Supplemental Material to the article

"Phase Diagram of the Two-orbital Model of Iron-based HTSC: Variational Cluster Approximation"

1. Variational cluster approximation. The variational cluster approximation is based on the Potthoff functional for a many-body Hamiltonian $H = T + V$ with the single-particle term V and the two-particle term T:

$$\Omega[\Sigma] = F_V[\Sigma] - \mathrm{Tr}\,\ln(G_0^{-1} - \Sigma). \tag{1}$$

Here $F_V[\Sigma]$ is the Legendre transform of the Luttinger–Ward functional; G_0 is the Green's function of the system without interaction; Σ is the self-energy. The functional $\Omega[\Sigma]$ is stationary at the physical self-energy of the system, and at this point it has the meaning of the grand potential of the system. Therefore, the problem reduces to the search for stationary points of the functional $\Omega[\Sigma]$. The functional $F_V[\Sigma]$ has the property of universality, i.e., it depends only on the interaction V, and not on T. This property allows one to associate the functional of the whole system with the functional of a reference system described by a Hamiltonian $H' = T' + V$ which differs from H only by its one-particle part:

$$\Omega[\Sigma] + \mathrm{Tr}\,\ln(G_0^{-1} - \Sigma) = \Omega'[\Sigma] + \mathrm{Tr}\,\ln({G'_0}^{-1} - \Sigma), \tag{2}$$

and, therefore,

$$\Omega[\Sigma] = \Omega'[\Sigma] - \mathrm{Tr}\,\ln(1 + (G_0^{-1} - {G'_0}^{-1})G') \tag{3}$$

The reference system is chosen in such a way that it is accessible to exact evaluation by numerical methods. The above equation is exact; however, it cannot be solved in this form, as the dependence $\Omega[\Sigma]$ is unknown. The idea of VCA is to replace the dependencies $\Omega[\Sigma]$ and $\Omega'[\Sigma]$ by approximated ones $\Omega[\Sigma']$ and $\Omega'[\Sigma']$, where Σ' is the self-energy of the reference system. This approximation becomes exact in the limit of infinite size of the reference system and is based on the assumption that the self-energy, in most general cases, is much more local quantity compared with, e.g., the Green's function. Since the size of the reference system is usually small enough because of the restrictions associated with the exponential growth of the dimension of the Hilbert space with the system size, it is not possible to observe directly the symmetry breaking corresponding to a phase transition by searching for the stationary point of $\Omega[\Sigma']$. Instead, one introduces fictitious one-particle Weiss fields W,

$$H = (T + W) + (V - W) \tag{4}$$

that are local to each reference system and represent the effect of the rest of the system without introducing distortions into the original Hamiltonian.

2. Polarization of orbitals in the two-orbital model

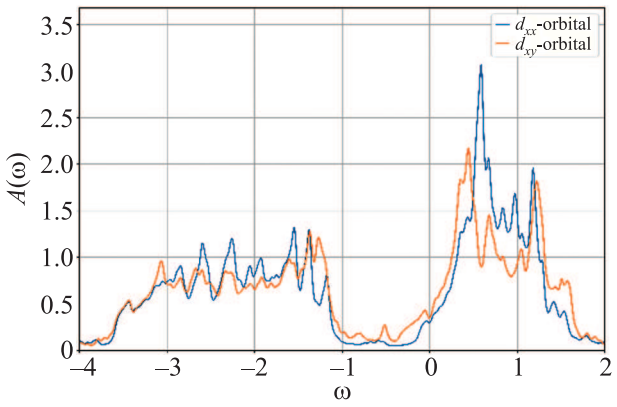

Figure 1: The polarization of the orbitals (nematic ordering) at doping $x = 1.1$ (a) and $x = 1.175$ (b). The coherent flat band below the Fermi level, which reflects antiferromagnetic correlations, disappears in the superconducting phase