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Publication Date

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UCRL-8560

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Lawrence Radiation Laboratory
Berkeley, California

Contract No. W-7405-eng-48

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David J. Thouless

December 18, 1958

Printed for the U. S. Atomic Energy Commission

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ABSTRACT

We have examined the ground state of the many-fermion system, using perturbation theory, with particular attention to Brueckner's method. A study of the single-particle propagators in the ground state of the system sheds some light on the relation between the single-particle energies used, for example, in the optical model of nuclear reactions, and Brueckner's self-consistent energies. This leads naturally to the use of a renormalization factor to allow for propagation off the energy shell. It is possible to formulate the perturbation theory entirely in terms of graphs with no fermion self-energy parts, and this method is used to examine the approximations used for this problem, and to relate more closely the calculations of the ground-state energy and of other properties of the ground state.

* Part of this work was included in a thesis submitted to the Cornell University Graduate Faculty in partial fulfillment of the requirements for the degree of Ph.D.

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1. INTRODUCTION

The method used by Brueckner and Gammel¹ for the nuclear many-body problem involves the determination of an effective interaction between particles, where the equation for the effective interaction has as its kernel a term given by a self-consistency requirement. The precise definition of this self-consistent energy denominator gives rise to a number of difficulties, in particular the off-energy-shell propagation problem, which was treated rather elaborately by Brueckner and Gammel.¹ This definition was discussed at some length in an earlier paper,² hereafter referred to as I, and the role of the self-consistency condition was examined. A rather different approach is used here, which considerably simplifies the discussion, and which leads to a clearer definition of the self-consistent energy. A similar approach to this problem has also been used by Prange and Klein.³

We use the time-dependent form of perturbation theory, and consider the propagators of single-particle excited states. In this paper, as in I, extensive use is made of the diagrammatic representation of perturbation theory introduced by Goldstone,⁴ and the notation here is the same as the notation explained in I.

To illustrate the use of this method, the Brueckner approximation is rederived, in a slightly altered and analytically much simpler form. The approximation involved in the use of a self-consistent energy denominator as a propagator is then simply displayed. The inclusion of the terms contributing to the single-particle energies, which were neglected by Brueckner and Gammel¹

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and discussed in detail in I and a number of other papers,⁵ makes the formulae less simple, but still manageable in an approximate form. A way of deriving the equations by a method similar to the perturbation theory developed in I, with the expansion in powers of the reaction matrix instead of the potential, is sketched in Section 6.

In Section 7 an attempt is made to obtain an approximation for the one-particle propagators; it is then shown how the properties of the propagators themselves, given by Galitskii and Migdal in a recent paper,⁶ can be used to find the ground-state energy in a more suitable manner than was possible by use of the linked-cluster expansion derived by Goldstone.⁴

2. TIME-DEPENDENT PERTURBATION THEORY

The time-dependent form of perturbation theory for a stationary-state problem was used by Goldstone in his original justification of the Brueckner theory,⁴ and its relation to the time-independent form has been clearly displayed in a recent paper by Bloch.⁷ It is equivalent to the time-independent form, but there are some results which it gives much more readily.

In this discussion, the unperturbed Hamiltonian will be taken to be just the kinetic energy operator, since the addition of a Hartree potential to the unperturbed Hamiltonian and its subtraction from the perturbation (the scheme used throughout I) is here an unnecessary complication. The perturbation is the interaction between the particles, and it will be treated by a Rayleigh-Schrodinger type of expansion. In the evaluation of the expectation value of some operator in the true ground state Ψ , a sum over graphs will have to be made, and the important feature of the time-dependent form is that each element of the graph contributes an independent factor. In the time-dependent theory, each vertex pair of the graph is labeled with a time t ,

and a particle line going from t_1 to t_2 gives a factor of $i \exp[i T(m)(t_1 - t_2)]$ for $t_2 > t_1$, and a factor of zero for $t_2 \leq t_1$; $T(m)$ is the kinetic energy of a particle of momentum m . A hole line from t_1 to t_2 gives a factor of zero for $t_2 > t_1$, and a factor of $-i \exp[i T(l)(t_1 - t_2)]$ for $t_2 \leq t_1$. This function, associated with each particle and hole line, is called the unperturbed propagator. Each vertex pair (a pair of vertices at the same level connected by an interaction line) gives a matrix element of the potential v as a factor. Each closed loop gives a factor -1 . The independence of these factors is destroyed by the integration over the time variables which leads to the time-independent theory, and so the time-dependent form can be handled more easily for some purposes.

One important difference between the time-dependent and the time-independent forms is that the vertex pairs in the time-independent form had to be regarded as ordered, and all possible orderings had to be taken into account. The different orderings possible are now taken into account automatically by an integration over an infinite range of all but one of the time variables, and so the vertex pairs are no longer considered as ordered. This does mean that factors have to be included to avoid counting the same graph twice, as was explained by Bloch,⁷ if the graph is symmetrical.

3. BEHAVIOR OF THE PROPAGATORS

The propagator of a hole or particle state, the one-particle Green's function, is given by the sum of all linked graphs with the state in consideration as the one and only external line, if formal perturbation theory gives the true ground state. This is a function of the initial and final times, or rather of the time interval between them. If we start with the true ground state, which is equivalent to the physical vacuum in this scheme, create a particle (or a hole)

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at time t_1 , and allow the new state to propagate freely until time t_2 , then the propagator is equal to i times the scalar product of this state with the state obtained from the ground state by creating the particle. The formula for the propagator of a particle state of momentum m is

$$\begin{aligned}
 S(m, t_1 - t_2) &= i \langle \Psi | \eta_m \exp [i(H - E_0)(t_1 - t_2)] \eta_m^\dagger | \Psi \rangle, \text{ for } t_2 > t_1 \\
 &= -i \langle \Psi | \eta_m^\dagger \exp [-i(H - E_0)(t_1 - t_2)] \eta_m | \Psi \rangle, \text{ for } t_2 < t_1.
 \end{aligned} \tag{1}$$

Here E_0 is the ground-state energy, η_m is the annihilation operator for the particle state, and $\eta_m^\dagger$ is the creation operator. Similarly, if η_ℓ is the creation operator for a hole state of momentum ℓ and $\eta_\ell^\dagger$ is the annihilation operator, its propagator is

$$\begin{aligned}
 S(\ell, t_1 - t_2) &= i \langle \Psi | \eta_\ell \exp [i(H - E_0)(t_1 - t_2)] \eta_\ell^\dagger | \Psi \rangle, \text{ for } t_2 > t_1 \\
 &= -i \langle \Psi | \eta_\ell^\dagger \exp [-i(H - E_0)(t_1 - t_2)] \eta_\ell | \Psi \rangle, \text{ for } t_2 < t_1.
 \end{aligned} \tag{2}$$

Now we consider any quantity which is given as a sum of all the linked graphs with particular external lines, such as the expectation value of a one- or two-particle operator, or even the propagator itself. A fermion line in such a graph can be replaced by any of the graphs which give the propagator of that state, and such a replacement is called an insertion into the fermion line. The sum of all such insertions is found by using the true propagator instead of the unperturbed propagator in the evaluation of the graph. Any graph with external lines has a unique skeleton, which cannot be obtained from a lower-order graph by making these insertions, and so the quantity can be calculated by taking all possible skeletons, and using the true propagator instead of the unperturbed

propagator. The calculation of the propagators themselves by this means gives a problem of self-consistency, which could also be expressed by a set of nonlinear integral equations. The propagators are given as a sum of skeleton graphs, but the propagators to be used in the evaluation of the graphs are the ones which we are trying to calculate. This idealized self-consistency problem is extremely complicated, even if approximations are made, but it is easier to handle if some physical interpretation of the propagators is used.

It is not possible to evaluate the ground-state graphs, which have no external lines, by enumerating the skeletons and using the true propagator, since a graph with no external lines has no uniquely determined skeleton. If we divide such a graph into two parts connected to each other only by two fermion lines, it is impossible to determine which part is the insertion and which includes the skeleton. This fact leads to some complications in the next section, and makes it desirable to find the ground-state energy by a method which does not involve these vacuum-vacuum graphs.

The asymptotic behavior of the propagators for large values of the time interval gives the parameters of the optical model. We had started from the ground state of nuclear matter and added one more particle (or removed one particle). There may be transient effects, but eventually the particle behaves like a wave which decays exponentially in time, if the optical model is correct. The wavelength gives the real part of the optical potential, and the decay gives the imaginary part. In this way, we find what was called the excitation energy of the state in I.

The behavior of the propagators for small time intervals also gives important information about the properties of the ground state, as was shown by Galitskii and Migdal.⁶ It will be noticed that the propagators are continuous in time except at the origin, where they have a discontinuity

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equal to i . The limit of the propagator as the time interval approaches zero from below is just $-i$ times the occupation number of the state to which the propagator refers, since the operator part of the expression is the number operator of the state. This can be used to calculate the expectation value of any single-particle operator; in particular, the kinetic energy can be calculated. It was also shown that the potential energy can be calculated from the first derivative of the propagator at zero time interval for this sort of interaction, and the value of the ground-state energy is given by

$$2 E_0 = \sum_k \lim_{t \rightarrow -0} \left\{ (ik^2/2M)S(k, t) - S'(k, t) \right\}. \quad (3)$$

The sum in this expression goes over all states, whether hole or particle states.

The Fourier transform of the propagator is regular except in the neighborhood of the real axis, and has a positive real part in the upper half plane, and a negative real part in the lower half plane. It is defined by a cut just below the real axis to the right of the chemical potential and above the real axis to the left of the chemical potential.⁶

4. THE BRUECKNER APPROXIMATION

This method is illustrated by deriving a form of the Brueckner approximation; the equations derived are similar in form to those given in Appendix A of the paper by Brueckner and Gammel.¹ The derivation here avoids the off-energy-shell troubles by introducing an extra parameter, and also suggests a treatment of the off-energy-shell effect which should simplify the calculations.

We start by assuming that we have approximate single-particle propagators $R(m, t)$ for particles and $R(l, t)$ for holes which allow for certain insertions, but which still have the property that particles can propagate only forwards in time and holes can propagate only backwards in time; this is not so for the true

propagators S . We can then write the equations for the propagation of two particles (not holes) with multiple scatterings between them, and this is

$$L(t) = P R_2(t) + i \int_t^0 P R_2(t') v L(t - t') dt' . \quad (4)$$

Here P is the projection operator which allows only states above the Fermi sea, R_2 is the product of the two (approximate) single-particle propagators, v is the potential matrix, and L is the two-particle propagator allowing for mutual scattering; all these operators are supposed to be defined in the space of antisymmetric two-particle wave functions. The equation just means that either the two particles can propagate without scattering each other, or the last scattering can take place at time t' , where t' is between t and 0 .

The particle propagator is made to allow for the sort of insertions shown in Fig. 1. The integral equation which this propagator satisfies is

$$\begin{aligned} R(m, t) = & i \exp [i T(m)t] + i \int_t^0 dt' R(m, t') \sum_{\ell < k_F} \langle m \ell | v | m \ell \rangle \exp[i T(m)(t-t')] \\ & - i \int_t^0 dt' \int_t^{t'} dt'' R(m, t') \sum_{\ell < k_F} \langle m \ell | v L(t'' - t') v | m \ell \rangle R(\ell, t' - t'') \\ & \exp [i T(m)(t - t'')] . \end{aligned}$$

(5)

The first term on the right of this equation represents the fact that the particle may propagate freely with kinetic energy $T(m)$. The second term comes from the possibility that the first insertion may be like Fig. 1(a) at time t' between t and 0 , and the third term from the possibility that the first insertion may be like Fig. 1(b) or 1(c), starting at time t'' and ending at

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time t' , with an indefinite number of scatterings of the two particles between these times.

The types of insertions which we allow for in the definition of the hole propagators are like Figs. 2(a), 2(b), and 2(d). We do not allow for insertions like Fig. 2(c), where the insertion goes above the top of the line in which it was inserted. This somewhat arbitrary restriction serves to determine uniquely which is the skeleton and which the insertion in a graph like Fig. 3; it also incidentally leads to the lack of off-energy-shell effects for hole states, as will be shown. The integral equation which the hole propagator satisfies is

$$\begin{aligned}
 R(\ell, t) = & -i e^{iT(\ell)t} - i \int_0^t dt' R(\ell, t-t') \sum_{\ell' < k_F} \langle \ell \ell' | v | \ell \ell' \rangle e^{iT(\ell)t'} \\
 & + i \int_0^t dt'' \int_{-\infty}^{t''} dt' R(\ell, t-t') \sum_{\ell' < k_F} \langle \ell \ell' | v | (t' - t'')v | \ell \ell' \rangle R(\ell', t''-t') e^{iT(\ell)t''}.
 \end{aligned}
 \tag{6}$$

The interpretation of this equation is similar to that of Eq. (5); it is the upper limit of the first integration in the third term on the right of (6) which is the artificial restriction to avoid ambiguities. This equation has the solution

$$R(\ell, t) = -i e^{iM(\ell)t}, \tag{7}$$

where

$$\begin{aligned}
 M(\ell) = & T(\ell) + \sum_{\ell' < k_F} \langle \ell \ell' | v | \ell \ell' \rangle \\
 & + i \int_{-\infty}^0 \sum_{\ell' < k_F} \langle \ell \ell' | v L(t) v | \ell \ell' \rangle e^{-i[M(\ell) + M(\ell')]t} dt.
 \end{aligned}
 \tag{8}$$

Equations (4), (5), (7), and (8) give a form of Brueckner's equations with the self-consistency requirement implicit. They have a more familiar form when we take Fourier transforms. We use the notation

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$$f(E) = -i \int_{-\infty}^{\infty} f(t) e^{-iEt} dt \quad (9)$$

to emphasize the relation between a function and its Fourier transform.

Equation (4) becomes

$$L(E) = PR_2(E) - P R_2(E) v L(E) , \quad (10)$$

where $R_2(E)$ is the convolution of two single-particle propagators, multiplied by $i/2\pi$. We write

$$G(E) = v - v L(E) v , \quad (11)$$

which then satisfies

$$G(E) = v - v P R_2(E) G(E) . \quad (12)$$

This is then the reaction matrix which forms the basis of Brueckner's work.

Equations (5) and (8) become

$$\begin{aligned} R(m, E) &= \\ &= i [E - T(m) + i\epsilon]^{-1} + R(m, E) \sum_{\ell < k_F} \langle m \ell | G[E + M(\ell)] | m \ell \rangle [E - T(m) + i\epsilon]^{-1} \\ &= i [E - T(m) - \sum_{\ell < k_F} \langle m \ell | G[E + M(\ell)] | m \ell \rangle + i\epsilon]^{-1} \end{aligned} \quad (13)$$

$$M(\ell) = T(\ell) + \sum_{\ell' < k_F} \langle \ell \ell' | G[M(\ell) + M(\ell')] | \ell \ell' \rangle . \quad (14)$$

In Eq. (13), ϵ is a positive number which tends to zero.

The off-energy-shell effect is exhibited by the dependence on E of the right side of Eq. (13), since E appears in the argument of the G matrix there.

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If we could solve the coupled set of Eqs (12), (13), and (14) we would have solved the Brueckner problem taking complete account of off-energy-shell effects. It looks as if we would have to solve the equations for all values of E , but in fact it is necessary only to solve for E greater than $2M(0)$, since we can use the analytic properties of the functions of E .

Both $R(m, E)$ and $G(E)$ are regular in the upper half plane.

$R(m, E)$ behaves asymptotically like iE^{-1} , and $G(E)$ like v ; $R(m, E)$ is pure imaginary for $E < M(k_F)$, and $G(E)$ is Hermitian for $E < 2M(k_F)$. To show these conditions are consistent, we use the relation

$$\text{Im } R(m, E) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{\text{Re } R(m, E')}{E - E'} dE' \quad (15)$$

This can be used to rewrite the two-particle propagator

$$\begin{aligned} \langle m_1 \ m_2 | R_2(E) | m_1 \ m_2 \rangle &= \\ &= -\frac{1}{2\pi i} \int_{-\infty}^{\infty} R(m_1, E') R(m_2, E - E') dE' \\ &= -\frac{1}{\pi^2} \mathcal{P} \int_{M(k_F)}^{\infty} \int_{M(k_F)}^{\infty} \frac{\text{Re } R(m_1, E') \text{Re } R(m_2, E'')}{E - E' - E''} dE' dE'' \\ &\quad + \frac{i}{\pi} \int_{M(k_F)}^{E - M(k_F)} \text{Re } R(m_2, E') \text{Re } R(m_2, E - E') dE' \quad , \end{aligned} \quad (16)$$

which shows immediately that $R_2(E)$ is real for $E < 2M(k_F)$, and so $G(E)$ is Hermitian. This also means that G can be calculated from Eq. (12) if only the real parts of the propagators are known for all values of $E > M(k_F)$. These in turn can be calculated if $G(E)$ is known for all $E > M(k_F) + M(0)$. To

solve (14), which is also required for self-consistency, $G(E)$ has to be known down to $E = 2M(0)$. The problem has been completely solved if the Eqs. (12), (13), (14), and (16) have been solved for all $E > 2M(0)$.

The ground-state energy is calculated in the usual way as a sum of diagonal elements of the kinetic energy operator and of G between states in the Fermi sea. It can therefore be directly obtained from the solutions of Eq. (14).

5. SIMPLIFICATION OF THE SELF-CONSISTENCY CONDITION

Equation (13) suggests an approximation which would simplify the calculation considerably, while keeping the better treatment of the off-energy-shell effect. It seems likely that the most important part of the propagator is where the denominator is small, and the real part has a zero given by

$$M(m) = T(m) + \sum_{\ell < k_F} \text{Re} \langle m \ell | G [M(m) + M(\ell)] | m \ell \rangle, \quad (17)$$

which is in the same form as Eq. (14). If we keep just the first two terms of the Taylor-series expansion of the matrix element of G about this zero, we get the propagator in the approximate form

$$R(m, E) = i \zeta(m) [E - M(m) + i \Gamma(m)]^{-1}, \quad (18)$$

where

$$\zeta(m) = \left\{ 1 - \sum_{\ell < k_F} \langle m \ell | G' [M(m) + M(\ell)] | m \ell \rangle \right\}^{-1}, \quad (19)$$

$$\Gamma(m) = - \zeta(m) \sum_{\ell < k_F} \text{Im} \langle m \ell | G [M(m) + M(\ell)] | m \ell \rangle. \quad (20)$$

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Substitution of Eq. (18) in (12) with the help of (15) gives

$$G(E) = v + \sum_{m_1 m_2 > k_F} v \begin{vmatrix} m_1 & m_2 \end{vmatrix} \frac{\xi(m_1) \xi(m_2)}{E - M(m_1) - M(m_2) + i\Gamma(m_1) + i\Gamma(m_2)} \langle m_1 m_2 | G(E) \rangle. \quad (21)$$

This equation must then be solved, and tested for self-consistency in (19) and (20).

The ground-state energy is found by substituting the solutions in (14). The sum in (21) is over all distinct pairs of particle states.

In this way the Brueckner equations are obtained in a form which allows approximately for off-energy-shell propagation. The renormalization factors ξ perform this task, and the derivative of $G(E)$ has to be known if one is to calculate ξ . It is not necessary, once the derivative is known, to calculate G off the energy shell, although the calculation may give a check on the reliability of the approximation (18).

It was pointed out in I and in a number of other papers⁵ that there are important terms neglected in the Brueckner approximation which contribute to the single-particle energies, and which should be taken into account in a self-consistent calculation. If these are taken into account the hole propagators are no longer pure exponentials, because of the appearance of off-energy-shell effects; the integral equations then become more complicated. The approximation (18) can, however, still be used, both for particle and hole propagators, to make the equations manageable. This is not treated in detail here, since a similar procedure is used in Section 7.

6. EXPANSION IN POWERS OF THE REACTION MATRIX

The method developed in I allows a formal expansion of the potential v in powers of the reaction matrix G to be made in the perturbation series, even if the expansion of v does not converge, so long as the resulting

perturbation expansion of the energy in powers of G converges. This result is used to express the expansion carried out in Sections 4 and 5 in terms of G instead of in terms of v . To be definite, we take $G(E)$ to be defined by Eq. (21), although some other definition could be used in a similar manner.

This G is a function of E , and so its Fourier transform is a function of the time interval t . The v which is used in the time-dependent perturbation theory is an instantaneous interaction of two particles, and has no reference to a time interval. To avoid the difficulty of expressing v in terms of G , we invent a noninstantaneous interaction which is, in fact, equal to $i v \delta(t)$. This function $v(t)$ can be expanded as a series in $G(t)$ by iteration of the Fourier transform of Eq. (21),

$$v(t) = G(t) + \sum_{m_1 m_2 > k_F} \int_t^0 dt' \int_{t'}^0 dt'' v(t-t') |m_1 m_2\rangle \zeta(m_1) \zeta(m_2) \\ \times e^{i[M(m_1) + M(m_2) - i\Gamma(m_1) - i\Gamma(m_2)](t' - t'')} \langle m_1 m_2 | G(t'') . \quad (22)$$

This method can be used to give a time-dependent perturbation expansion in terms of an interaction G smeared out in time, and it should be used if the potential is singular. As in I, the self-consistency requirement is reduced to the requirement that certain terms in the perturbation series should vanish or be small.

7. CALCULATION OF THE PROPAGATORS

The methods introduced in the first part of this paper are now used to calculate the propagators for a system of strongly interacting fermions, using a reaction matrix as the basis of the expansion. Approximate integral equations

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are written down for the propagators, which are the true propagators, not the restricted propagators used for the evaluation of the ground-state energy in Section 4. The graphs which were shown in I to be important for the evaluation of the excitation energy are all included.

The propagator of a state k has the form

$$S(k, E) = i [E - K_1(k, E) - K_2(k, E)]^{-1}, \quad (23)$$

where K_1 is a function of E regular in the upper half plane, and K_2 is regular in the lower half plane. Both functions go to a constant value at infinity. K_1 is defined by a cut just below the real axis from μ to $+\infty$, and K_2 by a cut just above the real axis from $-\infty$ to μ , where μ is the chemical potential. We also have

$$\begin{aligned} K_1(E^*) &= K_1^*(E), \\ K_2(E^*) &= K_2^*(E), \end{aligned} \quad (24)$$

except near the cuts. These properties follow from the form of the propagator,⁶ which is, from the Fourier transform of Eq. (1) or (2),

$$\begin{aligned} S(k, E) &= S_1(k, E) + S_2(k, E), \\ S_1(k, E) &= i \langle \Psi | \eta_k (E + E_0 - H + i\epsilon)^{-1} \eta_k^\dagger | \Psi \rangle, \\ S_2(k, E) &= i \langle \Psi | \eta_k^\dagger (E - E_0 + H - i\epsilon)^{-1} \eta_k | \Psi \rangle. \end{aligned} \quad (25)$$

We have here split the propagator into a part regular in the upper half plane and a part regular in the lower half plane, denoted respectively by S_1 and S_2 ; this is very convenient later.

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The propagators are calculated by summing over the skeleton graphs. It is assumed at first that the asymptotic behavior of the states for long times is like that of a hole for momentum $\ell < k_F$, and like that of a particle for momentum $m > k_F$. This means that we can solve the equations

$$\begin{aligned} E(\ell) &= K_1[\ell, E(\ell)] + \text{Re } K_2[\ell, E(\ell)] , \\ E(m) &= \text{Re } K_1[m, E(m)] + K_2[m, E(m)] \end{aligned} \quad (26)$$

to get the real parts of the excitation energies, and find the small imaginary parts by the equations

$$\begin{aligned} \Gamma(\ell) &= \zeta(\ell) \text{Im } K_2[\ell, E(\ell)] , \\ \Gamma(m) &= -\zeta(m) \text{Im } K_1[m, E(m)] , \end{aligned} \quad (27)$$

where

$$\zeta(k) = \{ 1 - K_1'[k, E(k)] - K_2'[k, E(k)] \}^{-1} . \quad (28)$$

We then expand the propagators by iterating the equation

$$\begin{aligned} S(k, E) &= i \zeta(k) \{ E - E(k) \mp i \Gamma(k) \}^{-1} \\ &= \zeta(k) \{ E - E(k) \mp i \Gamma(k) \}^{-1} [E - K_1(E) - K_2(E) \\ &\quad - \zeta(k)^{-1} \{ E - E(k) \mp i \Gamma(k) \}] S(k, E) , \end{aligned} \quad (29)$$

or, alternatively,

$$\begin{aligned} S(k, E) &= i \{ E - E(k) \mp i \Gamma(k) \}^{-1} \\ &= \{ E - E(k) \mp i \Gamma(k) \}^{-1} \{ E(k) \pm i \Gamma(k) - K_1(k, E) - K_2(k, E) \} S(k, E) . \end{aligned} \quad (30)$$

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For either of these expansions to converge at all points along the real axis, it is necessary to include the imaginary part of the energy, as we have done here, and to use approximately the correct excitation energy. Such convergence has not been shown to be necessary, but it does certainly give more freedom for possible reorderings of the perturbation series. We assume generally that the quantity in square brackets in Eq. (29) can be analytically continued across the cut, and that it vanishes and has zero derivative at $E = E(k) \pm i \Gamma(k)$.

The reaction matrix G we use is taken to satisfy Eqs. (21) and (22), with $M(m)$ replaced by $E(m)$. The lowest-order graphs for a particle state are those shown in Fig. 4. Figure 4(c) comes from the first iteration of Eq. (22), and cancels with a part of Fig. 4(b). The integral equation which includes all these graphs is

$$\begin{aligned}
 S(m, E) = & \int_{-\infty}^0 e^{iT(m)t - iEt} dt - \int_{-\infty}^0 dt_1 \int_{-\infty}^0 dt_2 \int_{-\infty}^0 dt_3 \\
 & S(m, t_3) \sum_{k_1} \langle m k_1 | G(t_2) | m k_1 \rangle S(k_1, -t_2) e^{iT(m)t_1 - iE(t_1 + t_2 + t_3)} \\
 & - \int_{-\infty}^0 dt_1 \int_{-\infty}^0 dt_2 \int_{-\infty}^0 dt_3 \int_{-\infty}^0 dt_4 \int_{-\infty}^0 dt_5 S(m, t_5) \sum_{k_1} \sum_{k_2 k_3} \langle m k_1 | G(t_4) | k_2 k_3 \rangle \\
 & S(k_1, -t_1 - t_2 - t_3) S(k_2, t_3) S(k_3, t_3) \langle k_2 k_3 | G(t_2) | m k_1 \rangle e^{iT(m)t_1 - iE(t_1 + t_2 + t_3 + t_4 + t_5)} \\
 & - \int_{-\infty}^0 dt_1 \int_{-\infty}^0 dt_2 \int_{-\infty}^0 dt_3 \int_{-\infty}^0 dt_4 \int_{-\infty}^0 dt_5 S(m, t_5) \sum_{k_1} \sum_{m_1 m_2 > k_F} \\
 & \langle m k_1 | G(t_4) | m_1 m_2 \rangle S(k_1, -t_2 - t_3 - t_4) \zeta(m_1) \zeta(m_2) \\
 & e^{i[E(m_1) + E(m_2) - i\Gamma(m_1) - i\Gamma(m_2)] t_3} \langle m_1 m_2 | G(t_2) | m k \rangle \\
 & e^{iT(m)t_1 - iE(t_1 + t_2 + t_3 + t_4 + t_5)}
 \end{aligned} \tag{31}$$

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With the aid of Eq. (23), this can be written as

$$\begin{aligned}
 K_1(m, E) = & T(m) - (2\pi)^{-1} \sum_{k_1} \int_{-\infty}^{\infty} \langle m k_1 | G(E_1) | m k_1 \rangle S_2(k_1, E_1 - E) dE_1 \\
 & + (2\pi)^{-2} i \sum_{k_1} \sum_{k_2 k_3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} | \langle m k_1 | G(E_1 + E_2) | k_2 k_3 \rangle |^2 \\
 & \times [S_2(k_1, E_1 + E_2 - E) S_1(k_2, E_1) S_1(k_3, E_2) + S_2(k_1, E_1 + E_2 - E) S_2(k_2, E_1) S_2(k_3, E_2)] dE_1 dE_2 \\
 & + (2\pi)^{-1} \sum_{k_1} \sum_{m_1 m_2 > k_F} \int_{-\infty}^{\infty} | \langle m k_1 | G(E_1) | k_2 k_3 \rangle |^2 S_2(k_1, E_1 - E) \\
 & \zeta(m_1) \zeta(m_2) [E - M(m_1) - M(m_2) + i \Gamma(m_1) + i \Gamma(m_2)]^{-1} dE_1
 \end{aligned}
 \tag{32}$$

$$\begin{aligned}
 K_2(m, E) = & (2\pi)^{-2} i \sum_{k_1} \sum_{k_2 k_3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} | \langle m k_1 | G(E_1 + E_2) | m_1 m_2 \rangle |^2 \\
 & S_1(k_1, E_1 + E_2 - E) S_2(k_2, E_1) S_2(k_3, E_2) dE_1 dE_2 .
 \end{aligned}
 \tag{33}$$

Exactly the same equation can be written for a hole state.

8. CALCULATION OF OBSERVABLE QUANTITIES

If the propagators are known, physical observables can be calculated.

The form of the propagator given by Eqs. (32) and (33) has very little justification, and the existence of a singularity of G near the Fermi surface

makes it doubtful that the approximation is useful in that neighborhood.⁸ For this reason we demonstrate how the excitation energy would be given by such a propagator, for comparison with the results obtained in I, and merely outline how other quantities of interest would be obtained; detailed expressions for these other quantities are quite easy to obtain, but do not seem to be of much value.

The excitation energy and damping are obtained by substitution of Eqs. (32) and (33) in (26) and (27). To evaluate this expression, it is necessary to expand the propagators on the right of Eqs. (32) and (33) by means of (29) or (30). Equation (29) should give the more rapid convergence, except that successive terms in its iteration all behave like E^{-1} as E goes to infinity. If there is a contribution to the integral being evaluated from infinity--or, in other words, unless there are further negative powers of E in the integrand--this expansion of the propagator is unsuitable because of the successive contributions at infinity. This difficulty can be avoided by using Eq. (30) to get $S(k, E)$ multiplied by a negative power of E , and then obtaining further terms in the expansion by iteration of Eq. (29).

To evaluate Eqs. (32) and (33) it is possible to use the iteration of (29) for all the terms except the second term on the right of (32), where it is necessary first to use (30); we keep two terms in the expansion of this particular term, and keep only the first term in the expansions of all the other terms. We thus get

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$$\begin{aligned}
K_1(k, E) &= T(k) + \sum_{\ell < k_F} \langle k \ell | G[E + E(\ell) + i\Gamma(\ell)] | k \ell \rangle \\
&- (2\pi)^{-1} i \sum_{\ell < k_F} \xi(\ell) \int_{-\infty}^{\infty} \langle k \ell | G(E_1) | k \ell \rangle \{ E_1 - E - E(\ell) - i\Gamma(\ell) \}^{-2} \\
&\times \{ K_1(\ell, E_1 - E) + K_2(\ell, E_1 - E) - E(\ell) - i\Gamma(\ell) \} dE_1 \\
&- (2\pi)^{-1} i \sum_{m > k_F} \xi(m) \int_{-\infty}^{\infty} \langle k m | G(E_1) | k m \rangle \{ E_1 - E - E(m) + i\Gamma(m) \}^{-2} \\
&\times K_2(m, E_1 - E) dE_1 + \sum_{\ell_1 < k_F} \sum_{\ell_2 \ell_3 < k_F} \xi(\ell_1) \xi(\ell_2) \xi(\ell_3) \\
&\times \left\{ \left| \langle k \ell_1 | G[E(\ell_2) + E(\ell_3) + i\Gamma(\ell_2) + i\Gamma(\ell_3)] | \ell_2 \ell_3 \rangle \right|^2 \right. \\
&\quad \left. - \left| \langle k \ell_1 | G[E + E(\ell_1) + i\Gamma(\ell_1)] | \ell_2 \ell_3 \rangle \right|^2 \right\} \\
&\times \{ E + E(\ell_1) - E(\ell_2) - E(\ell_3) + i\Gamma(\ell_1) - i\Gamma(\ell_2) - i\Gamma(\ell_3) \}^{-1} \quad (34)
\end{aligned}$$

$$\begin{aligned}
K_2(k, E) &= \sum_{m > k_F} \sum_{\ell_1 \ell_2 < k_F} \frac{\xi(m) \xi(\ell_1) \xi(\ell_2) \left| \langle k m | G[E(\ell_1) + E(\ell_2) + i\Gamma(\ell_1) + i\Gamma(\ell_2)] | \ell_1 \ell_2 \rangle \right|^2}{E + E(m) - E(\ell_1) - E(\ell_2) - i\Gamma(m) - i\Gamma(\ell_1) - i\Gamma(\ell_2)} \\
&\quad (35)
\end{aligned}$$

With some further approximations, it is possible to get an expression similar to that derived in I for the excitation energy and damping. The final term in Eq. (34) can be discarded, since it involves the difference between the squares of

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two G matrix elements with different arguments, and so is essentially of third order (we do keep some third-order terms, but these have a different structure, as will be seen). For the same reason, when we substitute Eq. (35) in (34), we see that the part of the third term on the right involving K_2 approximately cancels and can be discarded. Finally, we replace K_1 in Eq. (34) by its lowest-order approximation, which is linear in G , and use the expression for G' which is given by differentiating (21), which is

$$G'(E) = - \sum_{m_1 m_2 > k_F} G(E) | m_1 m_2 \rangle \frac{\zeta(m_1) \zeta(m_2)}{[E - E(m_1) - E(m_2) + i\Gamma(m_1) + i\Gamma(m_2)]^2} \langle m_1 m_2 | G(E) . \quad (36)$$

All this gives the excitation energy and damping as

$$\begin{aligned} E(k) \pm i\Gamma(k) &= T(k) + \sum_{\ell < k_F} \langle k \ell | G[E(k) + E(\ell) \pm i\Gamma(k) + i\Gamma(\ell)] | k \ell \rangle \\ &+ \sum_{\ell_1 \ell_2 < k_F} \sum_{m_1 m_2 > k_F} \frac{\zeta(\ell_1) \zeta(\ell_2) \zeta(m_1) \zeta(m_2)}{[E(k) + E(\ell_1) \pm i\Gamma(k) + i\Gamma(\ell_1) + E(\ell_2) + i\Gamma(\ell_2) - E(m_1) - E(m_2) - i\Gamma(m_1) - i\Gamma(m_2)]^2} \\ &\times \left\{ \langle k m_1 | G[E(k) + E(m_1) \pm i\Gamma(k) - i\Gamma(m_1)] | k m_1 \rangle \right. \\ &\quad \left. - \langle k \ell_1 | G[E(k) + E(\ell_1) \pm i\Gamma(k) + i\Gamma(\ell_1)] | k \ell_1 \rangle \right\} \\ &\times \{ E(m_1) + E(m_2) - E(\ell_1) - E(\ell_2) - i\Gamma(\ell_1) - i\Gamma(\ell_2) - i\Gamma(m_1) - i\Gamma(m_2) \}^{-2} \\ &+ \sum_{m > k_F} \sum_{\ell_1 \ell_2 < k_F} \frac{\zeta(m) \zeta(\ell_1) \zeta(\ell_2)}{[E(k) + E(m) \pm i\Gamma(k) - i\Gamma(m) + E(\ell_1) + E(\ell_2) + i\Gamma(\ell_1) + i\Gamma(\ell_2) - E(m_1) - E(m_2) - i\Gamma(m_1) - i\Gamma(m_2)]^2} \\ &\times \{ E(k) + E(m) - E(\ell_1) - E(\ell_2) \pm i\Gamma(k) - i\Gamma(m) - i\Gamma(\ell_1) - i\Gamma(\ell_2) \}^{-1} . \quad (37) \end{aligned}$$

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The terms included here are just the terms which were considered in I, although they have here a slightly different form because of the use of complex energies and of the renormalization factor ζ .

To obtain expressions for other quantities of physical interest, we proceed in a similar way. The occupation number for a state is found by integrating the propagator round a contour in the upper half plane. Use of Eqs. (30) and (29) gives the lowest-order terms for hole and particle states as

$$n(l) = 1 + \zeta(l) K_1' [l, E(l) + i\Gamma(l)] , \quad (38)$$

$$n(m) = -\zeta(m) K_2' [m, E(m) - i\Gamma(m)] .$$

These expressions can be used to calculate the average kinetic energy. The total potential energy can be written, in a form equivalent to Eq. (3), as

$$- \frac{1}{4\pi} \sum_k \int [K_1(k, E) + K_2(k, E) - k^2/2M] S(k, E) dE , \quad (39)$$

where the integral is taken along the infinite semicircle in the upper half plane. The total energy is, to lowest order,

$$E_0 = \sum_{l < k_F} \frac{l^2}{2M} + \sum_{l_1 l_2 < k_F} \langle l_1 l_2 | G[E(l) + E(l')] | l_1 l_2 \rangle , \quad (40)$$

which is the expression usually used in the calculations.

In general, the method of enumerating and evaluating higher-order terms in the perturbation expansion for a quantity is the following. First we take only skeleton graphs, and then we have to use the expansions of the propagators to evaluate these. In any line of a skeleton graph we can make any number of

insertions, corresponding to terms in the iteration of Eq. (29). For each insertion made, we must subtract its contributions to the excitation energy and to the renormalization factor; in time-dependent form, these subtractions are like δ and δ' functions of time.

9. CONCLUSIONS

The reformulation of the perturbation expansion in terms of graphs with no fermion self-energy parts has been shown to lead to some simplification, particularly because of the natural way in which the "excitation energies" and renormalization factors occur in approximations, rather than the "model energies," which are affected by off-energy-shell effects. This expansion, moreover, should still be useful even if the approximation used for the propagators, the quasi-particle assumption, is invalid. In order to study a system for which the quasi-particle assumption is invalid, it is necessary to study with particular care propagators in the neighborhood of the Fermi surface. The recent theories of superconductivity should be very helpful in making such a study.

FIGURE CAPTIONS

Figure 1: Some insertions allowed for in the definition (5) of the particle propagator $R(m, t)$.

Figure 2: Some possible insertions in a hole line. Figures 2(a), 2(b) and 2(d) are allowed for in the definition (6) of the hole propagator $R(l, t)$, but 2(c) is not.

Figure 3: An example of a ground state energy graph in which the distinction between the skeleton graph and the insertion is arbitrary.

Figure 4: The lowest order skeleton graphs used for evaluating the propagator $S(m, E)$ by Eq. (31).

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Fig. 1

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Fig. 2

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Fig. 3

(a)

(b)

(c)

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Fig. 4

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