

## Linearized Many-Body Problem\*

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The theory of an electron gas at high density is generalized so as to include the exchange scattering of a particle and hole in the singlet as well as in the triplet spin state. This approximation is the maximum possible linearization of a quantum-mechanical many-body problem, and corresponds to the theory of small-amplitude oscillations of a classical many-body system. The linearized Hamiltonian is that of Wentzel's meson pair theory, in which now two kinds of mesons are involved, one with spin zero corresponding to the singlet state of a particle and hole and the other with spin one corresponding to the triplet state. The correlation energy is shown to be the sum of the change in zero-point energies of the two-meson fields with correction only in the second-order term. The theory is then formulated in terms of Green's function, and it is proved explicitly that the linearized theory (or the random-phase approximation with exchange effects taken into account) is equivalent to the "ladder approximation" for the particle-hole scattering. The particle-particle scattering by means of the screened interaction is also discussed. The case of the  $\delta$ -function potential is explicitly solved, and it is shown that the correlation energy becomes complex in the region where the instability of the paramagnetic state occurs.

### 1. INTRODUCTION

AS is well known,<sup>1</sup> most important properties of many-body systems are determined by means of the dielectric constant  $\epsilon(\mathbf{k}, \omega)$  which in turn is obtained by the matrix element  $\langle n | \rho_{\mathbf{k}} | 0 \rangle$ ,  $\rho_{\mathbf{k}}$  being the Fourier transform of the density of particles. Since  $\rho_{\mathbf{k}}$  has the spin zero, only those excited states with the same property give the nonvanishing matrix elements for the paramagnetic ground state. In the conventional random phase approximation (RPA)<sup>2</sup> such excited states are scattering as well as bound states (plasmon) of a particle and hole in the singlet state; and even when we take into account exchange correlations, it is in principle sufficient to consider only this state, paying no attention to the triplet state.

However, when we are interested in the magnetic property of the system, the spin susceptibility  $\chi(\mathbf{k}, \omega)$  is determined by the matrix element  $\langle n | \mathbf{S}_{\mathbf{k}} | 0 \rangle$ ,  $\mathbf{S}_{\mathbf{k}}$  being the Fourier transform of the spin density. Since  $\mathbf{S}_{\mathbf{k}}$  has the spin one, the triplet state of a particle and hole comes into play in the excited states. We shall further notice that the spin-independent two-body potential energy  $H_I$  can be written in the following two forms:

$$H_I = \sum \frac{1}{2} v(\mathbf{k}) c_{\mathbf{p}+\mathbf{k}\sigma}^\dagger c_{\mathbf{p}'-\mathbf{k}\sigma'}^\dagger c_{\mathbf{p}'\sigma'} c_{\mathbf{p}\sigma} \\ = \frac{1}{2} \sum v(\mathbf{k}) (\mathbf{c}_{\mathbf{p}+\mathbf{k}}^\dagger \mathbf{c}_{\mathbf{p}}) (\mathbf{c}_{\mathbf{p}'}^\dagger \mathbf{c}_{\mathbf{p}'+\mathbf{k}}), \quad (1.1a)$$

$$= -\frac{1}{4} \sum v(\mathbf{p}'-\mathbf{p}) (\mathbf{c}_{\mathbf{p}'+\mathbf{k}}^\dagger \boldsymbol{\sigma} \mathbf{c}_{\mathbf{p}'}) (\mathbf{c}_{\mathbf{p}}^\dagger \boldsymbol{\sigma} \mathbf{c}_{\mathbf{p}+\mathbf{k}}) \\ -\frac{1}{4} \sum v(\mathbf{p}'-\mathbf{p}) (\mathbf{c}_{\mathbf{p}'+\mathbf{k}}^\dagger \mathbf{c}_{\mathbf{p}'}) (\mathbf{c}_{\mathbf{p}}^* \mathbf{c}_{\mathbf{p}+\mathbf{k}}), \quad (1.1b)$$

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<sup>1</sup> P. Nozières and D. Pines, *Nuovo Cimento* **1**, 470 (1958).

<sup>2</sup> K. Sawada, *Phys. Rev.* **106**, 372 (1957); K. Sawada, K. A. Brueckner, N. Fukuda, and R. Brout, *ibid.* **108**, 507 (1957).

disregarding some irrelevant terms. Here  $c_{\mathbf{p}\sigma}$  is the annihilation operator of a particle with momentum  $\mathbf{p}$  and spin  $\sigma$ , and

$$\mathbf{c}_{\mathbf{p}} = \begin{pmatrix} c_{\mathbf{p}+} \\ c_{\mathbf{p}-} \end{pmatrix}, \quad (1.2)$$

$\boldsymbol{\sigma}$  being the Pauli spin matrices. In Eq. (1.1a), the importance of the triplet state is not apparent, while in Eq. (1.1b) it appears explicitly together with that of the singlet state. The second term in Eq. (1.1b) leads to the exchange correction to the singlet state which was neglected in Ref. 2.

In order to obtain the singlet and triplet excited states, we have to solve an infinite set of Heisenberg's equations of motion for  $[\mathbf{c}_{\mathbf{p}}^\dagger(t) \mathbf{c}_{\mathbf{p}+\mathbf{k}}(t')]$ ,  $[\mathbf{c}_{\mathbf{p}}^\dagger(t) \boldsymbol{\sigma} \mathbf{c}_{\mathbf{p}+\mathbf{k}}(t')]$ , and their associated higher-order products of  $\mathbf{c}^\dagger$  and  $\mathbf{c}$ . In RPA<sup>2,3</sup> these equations are linearized only for the singlet operator  $[\mathbf{c}_{\mathbf{p}}^\dagger(t) \mathbf{c}_{\mathbf{p}+\mathbf{k}}(t)]$  disregarding the exchange correction and triplet states. The first correction to this approximation is to take into account the exchange term in the singlet state which is equivalent to including ladder-type exchange scatterings of a particle and hole in the first-order polarization diagram. This correction was approximately estimated by Hubbard and by Nozières and Pines,<sup>4</sup> and was shown to decrease the screening effect considerably for large momentum transfer.

Our linearized theory is to supplement each Gell-Mann and Brueckner diagram<sup>5</sup> by the whole set of ex-

<sup>3</sup> D. Bohm and D. Pines, *Phys. Rev.* **92**, 609 (1953).

<sup>4</sup> J. Hubbard, *Proc. Roy. Soc. (London)* **A243**, 336 (1957); P. Nozières and D. Pines, *Phys. Rev.* **111**, 442 (1958).

<sup>5</sup> M. Gell-Mann and K. A. Brueckner, *Phys. Rev.* **106**, 369 (1957).

changed diagrams, or stated otherwise, is to replace the direct potential by the direct minus exchange potential. All partially exchanged diagrams contribute only to the singlet state. If, however, we consider the totally exchanged diagram of a given Gell-Mann and Brueckner diagram, it is divided into two parts, one in which the particle and hole is in the singlet state and the other in the triplet state. The former is to be taken care of by the exchange correction to the singlet state, while the latter is nothing but the triplet contribution.

In order that the theory may be applicable even to a finite system, we shall consider the Hamiltonian in the Hartree-Fock representation given in the form:

$$H = E_{\text{HF}} + \sum_i \epsilon_i : c_i^\dagger c_i : + \frac{1}{2} \sum_{ijkl} v_{ij,kl} : c_i^\dagger c_j^\dagger c_l c_k : , \quad (1.3)$$

where  $E_{\text{HF}}$  is the Hartree-Fock energy,  $\epsilon_i$  the single-particle energy, and

$$v_{ij,kl} = \int dx dx' \varphi_i^\dagger(x) \varphi_j^\dagger(x') v(x, x') \varphi_k(x) \varphi_l(x') , \quad (1.4)$$

$\varphi_i(x)$  being the Hartree-Fock wavefunction. The spin variable is included in  $x$  and the integral sign means the integral over the coordinates as well as the sum over the spin variables. The symbol  $:\cdots:$  stands for the normal product with respect to the Hartree-Fock state. Let us consider an operator of the form

$$S = \sum_{ik} s_{ik} : c_i^\dagger c_k : , \quad (1.5)$$

and determine the coefficients such that

$$[S, H] = \omega S + Q_2 , \quad (1.6)$$

where  $\omega$  is a constant and  $Q_2$  a two-particle operator of the form  $:c^\dagger c^\dagger c c:$ . This leads to an eigenvalue equation<sup>6</sup>

$$(\epsilon_k - \epsilon_i) s_{ik} + \sum_{\alpha m} (V_{\alpha i, km} s_{m\alpha} + V_{m i, \alpha k} s_{\alpha m}) = \omega s_{ik} , \quad (1.7)$$

$$V_{ij,kl} = v_{ij,kl} - v_{ij,lk} .$$

Here and in the following, Greek indices  $(\alpha, \beta, \gamma)$  stand for occupied states which may be specified by 1 through  $N$ ,  $N$  being the total number of particles, and  $(m, n, p)$  for unoccupied states. If  $Q_2$  in Eq. (1.6) can be neglected,  $\omega$  gives the excited-state energy of the system. If, furthermore, the commutator of  $S$  and  $S^\dagger$  can be approximated by its expectation value, this approximation is called the linearized theory (or RPA including exchange effects). We shall assume henceforth that the Hartree-Fock state chosen at the beginning is stable.<sup>7</sup> Then it is shown that the system is equivalent to an

assembly of bosons with energy  $\omega$ . Equation (1.7) leads to coupled equations for  $s_{\alpha m}$  and  $s_{m\alpha}$  from which  $s_{\alpha\beta}$  and  $s_{mn}$  are determined algebraically. Introducing a function  $\psi_{ik}$  defined by

$$\begin{aligned} \psi_{ik} &= \theta(i, k) s_{ik} , & \theta(i, k) &= 1, \text{ for } i \leq N, k > N, \\ & & &= -1, \text{ for } i > N, k \leq N, \\ & & &= 0, \text{ otherwise,} \end{aligned} \quad (1.8)$$

we finally have

$$(\omega + \epsilon_i - \epsilon_k) \psi_{ik} = \theta(i, k) \sum_{jl} V_{ij,kl} \psi_{lj} . \quad (1.9)$$

If the interaction is spin-independent and the paramagnetic plane-wave representation is taken, Eq. (1.9) is separated into two parts, one for the singlet and the other for the triplet amplitude, as was explicitly shown in Ref. 6. In the ordinary RPA,<sup>2</sup> we have  $v_{ij,kl}$  instead of  $V_{ij,kl}$  in Eq. (1.9), as a result of which the triplet amplitude becomes that of a free particle and hole.

Thus we see that the ordinary RPA is formally extended to the linearized theory just by replacing  $v$  by  $V$ . However, the question arises whether this replacement is always permissible in calculating various physical quantities, without overestimating the contributions from certain diagrams under consideration. Such care should be taken since, for instance, the knowledge of the singlet amplitude is in principle sufficient to determine the dielectric constant and careless inclusion of the triplet contribution may easily lead to an overestimate. We shall show in this paper that in the linearized theory both contributions are always independent; e.g., the correlation energy is the sum of the change in zero-point energies of the singlet and triplet states, the overestimate appearing only in the second-order term.

In Sec. 2, Wentzel's model<sup>8</sup> (meson pair theory) equivalent to the ordinary RPA is extended to the linearized theory. For an infinite system, the new model deals with two kinds of mesons, one with spin zero corresponding to the singlet state of a particle and hole and the other with spin one (therefore with three components) corresponding to the triplet state. The two mesons are dynamically independent in the linearized theory. Then we calculate the change in the zero-point energies of the two fields, which is shown to be equal to the correlation energy obtained by replacing the Gell-Mann and Brueckner diagrams by the corresponding Hugenholtz diagrams.<sup>9</sup>

In Sec. 3, the method of Green's function for the particle and hole scattering is presented in the linearized theory. This formalism may be easier to handle for numerical computations. In Sec. 4, the single-particle and two-particle Green's functions are discussed in the same approximation, from which the single-particle distribution function and the generalized Bethe-

<sup>6</sup> N. Fukuda, Nucl. Phys. 44, 553 (1963).

<sup>7</sup> K. Sawada and N. Fukuda, Progr. Theor. Phys. (Kyoto) 25, 653 (1961); F. Iwamoto and K. Sawada, Phys. Rev. 126, 887 (1962); also see Ref. 6 and W. Kohn and S. J. Nettel, Phys. Rev. Letters 5, 8 (1960).

<sup>8</sup> G. Wentzel, Phys. Rev. 108, 1593 (1957).

<sup>9</sup> N. M. Hugenholtz, Physica 23, 481 (1957).

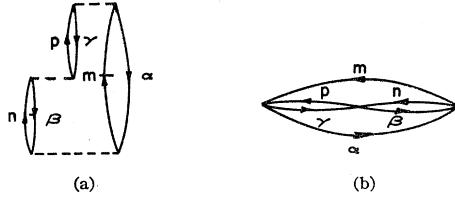


FIG. 1. (a) Gell-Mann and Brueckner diagram of third order (RPA). (b) Hugenholtz diagram corresponding to Fig. 1(a) (linearized theory).

Salpeter equation are derived. Sec. 5 is devoted to the application of the theory to the paramagnetic state of an infinite, uniform system. The case of the  $\delta$ -function potential is worked out, and it is shown that the correlation energy becomes complex in the region where the paramagnetic state is unstable. In the concluding remarks (Sec. 6), the limitation of the application is discussed in connection with the instability of the Hartree-Fock state.

In Appendix A, the instability of an electron gas with respect to spin-density fluctuations is demonstrated without introducing the repopulation of momentum space. This proof leads to the conclusion that the linearized theory makes no sense in the paramagnetic state of an electron gas. In Appendix B, the correlation energy is explicitly obtained up to third order, and in Appendix C, some properties of spin operators are summarized.

## 2. MESON PAIR THEORY EQUIVALENT TO THE LINEARIZED THEORY

We shall first write down the model Hamiltonian  $H_M$  which has the same excitation spectrum as in the linearized theory as follows:

$$H_M = \frac{1}{2} \sum_{\substack{\alpha \leq N \\ m > N}} (\epsilon_m - \epsilon_\alpha) (A_{\alpha m}^\dagger A_{\alpha m} + A_{\alpha m} A_{\alpha m}^\dagger) + \frac{1}{2} \sum_{ijkl} V_{ij,kl} (A_{ik} + A_{ki}^\dagger) (A_{jl} + A_{lj}^\dagger), \quad (2.1)$$

where the second summation is restricted so as to include only  $A_{\alpha m}$  and  $A_{\alpha m}^\dagger$  terms. The operator  $A_{\alpha m}$  is the annihilation operator of a meson in the state  $(\alpha, m)$  and satisfies the commutation relations

$$[A_{\alpha m}, A_{\beta n}] = 0, \quad [A_{\alpha m}, A_{\beta n}^\dagger] = \delta_{\alpha\beta} \delta_{mn}. \quad (2.2)$$

Since Eq. (2.1) is Hermitian, it is to be diagonalized by means of the normal mode operator  $S$  of the form

$$S = \sum_{\alpha m} (\psi_{\alpha m} A_{\alpha m} - \psi_{m\alpha} A_{\alpha m}^\dagger), \quad (2.3)$$

which is to satisfy

$$[S, H_M] = \omega S. \quad (2.4)$$

Then  $\psi_{ik}$  satisfies Eq. (1.9) which shows that the model Hamiltonian  $H_M$  has the same spectrum as in the linearized theory. Usually, the state  $(\alpha, m)$  has four different

spin states with the same orbital functions, which can be rearranged such that one is in the singlet and the other in the triplet state.

If the Hartree-Fock state is stable, the model Hamiltonian is positive definite<sup>6</sup> and makes it possible to obtain a complete set of normal modes  $S^{(r)}$  ( $r=1, 2, \dots$ ) which are assumed, without loss of generality, to satisfy the commutation relations:

$$[S^{(r)}, S^{(r')}] = 0, \quad [S^{(r)}, S^{(r')\dagger}] = \delta_{rr'}. \quad (2.5)$$

Then all eigenvalues  $\omega_r$  are positive and we finally have

$$H_M = \frac{1}{2} \sum_r \omega_r + \sum_r \omega_r S^{(r)\dagger} S^{(r)}. \quad (2.6)$$

The expansion theorem in the indefinite metric space, which was taken for granted in Ref. 6 [Eq. (4.26)], is thus completely equivalent to that in the Hilbert space associated with the positive definite Hermitian form.

A peculiar situation arises, however, when the instability of the Hartree-Fock state comes into play. If it only brings about the extra presence of zero frequency, it causes no mathematical difficulty; we are only concerned with the degenerate Hermitian form. As was discussed in Ref. 6, we usually have in this case either a complex value of  $\omega$ , although  $H_M$  is Hermitian, or a negative value of  $\omega$  in Eq. (2.6). This is because there exists no ground state of our model Hamiltonian.<sup>10</sup> Our linearized theory is thus meaningful if and only if the Hartree-Fock state is stable.

Now, it was already proved in Ref. 2 that if we replace  $V$  by  $v$  in Eq. (2.1), the sum of zero-point energies ( $\frac{1}{2} \sum \omega_r$ ) are essentially equal to the ground-state energy obtained by summing up Gell-Mann and Brueckner diagrams. As an illustration, let us consider the diagram of third order as shown in Fig. 1(a). The energy is given by

$$E_{\text{GBS}}^{(3)} = \sum v_{\gamma\alpha, \beta m} \frac{1}{\epsilon_\alpha + \epsilon_\gamma - \epsilon_m - \epsilon_\beta} \times v_{p\beta, \gamma n} \frac{1}{\epsilon_\alpha + \epsilon_\beta - \epsilon_m - \epsilon_n} v_{mn, \alpha\beta}. \quad (2.7)$$

The corresponding Hugenholtz diagram is shown in Fig. 1(b) and we have the energy

$$E_H^{(3)} = \sum V_{\gamma\alpha, \beta m} \frac{1}{\epsilon_\alpha + \epsilon_\gamma - \epsilon_m - \epsilon_\beta} \times V_{p\beta, \gamma n} \frac{1}{\epsilon_\alpha + \epsilon_\beta - \epsilon_m - \epsilon_n} V_{mn, \alpha\beta}. \quad (2.8)$$

<sup>10</sup> Such a model was studied by E. C. G. Sudarshan and H. J. Schnitzer, Phys. Rev. **123**, 2183, 2193 (1961). The simplest harmonic oscillator with  $H = \epsilon a^\dagger a + g(a^\dagger a^\dagger + a a)$ ,  $|g| > \epsilon > 0$ , is suggestive of this difficulty. This Hamiltonian can be diagonalized by a unitary transformation only for  $|g| \leq \epsilon$ . The  $\omega$  obtained by Eq. (2.4) becomes imaginary for  $|g| > \epsilon$ .

Since the linearized theory is equivalent to replacing  $v$  by  $V$  in the conventional RPA, this is to be equal to the zero-point energy of third order. Explicit demonstration is given in Appendix B. In general, the correlation energy in the linearized theory is given by the sum of Hugenholtz diagrams as shown in Fig. 2, i.e., in the ladder approximation for the particle and hole scattering. The time ordering of vertices between the end points may be arbitrary, but no interaction is allowed between the two ladder diagrams. In actual calculation, however, the summation of corresponding Feynman diagrams is easier to handle as is done in the next section, since the time ordering of vertices is automatically performed.

In second order we have

$$E_{\text{GBS}}^{(2)} = \frac{1}{2} \sum v_{\alpha\beta, mn} \frac{1}{\epsilon_\alpha + \epsilon_\beta - \epsilon_m - \epsilon_n} v_{mn, \alpha\beta}, \quad (2.9)$$

while the corresponding Hugenholtz diagram (exact in second order) gives

$$E^{(2)} = \frac{1}{4} \sum V_{\alpha\beta, mn} \frac{1}{\epsilon_\alpha + \epsilon_\beta - \epsilon_m - \epsilon_n} V_{mn, \alpha\beta}. \quad (2.10)$$

Therefore the replacement of  $v$  by  $V$  in Eq. (2.9) leads to the overestimate (factor 2) of the correct correlation energy. This comes from the situation that the two diagrams obtained by replacing one of the vertices in Fig. 3(a) by exchange interaction become identical as given in Fig. 3(b) and the diagram obtained by replacing both vertices by exchange interaction is identical to Fig. 3(a). It is easy to see that this overcounting is restricted to the second order and never occurs in higher orders. Therefore, in order to obtain, in the linearized theory, the correlation energy  $E_L^c$  which is of higher order than the second, we have to subtract the zeroth- and first-order terms from the zero-point energy and to correct the overestimate in second order. The zeroth- and first-order zero-point energies are given in Appendix B, and we finally have

$$E_L^c = \frac{1}{2} \sum_r \omega_r - \frac{1}{2} \sum_{\alpha m} (\epsilon_m - \epsilon_\alpha) - \frac{1}{2} \sum_{\alpha m} V_{\alpha m, m\alpha} - E^{(2)}. \quad (2.11)$$

It is to be noted that Eq. (2.5) and the completeness

FIG. 2. Hugenholtz diagrams to be summed up in the linearized theory.

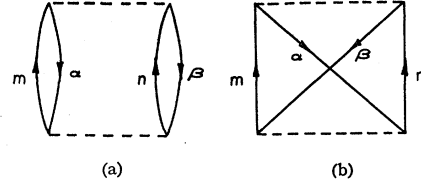
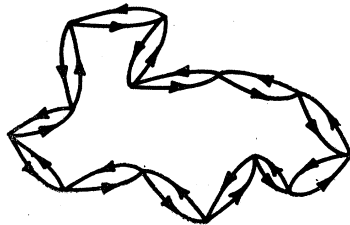


FIG. 3. (a) Gell-Mann and Brueckner diagram of second order. (b) Exchange diagram of second order.

condition for  $S^{(r)}$  are written as

$$\sum_{ik} \psi_{ik}^{(r)} \theta(i, k) \psi_{ki}^{(r')} = 0, \quad (2.12)$$

$$\sum_{ik} \psi_{ik}^{(r)*} \theta(i, k) \psi_{ik}^{(r')} = \delta_{rr'},$$

$$\sum_r \{ \psi_{ik}^{(r)} \psi_{ij}^{(r)*} - \psi_{ji}^{(r)} \psi_{ki}^{(r)*} \} = \delta_{il} \delta_{kj} \theta(i, k), \quad (2.13)$$

where the star stands for the complex conjugate. By multiplying Eq. (1.9) with  $\psi_{ik}^{(r)*} \theta(i, k)$  and summing over  $(ik)$ , we have

$$\frac{1}{2} \sum_r \omega_r = \frac{1}{2} \sum_{\alpha m r} (\epsilon_m - \epsilon_\alpha) \{ |\psi_{\alpha m}^{(r)}|^2 + |\psi_{m\alpha}^{(r)}|^2 \} + \frac{1}{2} \sum_{\substack{ikr \\ jl}} \psi_{ik}^{(r)*} V_{ij, kl} \psi_{lj}^{(r)}, \quad (2.14)$$

which is to be identical to the expectation value of  $H_M$  with respect to the ground state. In order to see this, we make use of the expansion theorem

$$A_{\alpha m} = \sum_r (\psi_{\alpha m}^{(r)*} S^{(r)} + \psi_{m\alpha}^{(r)} S^{(r)\dagger}), \quad (2.15)$$

which is inserted in Eq. (2.1) and leads to Eq. (2.6). Then we find that the first term on the right-hand side of Eq. (2.14) is the kinetic energy and the second the potential energy of the model Hamiltonian.

### 3. THE PARTICLE AND HOLE GREEN'S FUNCTION

In order to formulate the linearized theory introduced in Sec. 2 in the framework of field theory, let us introduce the Green's function,  $G(ik, jl; t-t')$ , for the particle and hole scattering according to

$$G(ik, jl; t-t') = -i \langle T [c_i^\dagger(t) c_k(t) c_i^\dagger(t') c_j(t')] \rangle, \quad (3.1)$$

where the bracket means the expectation value with respect to the true ground state of the Hamiltonian [Eq. (1.3)],  $T$  is the conventional chronological operator, and  $c_i(t)$  the Heisenberg operator defined by

$$c_i(t) = \exp(iHt) c_i \exp(-iHt), \quad (3.2)$$

the unit  $\hbar=1$  being chosen throughout this paper. We shall introduce, for the sake of convenience, the matrix propagator  $G(t-t')$  defined by

$$\langle ik | G(t-t') | jl \rangle = G(ik, jl; t-t'), \quad (3.3)$$

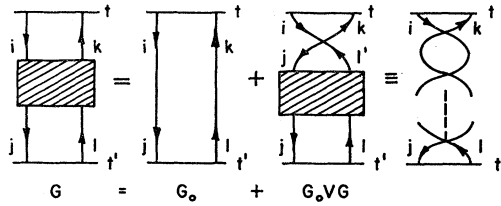


FIG. 4. Ladder approximation for the particle and hole scattering (Feynman diagrams).

The free propagator  $G_0(t-t')$  is easily calculated to give

$$\begin{aligned} G_0(ik, jl; t-t') &= -i\delta_{kl}\delta_{ij}\theta_N(i, k) \\ &\quad \times e^{-i(\epsilon_k - \epsilon_i)(t-t')}, \quad \text{for } t > t', \\ &= -i\delta_{kl}\delta_{ij}\theta_N(k, i) \\ &\quad \times e^{-i(\epsilon_k - \epsilon_i)(t-t')}, \quad \text{for } t < t', \end{aligned} \quad (3.4)$$

where

$$\begin{aligned} \theta_N(i, k) &= 1, \quad \text{for } i \leq N, k > N \\ &= 0, \quad \text{otherwise.} \end{aligned} \quad (3.5)$$

We shall now consider the ladder type scattering of a particle and hole as shown in Fig. 4. Then it is easily shown that the Green's function satisfies the integral equation of the form

$$G(t-t') = G_0(t-t') + \int_{-\infty}^{\infty} dt'' G_0(t-t'') V G(t''-t'), \quad (3.6)$$

where  $V$  is the interaction matrix defined by

$$\langle ik | V | jl \rangle = V_{kj, il}. \quad (3.7)$$

By introducing the Fourier transform of  $G(t)$  according to

$$\begin{aligned} G(t) &= 1/(2\pi) \int_{-\infty}^{\infty} d\omega G(\omega) e^{-i\omega t}, \\ G(\omega) &= \int_{-\infty}^{\infty} dt G(t) e^{i\omega t}, \end{aligned} \quad (3.8)$$

Eq. (3.6) is transformed into

$$G(\omega) = G_0(\omega) + G_0(\omega) V G(\omega). \quad (3.9)$$

Here  $G_0(\omega)$  is the diagonal matrix given by

$$G_0(ik, jl; \omega) = \delta_{ij}\delta_{kl} \frac{\theta(i, k)}{\omega + \epsilon_i - \epsilon_k + i\delta\theta(i, k)}, \quad (3.10)$$

$\delta$  being an infinitesimal positive number, with  $\theta(i, k)$  defined in Eq. (1.8).

The spectrum of a particle and hole, in the bound states as well as in the scattering or resonant states, is to be determined as the solution of the equation,

$$\det\{1 - G_0(\omega)V\} = 0, \quad (3.11)$$

since we are always allowed to contain the system in a

finite box.<sup>11</sup> The operator  $[1 - G_0(\omega)V]$  is the generalization of the dielectric constant in RPA. Equation (3.11) can be written explicitly as

$$\det\{\delta_{ij}\delta_{kl} - [\theta(i, k)/(\omega + \epsilon_i - \epsilon_k) V_{kj, il}]\} = 0, \quad (3.12)$$

which is identical to the secular equation of the complex conjugate of Eq. (1.9). Thus it is seen that the ladder approximation for a particle and hole scattering is equivalent to the linearized theory. It is to be noticed that Eq. (3.9) can be solved as

$$\begin{aligned} G(\omega) &= G_0(\omega) + G_0(\omega) \bar{V}(\omega) G_0(\omega), \\ \bar{V}(\omega) &= V[1/(1 - G_0(\omega)V)], \end{aligned} \quad (3.13)$$

which shows that  $G(\omega)$  is nothing but the value in the Born approximation in which  $V$  is replaced by the effective interaction  $\bar{V}(\omega)$ . The factor  $[1 - G_0(\omega)V]^{-1}$  is usually called the screening factor.

We can further show that the Bethe-Salpeter amplitude defined by

$$\psi_{ik}^{(r)}(t) = \langle r | c_k^\dagger(t) c_i(t) | 0 \rangle, \quad (3.14)$$

where  $|r\rangle$  is an arbitrary excited state, is, in the present approximation,<sup>12</sup> nothing but  $\psi_{ik}^{(r)}$  defined by Eq. (1.8), except for the time factor  $\exp(i\omega_r t)$ . In fact, we have

$$\begin{aligned} G(ik, jl; t-t') &= -i \sum_r \psi_{ik}^{(r)*}(t) \psi_{jl}^{(r)}(t'), \quad \text{for } t > t' \\ &= -i \sum_r \psi_{lj}^{(r)*}(t') \psi_{ki}^{(r)}(t), \quad \text{for } t < t', \end{aligned} \quad (3.15)$$

and by noticing that

$$\begin{aligned} [i(d/dt) + \epsilon_i - \epsilon_k] G_0(ik, jl; t-t') \\ = -i\theta(i, k)\delta(t-t'), \end{aligned} \quad (3.16)$$

the Gell-Mann and Low's method<sup>13</sup> leads easily to

$$[i(d/dt) + \epsilon_i - \epsilon_k] \psi_{ik}(t) = \theta(i, k) V_{ij, kl} \psi_{lj}(t). \quad (3.17)$$

For completeness, let us finally calculate the correlation energy in the present formalism. First of all, there holds an identity

$$\begin{aligned} \sum_{ijkl} (i/2) V_{il, kj} G(ik, jl; t=+0) \\ = \frac{1}{2} \sum_r \psi_{ik}^{(r)*} V_{ij, kl} \psi_{lj}^{(r)}, \end{aligned} \quad (3.18)$$

which is equal to the second term of Eq. (2.14), the potential energy of  $H_M$ . In order to prove Eq. (3.18), we

<sup>11</sup> For an infinite system, a cut is present along the real axis of the complex  $\omega$  plane, and we have to go over into the second Riemann sheet to get resonance energies.

<sup>12</sup> The normalization condition, Eq. (2.12), is to follow automatically as is seen in Appendix B.

<sup>13</sup> M. Gell-Mann and F. Low, Phys. Rev. **84**, 350 (1951).

notice that

$$G(ik, jl; \omega) = \sum_r \left\{ \frac{\psi_{ik}^{(r)*} \psi_{jl}^{(r)} \psi_{lj}^{(r)*} \psi_{ki}^{(r)}}{\omega - \omega_r + i\delta \quad \omega + \omega_r - i\delta} \right\}, \quad (3.19)$$

which follows from Eq. (3.15). By virtue of Eq. (3.8), we have

$$G(t=+0) = \lim_{t \rightarrow 0^+} \frac{1}{2\pi} \int_C d\omega G(\omega) e^{-i\omega t} = -i \sum_r \text{Res}^{(-)} \{G(\omega)\}, \quad (3.20)$$

where the contour  $C$  is the real axis and a large semi-circle in the lower half plane of complex  $\omega$ ,  $\text{Res}^{(-)}$  being the residue of  $G(\omega)$  inside the contour. Equation (3.20) leads to Eq. (3.18). Now, according to the well-known procedure,<sup>2</sup> we have

$$\frac{1}{2} \sum_r \omega_r - \frac{1}{2} \sum_{\alpha m} (\epsilon_m - \epsilon_\alpha) = \int_0^1 \frac{dg}{g} \left[ \sum_{ijkl} \frac{i}{2} g V_{il, kj} G(ik, jl; t=+0) \right], \quad (3.21)$$

where we have replaced the potential  $V$  by  $gV$ . From the form of Eq. (1.3), we may have anticipated the factor  $\frac{1}{4}$  instead of  $\frac{1}{2}$  in Eq. (3.21), but this is not the case.

We shall finally derive an alternative expression for Eq. (3.21) which is a simple generalization of Gell-Mann and Brueckner formula.<sup>5</sup> The ground-state energy is in general written as<sup>14</sup>

<sup>14</sup> N. Fukuda and Y. Wada, Progr. Theor. Phys. Suppl. **15**, 61 (1960).

$$E = \lim_{T \rightarrow \infty} (i/T) \langle \langle S \rangle_L - 1 \rangle, \quad (3.22)$$

where  $S$  is the  $S$  matrix and the bracket means linked vacuum diagrams. The constant  $T$  is the world time during which the total energy is conserved. The contribution of all diagrams shown in Fig. 2 is easily calculated to give

$$\begin{aligned} \sum_{n=2}^{\infty} E^{(n)} &= \sum_{n=2}^{\infty} \frac{i}{4\pi n} \int_{-\infty}^{\infty} d\omega \text{Tr} \{ [G_0(\omega)V]^n \} \\ &\quad - \frac{i}{16\pi} \int_{-\infty}^{\infty} d\omega \text{Tr} \{ [G_0(\omega)V]^2 \} \\ &= -\frac{i}{4\pi} \int_{-\infty}^{\infty} d\omega \{ \ln \det [1 - G_0(\omega)V] \\ &\quad + \text{Tr} [G_0(\omega)V] + \frac{1}{2} \text{Tr} [G_0(\omega)V]^2 \}, \quad (3.23) \end{aligned}$$

where the well-known identity

$$\text{Tr} \ln(1 - G_0(\omega)V) = \ln \det(1 - G_0(\omega)V) \quad (3.24)$$

is used. The last term in Eq. (3.23) is to cancel the over-



FIG. 5. Proper self-energy part in the linearized theory.

estimate (factor 2) of the second-order term. Since the integrand of Eq. (3.23) vanishes as  $1/\omega^2$  as  $\omega$  becomes infinite, we may connect a semicircle either in the upper or in the lower half plane. The evaluation of Eq. (3.23) is now straightforward to give directly

$$\sum_{n=2}^{\infty} E^{(n)} = \frac{1}{2} \left\{ \sum_r \omega_r - \sum_{\alpha m} (\epsilon_m - \epsilon_\alpha) - \frac{1}{2} \sum_{\alpha m} V_{\alpha m, m\alpha} - E^{(2)} \right\} \equiv E_L^e. \quad (3.25)$$

It is to be noted that the integral path in Eq. (3.23) usually can be deformed into the imaginary axis without crossing any singularity.

#### 4. THE SINGLE-PARTICLE AND PARTICLE-PARTICLE GREEN'S FUNCTION

The single-particle Green's function is defined by

$$S_F(ik; t-t') = -i \langle T [c_i(t) c_k^\dagger(t')] \rangle, \quad (4.1)$$

which satisfies, as is well known, the integral equation of the type

$$\begin{aligned} S_F(ik; t-t') &= S_F^{(0)}(ik; t-t') \\ &\quad + \sum_{i'k'} \int_{-\infty}^{\infty} dt'' dt''' S_F^{(0)}(ii'; t-t'') \\ &\quad \times \Sigma(i'k'; t''-t''') S_F(k'; t'''-t'). \quad (4.2) \end{aligned}$$

Here  $\Sigma$  is called the proper self-energy part, and  $S_F^{(0)}$  is the free Green's function satisfying

$$[i(d/dt) - \epsilon_i] S_F^{(0)}(ik; t-t') = \delta_{ik} \delta(t-t'). \quad (4.3)$$

By introducing the Fourier transforms of  $S_F(t)$  and  $\Sigma(t)$  according to Eq. (3.8), Eq. (4.2) can be written as

$$S_F(\omega) = S_F^{(0)}(\omega) + S_F^{(0)}(\omega) \Sigma(\omega) S_F(\omega), \quad (4.4)$$

where  $S_F$  and  $\Sigma$  are considered matrices. The single-particle energy is to be determined as the root of the equation

$$\det \{ 1 - S_F^{(0)}(\omega) \Sigma(\omega) \} = 0. \quad (4.5)$$

Let us now obtain  $\Sigma$  in the linearized theory, the cor-

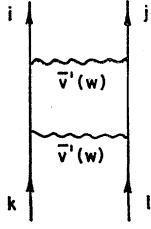


FIG. 6. Two-body propagator in the ladder approximation.

responding diagram being given in Fig. 5. We then have

$$\Sigma(i'k'; t-t') = i \sum_{jl} \langle ji' | VG(t-t') V | lk' \rangle S_F^{(0)}(jl; t-t'),$$

$$\Sigma(i'k'; \omega) = \frac{i}{2\pi} \int_{-\infty}^{\infty} \sum_{il} d\omega' \langle ji' | VG(\omega') \times V | lk' \rangle S_F^{(0)}(jl; \omega'), \quad (4.6)$$

where

$$S_F^{(0)}(ik; \omega) = \frac{\delta_{ik}}{\omega - \epsilon_i + i\epsilon(i)\delta}, \quad (4.7)$$

$$\epsilon(i) = 1, \quad \text{for } i > N,$$

$$= -1, \quad \text{for } i \leq N.$$

By introducing Eq. (3.19) into Eq. (4.6) and making use of Eq. (1.9), we can explicitly calculate the integral over  $\omega'$ . The result is

$$\Sigma(i'k'; \omega) = \sum_{rm} \frac{(\omega_r + \epsilon_m - \epsilon_{i'}) (\omega_r + \epsilon_m - \epsilon_{k'})}{\omega - \omega_r - \epsilon_m + i\delta} \psi_{mi'}^{(r)*} \psi_{mk'}^{(r)}$$

$$+ \sum_{r\alpha} \frac{(\omega_r - \epsilon_\alpha + \epsilon_{i'}) (\omega_r - \epsilon_\alpha + \epsilon_{k'})}{\omega + \omega_r - \epsilon_\alpha - i\delta} \psi_{k'\alpha}^{(r)*} \psi_{i'\alpha}^{(r)}. \quad (4.8)$$

The distribution function  $f_i$  is given by

$$f_i = -i S_F(ii; t=0) = -\frac{i}{2\pi} \int_C d\omega S_F(ii; \omega), \quad (4.9)$$

where the contour is the entire real axis and a large semi-circle in the upper half-plane. The free distribution function  $f_i^{(0)}$  is that of the Fermi distribution. Since the explicit calculation of Eq. (4.9) cannot be performed, we shall be content with the approximation in which  $S_F$  in the last term of Eq. (4.4) is replaced by  $S_F^{(0)}$ . Then we have

$$S_F(ii; \omega) = \frac{1}{\omega - \epsilon_i + i\delta\epsilon(i)} + \frac{1}{(\omega - \epsilon_i + i\delta\epsilon(i))^2}$$

$$\times \left\{ \sum_{rm} \frac{(\omega_r + \epsilon_m - \epsilon_i)^2}{\omega - \omega_r - \epsilon_m + i\delta} |\psi_{mi}^{(r)}|^2 \right.$$

$$\left. + \sum_{r\alpha} \frac{(\omega_r - \epsilon_\alpha + \epsilon_i)^2}{\omega + \omega_r - \epsilon_\alpha - i\delta} |\psi_{i\alpha}^{(r)}|^2 \right\}. \quad (4.10)$$

The contour integral of Eq. (4.9) is easily calculated to give

$$f_i = \sum_{r\beta} |\psi_{m\beta}^{(r)}|^2, \quad \text{for } i = m \text{ (unoccupied state),}$$

$$= 1 - \sum_{rn} |\psi_{n\alpha}^{(r)}|^2, \quad \text{for } i = \alpha \text{ (occupied state),}$$

$$\sum_i f_i = N, \quad (4.11)$$

where use has been made of Eq. (2.13).

The kinetic energy increase by means of this distribution function is given by

$$\sum_{m>N} \epsilon_m f_m - \sum_{\alpha \leq N} \epsilon_\alpha (1 - f_\alpha)$$

$$= \sum_{r\alpha m} (\epsilon_m - \epsilon_\alpha) |\psi_{m\alpha}^{(r)}|^2, \quad (4.12)$$

which is equal, by virtue of Eq. (2.13), to the first term of Eq. (2.14) minus  $\frac{1}{2} \sum_{\alpha m} (\epsilon_m - \epsilon_\alpha)$ , the zeroth-order zero-point energy. Therefore we may conclude that Eq. (4.11) gives the distribution function in the linearized theory.

We finally turn to the particle-particle Green's function which is defined by

$$D(ij, kl; t-t') = -\langle T[c_i(t)c_j(t)c_i^\dagger(t')c_k^\dagger(t')] \rangle. \quad (4.13)$$

Let us confine ourselves to the ladder approximation as shown in Fig. 6, where, however, the interaction is replaced by the screened one defined by Eq. (3.13). By introducing the matrices  $D$  and  $\bar{V}'$  according to

$$\lambda ij | D | kl \rangle = D(ij, kl), \quad (4.14)$$

$$\langle ij | \bar{V}' | kl \rangle = \langle ki | \bar{V} | jl \rangle \equiv \bar{V}'_{ij, kl},$$

the integral equation to be satisfied by  $D(\omega)$  is easily obtained as

$$D(\omega) = D_0(\omega) + (i/4) D_0(\omega) \bar{V}'(\omega) D(\omega), \quad (4.15)$$

where  $D_0(\omega)$  is the free Green's function given by

$$D_0(ij, kl; \omega) = -i(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk})$$

$$\times \frac{\epsilon(i, j)}{\omega - \omega_i - \omega_j + i\delta\epsilon(i, j)}, \quad (4.16)$$

$$\epsilon(i, j) = 1, \quad \text{for } i, j > N,$$

$$= -1, \quad \text{for } i, j \leq N,$$

$$= 0, \quad \text{otherwise.}$$

We may alternatively consider the Bethe-Salpeter equation for the amplitude defined by

$$\varphi_{ij}(t) = \langle 0 | c_i(t)c_j(t) | s \rangle = \varphi_{ij} e^{-i\Omega_s t}, \quad (4.17)$$

$\Omega_s$  being the excitation energy of the two-particle state  $|s\rangle$ . By means of Eq. (4.15), it is a routine job to derive

the Bethe-Salpeter equation<sup>15</sup>

$$(i(d/dt) - \epsilon_i - \epsilon_j) \varphi_{ij}(t) = \frac{1}{2} \sum_{kl} \int dt' \epsilon(i,j) \bar{V}_{ij,kl}(t-t') \varphi_{kl}(t'), \quad (4.18)$$

whose Fourier transform becomes

$$(\omega - \epsilon_i - \epsilon_j) \varphi_{ij}(\omega) = \frac{1}{2} \sum_{kl} \epsilon(i,j) \bar{V}_{ij,kl}(\omega) \varphi_{kl}(\omega). \quad (4.19)$$

Because of the factor  $\epsilon(i,j)$ , we may put

$$\varphi_{ij}(\omega) = 0, \text{ for } i \leq N, k > N, \text{ or } i > N, k \leq N \quad (4.20)$$

and Eq. (4.19) can be separated as

$$\begin{aligned} (\omega - \epsilon_m - \epsilon_n) \varphi_{mn} &= \frac{1}{2} \sum_{\alpha\beta} \bar{V}_{mn,\alpha\beta} \varphi_{\alpha\beta} \\ &\quad + \frac{1}{2} \sum_{m'n'} \bar{V}_{mn,m'n'} \varphi_{m'n'}, \\ (\omega - \epsilon_\alpha - \epsilon_\beta) \varphi_{\alpha\beta} &= -\frac{1}{2} \sum_{\alpha'\beta'} \bar{V}_{\alpha\beta,\alpha'\beta'} \varphi_{\alpha'\beta'} \\ &\quad - \frac{1}{2} \sum_{mn} \bar{V}_{\alpha\beta,mn} \varphi_{mn}. \end{aligned} \quad (4.21)$$

The scattering correction to the correlation energy  $E_L^c$  and the pair correlation function are obtained in terms of the Bethe-Salpeter amplitude in the usual way<sup>15</sup> with  $V$  replaced by  $\bar{V}$ .

5. APPLICATION TO AN INFINITE SYSTEM

Let us apply the present theory to an infinite system interacting through spin-independent potentials, under the assumption that the Fermi distribution (paramagnetic state) in momentum space is stable. The matrix element of the potential [Eq. (1.4)] becomes

$$V_{\mathbf{p}_1\sigma_1\mathbf{p}_2\sigma_2,\mathbf{p}_3\sigma_3\mathbf{p}_4\sigma_4} = \delta_{\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_3-\mathbf{p}_4} v(\mathbf{p}_1-\mathbf{p}_3) \delta_{\sigma_1\sigma_3} \delta_{\sigma_2\sigma_4}, \quad (5.1)$$

where the conservation of momentum is apparent in the first Kronecker's  $\delta$ -symbol and

$$v(q) = \frac{1}{\Omega} \int d^3x v(\mathbf{x}) e^{-iq \cdot \mathbf{x}}, \quad (5.2)$$

$\Omega$  being the normalization volume. If the exchange term is subtracted from Eq. (5.1) as in Eq. (1.7), we have

$$V_{\mathbf{p}_1\sigma_1\mathbf{p}_2\sigma_2,\mathbf{p}_3\sigma_3\mathbf{p}_4\sigma_4} = \delta_{\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_3-\mathbf{p}_4} \times \{v(\mathbf{p}_1-\mathbf{p}_3) \delta_{\sigma_1\sigma_3} \delta_{\sigma_2\sigma_4} - v(\mathbf{p}_1-\mathbf{p}_4) \delta_{\sigma_1\sigma_4} \delta_{\sigma_2\sigma_3}\}. \quad (5.3)$$

By considering  $V$  as a matrix with respect to spin indices and by making use of the identity in Appendix C,

$$\delta_{\sigma_1\sigma_4} \delta_{\sigma_2\sigma_3} = \frac{1}{2} \sum_{\lambda=0}^3 \langle \sigma_1\sigma_2 | \sigma_\lambda^{(1)} \sigma_\lambda^{(2)} | \sigma_3\sigma_4 \rangle, \quad (5.4)$$

with  $\sigma_0=1$ , and  $(\sigma_1,\sigma_2,\sigma_3)=\sigma$ , we have

$$V_{\mathbf{p}_1\mathbf{p}_2,\mathbf{p}_3\mathbf{p}_4} = \delta_{\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_3-\mathbf{p}_4} \times \{V_{\mathbf{p}_1\mathbf{p}_2,\mathbf{p}_3\mathbf{p}_4}^s + (\sigma^{(1)} \sigma^{(2)}) V_{\mathbf{p}_1\mathbf{p}_2,\mathbf{p}_3\mathbf{p}_4}^t\}, \quad (5.5)$$

<sup>15</sup> F. Iwamoto, Progr. Theoret. Phys. (Kyoto) 23, 871 (1960).

where

$$\begin{aligned} V_{\mathbf{p}_1\mathbf{p}_2,\mathbf{p}_3\mathbf{p}_4}^s &= v(\mathbf{p}_1-\mathbf{p}_3) - \frac{1}{2} v(\mathbf{p}_1-\mathbf{p}_4), \\ V_{\mathbf{p}_1\mathbf{p}_2,\mathbf{p}_3\mathbf{p}_4}^t &= -\frac{1}{2} v(\mathbf{p}_1-\mathbf{p}_4), \end{aligned} \quad (5.6)$$

which are called the singlet and triplet potentials, respectively. The potential energy is then written as

$$H_I = \frac{1}{4} \sum \delta_{\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_3-\mathbf{p}_4} \{ V_{\mathbf{p}_1\mathbf{p}_2,\mathbf{p}_3\mathbf{p}_4}^s : (\mathbf{c}_{\mathbf{p}_1}^\dagger \mathbf{c}_{\mathbf{p}_3}) (\mathbf{c}_{\mathbf{p}_2}^\dagger \mathbf{c}_{\mathbf{p}_4}) : + V_{\mathbf{p}_1\mathbf{p}_2,\mathbf{p}_3\mathbf{p}_4}^t : (\mathbf{c}_{\mathbf{p}_1}^\dagger \sigma \mathbf{c}_{\mathbf{p}_3}) (\mathbf{c}_{\mathbf{p}_2}^\dagger \sigma \mathbf{c}_{\mathbf{p}_4}) : \}. \quad (5.7)$$

Similarly, the particle-hole Green's function is split, because the Hamiltonian commutes with the total spin, as

$$\begin{aligned} \langle \mathbf{p}_1\sigma_1\mathbf{p}_2\sigma_2 | G(t-t') | \mathbf{p}_3\sigma_3\mathbf{p}_4\sigma_4 \rangle &= \frac{1}{4} \sum_{\lambda=0}^3 \langle \sigma_2\sigma_3 | \sigma_\lambda^{(1)} \sigma_\lambda^{(2)} | \sigma_1\sigma_4 \rangle \\ &\quad \times \langle \mathbf{p}_1\mathbf{p}_2 | G_\lambda(t-t') | \mathbf{p}_3\mathbf{p}_4 \rangle, \end{aligned} \quad (5.8)$$

where

$$\langle \mathbf{p}_1\mathbf{p}_2 | G_\lambda | \mathbf{p}_3\mathbf{p}_4 \rangle = -i \langle T [ \mathbf{c}_{\mathbf{p}_1}^\dagger(t) \sigma_\lambda \mathbf{c}_{\mathbf{p}_2}(t') \mathbf{c}_{\mathbf{p}_4}^\dagger \sigma_\lambda \mathbf{c}_{\mathbf{p}_3}(t') ] \rangle. \quad (5.9)$$

The proof is given in Appendix C. Since  $G_\lambda$  is to be the same for  $\lambda=1, 2, 3$ , we shall define the singlet and triplet Green's functions as

$$G^s \equiv G_0, \quad G^t \equiv G_1 = G_2 = G_3. \quad (5.10)$$

In this way we have succeeded in expressing the matrix  $G$  and the matrix  $V$  defined by Eq. (3.7) in terms of the direct products of spin and momentum matrices as follows:

$$\begin{aligned} G(t-t') &= \frac{1}{4} G^s + \frac{1}{4} (\sigma^{(1)} \cdot \sigma^{(2)}) G^t, \\ V &= V^s + (\sigma^{(1)} \cdot \sigma^{(2)}) V^t, \end{aligned} \quad (5.11)$$

where the rows and columns of spin matrices are re-shuffled according to Eq. (5.8). It is now an easy task to separate Eq. (3.6) into the two integral equations for the singlet and triplet Green's functions as

$$\begin{aligned} G^{s,t}(t-t') &= G^{(0)}(t-t') \\ &\quad + \int_{-\infty}^{\infty} dt'' G^{(0)}(t-t'') V^{s,t} G^{s,t}(t''-t'), \end{aligned} \quad (5.12)$$

where  $G^{(0)} = G_\lambda^{(0)}$  is independent of  $\lambda$ .

We shall now introduce the conservation of momentum explicitly in order to further reduce the momentum matrices. If we put

$$\mathbf{p}_1 = \mathbf{p}, \quad \mathbf{p}_2 = \mathbf{p} + \mathbf{q}, \quad \mathbf{p}_3 = \mathbf{p}', \quad (5.13)$$

the nonvanishing element of  $G$  and  $V$  necessitates

$$\mathbf{p}_4 = \mathbf{p}' + \mathbf{q}, \quad (5.14)$$

which allows us, as shown below, to consider the matrices  $G^{s,t}$  and  $V^{s,t}$  as having  $(\mathbf{p}, \mathbf{p}')$  elements with  $\mathbf{q}$



as a parameter:

$$\begin{aligned} \langle \mathbf{p}, \mathbf{p}+\mathbf{q} | G^{s,t} | \mathbf{p}', \mathbf{p}'+\mathbf{q} \rangle &\equiv \langle \mathbf{p} | G_q^{s,t} | \mathbf{p}' \rangle, \\ \langle \mathbf{p}, \mathbf{p}+\mathbf{q} | V^{s,t} | \mathbf{p}', \mathbf{p}'+\mathbf{q} \rangle &\equiv \langle \mathbf{p} | V_q^{s,t} | \mathbf{p}' \rangle, \\ \langle \mathbf{p} | V_q^s | \mathbf{p}' \rangle &= v(q) - \frac{1}{2}v(\mathbf{p}-\mathbf{p}'), \\ \langle \mathbf{p} | V_q^t | \mathbf{p}' \rangle &= -\frac{1}{2}v(\mathbf{p}-\mathbf{p}'). \end{aligned} \quad (5.15)$$

Then Eq. (5.12) is rewritten as

$$G_q^{s,t}(t-t') = G_q^{(0)}(t-t') + \int_{-\infty}^{\infty} dt'' G_q^{(0)}(t-t'') V_q^{s,t} G_q^{s,t}(t''-t'), \quad (5.16)$$

where  $G_q^{(0)}$  is a diagonal matrix whose Fourier transform is given by

$$\begin{aligned} \langle \mathbf{p} | G_q^{(0)}(\omega) | \mathbf{p}' \rangle &\equiv \delta_{\mathbf{p}\mathbf{p}'} G_q^{(0)}(\mathbf{p}; \omega), \\ G_q^{(0)}(\mathbf{p}; \omega) &= \frac{2\theta_q(\mathbf{p})}{\omega - \omega_q(\mathbf{p}) + i\theta_q(\mathbf{p})\delta}, \\ \theta_q(\mathbf{p}) &= 1, \quad \text{for } |\mathbf{p}| \leq p_f < |\mathbf{p}+\mathbf{q}|, \\ &= -1, \quad \text{for } |\mathbf{p}| > p_f \geq |\mathbf{p}+\mathbf{q}|, \\ &= 0, \quad \text{otherwise,} \end{aligned} \quad (5.17)$$

with

$$\begin{aligned} \omega_q(\mathbf{p}) &= \epsilon(\mathbf{p}+\mathbf{q}) - \epsilon(\mathbf{p}) = (\mathbf{p} \cdot \mathbf{q}/m) + (q^2/2m) \\ &+ \sum_{|\mathbf{p}'| < p_f} \{v(\mathbf{p}-\mathbf{p}') - v(\mathbf{p}+\mathbf{q}-\mathbf{p}')\}, \end{aligned} \quad (5.18)$$

$\epsilon(\mathbf{p})$  being the single-particle Hartree-Fock energy. It is easily shown that Eq. (3.11) determining the spectrum of a particle and hole is separated into

$$\begin{aligned} \det[1 - G_q^{(0)}(\omega) V_q^s] &= 0, \\ \det[1 - G_q^{(0)}(\omega) V_q^t] &= 0. \end{aligned} \quad (5.19)$$

We are now in a position to write down the correlation energy, Eq. (3.23), as the sum of the singlet and triplet contributions. We notice that

$$\begin{aligned} \langle \mathbf{p}\sigma_1\mathbf{p}+\mathbf{q}\sigma_2 | [G^{(0)}(\omega)V]^n | \mathbf{p}'\sigma_3\mathbf{p}'+\mathbf{q}\sigma_4 \rangle \\ = \frac{1}{2}\delta_{\sigma_1\sigma_2}\delta_{\sigma_3\sigma_4} \langle \mathbf{p} | [G_q^{(0)}(\omega)V_q^s]^n | \mathbf{p}' \rangle \\ + \frac{1}{2}\langle \sigma_2\sigma_3 | \boldsymbol{\sigma}^{(1)} \cdot \boldsymbol{\sigma}^{(2)} | \sigma_1\sigma_4 \rangle \langle \mathbf{p} | [G_q^{(0)}(\omega)V_q^t]^n | \mathbf{p}' \rangle, \end{aligned} \quad (5.20)$$

which is proved in Appendix C, from which follows

$$\begin{aligned} \text{Tr}\{[G^{(0)}(\omega)V]^n\} &= \sum_{\mathbf{q}} \text{Tr}\{[G_q^{(0)}(\omega)V_q^s]^n\} \\ &+ 3 \sum_{\mathbf{q}} \text{Tr}\{[G_q^{(0)}(\omega)V_q^t]^n\}. \end{aligned} \quad (5.21)$$

Therefore, by writing

$$E_L^c = E^s + 3E^t, \quad (5.22)$$

we have finally

$$\begin{aligned} E^{s,t} &= -\frac{i}{4\pi} \sum_{\mathbf{q}} \int_{-\infty}^{\infty} d\omega \{ \ln \det[1 - G_q^{(0)}(\omega)V_q^{s,t}] \\ &+ \text{Tr}[G_q^{(0)}(\omega)V_q^{s,t}] + \frac{1}{4} \text{Tr}[G_q^{(0)}(\omega)V_q^{s,t}]^2 \}. \end{aligned} \quad (5.23)$$

We may rearrange the second-order correction such that it appears only in the singlet contribution. If we neglect the triplet contribution and the exchange term in  $V^s$ , the result is identical to the Gell-Mann and Brueckner formula.<sup>5</sup>

Finally, we shall apply Eq. (5.23) to the case of the  $\delta$ -function potential

$$v(\mathbf{x}) = g\delta(\mathbf{x}), \quad v(q) = g/\Omega, \quad g > 0. \quad (5.24)$$

Then we have

$$\langle \mathbf{p} | V_q^s | \mathbf{p}' \rangle = g/2\Omega, \quad \langle \mathbf{p} | V_q^t | \mathbf{p}' \rangle = -g/2\Omega, \quad (5.25)$$

from which follows

$$\begin{aligned} \det[1 - G_q^{(0)}(\omega)V_q^s] &= 1 + (g/2\Omega) \sum_{\mathbf{p}} G_q^{(0)}(\mathbf{p}; \omega), \\ \det[1 + G_q^{(0)}(\omega)V_q^t] &= 1 - (g/2\Omega) \sum_{\mathbf{p}} G_q^{(0)}(\mathbf{p}; \omega). \end{aligned} \quad (5.26)$$

The integration path in Eq. (5.22) can be smoothly changed into the imaginary axis in the complex  $\omega$  plane. Then, by introducing the new variable  $u$  instead of  $\omega$  according to

$$\omega = i(qp_f/m)u, \quad (5.27)$$

we finally have, after replacing  $q$  by  $qp_f$ ,

$$\begin{aligned} E^s &= N \frac{3p_f^2}{8\pi m} \int_0^{\infty} dq q^3 \int_0^{\infty} du \\ &\times \{ \ln(1 + \gamma R) - \gamma R + \frac{1}{4}\gamma^2 R^2 \}, \end{aligned} \quad (5.28)$$

$$\begin{aligned} E^t &= N \frac{3p_f^2}{8\pi m} \int_0^{\infty} dq q^3 \int_0^{\infty} du \\ &\times \{ \ln(1 - \gamma R) + \gamma R + \frac{1}{4}\gamma^2 R^2 \}, \end{aligned} \quad (5.28)$$

where

$$\gamma = gm p_f / 2\pi^2, \quad (5.29)$$

and

$$\begin{aligned} R(u, q) &= q^{-1} \int_c^1 dt \int_{|a-b|}^{a+b} dp \frac{t p^3}{(pt)^2 + u^2}, \\ a &= \left[ 1 - \frac{q^2}{4}(1-t^2) \right]^{1/2}, \quad b = (\frac{1}{2})qt, \end{aligned} \quad (5.30)$$

$$c = 0, \quad \text{for } q \leq 2; \quad = q^{-1}(q^2-4)^{1/2}, \quad \text{for } q > 2,$$

which is positive and monotonically decreasing as a function of either  $u$  or  $q$ ;  $R(0,0) = 1$ . The correlation energy is well behaved for  $\gamma < 1$ , but at  $\gamma = 1$ , where the instability occurs with respect to spin density fluctuation,<sup>7</sup> the triplet correlation energy shows a singularity like  $(1-\gamma)^3 \ln(1-\gamma)$  and its analytic continuation makes no sense at all.

6. CONCLUDING REMARKS

The theory of the linearized many-body problem is presented here, with emphasis laid on the formal structure of the dynamical system. First of all, Wentzel's meson pair model is derived which is mathematically equivalent to this approximation. As compared to Ref. 8, two kinds of mesons are now involved, one with spin zero corresponding to the singlet state of a particle and hole and the other with spin one corresponding to the triplet state. Then the stability condition of the Hartree-Fock state with respect to an infinitesimal deformation of single-particle wavefunctions is equivalent to the positive definite character of the Hermitian model Hamiltonian, and the expansion theorem in the indefinite space<sup>6</sup> is transferred to that in the ordinary Hilbert space.

The linearized theory will be more or less workable provided that the potential is soft, repulsive, and probably of long range. However, the stability of the Hartree-Fock state is above all indispensable for this approximation to be valid, since otherwise the model Hamiltonian allows no ground state at all. We have explicitly shown in the case of the repulsive  $\delta$ -function potential that the correlation energy is a regular function of  $\gamma = mgp_f/2\pi^2$  for  $\gamma < 1$ , has a logarithmic singularity at  $\gamma = 1$ , and becomes complex for  $\gamma > 1$ , where the paramagnetic state is known to be unstable.<sup>7</sup> Such difficulty is always encountered whenever there occurs an instability of the starting Hartree-Fock state, and we are forced to start with the stable Hartree-Fock state in order that the linearized theory may have any meaning at all.

Now, the paramagnetic state of an electron gas is stable at high density with respect to density fluctuations but is always unstable with respect to spin density fluctuations as lately shown by Overhauser.<sup>16</sup> If it can be shown, and it actually is in Appendix A, that this is also unstable in the sense of Ref. 7, then the correlation energy arising from the triplet state is to be complex even at high density. In the conventional RPA, only the singlet state which is associated with density fluctuations comes into play and therefore the Wentzel's model Hamiltonian is positive definite. This is one of the reasons why the calculation in Ref. 2 is workable at high density. However, in the linearized theory which is supposed to be an improvement since the exchange corrections are taken into account consistently, the model Hamiltonian is no longer positive definite for the triplet meson field and allows no ground state. In our opinion, therefore, there might still be slight doubt about Gell-Mann and Brueckner's claim<sup>2,5</sup> that the triplet contribution, though complex, shall be discarded since it vanishes at high density.

<sup>16</sup> A. W. Overhauser, Phys. Rev. **128**, 1437 (1962).

APPENDIX A

Instability of an Electron Gas with Respect to Spin Density Fluctuation

We shall show that the paramagnetic state of an electron gas is always unstable with respect to an infinitesimal spin density fluctuation, even if we disregard the repopulation in momentum space for the occupied states. This is an alternative proof of the theorem due to Overhauser.<sup>16</sup>

The critical value of  $r_s$ , above which an electron gas becomes unstable, satisfies an inequality<sup>7</sup>

$$\frac{\alpha}{\pi} (r_s)_{\text{crit}} \leq N/(D_1 - D_2),$$

$$N = \frac{1}{(2\pi)^3} \int \int d^3\mathbf{k} |\psi(\mathbf{k})|^2 \mathbf{k} \cdot \mathbf{q}, \tag{A1}$$

$$D_1 = \frac{1}{(2\pi)^2} \int \int d^3\mathbf{k} d^3\mathbf{k}' \psi(\mathbf{k})^* \times \left\{ \frac{1}{|\mathbf{k} - \mathbf{k}'|} + \frac{1}{|\mathbf{k} + \mathbf{k}'|} \right\} \psi(\mathbf{k}'),$$

$$D_2 = \frac{1}{(2\pi)^2} \int \int d^3\mathbf{k} d^3\mathbf{k}' |\psi(\mathbf{k})|^2 \times \left\{ \frac{1}{|\mathbf{k} - \mathbf{k}'|^2} - \frac{1}{|\mathbf{k} + \mathbf{k}'|^2} \right\},$$

where the integration is to be carried out for  $|\mathbf{k} - \frac{1}{2}\mathbf{q}| \leq 1 \leq |\mathbf{k} + \frac{1}{2}\mathbf{q}|$ ; all momenta are measured with  $p_f$  as the unit. The momentum  $\mathbf{q}$  is arbitrary but is now chosen  $2(2p_f)$  in the direction of  $z$  axis. We shall choose the variational function as

$$\psi(\mathbf{k}) = 1/k_z, \text{ for } \mathbf{k} \text{ in } A, \tag{A2}$$

$$= 0, \text{ otherwise,}$$

where  $A$  is the shaded domain in Fig. 7.

We now proceed to the evaluation of integrals of Eq. (A1) by assuming that  $R$  and  $l$  are both infinitesimal and are related by

$$l = \lambda R, \quad 0 < \lambda < 1, \tag{A3}$$

where  $\lambda$  is a constant to be chosen properly later on. By introducing a variable  $\rho = (k_x^2 + k_y^2)^{1/2}$ , we have

$$N = \frac{1}{\pi} \left[ \int_0^{R^2/2} \frac{dk_z}{k_z} \int_0^{(2k_z)^{1/2}} d\rho \right. \\ \left. + \int_{R^2/2}^{l/2} \frac{dk_z}{k_z} \int_0^R d\rho \right] \int_0^{2\pi} d\varphi \\ = R^2 \{ \ln(1/R) + O(1) \}. \tag{A4}$$

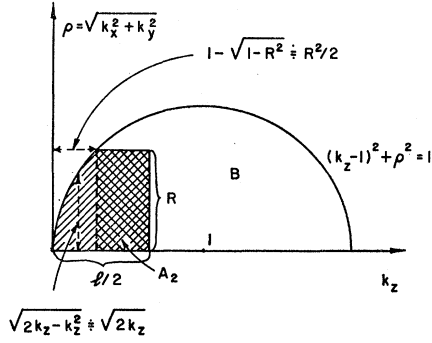


FIG. 7. The integral domain in  $k_z$  and  $\rho = (k_x^2 + k_y^2)^{1/2}$  space. The shaded domain is  $A$ .

In evaluating  $D_1$ , we notice that the integrand is positive definite and  $D_1$  is greater than the value integrated over the domain  $A_2$ . Then we have

$$D_1 > \frac{1}{(2\pi)^2} 2\pi \int_{R^2/2}^{1/2} \frac{dk_z}{k_z} \int_0^R d\rho \rho \int_{R^2/2}^{1/2} \frac{dk_z'}{k_z'} \int_0^R d\rho' \rho' \int_0^{2\pi} d\varphi$$

$$\times \left[ \frac{1}{\rho^2 + \rho'^2 - 2\rho\rho' \cos\varphi + (k_z - k_z')^2} + (k_z \rightarrow -k_z) \right]$$

$$= R^2 \{ [1 + (\lambda^2/4)] \ln[1 + (4/\lambda^2)] - 1 \} \left( \ln \frac{\lambda}{R} \right)^2,$$

$$[\ln(\lambda/R)]^2 = [\ln(1/R)]^2 + O[\ln(1/R)]. \quad (\text{A5})$$

The evaluation of  $D_2$  can be performed by making use of the familiar self-energy integral of an electron

$$\int_{A+B} \frac{d^3\mathbf{k}'}{|\mathbf{k} - \mathbf{k}'|^2}$$

$$= 2\pi \left[ \frac{1 - |\mathbf{k} - \mathbf{e}|^2}{2|\mathbf{k} - \mathbf{e}|^2} \ln \frac{|\mathbf{k} - \mathbf{e}| + 1}{|\mathbf{k} - \mathbf{e}| - 1} + 1 \right], \quad (\text{A6})$$

where  $\mathbf{e}$  is the unit vector of  $z$  axis. Since  $\mathbf{k}$  is in the domain  $A$ , we have

$$(\text{A6}) = 2\pi \{ 1 + k_z \ln(2/k_z) + O[R^2 \ln(1/R)] \}, \quad (\text{A7})$$

which leads to

$$D_2 = \frac{1}{(2\pi)^2} \int_A \frac{d^3\mathbf{k}}{k_z^2} \int_{A+B} \frac{d^3\mathbf{k}'}{|\mathbf{k} - \mathbf{k}'|^2} \frac{1}{|\mathbf{k} + \mathbf{k}'|^2}$$

$$= R^2 \frac{3}{2} [\ln(1/R)] \cdot \{ \ln(1/R) + O(1) \}. \quad (\text{A8})$$

We shall now choose the constant  $\lambda$  such that

$$\mu \equiv \frac{1}{4} \{ [1 + (\lambda^2/4)] \ln[1 + (4/\lambda^2)] - 1 \}$$

$$-\frac{3}{2} > 0, \quad 0 < \lambda < 1, \quad (\text{A9})$$

which is easily satisfied. Then we have

$$\frac{\alpha}{\pi} (r_s)_{\text{crit}} < \frac{1}{\mu \ln(1/R)} \left\{ 1 + O\left(\frac{1}{\ln(1/R)}\right) \right\}, \quad (\text{A10})$$

from which it is concluded that

$$(r_s)_{\text{crit}} = 0, \quad (\text{A11})$$

in agreement with the result of Overhauser. Since Eq. (A1) holds for any infinitesimal spin density fluctuation, the present proof shows that an electron gas is unstable not only with respect to a helical spin deformation but to a deformation generated by a term including  $\sigma_z$ , as was also noted by Overhauser.

## APPENDIX B

### Perturbation Theory in the Meson Pair Theory

We shall solve the eigenvalue problem [Eq. (1.9)] in perturbation theory, up to third order for  $\omega$ , and show that

$$\frac{1}{2} \sum_r \omega_r^{(3)} = \sum V_{\gamma\alpha, \beta m} \frac{1}{\epsilon_\alpha + \epsilon_\gamma - \epsilon_m - \epsilon_\beta}$$

$$\times V_{\beta\beta, \gamma n} \frac{1}{\epsilon_\alpha + \epsilon_\beta - \epsilon_m - \epsilon_n} V_{mn, \alpha\beta} \quad (\text{B1})$$

actually holds. Let us expand  $\psi_{ik}$  and  $\omega$  in powers of  $V$  as

$$\psi_{\alpha m} = \psi_{\alpha m}^{(0)} + \psi_{\alpha m}^{(1)} + \dots,$$

$$\psi_{m\alpha} = \psi_{m\alpha}^{(0)} + \psi_{m\alpha}^{(1)} + \dots, \quad (\text{B2})$$

$$\omega = \omega^{(0)} + \omega^{(1)} + \dots,$$

which are inserted in Eq. (1.9). Then we have

$$\omega^{(0)} = \epsilon_{m_0} - \epsilon_{\alpha_0}, \quad \psi_{\alpha m}^{(0)} = \delta_{\alpha\alpha_0} \delta_{m m_0}, \quad \psi_{m\alpha}^{(0)} = 0,$$

$$\omega^{(1)} = V_{\alpha_0 m_0, m_0 \alpha_0}, \quad \psi_{\alpha m}^{(1)} = \frac{V_{\alpha m_0, m \alpha_0}}{\epsilon_\alpha - \epsilon_{\alpha_0} - \epsilon_m + \epsilon_{m_0}},$$

$$\text{for } (\alpha m) \neq (\alpha_0 m_0), \quad (\text{B3})$$

$$\psi_{\alpha_0 m_0}^{(1)} = 0,$$

$$\psi_{m\alpha}^{(1)} = -\frac{V_{m m_0, \alpha \alpha_0}}{\epsilon_{\alpha_0} + \epsilon_\alpha - \epsilon_{m_0} - \epsilon_m},$$

where  $(\alpha_0, m_0)$  is a specified state into which the system goes over in the absence of interaction. The symbol  $(\alpha m) \neq (\alpha_0 m_0)$  means that  $(\alpha = \alpha_0, m = m_0)$  is excluded. These values of  $\psi_{ik}$  are identical to what are obtained

directly from Eq. (3.14). We further have

$$\omega^{(2)} = \sum_{(\beta n) \neq (\alpha_0 m_0)} \frac{V_{\alpha_0 n, m_0 \beta} V_{\beta m_0 n \alpha_0}}{\epsilon_\beta - \epsilon_{\alpha_0} - \epsilon_n + \epsilon_{m_0}} + \sum_{\beta n} \frac{V_{\beta \alpha_0, m_0 n} V_{n m_0 \alpha_0 \beta}}{\epsilon_{\alpha_0} + \epsilon_\beta - \epsilon_{m_0} - \epsilon_n},$$

$$\psi_{\alpha m}^{(2)} = \frac{1}{\epsilon_\alpha - \epsilon_{\alpha_0} - \epsilon_n + \epsilon_{m_0}} \{ V_{\alpha n, m \beta} \psi_{\beta n}^{(1)} - V_{\beta \alpha, m n} \psi_{n \beta}^{(1)} - \omega^{(1)} \psi_{\alpha m}^{(1)} \}, \quad (\text{B4})$$

for  $(\alpha m) \neq (\alpha_0 m_0)$ ,

$$\psi_{\alpha_0 m_0}^{(2)} = 0,$$

$$\psi_{m \alpha}^{(2)} = \frac{1}{\epsilon_{\alpha_0} + \epsilon_\alpha - \epsilon_{m_0} - \epsilon_n} \{ V_{m \beta, \alpha n} \psi_{n \beta}^{(1)} - V_{m n, \beta \alpha} \psi_{\beta n}^{(1)} + \omega^{(1)} \psi_{m \alpha}^{(1)} \}.$$

It is to be noted that from Eqs. (B3) and (B4) we have

$$\begin{aligned} \frac{1}{2} \sum_{\alpha_0 m_0} \omega^{(0)} &= \frac{1}{2} \sum_{\alpha m} (\epsilon_m - \epsilon_\alpha), \\ \frac{1}{2} \sum_{\alpha_0 m_0} \omega^{(1)} &= \frac{1}{2} \sum_{\alpha m} V_{\alpha m, m \alpha}, \\ \frac{1}{2} \sum_{\alpha_0 m_0} \omega^{(2)} &= \frac{1}{2} \sum_{\alpha m} V_{\alpha \beta, m n} \frac{1}{\epsilon_\alpha + \epsilon_\beta - \epsilon_m - \epsilon_n} V_{m n, \alpha \beta}. \end{aligned} \quad (\text{B5})$$

The third-order term is given by

$$\omega^{(3)} = \sum_{\beta n} (V_{\alpha_0 n, m_0 \beta} \psi_{\beta n}^{(2)} - V_{\beta \alpha_0, m_0 n} \psi_{n \beta}^{(2)}), \quad (\text{B6})$$

and we get

$$\begin{aligned} \frac{1}{2} \sum_{\alpha_0 m_0} \omega^{(3)} &= \frac{1}{2} \sum_{\alpha m} \sum_{(\beta n) \neq (\alpha m)} \frac{V_{\alpha n, m \beta}}{\epsilon_\beta - \epsilon_\alpha - \epsilon_n + \epsilon_m} \\ &\times \left\{ \sum_{(\gamma p) \neq (\alpha m)} \frac{V_{\beta p, n \gamma} V_{\gamma m, p \alpha}}{\epsilon_\gamma - \epsilon_\alpha - \epsilon_p + \epsilon_m} \right. \\ &+ \sum_{\gamma p} \frac{V_{\gamma \beta, n p} V_{p m, \alpha \gamma}}{\epsilon_\alpha + \epsilon_\gamma - \epsilon_m - \epsilon_p} \frac{V_{\alpha m, m \alpha} V_{\beta m, n \alpha}}{\epsilon_\beta - \epsilon_\alpha - \epsilon_n + \epsilon_m} \left. \right\} \\ &+ \frac{1}{2} \sum_{\alpha m} \sum_{\beta n} \frac{V_{\beta \alpha, m n}}{\epsilon_\alpha + \epsilon_\beta - \epsilon_m - \epsilon_n} \left\{ \sum_{\gamma p} \frac{V_{n \gamma, \beta p} V_{p m, \alpha \gamma}}{\epsilon_\alpha + \epsilon_\gamma - \epsilon_m - \epsilon_n} \right. \\ &+ \sum_{(\gamma p) \neq (\alpha m)} \frac{V_{n p, \gamma \beta} V_{\gamma m, p \alpha}}{\epsilon_\gamma - \epsilon_\alpha - \epsilon_p + \epsilon_m} \\ &\left. + \frac{V_{\alpha m, m \alpha} V_{n m, \alpha \beta}}{\epsilon_\alpha - \epsilon_\beta - \epsilon_m - \epsilon_n} \right\}. \quad (\text{B7}) \end{aligned}$$

The first term in the first braces, after performing cyclic permutation  $(\alpha \beta \gamma)(m n p)$ , is seen just to cancel the third term there. The sum of the second terms in the first and second braces, after performing cyclic permutation  $(\alpha \beta \gamma)(m n p)$  in the latter, gives the minus of the third term in the second braces and the same expression as the first term there. Thus we see that Eq. (B1) actually holds.

## APPENDIX C

### Some Properties of Spin Matrices

The total spin  $\mathbf{S}$  of the system is given by

$$\mathbf{S} = \frac{1}{2} \int d^3 \mathbf{x} \psi^\dagger(\mathbf{x}) \boldsymbol{\sigma} \psi(\mathbf{x}), \quad (\text{C1})$$

where  $\psi(\mathbf{x})$  is now the two-component field operator. A vector quantity  $\mathbf{Q}$ , defined by

$$\mathbf{Q} = \int d^3 \mathbf{x} d^3 \mathbf{x}' f(\mathbf{x}, \mathbf{x}') \psi^\dagger(\mathbf{x}) \boldsymbol{\sigma} \psi(\mathbf{x}'), \quad (\text{C2})$$

where  $f(\mathbf{x}, \mathbf{x}')$  is a  $c$ -number function, satisfies the commutation relation

$$[Q_i, S_j] = i \sum_k \epsilon_{ijk} Q_k,$$

$$\epsilon_{123} = 1,$$

$$\epsilon_{ijk} = 1, \text{ if } (ijk) \text{ is an even permutation of } (123),$$

$$= -1, \text{ if } (ijk) \text{ is an odd permutation of } (123),$$

$$= 0, \text{ otherwise.} \quad (\text{C3})$$

By introducing

$$Q_\pm = Q_1 \pm Q_2, \quad (\text{C4})$$

we have

$$[Q_\pm, S_3] = \mp Q_\pm, \quad [Q_3, S_3] = 0, \quad (\text{C5})$$

which means that  $Q_+$  and  $Q_-$  are the operators to increase and decrease the  $z$  component of the total spin by one, respectively. Since we get

$$[Q_i, S^2] = -2Q_i + 2i \sum_{kj} \epsilon_{ijk} Q_k S_j, \quad (\text{C6})$$

the state obtained by operating  $Q_i$  on a paramagnetic state,  $\Psi_0$ , has the spin one, representing a triplet state:

$$\begin{aligned} S^2(Q_i \Psi_0) &= 1(1+1)(Q_i \Psi_0), \\ S_3(Q_\pm \Psi_0) &= \pm(Q_\pm \Psi_0), \quad S_3(Q_3 \Psi_0) = 0. \end{aligned} \quad (\text{C7})$$

A scalar quantity  $Q_0$  defined by replacing  $\boldsymbol{\sigma}$  in Eq. (C2) by 1 commutes with  $S_i$  and  $Q_0 \Psi_0$  has spin zero, representing a singlet state.

We shall next make use of an important identity

$$|\sigma\rangle \langle \sigma'| = \frac{1}{2} \sum_{\lambda=0}^3 \langle \sigma' | \sigma_\lambda | \sigma \rangle \sigma_\lambda, \quad (\text{C8})$$

which is proved by taking the trace of both sides after

multiplying  $\sigma_\mu$ . This identity leads to

$$c_{p\sigma}^\dagger c_{p'\sigma'} = \frac{1}{2} \sum_{\lambda=0}^3 \langle \sigma' | \sigma_\lambda | \sigma \rangle (c_{p\sigma}^\dagger \sigma_\lambda c_{p'\sigma'}), \quad (C9)$$

by means of which the alternative proof of Eq. (5.7) is given. Equation (5.4) is a direct consequence of Eq. (C8). Introducing Eq. (C9) into Eq. (3.1), we get

$$\begin{aligned} & \langle \mathbf{p}_1 \sigma_1 \mathbf{p}_2 \sigma_2 | G(i-i') | \mathbf{p}_3 \sigma_3 \mathbf{p}_4 \sigma_4 \rangle \\ &= -i \frac{1}{4} \sum_{\lambda, \mu=0}^3 \langle \sigma_2 \sigma_3 | \sigma_\lambda^{(1)} \sigma_\mu^{(2)} | \sigma_1 \sigma_4 \rangle \\ & \quad \times \langle T [c_{p_1}^\dagger(i) \sigma_\lambda c_{p_2}(i) c_{p_4}^\dagger(i') \sigma_\mu c_{p_3}(i')] \rangle. \quad (C10) \end{aligned}$$

Because of Eq. (C7), the terms with  $\lambda \neq \mu$  vanish on the right-hand side if we refer to the paramagnetic ground state; this proves Eq. (5.8).

We shall now prove Eq. (5.20). For  $n=1$ , we have

$$\begin{aligned} & \langle \mathbf{p} \sigma_1 \mathbf{p} + \mathbf{q} \sigma_2 | [G^{(0)}(\omega) V] | \mathbf{p}' \sigma_3 \mathbf{p}' + \mathbf{q} \sigma_4 \rangle \\ &= \frac{1}{4} \sum_{\mathbf{p}' \sigma_5 \sigma_6 \lambda} \langle \sigma_2 \sigma_5 | \sigma_\lambda^{(1)} \sigma_\lambda^{(3)} | \sigma_1 \sigma_6 \rangle \langle \mathbf{p} | G_q^{(0)}(\omega) | \mathbf{p}' \rangle \\ & \quad \times \{ \langle \sigma_6 \sigma_3 | \sigma_5 \sigma_4 \rangle \langle \mathbf{p}' | V_q^s | \mathbf{p}' \rangle \\ & \quad + \langle \sigma_6 \sigma_3 | \boldsymbol{\sigma}^{(3)} \cdot \boldsymbol{\sigma}^{(2)} | \sigma_5 \sigma_4 \rangle \langle \mathbf{p}' | V_q^t | \mathbf{p}' \rangle \} \\ &= \frac{1}{2} \delta_{\sigma_1 \sigma_2} \delta_{\sigma_3 \sigma_4} \langle \mathbf{p} | G_q^{(0)}(\omega) V_q^s | \mathbf{p}' \rangle \\ & \quad + \frac{1}{2} \langle \sigma_2 \sigma_3 | \boldsymbol{\sigma}^{(1)} \cdot \boldsymbol{\sigma}^{(2)} | \sigma_1 \sigma_4 \rangle \langle \mathbf{p} | G_q^{(0)}(\omega) V_q^t | \mathbf{p}' \rangle, \quad (C11) \end{aligned}$$

where use has been made of

$$\text{Tr} \{ \sigma_\lambda \sigma_\mu \} = 2 \delta_{\lambda\mu}. \quad (C12)$$

This proof is sufficient to see that if Eq. (5.20) is valid for  $n$ , it is for  $n+1$ . Therefore by mathematical induction, Eq. (5.20) holds for any  $n \geq 1$ .

## Fluxoid Conservation by Superconducting Thin Film Rings\*

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A torque method for measuring the persistent current in superconducting rings has been used to investigate the conservation of the fluxoid originally predicted by London. The fluxoid through a superconducting ring is composed of two parts, one describing the mechanical angular momentum of the electrons and the other the magnetic flux trapped by the ring. The mechanical angular momentum depends on the penetration depth  $\lambda$  and therefore on the temperature. If the fluxoid is conserved, temperature variations should alter the balance between the mechanical and electromagnetic angular momenta. As a consequence, the amount of trapped flux, and hence the persistent current, should vary with temperature even though the ring remains at all times entirely within the pure superconducting state with zero resistance. Very thin films of tin have shown experimentally a decrease in persistent current with increasing temperature and an increase with decreasing temperature which agree with that to be expected on the basis of the fluxoid conservation predicted by London.

### I. INTRODUCTION

THE possibility of inducing persistent circulating currents in superconducting rings is one of the most intriguing and least understood consequences of the vanishing of electrical resistivity in superconductors. Such a persistent current loop possesses a magnetic moment and holds "trapped" a magnetic flux equal to the product of the self-inductance of the ring and the persistent current. While the current-carrying state is by no means the ground state of the system it is nevertheless extraordinarily stable. The earliest investigations of persistent currents were in fact directed toward use of this stability as a means of establishing an upper limit on the possible resistivity of the superconducting state.

Much recent interest has centered on investigation of the suggestion, first made by London, that the "fluxoid" or action integral, taken around the ring, of the canonical momentum of the superconducting electrons should be both conserved and quantized. The fluxoid contains one term in the mechanical angular momentum of the electrons and one in the magnetic flux trapped by the ring. In typical experiments performed with superconducting rings, the mechanical angular-momentum term makes only an extremely small perturbation on the much larger magnetic flux term. It may be noted in passing that the situation in atoms is just the converse with the magnetic flux acting as the small perturbation (Zeeman effect). Several investigators<sup>1,2</sup> using cylinders for which the mechanical angular-momentum term

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<sup>1</sup> R. Doll and M. Näbauer, *Phys. Rev. Letters* **7**, 51 (1961).

<sup>2</sup> B. S. Deaver and W. M. Fairbank, *Phys. Rev. Letters* **7**, 43 (1961).