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Strongly correlated electron system in the magnetic field

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ABSTRACT

In the range of hole concentrations $0.08 < x < 0.18$ the density of states of the two-dimensional t - J model reveals oscillations with changing the magnetic field. Oscillation frequencies correspond to large Fermi surfaces. However, the oscillations are modulated with a frequency which is smaller by an order of magnitude. The modulation is related to van Hove singularities in the Landau subbands, which traverse the Fermi level with changing the field. The singularities are connected with bending the subbands due to strong electron correlations. The frequency of the modulation is of the same order of magnitude as quantum oscillation frequencies in underdoped cuprates.

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1. Introduction

Theoretical investigations of systems of strongly correlated electrons in strong magnetic fields were started shortly after the discovery of the high- T_c superconductivity. A number of works was carried out on small clusters using the exact diagonalization (see, e.g., [1–3]). It is worth noting that due to the Peierls factor [4], the translation symmetry of the system is changed [5] – in the magnetic field the size of the elementary cell increases significantly. Clusters with sizes smaller than the size of this supercell violate the symmetry of the Hamiltonian and, therefore, it is difficult to extend the obtained results to larger crystals. Another approximation used for this problem is the mean-field approximation (see, e.g., [6–8]). The main shortcoming of this approximation is the neglect of the dynamic interaction of fermions with spin excitations. This interaction defines the fermion dispersion in the underdoped case.

The investigation of a system with strong electron correlations in the magnetic field is of interest in connection with the observation of quantum oscillations in the mixed state of underdoped yttrium cuprates [9–12]. Based on the Onsager–Lifshitz–Kosevich theory for metals [13] the observed decreased quantum oscillation frequencies were interpreted as a manifestation of small Fermi surface pockets [14], despite the fact that this interpretation seems to be in contradiction with numerous photoemission experiments. To explain the appearance of these small pockets proposals for various states with broken translational symmetry were suggested [15–17]. Other theories for explaining the decreased quantum oscillation

frequency suppose that it is connected with superconducting fluctuations [18,19] or use phenomenology of the marginal Fermi liquid [20].

Crystals, in which the decreased quantum oscillation frequencies were observed, belong to the underdoped region of the cuprate phase diagram, and, therefore, they are characterized by strong electron correlations. Theoretically the behavior of such crystals in strong magnetic fields is poorly known. In this work we use an approach, which allows us to overcome some limitations of the approximations used earlier for this problem. The approach provides a way to consider large enough clusters and moderate magnetic fields, taking into account the interaction of holes with spin excitations. We use the exact diagonalization of the kinetic term of the two-dimensional (2D) t - J model of Cu–O planes. The term contains the Peierls factor describing the influence of the homogeneous magnetic field perpendicular to the plane. As known [5,21,22], the energy spectrum of the kinetic term consists of the Landau subbands, which substitute the Landau levels in the lattice problem. The influence of strong electron correlations on these subbands is investigated using the Mori projection operator technique [23]. It should be noted that due to the complexity of the problem we were able to calculate only a few terms of the continued fraction of Green's function. Therefore, the obtained zero-field normal-state spectrum does not contain the pseudogap, which appears in other approaches both in the t - J and Hubbard models [24–26]. Since in the pseudogap the density of states (DOS) does not completely vanish, we nevertheless suppose that the used approximation gives at least qualitatively a correct picture of the normal-state energy spectrum of the t - J model in the perpendicular magnetic field.

In the used approximation, in the normal state the model has a large Fermi surface for the hole concentrations $x \gtrsim 0.06$. We found

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that in the range $0.08 < x < 0.18$ the density of hole states oscillates with frequency for a fixed field B and with $\frac{1}{B}$ at the Fermi level. The frequency of these latter oscillations with $\frac{1}{B}$ conforms with the large Fermi surface. However, the amplitude of these high-frequency oscillations is modulated with a frequency which is smaller by an order of magnitude. The appearance of this modulation is related to van Hove singularities in the Landau subbands, which traverse the Fermi level with changing B . These van Hove singularities are connected with bending the Landau subbands due to the influence of strong correlations. The frequency of the modulation is of the same order of magnitude as the quantum oscillation frequency observed in underdoped cuprates.

2. Main formulas

One of the main models used for the description of Cu-O planes of cuprate superconductors is the 2D t - J model. The Hamiltonian of this model in the magnetic field, which is perpendicular to the plane, reads

$$H = \sum_{\mathbf{I}\mathbf{I}'} t_{\mathbf{I}\mathbf{I}'} \exp\left(i \frac{e}{\hbar} \int_{\mathbf{I}}^{\mathbf{I}'} \mathbf{A}(\mathbf{r}) d\mathbf{r}\right) a_{\mathbf{I}\sigma}^\dagger a_{\mathbf{I}'\sigma} + \frac{1}{2} \sum_{\mathbf{I}\mathbf{I}'} J_{\mathbf{I}\mathbf{I}'} (s_{\mathbf{I}}^z s_{\mathbf{I}'}^z + s_{\mathbf{I}}^+ s_{\mathbf{I}'}^-) + g\mu_B B \sum_{\mathbf{I}} s_{\mathbf{I}}^z, \tag{1}$$

where 2D vectors \mathbf{I} and \mathbf{I}' label sites of a square plane lattice, $\sigma = \pm 1$ is the projection of the hole spin, $a_{\mathbf{I}\sigma}^\dagger = |\mathbf{I}\sigma\rangle\langle\mathbf{I}\sigma|$ and $a_{\mathbf{I}\sigma} = |\mathbf{I}\sigma\rangle\langle\mathbf{I}\sigma|$ are hole creation and annihilation operators with the empty $|\mathbf{I}\mathbf{0}\rangle$ and singly occupied $|\mathbf{I}\sigma\rangle$ site states. These three states form the complete set of hole states for the site \mathbf{I} in the t - J model. The first term of the Hamiltonian, the hole kinetic energy H_k , contains the hopping matrix element $t_{\mathbf{I}\mathbf{I}'}$ and the exponential factor with the Peierls phase [4], in which $\mathbf{A}(\mathbf{r})$ is the vector potential. The second term on the right-hand side of (1) is the exchange energy of localized spins with the exchange constant $J_{\mathbf{I}\mathbf{I}'}$ and the spin- $\frac{1}{2}$ operators $s_{\mathbf{I}}^z = \frac{1}{2} \sum_{\sigma} \sigma |\mathbf{I}\sigma\rangle\langle\mathbf{I}\sigma|$ and $s_{\mathbf{I}}^\pm = |\mathbf{I}, \pm 1\rangle\langle\mathbf{I}, \mp 1|$. The last, Zeeman term of the Hamiltonian contains the g -factor $g \approx 2$, the Bohr magneton μ_B and the magnetic induction B of the external magnetic field. It is supposed that this field is homogeneous and is only weakly disturbed by internal currents [27].

In the following consideration we shall suppose that only the nearest neighbor hopping and exchange constants are nonzero,

$$t_{\mathbf{I}\mathbf{I}'} = t \sum_{\mathbf{a}} \delta_{\mathbf{I}, \mathbf{I}'+\mathbf{a}}, \quad J_{\mathbf{I}\mathbf{I}'} = J \sum_{\mathbf{a}} \delta_{\mathbf{I}, \mathbf{I}'+\mathbf{a}},$$

where \mathbf{a} are four vectors connecting nearest neighbor sites. In cuprate perovskites, the exchange constant J is of the order of 100 meV. Comparing the interaction energy between a spin with its four neighbors (the second term of the Hamiltonian) and the energy of the spin in the external field (the third term of the Hamiltonian) one can ascertain that the former energy is two orders of magnitude larger than the latter even for fields of the order of 50 T. Therefore, the Zeeman term of the Hamiltonian can be neglected.

In the Landau gauge $\mathbf{A}_l = -Bl_y \mathbf{x}$, where l_y is the y component of the site vector \mathbf{I} and \mathbf{x} is the unit vector along the x axis (the 2D lattice is located in the xy plane, and the field is directed along the z axis). Hence the exponential in the kinetic term of the Hamiltonian can be written as

$$e^{i\kappa_{\mathbf{a}} \mathbf{l}}, \quad \kappa_{\mathbf{a}} = -\frac{e}{\hbar} B a_x \mathbf{y}. \tag{2}$$

In the following discussion we shall restrict our consideration to the fields satisfying the condition

$$\frac{e}{\hbar} B a^2 = \frac{2\pi}{n}, \tag{3}$$

where $a = |\mathbf{a}|$ and n is an integer. In this case the kinetic term of the Hamiltonian defines its translation properties – H_k is invariant with respect to translations by the lattice period along the x axis and by n lattice periods along the y axis. To retain this symmetry we apply the periodic Born-von Karman boundary conditions to the sample with N_x sites along the x axis and nN_y sites along the y axis. The boundary conditions define the set of allowed wave vectors with components $K_x = \frac{2\pi}{N_x a} n_x$ and $K_y = \frac{2\pi}{nN_y a} n_y$ with integer n_x and n_y . As can be seen from (2) and (3), the momenta $\kappa_{\mathbf{a}}$ coincide with one of the wave vectors in this net. Therefore, in H_k we can perform the usual Fourier transformation

$$a_{\mathbf{I}\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{K}} e^{-i\mathbf{K}\mathbf{I}} a_{\mathbf{K}\sigma},$$

using the known result $\frac{1}{N} \sum_{\mathbf{I}} e^{i\mathbf{K}\mathbf{I}} = \delta_{\mathbf{K}, \mathbf{Q}}$ for the wave vector \mathbf{K} on the net. Here $N = nN_x N_y$ and $\mathbf{Q} = (\frac{2\pi}{a} \nu_x, \frac{2\pi}{a} \nu_y)$ with integer ν_x and ν_y . After the Fourier transformation the kinetic term acquires the form

$$H_k = t \sum_{\mathbf{K}\mathbf{a}\sigma} e^{i\mathbf{K}\mathbf{a}} a_{\mathbf{K}-\kappa_{\mathbf{a}}, \sigma}^\dagger a_{\mathbf{K}\sigma}. \tag{4}$$

In deriving (4) we took into account that $\kappa_{\mathbf{a}} \mathbf{a} = 0$.

It is convenient to split the Brillouin zone into n stripes of the width $\frac{2\pi}{na}$, which are oriented parallel to the x axis. If we select one of these stripes, say, the lowest one with $-\frac{\pi}{a} < K_y \leq -\frac{\pi}{a} + \frac{2\pi}{na}$, and denote wave vectors in it as \mathbf{k} , momenta in the entire Brillouin zone can be described as $\mathbf{k} + j\kappa$. Here $0 \leq j \leq n-1$ and $\kappa = \frac{2\pi}{na} \mathbf{y}$. In these notations the kinetic energy acquires the form

$$H_k = \sum_{\mathbf{k}\sigma} \mathbf{A}_{\mathbf{k}\sigma}^\dagger \mathbf{h}_{\mathbf{k}} \mathbf{A}_{\mathbf{k}\sigma}, \tag{5}$$

where the summation over \mathbf{k} is performed over the selected stripe,

$$\mathbf{A}_{\mathbf{k}\sigma}^\dagger = (a_{\mathbf{k}\sigma}^\dagger, a_{\mathbf{k}+\kappa, \sigma}^\dagger, \dots, a_{\mathbf{k}+(n-1)\kappa, \sigma}^\dagger),$$

$$\frac{\mathbf{h}_{\mathbf{k}}}{t} = \begin{pmatrix} q_0 & e^{-ik_x a} & 0 & \dots & e^{ik_x a} \\ e^{ik_x a} & q_1 & e^{-ik_x a} & \dots & 0 \\ 0 & e^{ik_x a} & q_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ e^{-ik_x a} & 0 & \dots & e^{ik_x a} & q_{n-1} \end{pmatrix}, \tag{6}$$

and $q_j = 2 \cos(k_y a + \frac{2j\pi}{n})$.

The cyclic Hermitian matrix (6) can be diagonalized by the unitary transformation

$$a_{\mathbf{k}+j\kappa, \sigma} = \sum_{m=0}^{n-1} U_{\mathbf{k}jm} \alpha_{\mathbf{k}m\sigma},$$

$$\sum_{j'} h_{\mathbf{k}jj'} U_{\mathbf{k}j'm} = E_{\mathbf{k}m} U_{\mathbf{k}jm}. \tag{7}$$

This diagonalization gives the dispersion of the Landau subbands $E_{\mathbf{k}m}$ of uncorrelated carriers in the reduced Brillouin zone, which coincides with the above-mentioned lowest stripe. The applied procedure for deriving this dispersion is equivalent to the usually used approach, in which the magnetic supercell is introduced (see, e.g., [5,27]). The derivation of the kinetic-energy matrix (6) is simpler in our approach.

Since the kinetic energy defines symmetry properties of the total Hamiltonian (1), states corresponding to operators $\alpha_{\mathbf{k}m\sigma}$ in (7)

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