in every process of pair creation the system is required to remember how many pairs of each type it started with. Such considerations mitigate the initial physical attractiveness of the model due to its simplicity and help to indicate why the inconsistency described above arises.

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DIFFICULTY IN THE METHOD OF GREEN'S FUNCTIONS FOR A MANY-BODY SYSTEM*

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In the last few years, the method of Green's functions,[1] based on the infinite set (S) of coupled equations (with boundary conditions) satisfied by the sequence of n-particle Green's functions, has been used extensively[2-6] in the theory of superconductivity.[7] While (S) is a consequence of the Schrödinger equation, it is often believed, although not proved, that the converse is also true. In fact, we have shown, by solving an example exactly, that (S) may possess spurious solutions, some of which lead to an energy lower than the true ground-state energy, and so do not correspond to any state wave function. Thus the Green's function method as usually formulated is not a complete dynamical description of the system, and requires in addition some criterion to distinguish these extraneous solutions from the correct one.

This work was developed in order to choose between two contradictory theories[8-10] of the possible superfluid phase of He^3. These theories can be discussed in terms of the truncated pair Hamiltonian

$$H=\sum_{\vec{k}\sigma}(\epsilon_{\vec{k}}-\mu)a_{\vec{k}\sigma}^{\dagger}a_{\vec{k}\sigma}+\Omega^{-1}\sum_{\vec{k}\vec{k}'}V_{\vec{k}\vec{k}'}a_{-\vec{k}\downarrow}^{\dagger}a_{\vec{k}\uparrow}^{\dagger}a_{\vec{k}'\uparrow}a_{-\vec{k}'\downarrow}, \quad (1)$$

where $a_{\vec{k}\sigma}^{\dagger}$ creates a plane wave of momentum $\vec{k}$ and spin σ in the volume Ω. A model potential is chosen which vanishes unless $\vec{k}$ and $\vec{k}'$ lie inside a thin spherical shell centered on the Fermi surface, in which case

$$\Omega^{-1}V_{\vec{k}\vec{k}'}=-4\pi\lambda\sum_m Y_{2m}^{*}(\hat{k})Y_{2m}(\hat{k}'). \quad (2)$$

For the pair Hamiltonian (1), asymptotically exact solutions[5,6] of (S) can be found for which all correlation functions[3,6] of third and higher order vanish like Ω^{-1}. Two types of such solutions have been studied: One is the BCS type,[7-9] for which the second order correlation function is

$$C_2(\vec{k}\uparrow t_1, -\vec{k}\downarrow t_2; \vec{k}'\uparrow t_1', -\vec{k}'\downarrow t_2')=F(\vec{k}, t_1-t_2)F^{+}(\vec{k}', t_1'-t_2'); \quad (3)$$

the other, recently given by Gor'kov and Galitskii,[10] is based on the more general nonseparable form

$$C_2=\sum_m F_m(\vec{k}, t_1-t_2)F_m^{+}(\vec{k}', t_1'-t_2'), \quad (4)$$

where $F_m(\vec{k}, t)$ is proportional to $Y_{2m}(\hat{k})$. The BCS approach yields a ground state and an excitation spectrum which are anisotropic[8,9]; in contrast, the GG method leads to an isotropic system. Furthermore, the ground-state energy per unit volume W_{GG} obtained by GG is lower than W_{BCS}.

Indeed, it is even possible to find more than one solution of (S) satisfying (3), because the energy gap equation itself has more than one solution for a general $V_{\vec{k}\vec{k}'}$.[9,11] Since the energy gap equation can also be derived from a variational calculation,[7] these additional solutions correspond to stationary values of the average energy other than the absolute minimum; hence they can be discarded by appending a variational principle to the Green's function method.

If any GG-type solution corresponded to a wave function, then variational arguments could also be applied in this case, and would imply that the GG solution is the correct one. On the other hand, physical reasons[12-14] have been given to show that the BCS method yields the asymptotically exact solution of (1). Thus there exist two solutions, both of which seem admissible on physical grounds; since only one can be correct, further investigation is of importance to determine the validity of the methods involved. To gain some understanding of these problems, we have studied in detail a simple model Hamiltonian, for which the GG method again yields a lower ground-state energy than the BCS method. However, by constructing a lower bound to W for this Hamiltonian, we have proved that the BCS solution of lowest energy is asymptotically exact and that the GG type of solution of (S) must be rejected.

The model Hamiltonian we take is of the form (1) in the strong-coupling limit[15]; i.e., the kinetic energy $\epsilon_k - \mu$ is neglected. We choose a potential $V_{\vec{k}\vec{k}'}$ analogous to (2), but with a simplified angular dependence. We divide the spherical shell into four equal "orange segments" (each containing p pair states) labeled by the index $K = 1, 2, 3, 4$, and replace the continuously variable spherical harmonics by functions constant in each segment. Such a discrete space is spanned by four functions, so in order to simulate a partial wave of given angular momentum, we use only two functions $g_m(K)$ satisfying

$$\sum_{m=1,2} |g_m(K)|^2 = \text{independent of } K,$$

$$\sum_K g_m^*(K) g_{m'}(K) = \delta_{mm'}. \tag{5}$$

The interaction (2) is then replaced by

$$\Omega^{-1} V_{\vec{k}\vec{k}'} = -\lambda \sum_m g_m^*(K) g_m(K'), \tag{6}$$

where the $g_m(K)$ are given in Table I, and λ is of order Ω^{-1}.

Table I. Potential functions for the four-segment model and resulting solutions for the energy gap. The other two BCS solutions are obtained by the K interchange $1 \longleftrightarrow 3$, $2 \longleftrightarrow 4$.

K	1	2	3	4
$(10)^{1/2} g_1(K)$	1	2	1	2
$(10)^{1/2} g_2(K)$	2	i	-2	$-i$
$15\Delta_K^{(\text{BCS }1)}/\lambda p$	$4+2i\sqrt{5}$	$8+\sqrt{5}$	$4-2i\sqrt{5}$	$8-\sqrt{5}$
$15\Delta_K^{(\text{BCS }2)}/\lambda p$	$8+\sqrt{5}$	$2\sqrt{5}-4i$	$-8+\sqrt{5}$	$2\sqrt{5}+4i$
$15E_K^{(\text{GG})}/\lambda p$	15/2	15/2	15/2	15/2

The BCS and GG solutions for the ground state of this Hamiltonian are obtained straightforwardly. In the BCS formalism the single-particle energies are given by $E_{\vec{k}} = |\Delta(\vec{k})|$, with the usual gap equation

$$\Delta(\vec{k}) = -\tfrac{1}{2}\Omega^{-1} \sum_{\vec{k}'} V_{\vec{k}\vec{k}'} \Delta(\vec{k}')/E_{\vec{k}'}. \tag{7}$$

This equation has many solutions,[9-11] those of lowest total energy being listed in Table I. In contrast, the GG spectrum is

$$E_{\vec{k}} = \left(\sum_m |\Delta_m(\vec{k})|^2 \right)^{1/2},$$

where each $\Delta_m(\vec{k})$ satisfies Eq. (7). The resulting ground-state energies, $W = -\frac{1}{2}\sum_{\vec{k}} E_{\vec{k}}/\Omega$, are

$$W_{\text{BCS}} = -(14/15)\lambda p^2/\Omega, \quad W_{\text{GG}} = -\lambda p^2/\Omega, \tag{8}$$

where p, the number of pair states per shell segment, tends to infinity with Ω. It is interesting to note the fourfold degeneracy of the BCS ground state, corresponding to the four discrete rotations of the segmented shell; the BCS solutions of the He^3 problem also exhibit a rotational degeneracy. Similarly, our model reproduces the isotropy of the GG treatment of He^3. It is also worth emphasizing that in this model, W_{GG} is lower than W_{BCS}.

In order to find W exactly, we use the pseudo-spin formalism,[4,12,15] based on the fact that the operators

$$\vec{s}_{\vec{k}} \equiv (a_{\vec{k}\uparrow} a_{-\vec{k}\downarrow}^{\dagger}) \tfrac{1}{2}\vec{\sigma} \begin{pmatrix} a_{\vec{k}\uparrow}^{\dagger} \\ a_{-\vec{k}\downarrow} \end{pmatrix} \tag{9}$$

form a representation of an angular momentum

$\frac{1}{2}$. By defining

$$\vec{S}_K \equiv \sum_{\vec{k}\epsilon K} \vec{s}_{\vec{k}}, \tag{10}$$

the Hamiltonian becomes

$$H = -\lambda \sum_{mKK'} g_m^*(K) g_m(K') S_K^- S_{K'}^+. \tag{11}$$

The usual approximation for treating this Hamiltonian is to minimize it with respect to the $\vec{S}_K$ considered as four classical vectors of length $\frac{1}{2}p$. Since the magnitudes of the $\vec{S}_K$ are very large when $\Omega \to \infty$, it is plausible that this classical approximation is asymptotically exact. In fact, this approach is equivalent to the BCS method and thus yields an upper bound to W. However, a lower bound W_c may be constructed which tends to W_{BCS} as $\Omega \to \infty$.

To construct this bound, we first note that the $\vec{S}_K^2$ commute with (11) and have as their largest eigenvalue $\frac{1}{2}p(\frac{1}{2}p+1)$. In order to take a more precise account of these constants of the motion, it is then natural to modify the previous calculation by constraining all the $\vec{S}_K^2$ to retain this correct quantum mechanical value instead of $(\frac{1}{2}p)^2$; the minimum energy thus obtained is

$$W_c = -(14/15)\lambda p(p+2)/\Omega. \tag{12}$$

It is now possible to rewrite H in a form chosen to exhibit its lower bound. By defining $\vec{A}, \vec{B}, \vec{C}, \vec{D}$ as the transverse components of $\vec{S}_1 + \vec{S}_3$, $\vec{S}_1 - \vec{S}_3$, $\vec{S}_2 + \vec{S}_4$, $\vec{S}_2 - \vec{S}_4$, respectively, and

$$\tfrac{1}{2}R_K \equiv \tfrac{1}{2}p(\tfrac{1}{2}p+1) - \vec{S}_K^2 + S_{Kz}^2 \geq 0,$$

$$Q_{KK'} \equiv (S_{Kx} - S_{K'y})^2 + (S_{Ky} + S_{K'x})^2 \geq 0,$$

$$\vec{A}\times\vec{C} = A_x C_y - A_y C_x, \tag{13}$$

it is straightforward but tedious to verify the operator identity

$$H \equiv W_c\Omega + H_1 + H_2, \tag{14}$$

where

$$H_1 \equiv \tfrac{1}{2}\lambda\textstyle\sum_K [\frac{1}{2}p(\frac{1}{2}p+1) - \vec{S}_K^2 + (S_{Kz}+\frac{1}{2})^2] + [\frac{3}{10}\lambda/p(p+2)]\{(\vec{A}\times\vec{C} + \vec{B}\cdot\vec{D})^2$$
$$+ [\vec{A}\cdot\vec{C} - \vec{B}\times\vec{D} - \tfrac{2}{3}p(p+2)]^2 + \vec{A}^2\vec{D}^2 + (R_1 + R_3 + \vec{A}^2)(R_2 + R_4 + \vec{D}^2) + R_1Q_{24} + R_2Q_{31} + R_3Q_{42} + R_4Q_{13}\}, \tag{15}$$

$$H_2 \equiv -\tfrac{1}{2}\lambda + [\tfrac{3}{5}\lambda/p(p+2)](S_{1z} + S_{3z})(S_{2z} + S_{4z}). \tag{16}$$

Equations (13) and the form of (15) show that H_1 is a positive-definite operator. Furthermore, H_2, which results from commutators of the spin operators, is greater than $-(11/10)\lambda$, a quantity of order Ω^{-2} compared to $W_c\Omega$ and so completely negligible. Thus the classical minimum energy W_c is the desired lower bound, a result which can also be understood physically, since in this case quantum mechanical effects tend to raise the energy. The various terms of H_1 do not commute, and lead to a positive zero-point motion, analogous to that of a single particle in a potential well. In addition, the components of $\vec{S}_K$, being discrete quantum mechanically, do not assume the continuum of values which has been used for the classical minimization.

The above analysis demonstrates that for this simple model the BCS solution is asymptotically exact. Furthermore, there are strong indications that this treatment can be applied to a general Hamiltonian of the form (1), leading to the same conclusion. First, momentum space is divided into regions $K = 1, 2, \cdots, n$ (each containing p pair states), and $\epsilon_{\vec{k}}$ and $V_{\vec{k}\vec{k}'}$ are replaced by functions which are constant inside these regions. Next, pseudospins $\vec{S}_K$ are introduced and the $\vec{S}_K^2$ again commute with H. The Hamiltonian may now be minimized with respect to the directions of the $\vec{S}_K$, considered as classical vectors of length either $\frac{1}{2}p$, yielding W_{BCS}, or $[\frac{1}{2}p(\frac{1}{2}p+1)]^{1/2}$, yielding W_c. As a classical function then, H can be written as $W_c\Omega + H_{1c}$ where H_{1c} is non-negative; it is therefore reasonable to expect (although a proof has not been found) that, as an operator, H can be put in the form (14), where H_1 is a positive-definite operator having H_{1c} as its classical limit, and H_2 comes from the commutators and vanishes classically. Finally, we let Ω and n tend to infinity in such a way that p remains much larger than n. Then ϵ_K and $V_{KK'}$ again become continuous, H_2 can be neglected relative to $W_c\Omega$ since it is of lower order in p, and the upper and lower bounds W_{BCS} and W_c approach each other.

The general proof suggested above indicates that the BCS solution is asymptotically exact for the model (1), (2) used to describe He^3, and just as in the previous example, the GG solution[10] must be rejected.[16]

The example we have treated implies that the set of equations (S) does not specify the system uniquely. In particular, it yields solutions which do not correspond to any state vector, even though the properties of these solutions have intuitive physical appeal.[10] It is clearly necessary to find an additional criterion satisfied by the Green's functions to reject these solutions. Since they lead to too low a ground-state energy, a variational principle cannot be used. One possibility is that for the spurious solutions, contributions to the Green's functions usually neglected as being of lower order in the volume may not possess correct analytic properties. The normal solution below the critical temperature exhibits this behavior,[1] and in addition violates other necessary conditions[5] which might equally serve as the desired criterion. A further possibility is the "principle of vanishing correlation,"[14] which is not satisfied by the GG solution. Further investigation of this difficulty is needed before the method of Green's functions can be used without uncertainty.

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