The origin of the electron-hole asymmetry of the spin fluctuation and its effect on superconductivity in iron-based superconductors

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Development of the spin fluctuation has been considered as one of the important features of iron-based superconductors. One of the interesting observations is its electron-hole asymmetry. Namely, when electrons are doped like in $Ba(Fe_{1-x}Co_x)_2As_2$, the magnetic peaks in the neutron scattering experiments tend to deviate from the commensurate $(\pi, 0)$ to incommensurate positions toward (π, π) (in the unfolded BZ), while in the hole doped cases like KFe_2As_2 it deviates toward (0,0) [1].
In the present study, we first obtain a ten orbital model of $BaFe_2As_2$ and KFe_2As_2 from first principles calculation. We also obtain a five orbital model in the unfolded Brillouin zone, which can only be done approximately in 122 systems. We apply the random phase approximation to these models and obtain the spin susceptibility for various band fillings. The electron-hole asymmetry of the peak position of the spin fluctuations is nicely reproduced in the calculation, and its origin can be attributed to the different distribution of the orbital characters on the Fermi surface in electron and hole doped cases. We also discuss how these spin fluctuations affect the form of the superconducting gap.

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