On the phonon nature of a gap in high-temperature superconductors

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Abstract – The nature of the superconducting gap in high-temperature superconductors is a fundamental problem for understanding the mechanism of this phenomenon, however it has not been fully understood as yet. From the mid of the twentieth century when Bardeen, Cooper and Schrieffer constructed their theory it has been believed that a superconducting gap is a collective phenomenon of electron excitations. We show that in the framework of the translation-invariant bipolaron theory, for a superconducting gap, the angle-resolved photoemission spectroscopy method measures the phonon frequency for which the electron-phonon interaction is maximum. In the pseudogap phase the phonon mode associated with a bipolaron disappears when the bipolaron state breaks which leads to a failure of the pseudogap state.

One of a few direct methods providing information on the properties of a superconducting (SC) gap is angle-resolved single particle photoemission spectroscopy (ARPES) [1] together with a complementary scanning tunneling microscopy (STM) and related quasi-particle interference. There also double photoelectron spectroscopy technique has been developed which is the extension of ARPES to two particles in which two electrons are emitted and detected with well defined momentums \( \vec{k}_1 \) and \( \vec{k}_2 \) and energies \( E_1 \) and \( E_2 \) [2]. Despite a plenty of experimental data provided by ARPES, the physical nature of the gap in high-temperature superconductors (HTSC) is still to be understood. To a large extent this situation is caused by a lack of a unified theory of HTSC. If we proceed from the fact that the SC mechanism is based on Cooper pairing, then in the case of a strong Froehlich electron-phonon interaction this leads to a translation invariant (TI) bipolaron theory of HTSC [3]. In distinction from bipolarons with broken symmetry TI-bipolaron is delocalized in space and polarization potential well is lacking (zero polarization charge). TI-bipolaron is a compound bozon formed by two electrons with zero spin in singlet state and charge \( 2e \). TI-bipolaron gas being the charged Bose gas is able to experience Bose-Einstein condensation with high transition temperature. According to [2], a SC gap in TI-bipolaron theory has a purely phonon nature. In the translation-invariant bipolaron theory of superconductors bipolarons arise near the Fermi surface in the form of a gas of charged bosons whose condensation at the level which occurs lower the Fermi surface by the value equal to the bipolaron ground state energy, leads to a SC state. The spectrum of excitations of such a gas has a gap equal to the phonon frequency. The aim of this work is to show that in photoemission spectra obtained in ARPES is just the phonon frequency which is measured for the gap.

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The other gap is determined by the bipolaron energy and has nothing to do with the ARPES data.

We will proceed from the general expression for intensity $I(k, \omega)$ measured in an ARPES experiment:

$$I(k, \omega) = A(k, \omega) F(\omega) M(k, \omega)$$

In the ARPES intensity of TI-bipolaron the quantities involved in (1) differ from the example of electron photoemission. In the case of Bose-condensate under consideration \( \vec{k} \) is boson momentum, \( \omega \) - is boson energy with respect to Fermi level, \( A(k, \omega) \) - is the single-particle spectral function, \( F(\omega) \) - is the Bose-Einstein distribution function, \( M(k, \omega) \) - is the matrix element associated with the transition from the initial to final boson state.

In our case the role of charged boson taking part in light absorption is played by a bipolaron whose energy spectrum is given by the expression (2):

$$\epsilon_k = E_b \Delta_{k,0} + \left( E_b + \omega_0(\vec{k}) + \frac{k^2}{2M} \right) (1 - \Delta_{k,0}),$$

where $\Delta_{k,0} = 1$ if $k = 0$, $\Delta_{k,0} = 0$ if $k \neq 0$, and whose distribution function in Bose condensate is: $F(\omega) = \frac{1}{[\exp(\omega - \mu) - 1]^2}$.

For $k = 0$, a bipolaron is in the ground state with the energy $E_b$, while for $k \neq 0$, it is in the excited state with the energy $E_b + \omega_0(\vec{k}) + k^2/2M$, where $\omega_0$ is the phonon frequency, $M = 2m$, $m$ - is the electron effective mass.

For the following analysis, it is important that the energy of bipolaron excited states reckoned in eq. (2) from $E_b$ can be interpreted as the energy of a phonon $\omega_0$ and the kinetic energy of two electrons bounded to it. The latter in the scheme of extended zones has the form $(\vec{k} + \vec{G})^2/2M$ where $\vec{G}$ is the reciprocal lattice vector (Brillouin zone boundaries)(fig. 1).

The ARPES method measures the spectrum of the initial states. Since the kinetic energy corresponding to the reciprocal lattice vector (or a whole number of the reciprocal lattice vectors) is too large, then out of the whole bipolaron spectrum determined by eq. (2) we should take only $E_b(k = 0)$ and $E_b + \omega_0(\vec{k})$ ($k \neq 0$) to be the spectrum of the initial states. In other words, with spectral function $A(\omega, \vec{k}) = \frac{1}{\pi} Im G(\omega, \vec{k})$, where $G(\omega, \vec{k}) = (\omega - \epsilon_k - i\epsilon)^{-1}$ - is the Green function, the intensity $I(\vec{k}, \omega)$ will be written as:

\[p-2\]
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Fig. 2: Scheme of energy levels obtained by measuring the spectrum by ARPES method. The region of continuous spectrum is dashed.

\[ I(k, \omega) \sim \frac{1}{(\omega - E_b)^2 + \epsilon_1^2} \frac{1}{(\omega - E_b - \omega_0(k))^2 + \epsilon_2^2} \]  

which is a fit of Bose distribution function \( F \) with \( \mu = E_b \) and \( G \) with Lorentzian, where \( \epsilon_1, \epsilon_2 \) - determine the width of Bose distribution and the bipolaron level respectively (matrix element \( M(k, \omega) \) in eq. (1) has a smooth dependence on the energy and the wave vector).

Hence, as the light is absorbed by paired electrons, the ARPES method measures the kinetic energy of electrons with momentum \( k_e \) which escape from a sample to vacuum as a result of absorbing a photon with energy \( \hbar \nu \). The law of conservation of energy in this case has the form:

\[ \hbar \nu = \omega_0 + \left( \frac{k + \vec{G}}{2M} \right)^2 = \xi + \frac{k^2}{m_o} + \omega_0, \]

\[ \xi = 2\Phi_0 + |E_b|, \quad (4) \]

which is illustrated in fig. 2 where \( \Phi_0 \) is the work function of electrons (from the sample), \( m_0 \) - is the mass of a free electron in vacuum.

In the case under consideration, if bipolaron with energy \( \omega = \omega_0 = E_b + 2v_F(p_F - \vec{p}) \), lying in the region of existence of a bipolaron gas \( (2E_F + E_b, 2E_F) \), where \( E_F, p_F, v_F \) - are the energy, momentum, and velocity of a Fermi electron, respectively, \( p \) - is the electron momentum near the Fermi surface, absorbs the photon with energy \( \hbar \nu \) then the emerged phonon is fixed by ARPES as the gap \( \omega_0(k) \) and two electrons with kinetic energy \( k_e^2/m_0 \), determined by eq. (4), are emitted from the sample.

In this scenario in each act of light absorption, two electrons with similar momentum escape from the sample. This phenomenon could be detected by ARPES if the electron detector is placed just on the sample surface, i.e., the kinetic energy of the electron emission in vacuum (not compensated by the attraction potential in the bipolaron state) is several electron-volt.

Thus, ARPES measures the phonon frequency \( \omega_0(k) \), which is a SC gap and, consequently, in HTSC with \( d_{x^2-y^2} \) symmetry its angular dependence is given by the expression

\[ \omega_0(\vec{k}) = \Delta_0 |\cos k_x a - \cos k_y a| \]

which corresponds to the angular dependence of the intensity
Fig. 3: Schematic presentation of the angular dependence of the absorption intensity according to (3) for $\omega = \omega_i$.

$I(\omega_i, \vec{p}) \sim A(\omega_i, \vec{p})$ given by eq. (3) which is usually observed in ARPES experiments [1][4][5]. The form of $I(\omega_i, \vec{p})$ also suggests that there is a dependence of the absorption peaks on $\vec{p}$ which is symmetric about the position of the Fermi level. It is not shown in fig. 3 since in view of low population density, the intensity of absorption for $p > p_F$ will be very small [6].

Experimental testing of the effect of emission of TI-bipolarons as a whole is essential for understanding the pairing mechanism. Thus, according to [5], only one electron should escape from the sample, whose dispersion of initial states, for $k \neq 0$, is given by the formula $\epsilon_k^B = \sqrt{\frac{k^4}{4M^2} + \Delta^2(k)}$ (where $\epsilon_k^B$ is the spectrum of a Bogoliubov quasiparticle) which is different from spectrum (2). The use of spectra $\epsilon_k^B$ and (2) for describing the angular dependence of the absorption intensity may give a qualitative coincidence with modern ARPES data resolution. This experiment should give an answer to the question of whether a superconducting condensate of cuprates maintains a fermionic character of a Bose-Einstein condensate or TI-bipolarons?

It follows from the spectrum of $\omega_0(k)$ that in the nodal direction the coupling constant of the electron-phonon interaction becomes infinite, i.e., for bipolarons, the case of strong coupling is realized. fig. 4 shows a typical dependence of the absorption intensity $I(\omega_i, \vec{p})$ which is usually observed in ARPES experiments [4].

The dependence shown in fig. 4 follows from the expression for the intensity [4] with spectral function of a TI-bipolaron which corresponds to the spectrum of a TI-bipolaron [2] and cannot be obtained from spectral function [5] in paper [7] if the spectrum of a Bogoliubov particle $\epsilon_k^B$ and Fermi distribution function instead of Bose function $F(\omega)$ are used. This fact can be considered to be a good argument for TI-bipolaron mechanism of superconductivity in cuprates.

The above-considered peculiarities in the ARPES absorption spectra will also manifest themselves in tunnel experiments in the form of a thin structure (kinks) in measuring current-voltage characteristics. Compared to ARPES performed with traditional radiation sources ($\hbar \nu = 20 - 100 \text{ eV}$) the low-energy photons ($\hbar \nu = 6 - 7 \text{ eV}$) and improved momentum resolution are required to observe such singularities [7][10].

In paper [11] K.A. Kouzakov et al. also considered theoretically a possibility of emission of a Cooper pair for conventional SC in the course of ARPES experiment and, in particular, they demonstrated a peak in the emission current of Cooper pairs corresponding to zero
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The binding energy of an occupied two-electron state. The peak considered in [11] corresponds to the transition with $h\nu$ with binding energy $\sim 1$ meV which is at the boundary of accuracy of ARPES method. In the case of HTSC materials the binding energy is an order of magnitude higher which makes possible experimental checking of the effect. The main difference of our results from the data obtained in [11] is the angular dependence of the absorption peak (figs. 3, 4) characteristic for HTSC materials.

Now let us discuss briefly the temperature dependence of the intensity $I(\omega, \vec{p})$. According to eq. (1), it is determined by the temperature dependence $F(\omega)$. For $T < T_c$, where $T_c$ is the temperature of SC transition $F(\omega) \cong N_0(T)$ for $\omega = \epsilon_b$, where $N_0(T)$ is the number of bosons (bipolarons) in the condensate which determines the temperature dependence of absorption intensity. The value of $N_0$ decreases as $T$ grows and, generally speaking, vanishes at the temperature of SC transition. In fact, however, this will not happen since only the Bose-condensate part will become zero. According to the TI bipolaron theory of superconductors, for $T > T_c$, bipolarons still exist not only in the condensate state, but in the absence of the condensate as well. In this case the population density of the ground state of such bipolarons will decrease as $T$ increases and, finally, vanish at the temperature $T^*$ of transition from the pseudogap to normal phase state.

This conclusion is confirmed by ARPES experiments in the pseudogap and superconducting phases [12] which demonstrate that the angular dependence of the SC gap of $d$-type is similar to the angular dependence of the states density in the pseudogap phase. At the same time there are considerable differences between the ARPES data in the SC gap and pseudogap phases. In the SC phase the intensity of absorption has a peak below the Fermi level which corresponds to the sharp spectral peak of density states of Bose-condensate determined by eq. (3), while in the pseudogap phase this peak will be lacking because of the lack of the condensate [13]. In this case in view of the growth of the population density of excited bipolaron states, the intensity of the absorption peak in ARPES experiments will decrease as $T$ grows and reach minimum in the antinodal direction and maximum in the nodal one.

In this paper we have not characterized the mechanism of pairing of electrons or holes. Thus, for example, in Hubbard model as well as in t-J model in describing HTSC of copper oxide compounds the same holes take part in the formation of antiferromagnetic fluctuations and in hole pairing due to exchange by these fluctuations. If interaction of holes with magnetic fluctuations leads to formation of TI-magnetopolarons with the spectrum $\omega_0(k)$,
then this spectrum is also the spectrum of magnons renormalized by their interaction with holes (bound magnons). Exchange by such magnons can lead to pairing of holes, i.e., formation of a magnet TI-bipolaron whose spectrum, according to TI-bipolaron theory [4], is also determined by $\omega_0(k)$ spectrum, i.e., has $d$-symmetry. For this reason is valid the notion that RVB superconductor is simply a strong-coupling version of BCS superconductor [14].

Evidently, $d$-symmetry is specific for metal-oxide compounds and is not an indispensable attribute of HTSC. For example, in the $H_3S$ compound possessing a record temperature of superconducting transition with $T_c = 203$ K (under high pressure) in which electron-phonon interaction prevails, we can expect superconductivity of $s$-type, rather than $d$-type.

In conclusion it should be said that we leave open the question of the pairing mechanism. If this mechanism is an interaction of current carriers with magnetic fluctuations, then in our approach the particle which glues electrons into a pair should be a magnon rather than a phonon. In passing on from the pseudogap state to the normal one, this gluing mode disappears when a bipolaron decays into two individual electrons and the emitted phonon (magnon).

In the pseudogap phase there may be many gaps caused by phonon, magnon, plasmon and other types of elementary excitations. In this case the SC gap will correspond to a gap caused by an elementary excitation whose strength of interaction with electron excitations is maximum.

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