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# Calculation of Density of States for FeAs-based Superconductors

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*The spectral and the total density of states were calculated for two-dimensional FeAs-clusters within the limits of the two-orbital model, which is widely used for modeling iron-based superconductors. The spectra were restored by means of an asymptotically exact stochastic procedure, which was modified to restore the kernel of the integral equation relating the Matsubara Green's function and the spectral density. The data for Matsubara Green's function were obtained with the use of the generalized quantum world-line Monte Carlo algorithm adapted for the two-orbital model. The calculations were made for clusters with sizes up to 10×10 FeAs-cells. The data are presented for the distribution profiles along the main crystallographic directions and for the entire Brillouin zone. The analysis of the doped state revealed differences in the electron and hole states of the system that is correlated with known experimental data.*

*Keywords: FeAs-based superconductors, quantum Monte-Carlo algorithm, density of states, two-orbital model.*
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The discovery of high-temperature superconductors (HTSC) based on iron [1] was a new incentive to determination of nature of superconductivity in complex compounds with a layered structure. Compared to copper-based HTSC, the iron-based compounds have a more complex phase diagram, which includes antiferromagnetic, structural, and superconducting phase transitions [2, 3]. The key subject of the research now is the role of electron correlations in iron-based HTSC, which, generally, are crucial in the formation of physical properties of systems containing transition elements [4].

As well as copper-based HTSC, iron-based high-temperature superconductors are characterized by strongly expressed anisotropy, and have a structure, which consists of closely spaced atomic planes of Fe and As (for pnyctides). Estimates and ARPES experiment show that the quasiparticle spectrum forms a complex multi-band structure with hole and electron pockets in the Brillouin zone; the density of states near the Fermi level is the same for most of 122- and 1111-type compounds, and weakly depends on the interaction parameters [5].

The description of physical properties of these compounds within the limits of a two-dimensional tight-binding model such as the two [6, 7], three [8, 9] and five-orbital model [9, 10], which are typical generalized Hubbard models, do not provide the correct analysis in various approximations, including the mean-field approximation. The complexity of these models leads

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to the use of exact quantum calculation methods. Preliminary studies of electron correlations in large FeAs clusters developed earlier by the authors in a series of papers [11–15] with the use of quantum trajectory Monte Carlo algorithm that does not use the Wick's expansion and thus asymptotically exact, allowed to obtain results correlated with other experimental and calculated data. Calculations for FeAs clusters with the number of cells from $3 \times 3$ to $10 \times 10$ showed the presence of multi-band structure of the spectrum of the charge carriers; calculations of pair correlation functions demonstrated the possibility of effective attraction of carriers with $A_{1g}$ symmetry [11–13]. The present work is devoted to the analysis of the spectrum of elementary excitations, which determines the Fermi surface and the density of states.

The two-orbital model first proposed in [6] is the simplest model for iron-based HTSC, where the crystal structure of these compounds is taken into account and the main contribution to the density of states near the Fermi level comes from $3d$-states of iron atoms [7, 16]. The Hamiltonian of the model has the form

$$H = H_{int} + H_{kin}; \tag{1}$$

$$\begin{aligned}
H_{int} &= U \sum_{\boldsymbol{i}\alpha} n_{\boldsymbol{i}\alpha\uparrow} n_{\boldsymbol{i}\alpha\downarrow} + V \sum_{\boldsymbol{i}} n_{\boldsymbol{i}x} n_{\boldsymbol{i}y} - \mu \sum_{\boldsymbol{i}} n_{\boldsymbol{i}} - J \sum_{\boldsymbol{i}} (n_{\boldsymbol{i}x\uparrow} n_{\boldsymbol{i}y\uparrow} + n_{\boldsymbol{i}x\downarrow} n_{\boldsymbol{i}y\downarrow}) - \\
&- J \sum_{\boldsymbol{i}} \left( a^+_{\boldsymbol{i}x\downarrow} a_{\boldsymbol{i}x\uparrow} a^+_{\boldsymbol{i}y\uparrow} a_{\boldsymbol{i}y\downarrow} + a^+_{\boldsymbol{i}x\uparrow} a_{\boldsymbol{i}x\downarrow} a^+_{\boldsymbol{i}y\downarrow} a_{\boldsymbol{i}y\uparrow} + a^+_{\boldsymbol{i}x\uparrow} a_{\boldsymbol{i}y\downarrow} a^+_{\boldsymbol{i}x\downarrow} a_{\boldsymbol{i}y\uparrow} + a^+_{\boldsymbol{i}y\uparrow} a_{\boldsymbol{i}x\downarrow} a^+_{\boldsymbol{i}y\downarrow} a_{\boldsymbol{i}x\uparrow} \right); \\
H_{kin} &= -t_1 \sum_{\boldsymbol{i}\sigma} \left( a^+_{\boldsymbol{i}x\sigma} a_{\boldsymbol{i}+\boldsymbol{x},x\sigma} + a^+_{\boldsymbol{i}y\sigma} a_{\boldsymbol{i}+\boldsymbol{y},y\sigma} \right) - t_2 \sum_{\boldsymbol{i}\sigma} \left( a^+_{\boldsymbol{i}y\sigma} a_{\boldsymbol{i}+\boldsymbol{x},y\sigma} + a^+_{\boldsymbol{i}x\sigma} a_{\boldsymbol{i}+\boldsymbol{y},x\sigma} \right) - \\
&- t_3 \sum_{\boldsymbol{i}\sigma} \left( a^+_{\boldsymbol{i}x\sigma} a_{\boldsymbol{i}+\boldsymbol{x}+\boldsymbol{y},x\sigma} + a^+_{\boldsymbol{i}x\sigma} a_{\boldsymbol{i}+\boldsymbol{x}-\boldsymbol{y},x\sigma} + a^+_{\boldsymbol{i}y\sigma} a_{\boldsymbol{i}+\boldsymbol{x}+\boldsymbol{y},y\sigma} + a^+_{\boldsymbol{i}y\sigma} a_{\boldsymbol{i}+\boldsymbol{x}-\boldsymbol{y},y\sigma} \right) + \\
&+ t_4 \sum_{\boldsymbol{i}\sigma} \left( a^+_{\boldsymbol{i}x\sigma} a_{\boldsymbol{i}+\boldsymbol{x}-\boldsymbol{y},y\sigma} + a^+_{\boldsymbol{i}y\sigma} a_{\boldsymbol{i}+\boldsymbol{x}-\boldsymbol{y},x\sigma} - a^+_{\boldsymbol{i}x\sigma} a_{\boldsymbol{i}+\boldsymbol{x}+\boldsymbol{y},y\sigma} - a^+_{\boldsymbol{i}y\sigma} a_{\boldsymbol{i}+\boldsymbol{x}+\boldsymbol{y},x\sigma} \right) + h.c.
\end{aligned}$$

Here $a^+_{\boldsymbol{i}x(y)\sigma}(a_{\boldsymbol{i}x(y)\sigma})$ is the creation (annihilation) operator of an electron with the spin $\sigma$ at the $\boldsymbol{i}$th site and orbital $x(y)$; $t_i,\ i = 1, \ldots, 4$ are the amplitudes of hopping of electrons between the orbitals $x$ and $y$; the parameters $U$ and $V$ describe the Coulomb interaction inside the orbitals and between them, respectively; $J$ is the exchange integral; and $\mu$ is the chemical potential.

The minimalistic two-orbital model gives the opportunity to investigate it with a generalized quantum trajectory Monte Carlo algorithm; the coding of basis states and other features of the calculation of correlation functions are reported in detail in [11–13]. The parameters of $H_{kin}$ parameters in (1) were taken from [7]:

$$t_1 = 0.058, \quad t_2 = 0.22, \quad t_3 = -0.21, \quad t_4 = -0.08, \tag{2}$$

the connection between the interaction parameters in $H_{int}$ was defined as follows:

$$V = 0.5U; \quad J = 0.25U. \tag{3}$$

The Matsubara Green's function,

$$\left\langle T_\tau a_{\boldsymbol{i}\alpha\sigma}(\tau) a^+_{\boldsymbol{j}\beta\sigma'}(0) \right\rangle, \tag{4}$$

where $\boldsymbol{i}$ and $\boldsymbol{j}$ are the coordinates of iron atoms, $\alpha, \beta$ are orbitals, and $\sigma, \sigma'$ are spin projections, was calculated for clusters with dimensions up to $10 \times 10$ FeAs cells in the range of the interaction parameter $U = 2 \div 16$ under condition (3).

To correctly reconstruct the spectral function $A_\sigma(k,\omega)$ and the total density of states $N(\omega) = \sum_{k\sigma} A_\sigma(k,\omega)$, it is necessary to solve the integral equation relating the spectral function to the Matsubara Green's function:

$$G_\sigma(k,\tau) = -\int \frac{A_\sigma(k,\omega)\, e^{-\tau\omega}}{1+e^{-\beta\omega}} d\omega. \tag{5}$$

Equation (5) is a typical incorrect problem in the Hadamard sense; solving this problem is mathematically nontrivial. The method of direct iterations in this case usually does not give a correct result if the initial data on the form of the integrand are absent. In this work, to reconstruct the spectral function $A_\sigma(k,\omega)$ from Eq. (5), we used the method combining the gradient descent and Monte Carlo algorithms [17], which was adapted by us for this problem. It does not include sources of systematic errors because the space of the variable $\omega$ is not discretized.

Fig. 1 shows the total density of states at the half-filling depending on the interaction. The sharply defined electron and hole subzones are separated by a bridge; the spectral density slightly decreases in it with the increase of interaction, but not to zero. This non-zero density at the Fermi level indicates FeAs system as a metal [5]. The density of states in the absence of interaction (red line) is calculated analytically for comparison. The distance between the bands increases with an 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 somewhat more complicated than the conventional Hubbard term), which is typical for the generalized Hubbard model; with the growth of the interaction the bands are turning into narrow peaks, which leads to a reduction in the dispersion of excitations, and flattening of the momentum distribution.

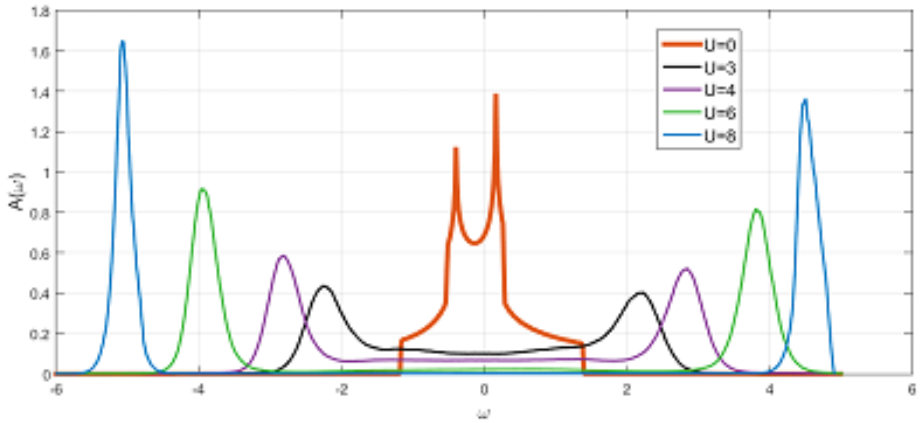


Fig. 1. The total density of states as a function of $U$. Cluster $8 \times 8$; $\beta = 1$. The red line shows the density of states for the free system at the same parameters

A clear picture of the flattening of dispersion and narrowing of the zones is also seen in the spectral density of states and excitations dispersion pattern shown in Fig. 2. It should be noted that the quasiparticle approximation for electron and hole excitations becomes increasingly valid as the interaction increases, since the half-width of the spectral peaks (and hence the decay) decreases with the increase of the energy of excitations.

Calculations of a two-dimensional Fermi system with the use of quantum Monte Carlo method, as is well known, are associated with a significant issue, the sign problem. This leads to the fact

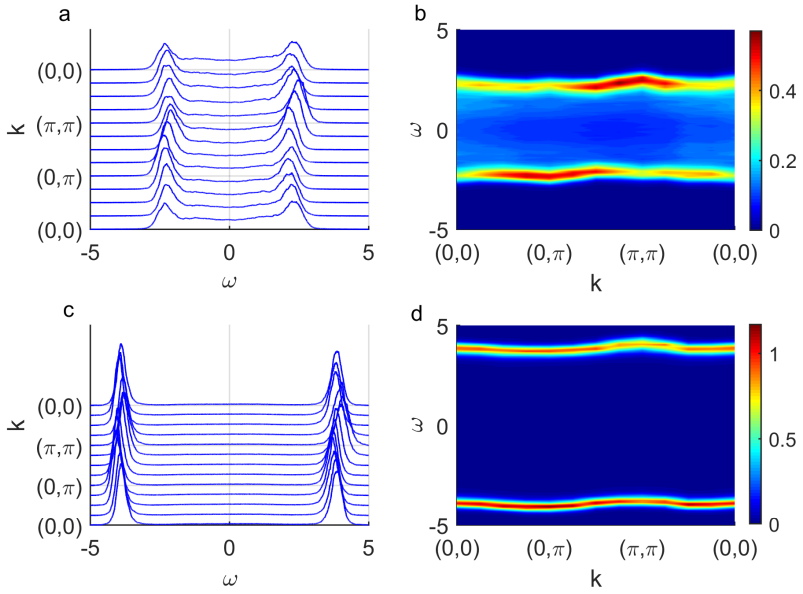


Fig. 2. The spectral density along the main crystallographic directions. The profiles of the spectral density (left); and dispersion (right). *a,b:* $U = 3$; *c,d:* $U = 6$

that the deviation from the half-filling does not allow to calculate the thermodynamic quantities, including the Green's function, with reasonable accuracy. This calculation is not an exception. Nevertheless, we can try to analyze the doped situation, assuming the normal filling of the zone by charge carriers while maintaining the calculated spectral density (the so-called "hard-zone" approximation). This description of strongly correlated systems is not entirely correct, but considering the fact that the profile of the Fermi surface, as shown by our results, is weakly dependent on the interaction parameter, near the half-filling it is possible to obtain data that can carry useful information, for example, about the features of the Fermi-liquid (or not) behavior of carriers [18]. We assume that near the Fermi surface the distortion of the zones by changing the carrier concentration $n$ at constant $U$ is weaker than by changing of $U$ with a constant density $n$.

As the exact density of states at the half filling is known, we can analyze the characteristics of the momentum distribution and the Fermi surface in the doped case. To do this, for the given $n$ and the known density of states $N(\omega)$ the chemical potential $\mu$ was numerically calculated:

$$n = \int \frac{N(\omega)}{1 + e^{\beta(\omega-\mu)}} d\omega, \tag{6}$$

and then the momentum distribution $n(k) = \int \frac{A_\sigma(k,\omega)}{1 + e^{\beta(\omega-\mu)}} d\omega$ was recalculated for the given $\mu$ for the entire Brillouin zone. Fig. 3 shows the momentum distribution for various fillings and interaction parameters for $8 \times 8$ cluster (analytical data are presented for $U = 0$ for clarity).

The first thing that should be noted is that nesting is observed in this model for electronic filling and finite interaction parameter, which is in agreement with the ARPES experiments [19–21]. The picture of the evolution of the Fermi surface at doping is close to that observed experimentally, for example, in $LiFe_{1-x}Co_x$ As system [21]. At the hole doping it can also be seen as carriers are localized near the regions $(0, \pm\pi)$, $(\pm\pi, 0)$, and in the case of electron doping

the central hole pocket drastically shrinks. Also, in the case of the electron doping the Fermi surface curvature in the corners (M) is close to a circle, somewhat flattened only at sufficiently large interaction, i.e. the invariance of this section of the Fermi surface maintains, even in the doped case. With increasing of the interaction, the boundaries of the Fermi surface increasingly blurred.

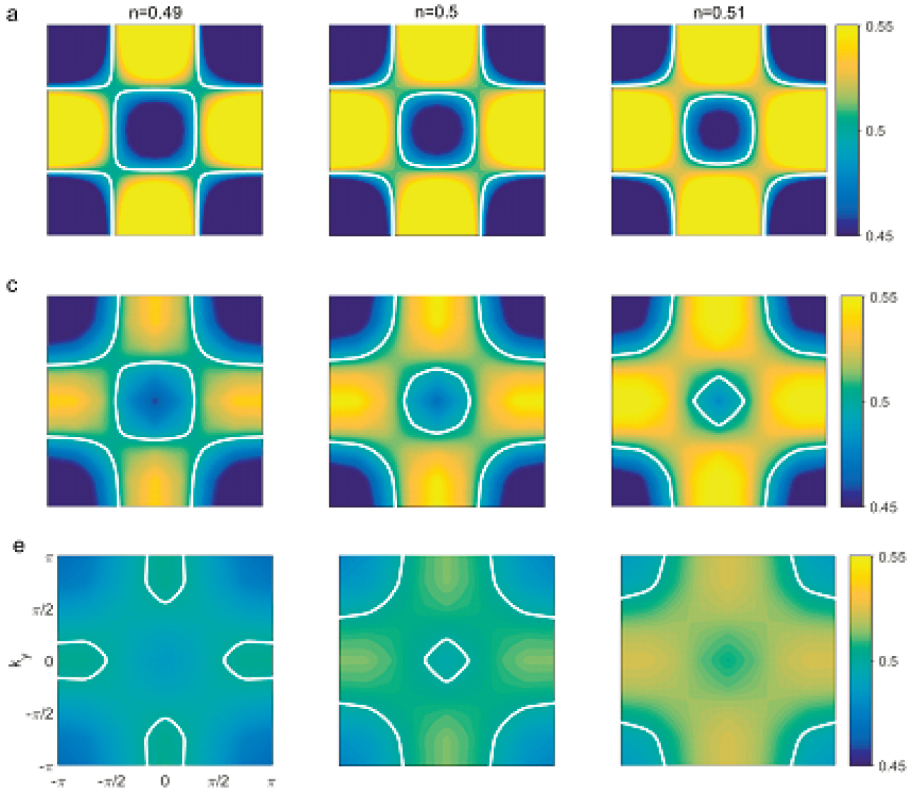


Fig. 3. Occupation number distribution. $U = 0$ (upper row); $U = 2$ (middle row); $U = 8$ (bottom row)

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## Расчет плотности состояний сверхпроводников на основе железа

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*Спектральная и полная плотности состояний были рассчитаны для двумерных FeAs-кластеров в рамках двухорбитальной модели, широко используемой для моделирования сверхпроводников на основе железа. Спектры были восстановлены при помощи асимптотически точной стохастической процедуры, которая была модифицирована для восстановления ядра интегрального уравнения, связывающего Мацубаровскую функцию Грина и спектральную плотность. Данные для Мацубаровской функции Грина были получены с использованием обобщенного квантового траекторного алгоритма Монте-Карло, адаптированного для двухорбитальной модели. Расчеты были проведены для кластеров размерами до 10x10 ячеек FeAs. Представлены данные для распределения плотности вдоль главных кристаллографических направлений для всей зоны Бриллюэна. Анализ допированного состояния выявил различия между электронными и дырочными состояниями системы, что находится в согласии с известными экспериментальными данными.*

*Ключевые слова: высокотемпературные сверхпроводники на основе железа, квантовые алгоритмы Монте-Карло, плотность состояний.*