In a search for a "simple" model of HTSC

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This letter is based on the belief that at the core of every phenomenon lies a set of clear principles which can be visualized by the use of a relatively "simple" model (for example, the essence of a photoelectric effect, properties of metals, super fluidity, superconductivity can be explained as a collision, by the Kronig-Penney model, a quasiparticle spectrum, Cooper pairs, the Bogolyubov transformation). The goal of this paper is to strengthen the search for a similar model which can be used to understand the fundamental properties of HTSC.

For two decades the problem of HTSC[1] has been eluding theorists; many mechanism[2] of HTSC has been offered but none of them succeeded to gather the support of the vast majority.

It is clear that in order to generate a superconductive current electrons must correlate demonstrating some effective attraction needed to overcome strong Coulomb repulsion. The question is what is the nature of that effective attraction?

One path is to follow the ideas behind BCS[3] theory and looking for an agent (phonons, magnons, excitons, etc.) which can lead to an attraction effectively stronger than a Coulomb repulsion (at least for some electrons).

A different path is to state that electrons do not need any "glue"[4] in the form of additional agents.

It is know that in HTSC electrons are strongly correlated, hence the electron-electron interactions cannot be seen as weak.

The simplest approach to account for a strong interaction would be using the Hartree approximation. In this approach calculation of a wave function and an energy spectrum of a single electron is based on a solution of a self-consistent equation similar to Eq.1 (for simplicity the system is assumed one dimensional, all common physical constants are set to unity; $m_e = -e = \hbar = 1$):

$$\{-\frac{1}{2}\frac{d^2}{dx^2}+U_L(x)+U_H(x)\}\psi_\xi=\varepsilon_\xi\psi_\xi \tag{1}$$

In Eq.1 $U_L(x)$ represents the potential of a lattice, and $U_H(x)=\int\frac{n(x')}{|x-x'|}\frac{dx'}{4\pi\varepsilon_0}$ is the Hartree potential calculated via electron density $n(x)=\sum|\psi_\xi|^2$. Since the lattice potential is periodic $U_L(x+a)=U_L(x)$ the wave functions of free electrons obey the Bloch theorem and $\psi_{0\xi}(x+a)=e^{ika}\psi_{0\xi}(x)$, but in general adding the Hartree potential might destroy this property for $\psi_\xi(x)$ functions. However, if electrons are localized close to the atomic sites one could expect that the electron density would have the same symmetry as the lattice has: $n(x+a)=n(x)$. In this case the symmetry of the Hartree potential mirrors the symmetry of the lattice potential: $U_H(x+a)=U_H(x)$ (meaning $\psi_\xi(x+a)=e^{ika}\psi_\xi(x)$, i.e. periodicity property is also self-consistent). One can conclude that a strong Coulomb repulsion helps electrons to be localized in an effective periodic potential $U_{Eff}(x)=U_p(x)+U_H(x)$ and essentially is not an interaction any more but a "tool" for a modification of an external lattice potential (similarly to a system of weakly interacting electrons where interactions lead to a modification of an electron mass into an effective electron mass).

If a Coulomb repulsion is not needed to be compensated any more, there is no need for an agent which would be used to generate an effective attraction between electrons - as long as electrons themselves experience some attraction.

If a HTSC is based on an antiferromagnetic material then the most of the electrons on the neighboring sites attract each other (when they have opposite spins – which a case for low temperatures), and this attraction (in the "absence" of Coulomb repulsion) is sufficient to present correlations needed for generating a new phase.

The "simplest" model that accounts for a strong on-site repulsion and describes electrons which are localized and exhibit an antiferromagnetic order is the Hubbard[5] 1-D model described by Eq.2.

$$H=-t\sum_{x,\sigma}(a^+_{x+1,\sigma}a_{x,\sigma}+a^+_{x,\sigma}a_{x+1,\sigma})+U\sum_{x}(a^+_{x,+}a_{x,+}a^+_{x,-}a_{x,-})-\mu\sum_{x,\sigma}(a^+_{x,\sigma}a_{x,\sigma}) \qquad (2)$$

There has been published a vast amount of work designated to study the properties of the model in general and its application to understanding properties of HTSC. The most of the complications are related to the facts that the model does not have a small parameter, and that the aspects of the electrons' behavior related to the real space are as important as the aspects related to the momentum space.

A simple model – if exists – should lead to a low temperature energy spectrum of a system, calculated as energy levels of a system of quasiparticles (or collective excitations). In this case there should be a canonical transformation connecting creation and annihilation operators of actual electrons with creation and annihilation operators of quasiparticles.

A well known Bogolyubov[6] transformation is an example of such approach. However the original transformation ($a_{\pm p\pm}=u_p b_{p\pm}\pm v_p b^+_{p\mp}$, etc.) acts only in the momentum space and cannot be a good candidate for being applied to the Hubbard model.

A similar transformation can be written for creation and annihilation operators acting in the real space (for example $a^+_{x\pm}=u_x b^+_{x\pm}\mp v_x b_{x\pm1\mp}$), however due to the translational invariance the coefficients for such transformation would have to be constants ($u_x = u$, $v_x = v$), hence this transformation most probably would not be helpful due to its extreme simplicity.

A canonical transformation which should unveil principal properties of the Hubbard model – if exists – should act simultaneously in the real and in the momentum spaces; it has to reflect the importance of the correlation between electrons occupying the neighboring sites, and at the same time introduce creation and annihilation operators of quasiparticles and acting in the momentum space.

Below Eq.3 describes a transformation which satisfies both conditions (note that it cannot be reduced to a Fourier transition from the original Bogolyubov transformation into the real space).

$$a^+_{x+} = \frac{1}{\sqrt{N}}\sum_p u_p b^+_{p+} e^{-ipx} - \frac{1}{\sqrt{N}}\sum_p v_p b_{p-} e^{ip(x+1)} \qquad a^+_{x-} = \frac{1}{\sqrt{N}}\sum_p u_p b^+_{p-} e^{-ipx} + \frac{1}{\sqrt{N}}\sum_p v_p b_{p+} e^{ip(x-1)} \quad (3)$$

In Eq.3 N represents the number of sites in a 1-D lattice with the lattice constant set to a unity. Real parameters u_p and v_p are connected by condition $u_p^2 + v_p^2 = 1$ (and each is an even function of p). Eq.4 demonstrates an example of the inversion of transformation set by Eq.3.

$$b^+_{p+} = \frac{u_p}{\sqrt{N}}\sum_x a^+_{x+} e^{ipx} + \frac{v_p}{\sqrt{N}}\sum_p a_{x+1-} e^{ipx} \quad (4)$$

As long as a transformation is defined, the following steps are well established and have been vastly used and described in the literature (the steps require routine calculations, which makes the model considered as "simple"). Namely, following the original work of Bogolyubov, one rewrites Hamiltonian (2) in terms of operators $b^+_{p\sigma}$ and $b_{p\sigma}$; all terms with four operators of the same kind (all four are $b^+_{p\sigma}$ or $b_{p\sigma}$) are being neglected; all other terms with four operators get simplified using a mean-field approach. Basically all terms are being divided into three categories; (a) terms which can be written in a form which includes products like b^+b but does not include products like b^+b^+ or bb (these terms become a part of the Hamiltonian written in terms of the energy levels of the quasiparticles $H \approx H_{eff} = E_0 + \sum \varepsilon_\eta b^+_\eta b_\eta$); (b) terms which include products like b^+b or bb but which can be exactly eliminated by setting a specific condition on the parameters of the transformation (for example, product $b^+_{p+}b^+_{-p-}$ is used as a common factor and the condition is derived by setting $b^+_{p+}b^+_{-p-} \times \{\ldots\} \equiv 0$); and (c) all other terms - which all are being neglected. In the end one has an expression for the ground state energy of the system, E_0, and for excitation energy levels, ε_η (there are other but mathematically equivalent approaches to arrive at Hamiltonian H_{eff}).

Here the goal is narrowed down to looking at a singular parameter, $\varepsilon_0 = \varepsilon_{\pi=0}$. If this parameter is not equal to zero the energy spectrum has a gap (different from the one characterizing Mott transition), which represents the presence of a new phase (however, in order for this phase to be a superconductive phase having this gap is not sufficient, also anomalous correlation functions have to be not equal to zero, $< a_{x\sigma} a_{x'\sigma'} > \neq 0$ for some of the values of x and σ).

Assuming that $u_0 = 1$ (i.e. for $p = 0$ operators $b^+_{0\sigma}$ from Eq.4 are not defined by operators $a_{x\sigma}$ - this assumption seems natural but is not critical for the approach), one finds that $\varepsilon_0 > 0$ if in Eq.2 Coulomb parameter U is large enough; specifically, $U > U_C$; where:

$$U_C = \frac{2t + \mu}{\frac{1}{N}\sum_p v_p^2 (1 - n_p) + \frac{1}{N}\sum_p u_p^2 \cos p\, n_p + \frac{1}{N}\left|\sum_p u_p v_p \cos p\, (1 - n_p)\right|}$$

and $b^+_{p\sigma} b_{p\sigma} | E_0 > = n_p | E_0 >$ ($| E_0 > = \prod_{|p| < p_F, \sigma} b^+_{p\sigma} | 0 >$ is the assumed ground state of the system with the vacuum state $| 0 >$ such that $b_{p\sigma} | 0 > = 0$; condition $N_e = < E_0 | \sum_{x,\sigma} a^+_{x\sigma} a_{x\sigma} | E_0 >$, with N_e is the number of electrons, relates chemical potential μ with other parameters).

This quick analysis supports three statements: (a) strongly correlated localized electrons do not need any additional “glue”-like agent in order to generate a state with a gap in the energy spectrum of the system; (b) the Hubbard model is sufficient to describe the appearance of a gap in the energy spectrum of a system of strongly correlated localized electrons; (c) there is a “simple” Bogolyubov-like transformation which acts simultaneously in real and momentum spaces and (supposedly) reflects the essential properties of the Hubbard model.

The following full analysis which includes application of transformation given by Eq. 3 to two sublattices (reflecting the antiferromagnetic order of the parent material) will reveal if the transformation set by Eq.3 is indeed sufficient to build a “simple” model describing fundamental properties of HTSC.

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