Generalized Hartree-Fock Method

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A variational principle is formulated to determine the single-particle states, their pairing, and the occupation number distribution for a trial state vector of the Bardeen, Cooper, Schrieffer type. The equations which are derived generalize those of the Hartree-Fock method obtained with a Slater determinant trial wave function. It is pointed out that in a suitable representation the vacuum state of a general quasi-particle transformation has such a trial form which exhibits directly the pairing of single-particle states. Another variational principle determines the excitation energies.

Two coupling cases are distinguished: the commutative case in which the self-consistent densities and energies are related to quantities which all commute, and the more general noncommutative case. The latter is of importance in critical-field phe-nomena. The equations for the commutative case can be written in a matrix form which retains its validity in the more general noncommutative case. The simple matrix commutator equations appear as direct generalizations of the density matrix form of the Hartree-Fock equations.

The equations for small oscillations have an equally simple form. Their connection with a diagonal representation of the quasi-particle energies is exhibited in a way which remains valid in the general coupling case. The "unphysical" solutions are excluded by the supplementary condition. The contact with the Green's function approach is established. The generalized matrix form of the Green's function equations shows especially clearly the symmetry properties of the method.

INTRODUCTION

THE theory of superconductivity of Bardeen, Cooper, and Schrieffer[1] has laid the foundations of a new approach to describe the behavior of an interacting fermion system. In a previous paper,[2] which will be referred to in the following as (F), the method was simplified by the introduction of a new kind of fermion variables, and new equations were derived for more general two-body interactions which show the independence of the main conclusions from the assumption of a constant interaction matrix element. The same new fermion variables were introduced independently by Bogoliubov[3] who derived equations directly from the interacting electron-phonon field problem. In a more recent paper[4] Bogoliubov worked out some of the consequences of considering a more general form of the quasi-particle transformation, and pointed out that this point of view leads to a simple way of describing the effect of an electromagnetic field in a gauge-independent manner. Many other works[5] contributed to a better understanding and to an extension of the theory. The subject is still in a state of vigorous development. Starting from the theory of superconductivity, the concepts of the method penetrated the domain of nuclear physics[6] and attempts are being made[7] to explore its consequences in the theory of elementary particles.

It has been pointed out previously[8] that the approximation of independent fermion excitations is related to a simple linearization of the matter field equations. A reference to a Hartree-like approximation can be found already in the paper of Bardeen, Cooper, and Schrieffer[1] in connection with the trial ground-state vector which is built up from independent commuting factors. Some further connections with the self-consistent field method of Hartree and Fock have been pointed out by Bogoliubov,[4] Nambu,[9] and others. The close connection between the two approaches will be made even more apparent in the present paper. The equations of the new method will appear as generalizations of the equations of the Hartree-Fock method, with a minimum generalization which takes into account the existence of a state of bound pairs of particles. Special care will be taken to show that the approximation method is really very simple, in spite of the impression one might obtain from some of the existing publications.

It has been shown in (F) that the approximate ground-state properties can be described in terms of the one-particle density matrix h and a pair field χ which is the expectation value of a pair of field operators. The new features of the approach are related to the existence of a nonvanishing χ in the case of appropriate attractive forces. The factorizable term contributed by the pair field χ to the two-body correlation function represents coherent long-range correlations. The approximation method attributes a

[1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. 108, 1175 (1957).

[2] J. G. Valatin, Nuovo cimento 7, 843 (1958), referred to in the text as (F).

[3] N. N. Bogoliubov, Nuovo cimento 7, 794 (1958).

[4] N. N. Bogoliubov, Uspekhi fiz. Nauk. 67, 549 (1959).

[5] Especially two main directions of development should be mentioned: the Green's function approach, started by the paper of L. P. Gorkov, J. Exptl. Theoret. Phys. U.S.S.R. 34, 735 (1958) [translation: Soviet Phys.—JETP 34(7), 505 (1958)], and the generalized random phase approximation of references 11, 12, and 13.

[6] A. Bohr, B. R. Mottelson, and D. Pines, Phys. Rev. 110, 936 (1958), and numerous more recent publications some of which are referred to in reference 10.

[7] Y. Nambu, Proceedings of the Midwest Conference, Purdue University, March, 1960 (unpublished).

[8] J. G. Valatin, Proceedings of the Low-Temperature Conference, Geneva, New York, 1958 (unpublished); J. G. Valatin and D. Butler, Nuovo cimento 10, 37 (1958).

[9] Y. Nambu, Phys. Rev. 117, 648 (1960).

special weight to this factorizable term which expresses then an effective condensation of pairs of particles in a single bound state.

Besides h and χ, it is convenient to introduce a self-consistent energy ν determined by h and a self-consistent pairing potential μ determined by χ. In the simple coupling case considered in (F), the quantities h, χ, ν, μ all commute, and the equations were derived in a representation in which they are all in a "diagonal" form. It will be convenient to refer to this case as the commutative coupling case, in contrast to the more general noncommutative case. The latter is of importance in critical magnetic field phenomena or in the analogous effect in rotating nuclei[10] where the electromagnetic interaction energy or the rotational coupling term does not commute with the pairing potential μ.

The simple equations of the commutative case will be cast in the present paper in a new matrix form which will retain its validity in the more general case. The simple pair structure of the ground-state vector also remains valid in the general case, though the representation which exhibits this will in general not lead to a diagonalization of the quasi-particle energy. Variational principles will be applied to determine the pair structure of the ground state, the excitation energies, and the matrix form of the equations. The new expressions obtained will not merely mean a considerable gain in the length of the equations but will lead to a deeper insight into the nature of the approximation. The whole approach should be looked at as a self-consistent zero-order approximation of a more general expansion procedure. The next approximation which leads to a natural extension of the method is provided by the generalized random phase approximation investigated by Bogoliubov,[11] Anderson,[12] and others.[13]

The notation will be kept close to that introduced in (F), and the reader is referred to this publication for details which will not be repeated here.

GROUND-STATE PAIRING AND VARIATIONAL PRINCIPLE

In terms of the quantized fermion field operator $\psi(x)$ and its adjoint $\psi^*(x)$, the Hamiltonian of a system with two-body interactions can be written in the form

$$H = \int dx\,dx'\,\psi^*(x)\epsilon(x,x')\psi(x')$$

$$+\frac{1}{2}\int dx\cdots dx_1'\,\psi^*(x)\psi^*(x')V(xx';x_1x_1')\psi(x_1')\psi(x_1).$$ (1a)

The letter x denotes the space coordinates, spin, isotopic spin, etc., of a single particle, and the integral sign includes the corresponding summations. The constant chemical potential which enters into the description because of approximations which do not conserve the number of particles is included in the single-particle energy ϵ. This may equally contain a contribution from interactions with an external field. The kernel of the two-body interaction V is chosen in a sufficiently general form to include velocity-dependent forces.

The trial ground-state vector of Bardeen, Cooper, and Schrieffer is of the form[14]

$$\Phi_0 = \prod_{\kappa>0}\left[(1-h_\kappa)^{\frac{1}{2}}+(h_\kappa)^{\frac{1}{2}}a_\kappa a_{-\kappa}\right],$$ (1b)

where the creation operators a_κ of a single-particle state $\varphi_\kappa(x)$ are related to $\psi^*(x)$ through

$$a_\kappa = \int dx\,\varphi_\kappa(x)\psi^*(x).$$ (1c)

The real number h_κ is the expectation value in Φ_0 of the number of particles in state κ,

$$h_\kappa = \langle a_\kappa a_\kappa{}^\dagger\rangle,$$ (1d)

and one has

$$0 \leqslant h_\kappa \leqslant 1, \quad h_\kappa = h_{-\kappa}.$$ (1e)

The values of h_κ are to be determined by minimizing the expectation value of the Hamiltonian (1a) with respect to the state (1b). The trial form of this state includes the possible choice

$$\begin{aligned}h_\kappa &= 1 \quad \text{for} \quad |\kappa| \leqslant |\kappa_0| \\ &= 0 \quad \text{for} \quad |\kappa| > |\kappa_0|.\end{aligned}$$ (1f)

For this number distribution, the state (1b) reduces to a simple product state which corresponds to a Slater determinant wave function in configuration space. The variational principle and stability considerations determine, according to the nature of the Hamiltonian (1a), if the ground state is better approximated by an occupation number distribution (1f) or by some other distribution h_κ.

In the original assumptions for an infinite system of electrons, it has been assumed that κ stands for a single-particle state with definite momentum and spin, and $-\kappa$ for a state with opposite momentum and opposite spin. The distribution (1f) is still a possible choice, and the variational principle is to determine the values of h_κ. In the Hartree-Fock method, the form (1f) of the number distribution is assumed, but the states

[10] B. Mottelson and J. G. Valatin, Phys. Rev. Letters **5**, 511 (1960).

[11] See reference 4 and other references given there, especially concerning the approach through the "method of approximate second quantization."

[12] P. W. Anderson, Phys. Rev. **112**, 1900 (1958).

[13] G. Rickayzen, Phys. Rev. **115**, 795 (1959); D. J. Thouless, Ann. Phys. **10**, 553 (1960); A. Bardasis and J. R. Schrieffer (to be published).

[14] An opposite convention $a \to a^*$, $a\dagger \to a$ is often used for creation and annihilation operators. Reasons for the present notation are explained in the author's Naples lectures, *Lectures on Quantum Field Theory*, edited by R. E. Caianiello (Academic Press, New York, 1960), p. 113. The state vector (1b) is written in an algebraic form. A more conventional notation would put behind the symbols a sign $|0\rangle$, indicating the state in which there is no particle present.

$\varphi_\kappa(x)$ are to be determined from the variational principle. The point to be made here is that assuming a trial state vector of the form (1b), with the single-particle states $\varphi_\kappa(x)$ the pairing κ, $-\kappa$ and the occupation numbers h_κ all unknown, the variational principle leads to a straightforward generalization of the Hartree-Fock method.

By introducing the fermion operators

$$\eta_\kappa = (1-h_\kappa)^{\frac{1}{2}} a_\kappa \mp (h_\kappa)^{\frac{1}{2}} a_{-\kappa}^\dagger$$
$$\eta_\kappa^\dagger = (1-h_\kappa)^{\frac{1}{2}} a_\kappa^\dagger \mp (h_\kappa)^{\frac{1}{2}} a_{-\kappa} \quad \text{for } \kappa>0 \text{ or } \kappa<0 \quad (2a)$$

the simple argument given in (F) shows that one has

$$\eta_\kappa^\dagger |\Phi_0 = 0 \tag{2b}$$

for all values of κ. The operators η_κ, $\eta_\kappa^\dagger$ satisfy the same anticommutation relations as a_κ, $a_\kappa^\dagger$. As explained in (F), a simple way to obtain expectation values of operators in the state Φ_0 is to express the operators in terms of η_κ, $\eta_\kappa^\dagger$ and to order the factors in each term in such a way that creation operators act after the annihilation operators.

One obtains in this way for the density matrix h the expression

$$h(x',x) = \langle \psi^*(x)\psi(x')\rangle = \sum_\kappa h_\kappa \varphi_\kappa(x')\varphi_\kappa^*(x), \tag{3a}$$

and for the pair field χ the expression

$$\chi(x',x) = \langle \psi(x)\psi(x')\rangle = \sum_\kappa \chi_\kappa \varphi_\kappa(x')\varphi_{-\kappa}(x), \tag{3b}$$

where

$$\chi_\kappa = +[h_\kappa(1-h_\kappa)]^{\frac{1}{2}} \quad \text{for } \kappa>0,$$
$$\chi_{-\kappa} = -\chi_\kappa. \tag{3c}$$

The summations extend over both positive and negative values of κ. From the definitions, one has

$$h(x,x') = h^*(x',x), \quad \chi(x,x') = -\chi(x',x). \tag{3d}$$

The self-consistent energy ν can be defined by

$$\nu(x,x') = \epsilon(x,x') + \int dx_1 dx_1' \{ V(xx_1; x'x_1')$$
$$- V(xx_1; x_1'x')\}h(x_1',x_1), \tag{4a}$$

and the self-consistent pairing potential μ by

$$\mu(x,x') = \int dx_1 dx_1' \, V(xx'; x_1x_1')\chi(x_1,x_1'). \tag{4b}$$

With a Hermitian single-particle energy ϵ, and a Hermitian and symmetric interaction energy V, one concludes from (3d) that

$$\nu(x',x) = \nu^*(x,x'), \quad \mu(x',x) = -\mu(x,x'). \tag{4c}$$

The expectation value $W_0 = \langle H \rangle$ of the Hamiltonian (1a) can be written in terms of h, χ, ν, μ as

$$W_0 = \frac{1}{2}\int dxdx'\{ (\epsilon(x,x')+\nu(x,x'))h(x',x)$$
$$-\mu(x,x')\chi^*(x',x)\}. \tag{4d}$$

The last expression has the form of a trace, and can be expressed in terms of the "diagonal" elements

$$\nu_\kappa = \nu_{\kappa\kappa} = \epsilon_\kappa + \sum_{\kappa'} \{(\kappa\kappa'|V|\kappa\kappa') - (\kappa\kappa'|V|\kappa'\kappa)\}h_{\kappa'}, \tag{5a}$$

$$\mu_\kappa = \mu_{\kappa,-\kappa} = \sum_{\kappa'} (\kappa, -\kappa|V|\kappa', -\kappa')\chi_{\kappa'} \quad \text{for } \kappa>0, \tag{5b}$$

with

$$\epsilon_\kappa = \epsilon_{\kappa\kappa} = \int dxdx' \, \varphi_\kappa^*(x)\epsilon(x,x')\varphi_\kappa(x'), \tag{5c}$$

$$(\kappa\kappa'|V|\kappa_1\kappa_1') = \int dx \cdots dx_1' \, \varphi_\kappa^*(x)\varphi_{\kappa'}^*(x')$$
$$\times V(xx'; x_1x_1')\varphi_{\kappa_1}(x_1)\varphi_{\kappa_1'}(x_1'). \tag{5d}$$

One obtains in this way

$$W_0 = \frac{1}{2}\sum_\kappa \{(\epsilon_\kappa+\nu_\kappa)h_\kappa+\mu_\kappa\chi_\kappa\}. \tag{5e}$$

Considering this expression as a function of h_κ, χ_κ, and $\varphi_\kappa(x)$, the expression is to be minimized under the supplementary condition

$$(1-2h_\kappa)^2 + (2\chi_\kappa)^2 = 1, \tag{5f}$$

which follows from the definition (3c), and under the constraints

$$\int dx\varphi_\kappa^*(x)\varphi_{\kappa'}(x) = \delta_{\kappa\kappa'}, \tag{5g}$$

which express the orthogonality and normalization of the one-particle states.

For a fixed system $\varphi_\kappa(x)$, one has

$$\nu_\kappa = \partial W_0/\partial h_\kappa, \quad \mu_\kappa = \partial W_0/\partial \chi_\kappa, \tag{6a}$$

and minimizing W_0 with respect to h_κ and χ_κ under the supplementary condition (5f), one obtains the equations

$$\nu_\kappa = \bar{E}_\kappa(1-2h_\kappa), \tag{6b}$$

$$\mu_\kappa = -\bar{E}_\kappa 2\chi_\kappa. \tag{6c}$$

An elimination of the Lagrangian multiplier $\bar{E}_\kappa$ gives the relationship

$$\nu_\kappa 2\chi_\kappa + \mu_\kappa(1-2h_\kappa) = 0, \tag{6d}$$

whereas for $\bar{E}_\kappa$ one obtains with the supplementary condition (5f)

$$\bar{E}_\kappa = (\nu_\kappa^2 + \mu_\kappa^2)^{\frac{1}{2}}. \tag{6e}$$

As shown in (F), in the commutative case this represents the energy of the independent quasi-particle excitations. In the more general case, $\bar{E}_\kappa$ is related only to the energy difference,

$$\bar{E}_\kappa = \nu_\kappa(1-2h_\kappa) - \mu_\kappa 2\chi_\kappa, \tag{6f}$$

between the expectation values of the Hamiltonian in the states $\eta_\kappa|\Phi_0$ and Φ_0. If the equations (6b, c) are satisfied, one obtains indeed from (6f), $\bar{E}_\kappa = \bar{E}_\kappa$.

If the states κ are known, the equations (5a, b, f) and (6b, c, e) determine h_κ and χ_κ.

For h_κ, χ_κ fixed, a variation of W_0 with respect to the functions φ_κ^* gives

$$\frac{\delta W_0}{\delta \varphi_\kappa^*(y)} = h_\kappa \int dx' \, \nu(y,x') \varphi_\kappa(x')$$

$$+ \chi_\kappa \int dx' \, \mu(y,x') \varphi_{-\kappa}^*(x') \quad (7a)$$

$$= \int dx \, K(y,x) \varphi_\kappa(x),$$

with

$$K(y,x) = \int dx' \{\nu(y,x') h(x',x) - \mu(y,x') \chi^*(x',x)\}, \quad (7b)$$

where the last equality is obtained by using the form (3a, b) of h and χ. With the constraints (5g), and Lagrangian multipliers $\lambda_{\kappa\kappa'}$, one obtains in this way the equations

$$\int dx \, K(y,x) \varphi_\kappa(x) = \sum_{\kappa'} \lambda_{\kappa\kappa'} \varphi_{\kappa'}(y). \quad (7c)$$

With the expressions (3a, b), (4a, b) of h, χ, μ, ν, these are nonlinear equations to determine the single-particle system $\varphi_\kappa(x)$. In the case that $\chi_\kappa = 0$ for all κ, they reduce to the Hartree-Fock equations.

From the expressions (3a, b, c) of h and χ, one obtains immediately the equations

$$h(x',x) - \int dy \{h(x',y)h(y,x) - \chi(x',y)\chi^*(y,x)\} = 0, \quad (8a)$$

$$\int dy \{h(x',y)\chi(y,x) - \chi(x',y)h^*(y,x)\} = 0. \quad (8b)$$

Apart from a change in notation which makes apparent the matrix character of these equations, these are the relationships derived by Bogoliubov[4] for the expectation values formed with respect to the vacuum state Φ_0 of the quasi-particle operators

$$\xi_\sigma = \sum_\kappa (u_{\kappa\sigma} a_\kappa + v_{\kappa\sigma} a_\kappa^\dagger),$$
$$\xi_\sigma^\dagger = \sum_\kappa (v_{\kappa\sigma}^* a_\kappa + u_{\kappa\sigma}^* a_\kappa^\dagger). \quad (8c)$$

The index κ stands in the present reference for an arbitrary system of one-particle states, and one has

$$\xi_\sigma^\dagger | \Phi_0 = 0. \quad (8d)$$

Bogoliubov has shown that the relationships (8a, b) express the necessary and sufficient condition for the quasi-particle transformation (8c) to be unitary.

The important point to note is that the relationships (8a, b) which follow from the form (3a, b) of h and χ imply conversely that h and χ can be brought simultaneously to that form, and that the vacuum state of the general quasi-particle transformation (8c) has the

simple pair structure (1b) of the trial state vector of Bardeen, Cooper, and Schrieffer. Indeed, the Hermitian matrix h can be brought to the diagonal form (3a), and assuming a more general form

$$\chi(x',x) = \sum_{\kappa\kappa'} \chi_{\kappa\kappa'} \varphi_{\kappa'}(x') \varphi_\kappa(x) \quad (8e)$$

for χ in this representation, one obtains from (8b)

$$(h_\kappa - h_{\kappa'})\chi_{\kappa\kappa'} = 0. \quad (8f)$$

If the eigenvalues h_κ of h are nondegenerate, apart from the twofold degeneracy $h_{-\kappa} = h_\kappa$, one concludes immediately $\chi_{\kappa\kappa'} = \chi_\kappa \delta_{\kappa,-\kappa'}$ for $\kappa > 0$. If there are other degeneracies, a further transformation in the subspace of degenerate eigenvalues h_κ might be needed to bring χ to this form[15] and to determine a pairing κ, $-\kappa$.

INDEPENDENT QUASI-PARTICLE EXCITATIONS

If the Hamiltonian (1a) is expressed in terms of the quasi-particle operators (2a), a part of the interaction energy can be separated[8] which after the ordering process of the quasi-particle creation and annihilation operators contains terms with genuinely four factors η, $\eta^\dagger$. The remaining part of the Hamiltonian[8,9] which contains the single-particle term of (1a) and terms resulting from the interaction energy by contractions represents a Hamiltonian for an independent quasi-particle motion. In terms of the particle creation and annihilation operators a_κ, $a_\kappa^\dagger$ it can be written as

$$\hat{H} = \text{const} + \frac{1}{2} \sum_{\kappa\kappa'} \{\nu_{\kappa\kappa'} a_\kappa a_{\kappa'}^\dagger - \nu_{\kappa\kappa'}^* a_\kappa^\dagger a_{\kappa'}$$

$$+ \mu_{\kappa\kappa'} a_\kappa a_{\kappa'} - \mu_{\kappa\kappa'}^* a_\kappa^\dagger a_{\kappa'}^\dagger\}. \quad (9a)$$

The linearized operator equations $i\dot{a}^\dagger = [a^\dagger, \hat{H}]$, $i\dot{a} = [a, \hat{H}]$, take the form

$$i\dot{a}_\kappa^\dagger = \sum_{\kappa'} (\nu_{\kappa\kappa'} a_{\kappa'}^\dagger + \mu_{\kappa\kappa'} a_{\kappa'}),$$
$$i\dot{a}_\kappa = \sum_{\kappa'} (-\mu_{\kappa\kappa'}^* a_{\kappa'}^\dagger - \nu_{\kappa\kappa'}^* a_{\kappa'}). \quad (9b)$$

In the case dealt with in (F), one can write $\nu_{\kappa\kappa'} = \nu_\kappa \delta_{\kappa\kappa'}$, $\mu_{\kappa\kappa'} = \mu_\kappa \delta_{\kappa,-\kappa'}$ for $\kappa > 0$, and the quasi-particle Hamiltonian (9a) is diagonalized by introducing the operators (2a). This will no longer hold in the general coupling case, and a further transformation

$$\xi_\sigma = \sum_\kappa C_{\sigma\kappa} \eta_\kappa, \quad \xi_\sigma^\dagger = \sum_\kappa C_{\sigma\kappa}^* \eta_\kappa^\dagger \quad (9c)$$

will be needed, where $C_{\sigma\kappa}$ is unitary, to bring $\hat{H}$ into a diagonal form

$$\hat{H} = W_0 + \sum_\sigma E_\sigma \xi_\sigma \xi_\sigma^\dagger. \quad (9d)$$

From Eq. (2b) a similar equation (8d) follows for the linear combinations (9c). The operators (9c), expressed in terms of a_κ, $a_\kappa^\dagger$ are of the form (8c), but represent now that special transformation which diagonalises the quasi-particle energy. The one-quasi-particle eigenstates

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[15] The conclusion that h and χ can be brought simultaneously to the form $h_{\kappa\kappa'} = h_\kappa \delta_{\kappa\kappa'}$, $\chi_{\kappa\kappa'} = \chi_\kappa \delta_{\kappa,-\kappa'}$ was pointed out independently by V. G. Soloviev (private communication).

of $\hat{H}$ will be given by

$$\xi_\sigma|\Phi_0=\sum_\kappa C_{\sigma\kappa}a_\kappa\Phi_0, \qquad (9e)$$

where Φ_0 is of the form (1b), and the definitions (2a), (9c) and the relationship $\eta_\kappa|\Phi_0=a_\kappa\Phi_0$ have been used. This represents a state with an additional unpaired particle in the sea of coupled bound pairs. Whereas (1b) can be considered as an approximation for the ground-state vector of a system with an even number of particles, the corresponding trial approximation for an odd number of particles will be of the form (9e).

Since the interaction terms of the difference $H-\hat{H}$ give zero expectation value in the state (9e), the eigenvalues W_0+E_σ of $\hat{H}$ can also be obtained by minimizing the expectation value of the Hamiltonian H with respect to a trial state vector of the form (9e). The expectation values h, χ can be expressed in terms of the unknown coefficients u, v of the quasi-particle wave function, and one obtains a set of self-consistent nonlinear equations. The self-consistency requirements become of importance in approximations to systems of finite size, as in the nuclear physics applications. For large systems with extended single-particle wave functions, as in the case of a metal, where the addition of one particle does not influence much the self-consistent fields, the values of h and χ obtained from the variational principle for a system with an even number of particles can be used in the equations to determine the excitation energies E_σ and wave function components u, v of an additional particle. The equations are then linear, and are simply the eigenvalue equations related to the linear operator $\hat{H}$ given by (8a). This relationship of the quasi-particle energies E_σ to a variational principle gives further justification for interpreting these quantities as excitation energies.[16]

MATRIX EQUATIONS

The quasi-particle transformation (2a) or (8c) introduces a single-particle space of twice as many dimensions formed by linear combinations of the wave functions $\varphi_\kappa(x)$ and their conjugate complex $\varphi_\kappa^*(x)$. According to a remark by Bogoliubov,[4] the subsidiary conditions (8a, b) for the quantities h and χ can be considered as expressing the projection operator character,

$$\mathcal{K}^2=\mathcal{K}, \qquad (10a)$$

of a matrix $\mathcal{K}$ defined in this space (φ,φ^*). With a compact notation and the simplification indicated after the equations (8a, b) one can write $\mathcal{K}$ in the form

$$\mathcal{K}=\begin{pmatrix} h & \chi \\ -\chi^* & 1-h^* \end{pmatrix}. \qquad (10b)$$

The aim of the present section is to show that by

introducing further quantities in the space (φ,φ^*), the equations obtain an extremely simple form. At the same time, they appear as direct generalizations of the commutator equations for the density matrix in the Hartree-Fock method.

The form (9b) of the linearized operator equations suggests the introduction of the Hermitian matrix,

$$\mathfrak{M}=\begin{pmatrix} \nu & \mu \\ -\mu^* & -\nu^* \end{pmatrix}, \qquad (11a)$$

in the (φ,φ^*) space. It follows from the symmetry of this matrix that if (u,v) is an eigenvector of $\mathfrak{M}$ with eigenvalue E_σ, then (v^*,u^*) is an eigenvector with eigenvalue $-E_\sigma$. The quasi-particle energies E_σ determined by the operator $\hat{H}$ are all positive. The matrix $\mathfrak{M}$ has twice as many eigenvalues $\pm E_\sigma$, the absolute values of which are the quasi-particle energies. The eigenvectors of $\mathfrak{M}$ determine the coefficients of the quasi-particle operators ξ_σ and $\xi_\sigma^\dagger$.

The variation of the expectation value (4d) of the Hamiltonian can be written in terms of $\mathfrak{M}$ and the variation $\delta\mathcal{K}$ as

$$\delta W_0=\tfrac{1}{2}\text{ Trace }\mathfrak{M}\delta\mathcal{K}. \qquad (11b)$$

Adding to this

$$\delta(\mathcal{K}^2-\mathcal{K})=\mathcal{K}\delta\mathcal{K}+\delta\mathcal{K}\mathcal{K}-\delta\mathcal{K}, \qquad (11c)$$

with a Lagrangian multiplier $-\tfrac{1}{2}\Lambda$, summed over the diagonal elements of the product, and equating the resulting expression with zero, one obtains the equation

$$\mathfrak{M}=\Lambda\mathcal{K}+\mathcal{K}\Lambda-\Lambda. \qquad (11d)$$

Because $\mathcal{K}^2=\mathcal{K}$, this means

$$\mathfrak{M}\mathcal{K}=\mathcal{K}\Lambda\mathcal{K}=\mathcal{K}\mathfrak{M}, \qquad (11e)$$

and gives the commutator equation

$$[\mathfrak{M},\mathcal{K}]=0. \qquad (11f)$$

If one varies the expectation value of the operator $i(\partial/\partial t)-H$, instead of the expectation value W_0 of the Hamiltonian H, one obtains the time-dependent equation

$$i\partial\mathcal{K}/\partial t=[\mathfrak{M},\mathcal{K}]. \qquad (11g)$$

The analogous equations of the Hartree-Fock method[17] in terms of the density matrix h are of the form

$$[\nu,h]=0, \qquad (12a)$$

and

$$i\partial h/\partial t=[\nu,h]. \qquad (12b)$$

The density matrix h is then given by the expression (3a) with a number distribution (1f), and the self-consistent energy ν by the corresponding expression (4a). For $\chi\equiv0$, the equations (11f, g) give a symmetrized version of these density matrix equations. The projection operator $\mathcal{K}$ defines in this case a new

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[16] A relationship of E_σ to a variational principle was indicated in the simpler commutative case by H. Koppe and B. Mühlschlegel, Z. Physik 151, 613 (1958).

[17] P. A. M. Dirac, Proc. Cambridge Phil. Soc. 26, 376 (1930).

vacuum state by interchanging the role of particles and holes.

Dirac's argument[17] given in connection with Eq. (12b) can be immediately extended to the present case to show that the energy expectation value (4d) is an integral of motion of the time dependent equation (11g), if ϵ and the interaction energy V in the Hamiltonian (1a) are time-independent. It is perhaps even simpler to refer to the expression (11b) for δW_0, which shows immediately that one has

$$\frac{d}{dt}W_0 = \tfrac{1}{2}\,\text{Trace }\mathfrak{M}\frac{\partial\mathfrak{K}}{\partial t}=0. \tag{13}$$

The last equality is a consequence of the equation (11g) and of the rule of permutation of factors in a trace.

Solutions of the stationary equation $[\mathfrak{M},\mathfrak{K}]=0$ can be built up from the projection operators of the spectral decomposition of $\mathfrak{M}$ which all commute with $\mathfrak{M}$. The quasi-particle excitation energies E_σ in the expression (9d) of $\hat{H}$ will be positive, if $\mathfrak{K}$ is chosen to be the projection operator of the negative energy spectrum of $\mathfrak{M}$. $\mathfrak{K}$ devides the space (φ,φ^*) into two subspaces and defines the approximate ground-state vector Φ_0.

If the notation is modified so that the matrix character of the equations is no longer recognizable, the components of the equations (11f, g) lead to the equations given by Bogoliubov.[4,18] The matrix commutator equations exhibit in a compact form the equations valid in the simpler commutative coupling case, and represent at the same time the form of the equations which remains valid in the more general case.

The more detailed form of the commutator equations becomes especially simple if a representation can be found in which all matrix elements are real. The following expressions will be given in such a representation. An illustration of the equations with a complex representation of $\mathfrak{K}$ and $\mathfrak{M}$ is provided by Eqs. (8a, b).

In such a real representation, $\mathfrak{K}$ and $\mathfrak{M}$ can be written in the form

$$\mathfrak{K}=\begin{pmatrix} h & \chi \\ -\chi & 1-h \end{pmatrix}, \quad \mathfrak{M}=\begin{pmatrix} \nu & \mu \\ -\mu & -\nu \end{pmatrix}. \tag{14a}$$

The matrix

$$1-2\mathfrak{K}=\begin{pmatrix} 1-2h & -2\chi \\ 2\chi & -(1-2h) \end{pmatrix} \tag{14b}$$

[18] A variational derivation of the equations was given by N. N. Bogoliubov and V. G. Soloviev, Doklady Akad. Nauk. U.S.S.R. 124, 1011 (1959) [translation: Soviet Phys.—Doklady 4, 143 (1959)], by expressing h and χ in the expression (4d) of W_0 by the coefficients u, v of a general quasi-particle transformation (8c) and varying u, v. Any transformation of the form (9c), with an arbitrary unitary $C_{\sigma\kappa}$ leads to the same h and χ, and there are infinitely many such transformations. As both W_0 and the resulting equations are independent of the arbitrary coefficients u, v, the introduction of these variables is obviously irrelevant in the argument. The same remark holds in connection with many expressions of published papers, where quantities which depend only on h and χ are expressed in terms of the coefficients u, v.

has eigenvalues ± 1, and in the stationary case when it commutes with $\mathfrak{M}$ its product with $\mathfrak{M}$ has positive eigenvalues E_σ instead of the negative eigenvalues $-E_\sigma$ of $\mathfrak{M}$.

The condition $\mathfrak{K}^2=\mathfrak{K}$ implies

$$(1-2\mathfrak{K})^2=\begin{pmatrix} (1-2h)^2-(2\chi)^2 & [(1-2h),-2\chi] \\ [(1-2h),-2\chi] & (1-2h)^2-(2\chi)^2 \end{pmatrix}=1, \tag{14c}$$

which gives the equations

$$(1-2h)^2-(2\chi)^2=1, \quad [h,\chi]=0. \tag{14d}$$

The first of these expresses the relationship (5f) in any nondiagonal representation which can be reached from the diagonal representation by means of a real orthogonal transformation. The additional minus sign comes from the anti-Hermitian character of χ. The second equation in (14d) indicates that h and χ can be diagonalized simultaneously.

The expression (14a) of $\mathfrak{M}$ gives

$$\mathfrak{M}^2=\begin{pmatrix} \nu^2-\mu^2 & [\nu,\mu] \\ [\nu,\mu] & \nu^2-\mu^2 \end{pmatrix}. \tag{15a}$$

If $[\nu,\mu]=0$, this form of $\mathfrak{M}^2$ shows that the eigenvalues of $\mathfrak{M}$ can be expressed as $\pm(\nu_\sigma^2+\mu_\sigma^2)^{\frac{1}{2}}$ in terms of the eigenvalues ν_σ and μ_σ of ν and $i\mu$. In the noncommutative coupling case when $[\nu,\mu]\neq 0$, the quasi-particle energies will be given in general by less simple expressions.[19]

For the commutator $[\mathfrak{M},\mathfrak{K}]$ of Eqs. (11f, g) one obtains with the expressions (14a, b)

$$[1-2\mathfrak{K},\mathfrak{M}]=2[\mathfrak{M},\mathfrak{K}]=2\begin{pmatrix} \mathfrak{B} & \mathfrak{A} \\ \mathfrak{A} & \mathfrak{B} \end{pmatrix}, \tag{15b}$$

where

$$2\mathfrak{A}=\{2\chi,\nu\}+\{(1-2h),\mu\}, \tag{15c}$$

$$2\mathfrak{B}=[(1-2h),\nu]+[2\chi,\mu], \tag{15d}$$

and the bracket $\{\ ,\ \}$ stands for the anticommutator of two quantities. The equation $[\mathfrak{M},\mathfrak{K}]=0$ is equivalent to

$$\mathfrak{A}=0, \quad \mathfrak{B}=0. \tag{15e}$$

In the diagonal representation of the commutative case, the equation $\mathfrak{A}=0$ reduces to the equation (6d) and $\mathfrak{B}=0$ is trivially satisfied. The time-dependent equation $i\partial\mathfrak{K}/\partial t=[\mathfrak{M},\mathfrak{K}]$ leads to the equations

$$i\partial\chi/\partial t=\mathfrak{A}, \quad i\partial h/\partial t=\mathfrak{B}. \tag{15f}$$

The contact with Bogoliubov's expressions[4] can be established through the quantities $\mathfrak{A}$ and $\mathfrak{B}$.

For the symmetrized product of $\mathfrak{M}$ and $1-2\mathfrak{K}$ one

[19] Such more general expressions for the quasi-particle energy have been worked out explicitly for simple models in connection with the work of reference 10.

obtains the expression

$$\{1-2\mathfrak{K},\ \mathfrak{M}\}=2\begin{pmatrix}\mathfrak{D} & \mathfrak{C}\\ \mathfrak{C} & \mathfrak{D}\end{pmatrix},\qquad(15g)$$

with

$$2\mathfrak{C}=[2\chi,\ \nu]+[(1-2h),\ \mu],\qquad(15h)$$

$$2\mathfrak{D}=\{(1-2h),\ \nu\}+\{2\chi,\ \mu\}.\qquad(15i)$$

In the commutative case, $\mathfrak{C}$ is zero and $\mathfrak{D}$ gives the expression (6f).

SMALL OSCILLATIONS

The equations of small oscillations about an equilibrium solution equally simplify with the compact form of the equations of motion given in the previous section. If one writes

$$\mathfrak{K}=\mathfrak{K}^{(0)}+\mathfrak{K}^{(1)},\quad \mathfrak{M}=\mathfrak{M}^{(0)}+\mathfrak{M}^{(1)},\qquad(16a)$$

in the time-dependent equation $i\partial\mathfrak{K}/\partial t=[\mathfrak{M},\mathfrak{K}]$, and assumes that $\mathfrak{K}^{(0)}$ is a solution of the stationary equation

$$[\mathfrak{M}^{(0)},\mathfrak{K}^{(0)}]=0,\qquad(16b)$$

small changes $\mathfrak{K}^{(1)}$ in the solution are determined by the equation

$$i\partial\mathfrak{K}^{(1)}/\partial t=[\mathfrak{M}^{(0)},\mathfrak{K}^{(1)}]+[\mathfrak{M}^{(1)},\mathfrak{K}^{(0)}],\qquad(16c)$$

which results by disregarding second-order terms. The corrections $\nu^{(1)}$, $\mu^{(1)}$ to the self-consistent potentials which determine $\mathfrak{M}^{(1)}$ are obtained by replacing h and χ by $h^{(1)}$ and $\chi^{(1)}$ in the definition of $\nu-\epsilon$ and μ. If $\mathfrak{K}^{(0)}$, $\mathfrak{M}^{(0)}$ are known, the equation (16c) is a linear equation in $\mathfrak{K}^{(1)}$. It is supplemented by the condition

$$\mathfrak{K}^{(0)}\mathfrak{K}^{(1)}+\mathfrak{K}^{(1)}\mathfrak{K}^{(0)}=\mathfrak{K}^{(1)},\qquad(16d)$$

which follows from $\mathfrak{K}^2=\mathfrak{K}$ and

$$\mathfrak{K}^{(0)2}=\mathfrak{K}^{(0)}.\qquad(16e)$$

The equations further simplify in a representation in which $\mathfrak{K}^{(0)}$ and $\mathfrak{M}^{(0)}$ are diagonal. With the notation

$$\begin{aligned}n_\sigma&=0\quad\text{for}\quad\sigma>0\\&=1\quad\text{for}\quad\sigma<0,\end{aligned}\qquad(17a)$$

one has in such a representation

$$\mathfrak{K}_{\sigma\sigma'}{}^{(0)}=n_\sigma\delta_{\sigma\sigma'},\qquad(17b)$$

$$\mathfrak{M}_{\sigma\sigma'}{}^{(0)}=(1-2n_\sigma)E_\sigma\delta_{\sigma\sigma'},\qquad(17c)$$

where $\sigma>0$ and $\sigma<0$ stand for the positive- and negative-energy eigenstates of $\mathfrak{M}^{(0)}$. The supplementary condition (16d) takes the form

$$(n_\sigma+n_{\sigma'}-1)\mathfrak{K}_{\sigma\sigma'}{}^{(1)}=0\qquad(17d)$$

which means that $\mathfrak{K}_{\sigma\sigma'}{}^{(1)}=0$ except for $n_\sigma+n_{\sigma'}=1$, that is, except for $\sigma>0$, $\sigma'<0$ or $\sigma<0$, $\sigma'>0$.

For the nonvanishing matrix elements one has

$$[\mathfrak{M}^{(0)},\mathfrak{K}^{(1)}]_{\sigma\sigma'}=\pm(E_\sigma+E_{\sigma'})\mathfrak{K}_{\sigma\sigma'}{}^{(1)},\qquad(18a)$$

$$[\mathfrak{M}^{(1)},\mathfrak{K}^{(0)}]_{\sigma\sigma'}=\pm\mathfrak{M}_{\sigma\sigma'}{}^{(1)},\qquad(18b)$$

where the $+$ sign holds for $\sigma>0$, $\sigma'<0$ and the $-$ sign for $\sigma<0$, $\sigma'>0$. Assuming a periodic solution in time with frequency ω, that is $i\partial\mathfrak{K}^{(1)}/\partial t=\omega\mathfrak{K}^{(1)}$, the equation (16c) gives, for $\omega\neq\pm(E_\sigma+E_{\sigma'})$, the relationships[19a]

$$\mathfrak{K}_{\sigma\sigma'}{}^{(1)}=-\frac{1}{E_\sigma+E_{\sigma'}-\omega}\mathfrak{M}_{\sigma\sigma'}{}^{(1)}\quad\text{for}\quad\sigma>0,\ \sigma'<0;$$

$$\mathfrak{K}_{\sigma\sigma'}{}^{(1)}=-\frac{1}{E_\sigma+E_{\sigma'}+\omega}\mathfrak{M}_{\sigma\sigma'}{}^{(1)}\quad\text{for}\quad\sigma<0,\ \sigma'>0.$$
$$(18c)$$

They represent a linear equation system to determine the collective oscillation frequencies ω and to investigate the stability of the solution $\mathfrak{K}^{(0)}$ of the self-consistent stationary equation (16b). The equations are written in a form in which they can be used, together with the definition of $\mathfrak{M}^{(1)}$, to give linear equations in $\mathfrak{M}^{(1)}$. If one multiplies with the denominators, they appear in the form of a linear two-particle wave equation to determine the two-quasi-particle wave function $\mathfrak{K}^{(1)}$. The term $\mathfrak{M}^{(1)}$ represents then an additional interaction between the two quasi-particles. The validity of this form of the equations in the more general coupling case is to be stressed.

The components of the equations (16c) are equivalent to the equations of the generalized random phase approximation,[11-13] if the expectation values of the linearized operator equations of the approximation are taken with respect to a state vector of the Bardeen, Cooper, Schrieffer type.

For $\sigma>0$, $\sigma'>0$ or $\sigma<0$, $\sigma'<0$, one has

$$[\mathfrak{M}^{(0)},\mathfrak{K}^{(1)}]_{\sigma\sigma'}=\pm(E_\sigma-E_{\sigma'}),\quad[\mathfrak{M}^{(1)},\mathfrak{K}^{(0)}]_{\sigma\sigma'}=0,\quad(19a)$$

which leads to solutions of the equation (16c) which satisfy

$$i\partial\mathfrak{K}_{\sigma\sigma'}{}^{(1)}/\partial t=\pm(E_\sigma-E_{\sigma'})\mathfrak{K}_{\sigma\sigma'}{}^{(1)}.\qquad(19b)$$

These correspond to the solutions called "unphysical" by Anderson[12] and are eliminated by the supplementary condition (16d), (17d).

GREEN'S FUNCTIONS

The symmetries of the representation become even more apparent in establishing the connection with the corresponding approximation of the Green's function equations. Positive and negative energy solutions contribute with a different sign in the time variable and the subspaces determined by $\mathfrak{K}$ and $1-\mathfrak{K}$ become related to the "negative" and "positive frequency part" Green's functions.

[19a] In order to obtain a Hermitian $\mathfrak{K}^{(1)}$, a linear combination of solutions with frequencies ω and $-\omega$ is to be taken.

In terms of the quantized field operators $\psi(x)$, $\psi^*(x)$, the linearized field equations can be written as

$$i\dot{\psi} = \nu\psi + \mu\psi^*, \qquad (20a)$$

$$i\dot{\psi}^* = -\mu^*\psi - \nu^*\psi^*, \qquad (20b)$$

where the kernels of the integral operators ν, μ are given by the expressions (4a, b). Equations (5b) give the detailed form of these equations in another representation. The letter x will now include the time variable, though with the simple form (4a, b) of ν, μ the integral sign in connection with these integral operators will indicate a summation over the variables excluding the time. The notation will, however, be suggestive to the form of the equations in further approximations where a multiplication with the self-energy operators involves also a time integration.

Introducing the Green's functions

$$
\begin{aligned}
G^{(-)}(x,x') &= \langle \psi^*(x')\psi(x) \rangle, \\
F^{(+)*}(x,x') &= \langle \psi^*(x')\psi^*(x) \rangle, \\
F^{(-)}(x,x') &= \langle \psi(x')\psi(x) \rangle, \\
G^{(+)*}(x,x') &= \langle \psi(x')\psi^*(x) \rangle,
\end{aligned}
\qquad (21a)
$$

where x and x' refer in general to two different time points, they satisfy the relationships

$$
\begin{aligned}
G^{(-)}(x,x') &= G^{(-)*}(x',x), & F^{(-)}(x,x') &= F^{(+)*}(x',x), \\
F^{(+)}(x,x') &= F^{(-)*}(x',x), & G^{(+)}(x,x') &= G^{(+)*}(x',x).
\end{aligned}
\qquad (21b)
$$

Multiplying the equations (20a, b) by $\psi^*(x')$ from the left and forming expectation values with respect to the state Φ_0, one obtains the equations

$$
\begin{aligned}
i\frac{\partial}{\partial t} G^{(-)}(x,x') &= \int dy\{\nu(x,y)G^{(-)}(y,x') \\
&\qquad + \mu(x,y)F^{(+)*}(y,x')\}, \\
i\frac{\partial}{\partial t} F^{(+)*}(x,x') &= \int dy\{-\mu^*(x,y)G^{(-)}(y,x') \\
&\qquad - \nu^*(x,y)F^{(+)*}(y,x')\}.
\end{aligned}
\qquad (21c)
$$

With the notation $\mathbf{\Psi}:(\psi,\psi^*)$, and the matrix form (11a) of $\mathfrak{M}$, the linearized field equations (20a, b) take the form

$$i\partial\mathbf{\Psi}/\partial t = \mathfrak{M}\mathbf{\Psi}. \qquad (22a)$$

Introducing the matrix

$$\mathcal{G}^{(-)} = \begin{pmatrix} G^{(-)} & F^{(-)} \\ F^{(+)*} & G^{(+)*} \end{pmatrix}, \qquad (22b)$$

the equations (21c) and the two similar equations obtained by multiplying the field equations (20a, b) from the left by $\psi(x')$ can be written in the matrix form

$$i\frac{\partial}{\partial t}\mathcal{G}^{(-)} = \mathfrak{M}\mathcal{G}^{(-)}. \qquad (22c)$$

Because of the symmetry properties of $\mathfrak{M}$, the conjugate complex of this equation can be written in the equivalent form

$$i\frac{\partial}{\partial t}\mathcal{G}^{(+)} = \mathfrak{M}\mathcal{G}^{(+)}, \qquad (22d)$$

where

$$\mathcal{G}^{(+)} = \begin{pmatrix} G^{(+)} & F^{(+)} \\ F^{(-)*} & G^{(-)*} \end{pmatrix}. \qquad (22e)$$

Besides the solutions $\mathcal{G}^{(+)}$, $\mathcal{G}^{(-)}$ of the homogeneous Green's function equation (22c, d) it may be of interest to consider the Green's function solutions $\mathcal{G}$, $\mathcal{G}_{(1)}$ related to the expectation value of anticommutators and commutators of field operators which are given by

$$\mathcal{G} = \mathcal{G}^{(+)} + \mathcal{G}^{(-)} = \begin{pmatrix} G & F \\ F^* & G^* \end{pmatrix}, \qquad (23a)$$

$$i\mathcal{G}_{(1)} = \mathcal{G}^{(+)} - \mathcal{G}^{(-)} = i\begin{pmatrix} G_{(1)} & F_{(1)} \\ F_{(1)}^* & G_{(1)}^* \end{pmatrix}, \qquad (23b)$$

with

$$G^{(+)} \pm G^{(-)} = \begin{cases} G \\ iG_{(1)} \end{cases}, \quad F^{(+)} \pm F^{(-)} = \begin{cases} F \\ iF_{(1)} \end{cases}, \qquad (23c)$$

where G, F are defined with the $+$ sign; $iG_{(1)}$, $iF_{(1)}$ with the $-$ sign. The retarded, advanced, and time-ordered solutions of the corresponding inhomogeneous Green's function equations with inhomogeneous δ-function terms can be constructed from these homogeneous solutions in the known way.

Apart from the inhomogeneous term, Eqs. (21c) give a generalized form of Gorkov's equations[5,20] and Eqs. (22c, d) establish the matrix form of these equations. The same equations can be obtained from the coupled system of Green's function equations by approximating the two-body Green's function by the sum of a contribution from an independent-particle motion described by G and of a factorizable term with factors F. This corresponds to the approximate form of the two-body correlation function[2] at equal times in which a dominant weight is attributed to a single factorizable term given by the product of two factors χ.

For $t = t'$ the Green's functions reduce to expressions considered in the previous sections. One has

$$\mathcal{G}^{(+)}(t=t') = \mathfrak{K}, \quad \mathcal{G}^{(-)}(t=t') = 1 - \mathfrak{K}, \qquad (24a)$$

$$\mathcal{G}(t=t') = 1, \quad \mathcal{G}_{(1)}(t=t') = 1 - 2\mathfrak{K}. \qquad (24b)$$

Through the relationship between $\mathfrak{M}$ and $\mathfrak{K}$, these initial conditions impose self-consistency requirements on the Green's function equations.

Because of $\nu(x,x') = \nu^*(x',x)$, $\mu(x,x') = -\mu(x',x)$, Eqs.

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[20] For use of the homogeneous Green's functions see also Yu. T. Grin', S. I. Drozdov, and D. F. Zaretzky, J. Exptl. Theoret. Phys. U.S.S.R. **38**, 222 (1960) [translation: Soviet Phys.—JETP **11**, 162 (1960)].

(20a, b) can be written in the alternative form

$$-i\dot{\psi}^*=\psi^*\nu-\psi\mu^*, \tag{25a}$$

$$-i\dot{\psi}=\psi^*\mu-\psi\nu^*. \tag{25b}$$

or with $\Psi^\dagger:(\psi^*,\psi)$ as

$$-i\partial\Psi^\dagger/\partial t=\Psi^\dagger\mathfrak{M}. \tag{25c}$$

For the matrix Green's functions (22b, e), (23a, b), this leads to equations of the form

$$-i\frac{\partial}{\partial t'}\mathcal{G}^{(-)}=\mathcal{G}^{(-)}\mathfrak{M}. \tag{25d}$$

Combining this with Eq. (22c), one obtains

$$i\left(\frac{\partial}{\partial t}+\frac{\partial}{\partial t'}\right)\mathcal{G}^{(-)}=[\mathfrak{M},\mathcal{G}^{(-)}]. \tag{25e}$$

With the initial condition (24a), this reduces for $t=t'$ to the equation

$$i\partial\mathcal{K}/\partial t=[\mathfrak{M},\mathcal{K}]. \tag{25f}$$

A somewhat different two-component notation has been considered by Anderson, Nambu,[9] and Schrieffer[21] in the case of electrons with a spin independent Hamiltonian. They consider the combination

$$\psi(x)=\begin{pmatrix}\psi_1(x)\\\psi_2^*(x)\end{pmatrix},$$

where ψ_1, ψ_2 refer to the two spin directions 1, 2, and introduce Pauli matrices in this notation.[22] There is no doubling of the single-particle states as in connection with the matrices $\mathcal{K}$, $\mathfrak{M}$. The connection between the two descriptions is established by the remark that in the case of a spin-independent Hamiltonian the quantities h, χ, ν, μ can be described by matrices of the form

$$h=\begin{pmatrix}h_{11}&0\\0&h_{22}\end{pmatrix},\quad \chi=\begin{pmatrix}0&\chi_{12}\\\chi_{21}&0\end{pmatrix},$$

$$\nu=\begin{pmatrix}\nu_{11}&0\\0&\nu_{22}\end{pmatrix},\quad \mu=\begin{pmatrix}0&\mu_{12}\\\mu_{21}&0\end{pmatrix}, \tag{26}$$

and the matrices $\mathcal{K}$, $\mathfrak{M}$ appear in a reduced form with respect to two invariant subspaces. In the case that there is no obvious *a priori* separation of the single-particle space into two independent subspaces, the more symmetric method of the present paper will still retain its validity.

ACKNOWLEDGMENT

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[21] J. R. Schrieffer (to be published).

[22] Schrieffer investigated an approximation scheme for the Green's functions which goes far beyond the zero-order approximation of the present paper.