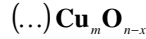


**Some thermodynamic non-Fermi liquid properties of correlated electron systems.**



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**Abstract**

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A mean-field Hamiltonian model has been used to investigate some thermodynamic properties of the normal states of non-Fermi liquid (NFL) systems,  $(\dots)Cu_mO_{n-x}$ . This Hamiltonian is like that of the Bardeen-Cooper-Schrieffer model [Phys. Rev. 108 (1957) 1175] but differs from the latter in (i) being multiband, (ii) the gap in energy being a function of the hopping integral and (iii) band energies of electrons being dependent upon spin orientation. The Hamiltonian is, therefore, similar to the Paring t-model [Physica C 258 (9166) 30] but differs from it in not incorporating hybridization term and hybrid pair superconductivity. The analysis of the model yields magnetic energy spectrum for  $Cu(3d)$  bands and non-magnetic energy spectrum for the  $O(2p)$  bands. Inverse temperature dependences of electronic specific heat ( $C_v$ ), entropy function ( $S$ ) and pair susceptibility ( $\chi^{\uparrow\downarrow}$ ) are computed and exhibited. The specific heat dependence upon inverse temperature shows a linear form at very high temperature. It displays inverse-square-law temperature dependence, approximately, for lower temperatures. In the very low temperature range, the actual curve of the theoretical specific heat with temperature is rather like that of the  $C_p$  versus  $T^{-2}$  curve obtained for  $Bi_4Cu_4O_{16+y}$  and  $Tl_2Ba_2Ca_{n-1}Cu_nO_{2n+4}$  down to millikelvin temperature. This is in contradistinction to the linear temperature dependence ( $C_v = \gamma T$ ) of Fermi liquid systems. The specific entropy dependence on temperature shows correct physical response of systems to order (disorder) with varying temperatures. The pair susceptibility is linear at very high temperature and constant ( $\chi = \chi_o$ ) at moderate/low temperatures. The latter is as in Fermi liquid systems, but the former is an NFL manifestation.

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**Keywords:** Mean-field model, Green's function, thermodynamic functions, inverse temperature.

## 1.0 Introduction

The new copper ceramic compounds<sup>1</sup>,  $(\dots)Cu_mO_{n-x}$  constitute very important members of a class of electronic systems known correlated electron (CES) [2]. One of the drawbacks to a better understanding of CES, in general, and copper oxide ceramics, in particular, is their non-Fermi liquid (NFL) [3] manifestation. Both their normal states which, for  $(\dots)Cu_mO_{n-x}$ , are strangely antiferromagnetic [4] and their excited states, which for the same ceramics, are superconducting<sup>5</sup>, show experimental NFL features [6] in their physical parameters. Since a

suitable theory to explain these novel features is yet not in place, it is the objective of this paper to attempt a theory of some NFL thermodynamic properties of these compounds.

The tow-band Bardeen-Cooper-Schrieffer (BCS) [7] model of superconductivity in these materials has been advanced by Animalu<sup>8</sup> and modified by Asomba<sup>9</sup>. We present, in Section 2, the pseudospin model of [9] modified to account for the NFL normal states of these compounds. In Section 3, the corresponding Green's function of the system Hamiltonian is deduced and the energy spectrum of the normal state is obtained. This leads, in Section 4, to the calculation of some of the thermodynamic parameters of the system, which are exhibited. Summary and concluding remarks are given in Section 5.

## 2.0 The two-band BCS pseudospin model

Because the properties of (...)  $Cu_m O_{n-x}$  are determined by  $CuO_2$  units of the system, the  $Cu(3d)$  and  $O(2p)$  bands need be incorporated in the system Hamiltonian model. The modification for the effective Hamiltonian of [9] is here advanced:

$$H = \sum_{ik\sigma} \epsilon_{ik\sigma} C_{ik\sigma}^+ C_{ik\sigma} + \sum_{ikk'\sigma} (\Delta_{ikk'\sigma} C_{ik\sigma}^+ C_{ik'\sigma}^+ + h.c) \quad (2.1)$$

In (2.1)  $\epsilon_{ik\sigma}$  is the kinetic energy of the  $i^{th}$  (=1 or 2 bands) electrons (holes) with crystal vector  $k$  and spin orientation  $\sigma$ ;  $C_{ik\sigma}^+$  ( $C_{ik\sigma}$ ) is the creation (annihilation) operator for the above electron and

$$\Delta_{ik\sigma} = -t_{ij} \langle C_{i-k\downarrow} C_{jk\uparrow} C_{jk\uparrow} \rangle \langle C_{j-k\downarrow} \rangle, i \neq j. \quad (2.2)$$

In Eq (2.1), and henceforth, the subscript  $k \downarrow$  implies  $-k \downarrow$  always where  $t_{ij}$  is the electron hopping energy from  $i \rightarrow j$ . This model is like the BCS model except in the definition of  $\Delta_{ikk'\sigma}$  and the multiband nature. It is also similar to the Paring t-Model of ref 9 except the absence of the mixing term and hybrid pair superconductivity in the case. This model can be written in this form

$$H = H'_k + H''_k$$

where

$$\begin{aligned} H'_k &= \epsilon_{1k\uparrow} C_{1k\uparrow}^+ C_{1k\uparrow} + \epsilon_{1k\downarrow} C_{1k\downarrow}^+ C_{1k\downarrow} + \epsilon_{2k\uparrow} C_{2k\uparrow}^+ C_{2k\uparrow} + \epsilon_{2k\downarrow} C_{2k\downarrow}^+ C_{2k\downarrow} \\ &= 1/2 [\epsilon_{1k\uparrow} + \epsilon_{1k\downarrow} + \epsilon_{2k\uparrow} + \epsilon_{2k\downarrow}] (C_{1k\uparrow}^+ C_{1k\uparrow} + C_{1k\downarrow}^+ C_{1k\downarrow} + C_{2k\uparrow}^+ C_{2k\uparrow} + C_{2k\downarrow}^+ C_{2k\downarrow} + \\ &- (\epsilon_{1k\uparrow} - \epsilon_{1k\downarrow}) (C_{1k\uparrow}^+ C_{1k\uparrow} - C_{1k\downarrow}^+ C_{1k\downarrow} + C_{2k\uparrow}^+ C_{2k\uparrow} - C_{2k\downarrow}^+ C_{2k\downarrow}) - (\epsilon_{1k\uparrow} + \epsilon_{1k\downarrow}) (C_{2k\uparrow}^+ C_{2k\uparrow} + C_{2k\downarrow}^+ C_{2k\downarrow}) \\ &- (\epsilon_{2k\uparrow} - \epsilon_{2k\downarrow}) (C_{1k\uparrow}^+ C_{1k\uparrow} + C_{2k\downarrow}^+ C_{2k\downarrow}) + (\epsilon_{1k\downarrow} - \epsilon_{1k\uparrow}) (C_{2k\uparrow}^+ C_{2k\uparrow} - C_{2k\downarrow}^+ C_{2k\downarrow}) + (\epsilon_{2k\downarrow} - \epsilon_{2k\uparrow}) \\ &(C_{1k\uparrow}^+ C_{1k\uparrow} - C_{1k\downarrow}^+ C_{1k\downarrow}) \end{aligned} \quad (2.3)$$

we define the four components vector wave function

$$\Psi_{k\sigma}^+ = (C_{1k\uparrow}^+ C_{1k\downarrow} + C_{2k\uparrow}^+ C_{2k\uparrow}) \quad (2.4)$$

And it's adjoint conjugate  $\Psi_{k\sigma}$ , alongside the  $4 \times 4$  parity and helicity operator [10]

$$\gamma_o = \begin{bmatrix} \sigma_o & 0 \\ 0 & -\sigma_o \end{bmatrix} \text{ and } \Gamma_i = \begin{bmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{bmatrix}, i=1,2,3 \quad (2.5)$$

where  $2 \times 2$  Pauli matrix. We obtain

$$H_k^1 = \sum_{k\sigma} \Psi_{k\sigma} [J_k + \xi_k \gamma_o + \vartheta_k \Gamma_3 \gamma_o] \Psi_{k\sigma} \quad (2.6)$$

where

$$J_k = 1/4 [(\epsilon_{1k\uparrow} - \epsilon_{1k\downarrow}) - (\epsilon_{2k\downarrow} - \epsilon_{2k\uparrow})] \quad (2.7)$$

$$\xi_k = 1/4 [(\epsilon_{2k\downarrow} - \epsilon_{2k\uparrow}) - (\epsilon_{1k\downarrow} - \epsilon_{1k\uparrow})] \quad (2.8)$$

$$\theta_k = 1/4 [(\epsilon_{1k\uparrow} + \epsilon_{1k\downarrow}) - (\epsilon_{2k\uparrow} + \epsilon_{2k\downarrow})] \quad (2.9)$$

$$\alpha_k = 1/4 [(\epsilon_{1k\uparrow} + \epsilon_{1k\downarrow}) - (\epsilon_{2k\uparrow} + \epsilon_{2k\downarrow})] \quad (2.10)$$

Equation (2.6) is the pseudospin model of the two-band kinetic term. Similarly,

$$H_k'' = \sum_{k'\sigma} \psi_{kk'\sigma} (\Delta_{kk'}^+ \Gamma_1 + \bar{\Delta}_{kk'} \Gamma_1 \gamma_o) \psi_{k'\sigma} \quad (2.11)$$

where

$$\Delta_{kk^1}^+ + \bar{\Delta}_{kk^1} = \Delta_{2kk^1} \quad (2.12)$$

$$\Delta_{kk^1}^+ + \bar{\Delta}_{kk^1} = \Delta_{1kk^1} \quad (2.13)$$

If in (2.6) and (2.11) we set  $\theta_k = \alpha_k = \Delta_k^+ = 0$ , the addition of (2.6) and (2.11) yields

$$H = \sum_{k'\sigma} \psi_{kk'\sigma} (\Delta_{kk'}^+ \Gamma_1 + \bar{\Delta}_{kk'} \Gamma_1 \gamma_o) \psi_{k'\sigma} \quad (2.14)$$

This is the NFL pseudospin Hamiltonian for the normal state in BCS-like formalism.

### 3.0 Energy spectrum

For the two-band non-Fermi liquid system, Equation (2.14), the particle propagator (green's function) has the structure, in Fourier space:

$$G(k, iw_n) = (iw_n - H)^{-1} \quad (3.1)$$

where  $k$  is a space co-ordinate and  $w$  is the time co-ordinate with  $w_n = \pi\beta^{-1}(2n+1)$ ,  $n \in Z$

$$\therefore G(k, iw_n) = \left[ XY + \left( \zeta_k Y + 2\zeta_k \bar{\Delta}_k^2 \right) \gamma_o + \left( \bar{\Delta}_k Y + 2\zeta_k^2 \bar{\Delta}_k^2 \right) \gamma_o \Gamma_1 + 2\zeta_k \bar{\Delta}_k X \Gamma_1 \right] D \quad (3.2)$$

where

$$X = iw_n - j_k, \quad (3.3)$$

$$Y = X^2 - \zeta_k^2 - \Delta_k^{-2} \quad (3.4)$$

$$D = Y^2 - 4\zeta_k^2 \Delta_k^{-2} \quad (3.5)$$

Now, taking  $\begin{pmatrix} \xi_k & \bar{\Delta}_k \\ \zeta_k & \Delta_k \end{pmatrix} = O$

$J_k = \zeta_k = -u/4$  and  $\bar{\Delta}_k = -t$  we have at the poles of the Green's function,  $D = 0$ , as

$$X^2 = \zeta_k^2 - \bar{\Delta}_k^2 = 0$$

$$\therefore (i\omega_n + u/4)^2 - \frac{u^2}{16} - t^2 = 0$$

$$(i\omega_n)^2 + u/2(i\omega_n) + u^2/16 - u^2/16 - t^2 = 0$$

$$E_k^2 + (u/2)E_k - t^2 = 0$$

where  $E_k = i\omega_n$ ,  $E_k = u/4 \pm 1/4(u^2 + 16t^2)^{1/2}$

There are the magnetic energy spectra of the  $Cu \uparrow$  and  $Cu \downarrow$  bands. The spectra of the  $0 \uparrow$  and  $0 \downarrow$  bands are  $u/2$  and are equal.

### 4.0 Some thermodynamic functions

In this Section, we proceed to present the inverse temperature dependence of the electronic specific heat ( $C_v$ ), inverse temperature dependence of the entropy function ( $S$ ) and the inverse temperature dependence of the magnetic spin susceptibility ( $\chi \uparrow \downarrow$ ). These will be displayed and discussed.

#### 4.1 Inverse temperature dependence of electronic specific heat ( $C_v$ ).

For the  $(\dots)Cu_m O_{n-x}$  compounds in the present work, the normal state single particle partition function is the trace ( $T_r$ ):

$$Z = T_r \exp(-\beta H) \quad (4.1)$$

where  $H$  is the pseudospin Hamiltonian of the system. Equation (4.1) is identical to the sum of the Boltzmann factor:

$$Z = \sum_i e^{-\beta E_i} \quad (4.2)$$

where  $E_i$  are the diagonal elements of  $H$  and constitute the energy spectra in these normal states of the system. Indeed, since the smallest units of the system are the  $E_{\rho k \uparrow}$  ( $E_{\rho k \downarrow}$ ) for the  $Cu$  ions. The latter ions are magnetic. Form the previous section; we have obtained the spectral energies as

$$E_{\rho k \uparrow} = E_{\rho k \downarrow} = -U/2 \quad (4.3)$$

$$E_{dk \uparrow} = -U/4 - 1/4(U^2 + 16t^2)^{1/2} \quad (4.4)$$

and

$$E_{dk \downarrow} = -U/4 + 1/4(U^2 + 16t^2)^{1/2} \quad (4.5)$$

We can then express the single particle partition functions as

$$Z = \exp\left[\frac{\beta U}{2}\right] + \exp\left[\frac{\beta U}{4}\right] + \exp\left[\beta\left(\frac{U}{4} + \frac{1}{4}(U^2 + 16t^2)^{1/2}\right)\right] + \exp\left[\beta\left(\frac{U}{4} - \frac{1}{4}(U^2 + 16t^2)^{1/2}\right)\right] \quad (4.6)$$

$$Z = \exp(a\beta)[2 \exp(a\beta) + \exp(b\beta) + \exp(-b\beta)] \quad (4.7)$$

where

$$a = U/4, b = U/4(U^2 + 16t^2)^{1/2} \quad (4.8)$$

This system can be considered as made up of  $N$  clusters of  $CuO_2$ . We may then seek the  $N$  cluster Halmholtz function.

$$F_N = -N/\beta \ln Z \quad (4.9)$$

$$\therefore F_N = -N/\beta [a\beta + \ln(2 \exp(a\beta) + \exp(b\beta) + \exp(-b\beta))]$$

The total internal energy of the system is therefore  $E_N = -\tau^2 \partial/\partial r [F_N/\tau] = -\partial/\partial \beta (\beta F_N)$  where  $\tau = \beta^{-1} = k_B T$ . The molar specific heat is

$$C_v = -k_B \beta^2 \frac{dE_N}{d\beta}$$

$$C_v = N_A k_B \beta^2 \frac{d}{d\beta} \left[ \frac{a}{1} + \frac{2a \exp(a\beta) + b \exp(b\beta) + b \exp(-b\beta)}{2 \exp(a\beta) + \exp(b\beta) + \exp(-b\beta)} \right]$$

$$C_v/R = 1/\tau^2 \left[ \frac{QP - X^2}{Q^2} \right] \quad (4.10)$$

where

$$Q = 2(\exp(a\beta) + \cosh(b\beta)) \quad (4.11a)$$

$$P = 2(a^2 \exp(a\beta) + b^2 \cosh(b\beta)) \quad (4.11b)$$

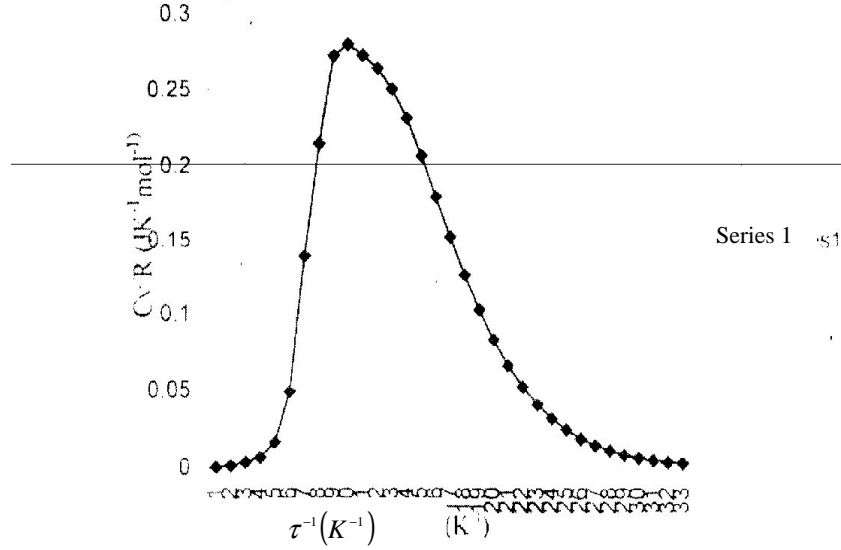
$$X = 2(a \exp(a\beta) + \sinh(b\beta)) \quad (4.11c)$$

and

$R = N_A K_B$  is the universal gas constant of thermodynamics.

Figure 1 is the inverse temperature dependence of electronic specific heat ( $C_v/R$ ) plotted against  $\tau^{-1}$  for  $a = 1.3eV, b = 0.72eV, t = 0.43V$  and  $5.4eV$

At very low inverse temperature range there is near linear relationship of  $C_v/R$  versus  $\tau^{-1}$  curve but no linear temperature relationship. A  $C_v/R = \gamma/\tau^{-1}$  relationship is deduced from this graph at high  $\tau^{-1}$  range. The theoretical curve is alike of the  $C_p$  versus  $T^2$  curve experimentally obtained for



**Figure1: The numerical values of electronic specific heat ( $C_v / R$ ) against inverse temperature ( $\tau^{-1}$ ).**  $Bi_4Ca_3Cu_4O_{16+y}$  by Villar et al [12] and for  $Tl_2Ba_2Ca_{n-1}Cu_nO_{2n+4}$  by Junod et all [13]. Down to millikelvein temperature. The inverse-square law temperature dependence of  $C_v / R$  is interpreted as resulting from Schottky contribution to the specific heat of the system. Indeed, out present temperature dependence of the specific heat closely resemble the expression for the Schottky heat capacity of a magnetic ion sub-system given by

$$C_m/R = \delta_1^2 / \tau^2 \frac{\left(\frac{g_o}{g_1}\right) e^{\delta_0 \tau}}{\left[1 + \left(\frac{g_o}{g_1}\right) e^{\delta_1 \tau}\right]^2} \approx \frac{\text{constant}}{\tau^2} \quad (4.12)$$

where  $g_o$  and  $g_1$  are the degeneracies of the available two energy levels to which lowest energy level of the system splits in the absence of an external magnetic field.  $\delta_1$  is a small energy value due to crystalline field interaction. It is clear from the above that there is no linear temperature dependence of  $C_v / R$  as in Fermi liquid systems.

#### 4.2 Inverse temperature dependence of entropy (S)

The entropy (S) is related to the Gibbs function given by

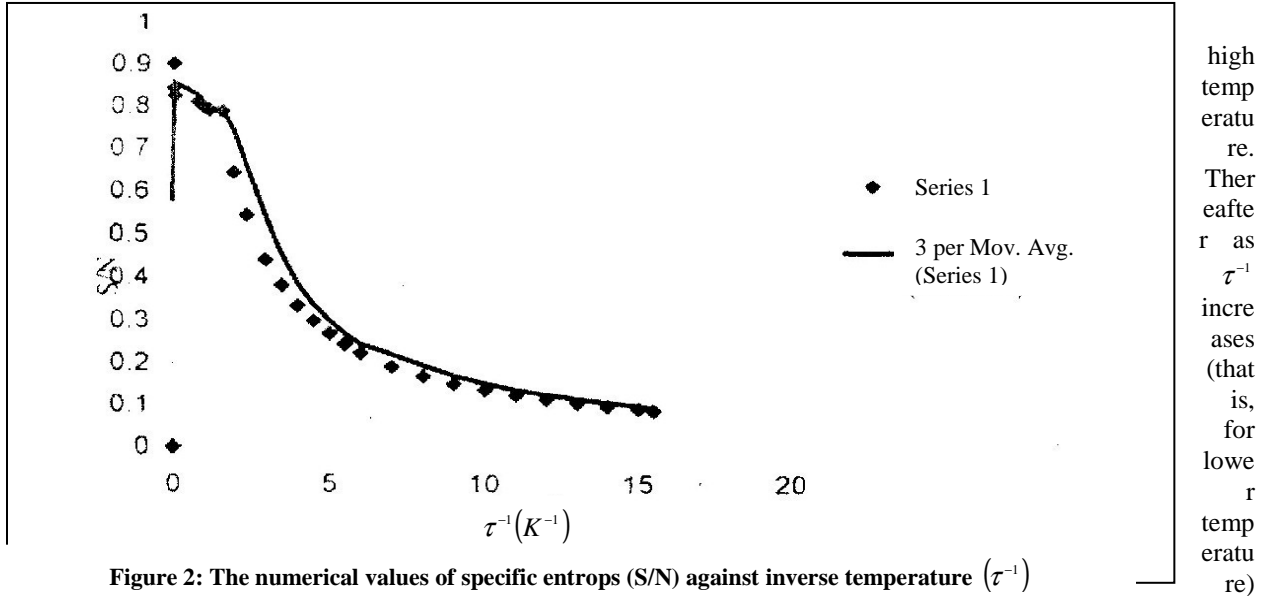
$$G = -NkT \ln Z \quad (4.13)$$

where  $Z$  is a partition function given by Equation (4.7). Therefore, the entropy function is

$$\begin{aligned} S &= -\frac{dG}{dT} = \frac{\partial NkT}{\partial T} \ln Z \\ S &= NkT \left[ \frac{a}{kT^2} + \frac{2a \exp(a\beta) + 2b \sinh(b\beta)}{2 \exp(a\beta) + 2 \cosh(b\beta)} \right] \\ S/N &= -ak\beta + \beta^{-1} \left[ \frac{a \exp(a\beta) + b \sinh(b\beta)}{\exp(a\beta) + \cosh(b\beta)} \right] \end{aligned} \quad (4.14)$$

This is the specific entropy and measure of the spin disorder in the system. The graph of  $S/N$  versus  $1/\tau$  is shown in fig. 2 for  $a = 1.3eV, b = 0.72eV, t = 0.43eV$  and  $u = 5.4eV$ .

As is evident from this graph,  $S/N$  versus  $\tau^{-1}$ , there is maximum entropy at  $\tau^{-1} = 0K$  corresponding to



the  $S/N$  which has the correct physical behaviour of the entropy function for varying temperature at very high temperature (maximum disorder) the entropy is high; at low temperature (minimum disorder) the entropy is least.

### 4.3 Inverse temperature dependence of spin pair susceptibility ( $\chi \uparrow \downarrow$ )

The pair susceptibility ( $\chi \uparrow \downarrow$ ) is given by  $\chi \uparrow \downarrow = \langle C_{2k\uparrow} C_{2k\downarrow} \rangle$ . Here  $\chi \uparrow \downarrow = \frac{1}{2} E_k \tanh(\frac{1}{2} \beta E_k)$

The graph of  $\chi (m^2 / mol)$  versus  $1/\tau (K^{-1})$  for  $a = 1.35eV, b = 0.72eV, t = 0.43eV$  and  $U = 5.4eV$  from equation. (4.15) is given in Figure 3.

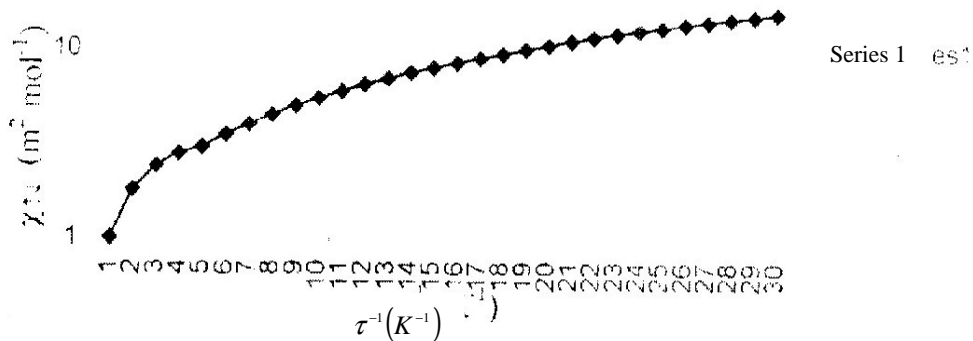


Figure 3: The numerical values of spin susceptibility  $\tau^{-1}(\chi \uparrow \downarrow)$  against inverse temperature ( $\tau^{-1}$ )

The essential feature of this graph is its ascent at low  $\tau^{-1}$  (high temperature T) and maintaining a quasi-plateau as T goes smaller. Indeed, the  $\chi \uparrow \downarrow$  behaviour as  $\tau^{-1}$  changes is similar to the magnetization curve for  $G_dBa_2Cu_3O_x$  polycrystals in the magnetic spin ordered phase.

The form of the susceptibility  $\chi \uparrow \downarrow$  versus  $\tau^{-1}$  plot shows novel similarity to the experimental plots of magnetization per magnetic dipole versus applied magnetic field per unit temperature for chromium potassium alum, iron ammonium alum and gadolinium sulphate which are magnetic ion sub-systems. These curves are also in agreement with the theoretical Brillouin function plots or odd half-integral J values [14]

In this case, the plateau in  $\chi$  as T goes very small, is a  $\chi = \chi_0$  feature of Fermi liquids while the ascent at high temperature is a non-Fermi liquid feature.

## 5.0 Summaries and conclusion

This paper set out to modify and apply the Bardeen-Cooper-Schrieffer model, which has been very successful in understanding superconductive pairing in Fermi liquid systems to non-Fermi liquid systems such as the copper oxide materials. These materials manifest both magnetic pairing in the normal state and superconductive pairing in the excited state. The interest in the non-Fermi liquid magnetic normal state of these materials.

In our generalization of the two-band BCS model to now cater for non-Fermi liquid systems we have tried to emphasize (1) the two different spin orientations, (2) a modification of the pairing potential which now depends upon the hopping and (3) the dominance of the kinetic term. This emphasis is new and important in the understanding of the new features. For the normal NFL system in the normal state, we transformed the Hamiltonian into the reduced mean-field two-band pseudospin representation. A Green's Function analysis of the Hamiltonian leads to magnetic and non-magnetic energy spectra. These are used to compute the electronic specific heat, the specific entropy and the magnetic pair susceptibility. These functions show NFL manifestations.

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