

FREQUENCY DEPENDENCE OF ELECTRONIC DENSITY OF STATES IN SUPERCONDUCTING (...) $\text{Cu}_m\text{O}_{n-x}$ SYSTEMS

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ABSTRACT

We have calculated and exhibited the frequency dependence of the superconducting electronic density of states (dos), normalized to the undoped state, in (...) $\text{Cu}_m\text{O}_{n-x}$ systems. This is achieved using our recently introduced Bardeen – Cooper – Schrieffer (BCS) – like pairing t-model (PtM) [Physica C258 (1996) 30] and first principles derivations. Presently, our calculations span negative and positive electronic energies (frequencies). The obtained results show dos irregularities. These are in sharp contrast with the behaviour of dos in the BCS model of superconductivity in Fermi liquid systems (e.g., simple metals). Our results are, surprisingly, consistent with experimental and band-structure determinations of the density of states in the cuprate systems. These results are, delightfully, in good qualitative agreement with the theoretical results by Charavarty et al. For $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ in the tunneling model by Anderson. We conclude that the PtM has successfully revealed the irregularities in the dos of non-Fermi liquid (NFL) (...) $\text{Cu}_m\text{O}_{n-x}$ systems: a feature widely experimentally established but only theoretically indicated by the tunneling model [Science 361 (1993)337], to the best knowledge of the present author. The present result goes further in establishing an NFL phase in our pairing t-model as a generalized BCS model of electron pairing and phase transitions.

1. INTRODUCTION

The experimental search by the Cambridge-Hiroshima [1,2] collaboration for Fermi liquid (FL) behaviour in hole-doped (...) $\text{Cu}_m\text{O}_{n-x}$ systems was very unsuccessful at all dopant levels (x). The Landau FL theory [3], we may recall, is characterized, among others, by (i) linear temperature dependent electronic specific heat: $C(T)=\gamma T$; (ii) temperature-independent magnetic susceptibility: $\chi(T)=\chi(0)$ and (iii) electrical resistivity that is partly constant and partly squared-temperature dependent: $\rho(T) = \rho_0 + AT^2$. An important underlying property of Fermi liquids is the weak interaction (coupling) among constituent electrons. This simple property formed the basis of the very successful Bardeen – Cooper- Schrieffer (BCS) [4] theory of electron pairing in the excited state of Fermi liquids. In our recent works [5,6] it was shown that the BCS theory could apply to electron pairing even in the normal state of a system of electrons. Indeed, the normal state depicts the serenity (coherence) of the constituent electrons of Fermi liquids.

The main conclusion from the above investigations [1,2] is that (...) $\text{Cu}_m\text{O}_{n-x}$ constitute non-Fermi liquid (NFL) systems. NFL systems are marked by strong interactions and electronic incoherence [7] bordering on disorder. These may lead to irregular density of states (dos) features. Indeed, the Landau FL theory has been

successful only in describing weakly interacting fermions with regular dos [8]. Irregularities in the density of states have been experimentally established [9] and band-structure determined [10] in (...) $\text{Cu}_m\text{O}_{n-x}$ systems. Only the tunneling model by Anderson [11,12] has theoretically revealed the experimental dos irregularities in these cuprate systems, to the best knowledge of the present author.

The purpose of the present work is to calculate the electronic density of states of non-Fermi liquid (...) $\text{Cu}_m\text{O}_{n-x}$ in the BCS-like pairing t-model (PtM) [5]. The objective is to further validate (invalidate) the PtM as an NFL model. To date, no consensus has been reached on non-Fermi liquid theoretical models. The results of current investigation could be of immense help in narrowing down the number and nature of plausible NFL models and theories of the future.

2. ENERGY SPECTRA OF NON-FERMI LIQUID (...) $\text{Cu}_m\text{O}_{n-x}$

The two-band model of the non-fermi liquid cuprate oxides as we proposed [5], in the mean-field approximation and Bloch representation, is the pairing t-model:

$$H = \sum_{ik\sigma} \varepsilon_{ik\sigma} C_{ik\sigma}^+ C_{ik\sigma} - \sum_{ijk\sigma, i \neq j} t_{ij} C_{ik\sigma}^+ C_{ik\sigma} + \sum_{ijk\sigma, i \neq j} \left(\Delta_{ij} C_{ik\downarrow}^+ C_{ik\uparrow} + h.c. \right) \quad (2.1)$$

In Eq.(2.1), $i(j) = d,p$, labels, $\text{Cu}(3d)$ and $\text{O}(2p)$ bands (and electrons) in (...) $\text{Cu}_m\text{O}_{n-x}$ systems and the wavefunctions of these bands overlap and hybridize. The first term of Eq.(2.1) is the kinetic (hopping) energy for i band elections with spin polarization $\sigma (= \uparrow \text{ or } \downarrow)$, wavevector k and unperturbed kinetic energy per electron $\varepsilon_{ik\sigma}$, measured relative to the Fermi level; $C_{ik\sigma}^+ (C_{ik\sigma})$ is the above-assigned electron creation (annihilation) operator. The second term is the band mixing (hybridization) energy with t_{ij} being the hopping matrix. Assuming $t_{ij} = t_{ji} = t$, the opposite spin pair interaction energy gap, in i band is

$$\Delta_{ii} = -t \langle C_{i\uparrow} C_{i\downarrow} \rangle \langle C_{i\downarrow} C_{i\uparrow} \rangle. \quad (2.2)$$

This Hamiltonian encompasses the normal and excited states of the system. Because the two phases are very distinct: one an antiferromagnetic normal state, the other the excited superconducting phase of the system, they can be separated, yielding different energy regimes for our calculations of the density of states.

A. Energy Spectrum of Undoped (...) $\text{Cu}_m\text{O}_{n-x}$

In this paper, the normal state (...) $\text{Cu}_m\text{O}_{n-x}$ is the undoped ($x = 0$) composition. Ordinarily, for these systems, this is the antiferromagnetic NFL state. The normal state Hamiltonian is excised from Eq.(2.1) by the kinetic energy imposition (where U and t are constants):

$$\varepsilon_{p\downarrow\sigma} = \varepsilon_{d\downarrow\sigma} = -\varepsilon_{d\uparrow\sigma} = -\frac{U}{2}, \quad (2.3)$$

$$\Delta_{dd} = -\Delta_{pp} = -t. \quad (2.4)$$

These guarantee [5] the experimental antiferromagnetic ordering in this state and lead to the NFL Hamiltonian of this regime, in pseudospin representation, as

$$\Pi_n = \sum \Psi_{k\sigma}^+ \left[\xi_k + \eta_k \gamma_0 + \bar{\Delta}_k \Gamma_1 \gamma_0 \right] \Psi_{k\sigma} \quad (2.5)$$

In Eq.(2.5),

$$\xi_k = \gamma_4 \left[\left(\varepsilon_{pk\uparrow} - \varepsilon_{pk\downarrow} \right) - \left(\varepsilon_{pk\downarrow} - \varepsilon_{pk\uparrow} \right) \right], \quad (2.6)$$

$$\eta_k = \gamma_4 \left[\left(\varepsilon_{dk\downarrow} - \varepsilon_{dk\uparrow} \right) - \left(\varepsilon_{pk\downarrow} - \varepsilon_{pk\uparrow} \right) \right], \quad (2.7)$$

$$\Gamma = (\Gamma_1, \Gamma_2, \Gamma_3) = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix} \quad (2.8)$$

$$\gamma_0 = \begin{pmatrix} \sigma_0 & 0 \\ 0 & -\sigma_0 \end{pmatrix} \quad (2.9)$$

$$\bar{\Delta}_k = \gamma_2 (\Delta_{dk} - \Delta_{pk}), \quad (2.10)$$

$$\Psi_{k\sigma}^+ = (C_{dk\uparrow}^+, C_{dk\downarrow}^+, C_{pk\uparrow}^+, C_{pk\downarrow}^+). \quad (2.11)$$

In the above, σ is the Pauli 2x2 matrix, σ_0 is the 2x2 unit matrix and $\Psi_{k\sigma}$ is the hermitian conjugate of $\Psi_{k\sigma}^+$.

The Fourier transform of the Greens function arising from the Hamiltonian, Eq. [2.5], is

$$G_n(k, i\omega_n) = (i\omega_n - \Pi_n)^{-1}, \quad (2.12)$$

where $\omega_n = \pi\beta^{-1}(2n+1)$ is the Matsuhara frequency ($n=0, \pm 1, \pm 2$)

It simplifies to

$$G_{nk}, i\omega_n = \frac{1}{D_n} \begin{bmatrix} XY+B & C+L & 0 & 0 \\ C+L & XY+B & 0 & 0 \\ 0 & 0 & XY-B & L-C \\ 0 & 0 & L-C & XY-B \end{bmatrix} \quad (2.13)$$

In Eq. (2.13)

$$X = i\omega_n - \xi_k, \quad (2.14)$$

$$Y = X^2 - \eta_k^2 - \bar{\Delta}_k^2 \quad (2.15)$$

$$D_n = Y^2 - 4\eta_k^2 \bar{\Delta}_k^2, \quad (2.16)$$

$$B = \eta_k Y + 2\eta_k \bar{\Delta}_k^2 \quad (2.17)$$

$$C = \bar{\Delta}_k (Y + 2\eta_k^2) \quad (2.18)$$

$$L = 2\eta_k \bar{\Delta}_k X \quad (2.19)$$

The poles ($D_n = 0$) of the Greens function, lead to

$$(i\omega_n)^2 - 2(i\omega_n)\xi_k + \xi_k^2 - \frac{U^2}{16} - t^2 = 0. \quad (2.20)$$

The energy spectrum $E_{k\pm} (= \pm i\omega_n)$ is obtained as solution of the above quadratics in $(i\omega_n)$:

$$E_{dk\pm} = -\frac{U}{4} \pm \frac{1}{4}(U^2 + 16t^2)^{1/2}, \quad (2.21)$$

where $\eta_k = \xi_k = -\frac{U}{4}$, (2.22)

and $\bar{\Delta}_k = -t$ (2.23)

$$E_{pk\sigma} = -\frac{U}{2}. \quad (2.24)$$

These are quite in accord with our earlier [5] results for these bands. They form the starting point for the calculation of the normal state (undoped system) density of states, in Sec. 3

B. Energy Spectrum of Doped (...)Cu_mO_{n-x}

The doped state of (...)Cu_mO_{n-x} is the $x \neq 0$ composition and is, indeed, the excited state of the system. The excited state is the superconducting phase. There are two superconducting regimes [6]: the $\epsilon_{ik\sigma} = \epsilon$ paired electron regime and the $\epsilon_{ik\sigma} \neq \epsilon_{jk\sigma}, i \neq j$, paired electron regime. It is the later regime that promises exceeding theoretical richness of interest to this author. Presently, however, we start by estimating the dos in the superconducting regime of the equikinetic singlet pairs of electrons. Thus the BCS energy criterion for pairing is here assumed, from the start.

In this case of energy equalization, the Hamiltonian of the system in pseudospin representation is [5]:

$$\Pi_s = \theta_k^* \Gamma_3 + \Delta^* \Gamma_1 - t \Gamma_3 \gamma_s, \quad (2.25)$$

where, $\epsilon_{ik\sigma} = \epsilon$

$$\theta^* = \epsilon; \Delta^* = \Delta \quad (2.26)$$

$$\gamma_s = \begin{pmatrix} 0 & \sigma_0 \\ \sigma_0 & 0 \end{pmatrix} \quad (2.27)$$

The Greens function solution of the above Hamiltonian follows the form of Eq. (2.12) such that

$$G_s(k, i\omega_n) = \frac{1}{D_s} (i\omega_n + \epsilon \Gamma_3 + \Delta \Gamma_1 - t \Gamma_3 \gamma_s) (Y' - 2t\epsilon \gamma_s). \quad (2.28)$$

In Eq. (2.28),

$$D_s = Y'^2 - 4\epsilon^2 t^2 \quad (2.29)$$

$$Y' = (i\omega_n)^2 - \epsilon^2 - \Delta^2 - t^2. \quad (2.30)$$

The pole analysis ($D_s = 0$) leads to

$$\left\{ (i\omega_n)^2 - \varepsilon^2 - \Delta^2 - t^2 \right\}^2 - 4\varepsilon^2 t^2 = 0. \quad (2.31)$$

Finally it yields the spectra:

$$E_{k\pm}^2 = (\varepsilon \pm t)^2 + \Delta_k^2. \quad (2.32)$$

Eq. (2.23) is the conventional BCS spectrum for a single band but now split by the hopping matrix, t . This is the spectrum of the superconducting (...) $\text{Cu}_m\text{O}_{n-x}$ in the equikinetical pairing electron regime. This is identical with our result [5] for a specified pairing symmetry of the system as the latter shifts by doping.

3. SUPERCONDUCTING ELECTRONIC DENSITY OF STATES

For our two-band (d-p) copper oxide compounds, (...) $\text{Cu}_m\text{O}_{n-x}$, the electronic density of states, at any phase, as a function of frequency (ω) is derived as

$$N(\omega) = (4\pi)^{-1} \sum_k \text{tr} \left[\left(\text{Im} G(k, i\omega_n \rightarrow \omega + i\delta) \right) \right]. \quad (3.1)$$

Here, $G(k, i\omega_n \rightarrow \omega + i\delta)$ is the analytic continuation of $G(k, i\omega_n)$. Now, because the density of states in the normal, undoped, state of our system is not constant but depends on electronic energy (frequency) spectrum, a more accurate picture of the superconducting dos is got by calculating the latter relative to the normal state value at any given frequency.

For the dos calculation, let us reinterpret the superconducting energy spectrum, Eq. (2.32), in the Cu ion plasma scenario [5]. So that we rewrite (2.32) as

$$E_k^2 = \bar{\varepsilon}_k^2 + \Delta_k^2, \quad (3.2)$$

$$\bar{\varepsilon}_k = \varepsilon_k \pm |t|. \quad (3.3)$$

Taking the upper limits of $\bar{\varepsilon}_k$ as approximating the Cu ion plasma energy

$$\bar{h}\omega_p = \bar{h}\omega_D + |t|, \quad (3.4)$$

we observe that in the absence of electron hopping (parameter t), the present theory reverts to conventional phonon (frequency ω_D) mediation of superconductivity which is the correct and expected limit.

It is now easy for one to carry through the prescription of Eq. (3.1) and obtain the ratio of the superconducting and normal state dos as

$$N_s(\omega) / N_n(\omega) = \left| \frac{\ln A}{\omega} \right|, \quad (3.5)$$

where, for low plasma frequencies as required, Bednorz and Muller [13];

$$A = \left| \frac{\omega_p}{\omega^2 - \omega_p} \right|. \quad (3.6)$$

The values of $y = N_s(\omega) / N_n(\omega)$ are plotted against frequency (ω), in fig. 1, for $\omega_p \approx 0.25, 0.5, 1.0, 2.0, 4.0$, in (...) $\text{Cu}_m\text{O}_{n-x}$. There exist striking similarities between the present plot and corresponding plots [10,12] for these systems.

4. SUMMARY AND CONCLUSION

The present paper set out to calculate and exhibit the electronic density of states of (...) $\text{Cu}_m\text{O}_{n-x}$ systems in the superconducting state. Since the value of dos depends on the energy spectrum of the state of interest this parameter is treated as a function of the electronic frequency. The superconducting state of the compound has a precursor normal state that has irregular energy spectrum and, hence, irregular dos. This informs that the calculation of the superconducting dos be relative to the normal state for a true cancellation of the effects of normal state on this excited state density of state. Our result shows irregularities in the density of states in accord with experiment [9,10], band-structure determination and a recent theory [11]. This reaffirms the proposal that (...) $\text{Cu}_m\text{O}_{n-x}$ is a non-Fermi liquid with irregular dos. What is most interesting in the present work is that the result has proceeded from a BCS-like model of pairing. This is unusual with this model.