The excitation energy spectrum for a system with electron pairs tunneling in a two-leg ladder has a doping depended gap

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A new model with a new Hamiltonian and a new canonical transformation is offered as the means for studying properties of a system of strongly correlated electrons. Consideration of the simplest possible situation, namely a system on non-interacting electrons in a two-leg ladder, leads to an expression for the excitation energy spectrum with no energy gap at the half-filling and with an energy gap away from the half filling.

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Since the time of the first high temperature superconductor was discovered[1], there is no yet a commonly accepted explanation of this phenomenon. Many publications on the matter start from some plausible reasoning leading to establishing of the model Hamiltonian and a discussion of the structure of the ground state. That plausible reasoning represents the physical view of the authors and, as long as the Hamiltonian and the ground state are set, the next step is using various mathematical methods to analyze the properties of the model. Many approaches are based on the Hubbard model[2]. The reason for using the Hubbard model is the fact that the parent state of a HTSC is an antiferromagnetic, which, when doped, exhibits many peculiar properties, including HTSC. However, the search for new models[3] is continuing and might lead to new insights on the matter and help to advance understanding of the nature of HTSC.

In this letter we offer a model based on the view that doping plays more important role than an initial antiferromagnetic order of the parent material.

At the half filling the charge density inside the material has the symmetry imposed by the symmetry of the lattice. Essentially, all locations "look alike". Let us assume that the number of electrons

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becomes less than the number of sites (this assumption does not affect further modelling). This leads to formation of a local zone with deficiency of electrons. A zone of this kind becomes a zone of attraction for electrons around. However, in order to reach that zone electrons have to overcome a potential barrier. Two electrons occupying neighboring sites and having opposite spins (due to the property of the parent material) might find themselves momentarily close to each other (which would not be possible to electrons with parallel spins) and form a bonded pair which – in turn – can tunnel into the zone with the deficiency of electrons. This tunneling is not restricted to low temperatures, hence might be happening even above the critical temperature of HTSC. The conclusion on the absence or presence of the superconductive phase has to be done based on the analysis of the excitation spectrum and the behavior of anomalous correlation functions.

Based on the presented view, one might assume that the ground state of the system should have the structure similar to the well know structure of the BCS[4] ground state, however paired electrons should not have opposite momenta (like in Cooper pairs) but instead, since they travel together, should have the same momentum.

To arrive at the Hamiltonian for the system, let us start from thinking of the Schrodinger equation for N_e electrons. To make a transition to a second quantization one has to select a set of one-electron wave functions as the means for constructing Slater determinant. However, in anticipation of the existence of pairs of bonded electrons one could construct determinant using $N_e - 2$ one-electron wave functions and one wave function describing a bonded pair. In this case the resulting Hamiltonian would have kinetic energy term related to the motion of individual electrons, but also a kinetic energy term related to the motion of pairs.

In this letter the Hamiltonian in Eq.1 is restricted to the simplest possible case of non-interacting electrons in a two-leg ladder. The importance of the antiferromagnetic order is preserved in the structure of the term describing tunneling electron pairs. The Hamiltonian neglects electron motion between the two chains, only the motion along each chain provides an input into the kinetic energy of the system.

In Eq.1, sites of a 2xN lattice are numerated with $k = 1, \ldots, N$ (in x – direction), and $n = 1, 2$ (in y – direction); $\sigma = \pm$ indicates the direction of the z-component of the electron spin; units are set with lattice constant $a = 1$, Boltzmann constant $k_B = 1$, and Planks constant $\hbar = 1$.

$$H = -t \sum_{k\,n\,\sigma} (a^+_{k+1\,n\,\sigma} a_{k\,n\,\sigma} + H.C) -$$

$$- v \sum_{k\,\sigma} (a^+_{k+1\,1\,\sigma} a^+_{k+1\,2\,-\sigma} a_{k\,2\,-\sigma} a_{k\,1\,\sigma} + H.C) - \mu \sum_{k\,n\,\sigma} a^+_{k\,n\,\sigma} a_{k\,n\,\sigma} .$$

(1)

In Eq.1 t is the hopping integral, v is the analog of the hopping integral for tunneling electron pairs, μ is chemical potential (the last term is to remove the restriction on the number of electrons in the system), and a-operators are creation and annihilation operators for the electrons in the lattice. Hamiltonian in Eq.1 has the structure very similar to the structure of the Hubbard model. This might be the reason for the Hubbard model to be able to describe certain features of HTSC. The similarity between the models also leads to a conclusion that the mathematical analysis of the presented model might be of the same level of elaborating as the Hubbard model (even with all the simplifications used to arrive at Eq.1). However, in order to just get the first impression of the viability of the model one can build on the offered above hypothesis about the ground state of the system. For example, using the ground state wave function one can calculate the expectation energy of the ground state for Hamiltonian (1).

Instead, we will use a different but an equivalent approach of defining new operators using a canonical transformation equivalent to the structure of the ground state wave function.

The first step is to make a transition into the momentum space using standard introduction of creation and annihilation operators (b – operators) acting in the momentum space, i.e. Eq.2.

$$a_{k\,n\,\sigma} = \frac{1}{\sqrt{N}} \sum_p b_{p\,n\,\sigma} e^{-ipk} \; ; \quad p = \pm \frac{2\pi m}{N}; \; m = 0,\, 1,\, ...,\, \frac{N}{2}$$

(2)

The new canonical transformation has to combine creation and annihilation operators for electrons with opposite spins but the same momentum by defining new creation and annihilation operators (c – operators); the assumed property of the new operators is that when an annihilation c – operator acts on the ground state vector of the system the result is zero.

This transformation, which is an equivalent of a well-known Bogolubov[5] canonical transformation, is described be Eq.3.

$$b_{p\,n+} = u_p c_{p\,n+} + w_p c^+_{p\,n-} \; , \quad b_{p\,n-} = u_p c_{p\,n-} - w_p c^+_{p\,n+} \; , \quad u_p^2 + w_p^2 = 1 .$$

(3)

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From this place the calculations become very routine since this approach has been known for decades and is described in numerous publications, including textbooks[6].

In short, when Hamiltonian (1) is written in terms of c – operators, terms with the structure of ccn (and H.C.) are exactly eliminated by setting a specific condition on the variables u_p and w_p (via an equation also involving excitation density $n_{pn\sigma}$); all other terms which are non–linear in terms of excitation density $n_{pn\sigma}$ are neglected due to an assumption that at low temperatures excitation density $n_{pn\sigma}$ is almost zero. Then the Hamiltonian takes a form of the one describing the system of non–interacting "particles", i.e. quasiparticles with a certain excitation energy spectrum, $\varepsilon(p)$. In particular, if $\varepsilon(p = 0) = 0$, the excitation energy spectrum has no energy gap, but otherwise the gap exists. If in addition to the existence of the energy gap the anomalous correlation functions for electrons are also not equal to zero, that is a strong indication of the existence of the superconductive phase.

For the model above for the expiation energy spectrum, $\varepsilon(p)$ calculations lead to Eq.4.

$$\varepsilon(p) = \frac{4v}{N}(2w_p^2 - 1)\sum_{\xi} \cos(p + \xi)\,[w_{\xi}^2 + (2w_{\xi}^2 - 1)n_{\xi}] \quad . \tag{4}$$

In Eq. 4 $n_p = < E_0 \left| c_{pn\sigma}^+ c_{pn\sigma} \right| E_0 >$ is the density of quasiparticles, which will be equal to zero at $T = 0$ K.

Calculation also shows that $w_p^2 = < E_0 \left| b_{pn\sigma}^+ b_{pn\sigma} \right| E_0 >$ is equal to the density of electrons (not quasiparticles) in the momentum space. Considering the simplest possible scenario, as the zeroth correction to the properties of the system, we can assume that all electrons (which are non-interacting in this model) occupy all momentum space below a certain momentum, p_F, so for $|p| > p_F$, $w_p^2 = 0$, and for $|p| < p_F$, $w_p^2 = 1$ (i.e. a standard step-function). In that case one finds that $p_F = \pi n_e/2$ ($n_e = N_e/(2N)$ is the electron density in a real space), and the energy spectrum (4) becomes $\varepsilon(p) = \frac{4v}{\pi}(1 - \sin\left(p + \frac{\pi}{2}n_e\right)$, with $\varepsilon(0) = \frac{4v}{\pi}(1 - \sin\left(\frac{\pi}{2}n_e\right)$. In this model, at the half filling when $n_e = 1$, $\varepsilon(0) = 0$, hence there is no gap. For small values of doping $x = n_e - 1$ we obtain an approximation, $\varepsilon(0) = \frac{\pi v}{2}x^2$, which means that doping in any directions should lead to development on the gap in the energy spectrum.

If we calculate anomalous correlation function $< E_0 \left| b_{pn+}^+ b_{pn-}^+ \right| E_0 > = w_p u_p$, condition $u_p^2 + w_p^2 = 1$ makes it to be equal to zero. However, it is naturally to expect that the actual electron distribution is not described by a simple step-function, for example due to electron interactions the distribution will be spread above and below momentum p_F. In that case in addition to the gap in the

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excitation energy spectrum the system also will have non-vanishing anomalous correlation functions. This understanding asserts the feasibility of the model as one of the prospective models for studying the properties of HTSC. The generalization to a square lattice is obvious and adding the interaction term should let the model to be much more realistic.

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