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High temperature superfluidity with abnormal fermionic occupancy

V.C. Aguilera-Navarro[1], M. de Llano[1]*, A. Plastino[1], R. Rossignoli[2]*****

[1] Instituto de Física Téorica, Universidad Estadual Paulista, R. Pamplona 145, 01405 São Paulo, Brazil
[2] Departamento de Física, Universidad Nacional de La Plata, C.C. 67, 1900 La Plata, Argentina

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We examine a Lipkin based two-level pairing model at finite temperature and in the thermodynamic limit. Whereas at $T=0$ the model exhibits a superconducting ground state for sufficiently high values of the coupling constant, a partially superconducting phase in which *some* of the particles are paired, is found to survive at high temperatures in a special treatment. This phase is a mixture of "abnormally-occupied" eigenstates, which lie at higher energy, of the interactionless model Hamiltonian.

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I. Introduction

Exactly soluble models such as the renowned Glick-Lipkin-Meshkov (GLM) model [1] have proved to be extremely valuable in studies concerning the validity and/or usefulness of diverse theoretical approaches developed to investigate many aspects of the quantum many-body problem for a finite number N of interacting spin-1/2 fermions. This model is based on the $SU(2)$ algebra associated with the so-called "quasispin" operators, and provides readily available exact solutions against which can be tested the results of different approximations. Quasispin operators were previously employed by Anderson [2] to reformulate the BCS theory of superconductivity.

Of the several multiplets associated with the possible eigenvalues of the relevant Casimir operator [1] only the one corresponding to the unperturbed ground state (*ugs*) of the system has been extensively dealt with in the literature. Cambiaggio and Plastino [3] have shown that the study and classification of *higher-energy* allows one to add a pairing-like interaction to the model without going beyond a $SU(2)\times SU(2)$ algebra. In this way, the notion of quasispin superfluidity can be incorporated into the model and treated exactly.

The thermodynamic limit ($N\gg 1$) of the GLM model and its extension to accommodate finite temperatures are the subject of an illuminating series of papers by Gilmore and Feng [4], and conveniently summarized in the book by Gilmore [4]. The corresponding treatment appropriate for dealing with quasispin superfluidity has been given by Rossignoli and Plastino [5], including the finite temperature mean field description.

In the present work we show that the higher energy multiplets referred to above lead to the concept of *abnormal occupancy* [6] of single particle states, and can be easily incorporated within an $SU(2)\times SU(2)$ framework. This in turn makes possible the construction of superconducting states which survive at high temperatures even for weak coupling.

II. The model

The GLM model deals with N spin 1/2 particles distributed in two 2Ω-fold degenerate single particle (s.p.) levels separated by the s.p. energy ε. We designate the 2Ω lower (upper) states by $|p,\mu=-1\rangle$ ($|p,\mu=-1\rangle$), with $p=1,\dots,2\Omega$. We introduce the so-called Lipkin quasispin operators [1],

$$\hat{J}_z=\tfrac{1}{2}\sum_{p,\mu}\mu C^+_{p\mu}C_{p\mu},\qquad \hat{J}_+=\sum_p C^+_{p+}C_{p-}=\hat{J}^+_-, \tag{1}$$

and the quasispin pairing operators [3]

$$\hat{Q}_0=\tfrac{1}{2}\sum_{p,\mu}C^+_{p\mu}C_{p\mu}-\Omega=\tfrac{1}{2}\hat{N}-\Omega,\qquad \hat{Q}_+=\sum_p C^+_{p+}C^+_{p-}=\hat{Q}^+_-, \tag{2}$$

* On leave from Physics Department, North Dakota State University, Fargo, ND 58105, USA
** On leave from Universidad Nacional de La Plata, Argentina
*** Member of the Scientist Research Career of CICBA, Argentina

where $\hat{N}$ stands for the number operator and the C's are ordinary fermion creation and destruction operators. Each set of operators (J and Q) separately obey angular-momentum-like commutation rules implying the group $SU(2)$. Moreover, every Q-operator commutes with each J-operator, implying a group structure $SU(2)\times SU(2)$. Obviously, $\hat{Q}_+$ creates, and $\hat{Q}_-$ destroys, two particles coupled to $J_z=0$. Thus, it becomes natural to introduce a quasispin "pairing" Hamiltonian

$$\hat{H}=\varepsilon \hat{J}_z-\tfrac{1}{2}\,|G|\,\hat{Q}_+\,\hat{Q}_- \tag{3}$$

with $|G|$ a coupling parameter. It is possible to form a complete orthogonal basis set characterized by the eigenvalues $J(J+1)$, $Q(Q+1)$, J_z, Q_0 of the operators $\hat{J}^2$, $\hat{Q}^2$, $\hat{J}_z$, $\hat{Q}_0$, say $|J, Q, J_z, Q_0\rangle$. There exists yet a further symmetry to be accounted for, as every J or Q operator commutes with any of the $2\Omega!$ operators that exchange the given p-spins [7]. This additional symmetry gives rise to a multiplicity $Y(J, Q)$ for a given state $|J, Q, J_z, Q_0\rangle$, essential to evaluate the entropy, specified [5] by

$$Y(J,Q)=\frac{(2\Omega+2)!\,(2\Omega)!\,(2J+1)\,(2Q+1)}{\begin{array}{c}(\Omega+J+Q+2)!\,(\Omega+J-Q+1)!\\ (\Omega-J+Q+1)!\,(\Omega-J-Q)!\end{array}}, \tag{4}$$

where the possible values of J and Q are constrained by the inequalities (for $N=$ even)

$$\begin{aligned}&0\leqq J\leqq \Omega-|Q_0|\,,\\ &|Q_0|\leqq Q\leqq \Omega\,,\\ &|Q_0|\leqq J+Q\leqq \Omega\,.\end{aligned} \tag{5}$$

In studying ground states, only the $J+Q=\Omega$ "band" needs to be considered. However, for nonzero temperature, a host of states belonging to other "bands" may become accessible to the relevant statistical ensemble [5].

A very useful concept is that of the quasispin seniority defined [3] as

$$v=2(\Omega-Q)\,, \tag{6}$$

which specifies the maximum possible number of "unpaired" particles compatible with a given value of Q. Following common usage, in this paper we set $N=2\Omega$, which from (2) implies $Q_0=0$, i.e., we will not consider states with $Q_0\neq 0$.

III. Zero temperature results

In order to meaningfully discuss the concept of abnormal occupancy, we shall digress from our central theme by briefly referring to the so-called monopole interaction [1]

$$\hat{V}=\tfrac{1}{2}\,\chi\,(\hat{J}_+^2+\hat{J}_-^2)\,, \tag{7}$$

with χ a coupling constant. The interaction (7) exhibits properties resembling those of the multipole-multipole (long-ranged) type often found in some microscopic nuclear models [8]. Adding this term to the hamiltonian (3) permits detailed studies [2] of the competition between short-ranged (pairing) and long-ranged interactions characteristic of many nuclear models at zero [3] or at finite [5] temperatures. It turns out that for $|\chi|\leqq \varepsilon/(N-1)\equiv\chi_c$ the *ugs* coincides [1,9] with the Hartree-Fock (HF) solution of

$$\hat{H}=-\varepsilon \hat{J}_z+\tfrac{1}{2}\,\chi\,(\hat{J}_+^2+\hat{J}_-^2)\,. \tag{8}$$

For $|\chi|>\chi_c$ the *ugs* becomes unstable against 2 particle-2 hole excitations and the HF solution becomes a linear combination of states with $J=N/2$ and $J_z=-N/2,\ldots,+N/2$, with coefficients specified [1,9] by the binomial distribution $\binom{N}{J_z+\frac{1}{2}N}$.

Actually, the intensive HF energy becomes independent of N as a function of $\chi'=\chi\,(N-1)$, so that the previous picture holds also in the thermodynamic limit ($N\gg 1$). Thus, the fact that the *ugs* coincides with the HF solution for a finite range of coupling values is also true in this case, where it is known [4–5] that HF yields exact intensive mean values (but not fluctuations [10]) in this type of model.

Similarly, a Fermi sphere of plane waves (PW) with k values filled up to the Fermi momentum k_F constitutes the lowest energy PWHF solution for a variety of two body interactions [6] modeling numerous neutral quantum fluids. Such a state has been called [6] the *normal occupancy state.* We here extend that designation to the *ugs* (Fig. 1, upper panel) denoted by $|J=N/2, J_z=-N/2, Q=Q_0=0\rangle$, which as we have seen, provides the lowest HF energy also for a finite range of coupling values. Thus, normal occupancy is associated within the GLM model with a complete absence of pairs of fermions coupled to $J_z=0$ ($Q=0$). At this point, having established this concept, we leave the subject of the monopole interaction [7].

In the same vein, a state with $Q\neq 0$ and $J_z=-v/2$ is the lowest-lying state of the multiplet $|J<N/2, Q, J_z, Q_0=0\rangle$ for an interactionless GLM system, but this state lies at an energy *higher* than that corresponding to the *ugs.* These states correspond to *abnormal* occupancy, in keeping with the terminology of [6], and which are typified by lower energy N-particle HF determinants possessing unoccupied s.p. states below the highest occupied s.p. state. Abnormal occupancy is thus characterized within the GLM model by the existence of *some* pairs of fermions coupled to $J_z=0$, namely, by a seniority v smaller than $v_{\max}\equiv N$, see Fig. 1, lowest panel. Abnormal occupancy becomes an important concept if, for some interacting many-body system, the concomitant "abnormal" states are energetically favored by the two body interaction [6]. This in fact is the situation here with the hamiltonian (3) as we shall see.

Indeed, one easily finds (the subscript zero indicates zero temperature) [3] that, for weak enough coupling, [see below, (13)],

$$E_0(ugs)=E_0(\text{normal})=-\tfrac{1}{2}\,\varepsilon N \tag{9}$$

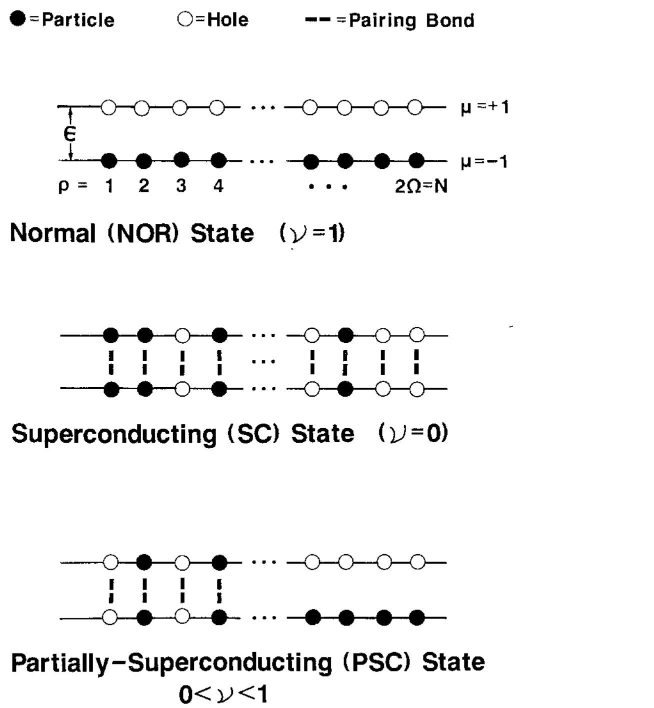

Fig. 1. Illustration of the GLM two-level model with 2Ω different states (labeled by p) occupied by $N(=2\Omega)$ particles, all in the lowest level (top panel); half in the lower and half in the upper level, and all paired (middle panel); and a mixed situation in which a certain fraction $0 < \nu < 1$, defined in (6) and (14) of the particles are unpaired (lowest panel)

represents the ground-state energy. On the other hand,

$$E_0(\text{abnormal}, v < N) = -\tfrac{1}{2}\,\varepsilon N + \tfrac{1}{2}\,\varepsilon\,(N-v) - \tfrac{1}{2}\,|G|\,[\tfrac{1}{2}(N-v)][\tfrac{1}{2}(N-v)+1], \tag{10}$$

so that

$$E_0(\text{abnormal}) \leqq E_0(ugs)$$

$$\text{for} \quad |G| > \frac{2\varepsilon}{\Omega + 1 - \frac{v}{2}} \equiv G_c^v \tag{11}$$

Analogously, the ordinary superconducting state (SC) (see Fig. 1, middle panel) is that associated with $v=0$ [8]. Thus [3]

$$E_0^{sc} = -\tfrac{1}{2}\,|G|\,\Omega\,(\Omega+1) \tag{12}$$

so that E_0^{sc} lies lower than $E_0(ugs)$ whenever

$$|G| > G_c^0 = \frac{2\varepsilon}{\Omega + 1 - \frac{v}{2}} \tag{13}$$

and where we note that $G_c^v > G_c^0$ for $v > 0$.

Let us consider now the thermodynamic limit. Appropriate scaling suggests introducing the following "intensive" quantities [4, 5]

$$r \equiv J/N, \quad q \equiv Q/N, \quad \nu \equiv v/N, \tag{14a}$$

$$g \equiv N|G|, \tag{14b}$$

and, if present, $\chi' = \chi\,(N-1)$, with ε remaining unscaled. The quantities (14a) can be regarded as continuous variables in this limit. Thus, ν is the maximum fractional number of particles which are unpaired. The coupling constant scalings are required in order to obtain finite intensive energies in the thermodynamic limit [4, 5]. With these scalings, the same qualitative conclusions as above hold in this limit, and equation (11) becomes $g > 4\varepsilon/(1-\nu) \equiv g_\nu^c$.

In case the monopole interaction (7) is present, the value of G_v^c is higher (see [3] for more details). In the thermodynamic limit, where the intensive HF energy is exact, we have $g_{\nu\chi'}^c = 4[\chi'(\nu/2)^2 + \varepsilon^2/4\chi']/(1-\nu)^2$.

It is important to stress that our abnormal states ar *partially superconducting* (PSC) states (see Fig. 1, lowest panel) with particles unpaired, but still characterized by the existence of pairs of fermions coupled to $J_z = 0$, which can be scattered by the $\hat{Q}_+\,\hat{Q}_-$ interaction term in (3) into doubly unoccupied states (p^+, p^-) (hole pairs). A flow (or "hopping") of pairs thus becomes possible in these PSC states, hampered only by the presence of the unpaired particles. We shall then find that, in addition to the ordinary $v=0$ superconductivity, the extended (pairing) GLM model exhibits other types of superconductivity, for all values of the coupling parameter.

IV. Finite temperature results

We now proceed to switch on the temperature. Two qualitatively different situations ensue: the finite N case and the thermodynamic limit. Without embarking into any explicit calculation, by recourse to the *crossover theorem* [4] for the present model, we can state that if our system undergoes a ground state ($T=0$) phase transition (from normal to ordinary superconducting) as we increase the coupling constant $|G|$, then the system will undergo the *reverse thermodynamic phase transition* at fixed G when T is increased.

Hence, noting that according to (11) and (13), $G_c^v > G_c^0$, which implies for the reverse thermal transition $T_c^v > T_c^0$, we reach the conclusion that the PSC phase survives at higher temperatures than the ordinary SC state. We next proceed to a detailed study in the thermodynamic limit, where we shall show that the PSC phase may survive at arbitrarily high temperature. This limit has been extensively studied in [4] and [5], and we employ throughout the notation of the latter reference. Earlier fundamental work, but related to the BCS model, can be found in [11].

We shall work in the present work within the "ground state band" [3]

$$r + q = \tfrac{1}{2}, \tag{15}$$

so that

$$r = \tfrac{1}{2}\,\nu, \quad q = \tfrac{1}{2}(1-\nu). \tag{16}$$

The entropy per particle [5] is

$$\lim_{2\Omega\to\infty} \frac{\ln[Y(J,Q)]}{2\Omega} = s(r,q) \equiv s(v) \tag{17}$$

which after employing Stirling's formula reads

$$s(v) = -k[(1-v)\ln(1-v) + v\ln v]. \tag{18}$$

This vanishes for $v=0$ and $v=1$, and is a maximum with value $k\ln 2$ for $v=1/2$. The free energy per particle can be expressed solely in terms of the intensive seniority v as

$$f = \lim_{2\Omega\to\infty} \langle \hat{H} \rangle / 2\Omega - Ts(v) \tag{19a}$$

$$= -\tfrac{1}{2}\varepsilon v - \tfrac{1}{8}g(1-v)^2$$

$$+kT[(1-v)\ln(1-v) + v\ln v], \tag{19b}$$

For fixed coupling g and fixed temperature T, $f(v)$ will possess an extremum if $f'(v)=0$, i.e., when

$$v = \{1 + \exp[\tfrac{1}{2}(g(1-v) - \varepsilon)/2kT]\}^{-1}$$

$$= \{1 + \exp[(\mathrm{d}E(v)/\mathrm{d}v)/kT]\}^{-1}, \tag{20}$$

where $E(v) = -\frac{1}{2}\varepsilon v - \frac{1}{8}g(1-v)^2$ is the intensive mean energy. Clearly, we get a Fermi distribution with zero chemical potential, where $\mathrm{d}E(v)/\mathrm{d}v$ is the energy required to change the seniority from v to $v+\mathrm{d}v$. The form (20) is expected since we are dealing throughout with the grand canonical formalism. This (exact) variational procedure can be shown to be equivalent to a (constrained) finite temperature BCS treatment [5, 12], with the accessible states restricted to the ground state band. Our extremum is also a minimum if $f''(v) > 0$, or when

$$[v(1-v)]^{-1} > g/(4T). \tag{21}$$

Whereas for $T=0$ (21) admits only $v=0$ or $v=1$, for $T>0$, $0<v<1$. Thus, three different situations or phases occur according to the value of v, namely,

a) $v=0$, ordinary superconducting (SC) phase, with

$$f(0) = -g/8 \tag{22}$$

b) $v=1$, normal (NOR) phase, with

$$f(1) = -\varepsilon/2 \tag{23}$$

and

c) $0<v<1$, partially superconducting (PSC) phase.

The latter includes the *maximum entropy* state, characterized by $v=\frac{1}{2}$. Therefore, from (19), this is the value which minimizes $f(v)$ at *infinite temperature*, demonstrating thus that the PSC phase survives at arbitrarily high temperatures. For $T=0$, (22) and (23) give $f(0) > f(1)$ for $g > 4\varepsilon$, implying that the SC phase is more stable in this region. Figure 2 summarizes the three phases in the $g-kT$ plane.

For finite N, the straightforward procedure is to evaluate the partition function [5] using the multiplicity factor (4). In the same way as before, for finite N the multiplicity is maximum for $v=N/2$ within the ground state band. Hence, a PSC state will become the most probable state as T increases for any $N=2\Omega$.

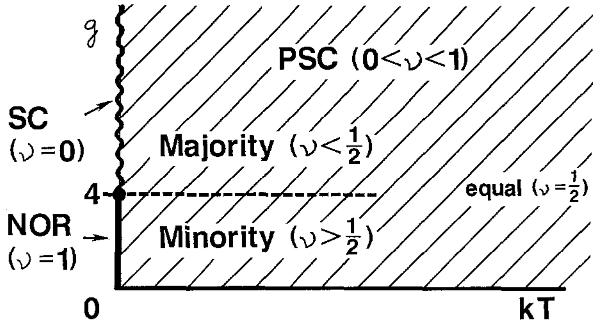

Fig. 2. Pairing GLM model N-body system phase diagram indicating regions where each of the three 'phases' described in Fig. 1 is most stable, as a function of the coupling g and temperature kT (both in units of ε, Fig. 1). The partially-superconducting (PSC) region is divided into three subregions where a majority, a minority or equal numbers of the N particles are unpaired in the lowest free-energy state as given by (19) minimized with respect to v

Table 1. Values of v which minimize the free-energy-per-particle (19) for typical values of g and kT (both in units of ε)

$g\backslash kT$	0.0	0.2	0.4	1.0	3.0	6.0	9.0
1	1	0.917	0.749	0.599	0.532	0.516	0.510
12	0	6×10^{-5}	0.002	0.100	0.391	0.453	0.470

Table 2. Values of $-\min_v f(v)$ for typical values of g and kT (both in units of ε), where $f(v)$ is the free-energy-per-particle (19)

$g\backslash kT$	0.0	0.2	0.4	1.0	3.0	6.0	9.0
0	0.5	0.516	0.601	0.975	2.34	4.41	6.49
1	0.5	0.517	0.608	0.994	2.37	4.44	6.52
4	0.5	0.521	0.652	1.07	2.45	4.53	6.61
10	1.25	1.25	1.25	1.40	2.67	4.73	6.81

In this paper we are especially interested in situation (c). Note that both the NOR and SC phases are highly ordered phases not ordinarily expected to survive high temperatures. We have calculated the minimum value of (19) for many pairs of values $(g/\varepsilon, kT/\varepsilon)$, for each of which the transcendental (20) was solved and the condition (21) verified as a check. Table 1 lists some typical v values minimizing f for $g/\varepsilon=1$ and 12. It clearly illustrates how for low temperatures and fixed $g/\varepsilon<4$, a *minority* $(v<\frac{1}{2})$ of the particles are paired, whereas for $g/\varepsilon>4$ a *majority* of particles are paired. For $T\to\infty$, we have an equal number of paired and unpaired particles $(v=\frac{1}{2})$. Table 2 gives some typical absolute values of the minimum free energy for several pairs of values $(g/\varepsilon, kT/\varepsilon)$.

V. Conclusions

Many quantitative and qualitative aspects of superconductivity are mimicked by a suitably extended version of the two-level GLM model, which has the advantage of being exactly soluble, so that no approximations are needed to deal with the facets of the superconducting problem of interest. Here we were looking for nonordinary superconducting phases, and it has been shown that the model indeed exhibits them. Furthermore, these partially superconducting phases survive at arbitrarily high temperatures in ground-state band calculations.

Our partially superconducting phase is a mixture of states with just *some* of the particles paired which, in the absence of interactions, are higher in energy compared with the normal state in which no particles are paired. The concomitant states can be regarded as abnormally occupied in the spirit of [6]. For weak coupling ,this phase consists of states where a minority of the particles are paired, whereas for coupling greater than a certain critical value it consists of states with a majority of the particles paired.

In both cases, as the temperature rises, this phase approaches a mixture of *equal* numbers of paired and unpaired fermions. The inherent mechanism responsible for the survival of this non-ordinary superconducting phase is the fact that in the ground state band the number of accessible states reaches a maximum for $v=\frac{1}{2}$. We conclude that abnormal occupancy and constrained statistics may be intimately connected with high-T_c superconductivity phenomena.

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