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Stationary property of the thermodynamic potential of the Hubbard model in strong coupling diagrammatic approach for superconducting state

V.A. Moskalenko[1,2], L.A. Dohotaru[3], D.F. Digor[1], and I.D. Cebotari[1]

[1]Institute of Applied Physics, Moldova Academy of Sciences, Chisinau 2028, Moldova
[2]The Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna 141980, Russia
[3]Technical University, Chisinau 2004, Moldova
E-mail: moskalen@thsun1.jinr.ru

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Diagrammatic analysis for normal state of Hubbard model proposed in our previous paper is generalized and used to investigate superconducting state of this model. We use the notion of charge quantum number to describe the irreducible Green's function of the superconducting state. As in the previous paper we introduce the notion of tunneling Green's function and of its mass operator. This last quantity turns out to be equal to correlation function of the system. We proved the existence of exact relation between renormalized one-particle propagator and thermodynamic potential which includes integration over auxiliary interaction constant. The notion of skeleton diagrams of propagator and vacuum kinds were introduced. These diagrams are constructed from irreducible Green's functions and tunneling lines. Identity of this functional to the thermodynamic potential has been proved and the stationarity with respect to variation of the mass operator has been demonstrated.

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1. Introduction

The present paper generalizes our previous work [1] on diagrammatic analysis of the normal state of the Hubbard model [2–4] to the superconducting state.

Now we shall assume the existence of pairing of charge carriers and non-zero Bogolyubov quasi-averages [5] and, consequently, of the Gor'kov anomalous Green's functions [6].

The central idea of standard BCS theory of conventional superconductivity is formation of Cooper pairs due to the presence of attractive interaction between electrons. Such attractive interaction can be of electron–phonon kind with mechanism based on the polarizability of ionic lattice in metal. After the discovery in 1986 of high-temperature superconductivity in cuprate compounds with layered perovskite structure begins the era of unconventional superconductivity with possible alternative mechanisms of superconductivity. One of such possible mechanism is spin fluctuation exchange [7] one based on the conception of spin polarization of electrons.

One of the most frequently used model for unconventional superconductivity is the Hubbard model. We shall discuss below its properties.

The main property of the Hubbard model consists in the existence of strong electron correlations and, as a result, of the new diagrammatic elements with the structure of Kubo cumulants and named by us as irreducible Green's functions. These functions describe the main charge, spin and pairing fluctuations of the system.

The new diagram technique for such strongly correlated systems has been developed in our earlier papers [8–18]. This diagram technique uses the algebra of Fermi operators and relies on the generalized Wick theorem which contains, apart from usual Feynman contributions, additional irreducible structures. These structures are the main elements of the diagrams.

In superconducting state, unlike the normal one, the irreducible Green's functions can contain any even number of fermion creation and annihilation operators, whereas in normal state the number of both kinds is equal. Therefore we need an automatic mathematical mechanism which takes into account all the possibilities to consider the interference of the particles and holes in the superconducting state.

With this purpose we use the notion of charge quantum number, introduced by us in [8] and called α-number, which has two values $\alpha = \pm 1$ according to the definition

$$C^{\alpha} = \begin{cases} C, & \alpha = 1; \\ C^{+}, & \alpha = -1, \end{cases} \quad (1)$$

were C is a fermion annihilation operator. In this new representation the tunneling part of the Hubbard Hamiltonian can be rewritten in the form

$$\begin{aligned} H' &= \sum_{\sigma}\sum_{\mathbf{xx}'} t(\mathbf{x}'-\mathbf{x}) C^{+}_{\mathbf{x}'\sigma} C_{\mathbf{x}\sigma} = \\ &= \frac{1}{2}\sum_{\alpha=-1,1}\sum_{\sigma}\sum_{\mathbf{xx}'} \alpha t_{\alpha}(\mathbf{x}'-\mathbf{x}) C^{-\alpha}_{\mathbf{x}'\sigma} C^{\alpha}_{\mathbf{x}\sigma}, \end{aligned} \quad (2)$$

with the definition of the tunneling matrix elements

$$\begin{aligned} &t_1(\mathbf{x}'-\mathbf{x}) = t(\mathbf{x}'-\mathbf{x}), \\ &t_{-1}(\mathbf{x}'-\mathbf{x}) = t(\mathbf{x}-\mathbf{x}'), \\ &t(\mathbf{x}=0) = 0. \end{aligned} \quad (3)$$

In this charge quantum number representation the operator H' has an additional multiple α for every vertex of the diagrams and additional summation over α. All the Green's functions depend of this number.

In interaction representation operator H' has a form

$$H'(\tau) = \frac{1}{2}\sum_{\alpha\sigma}\sum_{\mathbf{xx}'} \alpha t_{\alpha}(\mathbf{x}'-\mathbf{x}) C^{-\alpha}_{\mathbf{x}'\sigma}(\tau + \alpha 0^{+}) C^{\alpha}_{\mathbf{x}\sigma}(\tau). \quad (4)$$

The main part of the Hubbard Hamiltonian

$$\begin{aligned} &H = H^0 + H', \quad H^0 = \sum_i H_i^0, \\ &H_i^0 = -\mu\sum_{\sigma} C^{+}_{i\sigma} C_{i\sigma} + U n_{i\uparrow} n_{i\downarrow} \end{aligned} \quad (5)$$

contains the local part H^0, where μ is the chemical potential and U is the Coulomb repulsion of the electrons. This interaction is considered as a main parameter of the model and is taken into account in zero approximation of our theory. The operator H' describes electron hopping between lattice sites of the crystal and is considered as a perturbation.

We shall use the grand canonical partition function in our thermodynamic perturbation theory.

The paper is organized in the following way. In Sec. 2 we define the one-particle Matsubara Green's functions in terms of α representation and develop the diagrammatic theory in the strong coupling limit.

In Sec. 3 we establish relation between the full thermodynamic potential and the renormalized one-particle Green's function in the presence of additional integration over auxiliary constant of interaction λ and prove the stationarity theorem both for a special functional consisting of skeleton diagrams and for a renormalized thermodynamic potential shown to be its equivalent.

2. Diagrammatic theory

We shall use the following definition of the Matsubara Green's functions in the interaction representation

$$G^{\alpha\alpha'}(x \mid x') = -\left\langle T C^{\alpha}_{\mathbf{x}\sigma}(\tau) C^{-\alpha'}_{\mathbf{x}'\sigma'}(\tau') U(\beta)\right\rangle_0^c, \quad (6)$$

where x stands for $(\mathbf{x}, \sigma, \tau)$, index c of $\langle ... \rangle_0^c$ means the connected part of the diagrams and $\langle ... \rangle_0$ means thermal average with zero-order partition function

$$\mathrm{e}^{-\beta H^0} / \operatorname{Tr} \mathrm{e}^{-\beta H^0}.$$

We use the series expansion for the evolution operator $U(\beta)$ with some generalization because we introduce the auxiliary constant of interaction λ and use $\lambda H'$ instead H':

$$U_{\lambda}(\beta) = T \exp\left(-\lambda \int_0^{\beta} H'(\tau) d\tau\right), \quad (7)$$

with T as the chronological operator. At the last stage of calculation this constant λ will be put equal to 1.

The correspondence between definition (6) and usual one [13] is the following:

$$\begin{aligned} &G_{\lambda}^{1,1}(x \mid x') = -\left\langle T C_{\mathbf{x}\sigma}(\tau) \bar{C}_{\mathbf{x}'\sigma'}(\tau') U_{\lambda}(\beta)\right\rangle_0^c = \\ &= G^{\lambda}_{\sigma,\sigma'}(\mathbf{x}, \tau \mid \mathbf{x}', \tau'), \\ &G_{\lambda}^{1,-1}(x \mid x') = -\left\langle T C_{\mathbf{x}\sigma}(\tau) C_{\mathbf{x}'\sigma'}(\tau') U_{\lambda}(\beta)\right\rangle_0^c = \\ &= F^{\lambda}_{\sigma,\bar{\sigma}'}(\mathbf{x}, \tau \mid \mathbf{x}', \tau'), \\ &G_{\lambda}^{-1,1}(x \mid x') = -\left\langle T \bar{C}_{\mathbf{x}\sigma}(\tau) \bar{C}_{\mathbf{x}'\sigma'}(\tau') U_{\lambda}(\beta)\right\rangle_0^c = \\ &= \bar{F}^{\lambda}_{\bar{\sigma},\sigma'}(\mathbf{x}, \tau \mid \mathbf{x}', \tau'), \\ &G_{\lambda}^{-1,-1}(x \mid x') = -G_{\lambda}^{1,1}(x' \mid x). \end{aligned} \quad (8)$$

As a result of application of the generalized Wick theorem we obtain for propagator (6) the diagrammatic contributions depicted on the Fig. 1.

In superconducting state, unlike the normal state, the propagator lines do not contain arrows which determine the processes of creation and annihilation of electrons because indices α can take two values $\alpha = \pm 1$ and every vertex of the diagram describes different possibilities.

In Fig. 1 the diagram (a) is the zero order propagator, the diagram (b) and more complicated diagrams of such kind are of chain type. They correspond to the contribution of the ordinary Wick theorem and give the Hubbard I approximation. The contributions of the diagrams (c) and (d) of Fig. 1 are