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A field-theoretical approach to the extended Hubbard model

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ABSTRACT

We transform the quartic Hubbard terms in the extended Hubbard model to a quadratic form by making the Hubbard–Stratonovich transformation for the electron operators. This transformation allows us to derive exact results for mass operator and charge–charge and spin–spin correlation functions for *s*-wave superconductivity. We discuss the application of the method to the *d*-wave superconductivity.

1. Introduction

The Hubbard model predicts phase instabilities which give rise to a divergence of the charge and spin correlation functions, and therefore, it has been the focus of particular interest as a model for high-temperature superconductivity. The Hamiltonian of the standard Hubbard model contains only two terms representing the hopping of electrons between sites of the lattice and their on-site interaction. If the interaction between electrons on different sites of the lattice is included, the model is referred as the extended Hubbard model.

In what follows we study the following Hamiltonian:

$$H = -\sum_{ij,\sigma} \psi^{\dagger}_{i,\sigma}\psi_{j,\sigma} - \mu \sum_{i,\sigma} \hat{n}_{i,\sigma} + U \sum_{i} \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} - V \sum_{\langle i,j\rangle \sigma\sigma'} \hat{n}_{i,\sigma}\hat{n}_{j,\sigma'}, \qquad (1)$$

where μ is the chemical potential. The Fermi operator $\psi^{\dagger}_{i,\sigma}$ $(\psi_{i,\sigma})$ creates (destroys) a fermion on the lattice site i with spin projection $\sigma = \uparrow, \downarrow$ along a specified direction, and $\hat{n}_{i,\sigma} = \psi^{\dagger}_{i,\sigma}\psi_{i,\sigma}$ is the density operator on-site i. The symbol $\sum_{\langle ij\rangle}$ means sum over nearest-neighbor sites. The first term in (1) is the usual kinetic energy term in a tight-binding approximation, where t_{ij} is the single-electron hopping integral. Depending on the sign of U, the third term describes the on-site repulsive or attractive interaction between electrons with opposite spins. We assume that $V > 0$, so the last term is expect to stabilize the pairing by bringing in a nearest-neighbor attractive interaction. The lattice spacing is assumed to be $a = 1$ and the total number of sites is N.

The simplest method to study the possibility for the extended Hubbard model to show a superconducting instability is to apply mean-field analysis of pairing followed by general random phase approximation (GRPA) [1,2]. Going beyond the GRPA requires reliable approximation schemes to handle self-consistent relations between single- and two-particle quantities: the mass operator Σ depends on the two-particle Green function K, and the kernel of the Bethe–Salpeter (BS) equation $\delta\Sigma/\delta G$ for the spectrum of the collective excitations itself does depend on the mass operator. A possible approximation to this problem is the so-called two-particle self-consistent (TPSC) approach [3–15]. The TPSC approach is a method for closing the set of equations for single-particle mass operator and the two-body density matrix operator. The later can be factorized by introducing the so-called equal-time pair-correlation function $g_{\sigma\sigma'}(i,j)$ [12,13] which itself depends on the density–density correlation function. In other words, the TPSC approach goes beyond the GRPA for single-particle mass operator by establishing a self-consistency relation between single-particle and two-particle quantities. By setting $g_{\sigma\sigma'}(i,j) = 1$ one should recover the GRPA results for the mass operator and charge and spin correlation functions.

In what follows, we first obtain exact formulas for the electron self-energy (electron mass operator), the charge and spin correlation functions. We also briefly discuss how our approach could be generalized in order to include *d*-wave instabilities of the types examined in Refs. [16–20].

2. Field-theoretical approach to extended Hubbard model

The interaction part of the Hamiltonian (1) is quartic in the Grassmann fermion fields so the functional integrals cannot be

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evaluated exactly. However, it is convenient to transform the quartic Hubbard terms in (1) to a quadratic form by making the Hubbard–Stratonovich transformation for the electron operators:

$$\int \mu[A]\exp\left[\hat{\bar{\psi}}(y)\widehat{\Gamma}^{(0)}_{\alpha}(y;x|z)\hat{\psi}(x)A_{\alpha}(z)\right] = \exp\left\{-\frac{1}{2}\hat{\bar{\psi}}(y)\widehat{\Gamma}^{(0)}_{\alpha}(y;x|z)\hat{\psi}(x)D^{(0)}_{\alpha,\beta}(z,z')\hat{\bar{\psi}}(y')\widehat{\Gamma}^{(0)}_{\beta}(y';x'|z')\hat{\psi}(x')\right\}. \tag{2}$$

The symbol "hat" over any quantity O means that this quantity is a matrix. The functional measure $D\mu[A]$ is chosen to be:

$$\mu[A] = DAe^{\frac{1}{2}A_{\alpha}(z)D^{(0)-1}_{\alpha,\beta}(z,z')A_{\beta}(z')}, \quad \int \mu[A] = 1.$$

The Hubbard–Stratonovich transformation converts the quartic problem of interacting electrons to the more tractable quadratic problem of non-interacting Nambu fermion fields

$$\hat{\bar{\psi}}(y) = \left(\psi^{\dagger}_{\uparrow}(y)\psi_{\downarrow}(y)\right), \quad \hat{\psi}(x) = \begin{pmatrix}\psi_{\uparrow}(x)\\ \psi^{\dagger}_{\downarrow}(x)\end{pmatrix} \tag{3}$$

coupled to a Bose field $A_{\alpha}(z)$ where $\alpha = \uparrow, \downarrow$ is the spin degree of freedom which reflects the spin-dependent nature of the Hubbard interaction. The bare boson propagator in (2) provides an instantaneous spin-dependent interaction, and in accordance with the Hamiltonian (1), it should have the following form:

$$\begin{aligned} D^{(0)}_{\alpha\beta}(z,z') &= D^{(0)}_{\alpha\beta}(j,j';\nu-\nu') = \delta(\nu-\nu')\\ &\quad\left[U\delta_{jj'}\delta_{\alpha\bar{\beta}} - 2V_{\langle jj'\rangle}\left(\delta_{\bar{\alpha},\beta}+\delta_{\alpha\beta}\right)\right]\\ &= \frac{1}{N}\sum_{\mathbf{k}}\sum_{\omega_p} e^{\left\{\imath[\mathbf{k}.(\mathbf{r}_j-\mathbf{r}_{j'})-\omega_p(\nu-\nu')]\right\}}D^{(0)}_{\alpha\beta}(\mathbf{k};\imath\omega_p),\\ D^{(0)}_{\alpha\beta}(\mathbf{k};\imath\omega_p) &= U\delta_{\bar{\alpha},\beta} - V(\mathbf{k})(\delta_{\bar{\alpha},\beta}+\delta_{\alpha,\beta}). \end{aligned}$$

Here $\bar{\alpha}$ is complimentary of α, and $V(\mathbf{k}) = 4V\ (\cos k_x + \cos k_y)$ is the nearest-neighbor interaction in momentum space. The symbol $V_{\langle jj'\rangle}$ is equal to V if j and j' sites are nearest neighbors, and zero otherwise. We have used composite variables $y = \{\mathbf{r}_i, u\} = \{i, u\}$, $x = \{\mathbf{r}_{i'}, u'\} = \{i', u'\}$, $z = \{\mathbf{r}_j, \nu\} = \{j, \nu\}$ and $z' = \{\mathbf{r}_{j'}, \nu'\} = \{j', \nu'\}$, where $\mathbf{r}_i$, $\mathbf{r}_{i'}$, $\mathbf{r}_j$ and $\mathbf{r}_{j'}$ are the lattice site vectors. The symbol $\sum_{\omega_p}$ is used to denote $\beta^{-1}\sum_p$. For boson fields we have $\omega_p = (2\pi/\beta)p$; $p = 0, \pm1, \pm2, \ldots$.

After performing the Hubbard–Stratonovich transformation, the action of the system becomes

$$S = S^{(e)}_0 + S^{(A)}_0 + S^{(e-A)}, \tag{4}$$

where

$$S^{(e)}_0 = \hat{\bar{\psi}}(y)\widehat{G}^{(0)-1}(y;x)\hat{\psi}(x), \tag{5}$$

$$S^{(A)}_0 = \frac{1}{2}A_{\alpha}(z)D^{(0)-1}_{\alpha\beta}(z,z')A_{\beta}(z'), \tag{6}$$

$$S^{(e-A)} = \hat{\bar{\psi}}(y)\widehat{\Gamma}^{(0)}_{\alpha}(y,x|z)\hat{\psi}(x)A_{\alpha}(z). \tag{7}$$

The inverse Green function of free electrons $\widehat{G}^{(0)-1}(y;x)$ is diagonal with respect to the spin indices and has its usual form:

$$\begin{aligned} \widehat{G}^{(0)-1}(y;x) &= \begin{pmatrix} G^{(0)-1}(\uparrow,y;\uparrow,x) & 0\\ 0 & -G^{(0)-1}(\downarrow,y;\downarrow,x)\end{pmatrix}\\ &= \frac{1}{N}\sum_{\mathbf{k}}\sum_{\omega_m}\exp\{\imath\mathbf{k}.(\mathbf{r}_i-\mathbf{r}_{i'}-\omega_m(u-u')\}\\ &\quad\times\begin{pmatrix} G^{(0)-1}_{\uparrow,\uparrow}(\mathbf{k},\imath\omega_m) & 0\\ 0 & -G^{(0)-1}_{\downarrow,\downarrow}(\mathbf{k},\imath\omega_m)\end{pmatrix}, \end{aligned} \tag{8}$$

where $G^{(0)-1}_{\uparrow,\uparrow}(\mathbf{k},\imath\omega_m) = [\imath\omega_m - (\epsilon(\mathbf{k})-\mu)]^{-1}$, and $G^{(0)-1}_{\downarrow,\downarrow}(\mathbf{k},\imath\omega_m) = [\imath\omega_m + (\epsilon(\mathbf{k})-\mu)]^{-1}$. Here $\epsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y) - 4t'\cos k_x \cos k_y$ is the non-interacting dispersion on a square lattice, μ is the electron chemical potential, and the symbol $\sum_{\omega_m}$ is used to denote $\beta^{-1}\sum_m$. For fermion fields we have $\omega_m = (2\pi/\beta)(m+1/2)$; $m = 0, 1, 2, \ldots$.

The bare vertex $\widehat{\Gamma}^{(0)}_{\alpha}(y;x|z)$ is a 2×2 matrix defined as follows:

$$\begin{aligned} \widehat{\Gamma}^{(0)}_{\alpha}(y;x|z) &= \begin{pmatrix}\Gamma^{(0)}_{\alpha}(\uparrow,y;\uparrow x|z) & 0\\ 0 & -\Gamma^{(0)}_{\alpha}(\downarrow,y;\downarrow,x|z)\end{pmatrix},\\ \Gamma^{(0)}_{\alpha}(\sigma,y;\sigma,x|z) &= \Gamma^{(0)}_{\alpha}(\sigma,i,u;\sigma,i',u'|i'',\nu)\\ &= \delta(u-\nu)\delta(u-u')\delta_{\sigma,\alpha}\delta_{i,i'}\delta_{i,i''}. \end{aligned} \tag{9}$$

Since the electrons polarize the boson field, and the boson field acts onto the electrons, our approach describes the correlated motion of the electrons and the surrounding polarization field.

In field theory the expectation value of a general operator $\widehat{O}(u)$ is expressed as a functional integral over the boson field A and the Grassmann fermion fields $\hat{\bar{\psi}}$ and $\hat{\psi}$

$$\begin{aligned} \langle\widehat{T}_u(\widehat{O}(u))\rangle &= \frac{1}{Z[J,M]}\int D\mu[\hat{\bar{\psi}},\hat{\psi},A]\widehat{O}(u)\times\exp[J_{\alpha}(z)A_{\alpha}(z)\\ &\quad-\hat{\bar{\psi}}(y)\widehat{M}(y;x)\hat{\psi}(x)]|_{J=M=0}, \end{aligned} \tag{10}$$

where the symbol $\langle\ldots\rangle$ means that the thermodynamic average is made, and $\widehat{T}_u$ is an u-ordering operator. J, M are the sources of the boson and fermion fields, respectively. The functional $Z[J,M]$ is defined by

$$Z[J,M] = \int D\mu[\hat{\bar{\psi}},\hat{\psi},A]e^{[J_{\alpha}(z)A_{\alpha}(z)-\widehat{\bar{\psi}}(y)\widehat{M}(y;x)\hat{\psi}(x)]}, \tag{11}$$

where the functional measure $D\mu[\hat{\bar{\psi}},\hat{\psi},A] = DAD\hat{\bar{\psi}}D\hat{\psi}\exp(S)$ satisfies the condition $\int D\mu[\hat{\bar{\psi}},\hat{\psi},A] = 1$.

It is convenient to introduce complex indices $1 = \{\sigma_1, x_1\}$, $2 = \{\sigma_2, y_2\}, \ldots$, where, $\sigma_{1,2} = \{\uparrow,\downarrow\}$ and $x_1 = \{\mathbf{r}_{i_1}, u_1\}$, and $y_2 = \{\mathbf{r}_{i_2}, u_2\}$. We define a functional derivative $\delta/\delta M(1;2)$, and depending on the spin degrees of freedom σ_1 and σ_2, there are four possible derivatives:

$$\frac{\delta}{\delta M(\uparrow,y_2;\uparrow,x_1)}, \quad \frac{\delta}{\delta M(\uparrow,y_2;\downarrow,x_1)},$$
$$\frac{\delta}{\delta M(\downarrow,y_2;\uparrow,x_1)}, \quad \frac{\delta}{\delta M(\downarrow,y_2;\downarrow,x_1)}.$$

The reason to write the expectation value (10) as a functional integral is that all Green functions related to system under consideration can be expressed in terms of the functional derivatives of the generating functional of the connected Green functions $W[J,M] = \ln Z[J,M]$. By means of the functional $W[J,M]$, we define the following Green and vertex functions of the extended Hubbard model.

Boson Green function:

$$D_{\alpha\beta}(z,z') = -\frac{\delta^2 W}{\delta J_{\alpha}(z)\delta J_{\beta}(z')}. \tag{12}$$

The single-electron Green function $G(1;2) = -\delta W/\delta M(2;1)$ in the Hubbard model assumes the form: