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Charge and phase fluctuations in attractive Hubbard model

Grzegorz Litak *

Department of Mechanics, Lublin University of Technology, Ulica Nadbystrzycka 36, 20-618 Lublin, Poland

Abstract

Using the negative U Hubbard model we analyze normal state properties of a superconductor. In this model there exists a characteristic pairing temperature T_P above a superconducting critical temperature. Below T_P electrons start to form incoherent pairs. The fluctuations in charge and phase are precursors of charge density wave and superconductivity phases depending on band filling. They lead naturally to pseudogap opening in the density of states.

Keywords: Hubbard model; Fluctuations; Pseudogap; CDW

The pseudogap in electronic spectra of HTc superconducting cuprates has attracted a lot of attention [1]. The discussion on its origin and nature is not closed [2] however one of the possible explanations could be that it is a precursor of superconducting gap formation [2,3]. In this paper we will follow that mean and analyze the phase fluctuations of the superconducting order parameter [4] mediated by fluctuations of charge.

In this paper we employ the simplest purely electronic model which can lead to superconductivity, namely, the negative U Hubbard model [5]:

$$\widehat{H} = \sum_{ij\sigma} (-\mu\delta_{ij} - t_{ij})\hat{c}^{+}_{i\sigma}\hat{c}_{j\sigma} + \frac{1}{2}U\sum_{i}\hat{n}_{i\sigma}\hat{n}_{i-\sigma}, \qquad (1)$$

where i and j label the sites of a square lattice, t_{ij} are electron hopping integrals between nearest neighbor sites, $U<0$ describe attraction between electrons occupying the same site i, and μ is the chemical potential. The self-consistent Hartree–Fock–Gorkov (HFG) equation is:

$$\sum_j \begin{pmatrix} (E+\mu-\frac{Un_i}{2})\delta_{ij}+t_{ij} & \varDelta_i\delta_{ij} \\ \varDelta_i^*\delta_{ij} & (E+\mu+\frac{Un_i}{2})\delta_{ij}-t_{ij} \end{pmatrix} \mathbf{G}(j,k;E) = \mathbf{1}\delta_{ik}. \qquad (2)$$

In this case the superconducting order parameter $\varDelta_i$ and the local charge n_i at a finite temperature T ($\beta = 1/kT$) are given by following relations:

$$\varDelta_i = -\frac{U}{\pi}\int_{-\infty}^{\infty} \mathrm{d}E \frac{\mathrm{Im}G^{12}(i,i;E)}{\mathrm{e}^{\beta E}+1},$$
$$n_i = -\frac{2}{\pi}\int_{-\infty}^{\infty} \mathrm{d}E \frac{\mathrm{Im}G^{11}(i,i;E)}{\mathrm{e}^{\beta E}+1}. \qquad (3)$$

To go beyond the HFG we apply fluctuations of phase [4] and charge via Hubbard III approximation [6]. Thus the random local pairing potential gains a different phase Θ_i, $\varDelta_i \rightarrow \varDelta_i(\Theta_i) = |\varDelta|\mathrm{e}^{\mathrm{i}\Theta_i}$ dependent on lattice site i. The charge also changes randomly $n_i \rightarrow n_i = n \pm \delta n_i$ with lattice site i. In

* Tel.: +48-81-525-9061; fax: +48-81-525-0808.
E-mail address: litak@archimedes.pol.lublin.pl (G. Litak).

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such an approach the equation of motion has the following form:

$$\sum_j \begin{pmatrix} (E+\mu-\frac{Un_i}{2})\delta_{ij}+t_{ij} & |\Delta|e^{i\Theta_i}\delta_{ij} \\ |\Delta|e^{-i\Theta_i}\delta_{ij} & (E+\mu+\frac{Un_i}{2})\delta_{ij}-t_{ij} \end{pmatrix} \times \mathbf{G}(j,k;E) = \delta_{ik}. \quad (4)$$

Here the local pairing parameter Δ_i and the local charge n_i are given by self-consistent relations:

$$\Delta(\Theta_i) = \frac{-U}{\pi} \int_{-\infty}^{\infty} dE \frac{\mathrm{Im} G^{12}_{\Theta_i}(i,i;E)}{e^{\beta E}+1}, \quad (5)$$

$$\delta n = \frac{n_A - n_B}{2} = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \frac{\mathrm{Im}(G^{11}_A(i,i;E)) - (G^{11}_B(i,i;E))}{e^{\beta E}+1}, \quad (6)$$

where $\overline{\Delta}_i = 0$ and $\bar{n}_i = n$ ($n_A = n + \delta n$ and $n_B = n - \delta n$).

The set of above Eqs. (4)–(6) can be solved by means of coherent potential approximation (CPA) [4,7]. Single site condition for the coherent potential $\mathbf{\Sigma}(i,i,E) = \mathbf{\Sigma}(E)$ is defined by the zero value of an average T-matrix:

$$\langle \mathbf{T}_{\alpha,\Theta}(i,i;E) \rangle = \langle (\mathbf{V}_{\alpha,\Theta} - \mathbf{\Sigma}(E)) \times (\mathbf{1} - [\mathbf{V}_{\alpha,\Theta} - \mathbf{\Sigma}(E)]\overline{\mathbf{G}}(i,i;E))^{-1} \rangle, \quad (7)$$

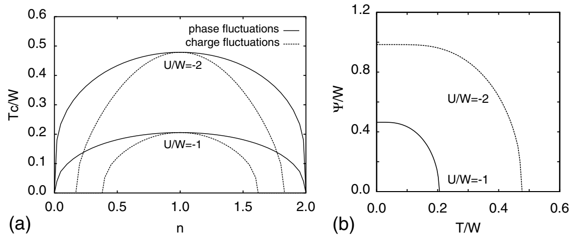

Fig. 1. (a) Characteristic temperature T_C for short range ordering: local phase and charge fluctuations versus band filling n, where $W = 8t$ is a band width. (b) Short range order parameter Ψ for half filled band ($n = 1$).

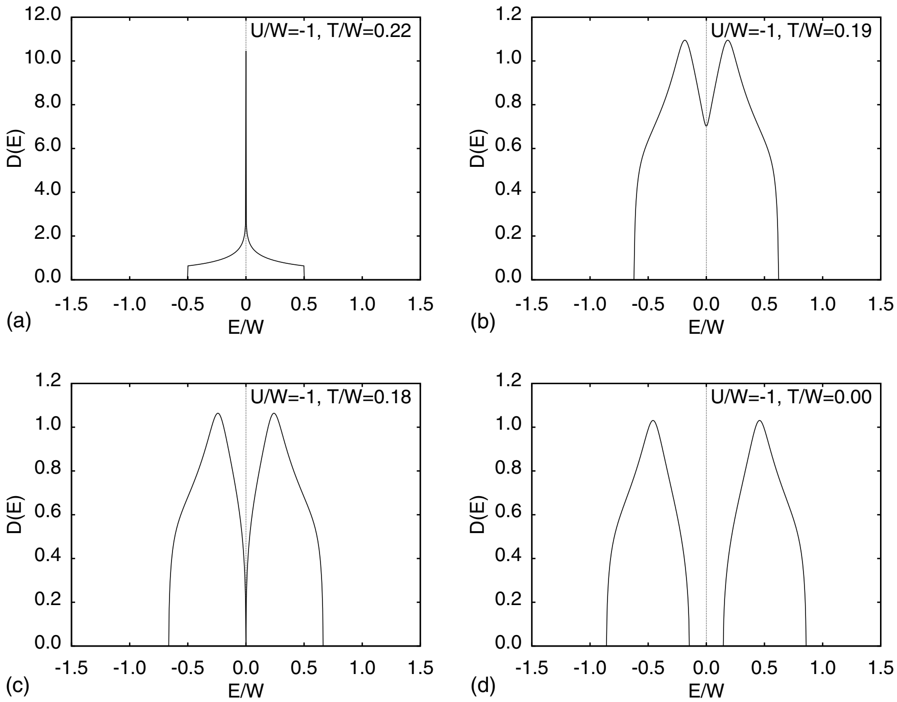

Fig. 2. Average densities at different temperatures and $n = 1$. Note, the formation of a pseudogap and a proper gap is caused by fluctuations in charge and phase below the critical temperatures of superconductivity and CDW.

where

$$V_{\alpha,\Theta} = \begin{bmatrix} \frac{Un_\alpha}{2} & -|\Delta|e^{i\Theta} \\ -|\Delta|e^{-i\Theta} & -\frac{Un_\alpha}{2} \end{bmatrix} \quad \text{and} \quad \alpha = A, B,$$
$$\Theta \in [0, 2\pi]. \tag{8}$$

Eqs. (5) and (6) can now be expressed through conditionally averaged Green functions:

$$\mathbf{G}_{\alpha,\Theta}(i,i;E)) = \overline{\mathbf{G}}(i,i;E) \times (\mathbf{1} - [\mathbf{V}_{\alpha,\Theta} - \mathbf{\Sigma}(E)]\overline{\mathbf{G}}(i,i;E))^{-1}. \tag{9}$$

The above model (Eqs. (4)–(9)) has been solved for a square lattice and large enough interaction $|U|/W = 1,2$ ($W = 8t$ is a band width). Fig. 1a shows characteristic temperatures T_C of phase (pairing temperature, T_P) and charge fluctuation appearance. Such fluctuations can be naturally related to precursors of long range order phases formation like superconductivity and charge density wave (CDW), respectively. Note that, fluctuations are characterized by different regions of band filling n. Charge fluctuations appear around half filled band ($n = 1$) while phase fluctuations are present for any n. Interestingly, for the particle-hole symmetric situation ($n = 1$) the characteristic temperatures T_C are the same for both fluctuations and they can coexist (Fig. 1a). In this case the state can be described by a generalized local order parameter $\Psi_i = (|\Delta|^2 + (U\delta n)^2)^{1/2}$ (Fig. 1b). It is similar to low temperature behaviour where superconductivity and CDW coexist [8]. However, in that case the CDW state was not stable in the presence of diagonal non-magnetic disorder [9–11]. The opening of a pseudogap above the superconducting critical temperature $T_C(\text{sup})$ [1] can be easily explained by such fluctuations. The corresponding densities of states for $U/W = -1$ are presented in Fig. 2. Note that, for smaller temperature $T < 0.18W$ (Fig. 2c) the pseudogap evolve into a proper gap in electronic spectrum. However to investigate transition into the superconducting state further one has to study the Kosterlitz–Thouless scenario [3].

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