Correlation properties and band structure of FeAs-based superconductors

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Abstract

The excitation spectrum is calculated for two-dimensional FeAs clusters modeling iron-based superconductors with the use of the quantum Monte Carlo algorithm in the framework of the full two-orbital model. The data for clusters of the size up to 10×10 FeAs cells are presented for the first time. The dependence of dispersion curves on temperature and interaction parameters is analyzed.

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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]. 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 [4–8].

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 assume the use of exact numerical quantum methods for the study of iron-based HTSC.

In this paper, we used the quantum continuous time world line Monte Carlo (MC) algorithm (CTWL-algorithm) [11] adapted for the full two-orbital model [12]. Already the first results of our calculations for a cluster consisting of 3×3 FeAs cells [13] showed the presence of a multi-gap structure of the spectrum of charge carriers, which is in qualitative agreement with [4, 14]. Further calculations of pair correlation functions for FeAs clusters with the number of cells from 4×4 to 10×10 [15, 16] at the half filling demonstrated the possibility of effective attraction of charge carriers that corresponds mainly to $A_{1g}$ symmetry, and to a lesser extent to $B_{2g}$ symmetry (according to the classification of [10, 17]).

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These data are in agreement both with the results of the exact diagonalization of the Hamiltonian matrix [10, 17-19], and with the data of variational [20] and determinant [21, 22] MC methods.

The present work continues the study of electron correlations in large FeAs clusters within the limits of the full two-orbital model and focuses the attention on the calculation of the spectrum of elementary excitations that determines the Fermi surface and the density of states. According to the experiments and calculations by DMFT and LDA techniques [4, 6, 14, 21-24], it is the quasiparticle spectrum which forms a complex multiple-gap band structure. It also follows from these calculations that the density of states near the Fermi level is almost entirely determined by the d-states of Fe, that suggests that all the phenomena associated with conducting and superconducting properties of these compounds are played out in a square lattice of the FeAs plane.

The algorithm developed in [12] allows us to calculate the Matsubara Green’s function that enables to obtain information about the quasiparticle spectrum and analyze its dependence on the system size and interaction parameters. Note that the calculations of Ref. 21, 22, 24-26 were carried out in the framework of the simplified model (the model with $S_4$-symmetry). Apparently, here we present the first data obtained by MC technique 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 follows from 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 [14, 23]. This gives the two-orbital model [9, 10] with the following Hamiltonian:

$$H = H_{\text{pot}} + H_{\text{kin}}$$

$$H_{\text{pot}} = U \sum_{i, \sigma} n_{i, \sigma \uparrow} n_{i, \sigma \downarrow} + V \sum_{i} n_{i, \sigma \uparrow} n_{i, \sigma \downarrow} - \mu \sum_{i} n_{i, \sigma \uparrow} + \mu \sum_{i} n_{i, \sigma \downarrow} - \mu \sum_{i} n_{i, \sigma \uparrow} + n_{i, \sigma \downarrow}$$

$$-J \sum_{i} \left( a_{i, \sigma \uparrow}^+ a_{i, \sigma \downarrow}^+ a_{i, \sigma \downarrow}^+ a_{i, \sigma \uparrow} + a_{i, \sigma \downarrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \downarrow} + a_{i, \sigma \uparrow}^+ a_{i, \sigma \downarrow}^+ a_{i, \sigma \downarrow}^+ a_{i, \sigma \uparrow} + a_{i, \sigma \downarrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \downarrow} + a_{i, \sigma \downarrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \downarrow} + a_{i, \sigma \downarrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \downarrow} + a_{i, \sigma \downarrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \downarrow} + a_{i, \sigma \downarrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \downarrow} + a_{i, \sigma \downarrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \uparrow}^+ a_{i, \sigma \downarrow} \right)$$

$$H_{\text{kin}} = -t_1 \sum_{i, \sigma} \left( a_{i, \sigma \uparrow}^+ a_{i+\delta, \sigma \downarrow} + a_{i+\delta, \sigma \downarrow}^+ a_{i+\delta, \sigma \uparrow} + a_{i, \sigma \downarrow}^+ a_{i+\delta, \sigma \uparrow} + a_{i+\delta, \sigma \uparrow}^+ a_{i, \sigma \downarrow} \right) + t_2 \sum_{i, \sigma} \left( a_{i, \sigma \downarrow}^+ a_{i+\delta, \sigma \uparrow} + a_{i+\delta, \sigma \uparrow}^+ a_{i, \sigma \downarrow} \right)$$

$$+ t_3 \sum_{i, \sigma} \left( a_{i, \sigma \uparrow}^+ a_{i+\delta, \sigma \downarrow} + a_{i+\delta, \sigma \downarrow}^+ a_{i, \sigma \uparrow} + a_{i, \sigma \downarrow}^+ a_{i+\delta, \sigma \uparrow} + a_{i+\delta, \sigma \uparrow}^+ a_{i, \sigma \downarrow} \right)$$

$$+ t_4 \sum_{i, \sigma} \left( a_{i, \sigma \uparrow}^+ a_{i+\delta, \sigma \downarrow} + a_{i+\delta, \sigma \downarrow}^+ a_{i, \sigma \uparrow} + a_{i, \sigma \downarrow}^+ a_{i+\delta, \sigma \uparrow} + a_{i+\delta, \sigma \uparrow}^+ a_{i, \sigma \downarrow} \right)$$

where operator $a_{i, \sigma \uparrow}^+ a_{i, \sigma \downarrow}^+ \left( a_{i, \sigma \downarrow}^+ a_{i, \sigma \uparrow}^+ \right)$ 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; $U$ 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 [11, 13, 15]. A realistic set of parameters of $H_{\text{kin}}$ in (1) was taken from [10] (all the parameters are normalized to 0.2 eV):

$$t_1 = 0.058; \quad t_2 = 0.22; \quad t_3 = -0.0208; \quad t_4 = -0.079$$

the relationship between the parameters of $H_{\text{pot}}$ was determined as

$$V = 0.5U; \quad J = 0.25U.$$

3. Results

The calculation of the Matsubara Green’s function

$$\langle T_{\tau} a_{i, \sigma \alpha} (r) a_{j, \beta \sigma}^+ (0) \rangle,$$
where $i, j$ are coordinates of Fe atoms; $\alpha, \beta$ are orbitals; $\sigma, \sigma'$ are spin projections, was carried out for clusters of sizes from 4x4 to 10x10 FeAs sells in the temperature range $\beta$ from 5 to 20, and the range of the interaction parameter $U$ from 2 to 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 1 shows typical Matsubara Green’s functions depending on the imaginary time $\tau$ for different interaction parameters.

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

$$G(k, \tau) \sim e^{-E(k)\tau}.$$  \hspace{1cm} (5)

It can be seen from Fig. 1b that the dependence (5) is realized with a reasonable accuracy. By analyzing these relationships, it is possible to calculate the quasiparticle dispersion $E(k)$.

Figure 2 shows the excitation spectra for 10x10 cluster.

According to our data, the temperature dependence is weak at $\beta \geq 10$. This is a sufficient condition for the realization of the asymptote of Green’s function (5) and the correct analysis of the dispersion.

The spectra of quasiparticles along the main crystallographic directions for various values of the interaction parameter $U$ are presented at Fig. 3. A typical electronic excitation branch can be seen. The upper branch for $U=8$ has the maximum at $k = (\pi, \pi)$, and the minimum is located in the region of zero momentum, while the lower branch has the maximum in the center of the band. Similar dispersion curves were obtained in the calculations in the framework of the simplified $S_4$ model [24-26].
Fig. 3. Excitation spectra depending on the value of the interaction parameter $U$ for $10\times10$ clusters. $\beta=15$.

The excitation spectra depend differently on the interaction parameter $U$. The minimum value for the upper branch (the center of the band) increases by about two times with increasing $U$, but at the edge of the band ($\pi, \pi$) this difference is minimal. Also, for $U=8$ a saddle region can be traced along the line $k=(\pi,0)-(-\pi,\pi)$, which may lead to a peak in the density of states near the Fermi level. Such features were noted also in [4, 6, 14, 21, 24]. For stronger interaction ($U=16$) the upper branch of the excitation spectrum undergoes a displacement in the direction to the point $k=(\pi,0)$, so that the maximum occurs at this point, and the non-dispersive region is not observed. A similar evolution of the lower branch is observed at the points $k=(\pi,0)$ and $k=(\pi,\pi)$, however, the non-dispersive region is maintained. In the center of the zone the dependence of the excitation energy on the interaction parameter is not observed.

4. Conclusion

Calculations of FeAs clusters with the number of cells up to $10\times10$ in the framework of the full two-orbital model were carried out by quantum MC algorithm at the half filling and at different temperatures and interaction parameters.

Apparently, for the first time the data obtained by MC technique on the excitation spectrum for FeAs clusters in the framework of the full two-orbital model, are presented. The results indicate the possibility of a peak in the density of states near the Fermi level, which correlates with the known experimental data and calculations.

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References

[1] Y.Kamihara, T. Watanabe, M. Hirano, and H. Hosono, J. Am. Chem. Soc., 130 (2008) 3296.
[2] Yu. Isyumov, E. Kurmaev. High-Tc Superconductors Based on FeAs Compounds. Springer, 2010.
[3] E. Dagotto, Rev. Mod. Phys. 85 (2013) 849.
[4] M.V. Sadovskii, Physics-Uspekhi 51 (2008) 1201.
[5] K. Ishida, Y. Nakai, and H. Hosono, J. Phys. Soc. Jpn. 78 (2009) 062001.
[6] M.V. Sadovskii, E.Z. Kuchinskii, I.A. Nekrasov, Journal of Magnetism and Magnetic Materials 324 (2012) 3481.
[7] M.V. Medvedev, I.A. Nekrasov, M.V. Sadovskii, JETP Lett. 95 (2012) 37.
[8] I.A. Nekrasov, M.V. Sadovskii, JETP Lett. 99(2014) 598.
[9] S. Raghu, Xiao-Liang Qi, Hao-Xing Liu et al., Phys. Rev. B 77 (2008) 220503(R).
[10] A. Moreo, M. Daghofer, J.A. Riera, and E. Dagotto, Phys. Rev. B 79 (2009) 134502.
[11] N.V. Prokof’ev, B.V. Svistunov, I.S. Tupitsyn, J. Exp. Theor. Phys. 114 (1998) 570.
[12] V.A. Kashurnikov, A.V. Krasavin, J. Exp. Theor. Phys. 111 (2010) 180.
[13] V.A. Kashurnikov, A.V. Krasavin, JETP Lett. 97 (2013) 333.
[14] K. Haule, J.H. Shim, G. Kotliar, Phys. Rev. Lett. 100 (2008) 226402.
[15] V.A. Kashurnikov, A.V. Krasavin, JETP Lett. 100 (2014) 16.
[16] V.A. Kashurnikov, A.V. Krasavin, JETP Lett. 100 (2014) 2894.
[17] Y. Wan and Q.-H. Wang, arXiv:0806.0923.
[18] A. Nicholson, W. Ge, X. Zhang et al., Phys. Rev. Lett. 106 (2011) 217002.
[19] M. Okumura, N. Nakai, H. Nakamura et al., Physica C 469 (2009) 932.
[20] K. Kubo, P. Thalmeier, J. Phys. Soc. Jpn. 80 (2011) SA121.
[21] Tianxing Ma, Hai-Qing Lin, Jiangping Hu, Phys. Rev. Lett. 110 (2013) 107002.
[22] Yang Wu, Guankin Liu and Tianxing Ma, EPL 104 (2013) 27013.
[23] I.A. Nekrasov, Z.V. Pchelkina, M.V. Sadovskii, JETP Lett. 88 (2008) 821; 88 (2008) 777.
[24] S. Liang, G. Alvarez, C. Sen, A. Moreo, and E. Dagotto, Phys. Rev. Lett. 109 (2012) 047001.
[25] S. Liang, A. Moreo, and E. Dagotto, Phys. Rev. Lett. 111 (2013) 047004.
[26] R. Applegate, Rajiv R.P. Singh, C.C. Chen, T.P. Devereaux, Phys. Rev. B, 85 (2012) 054411.