Momentum distribution in two-orbital Hubbard model: Quantum Monte Carlo approach

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Abstract. The two-dimensional two-orbital Hubbard model is studied with the use of world-line quantum Monte Carlo algorithm. Spectral functions and the density of states for various parameters of the model are obtained in both the undoped and low-doped regimes. The invariance of the Fermi surface with respect to the strength of the interaction is testified. Fermi-liquid parameters of the model are derived.

1. Introduction

The role of electron correlations in high-temperature superconductors (HTSC) based on iron [1] is decisive in the formation of physical properties of these systems. The effect of strong Coulomb interactions on the nature of superconductivity and the formation of a complex phase diagram including antiferromagnetic, structural and superconducting ordering, is a major focus of interest [2-3]. Like copper HTSC, iron-based superconductors are characterized by a strongly expressed anisotropy, and have a structure of closely spaced atomic planes of Fe and As (for pnictides). The main contribution to the band structure near the Fermi surface is provided by two orbitals, $d_{xz}$ and $d_{yz}$. Therefore, the simplest model Hamiltonian for iron-based HTSC, reflecting their crystal and electronic structure, is a two-dimensional generalized two-orbital Hubbard model [4], which has been intensively studied since the discovery of iron-based HTSC with the use of various approximate analytical and numerical methods. The applicability of finite-size cluster quantum Monte Carlo algorithms that allow, in principle, to obtain exact results, is limited in this case by the sign problem, which exponentially slows calculations at a sufficiently low temperature and/or away from the half-filling. In this work, with choosing specific basis states for the Hamiltonian of the two-orbital model and the use of CTWL-algorithm [5], we were able to overcome partly the sign problem and to obtain data for Matsubara Green's function at sufficiently low temperature in a wide range of model parameters. Using the relationship between Matsubara Green's function and the density of electron states, we have derived the Fermi liquid parameters of the model: quasi-particle weight ($Z$-factor), self-energy $\Sigma$, and scattering rate $\Gamma$, and studied the properties of the model under doping. The asymmetry in the behavior of $Z$-factor was observed at electron and hole doping, which reflects the asymmetry of the Hamiltonian. The evolution of the Fermi surface was studied at changing the model parameters and the level of doping; an increase of the volume of the Fermi surface with the growth of interaction was observed, which shows the deviation from the Luttinger theorem.
2. Two-orbital 2D Hubbard model

First introduced in [4], the minimum two-orbital model for iron-based HTSC takes into account the real crystal structure of these compounds, as well as the two-dimensional nature of physical properties, and has the following Hamiltonian:

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

\[ H_{\text{int}} = U \sum_{i \alpha} n_{i \alpha \uparrow} n_{i \alpha \downarrow} + V \sum_{i} n_{i \alpha \uparrow} n_{i \beta \downarrow} - \mu \sum_{i} n_{i \alpha \uparrow} - J \sum_{i} \left( n_{i \alpha \uparrow} n_{i \beta \uparrow} + n_{i \alpha \downarrow} n_{i \beta \downarrow} \right) - \]

\[ -J \sum_{i} \left( a_{i \alpha \uparrow}^{+} a_{i \alpha \downarrow}^{+} a_{i \beta \downarrow} a_{i \beta \uparrow}^{+} + a_{i \alpha \downarrow}^{+} a_{i \alpha \uparrow}^{+} a_{i \beta \downarrow} a_{i \beta \uparrow}^{+} + a_{i \alpha \downarrow}^{+} a_{i \beta \downarrow}^{+} a_{i \beta \uparrow} a_{i \alpha \uparrow}^{+} + a_{i \beta \downarrow}^{+} a_{i \beta \uparrow}^{+} a_{i \alpha \downarrow} a_{i \alpha \uparrow}^{+} \right); \]

\[ H_{\text{kin}} = -t_1 \sum_{i \alpha} \left( a_{i \alpha \uparrow}^{+} a_{i+1 \alpha \sigma} + a_{i \alpha \downarrow}^{+} a_{i+1 \beta \sigma} + a_{i \beta \uparrow} a_{i+1 \alpha \sigma}^{+} + a_{i \beta \downarrow} a_{i+1 \beta \sigma}^{+} \right) - t_2 \sum_{i \alpha} \left( a_{i \sigma \alpha}^{+} a_{i+1 \alpha \sigma} + a_{i \sigma \downarrow}^{+} a_{i+1 \beta \sigma} - a_{i \beta \sigma} a_{i+1 \alpha \sigma}^{+} - a_{i \alpha \sigma} a_{i+1 \beta \sigma}^{+} \right) - \]

\[ -t_3 \sum_{i \alpha} \left( a_{i \alpha \uparrow}^{+} a_{i+x \alpha \sigma} + a_{i \alpha \downarrow}^{+} a_{i+x \beta \sigma} + a_{i \beta \uparrow} a_{i+x \alpha \sigma}^{+} + a_{i \beta \downarrow} a_{i+x \beta \sigma}^{+} \right) + \]

\[ + t_4 \sum_{i \alpha} \left( a_{i \alpha \uparrow}^{+} a_{i-y \alpha \sigma} + a_{i \alpha \downarrow}^{+} a_{i-y \beta \sigma} + a_{i \beta \uparrow} a_{i-y \alpha \sigma}^{+} + a_{i \beta \downarrow} a_{i-y \beta \sigma}^{+} \right) + h.c. \]

Here operator \( a_{i \alpha \sigma}^{+} (a_{i \alpha \sigma}^{+}) \) creates (annihilates) an electron with spin projection \( \sigma \) on site \( i \) and orbital \( \chi (\gamma) \); \( t_1, j = 1, ..., \delta \) are hopping amplitudes between orbitals \( x(y) \); \( U, V, \) and \( J \) are Coulomb interaction terms; \( \mu \) is the chemical potential. In this work we used the quantum continuous time world-line Monte Carlo algorithm (CTWL-algorithm), adapted for the two-orbital model [5]. The parameters of \( H_{\text{kin}} \) in (1) were taken the same as in [6], \( t_1 = 0.058 \) (eV); \( t_2 = 0.22; \) \( t_3 = -0.21; \) \( t_4 = -0.08; \) and the relationships between Coulomb terms in \( H_{\text{int}} \) are \( V = 0.5U; \) \( J = 0.25U. \)

3. Momentum distribution

The momentum distribution \( n(k) \) can be obtained from the relation

\[ n(k) = G(k, \tau \rightarrow -0); \quad G(k, \tau) = \sum_{ij} G_{ij}(\tau) e^{ikr_{ij}}. \]

Here \( G_{ij}(\tau) \) is Matsubara Green’s function, \( G_{ij}(\tau) = -\langle T_a n_{i \sigma} (\tau) a_{j \beta \sigma}^{+} (0) \rangle \).

Direct approximation (2) in a numerical calculation leads to uncontrolled errors; therefore, we have used the following expression:

\[ n(k) = \int \frac{A_\sigma (k, \omega)}{1 + e^{(\omega - \mu)/T}} d\omega. \]

To calculate (3), the spectral function \( A_\sigma (k, \omega) \) and the total density of states \( A(\omega) = \sum_{\kappa \sigma} A_\sigma (k, \omega) \) were recovered with the use of a stochastic procedure [7] from the integral equation relating the spectral function with Matsubara Green's function,

\[ G_\sigma (k, \tau) = -\int \frac{A_\sigma (k, \omega) e^{-\tau (\omega - \mu)}}{1 + e^{-\beta (\omega - \mu)}} d\omega. \]

4. Half-filling

Figure 1 shows the profiles of the momentum distribution depending on the parameter \( U \) at half-filling. The data are presented for the inverse temperature \( \beta = 1 \). This is a reasonably low temperature as \( \beta t_{\text{max}} = \beta t_2 \approx 0.2; \) in addition, the sign problem does not allow lowering the temperature significantly. The flattening of the distribution with increase of the interaction is clearly visible, as well as
the presence of the hole pockets at the center (Γ) and the periphery (M) of the zone, the filling of which increases with U.

The total density of states (DOS) depending on the value of the interaction is shown in Figure 2. The calculations were performed at \( \beta = 1 \), so a thermal broadening of the zones takes place; however, we believe that it should not prevent to see the evolution of the zones with changing U. Such choice of temperature is associated with the convergence of quantum Monte Carlo algorithm, namely, with the sign problem. Only at this temperature we were able to perform the calculations at a series of values of the interaction parameters with sufficient accuracy. The interval between the bands increases with the increase of the interaction, and is close to the value of U, but not identical with it, since the interaction part of the Hamiltonian (1) is more complicated than the conventional Hubbard term. With the growth of the interaction the bands shrink turning into narrow peaks; this leads to a reduction of the dispersion and flattening of the momentum distribution.

![Figure 1.](image1)  
**Figure 1.** Momentum distribution in the first Brillouin zone as a function of U.

![Figure 2.](image2)  
**Figure 2.** The total DOS as a function of U. \( \beta=1 \).

![Figure 3.](image3)  
**Figure 3.** The evolution of the density of states with change of doping near the half-filling. \( U = 4; \beta = 2 \).

![Figure 4.](image4)  
**Figure 4.** Momentum distribution for various doping. \( U = 4; \beta = 2 \).

5. The doped case

The quantum Monte Carlo algorithm suffers from the minus-sign problem when calculating a two-dimensional Fermi system. This leads to the fact that the deviation from the half-filling may not afford calculation of thermodynamic average values, including the Green’s function, with the reasonable accuracy. We have managed to obtain a good convergence in the doped case only at several parameters of U and at temperatures not lower than \( \beta = 2 \). Figure 3 shows the total DOS at a low-level of electron and hole doping. The shape of the bands changes as the chemical potential moves from the electron to the hole doping region. The broadening of the bands is observed with increasing the level of doping (both hole and electron). The value of the density of states at the Fermi level increases slightly with increasing the hole doping. Therefore, the change of the number of carriers in the system is not equivalent to a simple filling of the bands (the so-called “hard-band approximation”), i.e., to a simple shift of the chemical potential at a constant density of states, which is the contribution of Coulomb
correlations in this typical generalized Hubbard model. Similar correlation effects were also observed in [8] for the Hubbard model in the low-doped regime.

Figure 4 shows the profiles of the momentum distribution along the main crystallographic directions in the first Brillouin zone for the same values of doping, as in Figure 3. The following can be noted. The profiles with different fillings are substantially equidistant, which means that the bands are filled with virtually no distortion as the concentration changes. The momentum distributions vary little with the change of the filling, which is consistent with the statement that the momentum distribution of quasiparticles has the same features (including the Fermi jump) as the total momentum distribution. Interaction blurs distribution gradients as well as at the half-filling case.

6. Fermi-liquid parameters

Studies of the Hubbard model [8, 9] and experimental data on FeAs-systems [10] may indicate non-Fermi liquid nature of these strongly correlated systems. To investigate this issue, we extracted the Fermi-liquid parameters of the model (1). In the quasiparticle approximation, the spectral density near the maximum of the peak for electron and hole excitations can be described as follows [11]:

$$A(k, \omega) = \frac{Z(k)}{-\pi \left(\omega - \epsilon(k) + \mu \right)^2 + \left(\Gamma(k, \omega)\right)^2}.$$  

(5)

Here $Z(k)$ is the quasiparticle weight or $Z$-factor, $\epsilon(k)$ is the excitation energy identified with the maximum of the spectral peak for a given point of the Brillouin zone; $\Gamma(k, \omega)$ is the quasiparticle scattering rate, $\Gamma(k, \omega) = -\text{Im} \left(\Sigma(k, \omega)\right)$; $\Sigma(k, \omega)$ is the self-energy; it is assumed that $|\epsilon(k) - \mu| \gg |\Gamma|$, so, the quasiparticle scattering rate is small.

The relation between the Green’s function and the $Z$-factor is given by

$$Z = \pi \frac{1}{\beta \text{Im} \left[\left(G(k, i\omega_0)\right)^{-1}\right]}; \quad G(k, i\omega_0) = \int_0^\beta G(k, \tau) e^{i\omega_0 \tau}.  \quad \text{(6)}$$

The renormalization of the $Z$-factor was observed with the increase of the interaction. The effect of doping on $Z$-factor is shown at Figure 5. $Z$-factor increases significantly even at low doping; this indicates growth of density of states at the Fermi-level. Note that similar results were obtained in [12] for the single-band Hubbard model.

![Figure 5. Z-factor as a function of doping.](image)

$U = 4; \beta = 2.$

Acknowledgments

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7. References

[1] Kamihara Y, Watanabe T, Hirano M and Hosono H 2008 J. Am. Chem. Soc. 130 3296
[2] Isyumov Yu, Kurmaev E 2010 High-$T_c$ Superconductors Based on FeAs Compounds Springer
[3] Dagotto E 2013 Rev. Mod. Phys. 85 849
[4] Raghu S et al 2008 Phys. Rev. B 77 220503(R)
[5] Kashurnikov V A, Krasavin A V 2013 JETP Lett. 97 333
[6] Moreo A, Daghofer M, Riera J A and Dagotto E 2009 Phys. Rev. B 79 134502
[7] Mishenko A S, Prokof’ev N V, Sakamoto A, Svistunov B V 2000 Phys. Rev. B 62 6317
[8] Gröber C, Eder R and Hanke W 2000 Phys. Rev. B 62 4336
[9] Korshunov M M, Ovchinnikov S G 2003 Phys. Solid State 45 1415
[10] Dai Y M et al 2015 Phys. Rev. X 5 031035
[11] Abrikosov A A, Gorkov L P, Dzyaloshinski I E 2012 Methods of Quantum Field Theory in Statistical Physics Dover Publications
[12] Arsenaulet L-F, Sémon P and Tremblay A-M S 2012 Phys. Rev. B 86 085133