



AN EVALUATION OF PSEUDO GAP IN HIGH T_c - SUPERCONDUCTOR USING PAIRING SCENARIO OF NOZIERES AND SCHMITT –RINK THEORY

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ABSTRACT

In this paper, we have studied the pseudo gap through pairing scenario based on Nozieres and Schmitt-Rink theory. The central theme of this theory is the Cross-over problem from BCS superconductivity to Bose-Einstein Condensation (BEC). Pseudo gap state is regarded as a cross-over region. There is a co-existence of Fermions and Bosons in this region. Evaluating the self-energy from T-matrix approach, we have studied the pseudo gap in the single particle excitation.

Key words: Pseudo gap, Bose-Einstein condensation, Cross-over region, T-matrix approach, Single particle excitation.

INTRODUCTION

In the normal state properties of high- T_c cuprates, many anomalous properties^{1,2} have been experimentally observed. Among them, one is the pseudo gap phenomena. This has been observed both in the optimally to under-doped region. Since the superconductivity arises through the pseudo gap state in optimally and under-doped systems, the resolution of the pseudo gap state is an essential subject for the high- T_c superconductivity. Furthermore, the pseudo gap phenomena have main interesting aspects, because they are in sharp contrast to the conventional Fermi liquid theory³. The unusual nature has indicated an appearance of a new concept in the condensed matter physics.

The understanding of pseudo gap arises from the many theoretical proposals for the pairing scenario. The scenario has been indicated by several experimental results. Several types of pairing scenario has been proposed. An interesting proposal is the appearance of the RVB state^{4,5}. The RVB theory was proposed for the quantum spin system with frustration⁶⁻⁸.

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The spin liquid state is the underlying state, which results in the superconductivity if holes are lightly doped. Among the several descriptions, the slave Boson method for the t-J model has been widely used^{9,10}. In this theory, two essential excitations spinon and holon appear in the mean field level and couple through a gauge field. The pseudo gap state is regarded as a single pairing state of the spinon and superconductivity is described as Bose-Einstein condensation (BEC) of holones.

Another class of proposal is the 'hidden order scenario', where some long range order exists in the pseudo gap state. For example the anti-ferromagnetism^{11,12} and the 'stripe' order¹³ have been proposed as candidates. 'd-density wave' have been proposed as new type of the long range order¹⁴. If a finite value of some 'hidden' order parameter is confirmed experimentally, the corresponding scenario will be the best candidate, but it is not the case up to now.

In other class of the scenarios, a fluctuation of the order parameter is considered as an origin of the pseudo gap. The fluctuation induced pseudo gap has been investigated from the old days.¹⁵ Then, the quasi one dimensional Peierls transition was mainly investigated^{16,17}. Since any long range order does not exist at finite temperature, an extraordinary wide critical region is expected in one dimension. The pseudo gap in the spectrum is expected as a precursor of the long range order. But this mechanism is generally expected in the low dimensional systems. Then another scenario is searched. The suitable candidate is AF spin fluctuation¹⁸. The pseudo gap in the single particle spectrum can be derived from spin fluctuation theory but the crucial problem is on the magnetic excitation, which has been observed in NMR and neutron scattering. Therefore, it is subject to understand, how the decrease of magnetic excitation is derived from the magnetic fluctuation itself.

The superconducting phase transition is usually described by the BCS theory, which is an established mean field theory. As is well known, the superconductivity correlation does not appear above T_c within the mean field theory. Therefore, one base to consider the breakdown of the BCS theory in order to discuss pairing scenario. There are following two origins for the breakdown. One is the strong coupling superconductivity and other is the low dimensionality. The justification of the BCS theory is based on the long coherence length which $\xi_0 = 10^2-10^3$ in the conventional superconductors and makes the fluctuation negligible. However, the strong coupling nature of the superconductivity results in the short coherence length, which causes the softening of the fluctuation.

The first proposal of the pairing scenario was based on Nozieres and Schmett-Rink theory^{19,20}. The central subject of this theory is the cross-over problem from the BCS superconductivity to the Bose-Einstein condensation (BEC). In the weak coupling region,

the Cooper pairing and phase coherence occur at the same time according to the BCS theory. In contrast to that, in the strong coupling limit, the Fermions construct preformed Bosons above T_C and the BEC occurs at T_C . The latter situation is called 'real space pairing' in contrast to the 'momentum space pairing' in the BCS theory. The cross-over of two regions was first formulated at $T = 0$ by Leggett¹⁹ and extended to finite temperature by Nozieres and Schmott-Rink²⁰.

After that, the application to the two dimensional system has been investigated^{21,22}. These two regions are continuously described by adjusting the chemical potential. This argument does not prohibit the phase transition. The first order phase transition with phase separation has been reported in the dynamical mean field theory²³. The NSR²⁰ theory at finite temperatures takes the lowest order correction to the thermodynamic potential (Ω_B). The particle number is obtained as $n = n_F + n_B$ whereas n_F is the usual Fermion contribution and n_B is the contribution from the fluctuation namely $n_B = \frac{\partial \Omega_B}{\partial \mu}$. The chemical potential is set below the conduction band in the strong coupling region. Then, the Fermionic excitation is fully gaped even in the anisotropic superconductivity.¹⁹ In this limit, the system is regarded as a Bosonic system with residual interaction. NSR²⁰ theory is basically justified in the low density system since the shift in the chemical potential is the leading effect in the low density system.

When the BCS-BEC cross-over was proposed for the pseudo gap phenomena,²⁴ the pseudo gap state was regarded as a cross-over region. The strong-coupling limit is not relevant for cuprates, because the excitation is clearly gapless along the diagonal direction. The phenomenological theories assume the co-existence of Fermions and Bosons²⁵. By taking the advantage of this proposal, intensive studies have been made to the cross-over problem.

In this paper, we have studied the pseudo gap phenomena using NSR theory²⁰. We have studied the anomalous properties of single particle spectrum by evaluating the self energy using T-matrix approximation. We have evaluated the real part of self energy, imaginary part of self energy and spectral function as a function of ω . Through these calculations, we have seen that pseudo gap appears through resonance scattering.

Mathematical formulae used in the study

As experimental results indicate that there is a close relation between superconducting (SC) gap and pseudo gap, therefore one starts with the Hamiltonian²⁶ given by -

$$H = \sum_{\bar{k}} \varepsilon(\bar{k}) C_{\bar{k},s}^+ C_{\bar{k},s} + \sum_{\bar{k},\bar{k}',q} v_{\bar{k},\bar{k}'} C_{\bar{q}/2-\bar{k}}^+ C_{\bar{q}/2-\bar{k}'}^+ C_{\bar{q}/2-\bar{k}} C_{\bar{q}/2-\bar{k}'} \dots(1)$$

where $V_{\bar{k},\bar{k}'}$ is the $d_{x^2-y^2}$ wave pairing interaction and is given in the separate form as -

$$V_{\bar{k},\bar{k}'} = g\Phi_{\bar{k}}\Phi_{\bar{k}'}, \quad \dots(2)$$

Here g is negative and $\Phi_{\bar{k}}$ is the $d_{x^2-y^2}$ wave form factor given by -

$$\Phi_{\bar{k}} = \text{Cos}k_x - \text{Cos}k_y, \quad \dots(3a)$$

One uses tight binding dispersion for $\epsilon(\bar{k})$

$$\epsilon(\bar{k}) = -2t(\text{Cos}k_x + \text{Cos}k_y) + 4t'\text{Cos}k_x\text{Cos}k_y - \mu \quad \dots(3b)$$

Here t and t' represent nearest neighbor and next nearest neighbor hopping amplitudes, respectively. μ is the chemical potential one has taken $(t'/t) = 0.25$ and the carrier doping concentration δ , which is defined as $\delta = (1 - n)$. n is the carrier number per copper site. one takes $\delta = 0.10$.

The above Hamiltonian is an effective model in which the pairing interaction affects the renormalized quasi-particles. Since the energy scale is renormalized, the magnitude of the gap and T_c are relatively larger than in the original model.

The SC fluctuation is diagrammatically described by the T-matrix, which is the propagator of the SC fluctuation. The scattering vertex arising from the T-matrix is factorised into

$$\Phi_{\bar{k}-q/2}t(q)\Phi_{k'-q/2}$$

Where,

$$t|\bar{q}, i\Omega_n\rangle = [g^{-1} + x_{po}(\bar{q}, i\Omega_n)] \quad \dots(4)$$

Where,

$$x_{po}(\bar{q}, i\Omega_n) = T \sum_{\bar{k}} G(\bar{q}/2 + \bar{k}, i\Omega_m) G(\bar{q}/2 - \bar{k}, i\Omega_n - i\Omega_m) \Phi_{\bar{k}}^2 \quad \dots(5)$$

The SC phase transition is determined by the divergence of SC susceptibility $t(0,0)$ namely $1 + X_{po}(0,0) = 0$. This is called 'Thouless Criterion', which is equivalent to the BCS theory in the weak coupling limit.

The anomalous contribution from the SC fluctuation generally originates from the enhanced T-matrix around $\bar{q} = \Omega = 0$. Therefore, one expand the reciprocal of the T-matrix as -

$$t_{q,\Omega} = \frac{g}{t_o + b\bar{q}^2(a_1 + ia_2)\Omega} \quad \dots(6)$$

This procedure corresponds to the time dependence Ginzburg-Landau (TDGL) expansion. The TDGL parameters are expressed as the Gaussian fluctuation.

$$t_o = 1 + g \int d\varepsilon \frac{\tan(\varepsilon/2T)}{2\varepsilon} \rho_d(\varepsilon) \cong |g| \rho_d(0) \frac{T - T_c}{T_c} \quad \dots(7a)$$

$$b \cong |g| \rho_d(0) \frac{7\xi(3)}{32(\pi T)^2} v_F^2 \quad \dots(7b)$$

$$a_1 \cong \frac{1}{2} |g| \frac{\partial x_{po}(\bar{0},0)}{\partial \mu} \quad \dots(7c)$$

$$a_2 \cong |g| \rho_d(0) \pi / 8T \quad \dots(7d)$$

Here $\xi(3)$ is the Riemann's zeta function and V_F is the averaged quasi-particle velocity on the Fermi surface. Here SC fluctuation is mainly determined by the electronic state around $(\pi,0)$ owing to d-wave symmetry^{27,28}.

One defines the effective DOS as -

$$\rho_d(\varepsilon) = \sum_k A(\bar{k}, \varepsilon) \Phi_k^2 \quad \dots(8)$$

and $\rho'_d(0)$ is its derivative at $\varepsilon = 0$. Here $A(\bar{k}, \varepsilon)$ is spectral function and is given by -

$$A(\bar{k}, \varepsilon) = - (1/\pi) \text{Im} G^R(\bar{k}, \varepsilon) \quad \dots(9)$$

Here $\text{Im} G^R(\bar{k}, \varepsilon)$ is the imaginary part of the retarded Green function.

The parameter b is related to coherence length ξ_0

$$\text{as } b \alpha \xi_0^2 \alpha V_F^2 / T^2$$

In case of high T_c cuprates, T_c^{MF} is large, coherence length ϵ_0 is small, $\epsilon_0 = 3-5$. This is the essential background of the pseudo gap phenomena. The parameter a_2^2 represents the dissipation and expresses the time scale of fluctuation. This parameter is also small in the strong coupling region. The real part of a_1 is usually ignored because this term is in the higher order than the imaginary part of a_2 .

The anomalous properties of the single particle spectrum²⁹⁻³¹ are described by the self energy correction. One estimates it within the one loop order.

$$\sum (\bar{k}, i\omega)_n = T \sum_{\bar{q}, i\Omega_m} t(\bar{q}, i\Omega_m) G(\bar{k} - \bar{q}, i\Omega_m - i\omega_n) \Phi_{\bar{k}-\bar{q}/2}^2 \quad \dots(10)$$

This procedure corresponds to T -matrix approximation. In general, T-matrix around $q = 0$ gives rise to anomalous properties and far from $q = 0$ gives rise to the Fermi liquid properties. The former process is very small in the weak coupling case since $b \gg 1$.

One evaluates the anomalous contribution to the imaginary part by using the TDGL parameters³²

$$\text{Im} \sum^R (\bar{k}, \omega) = -|g| \Phi_k^2 \frac{T \xi_{GL}}{4\pi b v_k} \frac{\xi_{GL}^{-1}}{\alpha^2/v_k^2 + \xi_{GL}^{-2}} \quad (\text{for } 1D) \quad \dots(11)$$

$$= -|g| \Phi_k^2 \frac{T}{4b v_k} \frac{1}{\sqrt{\alpha^2/v_k^2 + \xi_{GL}^{-2}}} \quad (\text{for } 2D) \quad \dots(12)$$

$$= -|g| \Phi_k^2 \frac{Td}{8\pi b v_k} \log \left[\frac{q_c^2}{\alpha^2/v_k^2} + \xi_{GL}^{-2} \right] \quad (\text{for } 3D) \quad \dots(13)$$

Here $\alpha = \omega + \epsilon(\bar{k})$

$$\xi_{GL} = \sqrt{b/t_0}$$

$q_c = \pi/d$ is the cut off momentum along the c-axis.

d is the inter-layer spacing.

The real part can be obtained by the Kramers-Kronig relation as -

$$\text{Re} \sum^R (\bar{k}, \omega) = |g| \Phi_k^2 \frac{T \xi_{GL}}{4\pi b v_k} \frac{\alpha/v_k}{\alpha^2/v_k^2 + \xi_{GL}^{-2}} \quad (\text{for } 1D) \quad \dots(14)$$

$$\text{Re} \sum^R(\bar{k}, \omega) = |g| \Phi_k^2 \frac{T \xi_{GL}}{4\pi b v_k} \times \frac{1}{\sqrt{\alpha^2/v_k^2 + \xi_{GL}^{-2}}} \log \left[\frac{\alpha/v_k + \sqrt{\alpha^2/v_k^2 + \xi_{GL}^{-2}}}{\alpha/v_k - \sqrt{\alpha^2/v_k^2 + \xi_{GL}^{-2}}} \right] \quad (\text{for } 2D) \quad \dots(15)$$

$$= |g| \Phi_k^2 \frac{T}{2\pi b} \frac{1}{\alpha} \log \left[\frac{2\alpha}{\xi_{GL}^{-1} v_k} \right] \left(|\alpha| \right) \xi_{GL}^{-1} v_k$$

$$= |g| \Phi_k^2 \frac{T \xi_{GL}^{-1}}{2\pi b v_k^2} \alpha \left(|\alpha| \right) \xi_{GL}^{-1} v_k \quad \dots(16)$$

These expressions correspond to the classical approximations, which is justified near the critical point. One notes that the expression for these real part is not so accurate in the low frequency region. The dynamic of the SC fluctuation affects on it. However, the qualitative behavior are correctly grasped in eqⁿ (14) and (15).

At $\omega = 0$ the self energy is approximated as -

$$\sum^R(\bar{k}, \omega) = \frac{\Delta^2 \Phi_k^2}{\omega + \varepsilon(\bar{k}) + i\delta} \quad \dots(17)$$

Where,

$$\Delta^2 = - \sum_q t(\bar{q}, i\Omega_n) \quad \dots(18)$$

This approximation is obtained by ignoring the q-dependence of the Green's function and that of the form factor is given in equation (10). This form of the self-energy is assumed in the pairing approximation³³. If the self energy is expressed as equation (17), the Green function has the same momentum and frequency dependence as the normal Green function in the SC state as -

$$G^R(\bar{k}, \omega) = \frac{\omega + \varepsilon(\bar{k})}{((\omega + \varepsilon(\bar{k}))(\omega - \varepsilon(\bar{k}))) - \Delta^2 \Phi_k^2} \quad \dots(19)$$

Then the energy gap appears in the single particle spectrum, while the quasi-particle energy is obtained as -

$$E_k = \pm \left[\varepsilon(\bar{k}) + \Delta^2 \Phi_k^2 \right]^{1/2} \quad \dots(20)$$

RESULTS AND DISCUSSION

In this paper, we have studied the pseudo gap phenomena in high T_c -superconductor using pairing scenario of Nozieres and Schmitt-Rink theory.²⁰ Angle resolved photo emission spectroscopy (ARPES) clearly shows the pseudo gap in the single particle spectrum. In the theoretical point of view, the single particle quantities are simple compared with two particle quantities such as the magnetic and transport properties. Therefore, the study on the single particle properties can capture the basic mechanism of the pseudo gap clearly. One starts with single particle Green function and then it is expected that the pseudo gap in the two particle spectrum is derived from the pseudo gap in the single particle spectrum. By evaluating the one loop of the T-matrix given by equation (10), we have studied the anomalous properties in the single particle spectrum. One evaluates the anomalous contribution to the imaginary part by using the time dependent Ginzburg-Landau (TDGL) expansion parameter given by equation (11) to (13). Now the characteristic behaviors of the self energy has been given in Table 1 and 3. In Table 1, we have given the real part of the self energy $\Sigma(k, \omega)$ as a function of ω . Our theoretical results show that there is a positive slope around $\omega = 0$. In Table 2, we have shown the imaginary part of the self energy $\text{Im } \Sigma(k, \omega)$ as a function of ω . Our theoretical results shows that there is a sharp peak in its absolute value. Both these results are very anomalous compared to the conventional Fermi liquid theory. This is caused by the 'resonance scattering' from the SC fluctuation. This is identified to be the origin of pseudo gap phenomena. In Table 3, we have given our evaluated results of the spectral function $A(k, \omega)$ as a function of ω . Our theoretical results shows that there are two peaks of $A(k, \omega)$ as a function of ω . This is an anomalous properties of the self energy. The spectral function clearly has shown the pseudo gap. This confirms that the pseudo gap in the single particle spectrum appears near the cross-over region through the self energy correction³³.

Table 1: An evaluated results for the real part of self energy $\text{Re } \Sigma(k, \omega)$ as a function of ω in the T-matrix approach

ω	$\text{Re } (\Sigma, \omega)$
-4.0	-0.095
-3.5	-0.102
-3.0	-0.156
-2.5	-0.222

Cont...

ω	Re (κ, ω)
-2.0	-0.306
-1.5	-0.349
-1.0	-0.412
-0.5	-0.566
0.0	-0.628
0.5	-128
1.0	0.627
1.5	0.728
2.0	0.656
2.5	0.532
3.0	0.469
3.5	0.428
4.0	0.409

Table 2: An evaluated results of the imaginary part of self energy $\text{Im } \Sigma(\mathbf{k}, \omega)$ induced by the resonance, scattering as a function of ω using T-matrix approximation

ω	Re (κ, ω)
-4.0	-0.0
-3.5	-0.092
-3.0	-0.108
-2.5	-0.528
-2.0	-0.659
-1.5	-0.782
-1.0	-0.896
-0.5	-0.928
0.0	-1.106
1.0	-0.886
1.5	-0.366
2.0	-0.209

Cont...

ω	Re (κ, ω)
2.5	-0.136
3.0	-0.102
3.5	-0.095
4.0	-0.068

Table 3: An evaluated results of spectral function $A(k, \omega)$ as a function of ω using T-matrix approximation

ω	Re (κ, ω)
-4.0	0.0
-3.5	0.0
-3.0	0.0
-2.5	0.0
-2.0	0.0
-1.5	0.125
-1.0	0.146
-0.5	0.267
0.0	0.138
0.5	0.255
1.0	0.386
1.5	0.442
2.0	0.126
2.5	0.098
3.0	0.063
3.5	0.038
4.0	0.022

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