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Low-frequency quantum oscillations due to strong electron correlations

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ABSTRACT

The density of states of the two-dimensional fermionic Hubbard model supplemented with perpendicular homogeneous magnetic field is calculated using the strong coupling diagram technique. The density of states at the Fermi level as a function of the inverse magnetic induction oscillates, and the frequency of these oscillations increases by an order of magnitude with the change of the deviation from half-filling from small to moderate values. This frequency variation is caused by the change of Landau subbands contributing to the density – in the former case they are at the periphery of the Landau spectrum, while in the latter case the dominant contribution is provided by bands near its center. With changing induction these groups of bands behave differently. For small deviations from half-filling the calculated oscillation frequency is comparable to that observed in quantum oscillation experiments in yttrium cuprates.

1. Introduction

Studies of systems with strong electron correlations in magnetic fields were started shortly after the discovery of the high-T_c superconductivity. One of the first theoretical approaches used for this purpose was the exact diagonalization of small clusters (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 moderate magnetic fields 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 exact-diagonalization results to larger crystals. Larger clusters can be considered in the mean-field approximation (see, e.g., [6–8]). However, in this approach the dynamic character of strong correlations is neglected.

The interest in this problem was revived with the observation of low-frequency quantum oscillations in the mixed state of underdoped yttrium cuprates [9–12]. Based on the Onsager–Lifshitz–Kosevich theory for metals [13] the decreased quantum oscillation frequencies were interpreted as a manifestation of small Fermi surface pockets [14]. To explain the appearance of these small pockets, proposals for various states with broken translational symmetry were put forward [15–17]. In [18,19] and [20] decreased quantum oscillation frequencies were related to superconducting fluctuations and to properties of the marginal Fermi liquid. To take proper account of strong electron correlations inherent in underdoped cuprates, in [21] the two-dimensional (2D) t–J model supplemented with perpendicular magnetic field was considered. Calculations were carried out using the Mori projection operator technique. Due to complicated commutation relations of the Hubbard operators only a few terms of the continued fraction representing Green's function were obtained. It was shown that the density of electron states (DOS) at the Fermi level oscillates with field strength. The oscillations have usual for large Fermi surfaces high frequencies, however, they are modulated by low-frequency components.

In this work we use the strong coupling diagram technique [22–27] for investigating the DOS of the 2D fermionic Hubbard model supplemented with perpendicular homogeneous magnetic field. This approach allows us to consider large enough clusters in fields of moderate intensities. It is known [5,28,29] that the energy spectrum of a weakly correlated metal consists of Landau subbands, which appear in the crystal potential instead of the Landau levels of free electrons. We found that, in the approximation of a site-independent irreducible part, each Landau subband forms strongly correlated bands independently of other subbands. Using for the irreducible part the Hubbard-I approximation [30] we revealed that the DOS at the Fermi level oscillates as a function of inverse magnetic induction. The frequency F of these oscillations increases by an order of magnitude when the deviation of the electron filling $\bar{n}$ from half-filling grows from a few percent to 25%. For a Hubbard repulsion $U = 8t$, t being the hopping constant, and an intersite distance $a = 4$Å, the frequency is of the order of 1 kT for small values of $|1 - \bar{n}|$. This frequency is close to those observed in experiments on quantum oscillations. The origin of the strong

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variation of the frequency with electron filling lies in the difference in Landau subbands contributing to the DOS at the Fermi level. In the case of small doping these subbands are located at the periphery of the spectrum, while for larger values of $|1-\bar{n}|$ the subbands near the central part of the spectrum make the main contribution. The behavior of these two groups of subbands as a function of magnetic induction is different. The influence of the Zeeman term on the DOS oscillations is also considered.

2. Main formulas

The Hamiltonian of the Hubbard model [30,31] supplemented with magnetic field reads

$$H = \sum_{\mathbf{l}\mathbf{l}'\sigma} t_{\mathbf{l}\mathbf{l}'} \exp\left(i\frac{e}{\hbar}\int_{\mathbf{l}'}^{\mathbf{l}} \mathbf{A}(\mathbf{r})d\mathbf{r}\right) a^{\dagger}_{\mathbf{l}'\sigma} a_{\mathbf{l}\sigma} + \frac{1}{2} g\mu_B B \sum_{\mathbf{l}\sigma} \sigma a^{\dagger}_{\mathbf{l}\sigma} a_{\mathbf{l}\sigma} + \sum_{\mathbf{l}\sigma}\left(\frac{U}{2} n_{\mathbf{l}\sigma} n_{\mathbf{l},-\sigma} - \mu n_{\mathbf{l}\sigma}\right), \quad (1)$$

where 2D vectors $\mathbf{l}$ and $\mathbf{l}'$ label sites of a square plane lattice, $\sigma = \pm 1$ is the spin projection, $a^{\dagger}_{\mathbf{l}\sigma}$ and $a_{\mathbf{l}\sigma}$ are electron creation and annihilation operators. The first (kinetic) term of the Hamiltonian contains the hopping matrix element $t_{\mathbf{l}\mathbf{l}'}$ and the exponential factor with the Peierls phase [4], in which $\mathbf{A}(\mathbf{r})$ is the vector potential. The Peierls description is valid for moderate fields, until the magnetic length becomes comparable to the spatial extent of the Wannier function [5,4]. The second (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 the field is directed perpendicularly to the plane, homogeneous and only weakly disturbed by internal currents [32]. The last term of Hamiltonian (1) involves the on-site Coulomb repulsion U, the electron number operator $n_{\mathbf{l}\sigma} = a^{\dagger}_{\mathbf{l}\sigma} a_{\mathbf{l}\sigma}$ as well as the chemical potential μ.

In the following the Landau gauge is used, in which $\mathbf{A}(\mathbf{l}) = -Bl_y\mathbf{x}$, where l_y is the y component of the site vector $\mathbf{l}$ and $\mathbf{x}$ is the unit vector along the x axis. If we suppose that only the nearest neighbor hopping constant is nonzero, $t_{\mathbf{l}\mathbf{l}'} = t\sum_{\mathbf{a}} \delta_{\mathbf{l},\mathbf{l}'+\mathbf{a}}$ where $\mathbf{a}$ are four vectors connecting nearest neighbor sites, the Peierls exponential in the kinetic term of the Hamiltonian can be written as

$$e^{i\boldsymbol{\kappa}_{\mathbf{a}}\mathbf{l}}, \quad \boldsymbol{\kappa}_{\mathbf{a}} = \frac{e}{\hbar} B a_x \mathbf{y}, \quad (2)$$

where a_x is the x component of the vector $\mathbf{a}$ and $\mathbf{y}$ is the unit vector along the y axis.

We will restrict ourselves to fields satisfying the condition

$$\frac{e}{\hbar} B a^2 = 2\pi \frac{n'}{n}, \quad (3)$$

where $a = |\mathbf{a}|$, n and $n' < n$ are integers with no common factor. In this case the kinetic term of Hamiltonian (1) defines its translation properties – the Hamiltonian 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 $\left(\frac{2\pi n_x}{N_x a}, \frac{2\pi n_y}{nN_y a}\right)$ with integers n_x and n_y. As can be seen from (2) and (3), the momenta $\boldsymbol{\kappa}_{\mathbf{a}}$ belong to this set of allowed wave vectors.

Let us consider the electron Green's function

$$G^{\sigma}(\mathbf{l}'\tau', \mathbf{l}\tau) = \langle \mathcal{T} \bar{a}_{\mathbf{l}'\sigma}(\tau') a_{\mathbf{l}\sigma}(\tau)\rangle, \quad (4)$$

where the statistical averaging denoted by the angular brackets and time dependencies of the operators

$$a_{\mathbf{l}\sigma}(\tau) = e^{H\tau} a_{\mathbf{l}\sigma} e^{-H\tau} \quad \text{and} \quad \bar{a}_{\mathbf{l}\sigma}(\tau) = e^{H\tau} a^{\dagger}_{\mathbf{l}\sigma} e^{-H\tau}$$

are determined by Hamiltonian (1). $\mathcal{T}$ is the time-ordering operator which arranges operators from right to left in ascending order of times τ. Hamiltonian (1) conserves the spin projection and, therefore, the Green's function (4) is diagonal in spin. To calculate this function we use the strong coupling diagram technique [22–27], in which it is expressed as a series expansion with the unperturbed Hamiltonian H_0 given by the last term of Hamiltonian (1). The role of perturbation, over which the power expansion is carried out, is played by the first two terms of this Hamiltonian. For brevity, the sum of these two terms is denoted as

$$H_1 = \sum_{\mathbf{l}\mathbf{l}'\sigma} T^{\sigma}(\mathbf{l}\mathbf{l}') a^{\dagger}_{\mathbf{l}'\sigma} a_{\mathbf{l}\sigma}.$$

Terms of the series expansion are constructed from on-site cumulants of the electron operators $a_{\mathbf{l}\sigma}(\tau)$ and $\bar{a}_{\mathbf{l}\sigma}(\tau)$ and hopping lines corresponding to the Hamiltonian H_1 (though the Zeeman term in H_1 does not lead to the transfer of an electron to another site, we retain the term hopping line used in this diagram technique). The averaging and time dependencies of operators in the cumulants are determined by the Hamiltonian H_0. As in the weak-coupling perturbation theory, the linked-cluster theorem allows one to discard disconnected diagrams and to carry out partial summations of the remaining connected diagrams.

The diagram is said to be irreducible if it cannot be divided into two disconnected parts by cutting some hopping line. The sum of all irreducible diagrams without external ends is termed the irreducible part $K^{\sigma}(\mathbf{l}'\tau', \mathbf{l}\tau)$. In terms of this quantity the equation for the Green's function reads

$$G^{\sigma}(\mathbf{l}'\tau', \mathbf{l}\tau) = K^{\sigma}(\mathbf{l}'\tau', \mathbf{l}\tau) + \sum_{\mathbf{l}_1\mathbf{l}'_1} \int_0^{\beta} K^{\sigma}(\mathbf{l}'\tau', \mathbf{l}_1\tau_1) \times T^{\sigma}(\mathbf{l}_1\mathbf{l}'_1) G^{\sigma}(\mathbf{l}'_1\tau_1, \mathbf{l}\tau) d\tau_1, \quad (5)$$

or, after Fourier transformations over space and time variables,

$$G^{\sigma}(\mathbf{q}'\mathbf{q}m) = K^{\sigma}(\mathbf{q}'\mathbf{q}m) + \sum_{\mathbf{q}_1\mathbf{q}'_1} K^{\sigma}(\mathbf{q}'\mathbf{q}_1 m) \times T^{\sigma}(\mathbf{q}_1\mathbf{q}'_1) G^{\sigma}(\mathbf{q}'_1\mathbf{q}m), \quad (6)$$

where $\beta = 1/T$ is the inverse temperature, m is an integer determining the Matsubara frequency $\omega_m = (2m+1)\pi T$ and

$$T^{\sigma}(\mathbf{q}\mathbf{q}') = t\Big[e^{iq'_x a}\delta_{\mathbf{q},\mathbf{q}'+\boldsymbol{\kappa}n'} + e^{-iq'_x a}\delta_{\mathbf{q},\mathbf{q}'-\boldsymbol{\kappa}n'} + 2\cos(q'_y a)\delta_{\mathbf{q}\mathbf{q}'}\Big] + \frac{1}{2} g\mu_B B\sigma\delta_{\mathbf{q}\mathbf{q}'}, \quad (7)$$

q_x and q_y are components of the wave vector $\mathbf{q}$, which belong to the first Brillouin zone, and $\boldsymbol{\kappa} = \frac{2\pi}{na}\mathbf{y}$. In the derivation of (7) we took into account that $\boldsymbol{\kappa}_{\mathbf{a}}$ in (2) belongs to the set of momenta determined by the chosen periodic boundary conditions. Equations (5) and (6) are forms of the Larkin equation [33]. Analogous equations were used for calculating the electron Green's function of the Hubbard model in the absence of the magnetic field [22–27].

In (6), $G^{\sigma}(\mathbf{q}'\mathbf{q}m)$ and $K^{\sigma}(\mathbf{q}'\mathbf{q}m)$ are not diagonal with respect to momenta due to the reduced translation symmetry of the problem. However, from symmetry arguments one can see that these