Properties of the One-Particle Green's Function for Nonuniform Many-Fermion Systems*

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(Received 24 May 1962)

In this paper we discuss some general properties of the one-particle Green's function, for nonuniform many-fermion systems and the associated single-particle interpretation of physical properties of such systems. We consider, in particular, the ground-state energy, the density of particles in the ground state, and the single-particle excitation spectrum. The investigation is restricted to the case of a static external field and a system at zero temperature. Various general approximation methods are studied starting from one in which the self-energy operator is replaced by an Hermitian and energy-independent operator.

1. INTRODUCTION

BY now, the theory of the Green's function approach to the analysis of uniform many-particle systems has been highly developed through the work of many authors.[1–6] In contrast, the extension of the theory to nonuniform systems, even in the simplest case of a static external potential, has only recently received attention[7–11] and has not yet been treated in a comprehensive manner.

It is true that the generalization of results to the nonuniform case usually turns out to be straightforward. One can fairly say that most of the hard questions—those connected with the specifically many-particle aspects of the problem—have already been answered by treating the uniform case.

Nevertheless, for the purposes of practical calculations on nonuniform systems and their physical interpretation, it is convenient to start from the more general formalism rather than modify the special case. Moreover, certain new qualitative features do arise for nonuniform systems, for example the occurrence of bound single-particle excitations in the presence of an attractive potential even though the interparticle forces are repulsive. In this case, one is concerned with the behavior of the one-particle Green's function alone.

It was, in fact, an example of just this kind—in connection with a perturbative calculation for a dense infinite electron gas in the presence of a point-positive charge[12]—that first drew the author's attention to the problems arising in the Green's function approach to nonuniform systems and to the incomplete nature of the existing treatment of the subject.

For the above reasons, we have thought it worthwhile to emphasize here some general features of the analysis of nonuniform many-fermion systems in terms of properties of the one-particle Green's function, for the case of a static external potential. In the following paper, some of these results and concepts are applied to the above-mentioned problem of the single-particle excitation spectrum of a dense electron gas with a positive point charge.

Let us recall that the one-particle Green's function is defined by

$$G(x,x')=G(x,t;x't')=-i\langle T\{\psi(x)\psi^\dagger(x')\}\rangle. \quad (1)$$

Here, $\psi(x)$ and $\psi^\dagger(x')$ are second quantized Heisenberg operators at the space-time points x,x'; T is the time-ordering operator and the brackets denote an expectation value with respect to the ground state of the many-body system.[13,14] $\psi(x)$ obeys the equation of motion[15]

$$-i\frac{d}{dt}\psi(x)=[H,\psi(x)], \quad (2)$$

where H is the Hamiltonian of the many-particle system.

In the case we are considering, H has the form

$$H=\int d^3x\,\psi^\dagger(x)[-\frac{\nabla_x^2}{2m}+V(x)]\psi(x)$$
$$+\tfrac{1}{2}\int\int d^3x d^3x'\,\psi^\dagger(x)\psi^\dagger(x')v(x-x')\psi(x')\psi(x), \quad (3)$$

* This research was supported in part by the U. S. Atomic Energy Commission.

[1] V. M. Galitskii and A. B. Migdal, J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 139 (1958); V. M. Galitskii, *ibid.* **34**, 151 (1958) [translations: Soviet Phys.—JETP **7**, 96 and 104 (1958)].

[2] P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959).

[3] A. Klein and R. Prange, Phys. Rev. **112**, 994 (1958).

[4] D. V. Dubois, Ann. Phys. (New York) **7**, 174 (1958); **8**, 24 (1959).

[5] V. Bonch-Bruevich and S. Kogan, Ann. Phys. (New York) **9**, 125 (1960).

[6] T. Kato, T. Kobayashi and M. Namiki, Suppl. Progr. Theoret. Phys. (Kyoto) No. 15, 3–60 (1960).

[7] The nonuniform case is discussed briefly in the fundamental papers of P. Martin and J. Schwinger (reference 2) and T. Kato, T. Kobayashi, and M. Namiki (reference 6). Some of the results of the present paper are closely related to those obtained in the article of Kato, Kobayashi, and Namiki.

[8] J. S. Langer, Phys. Rev. **124**, 997 (1961).

[9] J. S. Langer, Phys. Rev. **124**, 1003 (1961); **120**, 714 (1960).

[10] A. Abrikosov, J. Exptl. Theoret. Phys. (U.S.S.R.) **41**, 569 (1961); [translation: Soviet Phys.—JETP **14**, 408 (1962)].

[11] G. Baraff and S. Borowitz, Phys. Rev. **121**, 1704 (1961); G. Baraff, *ibid.* **123**, 2087 (1961).

[12] A. J. Layzer, Bull. Am. Phys. Soc. **6**, 447 (1961).

[13] For systems with degenerate ground states, we define the bracket symbol as including an additional average over the various degenerate ground states.

[14] Spin indices are suppressed. For spin-independent forces, G is diagonal in the spin coordinates and the diagonal elements are equal.

[15] We take $\hbar=1$.

where $v(x-x')$ is the interparticle potential and $V(x)$ is a static external potential.

It is sometimes convenient to regard G as an operator in four-dimensional space

$$G(x,t;x't')=\langle xt|G|x't'\rangle. \quad (4)$$

It is well known that the one-particle Green's function determines several important properties of the many-body system. For example, the density of particles at a given point of space and the ground-state energy are given (for fermions) by the expressions

$$\rho(x)=-iG(x,x+)\equiv -i\lim_{t'\to t+0} G(x,t;x,t'), \quad (5)$$

$$E_0=(-i)^{\frac{1}{2}}\int d^3r \lim_{x'\to x,\ t'\to t+0}\left[i\frac{\partial}{\partial t}-\frac{\nabla_x^2}{2m}+V(x)\right] \times G(x,t;x't'), \quad (6)$$

where $V(x)$ is the external potential.

$G(x,x')$ satisfies a very complicated inhomogeneous integro-differential equation of the form

$$\left[i\frac{\partial}{\partial t}+\frac{\nabla_x^2}{2m}-V(x)\right]G(x,x') - \int d^4z\,\Sigma(x,z)G(z,x')=\delta^4(x-x'), \quad (7)$$

where Σ is the so-called self-energy operator. Σ may be written in closed form by expressing it as a functional of $G(x,x')$ itself and the interaction potential and introducing a functional differentiation with respect to the external potential. This closed form of the equation is due to Schwinger in relativistic field theory and is usually called there the Schwinger equation for the one-particle Green's function.[16-18] The expression appropriate to the nonrelativistic many-body system with two-body interaction $v(x-x')$ has been obtained by Martin and Schwinger[2,19] and is given below in a slightly different form

$$V(x)\delta^4(x-z)+\Sigma(x,z)=\delta^4(x-z)\langle U(x)\rangle+M(x,z), \quad (8)$$

where

$$\langle U(x)\rangle\equiv U(x)-i\int d^3x''\,v(x,x'')G(x'',x'') \equiv U(x)+P(x), \quad (9)$$

$$t''=t+0,$$

and

$$M(x,z)=-i\int d^3x''\int d^4y\,v(x,x'')G(x,y)\frac{\delta G^{-1}(y,z)}{\delta U(x'')}. \quad (10)$$

The function $U(x)$ is an artificial time-dependent "source" which is to be set equal to the actual (static) external potential $V(x)$, following the functional differentiation.

A simple derivation of (7)-(10), of a conventional type,[17,18,5] proceeds through the functional differentiation with respect to the external source potential $U(x)$ of the important expression for $G(x,x')$ in the interaction representation.[20,21] The latter is of the general form:

$$\langle T\{\psi(x)\psi^\dagger(x')\}\rangle=\langle T\{\psi_I(x)\psi_I^\dagger(x')S\}\rangle_I/\langle S\rangle. \quad (11)$$

The subscript I refers to the interaction representation defined by arbitrarily breaking up the exact Hamiltonian H into "unperturbed" and "interacting" (Hermitian) parts, H_0 and H_1:

$$H_{\rm int}=H-H_0. \quad (12)$$

Accordingly, the expectation value on the right-hand side of (11) is with respect to the ground state of the unperturbed Hamiltonian, H_0. The symbol S in (11) refers to the "S matrix"

$$S=T\exp i\int_{-\infty}^{\infty} H_{\rm int}(t)dt, \quad (13)$$

where $H_{\rm int}(t)$ is the interaction Hamiltonian in the interaction representation.

To derive (7) one chooses

$$H_{\rm int}=\int\psi^\dagger(x)U(x)\psi(x)d^4x.$$

As an alternative to the closed form (7)-(10), Σ can be expanded in an infinite set of Feynman diagrams.[1,3,4,6] This can be thought of as a perturbation expansion of the Schwinger equation. (The structure of the diagrammatic expansion of Σ and the Feynman rules are for convenience reviewed in Sec. III of the present paper.)

A more conventional derivation of the Feynman diagram expansion is to use (11) once more, together with Wick's rules, this time with H_0 set equal to a suitable independent-particle Hamiltonian, usually the free-particle Hamiltonian. (This is the case considered in Sec. III).

[16] J. Schwinger, Proc. Natl. Acad. Sci. **37**, 452, 455 (1951)

[17] J. Anderson, Phys. Rev. **94**, 703 (1954).

[18] N. N. Bogoloubov and D. V. Shirkov, *Introduction to the Theory of Quantized Fields* (Interscience Publishers, Inc., New York, 1959), (translation from Russian), Chap. 5.

[19] A more detailed discussion of this equation and a much simpler derivation have been given by Kato, Kobayashi, and Namiki (reference 6). Still another derivation is indicated here.

[20] M. Gell-Mann and F. Low, Phys. Rev. **84**, 350 (1951).

[21] This relation is usually proved by making use of an adiabatic switching on the interaction. A physically more satisfactory limiting procedure which does not employ the adiabatic hypothesis is to go to the temperature zero limit of the analogous formula for the "temperature-propagator" formalism, in which the time variable is "rotated" to imaginary values, and then to go back to the time variables. The relation between the two formalisms has been discussed by A. Abrikosov, L. Gor'kov, and I. Dzyaloshinski, Soviet Phys.—JETP **36**, 636 (1959), who have also shown that in perturbation theory the result of this limiting procedure is the same as the usual interpretation of (11). [See also, J. Luttinger and J. Ward, Phys. Rev. **118**, 1417 (1960).] I would like to thank Professor B. Zumino for calling my attention to some of these points. From the above considerations, it would appear also that in the case of degenerate ground states, formula (11) should remain true provided that the bracket symbol includes an average over the degenerate ground states. (This is in accord with footnote 13).

Whether one uses a closed form for Σ or an infinite set of Feynman diagrams, the exact solution for the Green's function is a pretty hopeless task and one must resort, except in trivial examples such as the case of no interaction, to approximate methods, some of which are discussed here. The simplest of these is to expand Σ in Feynman diagrams involving powers of the interaction and also of the external source and then to keep only the lowest set of these diagrams. This is essentially the method used in the calculation of the following paper.[22]

Another important but harder to define piece of physical information provided by $G(x,x')$, one that is central to the investigation of the following paper, is the spectrum (and wave functions) of the so-called single-particle excitations; that is, the energies and lifetimes (and wave functions) of metastable quasi-particles or holes added to the ground state.

This information is supplied by the eigenvalues and eigenfunctions of the *homogeneous* equation corresponding to Eq. (7). A discussion of the relation of the Green's function approach to this concept has been given by Galitskii and Migdal,[1] Kato, Kobayashi, and Namiki[6] and others.[2–5] Further comments for the nonuniform case are given in the next section of the present paper along with a discussion of other aspects of the single particle picture of many-fermion system.

A "realistic" discussion of the concept of single-particle excitations would have to take into account the method of external excitation of the system. (See for example Low,[23] Englesberg,[24] and Glick and Ferrel.[25])

Such a discussion must necessarily be different for different concrete cases though, for general reasons, one expects that the energies and lifetimes of well-separated quasi-stable levels of the system correspond, at least approximately, to resonance energies and widths for external excitation, independently of the particular mode of excitation (cf. Dirac,[26] Brenig and Haag[27]).

Two general types of excitations may be distinguished: those in which the number of fermions is conserved, as in the stimulation of the system by a time-dependent external field, and those in which the number of fermions changes, say by ± 1, as in β decay or capture in the medium of an electron gas. In the latter case, the one-particle Green's function may be expected to yield direct physical information. In the former case one is more properly dealing with "resonances" of the two-particle Green's function but some of these resonances, of the noncollective type, may be regarded, at least approximately, as "products" of single-particle resonances (cf. Galitskii and Migdal[1]).

2. SOME REMARKS ON THE SINGLE-PARTICLE INTERPRETATION OF MANY-FERMION SYSTEMS

We wish to consider now some general properties of the one-particle Green's function $G(x,x')$ and their relation to physical properties of the many-particle system. We defer to the following section a detailed statement concerning the structure of the self-energy operator, Σ. The properties we have in mind are conveniently expressed in terms of single-particle approximations which we define below. The lowest order approximation, in addition to providing a conceptually clear model for the many-particle system, affords a starting point for more exact treatments as is shown.

In the case of a time-independent external potential, $G(x,x')$ and $\Sigma(x,x')$ are functions only of the time difference $\tau \equiv t'-t$ and are, therefore, diagonal in w space, where w is the energy variable conjugate to the time.[28] We introduce the diagonal elements $G(w)$, $\Sigma(w)$ by the relations

$$\begin{aligned}\langle xw|G|x'w'\rangle &= \langle x|G(w)|x'\rangle\delta(w-w'),\\ \langle xw|\Sigma|x'w'\rangle &= \langle x|\Sigma(w)|x'\rangle\delta(w-w').\end{aligned} \tag{14}$$

$G(w)$ is also the Fourier transform of $G(\tau)$

$$G(\tau)=\frac{1}{2\pi}\int dw\, e^{iw\tau}G(w), \tag{15}$$

where

$$\langle x|G(t'-t)|x'\rangle \equiv \langle xt|G|x't'\rangle. \tag{16}$$

From (7), $G(w)$ satisfies the operator equation, in ordinary 3-dimensional space,

$$[w-L(w)]G(w)=1, \tag{17}$$

where

$$L(w)\equiv (p^2/2m)+V(x)+\Sigma(w). \tag{18}$$

The corresponding homogeneous equation resembles a time-independent Schrödinger equation. It can, in fact, be interpreted as an effective Schrödinger equation for a single fermion moving in the field of the others. Mathematically, the "effective potential," $V(x)+\Sigma(w)$, differs from that of the usual type of Schrödinger equation in that $\Sigma(w)$ is non-Hermitian and w dependent or "energy dependent."[29] (It is also nonlocal in position space but this is not important for the present discussion.)

Information concerning the analytic properties of the exact operator $G(w)$ as a function of w is provided by a Lehmann type of spectral decomposition of $G(w)$, in the original form (1), in the many-particle Hilbert space according to a complete set of intermediate states of $N+1$ and $N-1$ particles.[1,2,5,6,8–10] This work shows

[22] However, due to the long range of the Coulomb potential it is necessary in that problem to sum over an infinite set of diagrams in order to avoid the "infrared divergence problem at small momentum transfers.

[23] F. Low, Phys. Rev. **88**, 53 (1952).

[24] S. Englesberg, Phys. Rev. **123**, 1130 (1961).

[25] A. Glick and R. Ferrel, Ann. Phys. (New York) **11**, 359 (1960).

[26] P. A. M. Dirac, *Principles of Quantum Mechanics* (Clarendon Press, Oxford, 1958), 4th ed., Chap. 8.

[27] N. Brenig and R. Haag, Fortshr. Physik **7**, 183–242 (1959).

[28] That is, $\langle w|t\rangle = \exp(+iwt)$.

[29] The non-Hermitian nature of $\Sigma(w)$ is related to the decay of single-particle excitations.

that on the "physical sheet" of the w plane (defined by the spectral decomposition), the matrix elements of $G(w)$ have two branch cuts from $w=\mu+0$ to $+\infty$ and from $\mu-0$ to $-\infty$ and are elsewhere analytic. Here, μ is the exact chemical potential defined as the difference between the ground-state energies of the $N+1$ and N-particle systems for large N. The "physical contour" of the w integration, necessary to obtain the Fourier transform $G(\tau)$, is along the lower side of the left cut and the upper side of the right cut. The spectral decomposition shows also that the non-Hermitian and w-dependent properties of $\Sigma(w)$ are intimately related.[30]

The h Approximation

To get a first approximation to the solution of (17), it is convenient to introduce an approximation for $L(w)$ called h, which is, in fact, Hermitian and independent of w. The most suitable choice for h will depend on the nature of the particular problem under consideration and the range of w to be approximated. We shall not pursue this question further, except to remark that in lowest order perturbation theory, with respect to the interaction coupling constant, $L(w)$ is indeed Hermitian and independent of w (see next section).

Letting G_h be the corresponding approximation to G, we have formally $G_h=(w-h)^{-1}$. Of course, $G_h(w)$ is not completely specified until a final boundary condition is given. This amounts to selecting a contour for the w integration. We do this by adding to h an infinitesimal imaginary part which is negative or positive according to whether w is greater or less than μ. This choice of contour is in agreement with the physical contour for the w integration of the exact $G(w)$ on the physical sheet. The (approximate) self-consistency of this specification within the framework of the h approximation will later become clear.

The complete specification of our approximation is then

$$G(w)\simeq G_h(w)\equiv[w-h+i\epsilon(w)]^{-1}, \tag{19}$$

where[31]

$$\epsilon(u)\equiv\theta(w-\mu)-\theta(\mu-w). \tag{20}$$

With respect to h we can introduce a complete orthonormal set of eigenfunctions u_n with corresponding eigenvalues ϵ_n. (We assume that the system is enclosed in a finite but arbitrarily large volume so that the index n is denumerable.) Thus, we have

$$hu_n=\epsilon_n u_n. \tag{21}$$

$G(w)$ then admits the usual type of diagonal bilinear expansion in terms of u_n and ϵ_n[32]:

$$G_h(w)=\sum_n u_n\rangle\langle u_n[w-\epsilon_n+i\epsilon(w)]^{-1}. \tag{22}$$

That is,

$$\langle x|G_h(w)|x'\rangle=\sum_n u_n(x)u_n^*(x')[w-\epsilon_n+i\epsilon(w)]^{-1}. \tag{23}$$

The spectrum of eigenvalues ϵ_n will have a quasi-continuous portion starting somewhere near $\epsilon_n=0$ and, if h has an attractive part, the spectrum may contain a discrete portion lying to the left of the quasi-continuous part and corresponding to bound single-particle states.[33]

The corresponding expression for $G_h(\tau)$ is a sum of oscillating terms

$$i\langle x|G_h(\tau)|x'\rangle=-\theta(\tau)\sum_{\epsilon_m<\mu}u_m(x)u_m^*(x')e^{i\epsilon_m\tau}+\theta(-\tau)\sum_{\epsilon_n>\mu}u_n(x)u_n^*(x')e^{i\epsilon_n\tau}. \tag{24}$$

Let us consider now expressions (5) and (6) for the number density $\rho(x)$ and the ground-state energy E_0. After a few elementary transformations, we obtain the following *exact* expressions for $\rho(x)$, E_0, and the total number of particles N.

$$E_0=\frac{1}{i}\frac{1}{2}\lim_{\tau\to+0}\mathrm{Tr}\left[-i\frac{d}{d\tau}+\frac{p^2}{2m}+V(x)\right]G(\tau)$$

$$=\frac{1}{2}\frac{1}{2\pi i}\int dw\, e^{iw0+}\,\mathrm{Tr}[w+p^2/2m+V(x)]G(w), \tag{25}$$

$$\rho(x)=\frac{1}{i}\lim_{\tau\to+0}\langle x|G(\tau)|x'\rangle=\frac{1}{2\pi i}\int dw\, e^{iw0+}\langle x|G(w)|x\rangle, \tag{26}$$

$$N=\int\rho(x)d^3x=\frac{1}{i}\lim_{\tau\to0+}\mathrm{Tr}G(\tau)=\frac{1}{2\pi i}\int dw\, e^{iw0+}\,\mathrm{Tr}G(w). \tag{27}$$

We have replaced the three-dimensional integration over coordinate space that occurs in the original expressions for E_0 and N by a trace operation, denoted by Tr. Replacing further the trace by a diagonal

[30] See the remarks at the end of this section. Physically speaking, the reason that the non-Hermitian and w-dependent properties of $\Sigma(w)$ are related is that the sign of the non-Hermitian part of the self-energy at a given w is associated with the direction of time for the decay of single-particle excitations of energy w, and holes (excitations of energy less than μ) propagate "backwards in time" [see Eq. (40)].

[31] Here $\theta(x)$ is the usual step function which assumes the values 0, 1 depending on whether x is less than or greater than unity.

[32] Instead of introducing the infinitesimal quantities $i\epsilon(w)$ to define the contour of the w integration, we could equally well modify the eigenvalues ϵ_n by the replacement $\epsilon_n\to\epsilon_n\pm i\eta$ where η is an infinitesimal positive quantity and the plus (minus) sign applies if μ is greater (less) than ϵ_n. This method is actually more general in that it leads to well-defined w integrations for products of the type $(w-\epsilon_n)^{-1}(w-u-\epsilon_{n'})^{-1}$ in cases where the $\epsilon(w)$ method leads to ambiguous expressions.

[33] This is the case in the problem of the following paper, where h includes a shielded Coulomb potential. The number of bound states is then finite. Another possible form of spectrum is the band structure which arises when there are several attractive centers.

summation with respect to the eigenfunctions u_n, we obtain the *exact* formulas:

$$E_0=\frac{1}{2\pi i}\left(\frac{1}{2}\right)\sum_n\int dw \times e^{iw0+}\langle n|[w+p^2/2m+V(x)]G(w)|n\rangle, \quad (28)$$

$$N=\frac{1}{2\pi i}\sum_n\int dw\, e^{iw0+}\langle n|G(w)|n\rangle. \quad (29)$$

We have also from (26)

$$\rho(x)=\sum_n\sum_{n'}u_n(x)u_{n'}^*(x)G_{nn'}, \quad (30)$$

where

$$G_{nn'}=\frac{1}{2\pi i}\int dw\, e^{iw0+}\langle n|G(w)|n'\rangle. \quad (31)$$

In the case of a uniform system with no external potential $\Sigma(w)$ is diagonal in momentum space, though, of course, still not Hermitian. Choosing plane-wave eigenstates $|p\rangle$ for the states $|n\rangle$ one obtains in that case well-known exact relations of the form (28) to (31) but with $G(w)$ replaced by its eigenvalue $G(w,p)$ and $G_{nn'}=G_{pp}\delta_{pp'}$.[1-6]

In the present nonuniform generalization, the momentum operator does not commute with $G(w)$ or $\Sigma(w)$ and we cannot specify a complete orthogonal set of states for which these operators are diagonal.[34]

Diagonalization is, of course, achieved in the h approximation. In this approximation, moreover, the w integration can be carried out easily and we obtain from (28)–(31):

$$E_0\simeq\sum_{\epsilon_n<\mu}\tfrac{1}{2}[\epsilon_n+\langle n|p^2/2m+V(x)|n\rangle], \quad (32)$$

$$N\simeq\sum_{\epsilon_n<\mu}1, \quad (33)$$

$$G_{nn'}\simeq\delta_{nn'}\theta(\mu-\epsilon_n). \quad (34)$$

These expressions are of the type one would expect in a single-particle picture of the many-fermion system. In particular, the expressions (32)–(34) for the ground-state energy or $\rho(x)$ in terms of single-particle states are of the same general form as in the Hartree-Fock approximation.[35] Indeed, the Hartree-Fock equation is a special case of the h approximation resulting from the approximation $\delta G^{-1}(y,z)/\delta U(x'')=-\delta^4(y-z)\delta^4(x-y)$ in the Schwinger equation, (7)–(10). This is a lowest order approximation for the quantity $\delta G^{-1}(y,z)/\delta U(x'')$ with respect to the interaction coupling constant.[36]

[34] For a spherically symmetric external potential $\Sigma(w)$ and $G(w)$ commute with the 3-space angular momentum operator $\mathbf{L}$ and are therefore diagonal with respect to L_z and L^2.

[35] See, for example, D. J. Thouless, *The Quantum Mechanics of Many-Body Systems* (Academic Press Inc., New York, 1961), Chap. I.

[36] For further remarks in this connection, see Sec. IV.

Single-Particle Excitations

To exhibit the relationship of the Green's function formalism to the concept of the single-particle excitations of the many-particle system, it is necessary to compare the expressions for $G(\tau)$ or $G(w)$ in three-dimensional space, involving the self-energy operator Σ, with the original defining expression (1) in the many-particle Hilbert space.

For this purpose, it is convenient to utilize an expansion of the wave-function operator $\psi(x)$ according to the complete orthonormal set u_n of eigenfunctions introduced in (21). Thus, we write

$$\psi(x)=\sum_k a_k u_k(x), \quad (35)$$

where the destruction operators a_k and their adjoints satisfy the anticommutation relations

$$[a_k,a_m^\dagger]_+=\delta_{km}. \quad (36)$$

Now, we have for the Green's function $G(\tau)$ and its transform $G(w)$ the following exact bilinear expressions:

$$G(x,x';\tau)=\sum_n\sum_{n'}u_n(x)u_{n'}^*(x')G_{nn'}(\tau), \quad (37)$$

$$G(x,x';w)=\sum_n\sum_{n'}u_n(x)u_{n'}^*(x')G_{nn'}(w). \quad (38)$$

$G_{nn'}$ can be expressed in two alternative forms. First, we have from (17)

$$G_{nn'}(w)=\langle n|[w-L(w)]^{-1}|n'\rangle. \quad (39)$$

Secondly, we have, using (35), from the defining Eq. (1) that

$$iG_{nn'}(\tau)=\theta(-\tau)\langle a_n e^{+i(H-E)\tau}a_{n'}^\dagger\rangle - \theta(\tau)\langle a_{n'}^\dagger e^{-i(H-E)\tau}a_n\rangle, \quad (40)$$

and, accordingly, from (15)

$$G_{nn'}(w)=-\langle a_n(H-E-w)^{-1}a_{n'}^\dagger\rangle + \langle a_{n'}^\dagger(H-E+w)^{-1}a_n\rangle. \quad (41)$$

We note, following Galitskii and Migdal,[1] that the diagonal element $\theta(-\tau)iG_{nn}(-\tau)$ is the probability amplitude that the system, if initially in the state $a_n^\dagger|\rangle$, with one particle in the state n added to the ground state will remain in that state after the time $-\tau$. A similar statement applies to $\theta(+\tau)G_{mm}(+\tau)$ with respect to the hole state $a_m|\rangle$. More generally, $\theta(-\tau)G_{n'n}(-\tau)$ is the probability amplitude for finding the system after the time $-\tau$ in the state $a_{n'}^\dagger|\rangle$ if initially it was in the state $a_n^\dagger|\rangle$ and similarly for hole to hole transitions.

Comparing (40) with (24) we see that *in the h approximation* single-particle or hole excitations $a_k^\dagger|\rangle$ or $a_m|\rangle$ are *stable*, and therefore eigenstates of H, and that $\epsilon_n(-\epsilon_m)$ is the energy difference between the ground-state energy of the system and the energy of the system with a single particle (hole) added in the state $k(m)$ to the ground state. In particular, the lowest added particle state corresponds to $\epsilon_n=\mu+0$ and,

therefore, is correctly determined as the energy difference between the ground state of the $N+1$ and N-particle systems.[37]

Furthermore, in this approximation a_n with $\epsilon_n > \mu$ or $a_m^\dagger$ with $\epsilon_m < \mu$ acting on the ground state gives zero. That is, the ground-state wave function, in this approximation, is an antisymmetrized product of the $u_n(x)$ with $\epsilon_n < \mu$ [there are N of these functions according to (33)].[38]

The Quasi-Particle Approximation

The h approximation has two important merits: It is diagonal in n,n' and it permits the w integration to be carried out in a simple manner, namely, by picking up residues of (simple) poles at $w=\epsilon_n$. These desirable features are retained, though with modified meanings, in a nonperturbative generalization of the h approximation usually called the quasi-particle (q-p) approximation, which allows for the instability of single-particle excitations by letting the spectrum of eigenvalues ϵ_n move into the complex plane.[39,1]

To define the q-p approximation more precisely, we first recall that in principle $G(w)$ admits of a diagonal bilinear expansion in the sets of eigenfunctions (assumed complete) $\phi_n(w), \psi_n(w)$ of $L(w)$ *and its adjoint* $L^\dagger(w)$ of the form,[40] for fixed w:

$$G(w)=\sum_n \phi_n(w)\rangle\langle\psi_n(w)[w-E_n(w)]^{-1}, \tag{42}$$

where

$$[L(w)-E_n(w)]\phi_n(w)=0, \tag{43a}$$

$$[L^\dagger(w)-E_m^*(w)]\psi_m(w)=0, \tag{43b}$$

and the sets (ϕ_n) and (ψ_n) are bi-orthogonal:

$$\langle\phi_m(w)|\psi_n(w)\rangle=\delta_{mn}. \tag{44}$$

In the spirit of the quasi-particle approximation, we shall *assume* that $G(w)$ has simple poles w_n lying near the real axis such that

$$w_n=E_n(w_n), \tag{45}$$

and that these simple poles form the dominant contribution to $G(w)$.[41] Thus, we neglect singularities due to the (possible) non-analytic form of $E_n(w)$, $\phi(w)$, or $\psi_n(w)$ as functions of w and also poles due to (possible) additional isolated roots of the equation $w=E_n(w)$. We assume also that w_n arises from a continuous displacement of the pole ϵ_n of the h approximation as the additional term $\lambda(L(w)-h)$ is "turned on," that is as λ grows from 0 to 1 continuously.

Furthermore, we shall assume that for $R(w_n)<\mu$ the imaginary part of w_n is positive and that for $R(w_n)>\mu$ it is negative, and that it is zero for $w=\mu$.[42]

Let us call the corresponding approximation to $G(w)$ $G_{\text{q-p}}(w)$. Then

$$G(w)\simeq G_{\text{q-p}}(w)=\sum_n g_n\phi_n\rangle\langle\psi_n(w-w_n)^{-1}, \tag{46}$$

where

$$\phi_n\equiv\phi_n(w_n), \tag{47a}$$

$$\psi_n\equiv\psi_n(w_n), \tag{47b}$$

$$g_n^{-1}=1-(d/dw)E_n(w)\,|_{w=w_n}. \tag{48}$$

g_n is the residue of $[w-E_n(w)]^{-1}$ at the pole $w_n=E_n(w_n)$. In terms of the time variable τ, $G(\tau)$ is a sum of damped exponentials:

$$iG(\tau)=\theta(-\tau)\sum_{R(\epsilon_n)>\mu} g_n\phi_n\rangle\langle\psi_n e^{iw_n\tau} - \theta(\tau)\sum_{R(\epsilon_n)<\mu} g_m\phi_m\rangle\langle\psi_n e^{iw_m\tau}. \tag{49}$$

The complex frequencies w_n are characteristic of the system and their real and imaginary parts may be interpreted as the energies (measured from the ground-state energy) and inverse lifetimes of metastable intermediate states of $N+1$ or $N-1$ particles.

The expressions for E_0, $\rho(x)$, and N in the q-p approximation as derived from (25) to (27) take a quite similar form to those in the h approximation given by (32)–(34). The differences are that the new "expectation values" have dual wave functions on the left and right instead of the same wave function and there is also an additional

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[37] The dual nature of the energies ϵ_n as excitation energies and as single-particle energies in the sense of (32) is well known in Hartree-Fock theory [D. J. Thouless, *The Quantum Mechanics of Many-Body Systems* (Academic Press Inc., New York, 1961), reference 35] and in the one-electron theory of solids, where it is usually known as Koopmans theorem. T. Koopmans, Physica **1**, 104, (1933); J. C. Phillips, Phys. Rev. **123**, 420 (1961).

[38] This interpretation of the h approximation in the many-particle space must itself be regarded as approximate. If one takes an antisymmetrized "ground state" of the form $g=\Pi_{m=1}^{N} a_m^\dagger|\rangle$ it is, in fact, impossible to choose the wave functions u_n such that the single-particle excitation states $a_m|g\rangle$, $a_n^\dagger|g\rangle$ are eigenstates of the *exact* Hamiltonian. Thouless has pointed out (reference 35) that if one merely diagonalizes H on the subspace of single-particle states $a_m|g\rangle$ and $a_n^\dagger|g\rangle$, one has already determined the wave functions u_n as solutions of the Hartree-Fock equations. But even when this is done, there will still be, in general, non-vanishing matrix elements of H between $a_n^\dagger|g$ and states of a higher (odd) number of excitations such as $a_r^\dagger a_s a_n^\dagger|g\rangle$.

[39] We refer to the review article of D. Pines for a further discussion of the quasi-particle approximation and for other references. (The concept was originally introduced by L. Landau.) D. Pines, *The Many-Body Problem* (W. A. Benjamin, Inc., New York, 1961) (collection).

[40] P. M. Morse and H. Fesbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, New York, 1953), Vol. 1, p. 884. I am indebted to Professor J. Percus for bringing this reference to my attention and for aid in rediscovering the bi-orthogonal expansion for Green's functions. Another derivation of (42) is as follows. Dropping the argument w of L, let us decompose L into its Hermitian and anti-Hermitian parts, L_1 and L_2: $L=L_1+iL_2$. Define the Hermitian operator $L(\lambda)=L_1+\lambda L_2$ for *real* λ. Then the Green's function $[w-L(\lambda)]^{-1}$ can be expanded in the usual diagonal bilinear expansion in terms of the eigenfunctions $\phi_n(\lambda)$, assumed complete, and (real) eigenvalues $E_n(\lambda)$. If we now "rotate" in this expansion λ to $+\lambda i$ in $\phi_n(\lambda)$, $\phi_n^*(\lambda)$, and $E_n(\lambda)$ and then set λ equal to unity we obtain the expansion (42) with the properties (43), (44).

[41] Since these poles of $G(w)$ lie off the real axis they are not on the physical sheet of the w plane but on a "second sheet" (or sheets). We assume, following Galitskii and Migdal (reference 1) that in the neighborhood of the real axis $G(w)$ on the physical sheet may be analytically continued onto the second sheet, across the branch cuts, such that the values of $G(w)$ on the physical contour agree with the values of $G(w)$ on the real axis of the second sheet.

[42] See the remarks at the end of this section.

factor of g_n for each state. We find, namely, that[43]

$$E_0(\text{q-p}) \simeq \sum_{R(\epsilon_n)<\mu} g_n \tfrac{1}{2}\left[w_n + \left\langle \psi_n \middle| \frac{p^2}{2m} + V(x) \middle| \phi_n \right\rangle \right], \quad (50)$$

$$N(\text{q-p}) \simeq \sum_{R(\epsilon_n)<\mu} g_n, \quad (51)$$

$$\rho(x)(\text{q-p}) \simeq \sum_{R(\epsilon_n)<\mu} g_n \phi_n(x) \psi_n^*(x). \quad (52)$$

If we calculate, in the usual manner, the eigenvalues w_n in lowest order perturbation theory, starting from the h approximation we obtain

$$w_n = \epsilon_n + W_n + i\Gamma_n, \quad (53)$$

where

$$W_n = RT_{nn}(\epsilon_n), \quad (54)$$

$$\Gamma_n = \text{Im}\, T_{nn}(\epsilon_n), \quad (55)$$

and

$$T_{nn'}(w) \equiv \langle n | L(w) - h | n' \rangle. \quad (56)$$

Similarly for the eigenfunctions ϕ_n and ψ_n in lowest order perturbation theory we obtain

$$\phi_n - u_n = \sum{}' \frac{T_{n'n}(\epsilon_n)}{\epsilon_n - \epsilon_{n'}} u_{n'}, \quad (57a)$$

$$\psi_n - u_n = \sum{}' \frac{T_{nn'}^*(\epsilon_n)}{\epsilon_n - \epsilon_{n'}} u_{n'}. \quad (57b)$$

Let us consider now the corresponding lowest order evaluation of the matrix elements $G_{nn'}$ of (37) and (38) within the framework of the q-p approximation. For the diagonal matrix elements G_{nn} we obtain[44] (for $\epsilon_n < \mu$ and $\tau > 0$)

$$iG_{nn}(\tau) \simeq -\bar{g}_n e^{-|\Gamma_n|\tau} e^{i(\epsilon_n + w_n)\tau}, \quad (58)$$

where

$$(\bar{g}_n)^{-1} = 1 - (d/dw)[T_{nn}(w)]_{w=\epsilon_n}. \quad (59)$$

For the nondiagonal elements $G_{nn'}$ one gets in the standard way for large times the familiar looking energy conserving transition rate[45]

$$(1/|\tau|)|G_{nn'}(\tau)|^2 \simeq 2\pi |T_{nn'}(\epsilon_n)|^2 \delta(\epsilon_n - \epsilon_{n'}). \quad (60)$$

[43] We have used the fact that $\text{Tr}\{A\rangle\langle B\} = \langle B|A\rangle$.

[44] Assuming that the interaction potential is proportional to a coupling constant g^2, the decay constant Γ_n is actually of order g^4 rather than g^2, in terms of the conventional perturbation expansion in powers of the coupling constant. This is because the non-Hermitian part, $\Sigma_2(w)$, of $\Sigma(w)$ is not present in lowest order. The lowest order Feynman graphs contributing to $\Sigma_2(w)$ are the "mass-operator" graphs M_f and M_g of Fig. 1. As is well known, these correspond to dissipation of the single-particle excitation through pair production out of the Fermi sea. This has been shown in detail by Kato, Kobayashi, and Namiki (reference 6). See also Dubois (reference 4).

[45] It is interesting to note that the rates $R_{nn'}$ and $R_{n'n}$ for the process $n \rightarrow n'$ and its inverse are not equal, due to the non-Hermitian part, Σ_2, of Σ. One finds that the difference $R_{nn'} - R_{n'n}$ is proportional to $\text{Im}\, M_{nn'}(\epsilon_n)(\Sigma_2)_{nn'}(\epsilon_n)$ where $M(w)$ is the Hermitian part of $L(w) - h$. This is of order g^6 in the coupling constant of interaction. (See footnote 44.)

Exact Perturbation Expansion

The lowest order perturbation results (58) and (60) can also be obtained by the expansion of $G(w)$ in terms of the unperturbed propagators $G_h \equiv [w - h + i\epsilon(w)]^{-1}$ provided that one assumes an exponential form for $G_{nn}(\tau)$. Thus, we have

$$G(w) = G_h + G_h(L(w) - h)G_h + \cdots, \quad (61)$$

and the first two terms of (61) give the same results (58) and (60).

The expansion (61) can, in principle, be used to determine the matrix elements of $G(w)$ to any degree of accuracy. The singularities due to the unperturbed propagators evidently lie on the real axis of the w plane. This is in agreement with the location of the singularities for the exact $G(w)$ on the physical sheet of the w plane. The contour of the w integration, for this expansion, specified by the infinitesimal imaginary quantity $i\epsilon(w)$, is in agreement with the physical contour along the real axis of the physical sheet, as defined earlier.

Spectral Properties of G

We conclude this section with a brief discussion of the relation of the spectral properties of $G(w)$ to the quasi-particle approximation for the nonuniform case. According to the usual spectral analysis, the diagonal elements $G_{nn}(\tau)$ of (40) can be written in the form[46]

$$G_{nn}(\tau) = -\frac{\theta(\tau)}{2\pi} \int_{-\infty}^{\mu} \Delta_{nn}^-(w) e^{iw\tau} dw + \frac{\theta(-\tau)}{2\pi} \int_{\mu}^{\infty} \Delta_{nn}^+(w) e^{iw\tau} dw, \quad (62)$$

where $\Delta_{nn}^-(\Delta_{nn}^+)$ is the discontinuity of $G_{nn}(w)$—upper minus lower values—across the left-hand (right-hand) cut on the real axis of the physical sheet of the w plane. $\Delta_{nn}^{\pm}$ has the properties that it is purely imaginary and, furthermore, $i\Delta_{nn}^{\pm}$ is positive:

$$i\Delta_{nn}^{\pm}(w) \equiv \rho_{nn}(w) \geq 0. \quad (63)$$

Indeed, from (41), $i\Delta_{nn'}(w)$ has the explicit form

$$i\Delta_{nn'}(w) = \pi\{\textstyle\sum_\alpha \langle a_n | N+1,\alpha\rangle\langle N+1,\alpha | a_{n'}^\dagger\rangle \delta(E_\alpha - E - w) + \sum_\beta \langle a_{n'}^\dagger | N-1,\beta\rangle\langle N-1,\beta | a_n\rangle \delta(E_\beta - E + w)\}.$$

For diagonal elements this yields the real positive expression[47]

$$\rho_{nn}(w) = i\Delta_{nn}(w) = \pi\{\textstyle\sum_\alpha |\langle N+1,\alpha | a_n^\dagger\rangle|^2 \delta(E_\alpha - E - w) + \sum_\beta |\langle N-1,\beta | a_n\rangle|^2 \delta(E_\beta - E + w)\}.$$

[46] This representation holds also for nondiagonal elements, but we are interested here mainly in the diagonal elements. The representation (62) follows immediately from a deformation of the physical contour to enclose the left or right-hand cut depending on the sign of τ, which determines whether the contour is closed from above or below.

[47] For nondiagonal elements, one can define the combinations $G_{nn'}' = G_{nn'} + G_{n'n}$ and $G_{nn'}'' = i(G_{nn'} - G_{n'n})$ for which the discontinuities are purely imaginary as in the diagonal case, but for which the corresponding $\rho_{nn'}$ are not necessarily positive.

The positive quantities ρ_{nn} are bounded by the relation

$$\int_{-\infty}^{\infty}\rho_{nn}(w)dw=2\pi, \tag{64}$$

which is a consequence of the equal time anticommutation relations applied to $G_{nn}(+0)-G_{nn}(-0)$.[48]

The discontinuity Δ can be expressed in terms of the anti-Hermitian part, $J(w)$ of $G(w)$. Thus, we write

$$G(w)=K(w)+iJ(w), \tag{65}$$

where

$$2K(w)=G(w)+G^{\dagger}(w)$$
$$=[w-L(w)]^{-1}+[w-L^{\dagger}(w)]^{-1}, \tag{66}$$

$$2J(w)=(-i)[G(w)-G^{\dagger}(w)]$$
$$=(-i)\{[w-L(w)]^{-1}-[w-L^{\dagger}(w)]^{-1}\}. \tag{67}$$

Then, we know that $K_{nn}(w)$, which is real, is continuous across the cuts and that

$$i\Delta_{nn}(w)=-2J_{nn}(w^{+})\geq 0, \tag{68}$$

where w^{+} denotes a value of w with an infinitesimal positive imaginary part.

Since the states n are arbitrary, it follows from (63) that for w *along the physical contour* of the physical sheet, or on the real axis of the second sheet,[41] $J(w)$ is a positive *operator*[49] for $w<\mu$ and a negative operator for $w>\mu$:

$$J(w)<0, \quad w>\mu, \tag{69a}$$

$$J(w)>0, \quad w<\mu. \tag{69b}$$

Furthermore, the matrix elements of $J(\mu)$ have been shown to vanish in every order of perturbation theory.[50,51]

Let us introduce also the Hermitian and anti-Hermitian parts Σ_1 and Σ_2 of the self-energy operator Σ:

$$\Sigma(w)=\Sigma_1(w)+i\Sigma_2(w). \tag{70}$$

Then, (69) implies also (for w on the physical contour of the physical sheet or on the real axis of the second sheet[41])

$$\Sigma_2(w)<0, \quad w>\mu, \tag{71a}$$

$$\Sigma_2(w)>0, \quad w<\mu. \tag{71b}$$

To prove (71) we multiply (67) on one side by $w-L(w)$ and on the other by $w-L^{\dagger}(w)$ to obtain

$$\Sigma_2(w)=[w-L^{\dagger}(w)]J(w)[w-L(w)], \tag{72}$$

or

$$\Sigma_2(w)=[G^{-1}]^{\dagger}J(w)G^{-1}. \tag{73}$$

Since for fixed w the expectation values of J are always, say, positive the same must be true of the combination on the right-hand side of (73). Furthermore, (73) shows that conversely (71) implies (69).

To show the relation of the above properties of $G(w)$ to the quasi-particle approximation, we first note that in the h approximation $\rho_{nn}(w)$ is simply $2\pi\delta(w-\epsilon_n)$ in agreement with (64). Comparing the spectral representation (62) for $G_{nn}(\tau)$ with the lowest order quasi-particle expression (58) [see also (49)] we see that they are in agreement provided that $\rho_{nn}(w)$ is narrowly peaked near ϵ_n at $w=\epsilon_n+W_n$ with a Lorentzian shape of width equal to Γ_n such that $|\Gamma_n/\epsilon_n|\ll 1$. Furthermore, (71) shows that the sign of the damping factor Γ_n in perturbation theory, as calculated from (55), comes out correctly, in accord with the *a priori* assumptions made in deriving the quasi-particle approximation.

3. STRUCTURE OF THE SELF-ENERGY OPERATOR

In this section we review briefly some essential facts concerning the structure of the self-energy operator in terms of Feynman diagrams.[1,3,4,6,18] At the same time we introduce a notation and a precise normalization that will be useful for the calculation of the following paper.

The Green's function $G(x,x')$ may be represented graphically as the sum of all connected Feynman diagrams with an electron line going from x to x' and it follows that the self-energy operator $\Sigma(x,x')$ is represented by the totality of strongly connected insertions, at x and x', in an electron line. By a "strongly connected" diagram in this context, we mean that the diagram cannot be split into two disconnected diagrams by breaking a single electron line.

The Feynman rules, in momentum space, for evaluating the "internal" portion of an arbitrary diagram for G or Σ, may be summarized in the following way: For every solid line labeled by p,w one has a factor $iG_0(p,w)$ where $G_0(p,w)$, the free-electron propagator, is given by

$$G_0(p,w)=\frac{\theta(p_F-p)}{w-p^2/2m-i\eta}+\frac{\theta(p-p_F)}{w-p^2/2m+i\eta}, \tag{74}$$

where p_F is the unperturbed Fermi momentum.[52]

For every horizontal dotted line labeled by q,p one has a factor $iv(q,w)=iv(q)$, the Fourier transform of the instantaneous interaction potential. A cross in an electron line represents the effect of the external source

[48] For nondiagonal elements the value of the corresponding integral must be zero.

[49] A positive operator is a Hermitian operator whose expectation values are always positive or equivalently whose eigenvalues are all positive. See F. Riesz and R. Sz.-Nagy, *Functional Analysis* (Frederick Ungar Company, New York, 1955), p. 262.

[50] J. Luttinger, Phys. Rev. 121, 942 (1961).

[51] J. S. Langer, reference 8.

[52] The discerning reader will note that due to the shift, $\delta\mu$, in the chemical potential caused by the interaction, the w integration in the definition (74) of $G_0(p,w)$ is not in accord with the physical contour. This well-known difficulty may be remedied by modifying the definition of G_0 in several ways: One can simply replace the contour of integration by the physical contour or one can shift the "unperturbed single-particle energies by the amount $\delta\mu(p^2/2m\rightarrow p^2/2m+\delta\mu)$ and perform the appropriate "mass-renormalization" subtractions. The latter procedure has the advantage that certain ambiguities associated with the singularity of the θ function at zero argument are eliminated. See J. Luttinger and J. Ward, Phys. Rev. 118, 1470 (1960); J. S. Langer, *ibid.* 120, 714 (1960).

potential and is accompanied by a factor $iV(q,w)=iV(q)\delta(w)$, where $V(q,w)$ is the Fourier transform of the (static) external potential. A closed loop has associated with it a minus sign and a factor $(2s+1)$ where s is the spin of the particle. (This is a simplification due to the spin independence of the interaction. In general, one has for closed loops a trace over the spin indices.) There is a factor of $(-i)^n$ for a diagram with n vertices.

At each vertex there is a four-dimensional delta function of momentum and energy conservation and a factor $(2\pi)^4$. One should integrate over all internal momenta and energy with a weight factor $d^3pdw/(2\pi)^4$.

In the above rules, the Fourier transform is normalized according to the definition

$$f(x)=\frac{1}{(2\pi)^4}\int d^4p\, f(p)e^{ip\cdot x}. \tag{75}$$

The final normalization necessary to obtain the operator $\Sigma(w)$ from the rules stated above is determined by the following additional prescription: Consider the subclass G' of diagrams of G with "external" lines labeled by p,w and p',w' and containing one and only one strongly connected insertion. Integrate over all momenta and energies except initial and final ones. The rules given above then yield the quantity

$$\begin{aligned}(2\pi)^4 i\langle pw|G'|p'w'\rangle&=(2\pi)^4 i\langle p|G'(w)|p'\rangle\delta(w-w')\\&=(2\pi)^4 iG_0(p,w)G_0(p',w')\langle p|\Sigma(w)|p'\rangle\delta(w-w').\end{aligned} \tag{76}$$

Diagrams for $\Sigma(x,x')$ fall naturally into two classes: those for which the insertion in an electron line is made at a single point $x=x'$, by a dotted line, and those for which the insertion is made at two distinct points x,x'. The former class of diagrams are called polarization diagrams and the totality of such diagrams will be called the polarization potential, P. Note that P is independent of w. Note also that P is a local potential in position space; that is, $P(x,x')=P(x)\delta^3(x-x')$. Some typical lowest order polarization diagrams are shown in Fig. 1 (a, b).

The polarization potential $P(x)$, in fact, agrees with the term $P(x)=\int v(x-x')\rho(x')d^3x'$ in the Schwinger equations (7)–(10), as may be verified by recalling that the sum of all closed loop electron diagrams at the point x is, in fact, the same as $\rho(x)$ (times the factor i). This clearly Hermitian term represents the "average classical field" potential acting on a single particle due to the average distribution of particles in the system, neglecting typical quantum effects associated with the Pauli principle and including an unwanted contribution from the density distribution of the particle itself.

The other category of diagrams of the general type shown in Fig. 1(c), corresponding to the term M of (8), are called mass operator or exchange diagrams (or potentials). The lowest order (second-order) diagram, Fig. 1(c) gives rise to the well-known lowest order exchange potential:

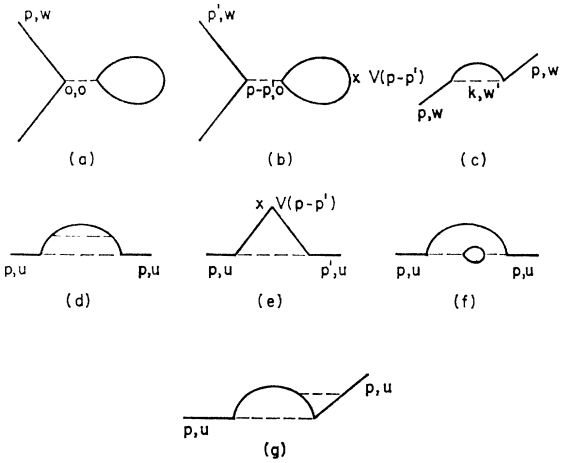

FIG. 1. Typical lowest order polarization diagrams (a), (b) and mass operator diagrams (c)–(g).

$$\begin{aligned}&\langle p|M_c|p'\rangle\\&\quad=(-)\frac{\delta^3(\rho-\rho')}{8\pi^3}\int d^3k\, v(k)\theta(p_F-|p-k|).\end{aligned} \tag{77}$$

Note that this lowest order diagram is Hermitian, w independent, and diagonal in momentum space (a function of $x-x'$ in position space). Higher order diagrams, however, are in general non-Hermitian, w dependent, and (incidentally) nondiagonal in momentum as well as position space. It is thus the mass operator part of the self-energy which is responsible for the unavoidably approximate nature of the h approximation discussed in the previous section.

4. SUMMARY AND DISCUSSION OF RESULTS

In the foregoing sections we have studied some mathematical properties of the one-particle Green's function $G(x,x')$ for nonuniform many-fermion systems and their implications for the single-particle interpretation of such physical properties as the ground-state energy, the density of particles in the ground state and single-particle excitations out of the ground state. For the most part, the results are generalizations of well-known counterparts for uniform systems. As we have seen, however, certain new problems arise, justifying a separate treatment of the more general nonuniform case.

We have taken as a starting point the exact non-homogeneous integro-differential equation for $G(x,x')$. This may be written in closed form [see Eqs. (7–10)] by introducing a functional differentiation with respect to an artificial time-dependent source U, which is to be set equal to the actual static external potential V, following the functional differentiation. The energy transform of this equation is of the operator form

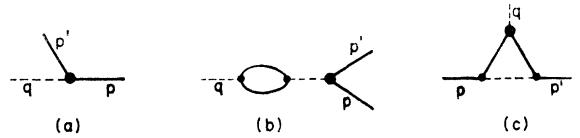

FIG. 2. Lowest order diagrams for the "improper vertex function $\partial G^{-1}/\partial U$. Diagram (a) is a simple point vertex, which yields the Hartree-Fock approximation.

$[L(w)-w]G(w)=1$, where $L(w)=\Sigma(w)+V$ and $\Sigma(w)$ is the so-called self-energy operator.

The corresponding homogeneous equation may be regarded as an effective Schrödinger equation for one-electron states, with $L(w)$ serving as an effective Hamiltonian. The non-Hermitian part $\Sigma_2(w)$ of $\Sigma(w)$ is associated with the instability of single-particle excitations. Indeed, in lowest order perturbation theory, the expectation value of $\Sigma_2(w)$ in the one-electron state in question is a measure of the inverse lifetime of the corresponding single-particle excitation. Consistently with this interpretation we have shown that for w greater (less) than μ, the exact chemical potential, $\Sigma_2(w)$ is a positive (negative) operator, which assures that the "direction of time" is that appropriate to particles or holes.

We have introduced a general and rather natural lowest order approximation, called the h approximation, in which $L(w)$ is replaced by an Hermitian and energy-independent operator, h. In the h approximation, single-particle excitations are *stable*.

The Hartree-Fock approximation was seen to be a special case of the h approximation in which the lowest order (with respect to the interaction) perturbation expression is employed for the "vertex function" $\partial G^{-1}/\partial U$ occurring in the closed expression (8)–(10) for the self-energy operator.

We remark here that this suggests a semiperturbative approximation scheme in which this vertex function is built up to any desired order of perturbation theory and the resultant nonlinear approximate equation for $G(x,x')$ is solved self-consistently after the manner of a Hartree-Fock equation. In this connection, we note that when written in the form (7)–(10), except for the quantity $\partial G^{-1}/\partial U$, $L(w)$ can be expressed as an operator functional of $G(w)$ alone. In particular, this is true of the polarization potential, as defined by (9), which in fact involves only the density of particles, the diagonal element of G in a position representation, (for equal times).

Feynman-diagramatically speaking, the expression $\partial G^{-1}/\partial U$ corresponds to an "improper" vertex which includes, in addition to the "proper" vertex, insertions in the adjacent dotted line. Lowest order diagrams for $\partial G^{-1}/\partial U$ are shown in diagrams (a), (b), and (c) of Fig. 2. These correspond respectively to the mass-operator diagrams (c), (f), and (g) of Fig. 1 with the important difference that in the present mass-operator diagrams the solid line exterior to the vertex should represent the unknown "exact" Green's function for which a solution is sought and which includes effects due to the interaction as well as effects due to the presence of the external source.

Analytic expressions, in momentum space, for the vertex diagrams (b) and (c) of Fig. 2 may be readily written down on the basis of related expressions given by Dubois[4] for the so-called density propagator, or bubble insertion in a dotted line. [Diagram (c) involves a straightforward modification of this treatment of the bubble insertion.]

We see that in our approximation scheme the lowest order is the Hartree-Fock approximation while the next order already goes beyond the h approximation and allows for the energy dependence of the effective Hamiltonian as well as for the instability of single-particle excitations.

The mathematical difficulties involved in solving the self-consistent equations of a given stage of the above approximation are similar to those involved in solving the Hartree-Fock equations, although new complications enter due to the non-Hermitian nature and energy dependence of the effective Hamiltonian. The question of the necessary mathematical treatment for this special approximation method is in fact related to some of the general formal developments of the preceding sections to the discussion of which we now return.

In the h approximation, the usual bilinear expansion of the Green's function affords a convenient explicit representation for $G(w)$ in terms of the eigenvalues and eigenfunctions of the homogeneous equation for $G(w)$. This is a sum over states expression with denominators $(w-\epsilon_n)$ where the ϵ_n are the one-electron eigenvalues. In the uniform case, where on symmetry grounds the eigenstates are plane wave states, this representation is valid even for the exact Green's function though the eigenvalues ϵ_n are w dependent. The resemblance to the h approximation is increased by employing the so-called quasi-particle approximation in which one assumes, as an approximation, that for each value of the momentum p, $G(w)$ has only the singularity of a simple isolated pole in the complex w plane, corresponding to an isolated complex root of the equation $w=\epsilon_n(w)$.

When one deals with the nonuniform case, this approach encounters a new obstacle: A complete orthogonal set of states diagonalizing the effective Hamiltonian, $L(w)$, cannot be given on the basis of symmetry alone.

We have proposed that one employ, to similar effect, the so-called bi-orthogonal expansion of $G(w)$ in terms of the eigenstates and eigenvalues of $L(w)$ itself and its *adjoint* operator L^+. (The biorthogonal expansion coincides with the usual bilinear expansion in the uniform case.) The quasi-particle approximation may then be introduced similarly to the uniform case: One assumes that $G(w)$ has only simple isolated poles in the complex w plane and that these "grow" out of *corresponding* poles of the h approximation, lying on the real

axis, as the non-Hermitian and w-dependent part of $L(w)$ is "turned on."

This representation allows one to maintain formally a single-particle interpretation of the basic physical properties of the system at the expense of introducing complex eigenvalues and non-orthogonal wave functions. Moreover, expectation values are replaced by "skew" expectation values involving also the dual wave function corresponding to the adjoint operator $L^+(w)$. [See Eqs. (50)–(52).] The imaginary part of an eigenvalue is, as usual, interpreted as the inverse lifetime of an associated single-particle excitation.

We emphasize that this formal use of the bi-orthogonal expansion and quasi-particle approximation is devoid of real content until a sufficiently careful analysis is made of the mathematical conditions necessary for its validity. In particular, as we have pointed out, the defining singularities of this expansion occur for values of w not on the "physical" sheet of the w plane, defined by a spectral decomposition of $G(w)$ in the many-particle Hilbert space, but rather on a hypothetical sheet (or sheets) defined by analytic continuation from the physical sheet across the branch cuts. It is necessary to prescribe the manner of this analytic continuation, to investigate the conditions under which it is possible and to ascertain the nature of the exact singulatiries.

We suggest (cf. footnote 40) that the analytic continuation may be effected by introducing a variable coefficient λ for $\Sigma_2(w)$, the non-Hermitian part of the self-energy operator and analytically continuing λ from real to imaginary values. One would thus solve a related problem with an Hermitian Hamiltonian and only at the last step would one transform the solution to that corresponding to the actual non-Hermitian problem. In this way one would "side-step" some of the difficulties mentioned above. But this too is a formal program which leaves unresolved the major methematical questions.

In any case, it is a rather attractive idea to try to maintain by means of a formal analytic continuation—whether in the energy variable w or the parameter λ—a single-particle interpretation in a region in which this interpretation has, in a strict sense, already broken down. One would therefore like to believe that the combination of bi-orthogonal expansion plus quasi-particle approximation, which in principle accomplishes this *tour de force*, will turn out to be a useful formalism.

ACKNOWLEDGMENTS

The author wishes to thank Professor J. Percus for aiding his acclimatization to many-particle theory and for many helpful discussions throughout the course of this work. Stimulating discussions with Professor J. Anderson and Professor B. Zumino are greatly appreciated.