Solid State Communications 258 (2017) 21–24

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Communication

Ladder approximation for the AC conductivity in the generalized two-dimensional Hubbard model

L.S. Lima

Departamento de Física e Matemática, Centro Federal de Educação Tecnológica de Minas Gerais, 30510-000 Belo Horizonte, MG, Brazil

A B S T R A C T

We calculate the optical conductivity of the generalized two-dimensional Hubbard model including vertex corrections, by using a ladder approximation in the diagrammatic expansion. We have obtained a superconductor behavior for this system at low temperature. Employing the ladder approach, we have included the influence of the electron-electron interaction on a previous result obtained in the mean field approximation. We have obtained the behavior of the optical conductivity, employing the ladder approximation, tending to zero in the DC limit. Since this approximation is better than the mean field approximation (it include information about the electron-electron interaction) then we have a better description to the behavior of the AC optical conductivity for the two-dimensional Hubbard model.

1. Introduction

Is well known that the conductivity of the two-dimensional Hubbard model is particularly relevant for high-temperature superconductors. Into this framework, vertex corrections are expected to be important because of strongly momentum-dependent self-energies [1]. Moreover, the superconductivity in hole-doped high-temperature superconductors is studied with emphasis on the connections among the Luttinger theorem, topological quantum field theories and critical theories involving change in the size of the Fermi surface [2]. The pseudogap phase have been described as a Higgs phase in a SU(2) gauge theory, where the Higgs field represents the local antiferromagnetism. Usually the superconductivity has been studied employing besides of the two-dimensional Hubbard model, the projected version of it, the t-J model [3–7]. However, recently, the utility of such modeling for high-temperature superconductors is highly questionable. In such system the gap is *d*-wave, i.e. there are regions in momentum space where the gap is zero. This has a strongly impact on the shape of the optical conductivity. On the other hand the superconductivity at high-temperature can be studied also using disordered spin systems modeled by the spin-1/2 two-dimensional Heisenberg antiferromagnet (AF) [8,9]. In general, is well known that the fact the electric conductivity tending to infinity, is not taken as the true definition of superconductivity. A material is superconducting if it presents the Meissner-Ochsenfeld effect. This effect is the fact that metals in the superconductor state are perfect diamagnets and hence expels a weak external magnetic field.

Is well known still that the type-II superconductivity cannot be explained using the standard BCS theory because this theory is valid only when the coupling constant between the par of electrons is small [2,10,11]. However, the Ginzburg-Landau theory was derived from the BCS theory by Gorkov long time ago. In materials such as ^{3}He there are two types of superfluidity depending on its pressure and its temperature. In a superconductor, electrons (fermions) form Cooper pairs in order to form bosons, which enables Bose-Einstein condensation. In ^{3}He, there is a similar situation: the ^{3}He atoms (which are fermions) pair up and form bosons too. However, in that case, they are not atoms vibrations that are responsible for the formation of pairs, but rather the fact that the atom magnetization become parallel to one another. The total magnetization of a pair of ^{3}He atoms taking part in superfluidity is in that case not equal to zero, contrary to the magnetization of a Cooper pair in the BCS theory.

One of the most important challenges in the study of high temperature superconductivity is to understand the relation between antiferromagnetism 2D with the superconductivity. There are many different families which include the iron-pnictides, electron-doped cuprates and heavy-fermion superconductors that are in close connection with the AFM phase [10]. Recently, there are a large number of measurements reported in iron-pnictide family as a function of the concentration of holes x [12,13].

The plan of this paper is the following. In Section 2 we describe the model, in Section 3 we describe the techniques to calculate the transport coefficients. In Section 4, we present our conclusions and final remarks.

2. The model

In this paper, we calculate the conductivity considering the influence of the electron-electron interaction on the superconductivity

E-mail addresses: lslima7@yahoo.com.br, lslima@des.cefetm.br.

http://dx.doi.org/10.1016/j.ssc.2017.04.012
Received 1 March 2017; Received in revised form 5 April 2017; Accepted 17 April 2017
Available online 18 April 2017

of the generalized two-dimensional Hubbard model. The model is given by the following Hamiltonian [14].

$$\mathcal{H} = -2t\sum_{\langle i,j\rangle}(c_i^\dagger c_j + h.\,c.\,) + U\sum_i n_{i\uparrow}n_{j\downarrow}, \tag{1}$$

where $\langle i, j\rangle$ stands for the sum over nearest-neighbors. Such model can be written in the form

$$\mathcal{H} = -2t\sum_{\langle i,j\rangle}(c_i^\dagger c_j + h.\,c.\,) - \frac{2U}{3}\sum_i(\vec{S_i})^2 + \frac{N_e U}{2}. \tag{2}$$

where $\vec{S_i} = \frac{\hbar}{2}c_\alpha^\dagger\sigma_{\alpha\alpha'}c_{\alpha'}$ with $\alpha = x, y, z$ and $\sigma_{\alpha\alpha'}$ are the three Pauli matrices. Therefore

$$\sum_i(\vec{S_i})^2 = \sum_i S_i^\alpha S_i^{\alpha'}. \tag{3}$$

By expanding the components and making use of the SU(2) identity

$$\sum_{\alpha=1,2,3}\sigma_{\beta\delta}^\alpha\sigma_{\mu\nu}^\alpha = 2\delta_{\beta\nu}\delta_{\delta\mu} - \delta_{\beta\delta}\delta_{\mu\nu} \tag{4}$$

one gets

$$\sum_i(\vec{S_i})^2 = \sum_i\left(\frac{3}{4}n_i - \frac{3}{2}n_{i\uparrow}n_{j\downarrow}\right) \tag{5}$$

Thus, we can write

$$\mathcal{H}_1 = U\sum_i n_{i\uparrow}n_{j\downarrow} = -\frac{2U}{3}(\vec{S_i})^2 + \frac{N_e U}{2}. \tag{6}$$

The last term is an additive constant. Thus, we have the model Eq. (1) is reduced to the model

$$\mathcal{H} = -2t\sum_{i,j,\alpha=\uparrow,\downarrow}(c_{i\alpha}^\dagger c_{j\alpha} + h.\,c.\,) + D\sum_i(\vec{S_i})^2. \tag{7}$$

We have calculated the vertex corrections for the conductivity in this model, where $D = -\frac{2U}{3}.\vec{S}(\vec{r})$ is the total spin of the band in $\vec{r}$. The system is SU(2) invariant on the spin rotations. For large values of U, i.e. $U/t \to \infty$, the local spin becomes as large as possible.

The single-particle fermionic spectrum is given as

$$\mathcal{H} = \sum_{\alpha=\uparrow,\downarrow}\int\frac{d^2k}{(2\pi)^2}\zeta_k c_{k\alpha}^\dagger c_{k\alpha}, \tag{8}$$

and thus the dispersion relation of the free Hamiltonian is

$$\zeta_k = \sqrt{\varepsilon_k^2 + \Delta^2}\,, \tag{9}$$

where Δ is the energy gap given as $\Delta = \sqrt{U/3}\,|\phi|$ and ε_k is the dispersion relation of free fermion

$$\varepsilon_k = -2t(\cos k_1 + \cos k_2). \tag{10}$$

From the solution of the analog BCS gap equation [15], we turn out that a number of different possible states can occur. The most important ones are the Anderson-Brinkman-Morrel state (ABM) and the Balain-Werthamer state (BW). The BW state has a gap, which has a constant magnitude over all the Fermi surface, rather like a BCS superconductor, while the ABM state has a gap which vanishes at the two points on the Fermi surface, $\vec{k} = (0, 0, \pm k_f)$. This difference leads to different physical properties. The ABM state is identified with ^{3}He-A-phase, while the BW state corresponds to the ^{3}He-B-phase. The B-phase is generally the more stable one, except in the high pressure region near to T_c [15].

3. Calculus of the transport coefficients

3.1. Kubo formalism of transport

The current operator for the two-dimensional Hubbard model is given by [14].

$$\mathcal{J}_i(\vec{n}, t) = -it\sum_{\alpha=\uparrow,\downarrow}(c_\alpha^\dagger(\vec{n}, t)c_\alpha(\vec{n} + \vec{x_i}, t) - h.\,c.) \tag{11}$$

where $c_n^\dagger$, (c_n) is a creation (annihilation) electron operator. We use the fermion model of two-dimensional Hubbard model [14] to determine the regular part of the spin conductivity (AC conductivity) or continuum conductivity and for the DC conductivity. The Superconductivity is the ability of fermions to form a persistent or non-dissipative current without an external field [13]. This does not happens in conventional metals where an electric current appears as response of the system to electric field, given by Ohm law, $\vec{\mathcal{J}} = \sigma\vec{E}$. Where $\vec{E}$ is an external electric field and σ is the electric conductivity. The linearly growing of the optical conductivity for large ω cannot satisfy in any way the f-sum rule [1], since the method used is accurate in the range of low ω.

In the Kubo formalism [16–20] the optical conductivity is given by the real part of the conductivity $\sigma(\omega)$, $\sigma'(\omega)$, being written in a standard form as [20].

$$\sigma'(\omega) = D_S\delta(\omega) + \sigma^{reg}(\omega), \tag{12}$$

where the Dirac delta term represents the DC contribution, where D_S is the Drude's weight

$$D_S = \pi[\langle\mathcal{K}\rangle + \Lambda'(\vec{k} = 0, \omega \to \vec{0})], \tag{13}$$

where it is given by two terms. The first term is given by the kinetic energy of the particles and the second term from $\Lambda'(k = 0, \omega \to 0)$ that is the real part of the current-current correlation function defined as

$$\Lambda(\vec{q}, \omega) = \frac{i}{\hbar N}\int_0^\infty dt e^{i\omega t}\langle[\mathcal{J}(\vec{q}, t), \mathcal{J}(-\vec{q}, 0)]\rangle. \tag{14}$$

$\sigma^{reg}(\omega)$, the regular part of $\sigma'(\omega)$, is given by [19].

$$\sigma^{reg}(\omega) = \frac{\Lambda''(\vec{q} = 0, \omega)}{\omega}, \tag{15}$$

where Λ'' is the imaginary part of the current-current correlation function. It represents the continuum contribution to the conductivity or AC conductivity. In the Eqs. (13) and (23), Λ' and Λ'' stand for the real and imaginary part of Λ.

After a long calculation we obtain the AC electric conductivity, neglecting electron-electron interactions, as

$$\sigma^{reg}(\omega) = \frac{\Lambda''(\vec{k} = 0, \omega)}{\omega} = \frac{(g\mu_B)^2}{\hbar}\int_0^\pi\int_0^\pi\frac{d^2k}{(2\pi)^2}\frac{\cos k(1 - e^{\zeta_k/T})f(\zeta_k)}{\zeta_k}\delta(\omega - 2\zeta_k). \tag{16}$$

where $f(\zeta_k) = (e^{\zeta_k/T} + 1)^{-1}$ is the Fermi-Dirac distribution.

3.2. Ladder approximation

The electron-electron interaction can be represented by the vertex function $\Pi_{kk'}$ which satisfies the Bethe-Salpeter equation [21].

$$\Pi_{kk'} = i\int_{-\infty}^\infty\frac{d\omega'}{2\pi}G_{\alpha\alpha}(\vec{k}, \omega + \omega')G_{\alpha\alpha}(\vec{k}, \omega')\Gamma_{kk'}(\omega, \omega'), \tag{17}$$

and

$$\Gamma_{kk'}(\omega, \omega') = \delta_{kk'} - \frac{2it}{\hbar N}\sum_{k_1}\int_{-\infty}^\infty\frac{d\omega_1}{2\pi}V_{kk_1k_1k}^{\alpha\alpha}(\omega', \omega_1)G_{\alpha\alpha}(\vec{k_1}, \omega + \omega_1)G_{\alpha\alpha}(\vec{k_1}, \omega_1)\Gamma_{kk'}(\omega, \omega_1). \tag{18}$$

The matrix $V_{kk_1k_1k}^{\alpha\alpha}(\omega', \omega_1)$ is the sum of all irreducible interaction parts. We take into account the electron-electron interaction to lowest order approximating $V^{\alpha\alpha}$ by its first-order irreducible interaction part [18,21].

$$V_{kk_1k_1k}^{\alpha\alpha}(\omega', \omega_1) = V_{kk_1k_1k}, \tag{19}$$

where we neglect all the contributions to $V^{\alpha\alpha}$ where two or more of the