Band structure and density of states in FeAs-based superconductors

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Abstract. The generalized quantum Monte Carlo algorithm was used to obtain one-particle excitation spectrum and electron density of states for two-dimensional FeAs-clusters modeling iron-based superconductors within the limits of the full two-orbital model. The calculations were performed for clusters with sizes up to 10×10 FeAs-cells. The excitation spectra were reconstructed from Matsubara Green's function. The spectral density of states and the total density of states near the Fermi level were obtained. The data are in accordance with known experimental results. The influence of the cluster size, temperature, and the interaction strength on the density of states was analysed.

1. Introduction
Iron-based high-temperature superconductors (HTSC) [1–3] are among the most interesting objects of research in the physics of superconductivity nowadays. As well as copper-based HTSC, these compounds have a layered structure. However, due to the features of the multi-gap band structure they have a complex phase diagram which includes antiferromagnetic, structural, and superconducting phase transitions [4–9].

Iron-based HTSC due to their pronounced anisotropy can be successfully described within the limits of two-dimensional tight-binding models. One of the most appropriate models for this purpose is the two-orbital model [10, 11] which is a typical multi-band generalized Hubbard model. The lack of expansion parameters for analytical approximations, and the presence of strong Coulomb correlations assume the use of exact numerical quantum methods for the study of iron-based HTSC.

The present work continues the study of electronic correlations in big FeAs-clusters and 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 (CTWL-algorithm) [12] was used to simulate the full two-orbital model [13, 14].

According to experimental data and calculations based on DMFT and LDA techniques [4, 6, 15-17], it is the quasiparticle spectrum which forms a complex multi-gap band structure. Furthermore, the density of states near the Fermi level is almost entirely determined by d-states of iron atoms, which gives reason to believe that all the phenomena associated with conducting and superconducting properties of these compounds are played on the FeAs-plane.

The quantum algorithm developed in [13] allows one to calculate the Matsubara Green’s function and to obtain the quasiparticle spectrum and its dependence on the system size and interaction parameters. The first data are presented on the excitation spectrum in the framework of the full two-orbital model for clusters with sizes up to 10×10 FeAs cells.
2. Model

The minimal electron model for FeAs-based HTSC is defined by the crystal structure of these compounds [1] and band structure calculations, that show that the largest contribution to the electronic density of states near the Fermi level give 3d-states of iron atoms [11, 17]. These reasons give the compounds [1] and band structure calculations, that show that the largest contribution to the electronic density of states near the Fermi level give 3d-states of iron atoms [11, 17]. The set density of states near the Fermi level give 3d-states of iron atoms [11, 17]. These reasons give the compounds [1] and band structure calculations, that show that the largest contribution to the electronic density of states near the Fermi level give 3d-states of iron atoms [11, 17]. These reasons give the compounds [1] and band structure calculations, that show that the largest contribution to the electronic density of states near the Fermi level give 3d-states of iron atoms [11, 17]. These reasons give the compounds [1] and band structure calculations, that show that the largest contribution to the electronic density of states near the Fermi level give 3d-states of iron atoms [11, 17].

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The Matsubara Green's function

\[ G(k,\tau)\sim e^{-E(k)\tau}. \]  

This dependence allows to derive the quasiparticle dispersion \( E(k) \). Figure 1b shows a typical excitation spectrum along the main crystallographic directions for the 10 \( \times \) 10 cluster. According to our data, the temperature dependence is weak at \( \beta \geq 10 \). This is the sufficient condition for realization of the asymptote of Green's function (5) and for the correct analysis of the dispersion. Furthermore, the

\[ H = H_{\text{int}} + H_{\text{kin}}. \]

\[ H_{\text{int}} = U \sum_{\ell,\sigma} n_{\ell,\sigma} n_{\ell,\sigma\uparrow} + V \sum_{\ell} n_{\ell x} n_{\ell y} - \mu \sum_{\ell} n_{\ell} - J \sum_{\ell} \left( n_{\ell x\uparrow} n_{\ell y\uparrow} + n_{\ell x\downarrow} n_{\ell y\downarrow} \right) \]

where operator \( a^+_i(x,y)\sigma(a_i(x,y)\sigma) \) 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 \( d_{xz} \) and \( d_{yz} \) orbitals defined as \( x \) and \( y \), respectively; parameters \( U \) and \( V \) describe the Coulomb interaction within and between orbitals, respectively; \( J \) is the exchange integral; \( \mu \) is the chemical potential.

The two-orbital model is quite complex to be studied by CTWL-algorithm; the encoding of the basis states, and the features of calculation of pair correlations are presented in detail in [14, 18, 19]. The set of parameters of \( H_{\text{kin}} \) in (1) was taken from [11]:

\[ t_1 = 0.058; t_2 = 0.22; t_3 = -0.0208; t_4 = -0.079. \]  

(2)

The relationship between the parameters of \( H_{\text{int}} \) was determined as

\[ V = 0.5U; J = 0.25U. \]  

(3)

All energy quantities are measured in 0.2 eV units.

3. Results

The Matsubara Green’s function

\[ \langle T_\tau a_{i\sigma}(\tau) a^+_{j\beta\sigma'}(0) \rangle, \]

where \( i,j \) are the coordinates of Fe atoms; \( \alpha, \beta \) are the orbitals; \( \sigma, \sigma' \) are the spin projections, was calculated for clusters of sizes from 4 \( \times \) 4 to 10 \( \times \) 10 FeAs-sells in the temperature range \( \beta = 5 \div 20 \), and the range of the interaction parameter \( U = 2 \div 16 \) while maintaining the relation (3). The data are presented for the half-filling; the typical number of MC steps for the convergence was \( \sim 10^{10} \).

Figure 1a shows typical Matsubara Green’s functions in logarithmic scale for various values of the interaction parameter.

Assuming that near the forbidden band the quasiparticle spectrum should be well resolved, the asymptotic behavior of the Matsubara Green’s function has the following form:

\[ G(k,\tau)\sim e^{-E(k)\tau}. \]  

(5)

This dependence allows to derive the quasiparticle dispersion \( E(k) \). Figure 1b shows a typical excitation spectrum along the main crystallographic directions for the 10 \( \times \) 10 cluster. According to our data, the temperature dependence is weak at \( \beta \geq 10 \). This is the sufficient condition for realization of the asymptote of Green's function (5) and for the correct analysis of the dispersion. Furthermore, the
comparison of the calculations for clusters of size $4 \times 4$, $6 \times 6$, $8 \times 8$, and $10 \times 10$ indicates that the size of the system $8 \times 8$ is big enough for obtaining results which are free of size effect. Similar dispersion curves were obtained under the simplified $S_4$-model [15, 20].

**Figure 1.** (a) Fourier component of the Matsubara Green’s function $G(k, \tau) = \sum G_{ij}(\tau) e^{ikr_{ij}}$, $G_{ij}(\tau) = \langle T_{t} a_{i \uparrow}(0) a_{j \uparrow}^{\dagger}(\tau) \rangle$, $k_{x}, k_{y} = 0$; (b) two branches of the excitation spectrum, $U = 4$. Cluster $10 \times 10$, $\beta = 15$.

**Figure 2.** Dispersion and constant-energy curves for $10 \times 10$ cluster. (a) $U = 4$; (b) $U = 8$; (c) $U = 16$. $\beta = 15$.

Figure 2 shows the excitation spectrum and Fermi surfaces for the upper mode at different interaction parameters for the entire Brillouin zone. It can be seen that the Coulomb interaction strongly changes the picture of the constant-energy curves.

With increasing the interaction strength peculiar hole pockets appear in the vicinity of regions $k_{x}, k_{y} = \pm \pi/2$; such behavior was also observed in calculations [4, 7, 8, 17] and experimentally [9].

**Figure 3** presents the results for the density of states $N(\omega) = \Sigma_{p\sigma} A_{\sigma}(p, \omega)$, where the spectral density $A_{\sigma}(p, \omega)$ was restored from the integral relation

$$G_{\sigma}(p, \tau) = - \int \frac{A_{\sigma}(p, \omega)e^{-\tau \omega}}{1 + e^{-\beta \omega}} d\omega. \quad (6)$$
The calculation of the kernel in (6) was carried out by direct iteration [21]. Problems with the convergence of the method for this typical ill-posed problem allowed us to introduce only preliminary data for the density of states, reliable mostly in the region of unoccupied states above the Fermi level. It can be seen that the total density of states is weakly dependent on the interaction parameter, and there is a gap in the spectrum in the range \((0 - 0.5)\) on the energy scale. The weak dependence of the density of states on the interaction parameters was also mentioned in several works [4, 6, 15, 16].

It should also be noted that even these preliminary results indicate a definite, though weak, peak at the Fermi level, confirming the experimental data on the metallic nature of the undoped FeAs systems [2, 4, 9, 22].

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 data obtained on the excitation spectrum and the density of states indicate the possibility of a strong correlation between the features of the spectrum and the value of the interaction, which is consistent with the known experimental data and calculations.

The preliminary data on the total density of states show the weak dependence on the parameters of the interaction. The gap in the excitation spectrum and the finite density of states at the Fermi level are observed, which confirms the supposition of the metallic state of undoped FeAs systems.

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