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BARDEEN-COOPER-SCHRIEFFER MODEL REVEALS POSSIBLE NON-FERMI LIQUID FEATURES

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ABSTRACT

The Bardeen-Cooper-Schrieffer (BCS) singlet pairing model, which newly incorporates particle states nonorthogonality, has revealed fractional exclusion of some electronic pair states. Fractional exclusion principle, as a generalisation of the Pauli exclusion principle, was recently discovered by Haldane in special spin-1/2 systems with extensive one-particle Hilber space dimension. This principle is freshly parameterized in our approximate mean-field BCS model and the latter is analysed via the matrix Greens function instrument. The results show possible non-equikinetic pair superconductivity and magnetic non-Fermi liquid (NFL) states, as recently observed in some correlated electron systems. Numerical predictions of the NFL specific heat and variation of the magnetic exchange with pair-kinetic-levels difference, $\varepsilon_{k\uparrow} - \varepsilon_{-k\downarrow}$, qualitatively agree with recent experiments on $Gd_{1-x}\ Y_x\ Ni_2\ Si_2$ and $Yba_2\ Cu_3\ 0_{6+y}$, which are well-known non-Fermi liquid systems.

1. INTRODUCTION

The conceptual simplicity of the electron (hole) pairing theory[1], in the Bardeen-Cooper-Schrieffer (BSC)[1] pairing model of superconductivity (SC), motives further exploration of that theory and model[1] for the possible understanding of the yet not-well-understood features of correlated electron systems (CES). This present as the basic issue raised by the discoveries[2] of novel SC and magnetism (both phase orders, perhaps, involving electron pairing) in CES, for example: the cuprates, the fullerides, the heavy fermions that constitute a large number of intermetallics that includes, the quaternary borocarbides.

With phonon mediation for pairing, intrinsic in the original BCS model, that model was intially regarded as inappropriate for understanding the new features, typically: high-temperature superconductivity[2], Bragg glass to vortex glass transition[3-5], and the ubiquity[6] of non-Fermi liquid (NFL)[7] states in CES. NFL states have, except as currently[8] by the present author, not been reported in the BCS model, to the best knowledge of this author. The generalisation of the BCS pairing theory and model to CES, enabling the latter to reveal the observed NFL states, is the challenge taken up in this paper. Newly in this paper, the non-Fermi liquid features are revealed in the electronic specific heat in addition to the already obtained NFL antiferromagnetism. The starting point for the calculations is the proposed MFL excitation energy spectrum.

Unmindful that the theoretic specifics for realising NFL states, along with other essential new features in different CES, pose serious and various conceptual problems, I first propose (in §2) some justification of a minimal modification of the original BCS

model to now explicitly obey the Pauli principle for spin energy levels. This will permit, in the model, the search (in §3) for its conformity with Haldane's[9] fractional exclusion principle for electronic pair-states. It will be found that the existence of this principle in the model, leads to the essential and novel realisation (in §4) of the magnetic NFL states and the non-Fermi liquid features of the electronic specific heat that experimentally exist in almost all CES, other features being, here, secondary. In §5, brief summary and concluding remarks are given.

2. BCS MODEL WITH PARTICLE-STATES NONORTHOGONALITY

Without loss of generality, I begin with correlated electron systems that have particle-states nonorthogonality[9]. The modelled CES is like a system of isolated unpaired spin -½ particles (spinous) in a singlet resonating valence bond background: a given spinon occupies its original site, moves (by hopping/flipping) to a vacant, isolated, single-particle site or a site that is part of a pair. Doubly-, singly- occupied, and vacant spin sites would result, these constituting the important entities of the model. The likelihood exists, of the appearance of bands with variable number of single-particle states in excess (deficit) of the mean particle number density of the 2- or 3-dimensional system. The likelihood exists, of the appearance of bands with variable number of single-particle state in excess (deficit) of the mean particle number density of the 2- or 3-dimensional system. The above ideas are alike of Laughlin "quasiparticles'[11] have the character of vortices with wave functions that are equivalent to the lowest Landau (LD)[12] level states. Fig. 1 schematically shows the propagation of single- and pair-particle states and vacancies in a system with nonorthogonal particle states. Single-particle hopping, (b) without spin flipping, and (c) with spin flipping, are illustrated starting with (a) as an arbitrary spin configuration of the fermion system.

An approximate BCS-like model, for these systems which, by virtue of single spin hopping/flipping, possess[0] extensive one- particle Hibert-space dimension, is the simple Hamiltonian:

$$H = \sum_{k\sigma} \varepsilon_{k\sigma} C^{+}_{k\sigma} C_{k\sigma} - \sum_{kk'} \left(V_{kk'} C^{+}_{k\uparrow} C^{+}_{-k'\downarrow} C_{-k'\downarrow} C_{k\uparrow} + h.c. \right). \qquad (2.1)$$

In eq. (2.1), $\varepsilon_{k\sigma}$ is the effective electronic kinetic energy measured relative to the chemical potential ($\mu \approx E_p$, Fermi energy), $C^{+}_{k\sigma}\left(C_{k\sigma}\right)$ is the creation (annihilation) operator for an electron with wave vector k and spin polarisation index $\sigma = \uparrow$ or $\downarrow$, while the subsript label $k\sigma$ means $-k'\downarrow$ for $\sigma = \downarrow$ with $-k'$ implied in all k', and the most general k- and k' -electron interaction is $V_{kk'}$. The Hamiltonian has the very simple form of the original BCS model, but differs from the latter in at least four important physical respects:

(a) There is dependence[13,14] here, of the electronic kinetic energy on spin, σ. Indeed, with the existence of single spin hopping/flipping, as may naturally be in a matrix of up- and down-spins, as guarantees the realisation of an extensive one-particle Hilbert space, and as manifests Haldane's nonorthogonality of the relevant three-site wave functions:

$$\left|1(23)>=\frac{1}{\sqrt{2}}\left[\left|2(13)>-\right|3(12)>\right],\right. \tag{2.2}$$

two spin-sublatice kinetic energies and interactions need be considered in the pairing theory.

(b) The magnetism, that may arise only by spin correlations and dynamics, as obtains[15]) in a Mott insulator, is intrinsic in the model by virtue of (a), with compliance to the Pauli principle. This possible magnetic state was absent in the original BCS model.

(c) The pair interaction $V_{kk'}$ in eq. (2.1), which was intrinsically only positive in the original BCS model, could presently be negative and of entirely different single or composite origin.

(d) By the consideration[16]) that the addition of an up- spin (say) in an arbitrary spin matrix, restricts the Hilbert space available to the existing down-spins, and the effective pair-interaction $V_{kk'}$ in such a system is basically statistical, the Landau level states pair-interaction[16]):

$$V_{kk'}^{LD}=\frac{.\eta\left|\epsilon_{k\uparrow}-\epsilon_{-k'\downarrow}\right|}{\left(k-k'\right)^{2}} \tag{2.3}$$

is (for $\eta > 0$) admissible in eq. (2.1). This would ordinarily not be admissible in the original pairing theory[1]) and model[1]).

3. CONFORMITY WITH HALDANE'S FRACTIONAL EXCLUSION

In order to elucidate the relevance of some of the above new features of the BCS model, I observe that the Frohlich[17]) pair-interaction:

$$V_{kk'}^{FR}=\frac{2\left|g_{k-k'}\right|^{2}\hbar\omega\,\theta\left(\hbar\omega-\Gamma-\left|\varepsilon_{k\uparrow}-\varepsilon_{-k'\downarrow}\right|\right)}{\left(\varepsilon_{k\uparrow}-\varepsilon_{-k'\downarrow}\right)^{2}-\left(\hbar\omega\right)^{2}}, \tag{3.1}$$

is, for SC, admissible in the form $-V_{kk'}^{FR}$ in eq. (2.1). With the functional arguments, $\left(\varepsilon_{k\uparrow}-\varepsilon_{-k'\downarrow}\right)$ and (k - k'), of $V_{kk'}^{FR}$ and $V_{kk'}^{LD}$, essentially the same, the realisation (eq.(2.3)) of the restatement[16]) of Haldane's fractional exclusion principle is expected to exist in eq. (3.1), in some related form.

This point may be clarified by noting that eq. (2.3) manifests unwanted singularity of $V_{kk'}^{LD}$, for k = k', and vanishes, for $\varepsilon_{k\uparrow}=\varepsilon_{k'\downarrow}$. These two undesirable conditions,

$$\varepsilon_{k\uparrow}=\varepsilon_{-k'\downarrow}, k=k', \tag{3.2}$$

are excluded in our physical system (i.e., in $V^{LD}_{kk'}$ of eq. (2.3), if eq. (2.3) is ever admissible, in eq. (2.1), for $V_{kk'}$,. Interestingly, the above conditions (eq. (3.2)) turn out as the most unwanted in the recent development[16,18,19]) of the theory of the so-called "tomographic Luttinger liquid", a fundamental NFL theory that hinges on eq. (2.3).

The admission of eq. (3.2), on the contrary, in $V_{kk'}^{FR}$, leads to the realisation o that potential not as null or as a singularity, but (for, $\theta(\hbar\omega - \Gamma) = 1$) as the simple constant value:

$$-V_{kk'}^{FR} = \left(\frac{2\left|g_{k-k'}\right|^2}{\hbar\omega} \right) \approx V_{BCS}. \tag{3.3}$$

Thus, for this admissibility, the potential $V_{kk'}$ of eq. (2.1) is necessarily $-V_{kk'}^{FR}$ for SC. It is then no coincidence, the complete accord of eq. (3.3) with the considerations by BCS[1)] in taking their $V_{kk'}$ to be a positive constant potential (V_{BCS}).

The above substitution of eq. (3.2) in eqs. (3.2) and (3.1), respectively, leads to two contrasting albeit complementary deductions from the $V_{kk'}^{FR}$ and statistical $V_{kk'}^{LD}$ considerations: what is excluded[16)] in one is included[1)] as essential in the other, and vice versa. On the basis of this simple paradigm, two questions are posed:

(i) What is the nature of $V_{kk'}$ in eq. (2.1), if it derives wholly or partly from the potential $V_{kk'}^{FR}$ with eq. (3.2) not holding?

(ii) What new realistions of a CES (as by eq. (2.1)) reveal in the new context of (i)?

The nature of the interaction, as (i) enquires, is straightforward: $V_{kk'}$ is no longer a constant as in the original BCS model. Additionally, this interaction could now be attractive or repulsive, depending on the condition:

$$\left|\varepsilon_{k\uparrow} - \varepsilon_{-k'\downarrow}\right| < \hbar\omega_c, \text{ or } \left|\varepsilon_{k\uparrow} - \varepsilon_{-k'\downarrow}\right| > \hbar\omega_c, \tag{3.4}$$

where ω_c is some characteristic boson (fermion) frequency (ω), as dictated by pairing mediation. The simplest valid deduction from eq. (3.4) is the new nonquikinetic-pair condition: $\varepsilon_{k\uparrow} \neq \varepsilon_{-k'\downarrow}$, for some allowed ω_c. It, immediately, leads to the conclusion that SC can exist in eq. (2.1) under such a condition that is clearly different from the original BCS (equikinetic-pair) condition, e.g. (3.2). Although the condition of eq. (3.4), with only "<", for SC, was, indeed, obtained by BCS, their starting criterion (eq. (3.2)) did not admit this new result (for $\varepsilon_{k\uparrow} \neq \varepsilon_{-k'\downarrow}$) as valid in their model, and it was missed out. For this important result to be accepted in the model[1)], the electronic kinetic energy ε_k, as in that model, must be generalised to a spin-dependent one: $\varepsilon_{k\sigma}$, as in eq. (2.1). This explicitly incorporates the necessary Pauli principle for fermions, and guarantees the physical realisations of (a) and (b) above.

The essential criterion for the possible nonquikinetic-pair superconductivity is that $V_{kk'}$ of eq. (2.1), under eq. (3.4), be positive for all boson (fermion) cutoff frequencies $\omega_c'(\omega_c'')$, where $\omega_c'' > \omega_c'$. This provides for possible joint boson-fermion mechanism of pairing in the CES of interest. For non-SC in the regime of eq. (3.4), on the other hand, the essential criterion is $V_{kk'} < 0$, in eq. (2.1). This, I suggest, is the condition for possible magnetic NFL states in CES. The on-set of nonequikinetic-pair SC arising from doping , as in $Yba_2Cu_3O_{6+y}$ ("123" system), is $V_{kk'} \approx 0$. This is co-terminus

with the disappearance of NFL non-SC states under eq. (3.4). Eq. (3.4) well agrees with the modification, of the BCS model, in eq. (2.1). it is really in this new scenario that one can investigate all the fringes of the correct answers to question (ii). In all cases, one considers singlet- pair states of general CES with states nonorthogonality and single spin dynamics (resulting from kinetic disorder) playing the most critical role. Recall that exclusive pair-hopping exists only in the equikinetic-pair regime of BCS, which excludes nonorthogonality and kinetic disorder.

In order to justify the above assertion, which seizes on the crux of the matter of question (ii),let me attempt a fresh understanding of eq. (2.1) in the context of the identification of the fractional exclusion principle (eq. (3.4)) rather as

$$\varepsilon_{k\uparrow} \neq \varepsilon_{-k'\downarrow} \quad k \neq k'. \tag{3.5}$$

My present interest is the application of eq. (3.5) in eq. (2.1) for all $V_{kk'}$ $\left(= V_{kk'}^{LD}, V_{kk'}^{FR}, \text{ or the combine}\right)$. The new NFL states, possibly derive from eq. (2.1) with eq. (3.5) in force. Should this be the case, eq. (3.5), would constitute the essential criterion for non-Fermi liquid states of the paired CES. Eqs. (3.2) and (3.5), which are complementary, would then constitute Haldane's fractional exclusion principle stated in terms of two key microscopic variables, $\varepsilon_{k\sigma}$ and kσ.

4. CHARACTERIZATION OF PROPOSED NFL STATES

By the above considerations, let me briefly analyze the possible NFL states, here proposed. Application of eq. (3.5) in eq. (2.1) leads to the mean-field Hamiltonian:

$$H = \frac{1}{2}\left\{ \sum_{k\sigma\sigma'} \varepsilon_{k\sigma'} C_{k\sigma}^{+} C_{k\sigma} - \sum_{kk'} \left(\varepsilon_{k\uparrow} C_{-k'\downarrow}^{+} C_{-k\uparrow} + \varepsilon_{-k'\downarrow} C_{k\uparrow}^{+} C_{k\uparrow} \right) \right\} - \sum_{kk'} \left(V_{kk'} \left\langle C_{-k'\downarrow} C_{k\uparrow} \right\rangle C_{k\uparrow}^{+} C_{-k'\downarrow}^{+} + h.c. \right). \tag{4.1}$$

This scheme is best, compactly written in pseudospin variables, as

$$H_{kk'} = \epsilon_{kk'} \propto_0 + \Delta_{kk'} \propto_1, \tag{4.2}$$

where

$$\epsilon_{kk'} = \frac{1}{2}\left(\varepsilon_{k\uparrow} - \varepsilon_{-k'\downarrow} \right), \quad \Delta_{kk'} = -V_{kk'} \left\langle C_{-k'\downarrow} C_{k\uparrow} \right\rangle, \tag{4.3}$$

$$\propto_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \propto_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4.4}$$

4.1 Excitation Energy Spectrum

In eq. (4.3), as in eq. (4.1), the expression <...> means the expectation value of the quantity in the angular brackets. Subsequent employment of the two-component wave function:

$$\Psi_{kk'}^{+} = \left(C_{k\uparrow}^{+} C_{-k'\downarrow} \right), \tag{4.5}$$

and the Hermitian conjugate, along with eqs. (4.2) – (4.4), recovers eq. (4.1) readily. A simple algebraic Green's function solution of eq. (4.2) is, in Fourier space, the matrix inverse:

$$G(k,k':i\omega_n) = (i\omega_n - H_{kk'})^{-1}, \tag{4.6}$$

in which $\omega_n (n = 0,\pm 1,\pm 2,...)$ is the fermonic Matsubara frequency. Substitution for $H_{kk'}$, in eq. (4.6), and simplification, lead to the excitation specturm:

$$E^{\pm}_{kk'} = \epsilon_{kk'} \pm J, \quad J = \Delta_{kk'} = J_{kk'}, \tag{4.7}$$

where the gap energy $(\Delta_{kk'})$ behaves as a magnetic exchange (J). By evaluating the pair functional, $\langle C_{-k'\downarrow} C_{k\uparrow} \rangle$, in eq. (4.3), the grand equation for J is obtained:

$$J - \frac{1}{2z_1 z_2}\{2(z_1 - J)J + z_1(n_1 z_1 + n_2 z_2)\}V_{kk'} = 0, \tag{4.8}$$

where,

$$z_1 = \epsilon_{kk'} + J, z_2 = \epsilon_{kk'} - J, n_i = n(z_i), \tag{4.9}$$

$$n(z) = (1 + \exp(\beta z))^{-1}. \tag{4.10}$$

I solve eq. (4.8), presently, for the typical occupancies $n_1 \approx 1$, $n_2 \approx 0$,, corresponding to $z_1 << T$ and $z_2 >> T$, respectively, under the constraints:

$$|\epsilon_{kk'}| > |J|, |V_{kk'}| > |\epsilon_{kk'}|, J, V_{kk'} \neq 0. \tag{4.11}$$

Ignoring terms $0(J^3)$, $0(1/V^2_{kk'})$, and higher orders, the real solutions are obtained as

$$J \approx \pm \frac{\epsilon^2_{kk'}}{V_{kk'}}. \tag{4.12}$$

These yield, in eq. (4.17), the new magnetic excitation spectrum for the possible NFL regime:

$$E^{\pm}_{kk'} \approx -\frac{V_{kk'}}{2} \pm \frac{at^2}{V_{kk'}}. \tag{4.13}$$

This has been so written by invoking the plausible approximation

$$-V_{kk'} \approx 2\epsilon_{kk'} \doteq ct. \tag{4.14}$$

The parameter t, in eq. (4.14), is the single spin hopping/flipping matrix, and the factors a and c are numerical constants. Eq. (4.13) has the form of the standard magnetic spectrum (for the Hubbard potential: $U \approx V_{kk'}$) of the Hubbard model[20], newly manifesting in the BCS pairing model.

The plots of the antiferromagnetic excitation energy, $E_{kk'}/t$, against pair-kinetic-levels difference, $(\varepsilon_{k\uparrow} - \varepsilon_{-k'\downarrow})/t$, are presented in Fig. 2, for various $\pm a$. the curves for our proposed NFL "quasiparticle" regime, exist only in the negative energy difference

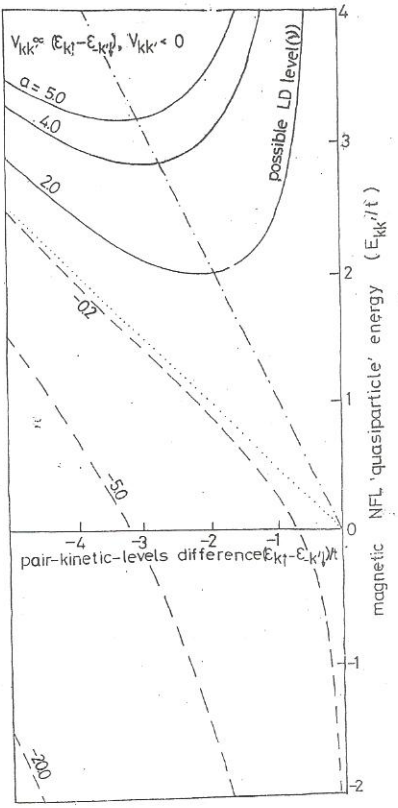


Fig.2 **Antiferromagnetic NFL excitation energy eq. (4.13) of a CES, $E^{-}_{kk'}/t$, against pair-kinetic-levels differences ($\left(\varepsilon_{k\uparrow} - \varepsilon_{-k'\downarrow}\right)/t$, for $V_{kk'} \propto \left(\varepsilon_{k\uparrow} - \varepsilon_{-k'\downarrow}\right)$ and a = ± 5.0, 4.0, 2.0, -0.2 and –20.0, as indicated. We have indicated +a (continuous), -a (dashed), trajectory of energy minima (dash-dot) and cutoff limit (dotted) Curves for integral ±a may correspond to the lowest Landau level states of index ν = ±a.**

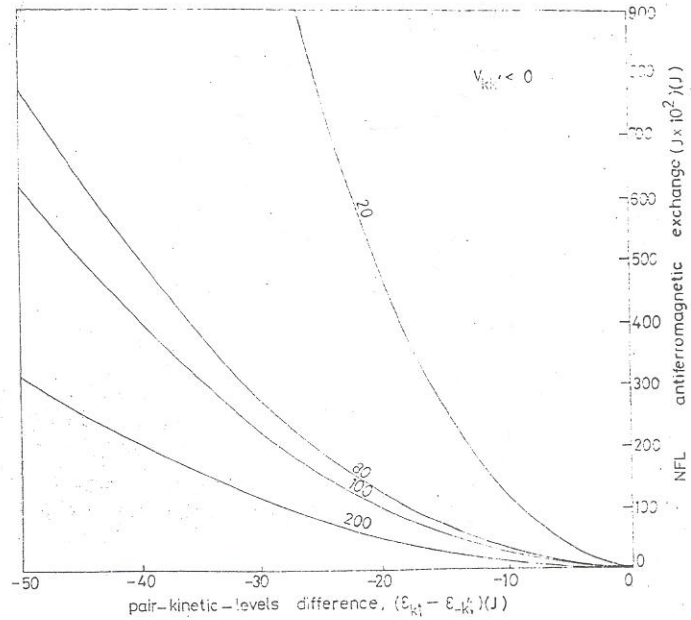


Fig. 3: **Anteferomagnetic NFL exchange (J) versus pair-kinetic- levels differences $\left(\varepsilon_{k\uparrow} - \varepsilon_{-k'\downarrow}\right)$ of eq. (4.12), for $|V_{kk'}| > |J|$. The curves are for $V_{kk'}$ constant (Joules indicated). These curves are in qualitative agreement with the experimental Neel temperature (T_N) versus oxygen parameter (y) plot[22] for the CES, $Yba_2Cu_3O_{6+y}$. incipient antiferromagnetism is deduced as the origin of the non-Fermi liquid behaviour of these systems.**

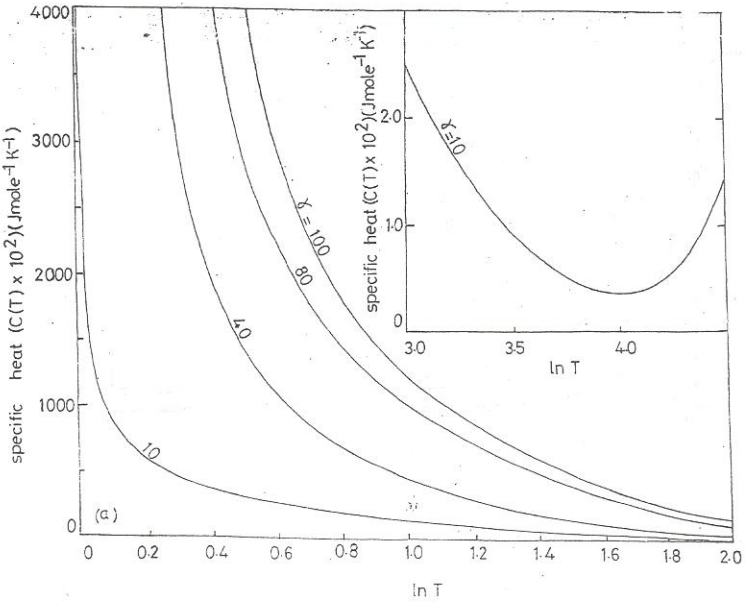
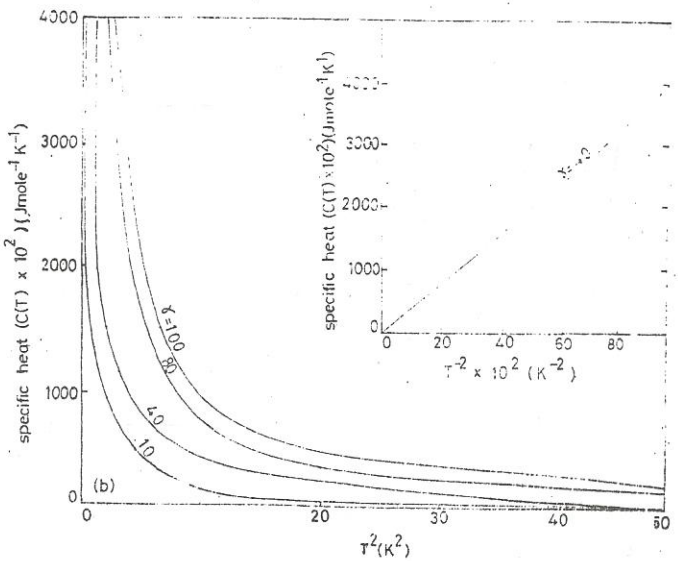


Fig. 4 Low-temperature specific heat variations in the general CES for constant γ (eq. (4.17)): (a) C(T) against lnT, (b) C(T) against T^2; inset: (a) C(T) against LnT revealing an upturn due to greater influence of J at higher low-temperature, for γ = 10 JK/mole, (b) C(T) against T^{-2} revealing linearity (γ=40 JK/mole) as for $Gd_{0.4}Y_{0.6}Ni_2Si_2$ by Sampathkumaran and Das[25].


specific heat (C(T) x 10^2){Jmole^-1 K^-1)
4000
3000
2000
1000
0
(b)
0
20
30
40
50
T^2(K^2)
θ=100
80
40
10
specific heat (C(T) x 10^2){Jmole^-1 K^-1)
3000
2000
1000
0
0
20
40
60
80
T^-2 x 10^2 (K^-2)

The obtained total molar internal energy of the system leads to the temperature- and exchange-energy-dependence of the electronic specific heat:

$$C(T,J) = \left\{\gamma(T,J) + 4J^2 / \left(1 + \exp(2J/T)\right)^2\right\} T^{\alpha} \qquad (4.17)$$

where $\alpha = -2$. I have, in eq. (4.17), set the Boltzmann constant $k_B = 1$, $J >> k_BT$, and γ is an aggregate function of T and J. This function (γ) may rather be regarded as slowly varying (or, indeed, approximated to a constant), the variations of C(T) are given in Fig. 4, for γ constant.

Fig. 4(a) shows the variation of C(T) with lnT for various γ, which is only illustrative (with the rough γ). There is C(T) divergence as $T \rightarrow 0$, as observed[24] in some CES. The inset, for $\gamma = 10$ JK/mole typically, exhibits an up-turn has been observed[25),26)] in CES and interpreted[26)], in systems as $Gd_{1-x}Y_xNi_2Si_2$[26)], as originating from short range magnetic correlations.

Fig. 4(b) is the C(T) versus T^2 variation. The inset of Fig. 4(6) is the C(T) versus T^{-2}, that manifests a linearity largely predicated on constant γ and $k_BT >> J$. Surprisingly the obtained linearity is consistent with Fig. 4(a) by Sampathkumaran and Das[25)] for $Gd_{0.4}Y_{0.6}Ni_2Si_2$. This result argues that an inverse-square-law temperature dependence: $C(T) \approx \gamma T^{-2}$ for γ constant, is not a bad approximation for some low-temperature CES, especially above a certain temperature. Below this minimum temperature, Schottky-like contribution to specific heat is deduced as by the experimental upturn in C/T versus T^2 in the high-T_c cuprates, $Bi_4Ca_3Sr_3Cu_40_{16+y}$[27)] and $Tl_2Ba_2Ca_{n-1}Cu_n0_{2n+4}$[28)], down to millikelvin temperatures.

5. SUMMARY AND CONCLUSION

A novel consideration of the Bardeen-Cooper-Schrieffer pairing model, in mean-field approximation, is presented and is applicable to a wide range of correlated electron systems. Haldane's fractional exclusion, as a generalization of the Pauli principle, is newly parameterized and employed in sifting out pair states of interest in correlated electron systems.

Some new criteria for isolating and investigating, in the simple BCS model, the largely complicated regimes of CES are thus pointed out. Possible non-Fermi liquid states that may be incipiently magnetic are revealed and briefly characterized. The presently obtained weak power-law temperature dependence of the electronic specific heat (in eq. (4.17)) and the inset (of Fig. (4b)) and the divergences (Fig. 4) in C(T) as $T \rightarrow 0$, are common indicatives of true NGL behaviour of the correlated electron systems cited. In my earlier paper[8)] only the behaviours of the magnetic exchange and Neel temperature were reported in the NFL regime.

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