection operator $\hat{P}$, (1.6*b*), which eliminates all configurations with d-sites. While in the derivation of the t-J model in subsect. 1·3 the projection was applied to the *Hamiltonian* itself, it appears here in conjunction with a *wave function*, which is used to calculate expectation values. The fully projected Gutzwiller wave function

$$|\Psi_G^{\infty}\rangle = \hat{P}|FS\rangle \tag{2.4}$$

is a wave function from the restricted Hilbert space $\mathscr{H}^{\text{restr}}$ where sites are only singly occupied. However, it is no longer a *variational* wave function, since it no longer contains free parameters. Hence the correlations in (2.4) are completely determined by those already contained in $|FS\rangle$ and cannot be further controlled. On the other hand, by replacing $|FS\rangle$ with a more general starting wave function this problem may be avoided. Even states with broken symmetry can be described, *e.g.*, by choosing an antiferromagnetic Hartree-Fock wave function («spin density wave»)

$$|SDW\rangle = \prod_{k,\sigma} [u_k \hat{a}_{k\sigma}^{+} + \sigma v_k \hat{a}_{k+Q,\sigma}^{+}] |0\rangle, \tag{2.5a}$$

where $\boldsymbol{Q}$ is half a reciprocal-lattice vector and $|0\rangle$ is the vacuum, or a BCS wave function

$$|BCS\rangle = \prod_{k} [u_k + v_k \hat{a}_{k\uparrow}^{+} \hat{a}_{-k\downarrow}^{+}] |0\rangle \tag{2.5b}$$

to obtain resonating-valence bond states [50, 51] (for a discussion of the latter see ref. [2]).

Exact analytic evaluations in terms of Gutzwiller-type wave functions have recently become possible in $d = 1$ and $d = \infty$ due to techniques developed by METZNER and the author [34, 52] (see also subsect. 2·4). These wave functions are now quite well understood [53]. In particular, for $n = 1$ and $U \gg t$ the GWF, (2.3), in $d = 1$ leads to the ground-state energy density [52]

$$E_G = -\left(\frac{4}{\pi}\right)^2 \frac{t^2}{U} \frac{1}{\ln U}, \tag{2.6}$$

where $\overline{U} = U/8|\varepsilon_0|$, with ε_0 as the energy of the noninteracting particles. Hence the exact result, $E \sim -t^2/U$, obtained from 2nd-order perturbation theory (see sect. 1), is found to be multiplied by a nonanalytic factor (this is the case even in dimensions $d > 1$ [54]); thus the ground-state energy E_G for the Hubbard model is not very good, as first noted by KAPLAN, HORSCH and FULDE [55]. Does this automatically imply that $|\Psi_G\rangle$ is a bad wave function in the strong-coupling limit? The answer is quite subtle: while it is true that the wave function is not very good for the *Hubbard* model at $U \gg t$, it is nevertheless an excellent wave function in $d = 1$ for the *effective* model at large U, *i.e.* the *t-J* model, where *d*-sites have been projected out. This can be seen from the spin-spin correlation function $C_j^{SS}(n, g)$, with $j \equiv |\boldsymbol{R}_j|$, which was evaluated exactly in terms of the GWF in $d = 1$ by GEBHARD and VOLLHARDT [56]. For $n = 1$, $g = 0$ one finds

$$C_{j>0}^{SS} = (-1)^j \frac{\mathrm{Si}(\pi j)}{\pi j} \overset{j\to\infty}{\sim} \frac{(-1)^j}{2j}, \tag{2.7}$$

where $\mathrm{Si}(\pi j)$ is the sine integral. The asymptotic behaviour implies a logarithmic divergence at momentum $\boldsymbol{Q}$, *i.e.* is of antiferromagnetic origin. Comparison with the exact result for the spin correlation function for the Heisenberg model in the case of $j = 1, 2$ and for large j, where [57] $C_j^{SS} \sim (-1)^j j^{-1} (\ln j)^{1/2}$, shows that $|\Psi_G^\infty\rangle$ yields excellent results in $d = 1$ [56]. The same is true for hole-hole correlations in the limit $n \lesssim 1$ and $U = \infty$. Subsequently HALDANE [58] and SHASTRY [59] recognized that (2.7) is, in fact, the exact result for a spin-1/2 Heisenberg model with an antiferromagnetic exchange coupling that falls off as $1/j^2$, and that $|\Psi_G^\infty\rangle$ is the *exact* ground-state wave function for this model. This peculiar exchange coupling leads to a partial frustration of the spin orientation, and hence the antiferromagnetic correlations are weaker than in the original Heisenberg model. Recently KURAMOTO and YOKOYAMA [60] showed that $|\Psi_G^\infty\rangle$ is exact even for $n < 1$, *i.e.* for the *t-J* model with $t_{ij} \sim 1/|i-j|^2$ at $t = J$. The investigation of the GWF thus led, and continues to lead [61, 62], to very interesting, new developments in the field of strongly correlated fermions.

We may now understand why the GWF, (2.3), which does not lead to a good energy for the Hubbard model at large but *finite* U, can nevertheless be an excellent wave function for the Heisenberg model [53]. Using the notation of (1.11) we have for $n = 1$

$$|\Psi_{HM}\rangle = |\Psi_{eff}\rangle + \frac{\alpha}{U} \hat{H}_{kin} |\Psi_{eff}\rangle + \mathcal{O}(t^2/U^2), \tag{2.8a}$$

where α is some constant. $|\Psi_{HM}\rangle$ has precisely one *d*-site, with one *e*-site next to it. By contrast, the GWF for $g \to 0$ has the form

$$|\Psi_G(g)\rangle = |\Psi_G^\infty\rangle + g_0 |\Psi^{(1)}\rangle + \mathcal{O}(g_0^2), \tag{2.8b}$$

where $|\Psi^{(1)}\rangle$ are the wave functions in $|FS\rangle$ with a single *d*-site (and one *e*-site

somewhere), and $g_0 = (\overline{U} \ln \overline{U})^{-1}$. The spatial correlation between d- and e-sites, described by the second terms in (2.8a), (2.8b), is seen to be strict in (2.8a), but is quite unspecific in (2.8b). But it is precisely $|\Psi^{(1)}\rangle$ which determines the ground-state energy of the *Hubbard* model at large but finite U ($|\Psi_G^\infty\rangle$ only yields zero energy). The logarithmic correction in (2.6) is, therefore, a consequence of the insufficient *density* correlations in $|\Psi^{(1)}\rangle$ [53, 55]. On the other hand, the calculation of the ground-state energy via the *effective* model using (2.8b) only involves $|\Psi_G^\infty\rangle$, *i.e.* is determined by the *spin* correlations which were found to be excellent in $d = 1$. Why are they so good? It seems that this is mainly a consequence of the spatial constraints caused by the low dimensionality. In $d = 1$ spatial correlations are even pronounced in the *Fermi gas* and the projector $\tilde{P}$ enhances them further. In higher dimensions the (spin) correlations in the GWF become weaker and weaker. Nevertheless, the main virtue of the GWF is its simplicity and explicitness. It is widely used in analytical and numerical treatments since it provides a straightforward starting point for investigations in the large-U limit. For example, the (in)stability of the Nagaoka state may be investigated by means of a fully projected wave function $|\Psi_G^\infty\rangle$, (2.4), where $|\mathrm{FS}\rangle$ is replaced by a ferromagnetic state with a single flipped spin. In this way SHASTRY, KRISHNAMURTHY and ANDERSON [63] obtained a value of $\delta_c^{\mathrm{upper}} = 0.49$ as an upper limit on the critical hole concentration δ_c above which the Nagaoka state is unstable on a square lattice. This approach has since been considerably refined. In particular, extensive numerical studies by VON DER LINDEN and EDWARDS [64] led to an improved estimate of $\delta_c^{\mathrm{upper}} = 0.29$. It appears that even this value can still be lowered considerably [65], such that the region of stability of the Nagaoka state becomes very small.

2·2. *The Gutzwiller approximation.* – Besides introducing the wave function (2.3), GUTZWILLER [6, 49] constructed a nonperturbative approximation scheme that allowed him to obtain an explicit expression for the ground-state energy of the Hubbard model in terms of (2.3). We will later see that this «Gutzwiller approximation» (GA), when used to calculate matrix elements in terms of the GWF, yields the *exact* result for $d = \infty$. The idea behind the GA may be easily understood [66] and will be illustrated below by calculating the norm $\langle \Psi_G | \Psi_G \rangle$. Working in configuration space the Fermi sea can be written as

$$|\mathrm{FS}\rangle = \sum_D \sum_{\{i_D\}} A_{i_D} |\Psi_{i_D}\rangle, \tag{2.9}$$

where $|\Psi_{i_D}\rangle$ is a spin configuration with D doubly occupied sites, with A_{i_D} as the corresponding amplitude. The sum extends over the whole set $\{i_D\}$ of different configurations with the same D and over all D. For a system with L lattice sites and N_σ σ-electrons, the number N_D of different configurations in $\{i_D\}$ is simply

given by

$$N_D = \frac{L!}{L_\uparrow ! L_\downarrow ! D! E!} , \tag{2.10}$$

where $L_\sigma = N_\sigma - D$ and $E = L - N_\uparrow - N_\downarrow + D$ are the number of singly occupied and empty sites, respectively. Since $\hat{D}$ is an eigenoperator of $|\Psi_{i_D}\rangle$, the norm of $|\Psi_G\rangle$ takes the form

$$\langle \Psi_G | \Psi_G \rangle = \sum_D g^{2D} \sum_{\{i_D\}} |A_{i_D}|^2 . \tag{2.11}$$

If now $|A_{i_D}|^2$ is assumed to be *independent* of the specific spin configuration (whereby spatial correlations are neglected), this quantity is given by the *classical* probability of finding any one of the possible spin configurations $\{i_D\}$ at $U = 0$, *i.e.*

$$\sum_{\{i_D\}} |A_{i_D}|^2 = P_\uparrow P_\downarrow N_D , \tag{2.12}$$

where $P_\sigma(L, N_\sigma) = 1/\binom{L}{N_\sigma} \simeq n_\sigma^{N_\sigma}(1 - n_\sigma)^{L-N_\sigma}$, with $n_\sigma = N_\sigma/L$. Hence (2.11) reduces to

$$\langle \Psi_G | \Psi_G \rangle = P_\uparrow P_\downarrow \sum_D g^{2D} N_D . \tag{2.13}$$

In the thermodynamic limit the sum in (2.13) is dominated by its largest term corresponding to a value $D = \overline{D}$, where $\overline{D}$ is determined by ($\overline{d} = \overline{D}/L$)

$$g^2 = \frac{\overline{d}(1 - n_\uparrow - n_\downarrow + \overline{d})}{(n_\downarrow - \overline{d})(n_\uparrow - \overline{d})} . \tag{2.14}$$

The result (2.14), obtained within the above «quasi-chemical approximation», is just the law of mass action, where g^2 (instead of the Boltzmann factor) regulates the dynamical equilibrium between the «concentrations» $[n_\uparrow - d]$ and $[n_\downarrow - d]$ of singly occupied sites, on one side of this «chemical reaction», and that of doubly occupied sites, $[\overline{d}]$, and holes, $[1 - n_\uparrow - n_\downarrow + \overline{d}]$, on the other side. (It is interesting to note that (2.14), with g^2 replaced by $\exp[-\beta U]$, is indeed an *exact* result in the case of the Hubbard model with *infinite-range* hopping [67].) Equation (2.14) uniquely relates $\overline{d}$ and g, such that g may be replaced by the quantity $\overline{d}$. The calculation of the expectation values of the kinetic and the interaction energy of the Hubbard model proceeds similarly [66]. The ground-state energy density as a function of the variational parameter $\overline{d}(g)$ is then found as

$$E[\overline{d}(g)]/L = \sum_\sigma q_\sigma(\overline{d}, n_\uparrow, n_\downarrow)\, \varepsilon_{0,\sigma} + U\overline{d} , \tag{2.15}$$

which has to be minimized with respect to $\overline{d}$. Here $\varepsilon_{0,\sigma}$ is the energy of noninter-

acting σ-electrons and $q \leqslant 1$ is an explicit function of $\bar{d}$ and n_σ, which may be viewed as a reduction factor of the hopping amplitude due to correlations; for $n_\uparrow = n_\downarrow$ one has $q_\sigma \equiv q = 2(1 - \delta - 2d)(\sqrt{d + \delta} + \sqrt{d})^2/(1 - \delta^2)$, where $\delta = 1 - n$. BRINKMAN and RICE [68] showed that in the special case $n_\sigma = 1/2$ (half-filled band) the minimization of (2.15) yields

$$q = 1 - \bar{U}^2 , \tag{2.16a}$$

$$\bar{d} = \frac{1}{4}(1 - \bar{U}), \tag{2.16b}$$

$$E/L = -|\varepsilon_0|(1 - \bar{U})^2 , \tag{2.16c}$$

where $\bar{U} = U/8|\varepsilon_0|$ and $\varepsilon_0 = \varepsilon_{0\uparrow} + \varepsilon_{0\downarrow}$. Equation (2.16c) says that the energy increases with U and *vanishes* at a *finite* critical value $U_c = 8|\varepsilon_0|$, since the density of doubly occupied sites $\bar{d}$ (and hence the reduction factor q) vanishes at this point. The fact that $E_{kin}, E_I \to 0$ for $U \to U_c$ means that the particles become localized, such that a charge current can no longer flow. So the GA, when used in conjunction with the GWF, describes a *metal-insulator transition* at a finite interaction strength («Brinkman-Rice transition»). This transition is due to a correlation-induced band narrowing and hence describes a *Mott-Hubbard* metal-insulator transition.

The Brinkman-Rice transition only occurs for $n_\sigma = 1/2$; for $n_\sigma \neq 1/2$ the quantities q and $\bar{d}$, and hence E, are finite for all $U < \infty$ and only vanish in the limit $U \to \infty$. Clearly, the transition to a localized state with $E = 0$ at a *finite* U_c, found in the case $n = 1$, does not describe the entire physics. We already know from sect. 1 that for $U \gg t$ the localized spins are coupled antiferromagnetically, which leads to a lowering of the energy $E = 0$ by an amount $E_{AF} \propto -t^2/U$. This effect is not included in the GA, since spatial correlations were explicitly neglected. (However, this approximation can be improved by using the antiferromagnetic Hartree-Fock starting wave function $|\Psi_0\rangle$ in (2.3).) Of course, the magnetic coupling is an *additional* effect (after all, it is obtained by 2nd-order perturbation theory from the localized state), *i.e.* is a *consequence* of the underlying correlation effects which lead to the localized state in the first place. Therefore, as long as one is not too close to $U = U_c$, the overall results of the GA are not invalidated by the appearance of magnetic coupling, and give important insight into the correlation-induced approach to the localized state.

2·3. *Connection to Fermi-liquid theory.* – The fact that the results of the GA describe a correlated, normal-state (*i.e.* paramagnetic) fermionic system allows one to make contact with Landau's Fermi-liquid theory [66, 68]. For example, a closer examination of the GA reveals that the «reduction factor» q in (2.15) is, in fact, the discontinuity of the momentum distribution n_k at the Fermi level and may thus be identified with the inverse effective-mass ratio $(m^*/m)^{-1}$. Since

$m^*/m = q^{-1} < \infty$ for $U < U_c$, the system is a Fermi liquid, *i.e.* is a metal, in this regime. At $U = U_c$ the effective mass diverges and the system becomes an insulator. This conclusion confirms the reasoning in subsect. 2·2, which was based on the vanishing of $\bar{d}$ at $U = U_c$.

One can also use (2.15) to calculate the spin susceptibility χ_s and compressibility κ within the GA [66, 68]. For $n_\sigma = 1/2$, where $m^*/m \equiv 1 + (1/3)F_1^s = 1/(1 - \bar{U}^2)$, the corresponding Fermi-liquid parameters are found as

$$F_0^a \simeq -1 + \frac{1}{(1+\bar{U})^2}, \tag{2.17a}$$

$$F_0^s \simeq \frac{1}{(1-\bar{U})^2} - 1, \tag{2.17b}$$

$$F_1^s = \frac{3\bar{U}^2}{1-\bar{U}^2}. \tag{2.17c}$$

Expanding (2.17) to second order in $\bar{U}$, we find $F_0^a(\bar{U}) = -2\bar{U} + 3\bar{U}^2$, $F_0^s(\bar{U}) = 2\bar{U} + 3\bar{U}^2$. This clearly shows the importance of two-particle correlation effects, which first enter at order U^2: they characteristically *change* the linear U behaviour suggested by Hartree-Fock theory. For $U \to U_c$, F_0^a levels off and saturates at $\simeq -3/4$, while F_0^s increases much stronger than linearly and eventually diverges. Qualitatively this behaviour is identical to the one found within self-consistent 2nd-order perturbation theory for the Hubbard model in $d = \infty$ [41]. Furthermore, for $U \to U_c$ the Wilson ratio

$$\frac{\chi_s/\chi_s^0}{m^*/m} = \frac{1}{1+F_0^a} \to \text{const}. \tag{2.18}$$

So the strong increase of χ_s as a function of U for $U \to U_c$ is mainly due to the strong increase of m^*/m and *not* due to an incipient ferromagnetic instability, which would demand $F_0^a \to -1$.

It was first pointed out by ANDERSON and BRINKMAN [69], and discussed in detail by VOLLHARDT [66], that the behaviour expressed by (2.17) and (2.18) is indeed observed in normal liquid ^{3}He, which is an isotropic, strongly correlated fermionic system of high density (the ^{3}He atom behaves as a spin-1/2 fermion due to the spin of the *nucleus*!). Namely, the effective mass m^* and the spin susceptibility χ_s are strongly enhanced, while the compressibility κ is strongly reduced. Normal liquid ^{3}He has, therefore, been called an «almost-localized» Fermi liquid [66, 69, 70].

A generalization of the above model to a lattice gas («cell») model, where the energy expression (2.15) is supplemented by a pressure term so that it allows for a *variable* density n, was developed by VOLLHARDT, WÖLFLE and ANDERSON [71] and applied to ^{3}He. In the case that the underlying lattice is taken as incompressible one finds that the particle density actually tends towards half-fil-

ling as the localization transition is approached (this was tacitly *assumed* in the above model). In this limit the compressibility now stays finite. If the lattice is given a finite compressibility itself (after all, even the solid is compressible), then the spurious localization transition disappears altogether. Thereby the (unphysical) singular features of the result of the model are removed, while the essential dependences of m^* and F_0^a, F_0^s on pressure, which are in good agreement with experiment, remain [71]. In particular, the high-magnetic-field behaviour is no longer singular, *i.e.* the magnetization $m(H)$ increases smoothly [72], but stronger than found in the experiment [73]. The static properties are nevertheless still determined by the «almost-localized» character of the system.

To model the entropy RICE *et al.* [74] and SEILER *et al.* [75] extended the Gutzwiller result (2.15) to finite temperatures T, using essentially phenomenological arguments. Within the model considered, there are two important temperature regimes: i) for $T \ll T_F$ the system is a Fermi liquid, while ii) for $T_F \lesssim T \lesssim U$ it shows classical behaviour, but is still strongly correlated. In the second temperature regime the entropy of the almost-localized fermions ($\bar{d} \simeq 0$) is bounded by $k_B \ln 2$ per ^{3}He atom, because the lattice sites are essentially *singly* occupied. However, due to the large effective mass m^*/m of the particles the entropy increases sharply at low temperatures

$$S(T) = \gamma T , \qquad T \ll T_F , \tag{2.19}$$

where $\gamma \propto m^*/m$. Hence the entropy reaches the bound $k_B \ln 2$ already at some *low* temperature $T_0 \ll T_F$, such that at higher temperatures $T_0 < T < U$ its increase must go on much slower. Consequently there must be a kink in $S(T)$ and in the specific heat $c_v(T)$ at $T \simeq T_0$. This feature, which is indeed observed in liquid ^{3}He at about 200 mK [76], is even more pronounced in two-dimensional films of ^{3}He at certain filling fractions [77] and seems to be a natural consequence of the almost-localized character of the particles.

2·4. *Derivation of the Gutzwiller approximation in $d = \infty$.* – To evaluate the expectation values $\langle \hat{H}_{kin} \rangle$ and $\langle \hat{H}_I \rangle$ in terms of the GWF *without* using the GA, we have to expand the product operator in (2.3*b*) as a sum. Since $\hat{D}_i$ is a purely local operator, the expectation value of an operator $\hat{\mathcal{O}}$ may be written as a sum over *different* lattice sites only and takes the form

$$\langle \hat{\mathcal{O}} \rangle = \sum_{m=0}^{\infty} \mathcal{O}_m (1 - g^2)^m , \tag{2.20}$$

where $1 - g^2 \leqslant 1$ is the expansion parameter. In the case of $\hat{H}_{kin}$ and $\hat{H}_I$ the coefficients $\mathcal{O}_m$ are given by expressions like $\langle \hat{D}_{i_1} \ldots \hat{D}_{i_m} \rangle_0, \langle \hat{D}_{i_1} \ldots \hat{c}^+_{i\sigma} \hat{c}_{j\sigma} \ldots \hat{D}_{i_m} \rangle_0$, which now have to be evaluated in the noninteracting state (notation $\langle \ldots \rangle_0$). In the two limits $d = 1$ and $d = \infty$ they can be calculated explicitly [34, 52]. This involves a diagrammatic theory which, in fact, is identical with the usual many-

body, Feynman-diagram perturbation theory for the Hubbard model (*i.e.* a ϕ^4 theory). The *lines* in a diagram correspond to the one-particle density matrix $g^0_{ij,\sigma} = \langle \hat{c}^+_{i\sigma} \hat{c}_{j\sigma} \rangle_0$, rather than the Green function $G^0_{ij,\sigma}(\omega)$, and vertices correspond to $g^2 - 1$, rather than U. The important point is that in the limit $d \to \infty$ the distance dependence of $g^0_{ij,\sigma}$ is *identical* to that of $G^0_{ij,\sigma}(\omega)$, (1.27). Hence the simplifications discussed in subsect. 1·5 for diagrams in terms of $G^0_{ij,\sigma}(\omega)$ occur here, too. In particular we have the same collapse phenomenon: if two vertices are connected by more than two separate paths they collapse, as shown in fig. 1.5. At the same time an additional simplification occurs, which is due to the fact that we are working with a ground-state variational wave function: there is no dynamics involved! So the nontrivial problem that remains in the many-body perturbation theory for the Hubbard model in $d = \infty$, namely the dynamics (expressed by the frequency dependence of $G^0_{ij,\sigma}(\omega)$), is absent here: $g^0_{ij,\sigma}$ does not depend on ω at all. As a consequence, the irreducible self-energy $\Sigma_{ij,\sigma}$ (or, rather, the diagrammatic quantity corresponding to $\Sigma_{ij,\sigma}$ in the present context) not only obeys (1.28*a*), *i.e.* is a local quantity, but is even *frequency-independent.* Using skeleton diagrams (*i.e.* fully dressed lines where self-energy insertions are included) the self-energy $\Sigma_{ii,\sigma}$ is then given by a sum of collapsed, flower-shaped diagrams with $m = 1, 3, 5$, etc. «petals» (see fig. 1.5 for $m = 3$) [34, 78]. This sum is a closed, self-consistent equation for $\Sigma_{ii,\sigma}$, which in principle can be solved for arbitrary starting wave function $|\Psi_G\rangle$. In the simplest case, *i.e.* that of the translational invariant GWF, (2.3), $\Sigma_{ii,\sigma}$ is translational invariant, too, and may easily be determined. For example, in the special case $n_\sigma = 1/2$ one finds $\Sigma_{ii,\sigma} = 1 - g$. This yields n_k and $\bar{d}$, which functionally depend on $\Sigma_{ij,\sigma}$. The ground-state energy E/L is then found to be given by (2.15), with $\bar{d} = \bar{d}(g)$, *i.e.* by the result obtained within the GA. So we discover that in the limit $d \to \infty$ the Gutzwiller approximation yields the correct evaluation of expectation values calculated in terms of the Gutzwiller wave function [34, 37]. Why? The answer lies in the large-d behaviour of the Fermi *gas* on which the GWF is based: already for nearest neighbours is its density-density (or spin-spin) correlation function of order $1/d$ small. This justifies the neglect of correlations in $d = \infty$ as assumed by the GA. It also shows that, in contrast to $d = 1$, the GWF does not describe correlations adequately in high dimensions. A detailed analysis of the correlation functions for large separations in dimensions $1 \leqslant d \leqslant \infty$ by VAN DONGEN *et al.* [79] shows that the Brinkman-Rice transition (*i.e.* the transition at a finite U_c) *only* occurs in $d = \infty$, but not in any finite dimension. Indeed, finite orders of perturbation theory in $1/d$ do not remove the transition. On the other hand, for $d = 3$ the results of the GA are found to be excellent if one is not too close to the transition [80]. Hence, in spite of the spurious transition, the results of the GA can be expected to be valuable even for *finite*-dimensional systems. This has been explicitly confirmed by its success in the description of liquid ^{3}He outlined in the previous subsection.

The equation for $\Sigma_{ii,\sigma}$ given by the sum of collapsed, flower-shaped diagrams

becomes quite difficult to solve—or even untractable—when it comes to calculating with generalized Gutzwiller-correlated wave functions of the form

$$|\Psi_G\rangle = g^{\hat{D}}\,|\Psi_0\rangle, \tag{2.21}$$

where $|\Psi_0\rangle$ is a somewhat more refined starting wave function. That has to do with the fact that, in spite of the considerable simplifications arising from the diagrammatic collapse in $d = \infty$, diagrams *do* survive. GEBHARD [80] showed that these problems vanish altogether when $|\Psi_0\rangle$ in (2.21) is written in the form

$$|\Psi_0\rangle = g^{-\sum_{i\sigma}\mu_{i\sigma}\hat{n}_{i\sigma}}\,|\tilde{\Psi}_0\rangle, \tag{2.22}$$

where $|\tilde{\Psi}_0\rangle$ is again an arbitrary, normalized one-particle wave function and the $\mu_{i\sigma}$ are explicit functions of g and the local densities $\tilde{n}_{i\sigma} = \langle\tilde{\Psi}_0\,|\hat{n}_{i\sigma}\,|\tilde{\Psi}_0\rangle$. The operator in (2.22) corresponds to a gauge transformation by which the local chemical potentials (*i.e.* the local fugacities) can be chosen such that all Hartree bubbles disappear in $d = \infty$. With this reinterpretation all diagrammatic calculations remain identical to the earlier ones—only the vertices are given a new value and lines now correspond to

$$\tilde{g}^0_{ij,\sigma} = g^0_{ij,\sigma}(1 - \delta_{ij}), \tag{2.23}$$

where now $\tilde{g}^0_{ii,\sigma} \equiv 0$, and hence $\Sigma_{ii,\sigma} \equiv 0$. Consequently, in $d = \infty$ diagrams vanish completely and results are obtained without the calculation of a single graph. So what remains in $d = \infty$ at all? First of all one finds that the «law of mass action», (2.14), is valid even *locally* and for arbitrary $|\tilde{\Psi}_0\rangle$ (even for those with long-range order). Secondly, the expectation value of the Hubbard Hamiltonian (1.4) in terms of (2.21), (2.22) assumes a *general* form for arbitrary $|\tilde{\Psi}_0\rangle$, *i.e.*

$$\langle\hat{H}\rangle = -t \sum_{\langle \boldsymbol{R}_i, \boldsymbol{R}_j\rangle} \sum_{\sigma} \sqrt{q_{i\sigma}}\sqrt{q_{j\sigma}}\, g^0_{ij,\sigma} + U \sum_i \bar{d}_i\,, \tag{2.24}$$

where $\bar{d}_i = \langle\hat{D}_i\rangle$ and $q_{i\sigma}$ is given by q_σ in (2.15) with n_σ replaced by $\tilde{n}_{i\sigma}$. In the simple, translationally invariant case $|\Psi_0\rangle \equiv |\mathrm{FS}\rangle$ the two wave functions $|\Psi_0\rangle$ and $|\tilde{\Psi}_0\rangle$ are the same up to a trivial factor, and $q_{i\sigma} \equiv q_i$; thus (2.15) is rederived.

The result (2.24) is identical with the saddle point solution of a slave-boson approach to the Hubbard model introduced by KOTLIAR and RUCKENSTEIN [81] (see sect. 3). In fact, one finds that in $d = \infty$ the general set of Gutzwiller-correlated wave functions (2.21) with (2.22) reproduce the full set of static saddle point equations of that approach. This provides a direct connection between two seemingly different approaches. So the results of this slave-boson approach are now known to obey the variational principle and to be valid for *arbitrary* $|\tilde{\Psi}_0\rangle$, *i.e.* not only for a paramagnetic or antiferromagnetic state [81]. Given an arbit-

rary $|\tilde{\Psi}_0\rangle$ the local densities $\tilde{n}_{i\sigma}$ are provided, too. This immediately leads to the ground-state energy $\langle \hat{H} \rangle$ in $d = \infty$. Finally we note that the simple «Gutzwiller counting» of spin configurations described in subsect. 2·2 may be used for arbitrary GWFs, including those with long-range order, *provided* that the latter is written in the form (2.22)[80]; of course, for $|\Psi_0\rangle = |\mathrm{FS}\rangle$ this is unimportant.

The formalism may be extended to finite dimensions $d < \infty$ by reversing the collapse of diagrams ($1/d$ expansion)[78,80]. In this way the large-d limit can be employed to obtain accurate variational results even for low dimensions ($d = 1, 2$). For this it is sometimes enough to simply insert the d-dimensional DOS into the $d = \infty$ result (whereby an infinite class of $1/d$ corrections is automatically included), as will be discussed in the next subsection.

2·5. *Projected wave functions for the periodic Anderson model.* – The approach described above is equally applicable to any other Hubbard-type model, *e.g.* the Anderson lattice model, which is referred to as the periodic Anderson model (PAM). This model is used to investigate basic properties of heavy-fermion and intermediate-valence systems. In its simplest form it is given by

$$\hat{H}_{\mathrm{PAM}} = \sum_{\boldsymbol{k},\sigma} \varepsilon_k \hat{n}^c_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{R}_i,\sigma} \left[\varepsilon_f \hat{n}^f_{i\sigma} + \frac{U}{2} \hat{n}^f_{i\sigma} \hat{n}^f_{i-\sigma} + \frac{V}{\sqrt{L}} \sum_{\boldsymbol{k}} (\exp[i\boldsymbol{k}\cdot\boldsymbol{R}_i] \hat{c}^+_{\boldsymbol{k}\sigma} \hat{f}_{i\sigma} + \mathrm{h.\,c.}) \right], \tag{2.25}$$

which describes a band of noninteracting conduction electrons ($\hat{c}_{\boldsymbol{k}\sigma}$), that hybridize via the matrix element V with static f-electrons ($\hat{f}_{i\sigma}$); the latter interact with each other by a Hubbard interaction and have a global energy ε_f. In (2.25) only an (unrealistic) twofold spin degeneracy has been assumed. The PAM is a straightforward generalization of the original *single-impurity* Anderson model (SIAM)[82] to a *lattice* of «impurities», *i.e.* localized f-electrons. It can be reobtained from (2.25) by restricting the sum over $\boldsymbol{R}_i$ to a single site, *e.g.* $\boldsymbol{R}_i = 0$, such that $\hat{f}_{i\sigma} \to \hat{f}_\sigma$. The SIAM is a model for an impurity in a metal which can develop a magnetic moment. In the so-called Kondo limit, *i.e.* for small hybridization V, strong repulsion U and an ε_f level well below the Fermi energy E_{F} such that $\varepsilon_f < 0$, $\varepsilon_f + U > 0$, a Schrieffer-Wolff transformation[14] of (2.25) leads to the famous Kondo model (for details see ref.[3]). In this model the spin of the conduction electrons at site $\boldsymbol{R}_i = 0$, $\boldsymbol{S}_0$, interacts with the spin $\boldsymbol{S}^{\mathrm{imp}}$ of the magnetic impurity at $\boldsymbol{R}_i = 0$ via the exchange interaction term $-2J\boldsymbol{S}_0 \cdot \boldsymbol{S}^{\mathrm{imp}}$, where $J = V^2/\varepsilon_f < 0$. The scattering of conduction electrons by an impurity whose spin can flip up and down, depending on the spin of the incoming conduction electron, leads to a genuine many-body problem, where *all* electrons enter via the Fermi distribution. Since $J < 0$, the conduction electrons and the impurity

spin wish to align antiferromagnetically at low temperatures («Kondo singlet»). Hence for $T \ll T_K$, where $T_K = (W/2k_B)\exp[-1/|J|N(0)]$ is the «Kondo temperature», the impurity spin has disappeared («Kondo screening»). Here W and $N(0)$ are the band width and the density of states at the Fermi energy of the conduction electrons, respectively. The energy $k_B T_K$ corresponds to the binding energy of the Kondo singlet. Hence, this singlet formation leads to a *lowering* of the ground-state energy of the system by a nonanalytically small amount $k_B T_K$.

For the periodic model, (2.25), RICE and UEDA [83] and BRANDOW [84] introduced a correlated wave function in direct analogy with the GWF for the Hubbard model as

$$|\Psi_{\mathrm{PAM}}\rangle = g^{\hat{D}^f} |\Psi_{\mathrm{PAM},0}\rangle, \tag{2.26a}$$

where $\hat{D}^f$ refers to the double occupancy of f-electrons and

$$|\Psi_{\mathrm{PAM},0}\rangle = \prod_k [1 + a^0_{k\sigma} \hat{f}^+_{k\sigma} \hat{c}_{k\sigma}] \, |\mathrm{cFS}\rangle \tag{2.26b}$$

is the ground-state wave function of the PAM for $U = 0$. Here $|\mathrm{cFS}\rangle$ is the Fermi sea of conduction electrons and

$$a^0_{k\sigma} = \frac{2V_k}{\varepsilon_f - \varepsilon_k + [(\varepsilon_k - \varepsilon_f)^2 + 4V_k^2]^{1/2}} \tag{2.27}$$

is a measure of the hybridization strength V_k (which is here taken to be k-dependent for generality); ε_k is the dispersion of the c-electrons. The choice of the wave function (2.26) is also inspired by the wave functions used in the case of the single-impurity model [85, 86]. Since the number of f-electrons is not conserved, the suppression of double occupancy would favour the transfer of f-electrons into the conduction band, thus changing the effective hybridization. Therefore, not only g but also the entire function $a^0_{k\sigma}$, (2.27), are used as variational quantities to optimize $|\Psi_{\mathrm{PAM}}\rangle$.

Within the Gutzwiller approximation (GA) the ground-state energy of $\hat{H}_{\mathrm{PAM}}$ in terms of (2.26) is found as [83, 87]

$$\frac{E_G^{\mathrm{PAM}}}{L} = \varepsilon_0 - \frac{U}{2} - \frac{W}{2} \exp\left[-\frac{UW}{8V^2}\right]. \tag{2.28}$$

Here ε_0 is the average energy of the noninteracting c-electrons, and we assumed the «symmetric case» $\varepsilon_f + U = -\varepsilon_f$, *i.e.* $\varepsilon_f = -U/2$, with $n^c = n^f = 1$ and hence the total density of electrons is given by $n = 2$ (half-filled band). The appearance of a nonanalytic term in the ground-state energy, *i.e.* of a binding energy that has the form known from the *single-impurity* Kondo problem, is remarkable. (In fact, the exponent differs by a factor 2 from the single-site exponent; this has been shown to be a genuine *lattice* effect [88].) The result in

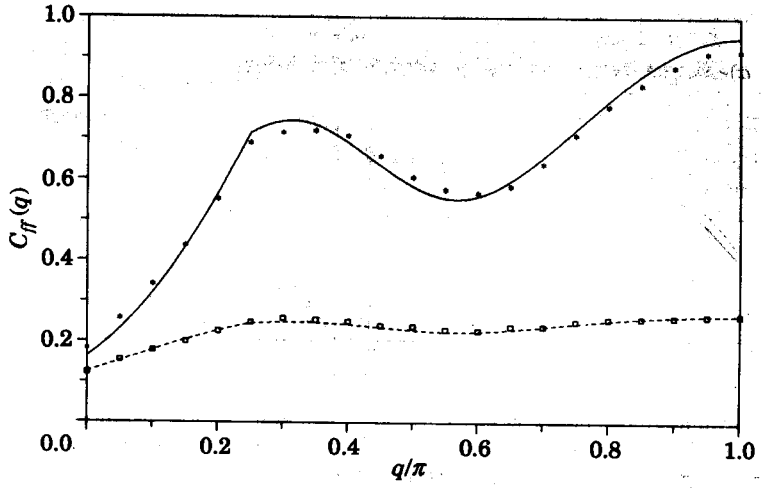

Fig. 2.1. – Evaluation of the spin-spin (C^{SS}) and density-density (C^{NN}) correlation functions of the f-electrons for the 1-dimensional PAM, using (3.30)[89]; the numerical data of Shiba[90] are shown for comparison; —— $C^{SS}(d=\infty$ result in $d=1)$, ····· C^{SS} (VMC in $d=1)$, - - - - - $C^{NN}(d=\infty$ result in $d=1)$, □□□ C^{NN} (VMC in $d=1)$, $n=1.75$, $U=\infty$, $\varepsilon_f=0$, $V=0.5$, $t=1$.

(2.28) agrees with that obtained by the exact evaluation of $\langle \hat{H}_{PAM} \rangle$ in terms of $|\Psi_{PAM}\rangle$ in $d=\infty$, *i.e.* the GA once again yields the correct evaluation for high dimensions[80].

It turns out that the $d=\infty$ result may even be used to obtain accurate results in the extreme opposite limit, *i.e.* $d=1$, by simply evaluating them with the one-dimensional DOS[89]. This is evident from fig. 2.1, where the results for the spin-spin and density-density correlation functions of the f-electrons in the PAM obtained in this way are shown in comparison with numerical data for $d=1$ by SHIBA[90]. The agreement is found to be excellent, particularly if ε_f is not too low. Even details like the Umklapp discontinuity at $q=2(\pi-k_F)$ are borne out.

These results clearly indicate that the expectation values derived in the $d=\infty$ limit may even be used to obtain *quantitatively* accurate results for low-dimensional systems. The reason for this appears to lie in the nature of the VWFs under investigation: they are usually rather simple, being characterized by only a small number of variational parameters, with the symmetry of the wave function more or less determined by construction. Therefore, a practical strategy for any investigation in terms of Gutzwiller-correlated wave functions is to first evaluate the quantities of interest in $d=\infty$ (which is always possible) and then use the exact d-dimensional DOS to obtain a good approximation for the expectation values in this particular dimension.

So far we have only shown that the d-dimensional ground-state properties of

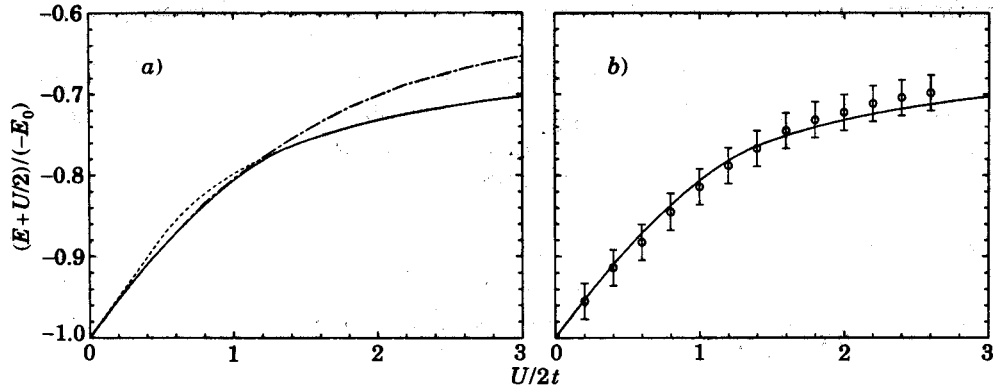

Fig. 2.2. – Ground-state energy E of the periodic Anderson model *vs.* interaction U, plotted as $(E - U/2)/(-E_0)$ with $E_0 \equiv E(U = 0)$, in $d = 1$: *a*) comparison of the results obtained from the paramagnetic Gutzwiller wave function (2.26*a*) and the spin density wave (2.32) with and without Gutzwiller projection: -·-·- Gutzwiller (paramagnetic), ----- SDW, —— Gutzwiller-correlated SDW, $V/2t = 0.375$; *b*) comparison of the results obtained from the projected spin density wave with quantum Monte Carlo results by BLANKENBECLER *et al.* [91]: ○ MC, —— Gutzwiller-correlated SDW, $V/2t = 0.375$.

the PAM, when calculated in terms of the wave function (2.26), can be determined accurately down to $d = 1$ by employing the limit $d = \infty$. This does not address the point of how good the results obtained with (2.26) are in absolute terms, *i.e.* in comparison with the *exact* ground-state wave function. In fig. 2.2*a*) the ground-state energy of the PAM in $d = 1$, measured relative to $\varepsilon_f = -U/2$, as obtained with the paramagnetic Gutzwiller wave function (2.26), is shown. It is compared with the results for a spin density wave function (see below) which becomes exact in the limits $U \to 0$ and $U \to \infty$. Obviously (2.26) yields good results only for *low* U, while at large U the energy is much higher than the exact asymptotic result. The origin for this discrepancy at large U is easily found: it is mainly due to the absence of the (negative!) contribution to the energy from second-order perturbation theory in the hybridization V. Indeed, in the symmetric case and for large U perturbation theory in V yields [91-93]

$$\frac{E^{\mathrm{PAM}}_{\mathrm{exact}}}{L} = \varepsilon_0 - \frac{U}{2} - \frac{2V^2}{L} \sum_{\substack{k \\ \varepsilon_k \geqslant 0}} \frac{1}{U/2 + \varepsilon_k} + \mathcal{O}(V^3), \tag{2.29a}$$

$$= \varepsilon_0 - \frac{U}{2} - \frac{2V^2}{U}, \qquad U \gg |\varepsilon_0|. \tag{2.29b}$$

This result does not depend on the explicit configuration of f-electrons when double occupancy is excluded. In fact, the term $\propto -V^2/U$ is even present for a

single f-spin and hence is not specific for the periodic model. Hence the second-order shift in (2.29a) does not contain any information about the magnetic state of the system—this only comes in at higher order, *i.e.* V^4/U^2. SHIBA and FAZEKAS [92] showed that the second-order contribution is automatically generated by a Schrieffer-Wolff transformation [14] that leads from (2.25) to an effective Hamiltonian (the Kondo lattice with antiferromagnetic coupling).

The overall features of the result for the ground-state energy of the PAM as obtained with the Gutzwiller-type wave function (2.26) are similar to those observed in the case of the Hubbard model [53]. Since the wave function introduces correlations into the *noninteracting* state, the energy comes out very well for weak interactions ($U \lesssim 3t$), but starts to deviate at larger values of U, where the wave function is no longer controlled by some exact limit. In both cases nonanalytic contributions are obtained for large U. The fact that the wave function (2.26) for the PAM does not yield the second-order shift $\propto -V^2/U$ (which is energetically important, but conceptually rather trivial) and only leads to a nonanalytically small, Kondo-like energy contribution (which is energetically unimportant, but conceptually significant) raises the question about the reliability of this wave function. In particular, it is not clear whether the exponentially small energy shift in (2.28) is a genuine feature of the finite-dimensional lattice model (PAM) at all, or whether it is simply an artefact of the approximation, *i.e.* is a residual feature of the single-impurity model on which the construction of the wave function is based. In spite of some indications supporting the Gutzwiller results [94], this is still an open question at present.

The failure of the Gutzwiller-type wave function $|\Psi_{\mathrm{PAM}}\rangle$ to describe the large-U limit of the ground-state energy (2.29a) correctly must obviously be attributed to the inadequacy of the starting wave function $|\Psi_{\mathrm{PAM},0}\rangle$. Any improvement, therefore, has to begin at the level of this starting wave function. For this purpose we will discuss a new type of (projected) wave function which yields a very good ground-state energy *already by itself*, such that the Gutzwiller projection only leads to a final improvement. Recently STRACK and the author [93] proposed a non-Gutzwiller-type wave function to describe the PAM with an antiferromagnetically ordered state of f-electrons. (Indeed we know from experiment [95] that there exist heavy-fermion systems, *e.g.* YbP, U_2Zn_{17}, UCd_{11}, UCu_5, which exhibit antiferromagnetic order in the ground state; due to the existence of a magnetic energy gap the exponentially small Kondo-like terms of the form discussed above will not be relevant then.) This projected wave function is given by

$$|\Psi^{(1)}_{\mathrm{PAM}}\rangle = \hat{C}|\mathrm{c\,FS}\rangle \otimes |\mathrm{f\,SDW}\rangle. \tag{2.30}$$

It has the general form (2.1) where the starting wave function is a product state of a Fermi sea of conduction electrons and a spin density wave of f-electrons (the product in (2.5a) extends over all $\boldsymbol{k}$ with $\varepsilon_{\boldsymbol{k}} \leqslant 0$), and the correlation opera-

tor $\hat{C} = \hat{C}_2 \hat{C}_1$ is given by

$$\hat{C}_1 = \exp\left[\sum_{k\sigma} \tilde{V}_k (\hat{f}^+_{k\sigma} \hat{c}_{k\sigma} + \hat{c}^+_{k\sigma} \hat{f}_{k\sigma})\right], \tag{2.31a}$$

$$\hat{C}_2 = \exp\left[\sum_{k\sigma} \tilde{\varepsilon}_k \hat{n}^f_{k\sigma})\right] \tag{2.31b}$$

with $\tilde{V}_k$ and $\tilde{\varepsilon}_k$ as k-dependent variational functions. In contrast to (2.26) the interactions are more or less already incorporated in the starting wave function, while the correlation operator $\hat{C}_1$ introduces the hybridization and $\hat{C}_2$ controls the quantum-mechanical motion of the f-electrons in $|\mathrm{f\,SDW}\rangle$ (note that $\ln \hat{C}_2$ has the form of a kinetic energy for the f-electrons). Since (2.30) is a two-particle product state, all expectation values in terms of $|\Psi^{(1)}_{\mathrm{PAM}}\rangle$ can be calculated analytically for arbitrary dimension d. The variational quantities u_k and v_k, with $u_k^2 + v_k^2 = 1$, $\tilde{\varepsilon}_k$ and $\tilde{V}_k$ have to be determined from the minimum of the ground-state energy. It is easy to see that the ground-state energy for the PAM obtained with $|\Psi^{(1)}_{\mathrm{PAM}}\rangle$ has the correct limiting behaviour at large U, *i.e.* contains the term $\propto -V^2/U$, as well as for small U [93]. However, at intermediate U-values the energy is higher than that found numerically [91]. BRENIG and MÜLLER-HARTMANN [96] noted that the wave function (2.30) can be improved by introducing an additional term so that the k-dependence of the c- and f-electrons is made symmetric. In this way they constructed the most general two-particle product state of the form (2.30). For the symmetric PAM it can be written in the form of a single Slater determinant SDW ground state

$$|\Psi^{(2)}_{\mathrm{PAM}}\rangle = \tag{2.32}$$

$$= \prod_{\substack{k \\ \varepsilon_k \leqslant 0}} \prod_{\sigma} \prod_{n=1}^{2} [\alpha_{k,n} \hat{c}^+_{k,\sigma} + \beta_{k,n} \hat{f}^+_{k,\sigma} + \sigma(\gamma_{k,n} \hat{c}^+_{k+Q,\sigma} + \delta_{k,n} \hat{f}^+_{k+Q,n})]\,|0\rangle,$$

where $\alpha_{k,n}, \beta_{k,n}, \gamma_{k,n}, \delta_{k,n}$ are variational functions and $n = 1, 2$ labels two orthogonal combinations. The expectation value of $\hat{H}_{\mathrm{PAM}}$ in terms of (2.32) can be expressed in closed form and the minimization can be performed in any dimension [96]. This provides an exact upper limit for the energy. The result for $d = 1$ obtained from the SDW, (2.32), is shown in fig. 2.2*a*). In comparison with the results obtained from $|\Psi^{(1)}_{\mathrm{PAM}}\rangle$ (not shown in the figure) the energy is found to be quite a bit lower at intermediate U-values. Its good overall agreement with the quantum Monte Carlo calculations by BLANKENBECLER *et al.* [91] is quite remarkable in view of the fact that (2.32) is only a single-particle wave function without true two-particle correlations.

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$$= \prod_{\substack{k \\ \varepsilon_k \leq 0}} \prod_{\sigma} \prod_{n=1}^{2} [\alpha_{k,n} \hat{c}^+_{k,\sigma} + \beta_{k,n} \hat{f}^+_{k,\sigma} + \sigma(\gamma_{k,n} \hat{c}^+_{k+Q,\sigma} + \delta_{k,n} \hat{f}^+_{k+Q,n})]\,|0\rangle,$$

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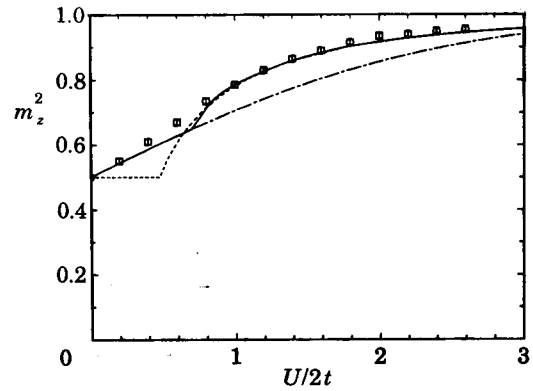


Fig. 2.3. – Square of the local magnetization, m_z^2, of the f-electrons in the periodic Anderson model *vs.* interaction in $d = 1$: the variational results [96, 97] (see fig. 2.2*a*)) are compared with Monte Carlo (MC) results [91]: –·–·– Gutzwiller (paramagnetic), ○ MC, ----- SDW, —— Gutzwiller-correlated SDW, $V/2t = 0.375$.

One may now proceed even further by considering $|\Psi_{\mathrm{PAM}}^{(2)}\rangle$ as a starting wave function *itself*, on which the Gutzwiller projector is applied. This leads to yet another improvement, namely the projected wave function [97]

$$|\Psi_{\mathrm{PAM}}^{(3)}\rangle = g^{\tilde{D}^f}\,|\Psi_{\mathrm{PAM}}^{(2)}\rangle, \tag{2.33}$$

where g is an additional variational parameter. Now exact analytic evaluations in terms of (2.33) can only be performed in $d = \infty$. However, from our earlier experience we may expect that, by evaluating the $d = \infty$ result with the d-dimensional DOS, accurate results can even be obtained down to $d = 1$, which is the most unfavourable limit for the $d = \infty$ approach. The results by GULÁCSI *et al.* [97] in fig. 2.2*a*), *b*) (full line) obtained in this way show that this is indeed the case. Of course, the improvement mainly concerns the intermediate U regime. In fact, the U^2 contribution, which is due to genuine two-particle correlations and hence is absent in the wave function (2.32), is now found to agree well with perturbation theory. Other, more sensitive, quantities like the local magnetization m_z of the f-electrons, where $m_z^2 = \langle(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2\rangle$, can also be calculated. In these cases the correlation factor in (2.33) is found to be important [97] and even leads to significant *qualitative* changes of the results obtained with the uncorrelated wave function (2.32) [96], as shown in fig. 2.3.

In view of the accuracy of the $d = \infty$ approach in dimensions as low as $d = 1$, one can be sure that the results for $d = 2, 3$ will be excellent [97]. These results may serve as a benchmark for future analytic or numerical works, such as quantum Monte Carlo calculations, which are very demanding in $d > 1$.

3. – Projection with auxiliary particles under slave conditions.

3·1. *Hubbard operators.* – The fact that in the strong-coupling limit the local constraints are stressed, forcing one to work in a restricted Hilbert space without doubly occupied sites, is clearly expressed in the projected Hubbard model (1.7). The use of *projected* local operators $\hat{X}_{i\sigma}$ as in (1.7*c*) leads to a seemingly simple form of the Hamiltonian. To exploit this simplicity HUBBARD [98] formulated an «atomic representation» of the Hubbard model in terms of local operators by starting from the atomic limit ($t = 0$), where

$$\hat{H}_{t=0} = \sum_{\boldsymbol{R}_i} \hat{h}_i \,, \qquad \hat{h}_i = \mu \sum_{\sigma} \hat{n}_{i\sigma} + U\hat{D}_i \,, \tag{3.1}$$

and the chemical potential has been explicitly included. The eigenstates of $\hat{h}_i$ are given by $\{|i\alpha\rangle\}$, where $\alpha = 0, \sigma, d$ corresponds to an empty site ($\alpha \equiv 0$), a simply occupied site ($\alpha \equiv \sigma = \uparrow, \downarrow$) or a doubly occupied site ($\alpha \equiv d$, or $\alpha \equiv 2$). The eigenvalue equation is defined by $\hat{h}_i |i\alpha\rangle = \varepsilon_{i\alpha} |i\alpha\rangle$. The atomic limit may be used as a starting point for a perturbation theory in the hopping t, which has recently been formulated in a systematic and computer-tractable way by METZNER [99].

The eigenstates $|i\alpha\rangle$ lead to the definition of the so-called Hubbard or X operators

$$\hat{X}_i^{\alpha\beta} = |i\alpha\rangle\langle\beta i| \tag{3.2}$$

which cause a transition from a state β to a state α of the «atom» at site $\boldsymbol{R}_i$, while leaving all other sites unchanged. These operators have the properties

$$(\hat{X}_i^{\alpha\beta})^+ = \hat{X}_i^{\beta\alpha} \,, \tag{3.3a}$$

$$\hat{X}_i^{\alpha\beta}\hat{X}_i^{\alpha'\beta'} = \delta_{\alpha'\beta}\hat{X}_i^{\alpha\beta'} \,, \tag{3.3b}$$

$$[\hat{X}_i^{\alpha\beta}, \hat{X}_j^{\alpha'\beta'}]_{\pm} = \delta_{ij}[\delta_{\alpha'\beta}\hat{X}_i^{\alpha\beta'} \pm \delta_{\alpha\beta'}\hat{X}_i^{\alpha'\beta}] , \tag{3.3c}$$

$$\sum_{\alpha} \hat{X}_i^{\alpha\alpha} = 1 \,. \tag{3.3d}$$

Clearly the X-operators obey a complicated, noncanonical algebra and are projection operators ($\hat{X}^2 = \hat{X}$) only if $\alpha = \beta$. The completeness relation (3.3*d*) allows one to express any local operator $\hat{\mathcal{O}}_i$ as

$$\hat{\mathcal{O}}_i = \sum_{\alpha,\beta} \langle i\alpha|\hat{\mathcal{O}}_i|\beta i\rangle \hat{X}_i^{\alpha\beta} \,, \tag{3.4}$$

e.g. $\hat{c}_{i\sigma} = \hat{X}_i^{0\sigma} + \sigma\hat{X}_i^{-\sigma d}$, $\hat{n}_{i\sigma} = \hat{X}_i^{\sigma\sigma} + \hat{X}_i^{dd}$ and $\hat{D}_i = \hat{X}_i^{dd}$. In particular, the projected c-operator in (1.7) is precisely given by $\hat{P}_i\hat{c}_{i\sigma}^+ = \hat{X}_i^{\sigma 0}$. In this representation the Hubbard interaction term $\hat{H}_{\mathrm{I}}$ reduces to a sum over $\hat{X}_i^{dd}$. In the limit

$U = \infty$, where d-sites are absent, the Hubbard model then takes the simple form

$$\hat{H}_t = -t \sum_{\langle R_i, R_j \rangle} \sum_{\sigma} \hat{X}_i^{\sigma 0} \hat{X}_j^{0\sigma} . \tag{3.5}$$

Of course, the simple form is deceptive in view of the complicated algebra for the X-operators.

Using this representation, HUBBARD [98] attempted to study the excitation spectrum of the model by linearizing the equation of motion for the X-operators. However, this decoupling is uncontrolled and leads to a violation of sum rules as has been explained by RUCKENSTEIN and SCHMITT-RINK [100]. These authors also showed that by introducing an N-fold spin degeneracy, $\sigma = 1, \ldots, N$, conserving approximations of the equation of motion can be performed in the limit of large N (see also ref. [35]).

3·2. *Slave bosons.* – The X-operators are based on a purely fermionic representation in terms of the original c-operators, *e.g.* $|i\sigma\rangle = \hat{c}_{i\sigma}^{+} |i0\rangle$, the reference state being the empty state $|i0\rangle$. Unfortunately the latter state cannot serve as a convenient starting point: there is no Wick's theorem for such states and hence the usual quantum field-theoretical methods cannot be applied. However, it is possible to express $\hat{X}_i^{\alpha\beta}$ *exactly* in terms of products of fermion and boson operators which obey *canonical* commutation rules, as first discussed by BARNES [101] and COLEMAN [102] in the context of the single-impurity Anderson model (SIAM). (The idea of a bosonic representation is quite old and originates in the work of Holstein and Primakoff and, of course, Schwinger on spin models; see Mattis' book [103].) In particular, the empty site itself is now created from a new, total vacuum $|\mathrm{vac}\rangle$ by application of a boson operator $\hat{e}_i^{+}$ as

$$|i0\rangle = \hat{e}_i^{+} |\mathrm{vac}\rangle , \tag{3.6a}$$

$$|i\sigma\rangle = \hat{f}_{i\sigma}^{+} |\mathrm{vac}\rangle , \tag{3.6b}$$

$$|id\rangle = \hat{d}_i^{+} |\mathrm{vac}\rangle , \tag{3.6c}$$

while singly occupied sites, having fermionic character, are described by fermion operators $\hat{f}_{i\sigma}^{+}$ as before and the d-sites, with their two electrons of opposite spin and total spin zero, are also created by bosonic operators $\hat{d}_i^{+}$. Accordingly, we have, for example,

$$\hat{c}_{i\sigma} \hat{P}_i \equiv \hat{X}_i^{0\sigma} = \hat{e}_i^{+} |\mathrm{vac}\rangle\langle\mathrm{vac}| \hat{f}_{i\sigma}^{+} \equiv \hat{e}_i^{+} \hat{f}_{i\sigma} \tag{3.7}$$

and the original electrons are represented by

$$\hat{c}_{i\sigma} = \hat{e}_i^{+} \hat{f}_{i\sigma} + \sigma \hat{f}_{i-\sigma}^{+} \hat{d}_i . \tag{3.8}$$

This shows that by the construction (3.6) the Hilbert space has been considerably enlarged. It now contains a bosonic part, leading to many unphysical

states. Since $\hat{e}_i$, $\hat{d}_i$ and $\hat{f}_{i\sigma}$ are supposed to obey canonical bosonic and fermionic commutation rules, (3.8) implies that these auxiliary operators must fulfil the *local* constraint (3.3*d*), *i.e.*

$$\hat{Q}_i \equiv \hat{n}_i^e + \sum_\sigma \hat{n}_{i\sigma}^f + \hat{n}_i^d - 1 = 0\,, \tag{3.9}$$

where $\hat{n}_i^e = \hat{e}_i^+ \hat{e}_i$, etc. Equation (3.9) guarantees that the site $\boldsymbol{R}_i$ is either empty, singly occupied or doubly occupied. Through this constraint the bosons are «slaved»—hence their name «slave bosons». In particular (3.9) does not allow them to form a macroscopic condensate as in the case of free bosons.

The *t-J* model, (1.9), then becomes

$$\hat{H}_{tJ} = \sum_{\langle \boldsymbol{R}_i, \boldsymbol{R}_j \rangle} \sum_\sigma \left[-t\hat{f}_{i\sigma}^+ \hat{f}_{j\sigma} \hat{e}_i \hat{e}_j^+ + \frac{J}{2} \sum_{\sigma'} \hat{f}_{i\sigma}^+ \hat{f}_{j\sigma} \hat{f}_{j\sigma'}^+ \hat{f}_{i\sigma'} \right]. \tag{3.10}$$

Since the *t-J* model is defined on the Hilbert space without *d*-sites, the constraint (3.9) reduces to $\hat{n}_i^e + \sum_\sigma \hat{n}_{i\sigma}^f = 1$ in this case.

Taking a lattice with one electron per site as a reference state, the creation of an empty site, $\hat{e}_i^+ |\text{vac}\rangle$, may also be viewed as the creation of a *hole* with spin zero and charge $(+e)$ («holon»); in this case $\hat{f}_{i\sigma}^+ |\text{vac}\rangle$ corresponds to the creation of a spin σ with charge zero («spinon»). The projected electron, (3.7), is, therefore, a composite object obtained by first removing a spin σ with zero charge and then creating a hole with charge $(+e)$ from the vacuum. Spin and charge degrees of freedom of the «real» electron are thus carried by separate fields and it is only through the constraint (3.9) that the necessary confinement of these fields for each physical electron is guaranteed. However, this separation is not unique since the above slave-boson representation is not the only one possible (see below); in fact, a «slave representation» may equally use Schwinger bosons for $|i\sigma\rangle$ and spinless fermions for $|i0\rangle$ and $|id\rangle$ [104, 105].

It is clear that the rewriting of $\hat{H}$ and $\hat{H}_{tJ}$ in terms of slave bosons does not solve (or even simplify) the actual many-body problem described by these models. (This is easily seen in the solution of a toy model, *e.g.* a *single* site without kinetic energy, which is simple to solve by standard methods [3] but becomes quite cumbersome in the slave-boson representation [106].) Indeed, one has traded a problem involving complicated operators by one that involves canonical operators tied by complicated *constraints*. One can only hope that, in analogy with the single-impurity Anderson model [82] discussed in sect. 2 (see [107]), reliable *approximations* now also become possible for these lattice models, *i.e.* that an approximation of the constraints involving many new particles (in particular the bosons, which are sometimes simpler to treat than fermions) is less radical and damaging than an approximation of the original fermionic problem.

It should be mentioned that approximate treatments of the t-J model, (3.10*b*), usually start from one of several possible mean-field decoupling schemes of the J-term and then include fluctuations around the mean-field solution. The relevant low-energy fluctuations are described by gauge fields; this important approach will not be discussed here and we refer the reader to ref. [2] and the work by IOFFE and LARKIN [108] and LEE and NAGAOSA [109].

3·3. *Application to the periodic Anderson model at* $U = \infty$. – Expressing the strongly correlated f-electrons in the PAM, (2.25), in terms of the auxiliary particles $\hat{e}_i, \hat{f}_{i\sigma}, \hat{d}_i$, while leaving the conduction electrons $\hat{c}_{i\sigma}$ unchanged, one finds in the limit $U = \infty$

$$\hat{H}_{\mathrm{PAM}} = \hat{H}^c_{\mathrm{kin}} + \sum_{\boldsymbol{R}_i,\,\sigma} [\varepsilon_f \hat{n}^f_{i\sigma} + V(\hat{c}^+_{i\sigma} \hat{f}_{i\sigma} \hat{e}^+_i + \mathrm{h.c.})], \tag{3.11}$$

where the local constraint (3.9) with $\hat{n}^d_i = 0$ has to be fulfilled. This constraint guarantees that a conduction electron can turn into an f-electron *only* if the f-level is empty. It may be included into (3.11) by introducting Lagrange multipliers $\hat{\lambda}_i$ (real scalar quantum fields) for each site as

$$\hat{H}'_{\mathrm{PAM}} = \hat{H}_{\mathrm{PAM}} + \sum_{\boldsymbol{R}_i} \hat{\lambda}_i \hat{Q}_i \,. \tag{3.12}$$

The constraint is enforced by demanding $\hat{\lambda}_i$ to be time-independent. We observe that $\hat{H}'_{\mathrm{PAM}} - \hat{H}_{\mathrm{hyb}}$, where $\hat{H}_{\mathrm{hyb}}$ is the hybridization term in (3.11), only depends bilinearly on $\hat{c}_{i\sigma}, \hat{f}_{i\sigma}, \hat{e}_{i\sigma}$ and can hence be immediately diagonalized. Indeed, the canonical commutation rules for these fields make the application of Wick's theorem possible *in spite* of the existence of strong interactions. However, the complications have only been shifted to $\hat{H}_{\mathrm{hyb}}$. It is now a *three*-particle interaction term, where c- and f-electrons are coupled by a bosonic field. As discussed in detail by AUERBACH and LEVIN [110], MILLIS and LEE [111] and COLEMAN [112], one may start to extract information from (3.11) by performing a mean-field approximation in analogy with the single-impurity model [107]. The bosons $\hat{e}_i$ are then assumed to be *classical* variables, which are replaced by their space- and time-independent expectation values, *i.e.* $\hat{e}_i \to \langle \hat{e}_i \rangle = \sqrt{n^e}$, and similarly $\hat{\lambda}_i \to \langle \hat{\lambda}_i \rangle = \lambda$ for the Lagrange multipliers. This means that the *local* constraint $\hat{Q}_i = 0$ is replaced by the much weaker, *global* one $\langle \hat{Q}_i \rangle = n^f + n^e - 1 = 0$ for the overall particle densities of bosons and fermions.

We note that, while the original Hamiltonian was symmetric under a simultaneous gauge transformation

$$\hat{f}_{i\sigma} \to \hat{f}_{i\sigma} e^{i\phi_i}, \qquad \hat{e}_i \to \hat{e}_i e^{i\phi_i}, \tag{3.13}$$

the above mean-field assumption breaks this symmetry. Hence the bosons now *do* form a macroscopic condensate: the relaxation of the local constraint to a global one «breaks the chains» of the slave bosons and hence allows them to

Bose-condense. At some temperature T_c^B there will then exist a transition to a normal state with $n^e = 0$ and the c- and f-electrons become completely decoupled. This is clearly an artefact of the mean-field approach where the (large!) fluctuations around $\langle \hat{e}_i \rangle$ are neglected. This will make it impossible to describe the crossover to high temperatures correctly. To introduce and control the fluctuations one may generalize the above model to include an arbitrary spin degeneracy $-J \leqslant \sigma \leqslant J$, with $N = 2J + 1$ states. For $N \to \infty$ fluctuations are suppressed, *i.e.* the mean-field theory becomes exact, while $1/N$ corrections destroy the spurious long-range order by fluctuations [113]. Most recently KROHA, HIRSCHFELD, MUTTALIB and WÖLFLE [114] showed that the unwanted Bose condensation is naturally inhibited if the Bose spectral function $A_e(\omega)$ is allowed to acquire spectral weight at $\omega < 0$, where it becomes negative itself, *i.e.*

$$n^e = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega A_e(\omega) f_{BE}(\omega) \overset{T \to 0}{\to} -\frac{1}{\pi} \int_{-\infty}^{0} d\omega A_e(\omega) > 0 \tag{3.14}$$

with f_{BE} as the Bose-Einstein distribution. Thereby the authors are able to separate the constraint problem from that involving the actual intrinsic dynamics. Using a self-consistent, conserving perturbation theory for the slave particles, they are then able to obtain a correct description of the single-impurity problem at low *and* high temperatures, including the crossover, for all degeneracies N.

Under the mean-field assumption the Hamiltonian (3.12) becomes

$$\hat{H}_{PAM}^{MF} = \hat{H}_{kin}^{c} + \sum_{R_i, \sigma} [\tilde{\varepsilon}_f \hat{n}_{i\sigma}^{f} + \tilde{V}(\hat{c}_{i\sigma}^{+} \hat{f}_{i\sigma} + \text{h.c.})] + \lambda L n^f , \tag{3.15}$$

which is precisely the *non*interacting model ($U = 0$) with renormalized parameters $\tilde{\varepsilon}_f = \varepsilon_f + \lambda$ and $\tilde{V} = \sqrt{1 - n^f} V$. It should be stressed that (3.15) may equally be obtained without the use of slave bosons. Indeed, on a pure mean-field level the latter are not essential here. The renormalization of V is just that given by Fermi's golden rule for the transition rate Γ between c- and f-states when the *average* probability for finding an unoccupied f-level is given by $1 - n_f$, *i.e.* $\Gamma = \pi \tilde{V}^2 N(0)$. The mean-field Hamiltonian (3.15) may easily be diagonalized (for details see ref. [3]). One obtains two renormalized quasi-particle bands

$$E_k^{\pm} = \frac{1}{2} \{ \varepsilon_k + \tilde{\varepsilon}_f \pm [(\varepsilon_k - \tilde{\varepsilon}_f)^2 + 4\tilde{V}^2]^{1/2} \} , \tag{3.16}$$

where $\tilde{\varepsilon}_f - \mu = \tilde{V}^2/(\varepsilon_{k_F} - \mu) \equiv \Delta E$ and $\mu \equiv E_{k_F}^{\pm}$ is the chemical potential. Hence the renormalized f-level is found to lie slightly above μ. Minimization of the free energy F_{PAM}^{MF} determines λ and n^f as $\lambda = 2N(0) V^2 \ln(\mu/\Delta E) \simeq |\varepsilon_f - \mu|$ and $n^f = 1 - \Delta E/2N(0) V^2$. The characteristic energy scale is then given by

$$\Delta E \equiv k_B T_0 \simeq \mu \exp[-|\varepsilon_f - \mu|/2N(0) V^2] . \tag{3.17}$$

For large negative $\varepsilon_f - \mu$ and small V^2 the associated characteristic temperature

T_0 is, therefore, seen to be much smaller than the Fermi temperature, $T_0 \ll T_F$, and can be viewed as the analogue of the Kondo temperature for the case of a lattice of impurities. In the ground state the system is hence found to *gain* an exponentially small energy, namely $k_B T_0$, by the hybridization. This ground state may be interpreted as one given by Kondo-screened spins, where the screening must necessarily be a *collective* effect.

The above results essentially reproduce those obtained from a (slave-boson) mean-field theory for the *single*-impurity model [107]. They become exact in the limit of large spin degeneracy, $N \to \infty$ [110-112]. Hence lattice effects appear to be suppressed in the large-N limit and enter explicitly only via a $1/N$ expansion. GEBHARD [88] showed that the ground-state results can equally be obtained from a Gutzwiller wave function, (2.26*a*), with spin degeneracy $N \to \infty$, which proves that the energy obeys variational bounds.

By calculating thermodynamic properties within the slave-boson approach one finds [110-112] that the linear specific-heat coefficient γ and the magnetic susceptibility χ_s are strongly enhanced by an effective-mass factor $m^*/m \sim \sim T_F/T_0 \gg 1$, while the Wilson ratio, (2.18), is equal to unity (in the $N \to \infty$ limit). This is, of course, just what is found in heavy-fermion systems, whose properties show many similarities with those of normal liquid ^{3}He discussed in sect. 2. Hence the above results seem to give a qualitative explanation of these striking features of heavy-fermion systems.

As far as the transport properties of heavy-fermion systems are concerned, it is a well-known experimental fact that the temperature dependences of the resistivity of individual heavy-fermion (HF) and intermediate-valence (IV) systems can be quite different, the two most characteristic dependences being schematically shown in fig. 3.1*a*). Both dependences are found in HF as well as IV systems. Hence a resistivity maximum, followed by a decrease of $\rho(T)$ for higher temperatures, is *not* characteristic for HF systems (where it is often interpreted as a remnant of the Kondo effect), but is also seen in IV systems. Similarly, the temperature dependence of the thermopower of individual HF/IV systems has any one of the typical dependences shown in fig. 3.1*b*).

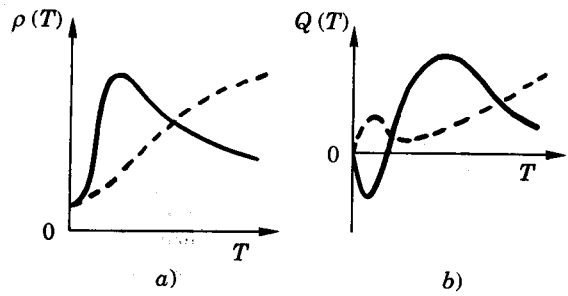


Fig. 3.1. – Typical temperature dependence of *a*) the resistivity and *b*) the thermopower of heavy-fermion and intermediate-valence systems.

(However, $Q(T)$ always has a large absolute value, always shows an extremum at some low temperature and may even change sign.) Hence the different T-dependences of $\rho(T)$ and $Q(T)$ observed do not distinguish between HF and IV systems.

In the above slave-boson mean-field theory the limit $U = \infty$ was taken from the beginning, and the strong renormalization of m^*/m etc. resulted from a Kondo-type screening of f-electrons. On the other hand, YAMADA and YOSIDA [115] showed that large mass enhancements m^*/m etc. are already obtainable in 2nd-order perturbation theory in U relative to the nonmagnetic Hartree-Fock state. Hence even the *weak*-coupling limit can lead to considerable insight into properties of (2.25) at large U. Employing self-consistent 2nd-order perturbation theory, so that Luttinger's sum rules are fulfilled, and exploiting the simplifications occurring in the large-dimension limit, SCHWEITZER and CZYCHOLL [116] recently calculated the d.c. conductivity $\sigma(T)$ and $Q(T)$ in $d = \infty$ from the Kubo formula. Current vertex corrections vanish in the limit $d = \infty$ (the current is odd in parity, while $\Sigma(\omega)$, which is purely local, is even [117]). Therefore, the two-particle propagator entering in the Kubo formula (1.20) reduces to a product of two one-particle propagators. The conductivity in a fixed direction and the thermopower are then given by

$$\sigma(T) = \frac{e^2 a^{2-d}}{2\pi\hbar} t^2 \int_{-\infty}^{\infty} \mathrm{d}E \left(-\frac{\partial f}{\partial E}\right) L(E), \tag{3.18a}$$

$$Q(T) = \frac{1}{eT} \int \mathrm{d}E \left(-\frac{\partial f}{\partial E}\right)(E-\mu) L(E) \Big/ \int \mathrm{d}E \left(-\frac{\partial f}{\partial E}\right) L(E), \tag{3.18b}$$

where

$$L(E) = \frac{2}{L} \sum_{(\boldsymbol{R}_i, \boldsymbol{R}_j)} \sum_{\sigma} \operatorname{Im} G^{\mathrm{c}}_{ij,\sigma}(E + i0^+) \operatorname{Im} G^{\mathrm{c}}_{ji,\sigma}(E + i0^+). \tag{3.19}$$

Here f is the Fermi function, a is the lattice constant and $G^{\mathrm{c}}_{ij,\sigma}$ is the Green function of the conduction electrons. (Note that because of the scaling (1.25) σ is formally of order $(1/d)$ small, since it is a two-point correlation function; however, σ/t^2 is finite.) For $\varepsilon_f = -0.5$, $U = 1$ and $V = 0.4$ (in units of t^*) and setting $d = 3$ in $t^2 = t^{*2}/2d$ there remains only one free parameter, n_{tot}, by which $\rho(T)$ and $Q(T)$ can be changed. The authors [116] then found that the limiting temperature dependences shown in fig. 3.1, as well as the full intermediate range, can be reproduced by only a slight variation of n_{tot}. Even the *absolute* magnitude comes out correctly in this way. These results show that the PAM can indeed account for the overall temperature dependence of transport properties of HF/IV systems. They also indicate that the relevant scattering mechanism responsible for this T-dependence is mainly due to scattering of conduction electrons from the correlated f-electrons (*i.e.* scattering from local spin fluctua-

tions). Clearly the large-d limit captures the essential aspects of transport phenomena even in *three*-dimensional systems.

Within the slave-boson theory the charge susceptibility is found to be almost unrenormalized. Furthermore, since the magnetic coupling (RKKY) between spins does not yet enter at order $1/N$ in a $1/N$ expansion (one has to include $1/N^2$ correction for that), the important *interplay* between Kondo screening and spin interaction can only enter at order $1/N^\alpha$, $\alpha \geqslant 3$. It is not clear whether such an expansion is tractable at all and, if so, whether it is sufficient to describe actual systems where $N = 2$. In fact, it seems reasonable to assume that an *infinite* number of $1/N$ corrections have to be included for that. This may, for example, be achieved within a self-consistent approach as worked out by KROHA *et al.* [114] (see eq. (3.14)). Thereby the authors are able to arrive at a correct description of the single-impurity model at all temperatures and all N.

3·4. *Labelling of fermionic spin and charge degrees of freedom with slave bosons.* – The origin for the asymmetry in the treatment of spin and charge fluctuations within a straightforward $1/N$ expansion may be traced back to the fact that, while *charges* are described by bosons, *spins* are exclusively decribed by fermions. This fundamental difference will generally come to light in an approximate treatment. A formulation without the above asymmetry, *i.e.* a representation of fermionic charge *and* spin degrees of freedom completely in terms of bosonic labels, was introduced by KOTLIAR and RUCKENSTEIN [81]. It was inspired by the ideas entering the Gutzwiller approximation (see subsect. 2·2) and the simplicity and quality of the results of this approximation for the ground-state energy (2.16) of the Hubbard model in terms of the Gutzwiller wave function. In this representation *four* auxiliary bosons $\hat{e}_i$, $\hat{p}_{i\sigma}$, $\hat{d}_i$ are introduced to label each one of the four local states $|i\alpha\rangle$ as

$$|i0\rangle = \hat{e}_i^+ \, |\mathrm{vac}\rangle , \tag{3.20a}$$

$$|i\sigma\rangle = \hat{f}_{i\sigma}^+ \hat{p}_{i\sigma}^+ \, |\mathrm{vac}\rangle , \tag{3.20b}$$

$$|id\rangle = \hat{f}_{i\uparrow}^+ \hat{f}_{i\downarrow}^+ \hat{d}_i^+ \, |\mathrm{vac}\rangle \tag{3.20c}$$

with $\hat{f}_{i\sigma}$ as (pseudo)fermion states. The squares of the *classical* values of these fields are supposed to give the occupation probabilities for the four states. Now one has even more auxiliar particles than in the Barnes/Coleman formulation presented in subsect. 3·3, *i.e.* the Hilbert space becomes even larger, and hence it is necessary to enforce more constraints to eliminate the unphysical states. In fact now there exist two local slave conditions

$$\hat{Q}_i^{(1)} \equiv \hat{n}_i^e + \sum_\sigma \hat{n}_{i\sigma}^p + \hat{n}_i^d - 1 = 0 , \tag{3.21a}$$

$$\hat{Q}_{i\sigma}^{(2)} \equiv \hat{n}_{i\sigma}^f - \hat{n}_{i\sigma}^p - \hat{n}_i^d = 0 . \tag{3.21b}$$

The first constraint, (3.21a), involves only bosons and may be viewed as their

completeness relation: a site is either empty, singly occupied or doubly occupied. The second constraint, (3.21*b*), links bosons with fermion states and expresses the fact that a site carrying an electron with spin σ can either be singly or doubly occupied. The physical electron described by $\hat{c}_{i\sigma}$ is then represented by

$$\hat{c}_{i\sigma} \to \hat{z}_{i\sigma}\hat{f}_{i\sigma}\,, \qquad \hat{z}_{i\sigma} = \hat{e}_i^{+}\hat{p}_{i\sigma} + \hat{p}_{i-\sigma}^{+}\hat{d}_i\,, \tag{3.22}$$

where $\hat{z}_{i\sigma}$ makes sure that the annihilation of a spin σ either leads to a state with a $(-\sigma)$-spin or to an empty site.

3·5. *Application to the Hubbard model.* – Using (3.21), (3.22) the Hubbard model (1.4) takes the form [81]

$$\hat{H} = -t\sum_{\langle \boldsymbol{R}_i, \boldsymbol{R}_j\rangle}\sum_{\sigma}\hat{f}_{i\sigma}^{+}\hat{f}_{j\sigma}\hat{z}_{i\sigma}^{+}\hat{z}_{j\sigma} + U\sum_{\boldsymbol{R}_i}\hat{n}_i^{d} + \sum_{\boldsymbol{R}_i}\Big(\hat{\lambda}_i^{(1)}\hat{Q}_i^{(1)} + \sum_{\sigma}\hat{\lambda}_{i\sigma}^{(2)}\hat{Q}_{i\sigma}^{(2)}\Big), \tag{3.23}$$

where the local constraints are enforced by three Lagrange multipliers $\hat{\lambda}_i^{(1)}$, $\hat{\lambda}_{i\sigma}^{(2)}$ per site (again real scalar quantum fields) which are required to be time-independent. We note that the complicated Hubbard interaction now has a very simple form (as in (3.10*a*)). The prize one has to pay for that is a complicated kinetic energy where fermions and bosons are coupled. However, the fermions $\hat{f}_{i\sigma}$ are seen to appear only bilinearly in (3.23), *i.e.* they do not interact with each other any more, since their interaction is carried entirely by bosonic fields. The fermions can, therefore, be eliminated from the problem («integrated out») as is easily done in a functional-integral formulation [81]. In this way the partition function $\mathcal{Z}$ for the d-dimensional Hubbard model—a model for interacting *fermions*—has been expressed exactly in terms of purely *bosonic* variables with a complicated interaction originating from the kinetic-energy operator. Since, loosely speaking, bosons are in general simpler to treat than fermions, one may now hope that, on an approximate level, the strong-coupling limit becomes more tractable.

We start again with a mean-field approximation, corresponding to a paramagnetic saddle point of the corresponding functional integral [81]. All bosons are replaced by real, site- and time-independent c-numbers as

$$\hat{e}_i \to \langle \hat{e}_i\rangle = \sqrt{n^e} = \sqrt{1 - n + \bar{d}}\,, \tag{3.24a}$$

$$\hat{p}_{i\sigma} \to \langle \hat{p}_{i\sigma}\rangle = \sqrt{n_\sigma^p} = \sqrt{n_\sigma - \bar{d}}\,, \tag{3.24b}$$

$$\hat{d}_i \to \langle \hat{d}_i\rangle = \sqrt{n^d} = \sqrt{\bar{d}}\,, \tag{3.24c}$$

and the same for the Lagrange multipliers: $\hat{\lambda}_i^{(1)} \to \lambda^{(1)}$, $\hat{\lambda}_{i\sigma}^{(2)} \to \lambda_\sigma^{(2)}$. In (3.24) we used the notion for the density of doubly occupied sites, $\bar{d}$, etc. introduced in subsect. 2·2. The local constraints are thereby again relaxed to global constraints: $\hat{Q}_i^{(1)} \to \langle \hat{Q}_i^{(1)}\rangle = 0$, $\hat{Q}_{i\sigma}^{(2)} \to \langle \hat{Q}_{i\sigma}^{(2)}\rangle = 0$. In particular, the constraint fac-

tors in the kinetic energy become

$$\hat{z}_{i\sigma} \to \langle \hat{z}_{i\sigma} \rangle = \sqrt{2\bar{d}(1-2\bar{d})}\,, \tag{3.25}$$

where we assumed $n_\sigma = 1/2$ for simplicity. At $U = 0$, where $\bar{d} = 1/4$, one, therefore, finds that the renormalization is given by $\langle \hat{z}_{i\sigma} \rangle = 1/2$, instead of unity. This is obviously an error caused by the decoupling approximation in which constraints are only fulfilled on average. This problem my be cured by noting that in the enlarged Hilbert space there exist many different Hamilton operators $\hat{H}$ which in the *physical* subspace all have the same properties [81]. Hence, by introducing additional normalization factors into the kinetic energy as

$$\hat{z}_{i\sigma} \to \hat{Z}_{i\sigma} = \frac{1}{\sqrt{1-\hat{n}_i^d-\hat{n}_{i\sigma}^p}}\,\hat{z}_{i\sigma}\,\frac{1}{\sqrt{1-\hat{n}_i^e-\hat{n}_{i-\sigma}^p}}\,, \tag{3.26}$$

the eigenvalue problem for $\hat{H}$, (3.23), is not changed, since in the physical subspace the additional factors in (3.26) have eigenvalues 1 and, therefore, play no role in any exact treatment of the constraints. This liberty may be exploited to ensure that on a mean-field level, where

$$\hat{Z}_{i\sigma} \to \langle \hat{Z}_{i\sigma} \rangle \equiv \sqrt{q_{i\sigma}} = \sqrt{\frac{8\bar{d}(1-2\bar{d})}{n(2-n)}} \tag{3.27}$$

for $n_\sigma = n/2$, one has $\langle \hat{Z}_{i\sigma} \rangle = 1$ for $U = 0$. Of course, the exact kinetic energy, *i.e.* the interaction *between* the bosons, is now exceedingly complicated.

The paramagnetic saddle point is seen to be identical to the result of the Gutzwiller approximation, (2.15), which becomes exact in $d = \infty$ [34, 80]. More generally, the set of all saddle point solutions is identical to the ground-state result (2.24) obtained with an *arbitrary* Gutzwiller wave function (2.21) [80, 88]. This conclusion is also valid for the PAM. Hence there is a direct connection between the above slave-boson representation and Gutzwiller wave functions: the saddle point solution with a given, built-in broken symmetry agrees with the results obtained in $d = \infty$ from the Gutzwiller wave function with the same broken symmetry. Both results may be applied to a d-dimensional system by evaluating the results with the d-dimensional density of states. This connection is not entirely surprising since the slave-boson formalism by KOTLIAR and RUCKENSTEIN [81] was modelled after the Gutzwiller results. We now learn that i) the Gutzwiller results can be obtained even *without* explicit wave functions (which, in principle, allows one to improve the theory systematically, and extend the theory to finite temperatures), and ii) in the ground state the saddle point solution satisfies variational bounds. From our experience with Gutzwiller-projected wave fucntions we can expect the quality of the mean-field results to be good. Indeed, LILLY, MURAMATSU and HANKE [118] found that for the Hubbard model in $d = 2$ the saddle point solution with broken A-B symmetry is in very

good agreement with quantum Monte Carlo results for local observables over a wide range of interactions ($0 < U \lesssim 20t$) and particle densities ($0 < n \leq 1$). Similarly, STRACK and VOLLHARDT [89] showed that the limit of high dimensions can be used to obtain accurate variational results even for low-dimensional ($d = 1, 2$) fermionic systems such as the Hubbard model and the PAM (see sect. 2).

The saddle point solution may also be used at $T > 0$ to obtain the corresponding partition function $\mathcal{Z}_{\mathrm{SP}} = \sum_n \exp[-\beta E_n]$, and thereby the free energy F_{SP}. The quality of $\mathcal{Z}_{\mathrm{SP}}$ was elucidated by GEBHARD [88], who showed that the energies E_n in the sum correspond to the energy expectation values

$$E_n = \frac{\langle \Psi_{\mathrm{G}}^{(n)} | \hat{H} | \Psi_{\mathrm{G}}^{(n)} \rangle}{\langle \Psi_{\mathrm{G}}^{(n)} | \Psi_{\mathrm{G}}^{(n)} \rangle} = \langle \Psi_n | \hat{H}^{\mathrm{eff}} | \Psi_n \rangle , \tag{3.28}$$

where $|\Psi_{\mathrm{G}}^{(n)}\rangle = g^{\hat{D}} |\Psi_n\rangle$ ($n = 0, 1, 2 \ldots$) with $|\Psi_{n=0}\rangle$ as the *exact* ground state of the noninteracting effective Hamiltonian $\hat{H}^{\mathrm{eff}}$, and $|\Psi_n\rangle$ are excited states of $\hat{H}^{\mathrm{eff}}$. The problem is that the $|\Psi_{\mathrm{G}}^{(n)}\rangle$ are not orthogonal (see also ref. [75]). Only low-lying excitations may be described in this way, while higher excitations (in particular charge excitations which are always suppressed by the correlation operator) cannot be described adequately. Hence the saddle point free energy is, at best, applicable at low T (Fermi-liquid regime) [88]. WÖLFLE and LI [119] showed that one-loop corrections to the saddle point solution provide a $T^3 \ln T$ spin fluctuation contribution to the specific heat. In this and other calculations it is important to employ a manifestly spin-rotation-invariant formulation of the Kotliar-Ruckenstein slave-boson theory [120], which in its original formulation [81] depends on the choice of the quantization axis (for a clear exposition, as well as a detailed derivation and discussion, see [121]). In particular, it requires the replacement of $\hat{p}_{i\sigma}$ by a scalar (spin 0) boson and a vector (spin 1) boson as

$$\hat{p}_{i\sigma}^{+} \to \hat{p}_{i\sigma\sigma'}^{+} = \frac{1}{\sqrt{2}} \sum_{\mu=0}^{3} \hat{p}_{i\mu}^{+} (\hat{\tau}_\mu)_{\sigma\sigma'} , \tag{3.29}$$

where τ_μ are the Pauli matrices.

3·6. *Local gauge symmetry.* – We wish to determine the symmetry of the Hubbard model, (3.23), under local gauge transformations of the four bosonic variables

$$\hat{b}_i \to \hat{b}_i e^{i\phi_i^b(\tau)} , \qquad b = e, d, p_\sigma . \tag{3.30}$$

Both the interaction term and the constraints are determined by pure densities $\hat{b}_i^{+} \hat{b}_i$ and are thus invariant under this transformation, implying a $U(1) \times \times U(1) \times U(1) \times U(1) \equiv U(1)^{\otimes 4}$ symmetry. However, the kinetic energy does not have this invariance and the substitution (3.30) leads to additional terms. JOLICOEUR and LE GUILLOU [122] noted that the latter can be absorbed into the

Lagrange multipliers $\lambda_i^{(1)}$, $\lambda_{i\sigma}^{(2)}$ as

$$\lambda_i^{(1)} \to \lambda_i^{(1)} - i \frac{\partial \phi_i^e}{\partial \tau}, \tag{3.31a}$$

$$\lambda_{i\sigma}^{(2)} \to \lambda_{i\sigma}^{(2)} + i \frac{\partial}{\partial \tau} (\phi_i^{p_\sigma} - \phi_i^e). \tag{3.31b}$$

However, since there are only *three* Lagrange multipliers, this requires that the phases obey the constraint $\phi_i^e + \phi_i^d = \sum_\sigma \phi_i^{p_\sigma}$. Hence the Hamiltonian (or the corresponding action) is only symmetric under the group $U(1)^{\otimes 3}$. This implies that the phases of the bosonic fields cannot all be chosen at wish (*e.g.*, zero) but only in the case of three of the bosons, while the fourth, *e.g.* $\hat{d}_i$, must remain complex [121, 122]. This is in contrast to the PAM at $U = \infty$, (3.11), where only a single $U(1)$ gauge symmetry exists which can then be used to eliminate the phase of the single boson $\hat{e}_i$. The above findings are not important for the saddle point mean-field solution itself. This approximation breaks the gauge symmetries anyway, *i.e.* assumes a Bose condensate at low T. (Note that this feature, *i.e.* the mean-field solution itself, again becomes exact in the limit of large spin degeneracy, $N \to \infty$, where fluctuations are suppressed [119].) However, they become crucial in the calculation of corrections to the saddle point, which now turn out be very complicated [122].

It should be stressed that for a given model of interacting electrons the results obtained by taking the $N \to \infty$ limit of an assumed spin degeneracy $\sigma = 1, \ldots, N$ greatly depend on the specific representation in terms of auxiliary particles. For example, in the case of the Hubbard model the $N \to \infty$ limit leads to different results depending on whether it is applied to the usual fermionic representation (1.4) or to the slave-boson version with $N \to \infty$ fermion fields $\hat{f}_{i\sigma}$, (3.23). (In fact eq. (1.4) always becomes trivial for $N \to \infty$, *i.e.* there exists no scaling of the parameters such that the kinetic *and* the interaction terms remain finite [35].) Only the *exact* solution for $N = 2$ of the model in the different representations will coincide. Hence, while an N-orbital slave-particle model does not necessarily correspond to a physical model of electrons, it nevertheless represents a well-defined model of quantum statistical mechanics [121].

4. – Construction of a comprehensive, dynamical mean-field theory for correlated fermions.

In the statistical theory of classical and quantum-mechanical systems mean-field theories (MFTs) play an extremely important role, since they are often able to provide a rough, overall description of the properties of a model. Such a nonperturbative approximation is particularly helpful when, as usual, exact solutions are not available. In the first three sections we already discussed several quite different MFTs. Although the term MFT is frequently used, the ac-

tual *meaning* of what a MFT is (or should be) is rather vague, because there is no unique prescription of how to construct such a theory. Hence every time one encounters the term «MFT», one should inquire about the potential reliability of this approximation, *i.e.* about its range of validity with respect to the input parameters (*e.g.*, the interaction strength, particle density, temperature, magnetic field, etc.), its thermodynamic consistency and, in particular, whether there exists a limit in which it becomes exact.

One of the best-known MFTs is the Weiss molecular-field theory for the Ising model. It is a prototypical *single-site* theory which becomes exact for infinite-range interaction, as well as in the limit $d \to \infty$. In the latter case the quantity $1/d$ is a small parameter which can be used to improve the MFT systematically. This MFT contains no unphysical singularities and is applicable for all values of the input parameters J, T and the magnetic field H. It is also diagrammatically controlled [33]. Insofar it is a very respectable approximation which sets very high standards for other MFTs.

Itinerant quantum-mechanical models, such as the Hubbard model and its generalizations, are naturally much more complicated than classical, Ising-type models. This is due to the additional energy transfer between the particles and the nontrivial algebra needed to describe these particles. Generally there do not even exist semi-classical approximations for such models that might serve as a promising starting point for further investigations. Under such circumstances the construction of a MFT with the comprehensive properties of the Weiss molecular-field theory for the Ising model will necessarily be much more complicated, too. There *do* exist useful, established mean-field approximation schemes, *e.g.* Hartree-Fock, random-phase approximation (RPA), saddle point evaluations of path integrals (see sect. 3), decoupling of operators, etc. However, these approximations are not MFTs in the spirit of statistical mechanics, since, on the pure mean-field level, they are not able to give a reliable, global description of a given model (*e.g.*, the phase diagram, thermodynamics, etc.) in the *entire range* of input parameters. In this situation the exact solution of a fermionic lattice model in the limit $d = \infty$ provides an ideal mean-field solution for these models which has all the desired features of a comprehensive MFT: it is a self-consistent, conserving approximation which is valid for all input parameters and can be systematically improved by taking $1/d$ corrections into account. In contrast to Hartree-Fock it is a dynamical MFT where two-particle correlations are explicitly included.

4·1. *Coherent potential approximation for disordered systems.* – To gain a deeper understanding of the mean-field features of the $d = \infty$ limit for interacting electrons, we first want to discuss the «coherent potential approximation» (CPA), which is known to provide a reliable, comprehensive mean-field approximation for single-particle quantities of noninteracting, *disordered* systems [123]; for reviews see ref. [124]. To be specific let us consider Anderson's

tight-binding Hamiltonian for electrons with local, *i.e.* «diagonal», disorder [125]

$$\hat{H}_{\mathrm{A}} = -\frac{t^*}{\sqrt{Z}} \sum_{\langle \boldsymbol{R}_i, \boldsymbol{R}_j \rangle} \hat{c}_i^+ \hat{c}_j + \sum_i V_i \hat{n}_i \,, \tag{4.1}$$

where V_i is a random variable drawn from some distribution function $P(V_i)$. The electrons described by (4.1) do not interact. Therefore, we deal with the problem of a *single particle* moving through a random medium. (Since there is no spin dependence one can suppress the spin index here and simply work with a spinless fermion as in (1.12).) The problem is made complicated by the randomness. It requires one to calculate the *average* of a physical quantity X (which is a function of all site energies V_i) with respect to $P(V_i)$ as

$$\langle X \rangle_{\mathrm{av}} := \prod_{\boldsymbol{R}_i} \int \mathrm{d}V_i \, P(V_i) X(V_1, \ldots, V_L) \,. \tag{4.2}$$

One may now proceed as follows:

1) The actual random medium, given by the local potentials V_i, is thought to be replaced exactly (!) by an (unknown) *effective* medium, described by a complex, frequency-dependent self-energy; this defines the self-energy.

2) Since the effective medium is required to yield an exact description of the random medium, we may remove the medium at a site $\boldsymbol{R}_i$, replace it by an actual potential V_i and then demand that, upon averaging, the scattering caused by the perturbation of the medium due to V_i vanishes identically. The self-consistency condition expressed in the last step actually *determines* the previously unknown self-energy.

Let $G_{ij}(z) \equiv G$ be the Green function of the electron in the random medium, with z as a complex frequency and G_0 as the unperturbed Green function; we suppress site indices for the moment [126]. The Lippmann-Schwinger equation for G is given by

$$G = G_0 + G_0 V G \quad \text{or} \quad G_0^{-1} G = 1 + VG \,. \tag{4.3}$$

We now introduce a self-energy $\Sigma_{ij}(z) \equiv \Sigma$ into (4.3), which plays the role of an additional, unknown potential

$$(G_0^{-1} - \Sigma) G = 1 + (V - \Sigma) G \,. \tag{4.4}$$

We *choose* Σ such that

$$\langle G \rangle_{\mathrm{av}} = (G_0^{-1} - \Sigma)^{-1} \,. \tag{4.5}$$

Multiplication of (4.4) by $\langle G\rangle_{\mathrm{av}}$ yields

$$G = \langle G\rangle_{\mathrm{av}} + \langle G\rangle_{\mathrm{av}}(V-\Sigma)G\,. \tag{4.6}$$

Here $V-\Sigma$ is a new scattering potential, whose effect can be described, as usual, by a T-matrix via

$$G = \langle G\rangle_{\mathrm{av}} + \langle G\rangle_{\mathrm{av}} T \langle G\rangle_{\mathrm{av}}\,, \tag{4.7}$$

where

$$T = \frac{V-\Sigma}{1-(V-\Sigma)\langle G\rangle_{\mathrm{av}}}\,. \tag{4.8}$$

Averaging of (4.7) yields

$$\langle T\rangle_{\mathrm{av}} = 0\,, \tag{4.9}$$

which is a self-consistent equation for Σ. Equation (4.9) demands that Σ is determined in such a way that the scattering due to the perturbation $V-\Sigma$ vanishes. If (4.9) could be solved exactly, the entire problem would be solved! However, an exact solution is usually not possible, so that an approximation has to be made to proceed further. At this stage CPA *assumes* the self-energy to be site diagonal

$$\Sigma_{ij}(\omega) = \Sigma(\omega)\delta_{ij}\,, \tag{4.10}$$

i.e. to be homogenous. Equation (4.10) is equivalent to a *single-site approximation* and corresponds to step 2) in the description of CPA below (4.2). Since $\Sigma(\omega)$ is homogeneous, it is a ***k-independent***, but frequency-dependent potential and thereby only adds to the frequency dependence of $(G_0)^{-1}$, *i.e.* the averaged local propagator is simply given by the unperturbed propagator with shifted frequency:

$$\langle G_{ii}\rangle_{\mathrm{av}} = G^0_{ii}(z-\Sigma)\,, \tag{4.11}$$

where

$$G^0_{ii}(z) = \int_{-\infty}^{\infty} \mathrm{d}E\,\frac{N(E)}{z-E} \tag{4.12}$$

is the local, unperturbed propagator, with $N(E)$ as the DOS of the unperturbed system. For *all* sites $\boldsymbol{R}_i$ the condition (4.9), therefore, reduces to $\langle T_i\rangle_{\mathrm{av}} = 0$, *i.e.*

$$\left\langle \frac{V_i-\Sigma(z)}{1-(V_i-\Sigma(z))\,G^0_{ii}(z-\Sigma(z))}\right\rangle_{\mathrm{av}} = 0\,. \tag{4.13}$$

Equation (4.13) implies that in the effective medium the average scattering from a single site («impurity») with potential $V_i-\Sigma$ vanishes. The single-site

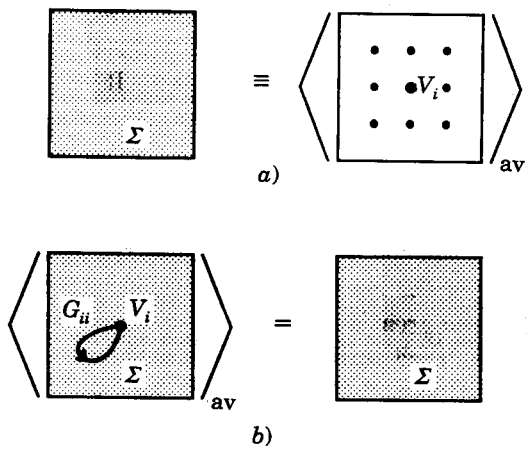


Fig. 4.1. – *a*) The random medium, described by local potentials V_i, is replaced by an unknown, but exact, effective potential Σ. *b*) By demanding the average scattering from a single site with potential $V_i - \Sigma$ to vanish Σ is determined self-consistently.

aspect underlying the CPA may, therefore, be visualized as shown in fig. 4.1 [124].

The CPA and its results have many attractive features: i) CPA is a nonperturbative, but very simple and self-consistent theory; ii) it may be considered as the best single-site approximation for the disorder problem as can be inferred from the above derivation; iii) it has the so-called «Herglotz properties», *i.e.* $\Sigma(z) = \Sigma^*(z^*)$ and $\mathrm{Im}\,(z - \Sigma(z)) \gtrless 0$ for $z \gtrless 0$ [127], which implies that it has the correct analytic properties (positive DOS, etc.); iv) it leads to very good qualitative and even quantitative results for the one-particle properties of disordered systems. The latter is true even in dimensions $d \leqslant 3$ and for parameter values of the disorder strength and the impurity concentration where CPA *cannot* be linked to perturbation theory. These properties have made CPA *the* approximation scheme for disordered systems although it cannot describe Anderson localization.

The single-site aspect of the CPA outlined above and, in particular, the property (4.10), which is identical with (1.28) for *interacting* lattice systems in $d = \infty$, suggest that the CPA will become exact in the limit of high coordination numbers Z. Using the scaling of t given by (1.25), which leads to identical diagrammatic simplifications as described in subsect. 1·6, VLAMING and VOLLHARDT [128] recently showed that this is indeed the case, irrespective of the lattice structure. In other words, CPA solves the disorder Hamiltonian (4.1) exactly in the limit $Z \to \infty$. This finding explains why for $Z < \infty$, *e.g.* finite dimensions on a regular lattice, the CPA can be so successful even for intermediate values of the input parameters (disorder strength, impurity concentration), *i.e.* in regions of parameter space where this can no longer be justified by perturba-

tion theory in these two parameters. We now see that there is an *additional* small parameter, namely $1/Z$, which allows for a perturbation expansion that is independent of the values of the input parameters. It is, therefore, not surprising that the CPA may give qualitatively and quantitatively correct results even in dimensions $d \lesssim 3$.

The CPA can also be derived *variationally* within a field-theoretical approach first discussed by JANIŠ [38, 129]. In this case the coherent potential, *i.e.* the self-energy, is determined from a stationary condition for the averaged free-energy functional of the corresponding single-site problem. This field-theoretical approach has the great advantage that it can be generalized to treat interacting lattice models, such as Hubbard-type models, *and* disorder models on the same basis. Furthermore, the physical idea behind this single-site theory is very transparent and may be explained in terms of the following simple picture [130]. To calculate the averaged free energy corresponding to a single site $\boldsymbol{R}_i$ of the system, we have to determine the energy density

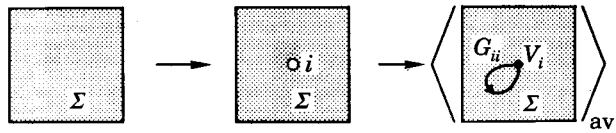
$$\langle \tilde{\Omega} \rangle_{\mathrm{av}} \equiv \langle \Omega_i \rangle_{\mathrm{av}} = \langle \Omega \rangle_{\mathrm{av}} / L \,, \tag{4.14}$$

where densities are indicated by a tilde. To this end we consider the second step of the CPA strategy outlined below eq. (4.2) and drawn schematically in fig. 4.2: i) we start from the homogeneous, effective medium with free-energy density $\tilde{\Omega}_{\mathrm{med}}$; ii) we remove the medium at site $\boldsymbol{R}_i$, *i.e.* subtract a corresponding energy density Ω_i, and iii) replace it by a site with a bare potential V_i, *i.e.* add a corresponding averaged energy density $\langle \Omega_i^{\mathrm{bare}} \rangle_{\mathrm{av}}$; so we have

$$\tilde{\Omega}_{\mathrm{av}} = \tilde{\Omega}_{\mathrm{med}} - \Omega_i + \langle \Omega_i^{\mathrm{bare}} \rangle_{\mathrm{av}} \,. \tag{4.15}$$

To calculate the contributions in (4.15) we make use of the trace-log formula $\ln \det \hat{A} = \mathrm{tr} \ln \hat{A}$ (see, for example, ref. [2]) for the free energy, which in the noninteracting case can be written as

$$\Omega_0 = -T \,\mathrm{tr} \sum_{k} \ln [G_k^0 (i\omega_n)]^{-1} \,. \tag{4.16}$$



a) b) c)

Fig. 4.2. – Steps to construct the exact averaged free-energy functional in $d = \infty$: *a*) homogeneous effective medium, *b*) medium is removed at site $\boldsymbol{R}_i$, *c*) hole in medium at site $\boldsymbol{R}_i$ is filled with the actual potential V_i; the amplitude for a particle from the medium to be at site $\boldsymbol{R}_i$ is given by the local propagator G_{ii}.

Here G_k^0, the propagator of the undisturbed system, is given by

$$G_k^0(z) = \frac{1}{z - \varepsilon_k + \mu}, \tag{4.17}$$

where $\omega_n = (2n + 1)\pi T$ are the Matsubara frequencies and the trace operation implies summation over all n and spin σ; in the present problem the spin is unimportant. Using (4.11), we find

$$\Omega_{\text{med}} = -T \operatorname{tr} \sum_k \ln [G_k^0(i\omega_n - \Sigma)]^{-1} = \tag{4.18}$$

$$= -LT \operatorname{tr} \int_{-\infty}^{\infty} dE\, N(E) \ln [i\omega_n - \Sigma + \mu - E]$$

and

$$\Omega_i = -T \operatorname{tr} \ln [G_{ii}^0(i\omega_n - \Sigma)]^{-1} = -T \operatorname{tr} \ln [\langle G_{ii} \rangle_{\text{av}}]^{-1}, \tag{4.19}$$

where $\Sigma \equiv \Sigma(i\omega_n)$. Finally, $\langle \Omega_i^{\text{bare}} \rangle_{\text{av}}$ can be obtained from

$$\Omega_i^{\text{bare}} = -T \ln \mathcal{Z}_i^{\text{bare}}, \tag{4.20}$$

where the local partition function is determined by the action A_i^{bare} as [131]

$$\mathcal{Z}_i^{\text{bare}} = \int \mathcal{D}\Psi \mathcal{D}\Psi^* \exp [A_i^{\text{bare}} \{\Psi, \Psi^*\}]. \tag{4.21}$$

Here Ψ, Ψ^* are Grassmann (anticommuting) variables. (It is not really necessary to use Grassmann variables in this problem, but they are very convenient because they make everything very simple; any reader who is not familiar with this technique can easily learn it by reading a few pages in the books by POPOV [131] or FRADKIN [2].) The action has the form of a Lagrangian

$$A_i^{\text{bare}} = \operatorname{tr} \Psi_n^* (\langle G_{ii} \rangle_{\text{av}})^{-1} \Psi_n - \operatorname{tr} \Psi_n^* (V_i - \Sigma) \Psi_n, \tag{4.22}$$

where the two terms correspond to the kinetic and potential energy, respectively. Since (4.22) is the expression for a noninteracting system (bilinear dependence on Ψ and Ψ^*), the functional integral in (4.21) is trivial. The trace-log formula yields

$$\ln \mathcal{Z}_i^{\text{bare}} = \operatorname{tr} \ln \{(\langle G_{ii} \rangle_{\text{av}})^{-1} - V_i + \Sigma\}, \tag{4.23a}$$

$$= \operatorname{tr} \ln (\mathcal{G}^{-1} - V_i), \tag{4.23b}$$

where we introduced an *effective* local propagator $\mathcal{G}$ by

$$\mathcal{G}^{-1} \equiv (\langle G_{ii} \rangle_{\text{av}})^{-1} + \Sigma. \tag{4.23c}$$

The $\mathcal{G}$ propagator describes the coupling between the medium and the site $\boldsymbol{R}_i$.

The averaged free energy, which is a functional of $\mathcal{G}^{-1}(\Sigma)$, then follows as

$$\langle\Omega\rangle_{\mathrm{av}} = -LT\,\mathrm{tr}\left\{\int \mathrm{d}E\, N(E)\,\ln[i\omega_n + \mu - \Sigma - E] - \ln(\mathcal{G}^{-1} - \Sigma) + \right. \tag{4.24}$$

$$\left. + \langle \ln(\mathcal{G}^{-1} - V_i)\rangle_{\mathrm{av}}\right\}.$$

By taking the variational derivative of (4.28) with respect to Σ, *i.e.* using the stationarity condition

$$\frac{\delta\langle\Omega\rangle_{\mathrm{av}}}{\delta\mathcal{G}^{-1}} = 0\,, \tag{4.25}$$

we obtain

$$\frac{1}{\mathcal{G}^{-1} - \Sigma} = \left\langle \frac{1}{\mathcal{G}^{-1} - V_i} \right\rangle_{\mathrm{av}}, \tag{4.26}$$

which, together with (4.11) and (4.23*c*), is seen to be identical with the self-consistent equation (4.13) for Σ. Given a value $\mathcal{G}^{-1}$ we obtain Σ from (4.26), which determines a new value $\mathcal{G}^{-1} = [G_{ii}^0(z-\Sigma)]^{-1} + \Sigma$, etc. Equation (4.26) expresses particularly clearly the single-site aspect of the CPA, as well as the role of Σ as a homogeneous effective potential that describes the effect of the original random potential V_i in the averaged system.

4·2. CPA *for interacting systems: exact solution of the Hubbard model in* $d = \infty$. – The CPA was extensively used in the 1970's—mostly in the investigation of disordered systems [124]. As such, it was also applied to interacting models, *e.g.* the Hubbard model, by first transforming the model (approximately) to a random-alloy problem («alloy analogy»). A new approach to the CPA, which makes use of field-theoretical functional-integral techniques in connection with explicit diagrammatic perturbation theory, was initiated by JANIŠ [38, 129]. Thereby the range of applicability of the CPA was extended to include *interacting* lattice systems (spin systems and itinerant systems) as well. Due to the insight gained from the investigation of fermionic lattice systems in the large-d limit [34, 41-43] we are now able to conclude that this generalized CPA approach becomes exact in $d = \infty$, just as the disorder CPA and the Weiss molecular-field theory become exact in this limit. In particular, this field-theoretical approach can be used to derive the exact free energy for fermionic models in $d = \infty$. This leads to a comprehensive mean-field theory for interacting fermionic models. Of course, this theory is necessarily much more complicated in detail than the previous MFTs since we now deal with a *dynamical* single-site problem in a fermionic bath.

The physical idea behind the approach is the same as that entering in the

CPA. Let us consider the motion of a particle on a lattice in $d = \infty$. The interaction with the other particles affects the motion. This change is exactly (!) described by a yet unknown complex, dynamical field $\Sigma_\sigma(\omega)$. (For simplicity we take $\Sigma_\sigma(\omega)$ to be homogeneous, *e.g.* consider the paramagnetic phase; in the case of an antiferromagnetic phase we would have to introduce sublattices, *e.g.* $\Sigma_\sigma \to \Sigma_\sigma^{A,B}$ [38].) Hence the original system with its *bare* interactions has been exactly replaced by an *effective* medium; the latter is simply a system of *non*interacting, itinerant electrons moving in a complex, homogeneous coherent potential $\Sigma_\sigma(\omega)$.

We will now use the generalized CPA described above [38, 40] to construct an exact expression for the free energy of the Hubbard model in $d = \infty$. We proceed as in the case of disordered systems (see subsect. 4·1 and fig. 4.2), with V_i replaced by $\hat{v}_{i\sigma} = U\hat{n}_{i,-\sigma}$—but, of course, we do not have to perform any impurity average now. The single-site free-energy density $\tilde{\Omega} = \Omega/L$ is then determined by

$$\tilde{\Omega} = \tilde{\Omega}_{\text{med}} - \Omega_i + \Omega_i^{\text{bare}} . \tag{4.27}$$

The three terms in (4.27) are given by (4.18)-(4.21), where now the propagators, the effective potential and the Grassmann numbers carry a spin index and the single-site action (4.22) has the form

$$A_i^{\text{bare}}\{\Psi_\sigma, \Psi_\sigma^*; \mathcal{G}_\sigma^{-1}\} = \tag{4.28}$$

$$= \operatorname{tr} \Psi_{\sigma,n}^* \mathcal{G}_\sigma^{-1} \Psi_{\sigma,n} - U \int_0^\beta \mathrm{d}\tau \, \Psi_\uparrow^*(\tau) \Psi_\uparrow(\tau) \Psi_\downarrow^*(\tau) \Psi_\downarrow(\tau).$$

An identical expression for the action A_i^{bare} of the effective single-site problem was obtained by GEORGES and KOTLIAR [39] within a rather different approach. They view the problem as an auxiliary *impurity* problem whose action is precisely given by (4.28) (see below); this equivalence was also pointed out by OHKAWA [132] and JARRELL [133].

The partition function $\mathcal{Z}_i^{\text{bare}}$ may be transformed [40] into a conventional functional integral over real, commuting variables by rewriting the Hubbard interaction in (4.28) using the Hubbard-Stratonovich transformation

$$\exp\left[-U \int_0^\beta \mathrm{d}\tau \, \Psi_\uparrow^*(\tau) \Psi_\uparrow(\tau) \Psi_\downarrow^*(\tau) \Psi_\downarrow(\tau)\right] = \tag{4.29a}$$

$$= \int \mathcal{D}\eta \, \mathcal{D}\xi \exp\left[-\frac{1}{2\beta} \int_0^\beta \mathrm{d}\tau \left[\eta^2(\tau) + \xi^2(\tau) - \right.\right.$$

$$-i\sqrt{2U\beta}\{\xi(\tau)[\Psi^*_\uparrow(\tau)\Psi_\uparrow(\tau)+\Psi^*_\downarrow(\tau)\Psi_\downarrow(\tau)]-$$

$$-i\eta(\tau)[\Psi^*_\uparrow(\tau)\Psi_\uparrow(\tau)-\Psi^*_\downarrow(\tau)\Psi_\downarrow(\tau)]\}\Big]\Big].$$

This is equivalent to the standard operator identity

$$\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}=\frac{1}{4}[(\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow})^2-(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})^2] \tag{4.29b}$$

for the Hubbard interaction, where the two terms on the r.h.s. correspond to charge and spin fluctuations, respectively. In (4.29*a*) the fluctuations are described by real fluctuating fields $\xi(\tau)$ and $\eta(\tau)$, respectively. Now that the interaction problem has been rewritten in terms of noninteracting particles in the presence of infinitely many fluctuating fields, the integration over the Grassmann variables in the expression for the partition function can be performed explicitly, yielding

$$\mathcal{Z}_i^{\text{bare}}=\int\mathcal{D}\eta\,\mathcal{D}\xi\exp[A_i^{\text{bare}}\{\eta,\xi;\mathcal{G}_\sigma^{-1}\}], \tag{4.30}$$

where now[40]

$$A_i^{\text{bare}}\{\eta,\xi;\mathcal{G}_\sigma^{-1}\}=-\frac{1}{2}\sum_{\nu=-\infty}^{\infty}(\xi_\nu^2+\eta_\nu^2)+\operatorname{tr}\ln\left[\hat{\mathcal{G}}_\sigma^{-1}-\sqrt{\frac{U}{2\beta}}(\sigma\hat{\eta}+i\hat{\xi})\right] \tag{4.31}$$

with $(\hat{\xi})_{mn}=\xi_{m-n}$, $(\hat{\eta})_{mn}=\eta_{m-n}$ and $(\hat{\mathcal{G}}_\sigma^{-1})_{mn}=\delta_{mn}[\mathcal{G}_\sigma(i\omega_n)]^{-1}$.

The total free energy (4.27) is then given by

$$\Omega=-LT\operatorname{tr}\left\{\int dE\,N(E)\ln[i\omega_n+\mu-\Sigma_\sigma-E]-\ln(\mathcal{G}_\sigma^{-1}-\Sigma_\sigma)\right\}-$$

$$-LT\ln\mathcal{Z}_i^{\text{bare}}. \tag{4.32}$$

The stationarity condition (4.25), $\delta\Omega/\delta\mathcal{G}_\sigma^{-1}=0$, leads to

$$\frac{1}{[\mathcal{G}_\sigma(i\omega_n)]^{-1}-\Sigma_\sigma(i\omega_n)}= \tag{4.33a}$$

$$=\frac{1}{\mathcal{Z}_i^{\text{bare}}}\int\mathcal{D}\Psi\,\mathcal{D}\Psi^*(\Psi_{\sigma,n}\Psi^*_{\sigma,n})\exp[A_i^{\text{bare}}\{\Psi_\sigma,\Psi^*_\sigma;\mathcal{G}_\sigma^{-1}\}]=$$

$$(4.33b) \quad = \frac{1}{\mathcal{Z}_i^{\text{bare}}} \int \mathcal{D}\eta\, \mathcal{D}\xi \left(\frac{1}{\hat{\mathcal{G}}_\sigma^{-1} - \sqrt{\frac{U}{2\beta}}\,(\sigma\hat{\eta} + i\hat{\xi})} \right)_{nn} \exp\left[A_i^{\text{bare}}\{\eta, \xi; \mathcal{G}_\sigma^{-1}\}\right] \equiv$$

$$(4.33c) \quad \equiv \left\langle \left(\frac{1}{\hat{\mathcal{G}}_\sigma^{-1} - \sqrt{\frac{U}{2\beta}}\,(\sigma\hat{\eta} + i\hat{\xi})} \right)_{nn} \right\rangle_{\eta, \xi}$$

with $\langle X \rangle_{\eta, \xi} = \left(\int \mathcal{D}\eta\, \mathcal{D}\xi X \exp\left[A_i^{\text{bare}}\right] \right) / \mathcal{Z}_i^{\text{bare}}$. Of course, the r.h.s. of (4.33*a*) is nothing but the very definition of the local propagator $G_{ii,\sigma}(i\omega_n)$ in terms of the action A_i^{bare}. Equation (4.33), together with

$$(4.34) \qquad [\mathcal{G}_\sigma(z)]^{-1} = [G^0_{ii,\sigma}(z - \Sigma_\sigma(z))]^{-1} + \Sigma_\sigma(z),$$

provides an *exact*, self-consistent set of equations for Σ_σ (or $\mathcal{G}_\sigma$) for the Hubbard model in $d = \infty$ [38-40, 133]. In contrast to Hartree-Fock this thermodynamically consistent MFT is valid for arbitrary values of the interaction parameter U and particle density n and explicitly contains two-particle correlation effects. Although it is mathematically much more complicated than the analogous expression (4.26) for the disorder problem without interactions, it can, in principle, again be solved by iteration: for given $\mathcal{G}_\sigma^{-1}$ we obtain Σ_σ from (4.33), which yields a new $\mathcal{G}_\sigma^{-1}$ via (4.34), etc. The exact local propagator is then provided by $G_{ii,\sigma} = (\mathcal{G}_\sigma^{-1} - \Sigma_\sigma)^{-1}$. As in the disorder case $G_{ii,\sigma}$ is completely expressed in terms of *effective* averaged quantities.

The expression used in (4.33*c*) brings out particularly clearly the similarities and differences between the (on-site) interaction problem and the analogous expression (4.25) for the disorder case without interactions: i) on the l.h.s. of (4.33) the self-energy Σ appears again as a (homogeneous) effective medium, which is obtained exactly from the original system by some averaging process; ii) however, this average is very different in the two cases: in the disorder problem it involves an integration over the actual disorder potentials V_i with a *given* disorder distribution $P(V_i)$, while in (4.33) it demands an integration over infinitely many fluctuating (random) fields η, ξ, which simulate the actual interaction; iii) the latter integration leads to a highly nontrivial *coupling* of the energies, *i.e.* Matsubara frequencies ω_n (note that this coupling even exists in the static limit, *i.e.* for $\eta_\nu = \xi_\nu = 0$ for $\nu \neq 0$), while in the disorder problem the corresponding equation (4.25) is diagonal in the frequency. This shows clearly that, although the interaction between electrons on different lattice sites has been reduced to an interaction of electrons with a mean field, the dynamics of the latter interaction is still nontrivial. Once more we observe that the many-body nature of the Hubbard model survives even in $d = \infty$, making an analytic evaluation of the local propagator $G_{ii,\sigma}$ from (4.33), (4.34) impossible.

It was pointed out by GEORGES and KOTLIAR [39, 134], as well as OHKAWA [132] and JARRELL [133], that the single-site problem emerging in the

limit $d \to \infty$, *i.e.* the fact that one obtains an *effective* problem of a single site with Hubbard interaction immersed in a noninteracting fermionic bath, is equivalent to an *actual* single-site problem, such as the Anderson impurity model [82] (see subsect. 2·5) or the Wolff model [135], supplemented by a self-consistency condition. (We note that such a connection, but *without* a self-consistency condition for the self-energy Σ, *i.e.* without a renormalization of the medium itself, was discussed already by EVENSON, WANG and SCHRIEFFER [136].) In the Wolff model

$$\hat{H}_{\mathrm{WM}} = \hat{H}_{\mathrm{kin}} + U\hat{n}_{0\uparrow}\hat{n}_{0\downarrow} , \tag{4.35}$$

where the kinetic energy $\hat{H}_{\mathrm{kin}}$ is given by (1.3*a*), the conduction electrons $\hat{c}_{i\sigma}$ can only interact on a single site $\boldsymbol{R}_0$. The Hubbard model (1.4*b*) is then a lattice generalization of (4.35) in analogy with the periodic Anderson model (2.25) which is a generalization of the single-impurity Anderson model to a lattice of *f*-orbitals. The mapping of the Hubbard model in $d = \infty$ onto one of the two models has the advantage that the form of the effective propagator $\mathcal{G}_\sigma$ is already known in these cases, namely

$$[\mathcal{G}_{\mathrm{SIAM}}(z)]^{-1} = z - \varepsilon_f + V^2 \int_{-\infty}^{\infty} \mathrm{d}E \, \frac{\Delta(E)}{z - E} , \tag{4.36a}$$

where $\Delta(E) = \sum_k \delta(E - \varepsilon_k)$, and

$$[\mathcal{G}_{\mathrm{WM}}(z)]^{-1} = \int_{-\infty}^{\infty} \mathrm{d}E \, \frac{\Delta(E)}{z - E} . \tag{4.36b}$$

In the present case the function $\Delta(E)$ has to be determined self-consistently. This relation, together with the extensive numerical experience that has accumulated in the treatment of impurity models, makes a numerical solution of the self-consistency problem (4.33), (4.34) tractable. Indeed, it is exciting to see that at this very moment the first explicit, numerically exact results for the phase diagram obtained by quantum Monte Carlo techniques become available [137-139]; they all find evidence for a Mott-Hubbard insulating state above a critical value of U.

The generalized CPA approach can also be used to derive the exact averaged free energy of Hubbard-type models with local disorder [130]. On the level of 2-particle (and higher) correlation functions the simultaneous existence of interactions and disorder leads to a new coupling of quantum degrees of freedom which have no counterparts in noninteracting, disordered, or pure, interacting systems. This coupling requires the self-energy for the nonrandom model to be frequency-dependent. Hence it is a genuine correlation effect which is lost in any Hartree-Fock treatment.

4·3. *The Falicov-Kimball model.* – An exact evaluation of the free energy Ω and hence of the phase diagram becomes possible in the absence of the Hubbard interaction (as in the case of spinless fermions, (1.12), with or without disorder [17]) or when there is no coupling between the frequencies, *e.g.* when one species of particles is decoupled from the surrounding medium. This is the case in the so-called «simplified Hubbard model», where only one of the two spin species is allowed to hop (*e.g.*, $t_\uparrow = -t$, $t_\downarrow = 0$). This simplification was first discussed by HUBBARD [5] and GUTZWILLER [49] as an approximation to the full model. It was then considered by FALICOV and KIMBALL [140] as a model for a semiconductor-metal transition in systems like SmB_6, V_2O_3 and Ti_2O_3, taking the mobile and fixed particles to be spinless d- and f-electrons, respectively. Later LIEB and KENNEDY [141] investigated it as a model for crystallization in terms of mobile electrons and immobile nuclei. The Hamiltonian for this «simplified Hubbard model« (which is referred to as «Falicov-Kimball model» in the rare-earth community) may, therefore, be written in different forms:

$$\text{(4.37}a\text{)} \qquad \hat{H}_{\text{simp}} = -t \sum_{\langle R_i, R_j \rangle} \hat{c}_{i\uparrow}^{+} \hat{c}_{j\uparrow} + U \sum_{R_i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \sum_{R_i, \sigma} \mu_\sigma \hat{n}_{i\sigma} ,$$

$$\text{(4.37}b\text{)} \qquad = -t \sum_{\langle R_i, R_j \rangle} \hat{d}_i^{+} \hat{d}_j + U \sum_{R_i} \hat{n}_i^d \hat{n}_i^f - \sum_{R_i} (\mu_d \hat{n}_i^d + \mu_f \hat{n}_i^f) .$$

Due to the immobility of one of the fermion species there is no energy transfer between the two species $\uparrow$, $\downarrow$ (or d, f), *i.e.* they are *dynamically uncoupled.* (Note that, although the immobile spins have no explicit dynamics, they are not fixed at given positions; hence an ensemble average over all particles will decide on the optimal spatial distribution of the fixed particles—this is similar to the case of Ising spins.)

In spite of the additional simplification involved in (4.37) this model is still complicated—especially away from half-filling. However, an exact solution is possible in $d = \infty$, which was first obtained by BRANDT and MIELSCH [142]. The free energy for the model can also be derived within the generalized CPA approach [38]. The effective propagator for the fixed spins in (4.32) is now given by $\mathcal{G}_\downarrow = (i\omega_n + \mu_\downarrow)^{-1}$ and the static approximation becomes exact! This is due to the separation of the dynamics of the two spin species, as can be demonstrated in a diagrammatic perturbation expansion. There is no energy transfer at vertices between up and down spins due to the δ-function dispersion of fixed electrons. Effectively this means that closed loops factorize and thus contribute only globally. The perturbation theory can then be summed explicitly to all orders. For the special case of half-filling the phase diagram of the simplified Hubbard model in $d = \infty$ is shown in fig. 4.3. For values of T and U below the curve, the system is in an ordered state (charge density wave), above that it is in a homogeneous phase. For $U \gg t$ one has $T_c \sim t^2/U$ as in the full Hubbard model (in fact,

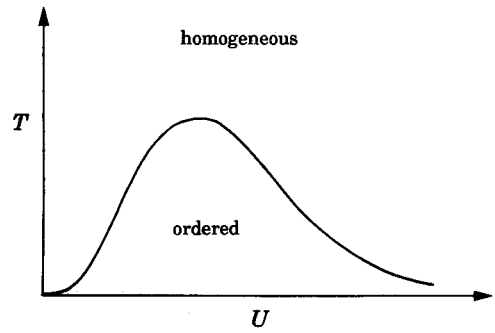


Fig. 4.3. – Phase diagram of the Falikov-Kimball model at half-filling.

the two models coincide for half-filling and large U). The phase boundary is very similar to that in $d < \infty$ [141].

As mentioned at the end of subsect. 4·2, the addition of disorder to Hubbard-type models leads to a new, nontrivial coupling of the quantum degrees of freedom. This can be shown explicitly in the case of the Falikov-Kimball model [130], since the exact solution of the nondisordered model is known. In particular one finds that in the ordered phase the average free energy depends on $\langle n_{i\downarrow}^{\alpha} \ln n_{i\downarrow}^{\alpha} \rangle_{\mathrm{av}}$, where $\alpha = A, B$ refers to the sublattice, *i.e.* depends on *infinitely many* averaged quantities $\langle (n_{i\downarrow}^{\alpha})^k \rangle_{\mathrm{av}}$, $k = 1, 2, 3$, etc. Such a dependence is reminiscent of the configuration-dependent mean-field free energy of Thouless, Anderson and Palmer [143] in the classical spin glass problem. This enables one now to investigate the transition to phases with broken ergodicity even in quantum systems.

* * *

I am extremely grateful to my collaborators and colleagues for countless discussions on the material presented in these lecture notes, particularly to G. CZYCHOLL, F. GEBHARD, P. VAN DONGEN, V. JANIŠ, W. METZNER, E. MÜLLER-HARTMANN, R. STRACK, G. UHRIG, R. VLAMING and especially P. WÖLFLE. I also would like to thank Mrs. G. KRAMP-SALECKER for her patience in preparing the manuscript. This work was supported in part by the Sonderforschungsbereich Nr. 341 of the Deutsche Forschungsgemeinschaft.

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