Generalized Self-Consistent-Field Theory: Gor'kov Factorization*

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(Received 3 August 1964)

Gor'kov factorization, $\langle\psi^\dagger(1)\psi^\dagger(2)\psi(3)\psi(4)\rangle \to \langle\psi^\dagger(1)\psi^\dagger(2)\rangle\langle\psi(3)\psi(4)\rangle$, is made the basis of a generalized self-consistent-field (SCF) theory precisely analogous to that previously developed for Hartree factorization, $\langle\psi^\dagger(1)\psi^\dagger(2)\psi(3)\psi(4)\rangle \to \langle\psi^\dagger(1)\psi(4)\rangle\langle\psi^\dagger(2)\psi(3)\rangle$. The generalized SCF method is reviewed in the context of Gor'kov factorization. The corresponding simple SCF theory is developed to illustrate the method and is shown to give a simple Hamiltonian version of the Bardeen-Cooper-Schrieffer theory of superconductivity and, more generally, of coherent pairing. The notion of an external pairing field is introduced and the corresponding response functions developed via a formalism like that of Kubo. General fluctuation-dissipation theorems are proved for the response functions. An equation of state is then obtained by a formulation analogous to the dielectric formulation. The insertion of the simple SCF approximation to the response function into the equation of state yields a generalization of the usual low-density (or short-range) evaluation of the grand potential to arbitrary temperatures. Screening the bare interaction with this approximate response function converts the former into the t matrix of the independent-pair approximation. The entire analysis gives an underlying unity to the currently disparate treatments of superconductivity, of long-range correlations, and of short-range correlations.

I. INTRODUCTION

THROUGH the introduction of appropriate self-consistent fields, Gor'kov[1] and Nambu[2] have elegantly and compactly reformulated the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity.[3] Gor'kov, in particular, introduced into the equation of motion of the single-particle Green's function the basic approximation

$$\langle\psi^\dagger(1)\psi^\dagger(2)\psi(3)\psi(4)\rangle \to \langle\psi^\dagger(1)\psi^\dagger(2)\rangle\langle\psi(3)\psi(4)\rangle, \quad (1.1)$$

which we call Gor'kov factorization. Here the $\psi^\dagger(i)$ and $\psi(j)$ are fermion creation and destruction operators, and the angular brackets indicate an appropriate ensemble average. Gor'kov rationalized the number-nonconserving character of the approximation (1) by noting that the exact average $\langle\psi^\dagger(1)\psi^\dagger(2)\psi(3)\psi(4)\rangle$ contained, e.g., the important terms $\langle N|\psi^\dagger(1)\psi^\dagger(2)|N-2\rangle \times\langle N-2|\psi(3)\psi(4)|N\rangle$ which are kept in the approximation (1.1).

In an earlier paper,[4] we made Hartree factorization,

$$\langle\psi^\dagger(1)\psi^\dagger(2)\psi(3)\psi(4)\rangle \to \langle\psi^\dagger(1)\psi(4)\rangle\langle\psi^\dagger(2)\psi(3)\rangle, \quad (1.2)$$

the basis of a fairly complete formulation of a generalized self-consistent-field (SCF) theory. In the present paper, we make the Gor'kov factorization the basis of an analogous theoretical development.

For uniform systems the Hartree SCF vanishes. The generalized Hartree SCF method is then suitable for discussing exchange and correlation corrections to the simple SCF theory via a dielectric formulation[4,5] useful at high densities for long-range interactions (Ref. 4 is designated as I here). For nonuniform systems, the Hartree factorization plus dielectric formulation is convenient for the study of the interrelation of exchange and correlation with the nonuniformity.[6]

Correspondingly, for normal systems the Gor'kov SCF vanishes. The generalized Gor'kov SCF method is then, as we shall see, suitable for discussing exchange and correlation corrections via an analog of the dielectric formulation, but now it becomes useful at low densities or for short-range interactions. For systems with coherent pairing of the first and second kinds,[7,8] the Gor'kov field does not vanish. Our SCF procedure then permits the development of a Hamiltonian formulation of, e.g., the theory of superconductivity which is simple, convenient, and, because it is a Hamiltonian formulation, of wider general utility than the Green's function theory of Gor'kov. Our procedure, in a sense, provides a bridge between the Hamiltonian formulation of Bogoliubov[9] and the Green's function formulation of Gor'kov. One can proceed forward with the SCF theory by putting it into a single-particle-like form which resembles somewhat Anderson's pseudospin theory[10] or Nambu's spinor theory.[2] The new form which will be discussed in a separate publication, looks promising in relation to the general problem of developing transport equations for superconductors.[11] Alternatively, one can

* This work has received direct partial support from National Aeronautic and Space Agency and the National Science Foundation.

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TABLE I. Restrictions on the interaction.

	Restriction	Origin
1.	$v_{\mathbf{q}}(\mathbf{p},\mathbf{p}')_{\sigma_1\sigma_1',\sigma_2'\sigma_2}=(v_{\mathbf{q}}(\mathbf{p},\mathbf{p}')_{\sigma_1\sigma_1',\sigma_2'\sigma_2})^*$	Convenience
2.	$=v_{\mathbf{q}}(\mathbf{p},\mathbf{p}')_{-\sigma_1-\sigma_1',-\sigma_2'-\sigma_2}$	Spin-rotation invariance
3.	$=v_{-\mathbf{q}}(\mathbf{p}+\mathbf{q},\mathbf{p}'-\mathbf{q})_{-\sigma_2-\sigma_2',-\sigma_1',-\sigma_1}$	Time-reversal invariance
4.	$=v_{-\mathbf{q}}(-\mathbf{p},-\mathbf{p}')_{\sigma_1\sigma_1',\sigma_2'\sigma_2}$	Inversion invariance
5.	$=v_{-\mathbf{q}}(\mathbf{p}',\mathbf{p})_{\sigma_1'\sigma_1,\sigma_2\sigma_2'}$	Identity of particles
6.	$=f(p,p',q,\mathbf{p}\cdot\mathbf{q},\mathbf{p}'\cdot\mathbf{q})$	Spatial-rotation invariance
7.	$=0$ unless $\sigma_1+\sigma_1'=\sigma_2+\sigma_2'$	Spin-rotation invariance
8.	$v_{\uparrow\uparrow\uparrow\uparrow}=v_{\uparrow\downarrow\downarrow\uparrow}+v_{\uparrow\downarrow\uparrow\downarrow}$	Spin-rotation invariance

work towards going beyond the BCS theory with the aid of the "dielectric" formulation in order to shed light on the nature of the superconducting to normal phase transition.[12] Finally, we have already used the SCF theory described herein as a basis for studying the relative stability of normal and coherently paired states.[7,13]

In Sec. II, we apply the generalized SCF method to the present case of Gor'kov factorization. In Sec. III, we illustrate the theory in its simplest form by applying it to the familiar case of a coherently paired state (e.g., the superconducting state). In Sec. IV, we study the response of the system to an external pairing potential, and, in Sec. V, derive the corresponding fluctuation-dissipation theorems. An equation of state is then developed in Sec. VI which is analogous to the dielectric formulation of Ref. 5. These results are simplified in Sec. VII by the application of various symmetry and related considerations. An approximate study of the equation of state valid for low densities or short-range interactions illustrates the relation of the present theory to other methods.

Although the theory has been presented herein only for fermions, all general results hold equally well for bosons, to which they may be applied simply by eliminating the spin indices and substituting symmetrizing for antisymmetrizing wherever the latter is indicated.

After this work was completed, it came to the author's attention that a closely related use of Gor'kov factorization has been made by Emery.[14] Emery introduces an external pairing field and the corresponding generalized response functions. He then developes an equation of state analogous to the dielectric formulations of Nozieres and Pines[5] and of Brout and Englert[5] by integrating over the strength of the particle interaction. A simple Gor'kov SCF theory analogous to that of Sec. III is then introduced to give a result for the response function and grand potential analogous to the $\xi=0$ result of Sec. VIII. The philosophy followed is thus related more closely to that of Ehrenreich and Cohen[15] than to that of the present paper and of I.

II. THE GENERALIZED SCF METHOD

We consider a collection of N interacting fermions confined within a volume $V(N\to\infty,\ V\to\infty,\ \rho=N/V$ remains finite). Because we work with the grand canonical ensemble, we use the "thermodynamic" Hamiltonian to govern the motion of the system:

$$\mathcal{H}_{TH}=\mathcal{K}+\mathcal{V}_I. \tag{2.1}$$

Here $\mathcal{K}$ is the kinetic energy K measured relative to the Gibbs free energy μN, where μ is the chemical potential, or Fermi energy. Upon introducing second quantization, with $\psi_{\mathbf{p}\sigma}^\dagger$ the creation operator for a state of momentum $\mathbf{p}$ and spin direction σ, $\mathcal{K}$ may be written

$$\mathcal{K}=K-\mu N=\sum_{\mathbf{p}\sigma}\epsilon_p\psi_{\mathbf{p}\sigma}^\dagger\psi_{\mathbf{p}\sigma}, \tag{2.1a}$$

$$\epsilon_p=(p^2/2m)-\mu. \tag{2.1b}$$

Correspondingly, $\mathcal{V}_I$ is the interaction potential, which may be written generally as

$$\mathcal{V}_I=\tfrac{1}{2}\sum_{\substack{\mathbf{qp},\mathbf{p}'\\ \sigma_1,\sigma_1';\sigma_2,\sigma_2'}} v_{\mathbf{q}}(\mathbf{p},\mathbf{p}')_{\sigma_1\sigma_1',\sigma_2'\sigma_2}\times\psi_{\mathbf{p}+\mathbf{q}\sigma_1}^\dagger\psi_{\mathbf{p}'-\mathbf{q}\sigma_1'}^\dagger\psi_{\mathbf{p}'\sigma_2'}\psi_{\mathbf{p}\sigma_2}. \tag{2.2}$$

In (2.2), $v_{\mathbf{q}}(\mathbf{p},\mathbf{p}')_{\sigma_1\sigma_1',\sigma_2'\sigma_2}$ is the matrix element of the interaction for the scattering of a pair of particles from the states $\mathbf{p}\sigma_2$ and $\mathbf{p}'\sigma_2'$ to the states $\mathbf{p}+\mathbf{q}\sigma_1$ and $\mathbf{p}'-\mathbf{q}\sigma_1'$; $\hbar\mathbf{q}$ is the associated momentum transfer. We have allowed for momentum and spin dependence of the interaction for later application to off-the-energy-shell interactions of Landau quasiparticles.[16] The restrictions imposed on $v_{\mathbf{q}}(\mathbf{p},\mathbf{p}')_{\sigma_1\sigma_1',\sigma_2'\sigma_2}$ by symmetry or convenience are listed in Table I.

It is convenient to introduce pair-field operators $d^\pm(\mathbf{p},\mathbf{p}')$ and to resolve them into singlet $d_s^\pm$ and triplet

[12] That the BCS theory may need augmenting in the vicinity of the transition temperature is suggested by the specific-heat measurements of D. C. Rorer, H. Meyer, and R. C. Richardson, Z. Naturforsch. **18**, 130 (1963), and of D. C. Hopkins, Ph.D. thesis, University of Illinois, 1962 (unpublished), both for Al. I am grateful to Professor D. H. Douglass for calling this work to my attention and for detailed discussions of these and related matters.

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components $d_m^{\pm}$, $m=0, \pm 1$. The latter resolution is made by observing that $\psi_{p\uparrow}^{\dagger}$ and $-\psi_{p\downarrow}$ transform as the $m=\frac{1}{2}$ component of a spinor and $\psi_{p\downarrow}^{\dagger}$ and $\psi_{p\uparrow}$ as the $m=-\frac{1}{2}$ component under spin rotation. We have, then,

$$d_s^-(\mathbf{p},\mathbf{p}')=(1/\sqrt{2})(\psi_{p\downarrow}\psi_{p'\uparrow}-\psi_{p\uparrow}\psi_{p'\downarrow}); \quad d_s^-(\mathbf{p},\mathbf{p}')\equiv d_s^-(\mathbf{p}',\mathbf{p}), \tag{2.3a}$$

$$d_s^+(\mathbf{p},\mathbf{p}')=(1/\sqrt{2})(\psi_{p\uparrow}^{\dagger}\psi_{p'\downarrow}^{\dagger}-\psi_{p\downarrow}^{\dagger}\psi_{p'\uparrow}^{\dagger}); \quad [d_s^-(\mathbf{p}',\mathbf{p})]^{\dagger}\equiv d_s^+(\mathbf{p},\mathbf{p}'), \tag{2.3b}$$

$$d_1^-(\mathbf{p},\mathbf{p}')=\psi_{p\downarrow}\psi_{p'\downarrow}, \quad d_1^+(\mathbf{p},\mathbf{p}')=\psi_{p\uparrow}^{\dagger}\psi_{p'\uparrow}^{\dagger},$$

$$d_0^-(\mathbf{p},\mathbf{p}')=(1/\sqrt{2})(\psi_{p\uparrow}\psi_{p'\downarrow}+\psi_{p\downarrow}\psi_{p'\uparrow}), \quad d_0^+(\mathbf{p},\mathbf{p}')=(1/\sqrt{2})(\psi_{p\uparrow}^{\dagger}\psi_{p'\downarrow}^{\dagger}+\psi_{p\downarrow}^{\dagger}\psi_{p'\uparrow}^{\dagger}), \tag{2.4a}$$

$$d_{-1}^-(\mathbf{p},\mathbf{p}')=\psi_{p\uparrow}\psi_{p'\uparrow}, \quad d_{-1}^+(\mathbf{p},\mathbf{p}')=\psi_{p\downarrow}^{\dagger}\psi_{p'\downarrow}^{\dagger},$$

$$d_m^-(\mathbf{p},\mathbf{p}')\equiv -d_m^-(\mathbf{p}',\mathbf{p}), \quad [d_m(\mathbf{p}',\mathbf{p})]^{\dagger}\equiv d_{-m}^+(\mathbf{p},\mathbf{p}'). \tag{2.4b}$$

Substitution of (2.3) and (2.4) into (2.2) yields for $\mathcal{U}_I$ after use of Table I,

$$\mathcal{U}_I=\tfrac{1}{2}\sum_{\substack{\mathbf{q},\mathbf{p},\mathbf{p}'\\ m}}[v_q(\mathbf{p},\mathbf{p}')_s d_s^+(\mathbf{p}+\mathbf{q},\mathbf{p}'-\mathbf{q})d_s^-(\mathbf{p}',\mathbf{p}) + v_q(\mathbf{p},\mathbf{p}')_t d_m^+(\mathbf{p}+\mathbf{q},\mathbf{p}'-\mathbf{q})d_{-m}^-(\mathbf{p}',\mathbf{p})], \tag{2.5}$$

where v_s and v_t are the singlet and triplet interaction potentials,

$$v_s=v_{\uparrow\downarrow\downarrow\uparrow}-v_{\uparrow\downarrow\uparrow\downarrow}, \tag{2.6a}$$

$$v_t=v_{\uparrow\uparrow\uparrow\uparrow}=v_{\uparrow\downarrow\downarrow\uparrow}+v_{\uparrow\downarrow\uparrow\downarrow}. \tag{2.6b}$$

It is convenient to abbreviate (2.5) still further by writing

$$\mathcal{U}_I=\tfrac{1}{2}\sum_{\mathbf{q},\mathbf{p},\mathbf{p}',\alpha} v_q(\mathbf{p},\mathbf{p}')_\alpha d_\alpha^+(\mathbf{p}+\mathbf{q},\mathbf{p}'-\mathbf{q})d_{-\alpha}^-(\mathbf{p}',\mathbf{p}), \tag{2.7}$$

where α stands for s, t, and/or m in turn.

We have to do with the average of $\mathcal{H}_{TH}$ in the formulation of the variational principles of quantum mechanics,

$$U'=\langle \mathcal{H}_{TH}\rangle, \tag{2.8}$$

which is the difference between the internal energy U and the Gibbs free energy $G=\mu\langle N\rangle$. In U', the average interaction energy $\langle \mathcal{U}_I\rangle$ contains averages of products like $\langle d_\alpha^+ d_{-\alpha}^-\rangle$. The starting point of the generalized SCF method introduced in I is to modify all such quantities,

$$\langle d_\alpha^+ d_{-\alpha}^-\rangle \rightarrow (1-\xi)\langle d_\alpha^+\rangle\langle d_{-\alpha}^-\rangle+\xi\langle d_\alpha^+ d_{-\alpha}^-\rangle, \tag{2.9}$$

wherever they enter U' but otherwise to maintain the usual variational principles unchanged. The parameter ξ, which varies between zero and unity may be regarded as a correlation coupling parameter. When ξ is zero, we have a *simple* SCF theory, and (2.9) reduces to Gor'kov factorization. When ξ is unity, we recapture the exact problem. At intermediate values of ξ, we have a *generalized* SCF theory.

In thermodynamic equilibrium, the grand potential,

$$\Omega=U'-TS=-pV, \tag{2.10}$$

is a minimum for arbitrary variation of the density matrix P, subject to normalization of P and constancy of T, μ, and V. This variational principle together with (2.9) leads immediately to

$$P_0=\exp[(\Omega'-\mathcal{H}_s^0)/k_BT] \tag{2.11}$$

for the density matrix in equilibrium. The SCF Hamiltonian $\mathcal{H}_s^0$ in equilibrium

$$\mathcal{H}_s^0=\mathcal{K}+(1-\xi)\mathcal{U}_G^0+\xi\mathcal{U}_I, \tag{2.12}$$

now contains a SCF term $\mathcal{U}_G$;

$$\mathcal{U}_G=\sum_{\mathbf{p},\mathbf{p}',\alpha}[V_{G\alpha}^+(\mathbf{p},\mathbf{p}')d_{-\alpha}^-(\mathbf{p}',\mathbf{p}) + V_{G\alpha}^-(\mathbf{p},\mathbf{p}')d_{-\alpha}^+(\mathbf{p}',\mathbf{p})]. \tag{2.13}$$

In (2.13) $V_{G\alpha}$ is the Gor'kov field, i.e., the self-pairing field of the system,

$$V_{G\alpha}^-(\mathbf{p},\mathbf{p}')=\tfrac{1}{2}\sum_{\mathbf{q}} v_q(\mathbf{p},\mathbf{p}')_\alpha\langle d_\alpha^-(\mathbf{p}+\mathbf{q},\mathbf{p}'-\mathbf{q})\rangle, \tag{2.14a}$$

$$V_{G\alpha}^+(\mathbf{p},\mathbf{p}')=\tfrac{1}{2}\sum_{\mathbf{q}} v_q(\mathbf{p},\mathbf{p}')_\alpha\langle d_\alpha^+(\mathbf{p}+\mathbf{q},\mathbf{p}'-\mathbf{q})\rangle, \tag{2.14b}$$

$$[V_{G\alpha}^-(\mathbf{p},\mathbf{p}')]^*=V_{G,-\alpha}^+(\mathbf{p}',\mathbf{p}). \tag{2.14c}$$

The Gor'kov fields are to be determined self-consistently by averaging d^- or d^+ in (2.14) with P_0, (2.11), which in turn depends on the Gor'kov fields.

For time-dependent problems, the equation of motion of the density matrix is

$$i\hbar\dot{P}=[\mathcal{H}_s,P], \tag{2.15}$$

which is to be solved self-consistently with the defining equations of the Gor'kov fields (2.14).

III. SCF THEORY OF COHERENTLY PAIRED STATES

To illustrate the formalism, we discuss briefly in the present section the thermal equilibrium theory of coherently paired states in the $\xi=0$ limit (simple SCF theory). The SCF Hamiltonian is now

$$\mathcal{H}_s^0=\sum_{p\sigma}\epsilon_p\psi_{p\sigma}^{\dagger}\psi_{p\sigma} + \sum_{\mathbf{p},\mathbf{p}',\alpha}[V_{G\alpha}^+(\mathbf{p},\mathbf{p}')d_{-\alpha}^-(\mathbf{p}',\mathbf{p})+\text{conj.}]. \tag{3.1}$$

We restrict ourselves to uniform, isotropic, and nonmagnetic states of the system. Elementary symmetry arguments show that

$$\langle d_\alpha^-(\mathbf{p},\mathbf{p}')\rangle=0 \quad \text{unless} \quad \mathbf{p}=-\mathbf{p}' \quad \text{and} \quad \alpha=s, \tag{3.2}$$

and similarly for V_G^+, V_G^-, and $\langle d^+\rangle$. Moreover, $\langle d_s^-(-\mathbf{p},\mathbf{p})\rangle$ depends only on p; we thus have s wave, singlet pairing as supposed in the original BCS theory.

The SCF Hamiltonian simplifies further to

$$\mathcal{H}_s^0=\sum_{\mathbf{p}}[\epsilon_p(\psi_{\mathbf{p}\uparrow}^\dagger\psi_{\mathbf{p}\uparrow}+\psi_{\mathbf{p}\downarrow}^\dagger\psi_{\mathbf{p}\downarrow} +\Delta_{\mathbf{p}}\psi_{\mathbf{p}\uparrow}^\dagger\psi_{-\mathbf{p}\downarrow}^\dagger+\Delta_{\mathbf{p}}^+\psi_{-\mathbf{p}\downarrow}\psi_{\mathbf{p}\uparrow}], \tag{3.3}$$

where

$$\Delta_{\mathbf{p}}=\Delta_p=(\Delta_{\mathbf{p}}^+)^*=\sum_{\mathbf{q}} v_{\mathbf{q}}(\mathbf{p},-\mathbf{p})_s\langle\psi_{-\mathbf{p}-\mathbf{q}\downarrow}\psi_{\mathbf{q}+\mathbf{p}\uparrow}\rangle \tag{3.4}$$

is the energy-gap parameter and is to be determined self-consistently. At this point, one makes the Bogoliubov transformation to diagonalize the Hamiltonian and quickly recaptures all the familiar results of superconductivity theory. The Bogoliubov transformation is[9]

$$\begin{aligned}&\psi_{\mathbf{p}\uparrow}^\dagger=u_p c_{\mathbf{p}\uparrow}^\dagger+v_p c_{-\mathbf{p}\downarrow}, \qquad \psi_{\mathbf{p}\downarrow}=u_p^* c_{\mathbf{p}\uparrow}+v_p^* c_{-\mathbf{p}\downarrow}^\dagger,\\ &\psi_{-\mathbf{p}\downarrow}=u_p c_{-\mathbf{p}\downarrow}-v_p c_{\mathbf{p}\uparrow}^\dagger, \quad \psi_{-\mathbf{p}\downarrow}^\dagger=u_p^* c_{-\mathbf{p}\downarrow}^\dagger-v_p^* c_{\mathbf{p}\uparrow},\end{aligned} \tag{3.5}$$

$$|u_p|^2+|v_p|^2=1,$$

where the $c_{\mathbf{p}\sigma}$ are the Bogoliubov quasiparticle operators. The diagonalization requirement gives Δ_p real and, together with the requirement that the lowest eigenvalue of $\mathcal{H}_s^0$ correspond to no quasiparticles excited, gives also that

$$|u_p|^2=\tfrac{1}{2}(1+\epsilon_p/E_p), \tag{3.6a}$$

$$|v_p|^2=\tfrac{1}{2}(1-\epsilon_p/E_p), \tag{3.6b}$$

$$E_p=(\epsilon_p^2+\Delta_p^2)^{1/2}, \tag{3.7}$$

$$\mathcal{H}_s^0=\sum_{\mathbf{p}}\{(\epsilon_p-E_p)+E_p[c_{\mathbf{p}\uparrow}^\dagger c_{\mathbf{p}\uparrow}+c_{\mathbf{p}\downarrow}^\dagger c_{\mathbf{p}\downarrow}]\}. \tag{3.8}$$

If the sign of v_p is taken as positive, the sign of u_p is opposite to that of Δ_p. Finally, the self-consistency requirement (3.4) gives the BCS integral equation for the energy-gap parameter,

$$\Delta_p=-\tfrac{1}{2}\sum_{\mathbf{q}} v_{\mathbf{q}}(\mathbf{p},-\mathbf{p})\frac{\tanh\frac{1}{2}\beta E_{|\mathbf{p}+\mathbf{q}|}}{E_{|\mathbf{p}+\mathbf{q}|}}\Delta_{|\mathbf{p}+\mathbf{q}|}. \tag{3.9}$$

It should be noted that

$$\langle\mathcal{H}_s^0\rangle=\sum_{\mathbf{p}}[(\epsilon_p-E_p)+E_p(f_{p\uparrow}+f_{p\downarrow})], \tag{3.10}$$

where

$$f_{p\sigma}=[e^{\beta E_p}+1]^{-1}, \tag{3.11}$$

is not the value of U'. Instead, we have

$$U'=\langle\mathcal{H}_s^0\rangle-\tfrac{1}{2}(1-\xi)\langle\mathcal{U}_G^0\rangle \tag{3.12}$$

in general. For our present $\xi=0$ case, (3.12) gives

$$U'=\sum_{\mathbf{p}}(\epsilon_p-E_p)|v_p|^2+\sum_{\mathbf{p}\sigma}E_p f_{p\sigma}, \tag{3.13}$$

which is the usual result for the total energy.

We see that the present version of Gor'kov SCF theory gives a simple Hamiltonian formulation for superconductors (or for CP II[8]) at thermal equilibrium. The particular advantages of the present scheme, however, manifest themselves much more clearly for nonequilibrium problems, which we have studied to some extent but which cannot be dwelled upon here.

IV. RESPONSE TO AN EXTERNAL PAIRING FIELD

We return now to the generalized SCF theory, $\xi\neq0$, and add to the Hamiltonian an interaction $\mathcal{U}_0$ between the system and its environment which transfers a pair of electrons simultaneously from one to the other:

$$\mathcal{U}_0=\sum_{\mathbf{p}\mathbf{p}',\sigma\sigma'}[V_0^-(\mathbf{p}',\mathbf{p})_{\sigma'\sigma}\psi_{\mathbf{p}\sigma}^\dagger\psi_{\mathbf{p}'\sigma'}^\dagger +V_0^+(\mathbf{p},\mathbf{p}')_{\sigma\sigma'}\psi_{\mathbf{p}'\sigma'}\psi_{\mathbf{p}\sigma}]. \tag{4.1}$$

We are interested in the linear response of the system to the (in general, time-dependent) external pairing potentials, or pairing fields, V_0^- and V_0^+, which may be considered independent. Once again, it is convenient to resolve V_0^- and V_0^+ into their singlet and triplet components as in (2.3), (2.4), and (2.7):

$$\mathcal{U}_0=\sum_{\mathbf{p},\mathbf{p}',\alpha}[V_0^-(\mathbf{p}',\mathbf{p})_\alpha d_{-\alpha}^+(\mathbf{p},\mathbf{p}') +V_0^+(\mathbf{p},\mathbf{p}')_\alpha d_{-\alpha}^-(\mathbf{p}',\mathbf{p})]. \tag{4.2}$$

The total SCF Hamiltonian which governs the evolution of the system in time is now

$$\mathcal{H}_s=\mathcal{K}+(1-\xi)\mathcal{U}_G+\xi\mathcal{U}_I+\mathcal{U}_0. \tag{4.3}$$

The external pairing field $\mathcal{U}_0$ induces a departure $\Delta\mathcal{U}_G$ of the self-pairing field $\mathcal{U}_G$ from its equilibrum value $\mathcal{U}_G^0$,

$$\mathcal{U}_G=\mathcal{U}_G^0+\Delta\mathcal{U}_G. \tag{4.4}$$

The SCF Hamiltonian correspondingly changes from its equilibrium counterpart to

$$\mathcal{H}_s=\mathcal{H}_s^0+\mathcal{U}_\xi, \tag{4.5}$$

$$\mathcal{U}_\xi=(1-\xi)\Delta\mathcal{U}_G+\mathcal{U}_0. \tag{4.6}$$

The entity $\mathcal{U}_\xi$ is the effective pairing field accompanying $\mathcal{U}_0$. It is necessary to introduce also the total internal pairing field $\mathcal{U}$ accompanying $\mathcal{U}_0$:

$$\mathcal{U}=\Delta\mathcal{U}_G+\mathcal{U}_0. \tag{4.7}$$

The corresponding entities V_ξ, V, V_0 are analogous to the Lorentz local field, the electric field $\mathbf{E}$, and Maxwell's displacement field $\mathbf{D}$, respectively, in problems of longitudinal electromagnetic disturbances (cf. also I).

In computing linear responses, we restrict ourselves to evaluating ΔV_G, and hence V and V_ξ, to first order in V_0. There must result a linear relation between V_0 and V after all the mechanics of self-consistency are worked out. In analogy with the relation $D=\epsilon E$ of electromagnetism, it is convenient to express this linear relationship schematically as

$$V_0=\epsilon V, \tag{4.8}$$

where all variables specifying the components of V_0, ϵ, and V have been suppressed for clarity.[17] The response function ϵ is thus analogous to the dielectric function of I. The task of the present section is to derive expressions for the response function analogous to those derived for the dielectric function in I.

The procedure we follow is similar to that systematized by Kubo.[18] We order the calculation in powers of $\mathcal{V}_0$ and keep only first-order terms. For the density matrix we have, then,

$$P=P_0+P_1, \tag{4.9}$$

$$i\hbar\dot{P}_1=[\mathcal{H}_s^0,P_1]+[\mathcal{V}_\xi,P_0]. \tag{4.10}$$

Requiring that $\mathcal{V}_0$ and P_1 vanish in the remote past, the solution of (4.10) is

$$P_1(t)=\frac{1}{i\hbar}\int_{-\infty}^{t}\left[\exp\left(\frac{i}{\hbar}\mathcal{H}_s^0(t'-t)\right)\mathcal{V}_\xi(t')\times\exp\left(-\frac{i}{\hbar}\mathcal{H}_s^0(t'-t)\right)P_0\right]dt'. \tag{4.11}$$

It should be noted that (4.11) is written in the Schrödinger and not in the Heisenberg picture.

To proceed further at this point by evaluating the SCF implicitly contained in (4.11) through $\mathcal{V}_\xi$ would get us involved with a very heavy notation. Accordingly we now introduce a compact, abstract vector and matrix notation for the entities we deal with here. Let the superscript τ stand for the superscript $\pm$ of the pair fields d and pairing fields V_ξ, V, V_0. Regard $X(\mathbf{p}_1,\mathbf{p}_2)_\alpha{}^\tau$ for any such quantity X as the $\mathbf{p}_1$, $\mathbf{p}_2$, α, τ component of the column vector $\mathbf{X}$ in an appropriate Hilbert space. The row vector $\mathbf{X}^\dagger$ which is the Hermitian conjugate to $\mathbf{X}$ is

$$X^\dagger(\mathbf{p}_1,\mathbf{p}_2)_\alpha{}^\tau=X(\mathbf{p}_2,\mathbf{p}_1)_{-\alpha}{}^{-\tau}. \tag{4.12}$$

For convenience, we can specify the entire collection of variables specifying a component of $\mathbf{X}$ or $\mathbf{X}^\dagger$ by the subscript i,

$$X_i \Leftrightarrow X(\mathbf{p}_1,\mathbf{p}_2)_\alpha{}^\tau. \tag{4.13}$$

We now define the scalar product P of two vectors $\mathbf{X}$ and $\mathbf{Y}$ to be

$$P=\mathbf{X}\cdot\mathbf{Y}=\sum_i X_i^\dagger Y_i=\sum_i X_i Y_i^\dagger=\mathbf{Y}\cdot\mathbf{X}. \tag{4.14}$$

We see from (2.13), (4.2), (4.6), (4.12), and (4.14) that $\mathcal{V}_\xi$ may be written as

$$\mathcal{V}_\xi=\mathbf{d}\cdot\mathbf{V}_\xi. \tag{4.15}$$

Similarly, we see that ϵ defined through the relationship (4.8) must be a matrix $\boldsymbol{\epsilon}$ in the same sense that $\mathbf{V}_0$ and $\mathbf{V}$ are vectors

$$\mathbf{V}_0=\boldsymbol{\epsilon}\cdot\mathbf{V} \quad \text{or} \quad (V_0)_i=\sum_j \epsilon_{ij}V_j. \tag{4.16}$$

This completes the introduction of the compact notation; we now turn back to the calculation of $\boldsymbol{\epsilon}$.

We start by evaluating

$$\langle d_i\rangle^{(1)}=\mathrm{tr}d_iP_1. \tag{4.17}$$

Putting (4.15) into (4.11) and the result into (4.17) leads to

$$\langle\mathbf{d}\rangle^{(1)}=\int_{-\infty}^{\infty}\mathbf{A}(t-t')\cdot\mathbf{V}_\xi(t')dt'. \tag{4.18}$$

The entity $\mathbf{A}(t-t')$ is a matrix in the same sense that $\boldsymbol{\epsilon}$ is a matrix in (4.16). It is causal and has the elements

$$A_{ij}(t-t')=\langle\langle d_i(t),d_j^\dagger(t')\rangle\rangle, \quad t\geq t' \qquad =0, \quad t<t'. \tag{4.19}$$

The bracket symbol used in (4.19) stands explicitly for

$$\langle\langle a(t),b(t')\rangle\rangle=(1/i\hbar)\,\mathrm{tr}[a(t),b(t')]P_0, \tag{4.20}$$

where $a(t)$ and $b(t')$ are second-quantized operators in the Heisenberg picture generated by $\mathcal{H}_s^0$. In (4.19), in particular, the Hermitian conjugation $\mathbf{d}\rightarrow\mathbf{d}^\dagger$ is to be taken according to (4.12) *before* passing into the Heisenberg picture.

It is convenient to specialize the time dependence of V_0, etc., to $\exp(-i\omega^+t)$, $\omega^+=\omega+i\alpha$, $\alpha\rightarrow 0^+$, in which case (4.18) becomes

$$\langle\mathbf{d}(t)\rangle^{(1)}=\mathbf{A}(\omega^+)\cdot\mathbf{V}_\xi(t), \tag{4.21}$$

where

$$\mathbf{A}(\omega^+)=\int_{-\infty}^{\infty}e^{i\omega^+(t-t')}\mathbf{A}(t-t')dt'. \tag{4.22}$$

In the representation based on the functions Ψ_m diagonalizing $\mathcal{H}_s^0$,

$$\mathcal{H}_s^0\Psi_m=E_m\Psi_m, \tag{4.23}$$

$$P_{mm'}{}^0=\mathcal{P}_m\delta_{mm'}, \quad \mathcal{P}_m=-e^{-\beta E_m}/\sum_{m'}e^{-\beta E_{m'}}, \tag{4.24}$$

Eqs. (4.19) and (4.22) imply the following explicit

[17] The symbolic product in (4.8) must be regarded as nonlocal in time as well, except in the case of harmonic time dependence, *vid.* Eqs. (4.14), (4.17), (4.23), and (4.24).

[18] R. Kubo, J. Phys. Soc. Japan **12**, 570 (1957).

expressions for $\mathbf{A}$:

$$\mathbf{A}(\omega^+)=\sum_{mm'}\mathcal{P}_m\left[\frac{\mathbf{d}_{mm'}\mathbf{d}_{m'm}{}^\dagger}{E_m-E_{m'}+\hbar\omega^+}+\frac{d_{m'm}d_{mm'}{}^\dagger}{E_m-E_{m'}-\hbar\omega^+}\right]. \quad (4.25)$$

We now symbolize the particle interaction $v_{\mathbf{q}}(\mathbf{p},\mathbf{p}')$ of (2.2) and (2.7) as a matrix $\mathbf{v}$ and indicate the contraction (summation over $\mathbf{q}$) involved in obtaining V_G from $\langle\mathbf{d}\rangle$, Eq. (2.14), by

$$V_G=\tfrac{1}{2}\mathbf{v}\cdot\langle\mathbf{d}\rangle. \quad (4.26)$$

Inserting (4.21) into (4.22) and recalling the definitions (4.6)–(4.8) leads, then, to the reciprocal relations between $\boldsymbol{\varepsilon}$ and $\frac{1}{2}\mathbf{v}\cdot\mathbf{A}$:

$$\boldsymbol{\varepsilon}(\omega^+)=\mathbf{I}-[\mathbf{I}+\xi\tfrac{1}{2}\mathbf{v}\cdot\mathbf{A}(\omega^+)]^{-1}\cdot\tfrac{1}{2}\mathbf{v}\cdot\mathbf{A}(\omega^+), \quad (4.27)$$

$$\tfrac{1}{2}\mathbf{v}\cdot\mathbf{A}(\omega^+)=-[\boldsymbol{\varepsilon}(\omega^+)-\mathbf{I}]\cdot[\mathbf{I}+\xi(\boldsymbol{\varepsilon}(\omega^+)-\mathbf{I})]^{-1}. \quad (4.28)$$

This derivation of Eqs. (4.27) and (4.28) completes the task of this section.

V. FLUCTUATION-DISSIPATION THEOREM

In the following, we develop the theory of the dissipation of the energy of the external system caused by the interaction between the external system and the system proper, $\mathcal{V}_0$. We then go on to examine fluctuations in the system proper *via* the causal matrix $\mathbf{A}$, and, finally, to establish the connection between the fluctuations and the dissipation–the required fluctuation-dissipation theorem for generalized SCF theory.

The time rate of change of the U', Eq. (2.8) *et seq.*, of the system proper is given by

$$\dot{U}'=\mathrm{tr}\frac{\delta U'}{\delta P}\dot{P}+\frac{\partial U'}{\partial t}, \quad (5.1)$$

where $\partial U'/\partial t$ is the contribution of the explicit time dependence of the external fields. From the basic equations of the SCF method, Eq. (2.15), and

$$\delta U'/\delta P=\mathfrak{IC}_s, \quad (5.2)$$

it follows that the first term in (5.1) vanishes:

$$\mathrm{tr}\frac{\delta U'}{\delta P}\dot{P}=\frac{1}{i\hbar}\,\mathrm{tr}\mathfrak{IC}_s[\mathfrak{IC}_s,P]=0. \quad (5.3)$$

We have, then, from (4.2)

$$\dot{U}'=\partial U'/\partial t=\dot{\mathbf{V}}_0\cdot\langle\mathbf{d}\rangle. \quad (5.4)$$

We now give a more concrete meaning to the external pairing field $\mathbf{V}_0$ by supposing it to arise from a "classical" fermion pair field $\mathbf{d}_0$ and $\mathbf{d}_0{}^+$ external to and independent of the system proper:

$$\mathbf{V}_0=\tfrac{1}{2}\mathbf{v}\cdot\mathbf{d}_0. \quad (5.5)$$

We mean by the term "classical" that the individual components of $\mathbf{d}_0$ are c numbers, whereas those of $\mathbf{d}$ are q numbers, i.e., operators in Fock space. We suppose also the existence of a self-interaction energy for the pair fields of the external system

$$\mathcal{V}_{00}=k(\mathbf{v}\cdot\mathbf{d}_0)\cdot\mathbf{d}_0=\tfrac{1}{2}\mathbf{d}_0\cdot\mathbf{V}_0, \quad (5.6)$$

the time rate of change of which is

$$\dot{\mathcal{V}}_{00}=\dot{\mathbf{d}}_0\cdot\mathbf{V}_0. \quad (5.7)$$

If we substitute (5.5) for $\mathbf{V}_0$ in (5.4), we can transfer the $\mathbf{v}\cdot$ from $\mathbf{d}_0$ to $\mathbf{d}$ by virtue of the symmetry properties of v, Table I,

$$\dot{U}'=\dot{\mathbf{d}}_0\cdot\mathbf{V}_G. \quad (5.8)$$

We can now express $\mathbf{V}_G$ to first order in $\mathbf{V}_0$ through the definition (4.7) and (4.8):

$$\dot{U}'=[\dot{\mathbf{d}}_0\cdot\boldsymbol{\varepsilon}^{-1}\cdot\mathbf{V}_0-\dot{\mathbf{d}}_0\cdot\mathbf{V}_0]. \quad (5.9)$$

The sum of the field energy of the external system and the U' of the system proper, which includes the interaction between the two, varies with time as[17]

$$d(\mathcal{V}_{00}+U')/dt=[\dot{\mathbf{d}}_0\cdot\boldsymbol{\varepsilon}^{-1}\cdot\mathbf{V}_0]. \quad (5.10)$$

This result is of complete generality; it is valid for all problems of second-order perturbation of one system by another and is, of course, not peculiar to our present generalized SCF theory with Gor'kov factorization. Only in the present context can it be regarded as a new result. It is implicit in (5.10) that the interaction $\mathcal{V}_0$ vanishes in the remote past and is subsequently turned on adiabatically. Integration then yields for the second-order energy change the same result as would be obtained by direct calculation,

$$\Delta(\mathcal{V}_{00}+U')=\tfrac{1}{2}\mathbf{d}_0\cdot\boldsymbol{\varepsilon}^{-1}\cdot\mathbf{V}_0. \quad (5.11)$$

One sees from (5.11) that pairing interactions are screened by the linear response function $\boldsymbol{\varepsilon}$ in precisely the same way that the Coulomb interaction is screened by the dynamical dielectric function. As we shall see later, this result provides a convenient basis for making contact with the more familiar pair scattering-matrix approach to pair interactions.

The part of $d(\mathcal{V}_{00}+U')/dt$ which is $\pi/2$ out of phase with $\Delta(\mathcal{V}_{00}+U')$ is stored, and that part of it which is in phase is dissipated. Thus $(1/2i)\{\boldsymbol{\varepsilon}^{-1}(\omega^+)-[\boldsymbol{\varepsilon}^{-1}(\omega^+)]^\dagger\}$ determines the dissipation for arbitrary $\mathbf{d}_0$, or $\mathbf{V}_0$, through (5.10). Inasmuch as the chemical potential μ is kept as a constant explicitly entering the effective Hamiltonian governing the motion of the system, it is clear that only processes in which the chemical potential is unchanged are embraced here. The system remains open to, and in equilibrium with in regard to transfer of particles, a large, unchanging reservoir of particles. If, in addition, we restrict $\mathbf{d}_0{}^-$ and $\mathbf{d}_0{}^+$ in such a way that $\langle N\rangle$ remains constant, we can identify $\dot{U}'$ and $\Delta U'$ with $\dot{U}$ and ΔU, U being the internal energy of the system

proper. $\mathrm{Im}[\boldsymbol{\varepsilon}^{-1}(\omega^+)]$ then determines the usual dissipation of energy by transfer from the external system to the system proper, where it is ultimately converted to heat. If, on the other hand, $\langle\dot{N}\rangle$ is nonzero, $\dot{U}'$ contains the term $-\mu\langle\dot{N}\rangle$ in addition to $\dot{U}$, $-\mu\langle\dot{N}\rangle$ being the rate of change of the internal energy of the particle reservoir. $\mathrm{Im}[\boldsymbol{\varepsilon}^{-1}(\omega^+)]$ then determines the dissipation of energy by transfer from the external system to both the system proper and the particle reservoir.

We now turn from the study of dissipation to the study of fluctuations in the pair fields at thermal equilibrium. We define the correlation matrix $\mathbf{C}(t-t')$ to be

$$\mathbf{C}(t-t')=(1/\hbar)\langle\mathbf{d}(t)\mathbf{d}^\dagger(t')\rangle=(1/\hbar)\,\mathrm{tr}\mathbf{d}(t)\mathbf{d}^\dagger(t')P_0 \quad (5.12)$$

with $\mathbf{d}(t)$ and $\mathbf{d}^\dagger(t')$ in the Heisenberg picture generated by $\mathfrak{IC}_s^0$ and with Hermitian conjugation applied before entering the Heisenberg picture. We see by comparing (5.12) with (4.19) that $\mathbf{A}(t-t')$ is $(-i)$ times the causal antisymmetric part of $\mathbf{C}(t-t')$. The Fourier transform of $\mathbf{C}(t-t')$,

$$\mathbf{C}(\omega)=(1/2\pi)\int_{-\infty}^{\infty}\mathbf{C}(t-t')e^{i\omega(t-t')}dt', \quad (5.13)$$

is proportional to the spectral distribution function for $\mathbf{d}(t)$. In explicit matrix form, $\mathbf{C}(\omega)$ is

$$\mathbf{C}(\omega)=\sum_{mm'}\mathcal{P}_m\mathbf{d}_{mm'}\mathbf{d}_{m'm}^\dagger\delta(E_m-E_{m'}+\hbar\omega). \quad (5.14)$$

It follows from (4.25) that

$$\mathbf{A}(\omega^+)-[\mathbf{A}(\omega^+)]^\dagger=-2\pi i(1-e^{-\beta\hbar\omega})\times\sum_{mm'}{}'\mathcal{P}_m\mathbf{d}_{mm'}\mathbf{d}_{m'm}^\dagger\delta(E_m-E_{m'}+\hbar\omega). \quad (5.15)$$

Equations (5.15) and (5 14) together yield

$$\frac{1}{2\pi i}\frac{\mathbf{A}(\omega^+)-[\mathbf{A}(\omega^+)]^\dagger}{1-e^{-\beta\hbar\omega}}=\mathbf{C}(\omega)-\sum_m\mathcal{P}_m\mathbf{d}_{mm}\mathbf{d}_{mm}^\dagger\delta(\hbar\omega). \quad (5.16)$$

In the absence of coherent pairing, $\mathbf{d}_{mm}$ vanishes; otherwise, $\Sigma_m\,\mathcal{P}_m\mathbf{d}_{mm}\mathbf{d}_{mm}^\dagger$ differs from $\langle\mathbf{d}\rangle\langle\mathbf{d}^\dagger\rangle$ by a quantity which vanishes in the limit $N\to\infty$ [cf. the discussion following Eqs. (IV.18′) and (IV.19′) in I]. In either event, we have

$$\mathbf{C}(\omega)-\langle\mathbf{d}\rangle\langle\mathbf{d}^\dagger\rangle\delta(\hbar\omega)=-\frac{1}{2\pi i}\frac{\mathbf{A}(\omega^+)-[\mathbf{A}(\omega^+)]^\dagger}{1-e^{-\beta\hbar\omega}}. \quad (5.17)$$

The left-hand side of (5.17) is the unnormalized spectral distribution function of the fluctuations in $\mathbf{d}(t)$; the right-hand side is related to the dissipation through (4.28).

Let us now consider the joint fluctuations in the Gor'kov field operator,

$$\mathbf{V}_G{}^{\mathrm{op}}=\tfrac{1}{2}\mathbf{v}\cdot\mathbf{d}, \quad (5.18)$$

and the pair operator $\mathbf{d}$. We introduce the notation $\{\mathbf{M}\}_a$; for the anti Hermitian part of the matrix $\mathbf{M}$. From (5.17) it follows that

$$\langle\mathbf{V}_G{}^{\mathrm{op}}\mathbf{d}\rangle_\omega-\mathbf{V}_G{}^0\langle\mathbf{d}\rangle^0\delta(\hbar\omega)=-\frac{1}{\pi i}\frac{\{\frac{1}{2}\mathbf{v}\cdot\mathbf{A}(\omega^+)\}_a}{1-e^{-\beta\hbar\omega}}. \quad (5.19)$$

We re-express the right-hand side of (5.19) through (4.28):

$$\langle\mathbf{V}_G{}^{\mathrm{op}}\mathbf{d}\rangle_\omega-\mathbf{V}_G{}^0\langle\mathbf{d}\rangle^0\delta(\hbar\omega)=\frac{1}{\pi i}\frac{\{(\boldsymbol{\varepsilon}(\omega^+)-\mathbf{I})\cdot[\mathbf{I}+\xi(\boldsymbol{\varepsilon}(\omega^+)-\mathbf{I})]^{-1}\}_a}{1-e^{-\beta\hbar\omega}}. \quad (5.20)$$

Equation (5.20) is the desired fluctuation-dissipation theorem in its most general form. We can derive from it the equal-time fluctuation-dissipation theorem by integration over frequency

$$\langle\mathbf{V}_G{}^{\mathrm{op}}\mathbf{d}\rangle^0-\mathbf{V}_G{}^0\langle\mathbf{d}\rangle^0=\frac{\hbar}{\pi i}\int_{-\infty}^{\infty}d\omega\frac{\{(\boldsymbol{\varepsilon}(\omega^+)-\mathbf{I})\cdot[\mathbf{I}+\xi(\boldsymbol{\varepsilon}(\omega^+)-\mathbf{I})]^{-1}\}_a}{1-e^{-\beta\hbar\omega}}. \quad (5.21)$$

Equation (5.21) provides the basis for the derivation of an equation of state in the next section.

VI. AN EQUATION OF STATE

In thermal equilibrium, the fundamental thermodynamic variables of our system are T, μ, and V. The grand potential then depends on T, μ, and V; for fixed T, μ, V, it depends on ξ as well:

$$\Omega=\Omega(T,\mu,V;\xi). \quad (6.1)$$

The total derivative of Ω with ξ for fixed T, μ, V, is

$$\left(\frac{\partial\Omega(\xi)}{\partial\xi}\right)_{T,\mu,V}=\mathrm{tr}\left[\left(\frac{\delta\Omega}{\delta P_0}\right)_{T,\mu,V}\left(\frac{\partial P_0}{\partial\xi}\right)_{T,\mu,V}\right]+\left(\frac{\partial\Omega}{\partial\xi}\right)_{P_0,T,\mu,V}. \quad (6.2)$$

The basic variational principle of the generalized SCF theory for equilibrium problems is that Ω is stationary with respect to variations of the density-matrix P_0,

$$\left(\frac{\delta\Omega}{\delta P_0}\right)_{T,\mu,V}=0, \quad (6.3)$$

or

$$\left(\frac{\partial\Omega(\xi)}{\partial\xi}\right)_{T,\mu,V}=\left(\frac{\partial\Omega}{\partial\xi}\right)_{P_0,T,\mu,V}. \quad (6.4)$$

The explicit dependence of ξ on Ω arises from the presence of ξ in U', through the replacement (2.9).

The compact notation of Sec. IV needs a slight expansion at this point. The indices τ or τ' $(=\pm)$, indicating whether one is dealing with a particle pair $(+)$ or a hole pair $(-)$, must be made explicit at this point. This we do and suppress the remaining variables in a

submatrix notation (cf. the introductory paragraph of Sec. VII). Equations (6.4) and (2.9) then lead to

$$\frac{\partial\Omega(\xi)}{\partial\xi}\Big)_{T,\mu,V}=[\langle(\mathbf{V}_G{}^{\mathrm{op}})^+\cdot\mathbf{d}^+\rangle^0-(\mathbf{V}_G{}^0)^+\cdot\langle\mathbf{d}^+\rangle^0] \quad (6.5)$$

in the current notation, recalling that the scalar product in (6.5) is a Hermitian product. The ξ derivative of the grand potential is thus one-half of the fluctuation in the interaction of the Gor'kov field of the system $(V_G{}^{\mathrm{op}})^+$ with the pair field $\mathbf{d}^-$.

In the last section, we derived a general fluctuation-dissipation theorem relating such fluctuations as (6.5) to the response matrix $\boldsymbol{\varepsilon}$, Eq. (5.21). Insertion of (5.21) into (6.5), followed by integration over ξ from 0 to 1 leads to

$$\Omega(T,\mu,V;1)=\Omega(T,\mu,V;0)+\frac{\hbar}{\pi i}\int_0^1 d\xi \times\mathrm{tr}\int_{-\infty}^{\infty}d\omega\frac{\{(\boldsymbol{\varepsilon}(\omega^+)-\mathbf{I})\cdot[\mathbf{I}+\xi(\boldsymbol{\varepsilon}(\omega^+)-\mathbf{I})]^{-1}\}_{\alpha}{}^{++}}{1-e^{-\beta\hbar\omega}}. \quad (6.6)$$

Equation (6.6) relates the grand potential for the actual system $\Omega(\xi=1)$ to the grand potential for the system treated in the simple SCF approximation $\Omega(\xi=0)$. The trace in (6.6) means simply that the diagonal elements of the $++$ submatrix in the curly brackets are to be summed: i.e., the trace is taken with respect to the orbital and spin variables and not the particle versus hole variables. The relation (6.6) is seen to be an equation of state through (2.10); it gives the functional dependence of the pressure p on T, μ, and V.

VII. SIMPLIFICATION BY SYMMETRY AND OTHER CONSIDERATIONS

The compact notation we have used from Sec. IV onward greatly simplifies the writing of the fairly complex relations we have developed thus far. At the same time, however, it obscures the interrelations among the individual components of, e.g., the matrix $\mathbf{A}$, (4.19) and (4.22), which may be regarded as a kind of susceptibility, cf. (4.18). These interrelations are imposed by a variety of symmetry and other considerations like those leading to Table I for v. To facilitate application of these symmetry arguments, we first write out a matrix equation in complete detail, Eq. (4.21) in particular, in order to exhibit all of the indices, and then introduce a submatrix notation adapted to the symmetry arguments. In detail, then, Eq. (4.21) reads

$$\langle d(\mathbf{p}_1,\mathbf{p}_2)_{\alpha}{}^{\tau}\rangle^{(1)}=\sum_{\substack{\mathbf{p}_1'\mathbf{p}_2'\\ \alpha',\tau'}}A(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1'\mathbf{p}_2';\omega^+)_{\alpha}{}^{\tau};{}_{\alpha'}{}^{\tau'}V_{\xi}(\mathbf{p}_1',\mathbf{p}_2')_{\alpha'}{}^{\tau'}. \quad (7.1)$$

The detailed definition of $\mathbf{A}$ emerges most clearly from the form (4.25):

$$A(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1',\mathbf{p}_2';\omega^+)_{\alpha}{}^{\tau};{}_{\alpha'}{}^{\tau'}=\sum_{mm'}\mathcal{P}_m\left[\frac{(d(\mathbf{p}_1,\mathbf{p}_2)_{\alpha}{}^{\tau})_{mm'}(d(\mathbf{p}_2',\mathbf{p}_1')_{-\alpha'}{}^{-\tau'})_{m'm}}{E_m-E_{m'}+\hbar\omega^+}+\frac{(d(\mathbf{p}_1,\mathbf{p}_2)_{\alpha}{}^{\tau})_{m'm}(d(\mathbf{p}_2',\mathbf{p}_1')_{-\alpha'}{}^{-\tau'})_{mm'}}{E_m-E_{m'}-\hbar\omega^+}\right]. \quad (7.2)$$

In the remainder of this section, we shall suppress all indices not directly relevant to any given argument, including the dependence on ω^+, leaving us with a submatrix notation of varying degrees of completeness. For example, we can suppress all but the destruction/creation indices, leaving $\mathbf{A}^{\tau\tau'}$ (already used in Sec. VI), or all but the spin indices, leaving $\mathbf{A}_{\alpha\alpha'}$, etc.

Number conservation. In the normal state at thermal equilibrium, $\mathbf{V}_G{}^0$ and $\langle\mathbf{d}\rangle^0$ vanish; there is number conservation. As a consequence, those components $\mathbf{A}^{\tau\tau'}$ which do not conserve number, i.e., $\mathbf{A}^{+-}$ and $\mathbf{A}^{-+}$, must vanish. Fields of $(+)$-type and $(-)$-type are uncoupled in the normal state. For coherently paired states with $\xi<1$, on the other hand, $\mathbf{V}_G{}^0$ does not vanish so that $\mathcal{K}_s{}^0$ is not number conserving; $\mathbf{A}^{+-}$ and $\mathbf{A}^{-+}$ do not vanish when coherent pairing (CP) occurs.

Spin-rotation invariance. In an unmagnetized state, i.e., a total spin singlet, the system is completely invariant under change of the axis of spin quantization, neglecting spin-orbit coupling. There can be no singlet-triplet coupling, and the triplet-triplet submatrix of $\mathbf{A}_{\alpha\alpha'}$, $\mathbf{A}_{mm'}$, must be of the form $(\mathbf{A}_t)\delta_{mm'}$. We have left of $\mathbf{A}_{\alpha\alpha'}$, then, only $(\mathbf{A}_{\alpha})\delta_{\alpha\alpha'}$, $\mathbf{A}_{\alpha}=\mathbf{A}_s$ or $\mathbf{A}_t$. For simplicity, we can use $\mathbf{A}_{11}$ for $\mathbf{A}_t$.

Translation invariance. The translation invariance of a uniform system requires that

$$\mathbf{A}(\mathbf{p}_1\mathbf{p}_2;\mathbf{p}_1'\mathbf{p}_2')^{\tau\tau'}=0 \quad \text{unless} \quad \tau(\mathbf{p}_1+\mathbf{p}_2)=\tau'(\mathbf{p}_1'+\mathbf{p}_2'). \quad (7.3)$$

The restriction (7.3) (i.e., conservation of momentum) makes it convenient to introduce the total momentum and the momentum relative to the c.m., $\mathbf{P}$ and $\mathbf{p}_r$, respectively, in place of the two momenta $\mathbf{p}_1$ and $\mathbf{p}_2$ of the pair operator $d(\mathbf{p}_1,\mathbf{p}_2)_{\alpha}{}^{\tau}$ via the transformations

$$\mathbf{P}=\tau(\mathbf{p}_1+\mathbf{p}_2), \quad \mathbf{p}_r=\tfrac{1}{2}\tau(\mathbf{p}_1-\mathbf{p}_2). \quad (7.4)$$

The detailed product (7.1) becomes, then,

$$\langle\mathbf{d}(\mathbf{P},\mathbf{p}_r)_{\alpha}{}^{\tau}\rangle^{(1)}=\sum_{\mathbf{p}_r',\tau'}A(\mathbf{P},\mathbf{p}_r;\mathbf{P},\mathbf{p}_r')_{\alpha}{}^{\tau\tau'}V_{\xi}(\mathbf{P},\mathbf{p}_r')_{\alpha}{}^{\tau'}; \quad (7.5)$$

momentum conservation thus decouples different total momenta. We are left with a functional dependence of A on $\mathbf{P}$, ω^+, and α and a matrix dependence on $\mathbf{p}_r$ and τ, $A(\mathbf{P},\omega^+;\mathbf{p}_r,\mathbf{p}_r')_{\alpha}{}^{\tau\tau'}$, where [cf. (7.2)]

$$A(\mathbf{P},\omega^+;\mathbf{p}_r,\mathbf{p}_r')_{\alpha}{}^{\tau\tau'}\equiv A(\tau(\mathbf{p}_r+\tfrac{1}{2}\mathbf{P}),\tau(-\mathbf{p}_r+\tfrac{1}{2}\mathbf{P});\tau'(\mathbf{p}_r'+\tfrac{1}{2}\mathbf{P}),\tau'(-\mathbf{p}_r'+\tfrac{1}{2}\mathbf{P});\omega^+)_{\alpha}{}^{\tau\tau'}. \quad (7.6)$$

The definition of $\mathbf{V}_G$, (2.14), becomes

$$V_G(\mathbf{P},\mathbf{p}_r)_\alpha{}^\tau=\tfrac{1}{2}\sum_{\mathbf{q}} v_{\mathbf{q}}(\mathbf{P},\mathbf{p}_r)_\alpha\langle d(\mathbf{P},\mathbf{p}_r+\mathbf{q})_\alpha{}^\tau\rangle \quad (7.7)$$

in total and relative momenta; one sees again the conservation of total momenta, i.e., decoupling of different $\mathbf{P}$.

Simplified equation of state. In the absence of coherent pairing and magnetism, the results obtained thus far in the present section permit writing the equation of state (6.6) in a more explicit form. We need consider $\boldsymbol{\epsilon}$ as a matrix, or better operator, only with regard to the relative coordinate $\mathbf{r}$ and momentum $\mathbf{p}_r$ in the c.m. frame of a pair, $\boldsymbol{\epsilon}(\mathbf{P},\omega^+)_\alpha{}^{++}$. The simplified equation of state is

$$\begin{aligned}&\Omega(T,\mu,V;1)=\Omega(T,\mu,V;0)\\&+\frac{\hbar}{\pi i}\int_0^1 d\xi\sum_{\mathbf{P}}\mathrm{tr}\int_{-\infty}^{\infty}d\omega[1-e^{-\beta\hbar\omega}]^{-1}\\&\times\{(\boldsymbol{\epsilon}(\mathbf{P},\omega^+)_s{}^{++}-\mathbf{I})\cdot[\mathbf{I}+\xi(\boldsymbol{\epsilon}(\mathbf{P},\omega^+)_s{}^{++}-\mathbf{I})]^{-1}\\&+3(\boldsymbol{\epsilon}(\mathbf{P},\omega^+)_t{}^{++}-\mathbf{I})\cdot[\mathbf{I}+\xi(\boldsymbol{\epsilon}(\mathbf{P},\omega^+)_t{}^{++}-\mathbf{I})]^{-1}\}_\alpha. \quad (7.8)\end{aligned}$$

The trace and operator products in (7.8) now refer only to the relative coordinates.

Time-reversal invariance. Time-reversal invariance imposes restrictions on the entities $\mathbf{A}$ and $\boldsymbol{\epsilon}$ viewed as operators in the relative coordinates. For nonmagnetic states, complex conjugation is equivalent to time reversal, yielding

$$\mathbf{A}(\omega^+)=\mathbf{A}^\dagger(\omega^-). \quad (7.9)$$

In (7.9), Hermitian conjugation is applied to the entire matrix $\mathbf{A}$. Let us now introduce the complex frequency z. It follows from (7.9) and (4.28) that the frequency integral in the equal-time fluctuation-dissipation theorem (5.21), and all results derived from it, such as the equation of state (6.6) or (7.8), can be re-expressed as an integral along a contour around the real axis enclosing none of the poles of $[1-e^{-\beta\hbar z}]$ on the imaginary axis, cf. Fig. 1,

$$\begin{aligned}&\langle\mathbf{V}_G{}^{\mathrm{op}}\mathbf{d}\rangle^0-\mathbf{V}_G{}^0\langle\mathbf{d}\rangle^0\\&=-\frac{\hbar}{2\pi i}\oint\frac{(\boldsymbol{\epsilon}(z)-\mathbf{I})\cdot[\mathbf{I}+\xi(\boldsymbol{\epsilon}(z)-\mathbf{I})]^{-1}}{1-e^{-\beta\hbar z}}dz, \quad (7.10)\end{aligned}$$

where only the principle part of $[1-e^{-\beta\hbar z}]^{-1}$ is to be taken.

The equation of state (7.8) may be similarly re-expressed as

$$\begin{aligned}&\Omega(T,\mu,V;1)=\Omega(T,\mu,V;0)\\&-\int_0^1 d\xi\sum_{\mathbf{P}}\mathrm{tr}\frac{\hbar}{2\pi i}\oint[1-e^{-\beta\hbar z}]^{-1}\\&\times\{(\boldsymbol{\epsilon}(\mathbf{P},z)_s{}^{++}-\mathbf{I})\cdot[\mathbf{I}+\xi(\boldsymbol{\epsilon}(\mathbf{P},z)_s{}^{++}-\mathbf{I})]^{-1}\\&+3(\boldsymbol{\epsilon}(\mathbf{P},z)_t{}^{++}-\mathbf{I})\cdot[\mathbf{I}+\xi(\boldsymbol{\epsilon}(\mathbf{P},z)_t{}^{++}-\mathbf{I})]^{-1}\}dz. \quad (7.11)\end{aligned}$$

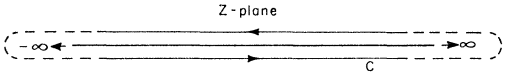

FIG. 1. The contour C for the integral of Eqs. (7.10), (7.11), and Sec. VIII.

One can alternatively inquire as to the response to a time-reversed external field, $\omega^+\rightarrow-\omega^+$, with the result that

$$\mathbf{A}(\mathbf{P},-\omega^+;\mathbf{p}_r,\mathbf{p}_r')=\mathbf{A}(-\mathbf{P},\omega^+;\mathbf{p}_r',\mathbf{p}_r). \quad (7.12)$$

Statistics. Fermi statistics impose restrictions on $\mathbf{A}$ and $\boldsymbol{\epsilon}$ through the commutation relations satisfied by the field operators, which amount to relations between spin and parity:

$$\begin{aligned}d_s(\mathbf{P},\mathbf{p}_r)^\tau&=d_s(\mathbf{P},-\mathbf{p}_r)^\tau,\\d_t(\mathbf{P},\mathbf{p}_r)^\tau&=-d_t(\mathbf{P},-\mathbf{p}_r)^\tau,\end{aligned} \quad (7.13)$$

i.e., all singlet fields must be even in the relative momentum or coordinate and all triplet fields odd. Equation (7.13) implies

$$\begin{aligned}\mathbf{A}(\mathbf{p}_r,\mathbf{p}_r')_\alpha&=\mp\mathbf{A}(-\mathbf{p}_r,\mathbf{p}_r')_\alpha\\&=\mp\mathbf{A}(\mathbf{p}_r,-\mathbf{p}_r')_\alpha=\mathbf{A}(-\mathbf{p}_r,-\mathbf{p}_r')_\alpha,\end{aligned} \quad (7.14)$$

where the upper sign goes with $\alpha=t$ and the lower with $\alpha=s$.

Inversion symmetry. We infer immediately from inversion symmetry that

$$\mathbf{A}(\mathbf{P};\mathbf{p}_r,\mathbf{p}_r')=A(-\mathbf{P};-\mathbf{p}_r,-\mathbf{p}_r'). \quad (7.15)$$

Equations (7.14) and (7.15) together give

$$\mathbf{A}(\mathbf{P})=\mathbf{A}(-\mathbf{P}). \quad (7.16)$$

Equations (7.16) and (7.12) together give

$$A(\mathbf{P},-\omega^+;\mathbf{p}_r,\mathbf{p}_r')_\alpha{}^{\tau\tau'}=A(\mathbf{P},\omega^+;\mathbf{p}_r',\mathbf{p}_r)_\alpha{}^{-\tau',-\tau}. \quad (7.17)$$

Orbital-Rotation invariance. Isotropy of the system requires that

$$\mathbf{A}=\mathbf{A}(P;p_r,\hat{P}\cdot\hat{p}_r;p_r',\hat{P}\cdot\hat{p}_r'). \quad (7.18)$$

Equations (7.14) and (7.18) together state that only odd Legendre polynomials in $\hat{P}\cdot\hat{p}_r$ or $\hat{P}\cdot\hat{p}_r'$ enter A_t whereas only even enter A_s.

VIII. THE $\xi=0$ APPROXIMATION FOR $\boldsymbol{\epsilon}$

As in the case of Hartree factorization in I, the obvious first approximation to use for $\boldsymbol{\epsilon}(\xi)$ in the equation of state (7.8) is the $\xi=0$ approximation, $\boldsymbol{\epsilon}(\xi=0)$. The integration over ξ can now be performed immediately after interchanging it with all other sums and integrals,

$$\begin{aligned}&\Omega(T,\mu,V;1)=\Omega(T,\mu,V;0)\\&-\sum_{\mathbf{P}\alpha}\mathrm{tr}\frac{\hbar}{2\pi i}\oint\frac{\ln[\boldsymbol{\epsilon}(\mathbf{P},z;\xi=0)_\alpha{}^{++}]}{1-e^{-\beta\hbar z}}dz. \quad (8.1)\end{aligned}$$

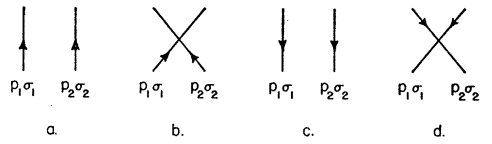

FIG. 2. The diagrams which contribute to $\mathbf{A}^{++}$: (a) particle pair, direct; (b) particle pair, exchange; (c) hole pair, direct; (d) hole pair, exchange. To each pair, the pair propagator $[E(p_1)+E(p_2)+\hbar\omega^+]^{-1}$ is attached. To each particle line the factor $(1-n(p_i))$ is attached; to each hole line, $n(p_i)$. The sign is negative for a direct particle pair, positive for a direct hole pair, and exchange reverses the sign.

In (8.1) $\boldsymbol{\varepsilon}$ and $\ln\boldsymbol{\varepsilon}$ are operators in the relative coordinates, and tr $\ln\boldsymbol{\varepsilon}$ refers then to the relative coordinates.

Before we can relate (8.1) to previous results for the grand potential, it is necessary to evaluate $\boldsymbol{\varepsilon}(\xi=0)$ and to explore its meaning. Setting $\xi=0$ is equivalent to working in the simple, as opposed to generalized, Gor'kov SCF theory. We are concerned with the dynamical version for no coherent pairing of the equilibrium theory of coherent pairing given in Sec. III. From (4.28) it follows that

$$\boldsymbol{\varepsilon}(\xi=0)=\mathbf{1}-\tfrac{1}{2}\mathbf{v}\cdot\mathbf{A}(\xi=0). \tag{8.2}$$

We have assumed that no coherent pairing occurs so that $V_G{}^0=0$ and $\mathfrak{IC}_s{}^0$ is the free-particle Hamiltonian. The evaluation of $\mathbf{A}$ by the standard methods of quantum-field theory is then straightforward. The four diagrams which contribute to $\mathbf{A}^{++}$ are shown in Fig. 2, and their contributions are described in the figure caption. There results for $\mathbf{A}^{++}$,

$$A(\mathbf{P},\omega^+;\mathbf{p}_r,\mathbf{p}_r')_\alpha{}^{++}=-[(1-f_1-f_2)/(E_1+E_2+\hbar\omega^+)]\times(1\pm\mathcal{I}_r')\delta_{\mathbf{p}_r,\mathbf{p}_r'}. \tag{8.3}$$

Here $\mathbf{p}_1=\mathbf{p}_r+\frac{1}{2}\mathbf{P}$; $\mathbf{p}_2=-\mathbf{p}_r+\frac{1}{2}\mathbf{P}$; E_1, E_2 and f_1, f_2 are the corresponding single-particle energies and Fermi factors; $\mathcal{I}_r'$ is the inversion operator for relative coordinates, the prime signifying that its acts in (8.3) only on $\mathbf{p}_r'$; the plus sign goes with $\alpha=s$, and the minus with $\alpha=t$. The corresponding expression for $\boldsymbol{\varepsilon}$, with the multiplication of $\mathbf{v}$ in (8.2) carried out in relative coordinates and with $\boldsymbol{\varepsilon}$ regarded as an operator in the relative coordinates, is

$$\boldsymbol{\varepsilon}(\mathbf{P},\omega^+)_\alpha{}^{++}=1+[v(1,2)\tfrac{1}{2}(1\pm\mathcal{I}_r)(1-f_1-f_2)/(E_1+E_2+\hbar\omega^+)]. \tag{8.4}$$

Equation (8.4) is the desired result for the $\xi=0$ approximation to the response function.

The physical significance of $\boldsymbol{\varepsilon}(\xi=0)$ becomes apparent if we introduce for arbitrary ξ the matrix

$$t(\mathbf{P},\omega^+)_\alpha=[\boldsymbol{\varepsilon}(\mathbf{p},\omega^+)_\alpha{}^{++}]^{-1}\cdot\mathbf{v}. \tag{8.5}$$

In the $\xi=0$ limit, we may rewrite this as the operator equation

$$t(\mathbf{P},\omega^+)_\alpha=v(1,2)-v(1,2)\tfrac{1}{2}(1\pm\mathcal{I}_r)\times[(1-f_1-f_2)/(E_1+E_2+\hbar\omega^+)]t(\mathbf{P},\omega^+). \tag{8.6}$$

It follows from (8.5) and (8.6) that screening the bare interaction v by the response function $\boldsymbol{\epsilon}$ converts v to the usual scattering operator or t matrix. The t matrix of (8.5) and (8.6) represents the exact solution of the Bethe-Salpeter equation in the low-density limit (with causal boundary conditions); it gives the scattering of a pair of electrons or of holes, computed in the independent-pair approximation, but including all exchange and exclusion effects.[19]

It should now be clear from the structure of (7.8) and (8.1) and from the above discussion of the $\xi=0$ approximation for $\boldsymbol{\epsilon}$ that the approximate equation of state (8.1) is the same as would be obtained by carrying out the semi-invariant expansion[20] of the grand potential in powers of the interaction v and summing all terms which correspond to all ladders obtained by iterating the four prototype diagrams of Fig. 2 among themselves. Previous results of a related nature are reviewed and discussed by Bloch[21] and include the work of Brueckner[22] and the binary collision approximation of Yang and Lee.[23]

The relationship between the $\xi=0$ approximation of the present formalism and earlier work becomes clearer still after carrying out the integration over frequency in (8.1). Integrating by parts, with $s=\hbar z$, gives

$$-\frac{1}{2\pi i}\oint ds\frac{\ln\boldsymbol{\varepsilon}}{1-e^{-\beta s}}=\frac{k_BT}{2\pi i}\oint ds\ln(1-e^{\beta s})\frac{d\ln\boldsymbol{\varepsilon}}{ds}. \tag{8.7}$$

One simple way of evaluating the derivative of $\ln\boldsymbol{\varepsilon}$ in (8.7) is to carry out the formal expansion of $\ln\boldsymbol{\varepsilon}$ in powers of v by use of (8.4):

$$\ln\boldsymbol{\varepsilon}=\sum_{n=1}^{\infty}\frac{1}{n}-\{v(1,2)\tfrac{1}{2}(1\pm\mathcal{I}_r)(1-f_1-f_2)\times[E_1+E_2+s]^{-1}\}^n. \tag{8.8}$$

Differentiating the nth term of the right-hand side of (8.8) generates n separate terms in each of which the factor $[E_1+E_2+s]^{-1}$ is replaced by $-[E_1+E_2+s]^{-2}$ in all n possible orderings. However, we use $d\ln\boldsymbol{\varepsilon}/ds$ only in a trace so that the ordering is irrelevant. The $(1/n)$ in (8.8) can be canceled and the extra factor of $[E_1+E_2+s]^{-1}$ moved to the left. We can thus make in (8.7) the replacement

$$d\ln\boldsymbol{\varepsilon}/ds\rightarrow[E_1+E_2+s]^{-1}\{[1-v(1,2)\tfrac{1}{2}(1\pm\mathcal{I}_r)\times(1-f_1-f_2)[E_1+E_2+s]^{-1}]-1\}. \tag{8.9}$$

[19] For references and discussion see, e.g., C. B. Duke, thesis, Princeton University, 1963 (unpublished); and to be published.
[20] R. Kubo, J. Phys. Soc. Japan **17**, 1100 (1962).
[21] C. Bloch, in *Studies in Statistical Mechanics, III*, edited by J. de Boer and G. E. Uhlenbeck (North-Holland Publishing Company, Amsterdam, to be published).
[22] K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958); K. A. Brueckner, in *The Many-Body Problem* (Les Houches, 1958, John Wiley & Sons, Inc., New York, 1959).
[23] T. D. Lee and C. N. Yang, Phys. Rev. **113**, 1165 (1959); **117**, 22 (1960).

Moreover, since we are again dealing only with a trace, we need only consider the symmetrized part of $v(1,2)\frac{1}{2}(1\pm\vartheta_r)(1-f_1-f_2)$. This leads to the further replacement,

$$d\ln\varepsilon/ds \rightarrow [\mathcal{H}_2'+s]^{-1}-[\mathcal{H}_{20}+s]^{-1}, \quad (8.10)$$

where

$$\mathcal{H}_2'=\mathcal{H}_{20}+\hat{v}(1,2)\tfrac{1}{2}(1\pm\vartheta_r), \quad (8.11)$$

$$\mathcal{H}_{20}=E_1+E_2, \quad (8.12)$$

$$\hat{v}(1,2)=(f_1+f_2-1)^{1/2}v(1,2)(f_1+f_2-1)^{1/2}. \quad (8.13)$$

It is unnecessary to symmetrize the factor $\frac{1}{2}(1\pm\vartheta_r)$ because it commutes with $v(1,2)$ (cf. Table I) and (f_1+f_2-1). The entity $\mathcal{H}_{20}$ is the Hamiltonian for two free particles except that in it energies are measured relative to the chemical potential. Correspondingly, $\mathcal{H}_2'$ is the Hamiltonian for two particles interacting via the potential $\hat{v}(1,2)$. The eigenvalues of both $\mathcal{H}_{20}$ and $\mathcal{H}_2'$ are all on the real axis. Hence the contour C of (8.7) surrounds all poles of $d\ln\varepsilon/ds$ and (8.7) may be evaluated by the residue theorem for operator-valued functions

$$-\frac{1}{2\pi i}\oint ds\frac{\ln\varepsilon}{1-e^{-\beta s}} \rightarrow$$

$$k_BT[\ln(1-e^{-\beta\mathcal{H}_2'})-\ln(1-e^{-\beta\mathcal{H}_{20}})]. \quad (8.14)$$

Matrix elements of the right-hand side of (8.14) vanish unless the two-particle wave functions involved are totally antisymmetric, including both space and spin. Thus we can collect the sum over the spin index α, the sum over the center-of-mass momentum $\mathbf{P}$, and the trace over the relative coordinates into a single trace denoted by tr_{2a}, which signifies taking the trace with respect to antisymmetric two-particle wave functions depending on both space and spin variables. It is then possible to drop the projection operator $\frac{1}{2}(1\pm\vartheta_r)$. We obtain, finally,

$$\Omega(1)=\Omega(0)+k_BT \times\mathrm{tr}_{2a}[\ln(1-e^{-\beta\mathcal{H}_2})-\ln(1-e^{-\beta\mathcal{H}_{20}})], \quad (8.15)$$

where

$$\mathcal{H}_2=E_1+E_2+\hat{v}(1,2)=\mathcal{H}_{20}+\hat{v}(1,2). \quad (8.16)$$

Recalling that coherent pairing is excluded from the present considerations we see that the exponentials in (8.15) are small at low temperatures so that the logarithms can be expanded, yielding

$$\Omega(1)=\Omega(0)-k_BT\,\mathrm{tr}_{2a}[e^{-\beta\mathcal{H}_2}-e^{-\beta\mathcal{H}_{20}}], \quad T\rightarrow 0. \quad (8.17)$$

The result (8.17) is usually obtained directly by the summation of ladder diagrams (cf. Ref. 21), and stated to be valid at low densities. We see here that low temperatures are also required for its validity.

The analysis of the present section has shown that Gor'kov factorization gives results via the $\xi=0$ approximation for ϵ in the equation of state which are correct for low densities or short-range interactions. There is a simple explanation for this. The Gor'kov factorization $\langle\psi^\dagger\psi^\dagger\rangle\langle\psi\psi\rangle$ means that the motion of a given pair of particles after a collision is treated as independent of the motion before collision. The motion consists thus of a sequence of binary collisions, each one independent of the last, so that Gor'kov factorization gives a compact and elegant mathematical formulation of the binary collision idea.

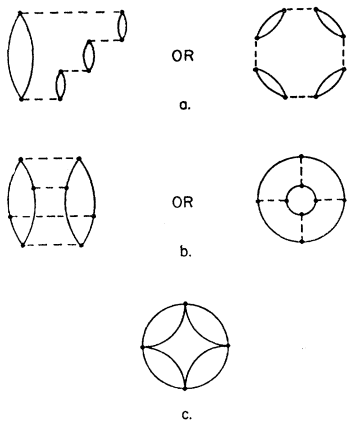

FIG. 3. Representative fourth-order diagrams: (a) a conventional polarization graph; (b) a conventional ladder graph; (c) a Hugenholtz graph in which the conventional interaction line terminating in two-propagator vertices is replaced by a single four-propagator vertex. It is evident that (a) and (b) are different special cases of (c).

Inasmuch as the low-temperature, low-density result (8.17) can now be obtained almost trivially through the semiinvariant techniques of Kubo,[20] its rederivation here provides no justification for the introduction of all the preceding formal machinery. Rather, the present work should be regarded as an attempt at demonstrating the underlying unity of the presently disparate theories of coherent pairing, of short-range correlations at low densities and of long-range correlations at high densities. Here we have used generalized SCF theory for all three, the Gor'kov factorization for the first two and the Hartree factorization for the latter.

The close similarity thus demonstrated of treatments of long-range correlation by summation of polarization graphs, Fig. 3(a), and short-range correlation by summation of ladder graphs, Fig. 3(b), may be further understood by recognizing that each is a subclass of the same class of Hugenholtz graphs,[24] Fig. 3(c).

We have thus far restricted ourselves to the case of no coherent pairing. However, the $\xi=0$ approximation to the response function can still be made in the presence of coherent pairing and would result in an appropriate generalization of (8.15). All four components of $\epsilon^{\tau\tau'}$ would be nonzero, but otherwise the structure of the calculation is not greatly changed.

ACKNOWLEDGMENTS

In addition to its direct support by NASA and the NSF, this research has benefited indirectly from support of the Institute for the Study of Metals by NSF and ARPA.

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