Restoration of density of states for FeAs-based superconductors

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Abstract. The spectral and total electron density of states were calculated for two-dimensional FeAs-clusters modeling iron-based superconductors, with use of the generalized quantum Monte Carlo algorithm within the limits of the two-orbital model. The spectra have been obtained by means of the stochastic procedure, which was modified to restore the kernel of the integral equation relating the Matsubara Green's function and the spectral density. The calculations were made for clusters with sizes up to 10×10 FeAs-cells. The data on the total density of states near the Fermi level are obtained. There are two branches of the quasiparticle spectrum on both sides of the Fermi level. The effect of the values of the interaction parameter, the cluster size and temperature on the excitation spectra is discussed.

1. Introduction

One of the most interesting objects of research in the physics of superconductivity nowadays is iron-based high-temperature superconductors (HTSC) [1–3]. Similar to the copper-based HTSC, these compounds have a layered structure. However, due to the features of the multi-gap band structure their phase diagram is more complicated and includes antiferromagnetic, structural, and superconducting phase transitions [4–8].

The pronounced anisotropy of iron-based HTSC allows applying two-dimensional tight-binding models for their description. One of the most appropriate model for these compounds is the two-orbital model [9, 10], which is a typical multi-band generalized Hubbard model. The lack of expansion parameters for analytical approximations, and the presence of strong Coulomb correlations require the use of exact numerical quantum methods for the study of iron-based HTSC.

The present work focuses on the calculation of the spectrum of elementary excitations which determines the Fermi surface and the density of states. The quantum continuous time world line Monte Carlo (MC) algorithm (CTWL-algorithm) was used to simulate the full two-orbital model [11], which allows calculation of the Matsubara Green's function and obtaining the quasiparticle spectrum and its dependence on the system size and interaction parameters.

2. Model

The Hamiltonian of the two-orbital model is as follows [9, 10]:

\[ H = H_{\text{in}} + H_{\text{kin}} \]  \hfill (1)
\begin{equation}
H_{in} = U \sum_{i, \alpha} n_{i, \alpha} n_{i, \alpha, \downarrow} + V \sum_{i, \alpha} n_{i, \alpha} n_{i, \alpha, \uparrow} - \mu \sum_{i, \alpha} n_{i, \alpha} - J \sum_{i} \left( a_{i, \alpha, \uparrow}^+ a_{i, \alpha, \downarrow} + a_{i, \alpha, \downarrow}^+ a_{i, \alpha, \uparrow} + a_{i, \alpha, \uparrow}^+ a_{i, \alpha, \uparrow} + a_{i, \alpha, \downarrow}^+ a_{i, \alpha, \downarrow} \right)
- J \sum_{i} \left( a_{i, \alpha, \uparrow}^+ a_{i, \alpha, \uparrow} + a_{i, \alpha, \downarrow}^+ a_{i, \alpha, \downarrow} \right)
\end{equation}

\begin{equation}
H_{kin} = -t_{1} \sum_{i, \sigma} \left(a_{i, \sigma}^+ a_{i+x, \sigma} + a_{i-x, \sigma}^+ a_{i, \sigma} + a_{i+y, \sigma}^+ a_{i, \sigma} + a_{i, \sigma}^+ a_{i+y, \sigma}\right)
- t_{2} \sum_{i, \sigma} \left(a_{i, \sigma}^+ a_{i+x, \sigma} a_{i, \sigma} + a_{i, \sigma}^+ a_{i+y, \sigma} a_{i, \sigma}ight)
+ t_{4} \sum_{i, \sigma} \left(a_{i, \sigma}^+ a_{i+x, \sigma} a_{i, \sigma} + a_{i, \sigma}^+ a_{i+y, \sigma} a_{i, \sigma}\right)
+ h.c.
\end{equation}

Here \( a_{i, x(y), \sigma}^+ \) creates (annihilates) an electron with spin \( \sigma \) on site \( i \) and orbital \( x(y) \); \( t_{i}, i=1,\ldots,4 \) are the hopping amplitudes between \( d_{x^2-y^2} \) and \( d_{y^z} \) orbitals defined as \( x \) and \( y \), respectively; \( U \) and \( V \) are the parameters of the Coulomb interaction within and between orbitals; \( J \) is the exchange integral; \( \mu \) is the chemical potential.

The parameters of \( H_{kin} \) in (1) were chosen similarly to [10]:

\begin{equation}
t_{1} = 0.058; \quad t_{2} = 0.22; \quad t_{3} = -0.0208; \quad t_{4} = -0.079;
\end{equation}

the relationship between the parameters of \( H_{in} \) was defined as following:

\begin{equation}
V = 0.5U; \quad J = 0.25U.
\end{equation}

Hereafter, all the energy parameters are normalized to the value of 0.2 eV.

3. Results

The Matsubara Green’s function

\begin{equation}
\langle T_{\tau} a_{i, \alpha, \sigma}^\dagger(0) a_{j, \beta', \sigma'}(0) \rangle,
\end{equation}

where \( i, j \) are coordinates of iron atoms; \( \alpha, \beta \) are orbitals; \( \sigma, \sigma' \) are spin projections, was calculated for clusters of sizes up to \( 10^4 \times 10 \) FeAs cells. To properly restore the spectral density \( A_{\sigma}(k, \omega) \) from data on the Matsubara Green’s function, and to calculate the total density of states \( N(\omega) = \sum_{k, \sigma} A_{\sigma}(k, \omega) \) we must determine the kernel of the integral equation

\begin{equation}
G_{\sigma}(k, \omega) = -\int \frac{A_{\sigma}(k, \omega) e^{-i\omega}}{1 + e^{-\beta \omega}} d\omega,
\end{equation}

\( \beta = 1/T \), \( T \) is the temperature. The problem (5) is a typical ill-posed problem; its solution is a non-trivial mathematical task, and a method of direct iterations usually does not give the correct result if no information about a kernel is provided.

The density of states \( N(\omega) \) was restored for the whole Brillouin zone using the combined method “Monte Carlo + gradient descent”, first introduced in [12] and adapted by us for the Green’s function of the two-orbital model. The input parameter for (5) were the data for the Matsubara Green’s function
(4), obtained with the use of the CTWL-algorithm [11]. It was found that for clusters with sizes greater than 4×4 the results are no longer dependent on the size of the system, which suggests the applicability of the data presented for the analysis of the properties of a macroscopic system.

Figure 1. The dependence of the electron states density on the value of the interaction parameter $U$ calculated for cluster 8×8 and temperature $\beta = 20$.

Figure 2. The dependence of the electron states density on temperature calculated for cluster 6×6 and $U = 8$.

Figure 1 shows the dependence of the density of states on the interaction parameter $U$ of the model (3). The Fermi energy corresponds to zero on the energy scale. There are two zones above and below the Fermi level. The density of states is weakly dependent on the interaction parameter near the Fermi level. The increase of the interaction parameter almost does not change the electron zone above the Fermi level, only slightly smoothing the sharp peak at the maximum. For the hole zone located substantially lower on the energy scale, the changes are more significant. The maximum is smoothed and shifted by the value of $-U$ down the energy scale, the zone itself is broadened, and the gap in the spectrum increases. Similar behavior is observed for the upper and lower zones in the standard Hubbard model, which is also mentioned in LDA + DMFT calculations [13]. From this perspective, it can be assumed that FeAs compounds belong to the strongly correlated systems.

Figure 2 shows the dependence of the density of states as a function of temperature. The zones are separated by the “gap”, a quite pronounced decrease in the value of the total density. In the gap, however, the total density differs from zero, indicating that undoped FeAs are metals; this fact is confirmed...
experimentally [4, 14]. The dependence of the total density of states on temperature at $\beta \leq 10$ is weak. When the temperature rises above this value, the “gap” begins to close.

4. Conclusions
Calculations of FeAs clusters of size up to $10 \times 10$ within the limits of the full two-orbital model were performed using quantum Monte Carlo algorithm at half-filling and different values of temperature and the interaction parameter. The spectral density was restored from Matsubara Green's function with the use of the combined method “Monte Carlo + gradient descent”. The obtained data on the excitation spectra and the density of states indicate the possibility of a strong correlation between characteristics of the spectrum and the strength of interaction, in qualitative agreement with the available experimental data and results of other calculations.

It is shown that the density of states weakly depends on the parameters of the model near the Fermi level, but it is strongly dependent on the interaction far from it for the case of hole filling. There is a “gap” in the spectrum; at the Fermi level between the zones the density of electron states decreases sharply, remaining, however, finite, which indicates the metallic state of undoped FeAs-systems.

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