Quantum Monte-Carlo simulation of FeAs-based superconductors

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Abstract. The generalized quantum Monte Carlo algorithm is developed and used to calculate the energy, occupation numbers, and correlation functions of finite FeAs clusters in the two-orbital model at finite temperatures. The coding of quantum states made it possible to take into account complex exchange terms between the orbitals. The results for the calculation of the thermodynamic characteristics of finite two-dimensional FeAs clusters simulating iron-based superconductors have been obtained.

1. Introduction

A new class of high-temperature superconductors in FeAs compounds uncovered in 2008 [1] has a layered structure of closely located atomic planes consisting of Fe and As atoms. Similar to copper oxide high-temperature superconductors, they have pronounced anisotropy; consequently, these systems can be adequately described by two-dimensional strong coupling models.

The features of the multigap band structure, anomalous magnetic properties, and pronounced presence of strong correlations, which follow from numerous experimental data (see, e.g. reviews [2-4] and references therein), indicate that the description of the system requires not only analytical approximations but also accurate numerical calculations. The existing strong coupling models for these compounds such as two- [5,6], three- [7,8], and five-orbital [8,9] are typical generalized Hubbard models and cannot provide a correct analysis in various approximations, including the mean-field approximation. The complexity of these models requires the application of accurate quantum calculation methods for the study of iron-based high-temperature superconductors.

One of the most efficient methods for the study of strongly correlated systems is the quantum Monte Carlo continuous-time worldline (CTWL) algorithm [10], which makes it possible to calculate the characteristics of systems with various sizes, dimensions, and statistics, as well as to take into account the sign problem. Although the CTWL algorithm is quite general for the characteristics of the systems under study, it requires modification for each specific problem. The initial modification of the CTWL algorithm for the problem considered in this work is the generalized algorithm [11] that allows a convenient coding of states for Monte Carlo procedures.
2. Model

The choice of an adequate strong coupling model for FeAs superconductors is determined by two circumstances. The first circumstance is the crystal structure of compounds, and the second is the complexity of the model in applicability to the analytical and numerical investigation of superconducting compounds. On one hand, the two-orbital model proposed in [5] can reproduce the significant physics of electron interactions in new compounds. On the other hand, it reaches the limit of complexity for the implementation of algorithms for the study of new superconductors on the basis both of quantum Monte Carlo methods and of methods of exact diagonalization of the Hamilton matrix. The properties of the two-orbital model were studied in detail in [6,12] using the exact diagonalization method. However, those studies were performed only for a \(8 \times 8\) cluster including eight iron atoms, because the size of the Hamilton matrix increases rapidly with the number of atoms.

The Hamiltonian of the two-orbital model has the form [5]

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

where

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

\[
H_{\text{kin}} = -t_1 \sum_{i, \sigma} \left( a_{i+\hat{x}, \sigma}^+ a_{i, \sigma} + a_{i, \sigma}^+ a_{i+\hat{x}, \sigma}^+ a_{i+\hat{y}, \sigma} + a_{i+\hat{y}, \sigma}^+ a_{i, \sigma}^+ a_{i+\hat{y}, \sigma} + a_{i, \sigma} a_{i+\hat{y}, \sigma}^+ a_{i+\hat{y}, \sigma} + h.c. \right) - t_2 \sum_{i, \sigma} \left( a_{i+\hat{x}, \sigma}^+ a_{i+\hat{y}, \sigma}^+ a_{i+\hat{y}, \sigma} a_{i+\hat{x}, \sigma} + h.c. \right) - t_3 \sum_{i, \sigma} \left( a_{i+\hat{x}, \sigma}^+ a_{i+\hat{x}, \sigma}^+ a_{i+\hat{y}, \sigma} + a_{i, \sigma}^+ a_{i+\hat{y}, \sigma}^+ a_{i+\hat{y}, \sigma} + a_{i, \sigma} a_{i+\hat{y}, \sigma}^+ a_{i+\hat{y}, \sigma} + h.c. \right) - t_4 \sum_{i, \sigma} \left( a_{i+\hat{x}, \sigma}^+ a_{i+\hat{x}, \sigma}^+ a_{i+\hat{y}, \sigma} + a_{i, \sigma}^+ a_{i+\hat{y}, \sigma}^+ a_{i+\hat{y}, \sigma} + h.c. \right) + t_5 \sum_{i, \sigma} \left( a_{i+\hat{x}, \sigma}^+ a_{i+\hat{x}, \sigma}^+ a_{i+\hat{y}, \sigma} + a_{i, \sigma} a_{i+\hat{y}, \sigma}^+ a_{i+\hat{y}, \sigma} + h.c. \right).
\]

Here, \(a_{i, x, \sigma}^+ (a_{i, x, \sigma})\) is the creation (annihilation) operator of an electron with the spin \(\sigma\) at the \(i\)th site and orbital \(x\); \(t_i (i = 1, ..., 4)\) are the electron hopping amplitudes between the \(d_{xz}\) and \(d_{yz}\) orbitals (denoted as \(x\) and \(y\), respectively, figure 1); \(U\) and \(V\) describe the Coulomb interaction; \(J\) is the Hund coupling term; and \(\mu\) is the chemical potential.

![Figure 1. Electron hoppings between orbitals taken into account in the two-orbital model.](image)
3. Method

The character of the interaction between the orbitals following from the experimental data [13] indicates that pair hopping of electrons from one orbital to another should be taken into account; this is a very nontrivial problem in Monte Carlo algorithms.

In this work, the worldline quantum Monte Carlo algorithm is modified so that it can ensure the calculation of the Hamiltonian of the general form [11]

\[
H = \sum_{k} \sum_{n_1, n_2} A_{k}^{n_1 n_2} A_{k}^{n_1 n_2} + h.c. + \sum_{k} B_{k}^{n_1 n_2} A_{k}^{n_1 n_2} + h.c. + \sum_{k} C_{k}^{n_1 n_2} A_{k}^{n_1 n_2}
\]  

(4)

Here, \( A_{k}^{n_1 n_2} \) are the off-diagonal transition matrix elements between the states \( n_1 \) and \( n_2 \) at the \( k \)th site; \( N_{k}^{n} \) is the particle number operator in the state \( n \) at the \( k \)th site; and \( t, B, C, \) and \( D \) are the corresponding interaction amplitudes. The two-orbital model allows the description with the general Hamiltonian given by (4) with the coding of states at sites presented in the table 1.

| Table 1. Coding of site states in the two-orbital model |
|--------------------------------------------------------|
| State no. | Orbital \( y \) | Orbital \( x \) | State no. | Orbital \( y \) | Orbital \( x \) |
|-----------|----------------|----------------|-----------|----------------|----------------|
| 0         | \( |0\rangle \)  | \( |0\rangle \)  | 8         | \( \downarrow \rangle \) | \( |0\rangle \)  |
| 1         | \( |0\rangle \)  | \( |\uparrow\rangle \) | 9         | \( \downarrow \rangle \) | \( |\uparrow\rangle \) |
| 2         | \( |0\rangle \)  | \( |\downarrow\rangle \) | 10        | \( \downarrow \rangle \) | \( |\downarrow\rangle \) |
| 3         | \( |0\rangle \)  | \( |\uparrow\downarrow\rangle \) | 11        | \( \downarrow \rangle \) | \( |\uparrow\downarrow\rangle \) |
| 4         | \( |\uparrow\rangle \) | \( |0\rangle \)  | 12        | \( |\uparrow\downarrow\rangle \) | \( |0\rangle \)  |
| 5         | \( |\uparrow\rangle \) | \( |\uparrow\rangle \) | 13        | \( |\uparrow\downarrow\rangle \) | \( |\uparrow\rangle \) |
| 6         | \( |\uparrow\rangle \) | \( |\downarrow\rangle \) | 14        | \( |\uparrow\downarrow\rangle \) | \( |\downarrow\rangle \) |
| 7         | \( |\uparrow\rangle \) | \( |\uparrow\downarrow\rangle \) | 15        | \( |\uparrow\downarrow\rangle \) | \( |\uparrow\downarrow\rangle \) |

Figure 2 illustrates the correspondence of the pattern of worldliness in the new generalized coding and in the standard coding of the CTWL algorithm for some terms of the Hamiltonian of the two-orbital model.
Figure 2. Worldlines of particles for the terms (left) \( a_{y,i}^+ a_{y,i} a_{x,i} a_{x,i}^+ \) and (right) \( a_{y,x,i}^+ a_{y,x,i} a_{x,i} a_{x,i}^+ \) of the Hamiltonian of the two-orbital model. The action of these operators is given in the (a) second quantization representation, (b) generalized Monte Carlo coding, and (c) standard worldline Monte Carlo algorithm.

4. Results

The new algorithm was tested in the calculation of a 3×3 cluster with a small number of particles. The results calculated for the energy of the system and average occupation numbers of the sites with various model parameters show the complete coincidence with the data obtained by the method of exact diagonalization of the Hamilton matrix for the same clusters.

The main problem in the quantum Monte Carlo study of fermion systems is the sign problem [14]. It appears because the statistical weights of configurations over which summation is performed in the algorithm operation process can have any sign. The mean value of an arbitrary operator \( A \) is calculated by the formula

\[
\langle A \rangle = \frac{\sum_n A_n |W_n| \text{sgn} W_n}{\sum_n |W_n| \text{sgn} W_n} = \frac{\sum_{MC} A n \text{sgn} W_n'}{\sum_{MC} \text{sgn} W_n'},
\]

where \( W_n' \) is the statistical weight of the \( i \)th configuration. The sign problem is primarily due to the antisymmetry of the fermion wavefunction; correspondingly, the calculation of mean values involves the summation of sign-alternating series, which strongly increases statistical errors and calculation time. The effect of the sign problem on the calculation convergence rate depends on many factors. In particular, it is determined by the choice of the basis states of the system. For more efficient convergence and partial suppression of the sign problem, the scheme was supplemented by the off-diagonal term in the form

\[
-\alpha \sum_{k,n_1,n_2} \left( A_{k,n_1,n_2}^* + h.c. \right).
\]
Here, $\alpha \sim 0.005$. On one hand, such an addition to the Hamiltonian does not change the results of calculation within the achieved accuracy. On the other hand, the introduction of such a controlled off-diagonal term significantly “enlives” the statistics and increases the convergence rate.

As will be seen below, the basis presented in the table 1 is quite successful and allows the calculations of the two-orbital with the necessary accuracy.

The experimental investigations of iron-based high-temperature superconductors, as well as the calculations of the band structure (see, e.g., [6] and references therein), provide various possible sets of parameters of the Hamiltonian of the two-orbital model that make it possible to qualitatively describe the observed electronic properties of these compounds. To reveal the capabilities of the new developed method, we chose the following two sets of parameters for a $3 \times 3$ square cluster consisting of nine iron atoms with periodic boundary conditions (here and below, all energy quantities are given in electronvolts [6]):

\[
U = 1; \quad V = 1; \quad J = 0.25; \quad t_1 = 0.058; \quad t_2 = 0.22; \quad t_3 = -0.0208; \quad t_4 = -0.079; \quad (7)
\]

\[
U = 8; \quad V = 4; \quad J = 2; \quad t_1 = 0.058; \quad t_2 = 0.22; \quad t_3 = -0.0208; \quad t_4 = -0.079. \quad (8)
\]

The dependences of the number of particles in the system, the energy of the system, and the average sign of configurations on the chemical potential $\mu$ were calculated using the quantum Monte Carlo algorithm with sets (7) and (8) of parameters.

![Figure 3](image)

**Figure 3.** Average sign $S$ of the configurations, energy $E$, and filling factor versus the chemical potential $\mu$ for the $3 \times 3$ cluster, the parameters of the model given by (8), and the temperature $\beta = 1/T = 10$.

Figure 3 shows the dependences of the indicated quantities on the chemical potential for the parameters of the Hamiltonian given by (8) (here and below, all errors of the calculated values are smaller than the sizes of the symbols). According to the figure, the physical quantities for a $3 \times 3$ cluster can be calculated in the chosen basis almost without the sign problem. The dependences of the energy and number of particles on $\mu$ exhibit flat segments in the ranges $\mu_{11} < \mu < \mu_{12}$, $\mu_{21} < \mu < \mu_{22}$, and $\mu_{31} < \mu < \mu_{32}$. They can be attributed to the regions of the dielectric phase. The widths of the energy gaps are $\Delta_1 = \mu_{12} - \mu_{11}$, $\Delta_2 = \mu_{22} - \mu_{21}$, and $\Delta_3 = \mu_{32} - \mu_{31}$. Thus, at $n_1 = 0.25$, $n_2 = 0.5$, and $n_3 = 0.75$, three dielectric regions are observed. It is noteworthy that the average sign magnitude is close to unity in the dielectric phase and decreases sharply in the transit regions. Convergence in this case usually takes about $10^{11}$ elementary Monte Carlo steps.
The spin susceptibility

$$\chi(q) = \int_0^\beta d\tau \sum_{ij} e^{i\omega(i-j)} \left\langle m_{ij}(\tau)m_{ji}(0) \right\rangle,$$  (9)

where $\alpha, \beta = x, y$ are orbitals; $m_{ij} = \frac{1}{2}(n_{i,\alpha,\uparrow} - n_{i,\alpha,\downarrow})$, was calculated for various cluster sizes and sets of parameters of the Hamiltonian. The results for the $6 \times 6$ cluster are presented in figure 4.

Figure 4. Spin susceptibility for the $6 \times 6$ cluster. Hopping terms are given by (8).

As can be seen, with the decrease of temperature the peaks at points $(\pi,0)$ and $(\pi,\pi)$ emerge which indicate the growth of antiferromagnetic correlations. To clarify the possible channels of pairing the correlation functions $P_2$ and $P_9$ were calculated (notations are in accordance with [6]):

$$P_2 = \int_0^\beta d\tau \sum_{ij} \left\langle \Delta_2(i,\tau)\Delta_2^*(j,0) \right\rangle,$$  (10)

$$P_9 = \int_0^\beta d\tau \sum_{ij} \left\langle \Delta_9(i,\tau)\Delta_9^*(j,0) \right\rangle,$$  (11)

$$\Delta_2 = \frac{1}{2N} \sum_{ijkl} (a_{i,\alpha,\uparrow}a_{j,\beta,\downarrow} - a_{i,\alpha,\downarrow}a_{j,\beta,\uparrow}),$$  (12)

$$\Delta_9 = \frac{1}{2N} \sum_{ijkl} (a_{i,\pi,\uparrow}a_{j,\pi,\downarrow} - a_{i,\pi,\downarrow}a_{j,\pi,\uparrow}).$$  (13)

Here $\mu$ is the vector to the nearest neighbour site; and $N$ is the number of sites in the cluster. The function $P_2$ characterizes the pairing on the same orbitals of nearest neighbour sites and the function $P_9$ characterizes the pairing on the different orbitals. Figure 5 shows the results for the $10 \times 10$ cluster. Correlations grow with the decreasing of temperature for both correlation functions; to reveal the correlation properties the values $\overline{P}_2$ and $\overline{P}_9$ were subtracted from $P_2$ and $P_9$, where $\overline{P}_2$ and $\overline{P}_9$ are determined by the Wick’s decomposition of the type

$$\langle a_{i,1}a_{i,2}a_{i,3}a_{i,4} \rangle = \langle a_{i,1} \rangle \langle a_{i,2} \rangle \langle a_{i,3} \rangle \langle a_{i,4} \rangle - \langle a_{i,1} \rangle \langle a_{i,2} \rangle \langle a_{i,3} \rangle \langle a_{i,4} \rangle.$$  (14)
5. Conclusions

We developed the generalized quantum Monte Carlo algorithm that allowed the calculation of thermodynamic and correlation properties of FeAs clusters modeling iron-based superconductors within the two-orbital model at finite temperatures. The coding of quantum states made it possible to take into account complex exchange terms between the orbitals. The exact inclusion of off-diagonal terms in (2) which can play a key role in the pairing of charge carriers and, therefore, cannot be neglected, is the main feature of the presented algorithm.

Further investigations will make it possible to determine the region of the parameters of the model that corresponds to the effective attraction between electrons, and also to calculate the Matsubara Green’s function and to reconstruct the spectral density of states, which is possible using the described method.

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