MAGNETIC AND SUPERCONDUCTIVE STATES IN THE REPULSIVE HUBBARD MODEL

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Dedicated to L. D. Faddeev
on the occasion of his 60th birthday

It is shown that antiferromagnetic, ferromagnetic, and superconductive states are possible in the repulsive Hubbard model. The role of small denominators of the Green functions and the Van Hove saddle points in the phase transitions is discussed. It is shown that superconductivity is possible if and only if one of the Van Hove saddle points is situated near the Fermi level. The Cooper pairing arises in channels with odd angular momenta. (It is the p-pairing in the first approximation.) The optimal mutual position of the Van Hove saddle point and the Fermi level corresponding to the maximal critical temperature is found. The problem of the coexistence of superconductivity and ferromagnetism is discussed. Bibliography: 25 titles.

1. INTRODUCTION

High temperature superconductivity (HTSC) was discovered more than six years ago [1], but up to now we have no clear theoretical explanation for this phenomenon. At present, the Hubbard model is very popular as the most favorite candidate for a model of HTSC [2–4]. The Hamiltonian of the model looks as follows:

\[ \hat{H} - \mu \hat{N} = - \sum_{s, (ij)} t_{ij} a_{is}^{\dagger} a_{js} + U \sum_i \hat{n}_{i1} \hat{n}_{i1} - \mu \sum_{i,s} \hat{n}_{is}. \]  

(1)

Here \( a_{is}^{\dagger} \) and \( a_{js} \) are the creation and annihilation operators of fermions with spin \( s = \uparrow \) or \( \downarrow \) on the lattice site \( i \) and \( \hat{n}_{is} = a_{is}^{\dagger} a_{is} \). The first term in (1) describes the hopping of electrons, and \( t_{ij} \) is the hopping amplitude between sites \( i \) and \( j \). The second term in (1) is due to the repulsion between two electrons on the same site, and the third term contains the chemical potential \( \mu \), which plays the role of the Lagrange multiplier.

The Hamiltonian (1) is a finite-dimensional matrix for a finite lattice. Its dimension is \( 4^N \), where \( N \) is the number of lattice sites.

Some authors try to explain HTSC using the topologically nontrivial effective action containing the Chern–Simons terms [5–9].

We have investigated another possible approach, using the Cooper pairing with nonzero angular momenta [10–15]. Here we mainly discuss the two-dimensional (\( D = 2 \)) repulsive (\( U > 0 \)) Hubbard model with \( t_1 \neq t_2 \). It turns out that an effective attraction arises between electrons with momenta near the saddle points of the energy function \( \varepsilon(\vec{k}) \) of the electron in the momentum space if the Fermi surface \( \varepsilon(\vec{k}) = 0 \) is close to one of the saddle points (such a saddle point is a special case of the so-called Van Hove points where \( d\varepsilon(\vec{k}) = 0 \) [16]). Thus, the vicinities of the saddle Van Hove points play the main role in the mechanism of superconductivity. The Cooper pairing arises in channels with odd angular momenta, and such a pairing may be approximately considered as a \( p \)-pairing. Taking \( t_1 \neq t_2 \) we can separate the domain in the phase diagram where antiferromagnetism exists from the domain where superconductivity is more preferable.

It should be mentioned that the simplest Hubbard model with Hamiltonian (1) can be regarded only as a toy model of HTSC. More realistic is the so-called three-band model (the Emery model) describing the hopping of electrons between copper and oxygen atoms.

This model has also been investigated by C. Malyshev and myself [13] within the framework of the temperature Green method, which is applied to the simplest Hubbard Hamiltonian (1) in this paper.

The paper is organized as follows. In Sec. 2 the formalism of the temperature Green functions is constructed for the Hubbard model. In Sec. 3 we discuss the role of small denominators and the Van Hove saddle points in the phase transitions. In Sec. 4–6 antiferromagnetic, superconductive, and ferromagnetic states in the repulsive Hubbard model are described within the framework of the Green functions. Section 7 is devoted to the problem of the coexistence of ferromagnetism and superconductivity.

2. TEMPERATURE GREEN FUNCTION METHOD

This method [17] can be explained in the shortest way by using the functional integration formalism [18]. We define the temperature Green function

$$G_s(p) = -\langle a_s(p) a^*_s(p) \rangle = -\frac{\int a_s(p) a^*(p) e^S D\mu}{\int e^S D\mu}$$

as a (formal) ratio of two functional integrals, where

$$S = \int_0^\beta d\tau \sum_{i,s} \frac{\partial a^*_i(\tau)}{\partial \tau} a_i(\tau) - \int_0^\beta d\tau (H(\tau) - \mu N(\tau))$$

is the action functional corresponding to the Hubbard Hamiltonian (1). Here $\tau \in [0, \beta]$, $\beta = T^{-1}$ is the inverse temperature, and $H(\tau) - \mu N(\tau)$ can be obtained from (1) by changing $a_i \rightarrow a_i(\tau), a^*_i \rightarrow a^*_i(\tau)$. The anticommuting functions $a_i(\tau), a^*_i(\tau)$ can be written as the Fourier series

$$a_i(\tau) = (\beta N)^{-1/2} \sum_p e^{i(\vec{k}) - \omega \tau} a_s(p), \quad a^*_i(\tau) = (\beta N)^{-1/2} \sum_p e^{-i((\vec{k}) - \omega \tau)} a^*_s(p).$$

Here $p = (\omega, \vec{k})$ has the meaning of the four-momentum, $\omega = \pi T(2n + 1)$ is the Matsubara frequency, and $|k_i| \leq \pi$, $i = 1, \ldots, D$. The Fourier coefficients $a_s(p), a^*_s(p)$ can be considered as anticommuting generators of the Grassmann algebra, and on the right-hand side of Eq. (2) we have the ratio of two integrals (Berezin integrals) with the measure

$$D\mu = \prod_{p,s} da^*_s(p) da_s(p).$$

Substituting the Fourier series (4) in (3), we can express the action $S$ via the generators $a_s(p), a^*_s(p)$,

$$S = \sum_{p,s} (i\omega - \varepsilon_0(\vec{k}) + \mu)a_s(p)a^*_s(p) - \frac{4}{\beta N} \sum_{p_1+p_2=p_3+p_4} a^*_1(p_1)a^*_2(p_2)a_4(p_3)a_1(p_4).$$

Here

$$\varepsilon_0(\vec{k}) = -2 \sum_{i=1}^D t_i \cos k_i$$

is the “bare” electron energy in the momentum space if we take into account only the hoppings of electrons between the nearest neighbors.

In what follows we use the perturbation theory which can be constructed if we take the quadratic form in $a_s(p), a^*_s(p)$ in (6) as a “bare” (unperturbed) action and the quartic term in (6) as a perturbation. Such a perturbation theory can be formulated in terms of diagrams with elements of the form

$$G_0(p) = (i\omega - \varepsilon_0(\vec{k}) + \mu)^{-1}$$