Momentum distribution of occupation numbers in FeAs-based superconductors

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Abstract. The momentum distribution of charge carriers in two-dimensional FeAs-clusters modeling iron-based superconductors was calculated within the limits of the two-orbital model. The calculation was implemented by use of quantum world-line Monte Carlo algorithm. Matsubara Green's function was calculated for clusters with sizes up to 10×10 FeAs-cells. Profiles of the distributions are presented for the entire Brillouin zone. The data indicate the presence of a jump near the Fermi level, which is the evidence of the Fermi-type distribution. The influence on the momentum distribution of the value of the interaction parameter is discussed.

1. Introduction
The form of the momentum distribution function of charge carriers, the presence or absence of the Fermi jump, can provide additional information for the study of electron correlations in high-temperature superconductors (HTSC) based on iron [1-4]. Clarification of the issue of the nature of a strongly correlated system, whether it is of Fermi type, or has Luttinger liquid features, will allow properly analyzing experimental and calculated data on various spectral characteristics of these compounds.

The description of physical properties of iron-based HTSC in the framework of the two-dimensional tight-binding model, such as the two- [5, 6], three- [7, 8], and five-orbital models [8, 9], which are typical generalized Hubbard models, virtually does not allow a correct analysis in the framework of various approximations, including the mean-field approximation. The complexity of these models leads to the use of exact quantum calculation methods to study iron-based HTSC.

Preliminary studies of electron correlations in large FeAs clusters developed earlier by the authors in a series of papers [10-14] with the use of the quantum world-line Monte Carlo algorithm (CTWL-algorithm) within the limits of the full two-orbital model, yielded a number of results correlated with other experimental and theoretical work.

The present work is devoted to the study of the momentum distribution of charge carriers and the analysis of possible Fermi nature of the distribution near the Fermi surface. Quantum algorithm developed in [10] allows the calculation of the Matsubara Green's function and the off-diagonal density matrix, which, in turn, allows the calculation of the momentum distribution and analyzing its dependence on the size of the system, the temperature and the interaction parameters.

We present data on the calculation of the charge carrier distribution function within the full two-orbital model for the clusters with sizes up to 10×10 FeAs cells. The profile of the distribution function for the entire Brillouin zone is obtained, and the jump of the distribution near the Fermi level is analyzed. There is a strong dependence on the value of the interaction parameters.
2. Model

The minimal two-orbital model for FeAs-based HTSC takes into account the real crystal structure of these compounds, as well as anisotropy of physical properties. Since 3d-states of iron atoms provide the main contribution to the formation of the band structure near the Fermi level [5, 6], the Hamiltonian of the model is presented as follows:

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

\[ H_{\text{int}} = U \sum_{l,a,i} n_{l,i,a,\uparrow} n_{l,i,a,\downarrow} + V \sum_{l} n_{l,x} n_{l,y} - \mu \sum_{l} n_{l,x} - J \sum_{(a_{l,x,\uparrow} + a_{l,x,\downarrow}^+)^2}, \]

\[ H_{\text{kin}} = -t_1 \sum_{l,\sigma} (a_{l,x,\sigma}^+ a_{l+xx,\sigma} + a_{l,y,\sigma}^+ a_{l+yy,\sigma} + h.c.) - t_2 \sum_{l,\sigma} (a_{l,y,\sigma}^+ a_{l+xy,\sigma} + a_{l,x,\sigma}^+ a_{l+yx,\sigma} + h.c.) \]

\[ -t_3 \sum_{l,\sigma} (a_{l,x,\sigma}^+ a_{l+xx,\sigma} + a_{l,y,\sigma}^+ a_{l+yy,\sigma} + a_{l,y,\sigma}^+ a_{l+xy,\sigma} + a_{l,x,\sigma}^+ a_{l+yx,\sigma} + h.c.) \]

\[ -t_4 \sum_{l,\sigma} (a_{l,x,\sigma}^+ a_{l+xx,\sigma} + a_{l,y,\sigma}^+ a_{l+yy,\sigma} + a_{l,y,\sigma}^+ a_{l+xy,\sigma} + a_{l,x,\sigma}^+ a_{l+yx,\sigma} + h.c.) \]

(1)

where operator \( a_{l,x(y),\sigma}^+ (a_{l,x(y),\sigma}) \) creates (annihilates) an electron with spin \( \sigma \) on site \( l \) and orbital \( x(y) \); \( t_i, i = 1, ..., 4 \) 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.

As our research shows, namely the exchange term is important for the correct description of the correlation properties of the system and for implementation of a certain type of symmetry pairing of charge carriers. But at the same time it is this term which distinguishes the model (1) from the usual generalized Hubbard model and leads to difficulties in the implementation of quantum Monte Carlo algorithm. All the features of the numerical modeling, coding of basic states, and calculation of Green's and correlation functions in the framework of CTWL-algorithm are described in detail in [10, 11].

The set of realistic parameters of \( H_{\text{kin}} \) in (1) was taken from [10–12]:

\[ t_1 = 0.058; t_2 = 0.22; t_3 = -0.0208; t_4 = -0.079. \] (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. Matsubara Green’s function and momentum distribution

The Matsubara Green’s function

\[ G_{ij,\sigma,\sigma'}(\tau) = \langle T_{\tau} a_{i,\sigma,\sigma'}(\tau) a_{j,\sigma',0}^+ \rangle, \]

(4)

where \( i, j \) are the coordinates of Fe atoms; \( \alpha, \beta \) are the orbitals; \( \sigma, \sigma' \) are the spin projections, was calculated for the analysis of the momentum distribution for clusters of sizes up 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).

Momentum distribution can be obtained from the data for the Matsubara Green’s functions as follows:

\[ n(\vec{k}) = -G(\vec{k}, \tau \to -0); \]

\[ G(\vec{k}, \tau) = \sum_{ij} G_{ij,\sigma,\sigma'}(\tau) e^{i\vec{k}\vec{r}_{ij}}. \] (5)
The distribution $n(k)$ was normalized according to average occupation numbers of orbitals calculated independently. The values of the chemical potential were chosen so that the calculation was carried out at half filling.

4. Results
It should be noted that the results for clusters of size $6 \times 6$ and greater are no longer depend on the size of the system, indicating the possibility of the applicability of the data obtained for the analysis of the properties of a macroscopic system.

Figure 1 (a) shows the profiles of the momentum distribution along the main crystallographic directions for $8 \times 8$ cluster, depending on the interaction parameter $U$. The "jump" in the occupation numbers is clearly visible. We define the Fermi level as the point of the maximum gradient of the distribution. The interaction significantly blurs the distribution profile, and there are no completely filled or empty areas. According to our results, the distribution weakly depends on temperature at $1/T \geq 5$ near the Fermi level. Figure 1 (b) also shows the profiles of the electron density of states along the main crystallographic directions, calculated from data on the Green's function by the method presented in [16].

![Graph showing the distribution](image)

**Figure 1.** (a) Profile of the momentum distribution along the main crystallographic directions depending on the interaction parameter $U$. Temperature $1/T = 5$; cluster $8 \times 8$. (b) The density of electronic states for the same cluster; $U = 2$. 
Figure 2 shows the distribution for the entire Brillouin zone. The Fermi surface corresponding to the half-filling is displayed in white. Note that the lines corresponding to different occupation numbers reflect the picture of the possible profiles of the Fermi surface for other fillings, assuming normal zone filling while maintaining the calculated distribution profile. The line of the maximum gradient corresponds to the half-filling. At $U = 8$ the dependence on the interaction is saturated, and for greater values of $U$ the distribution profile does not change.

![Figure 2](image)

**Figure 2.** (a) The evolution of the momentum distribution for the entire Brillouin zone with the change the interaction parameter $U$. (b) The same in the projection on the $xy$ plane. The Fermi surface is shown in white. Cluster $8 \times 8$; temperature $1/T = 5$.

5. Conclusions
Calculations of FeAs clusters of size up to $10 \times 10$ within the limits of the full two-orbital model were performed using generalized quantum Monte Carlo algorithm at half-filling and different values of temperature and the interaction parameter. The momentum distribution of charge carriers is restored from the Matsubara Green's function. The data for the distribution profile along the main crystallographic directions and for the entire Brillouin zone are presented. The jump of the distribution of occupation numbers is obtained, indicating the Fermi-liquid nature of the electronic ensemble. It is shown that this jump is sensitive to the interaction parameters.

Acknowledgements
The work was supported by Russian Found for Basic Research (projects # 14-08-00509 and # 15-02-02764).
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