Assuming that $r_0 \gg r_{ij}$ (for all i and j), one sets

$$f \approx [1+(\sum \alpha_i)/r][1+(\sum \beta_i/r)], \tag{29}$$

and obtains from (26)

$$r_0^2=(\sum \alpha_i)(\sum \beta_i)=\tfrac{1}{4}(m_{N+1}^2-q_{N+1}^2). \tag{30}$$

Hence, this additional minimal surface exists (and is nearly spherical) whenever the inequalities

$$m_{N+1} \gg r_{ij}, \quad m_{N+1} \gg |q_{N+1}|, \tag{31}$$

are satisfied. The remaining N sheets also have their associated minimal surfaces; however, these are highly distorted, so that one must resort to numerical solution of the variational principle (24) to locate them. Figures 4 and 5 display the results of such a numerical investigation for the special case $N=2$ and $m_1=m_2$, $q_1=q_2=0$.

It can be shown that the minimal surfaces are elongated slightly along the lines joining them.[10] This type of distortion is just what one might expect by analogy with Newtonian tidal forces; indeed, the magnitude of the distortion is inversely proportional to the cube of the separation distance r_{ij} in the Newtonian limit, and increases as the ratio of mass to separation distance is increased. Thus, the deviation of each minimal surface from spherical symmetry provides another way to estimate the interaction between the N particles.

ACKNOWLEDGMENTS

We are grateful to Professor J. A. Wheeler and Professor C. W. Misner for many interesting discussions. One of us (DRB) wishes to thank Professor F. Rohrlich and Professor M. Dresden of the State University of Iowa for their kind hospitality while part of this work was in progress.

[10] J. A. Wheeler, Rev. Mod. Phys. **33**, 63 (1961).

PHYSICAL REVIEW VOLUME 131, NUMBER 1 1 JULY 1963

Solutions of the Density Matrix-Pairing Tensor Equations of Superconductivity Theory*

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(Received 25 February 1963)

An algorithm is provided for writing down explicitly all solutions of the density matrix-pairing tensor equations which arise in the generalized Bogoliubov-Valatin transformation approach to superconductivity theory. Certain simpler special cases are then examined. Finally reasons are given indicating that our solutions should provide a practical computational tool in many-body theory.

1. INTRODUCTION

A GENERALIZED Hartree-Fock method has been proposed by Bogoliubov[1] and Valatin[2] for investigating the quantum-mechanical problem posed by certain Hamiltonians of the form

$$H=\int dxdx'\psi^*(x)\epsilon(xx')\psi(x')+\frac{1}{2}\int dxdx'dx_1dx_1' \times\psi^*(x)\psi^*(x')W(xx'x_1x_1')\psi(x_1')\psi(x_1). \tag{1}$$

The letter x denotes the space and spin coordinates of a single particle, while ψ is the usual field operator which may be written

$$\psi=\xi^T a, \tag{2}$$

where ξ is a column vector of orthonormal single-particle wave functions and a is a column vector of the corresponding destruction operators. We use the notation that ξ^T denotes the transpose of ξ.

In the approach of Bogoliubov one specifies a set ξ and introduces a new set of creation and destruction operators through the transformation

$$a=U\alpha+V\alpha^\dagger, \tag{3}$$

where U and V denote matrices operating on column vectors of destruction and creation operators as indicated. The requirements that the a's and the α's both satisfy the usual fermion anticommutation rules lead to certain conditions on U and V which may be written simply in the present notation as

$$UU^{*T}+VV^{*T}=\mathrm{I}, \quad UV^T+VU^T=0. \tag{4}$$

The procedure is then to define a trial variational wave function $\Psi(U,V)$ through

$$\alpha\Psi=0, \tag{5}$$

and calculate the corresponding energy. The latter

* This work was supported by the U. S. Atomic Energy Commission.
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[1] N. N. Bogoliubov, Dokl. Akad. Nauk. S.S.S.R. **119**, 244 (1958); N. N. Bogoliubov and V. G. Soloviev, *ibid.* **124**, 1011 (1959) [translation: Soviet Phys.—Dokl. **3**, 292 (1958); **4**, 143 (1959)]. N. N. Bogoliubov, Usp. Fiz. Nauk. **67**, 549 (1959) [translation: Soviet Phys.—Usp. **2**, 236 (1959)].
[2] J. G. Valatin, Phys. Rev. **122**, 1012 (1961).

turns out to be

$$(\Psi,H\Psi)=\sum_{\kappa,\kappa'}\epsilon(\kappa\kappa')F_{\kappa\kappa'}+\tfrac{1}{2}\sum W(\kappa_1\kappa_2\kappa_1'\kappa_2')$$

$$\times[F_{\kappa_1\kappa_1'}F_{\kappa_2\kappa_2'}-F_{\kappa_2\kappa_1'}F_{\kappa_1\kappa_2'}+\Phi_{\kappa_1\kappa_2}{}^*\Phi_{\kappa_1'\kappa_2'}], \quad (6)$$

where $\epsilon(\kappa\kappa')$ and $W(\kappa_1\kappa_2\kappa_1'\kappa_2')$ are matrix elements computed with respect to the orbitals of ξ in the standard way while

$$F=V^*V^T, \quad \Phi=UV^T. \quad (7)$$

The important point to note at this stage is that F and Φ, respectively, the density matrix and the pairing tensor,[3] conveniently specify the energy and are, therefore, more desirable to work with than U and V. It, thus, becomes necessary to replace the conditions (4) by equivalent requirements on F and Φ. These turn out to be[1,3] the symmetry properties

$$F^T=F^*, \quad \Phi^T=-\Phi, \quad (8)$$

together with the conditions

$$\Phi^*\Phi=F^2-F, \quad \Phi F=F^*\Phi. \quad (9)$$

The latter are alternatively written as

$$\mathrm{K}^2=\mathrm{K}, \qquad \mathrm{K}=\begin{pmatrix}\mathrm{I}-F^* & \Phi\\ -\Phi^* & F\end{pmatrix}. \quad (9')$$

On the other hand, the point of view put forward by Valatin is that the transformations can be greatly simplified by judicious choice of basic set and he uses the special Bogoliubov-Valatin[4] transformation but also allows the variation of the orbitals. The essential equivalence of the two methods has been demonstrated generally in the recent paper of Bloch and Messiah[3] using transformation theory based on (2) and (7).

The present work is motivated by the observation that in either Bogoliubov's or Valatin's approach, the solution of the Euler equations resulting from minimization of the energy is bedevilled by awkward subsidiary conditions. This must surely be the reason why no applications seem yet to have been reported. It would be desirable then to be able to write down explicitly F's and Φ's automatically satisfying (8) and (9). The minimization of (6) could then be carried out without restriction. Our intention, therefore, is to investigate solutions of (8) and (9) for an arbitrary fixed basis.

The crucial step which does not seem to have been taken hitherto is to observe that the requirements (4) can be replaced by the unitarity condition

$$\begin{pmatrix}U & V\\ V^*U^*\end{pmatrix}\begin{pmatrix}U & V\\ V^*U^*\end{pmatrix}^{*T}=\begin{pmatrix}\mathrm{I} & 0\\ 0 & \mathrm{I}\end{pmatrix}. \quad (4')$$

Quite apart from its use for our stated objective, the latter is a simplifying tool in the general theory. As an example of this, it has been thought worthwhile at this point to establish the asserted equivalence of (4) to (8) and (9), thus making our account self contained.

2. THE STATUS OF THE DENSITY MATRIX-PAIRING TENSOR EQUATIONS

First, let us suppose (4) holds and F and Φ are defined by (7). Then $F^T=F^*$ follows from the definition, while $\Phi^T=-\Phi$ results almost as easily using the second of Eqs. (4). Finally, since $\begin{pmatrix}U & V\\ V^*U^*\end{pmatrix}$ is unitary and $\begin{pmatrix}\mathrm{I} & 0\\ 0 & 0\end{pmatrix}$ is idempotent, then

$$\begin{pmatrix}U & V\\ V^*U^*\end{pmatrix}\begin{pmatrix}\mathrm{I} & 0\\ 0 & 0\end{pmatrix}\begin{pmatrix}U & V\\ V^*U^*\end{pmatrix}^{*T}=\begin{pmatrix}U\,U^{*T} & U\,V^T\\ V^*U^{*T} & V^*V^T\end{pmatrix} \quad (10)$$

is also idempotent. The latter, however, on using (4) turns out to be just K as given by (9') and this completes half the proof.

Now suppose (8) and (9) hold. We wish to show then that there exist suitable matrices U and V satisfying (4) and such that F and Φ can be written in the form (7). We begin by observing that since K is idempotent its only eigenvalues are 0 or 1. Furthermore, there is a one-one correspondence between the latter, since

$$\begin{pmatrix}\mathrm{I}-F^* & \Phi\\ -\Phi^* & F\end{pmatrix}\begin{pmatrix}A\\ B\end{pmatrix}=1\begin{pmatrix}A\\ B\end{pmatrix} \quad (11)$$

is equivalently written as

$$\begin{pmatrix}\mathrm{I}-F^* & \Phi\\ -\Phi^* & F\end{pmatrix}\begin{pmatrix}B\\ A\end{pmatrix}=0\begin{pmatrix}B\\ A\end{pmatrix}, \quad (12)$$

the assumption $A=B$ leading to a contradiction. Thus, since K is easily seen to be Hermitian it has the canonical form $\begin{pmatrix}\mathrm{I} & 0\\ 0 & 0\end{pmatrix}$ introduced previously under unitary transformation. In an obvious partitioning we may introduce the matrices U, V, P, and Q through the identity

$$\begin{pmatrix}\mathrm{I}-F^* & \Phi\\ -\Phi^* & F\end{pmatrix}=\begin{pmatrix}U & P\\ V^* & Q\end{pmatrix}\begin{pmatrix}\mathrm{I} & 0\\ 0 & 0\end{pmatrix}\begin{pmatrix}U & P\\ V^* & Q\end{pmatrix}^{*T}. \quad (13)$$

Multiplying out the latter gives just the right-hand side of (10) and comparison of elements leads to (8) and (4).

3. SOLUTIONS OF THE DENSITY MATRIX-PAIRING TENSOR EQUATIONS

In the present development we have emphasized that the Bogoliubov conditions (4) can be replaced by (4'). It is the latter unitarity condition which provides us with an algorithm for writing down all solutions of

[3] C. Bloch and A. Messiah, Nucl. Phys. **39**, 95 (1962).

(8) and (9). Quite generally, we have

$$\begin{pmatrix} U & V \\ V^* & U^* \end{pmatrix} = \exp\begin{pmatrix} \theta & \phi \\ \phi^* & \theta^* \end{pmatrix}, \tag{14}$$

where

$$\theta^{*T} = -\theta, \quad \phi^T = -\phi. \tag{15}$$

The general character of these equations follows from unitarity, while the particular symmetry of the left side of (14) determines that of the right. The procedure, then, is to choose any θ and ϕ consistent with (15), calculate $U(\theta,\phi)$ and $V(\theta,\phi)$ from (14) and then $F(\theta,\phi)$ and $\Phi(\theta,\phi)$ from (7). The first few terms of such developments may be written

$$U = \mathrm{I} + \theta + \frac{1}{2!}(\theta^2 + \phi\phi^*) + \cdots, \quad V = \phi + \frac{1}{2!}(\theta\phi + \phi\theta^*) + \cdots, \tag{16}$$

and

$$F = -\phi^*\phi + \frac{1}{2!}(\phi^*\phi\theta^* - \theta^*\phi^*\phi) + \cdots,$$

$$\Phi = -\phi + \frac{1}{2!}(\phi\theta^* - \theta\phi) + \cdots, \tag{17}$$

and clearly as many terms can be evaluated as required. (Throughout, convergence of infinite series has been assumed whenever necessary.)

The remainder of this section is concerned with special cases where analytical treatment can be carried further. Let us begin by considering what happens if one of θ and ϕ vanishes. The case $\phi = 0$ is uninteresting since this gives a no-particle system in which F and Φ vanish.

The case $\theta = 0$, however, is of considerable interest. Here, we have

$$U^0 = \mathrm{I} + \frac{1}{2!}\phi\phi^* + \frac{1}{4!}(\phi\phi^*)^2 + \cdots \equiv \cosh(\phi\phi^*)^{1/2} \tag{18}$$

and

$$V^0 = \phi + \frac{1}{3!}\phi\phi^*\phi + \frac{1}{5!}\phi\phi^*\phi\phi^*\phi + \cdots \equiv [\sinh(\phi\phi^*)^{1/2}](\phi/\phi^*)^{1/2} \tag{19}$$

and, thus,

$$F^0 = -\sinh^2(\phi^*\phi)^{1/2},$$

$$\Phi = -\tfrac{1}{2}[\sinh 2(\phi\phi^*)^{1/2}](\phi/\phi^*)^{1/2}. \tag{20}$$

The interpretation of these equations is straightforward when ϕ is real. In the complex case a little care has to be exercised.

It is readily seen that the usual special pairing description[4] is included in the treatment of the previous paragraph, for if we make the particular choice

$$\phi_{\kappa\kappa'} = \delta_{\kappa,-\kappa'}\phi_\kappa, \quad \phi_{-\kappa} = -\phi_\kappa, \tag{21}$$

one may check without difficulty that the series (18) and (19) can be summed and one finds the results

$$F_{\kappa\kappa'}{}^0 = \delta_{\kappa\kappa'}\sin^2|\phi_\kappa|,$$

$$\Phi_{\kappa\kappa'}{}^0 = -\delta_{\kappa,-\kappa'}\tfrac{1}{2}\sin 2|\phi_\kappa|\,\exp(i\arg\phi_\kappa). \tag{22}$$

These fairly standard results are usually quoted in real form but seem always to be taken as above in the literature[5] on the proposed superfluid phase of He^3, for example, where use of the complex case appears to be mandatory.

The case $\phi \neq 0$ is, thus, seen to be necessary in the class of problem we have in mind. The further question then remains of how to choose $\theta \neq 0$ so as to proceed beyond the approximation (20). We have obtained the following result which tells us rather how *not* to choose θ.

Suppose both θ and ϕ are nonvanishing but $\theta\phi = \phi\theta^*$. Then we assert that the class (20) is obtained once more, the results being independent of θ. Before proceeding to the proof a comment on this result is in place. Broadly speaking, it blocks a large number of *prima facie* promising avenues. To mention but one, the use of antisymmetric matrices in the construction of orthogonal matrices is well known. It might, therefore, seem reasonable when dealing with real matrices to choose θ and ϕ as arbitrary odd functions of an arbitrary antisymmetric matrix, the conditions (15) then being fulfilled. Unfortunately so is the commutative property and our result applies.

Our assertion is proved by observing that by our hypothesis $\begin{pmatrix} \theta & 0 \\ 0 & \theta^* \end{pmatrix}$ and $\begin{pmatrix} 0 & \phi \\ \phi^* & 0 \end{pmatrix}$ commute and, thus, the right side of (14) may be written as

$$\exp\begin{pmatrix} 0 & \phi \\ \phi^* & 0 \end{pmatrix}\exp\begin{pmatrix} \theta & 0 \\ 0 & \theta^* \end{pmatrix} = \begin{pmatrix} U^0 & V^0 \\ V^{0*} & U^{0*} \end{pmatrix}\begin{pmatrix} \exp\theta & 0 \\ 0 & \exp\theta^* \end{pmatrix}. \tag{23}$$

This leads to values for U and V of $U^0\exp\theta$ and $V^0\exp\theta^*$, respectively. On computing the corresponding F and Φ and invoking the anti-Hermitian property (15) of θ we obtain once more the forms (20).

4. FURTHER QUESTIONS

In view of past experience in many-body perturbation theory,[6] it is fair to ask whether in any application,

[4] N. N. Bogoliubov, Nuovo Cimento **7**, 795 (1958); J. G. Valatin, *ibid.* **7**, 843 (1958).

[5] See, for example, P. W. Anderson and P. Morel, Phys. Rev. **123**, 1911 (1961).

[6] One might mention, for example, the well-known divergencies in the perturbation series for a high-density electron gas which are only removed after reclassification and resummation of terms drawn from all orders [M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957)]. Besides this, there exists the unresolved question of the effect perturbation theory has on the analytical properties of the momentum-distribution function [L. Van Hove, Suppl. Physica **26**, 200 (1960)].

the termination of the series (17) after only a finite number of terms is likely to affect profoundly the analytical nature of our solution. Furthermore, even if this does not happen, are we likely to obtain quantitatively reasonable results? We believe that both these questions can be answered optimistically and support this viewpoint by taking the one example—the original case considered by Bardeen, Cooper and Schrieffer[7] (B.C.S.)—where the above kind of treatment when infinite sums are taken is known[8] to furnish essentially the exact solution, and calculating what happens by terminating our series at an early stage.

The details of this problem have been extensively discussed and need not be dwelt on. We simply state that we are considering the reduced Hamiltonian characterized by single-particle energies ϵ_κ measured relative to the Fermi level and a constant average attractive matrix element $-V/\Omega$ for pairs $(\kappa, -\kappa)$ making transitions in the energy region $|\epsilon|<\hbar\omega$. The exact solution is got using (22) in real form. One finds the well-known physical situation characterized by a gap in the single-particle excitation spectrum of size 2Δ where

$$N(0)V\sinh^{-1}(\hbar\omega/\Delta)=1. \tag{24}$$

Here $N(0)$ is the familiar density-of-states factor evaluated at the Fermi surface.

On the other hand, suppose we attempt to assess the situation by cutting off terms in (20) and working consistently to second order. Then (22) is replaced by

$$F_{\kappa\kappa'}{}^0=\delta_{\kappa\kappa'}(\phi_\kappa{}^2+\cdots),$$
$$\Phi_{\kappa\kappa'}=-\delta_{\kappa-\kappa'}(\phi_\kappa-\tfrac{2}{3}\phi_\kappa{}^3+\cdots), \tag{22'}$$

and these lead to the Euler equation

$$\frac{2\phi_\kappa}{1-2\phi_\kappa{}^2}=\frac{V}{\Omega\epsilon_\kappa}\sum_{|\epsilon_{\kappa'}|<\hbar\omega}|\phi_{\kappa'}|\equiv\frac{\Delta}{\epsilon_\kappa}, \tag{25}$$

this integral equation serving also to define a quantity Δ now, however, no longer equal to that of (24). Nevertheless, following closely the analysis of B.C.S., we find that 2Δ again represents the energy gap in the present approximation and that the same qualitative physical picture emerges. The value of Δ is straightforwardly shown to be given by

$$N(0)V[-x^2+x(1+x^2)^{1/2}+\sinh^{-1}x]=1,$$
$$x=\hbar\omega/\sqrt{2}\Delta. \tag{26}$$

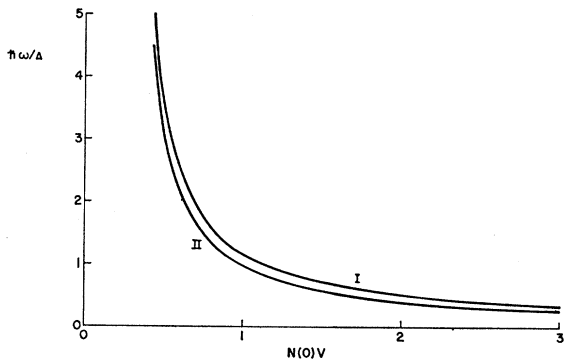

FIG. 1. Indication of the variation of energy gap Δ with coupling $N(o)V$ for the B.C.S. model. Curve I is exact while curve II is our first order approximation to it.

To assess the quantitative accuracy of the approximation we need only compare (24) and (26). In the large x region of interest in superconductors, the agreement is remarkable considering the quite crude nature of our approximation. We have

$$\sinh^{-1}(\hbar\omega/\Delta)=\ln x+1.04+1/(8x^2)+O(x^{-4}), \tag{27}$$

while

$$-x^2+x(1+x^2)^{1/2}+\sinh^{-1}x$$
$$=\ln x+1.19+1/(8x^2)+O(x^{-4}). \tag{28}$$

Outside this region good results are again obtained as the graph indicates.

Our conclusion is, therefore, that our solutions (17), quite apart from solving a general theoretical problem in principle, provide us also with a promising computational tool. The need now is to apply them in their generality to some specific problem and this matter is under consideration.

ACKNOWLEDGMENTS

The writer would like to thank Professor P. A. Carruthers and Professor J. A. Krumhansl for the hospitality he has enjoyed at this laboratory. A stimulating correspondence with Dr. D. Parsons is also acknowledged.

[7] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
[8] N. N. Bogoliubov, Suppl. Physica **26**, 1 (1960).