Self-Consistent Approximations in Many-Body Systems

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This paper investigates the criteria for maintenance of the macroscopic conservation laws of number, momentum, and energy by approximate two-particle correlation functions in many-body systems. The methods of generating such approximations are the same as in a previous paper. However, the derivations of the conservation laws given here clarify both why the approximation method works and the connection between the macroscopic conservation laws and those at the vertices.

Conserving nonequilibrium approximations are based on self-consistent approximations to the one-particle Green's function. The same condition that ensures that the nonequilibrium theory be conserving also ensures that the equilibrium approximation has the following properties. The several common methods for determining the partition function from the one-particle Green's function all lead to the same result. When applied to a zero-temperature normal fermion system, the approximation procedure maintains the Hugenholtz-Van Hove theorem. Consequently, the self-consistent version of Brueckner's nuclear matter theory obeys this theorem.

I. INTRODUCTION

IN an earlier paper[1] we underlined the importance, in developing a quantum theory of transport phenomena, of making approximations to two-particle correlation functions in a manner that preserves the conservation laws for particle number, momentum, and energy. We described a method for generating such conserving approximations, but the connection between the conservation laws at the vertices and the macroscopic conservation laws was somewhat obscure. A question raised is how can a diagrammatic type approximation maintain the conservation laws at the vertices and yet not conserve number, momentum, and energy over all? One purpose of this paper is to illuminate the relation of the over-all conservation laws to those at the vertices. In doing this, we shall discover that the three criteria given in I for an approximation to be conserving can be condensed to one simple criterion.

The basic point is that to have the macroscopic conservation laws obeyed, the two-particle correlation function

$$L(12,1'2') = G_2(12,1'2') - G(1-1')G(2-2') \quad (1)$$

must be the variational derivative of the one-particle Green's function $G(1,1')$ with respect to an external potential $U(2',2)$ nonlocal in space and time:

$$L(12,1'2') = \pm [\delta G(1,1')/\delta U(2',2)]_{U=0}. \quad (2)$$

The U dependence of G is given in the equation of motion

$$\int [G_0^{-1}(1,\bar{1}) - U(1,\bar{1})]G(\bar{1},1';U)$$

$$= \delta(1-1') \pm i \int V(1-\bar{3})G_2(1\bar{3},1'\bar{3}^+;U). \quad (3a)$$

Here $V(1-2)$ means $v(\mathbf{r}_1 - \mathbf{r}_2)\delta(t_1 - t_2)$.

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[1] G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 287 (1961), hereafter referred to as I. The present notation shall be the same as in that paper.

Our prescription for generating conserving approximations is to replace the VG_2 term in Eq. (3a) by a functional of G the Green's function itself and V, i.e.,

$$\pm i \int V(1-\bar{3})G_2(1\bar{3},1'\bar{3}^+;U) \rightarrow$$

$$\int \Sigma(1,\bar{2})G(\bar{2},1';U), \quad (4)$$

where the self-energy Σ is a functional of $G(U)$ and V. This functional dependence is to be given by a sum of diagrams constructed of G and V—some subset of terms in a complete expansion[2] of Σ in G and V. The self-consistent Hartree and Hartree-Fock approximations are examples in which Σ is of the first order in its explicit V dependence. A possible such term of second order in its explicit V dependence is

$$\Sigma(1,2) = \mp \int d\bar{1}d\bar{2}\, V(1-\bar{1})V(2-\bar{2})G(1,2)G(\bar{1},\bar{2})G(\bar{2},\bar{1}).$$

This is illustrated in Fig. 1(c) on the right.

In these approximations, Σ is taken to be a functional of $G(U)$, and therefore it depends on U through the U dependence of G. Inclusion of the U dependence of Σ, through expanding Σ in terms of $G(U)$ and not just $G(U=0)$ is fundamentally what leads to the conservation laws. This will become more clear later. The Green's function $G(U)$ is then to be determined self-consistently from the equation

$$\int d\bar{1}[G_0^{-1}(1,\bar{1}) - U(1,\bar{1}) - \Sigma(1,\bar{1})]$$

$$\times G(\bar{1},1') = \delta(1-1'). \quad (5a)$$

It directly follows that G also obeys

$$\int d\bar{1}G(1,\bar{1})[G_0^{-1}(\bar{1},1') - U(\bar{1},1') - \Sigma(\bar{1},1')]$$

$$= \delta(1-1'). \quad (5b)$$

[2] Such an expansion may readily be constructed along the lines set forth by J. Schwinger in Proc. Natl. Acad. Sci. U. S. **37**, 452 (1951).

That G obeys this equation in addition to (5a) is a much weaker statement than condition A in I. Condition A requires that G also obey the "left-hand" equation of motion

$$\int d\bar{1}\, G(1,\bar{1})[G_0^{-1}(\bar{1},1')-U(\bar{1},1')]$$

$$=\delta(1-1')\pm i\int G_2(1\bar{3}^-,1'\bar{3})V(1'-\bar{3}), \quad (3b)$$

where G_2 is approximated by the same functional of G and V as it is in (4). In general, Eq. (3b) differs from Eq. (5b). It shall turn out that one condition to be placed later on the functional form of Σ will imply that (3b) and (5b) are the same, i.e., that condition A is satisfied by the approximation. At this point we write approximations only to the "right-hand" equation of motion (3a), and place no further restrictions on the functional dependence of VG_2 in this equation.

II. CONSERVATION LAWS FOR L

Just demand that Σ be a functional of $G(U)$ ensures that the approximation for $L(12,1'2')$, generated by Eq. (2), obeys the over-all conservation laws in the 2, 2′ variables. We shall now show how this follows. In order that L be conserving in the 1, 1′ variables also, it will be necessary to place one restriction on the possible functional dependence of Σ on G.

For now we must notice that in a diagrammatic type expansion of Σ in terms of G and V, the conservation laws at the vertices are obeyed. At each vertex in $\Sigma(1,2)$, except at the exterior vertices 1 and 2, there is one interaction line, two particles entering and two particles leaving—thus there is particle conservation at the vertices. The intermediate points are integrated over all space. This, in the absence of any external disturbances, leads to momentum conservation. Also, the intermediate times are integrated over the range 0 to $-i\beta$, consistent with the periodic boundary conditions, and this, in the absence of external disturbances, leads to the appropriate form of energy conservation at the vertices.

We shall first show that the approximate

$$L=\pm(\delta G/\delta U)_{U=0}$$

obeys the differential number conservation law.[3] To do this, let us consider G in the presence of a U that corresponds to a gauge transformation. This external disturbance is local in time and given by

$$\int\int_0^{-i\beta}\psi^\dagger(1)U(1,1')\psi(1')d1d1'$$

$$=\int_0^{-i\beta}d1\left[\boldsymbol{\nabla}\Lambda(1)\cdot\left(\mathbf{j}(1)+\frac{1}{2m}\boldsymbol{\nabla}\Lambda(1)\rho(1)\right)\right.$$

$$\left.+\frac{\partial\Lambda(1)}{\partial t_1}\rho(1)\right]. \quad (6)$$

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[3] This proof was suggested to me by Dr. L. P. Kadanoff.

With this U, Eq. (3a) becomes

$$\{i\partial/\partial t_1-\partial\Lambda(1)/\partial t_1+(1/2m)[\boldsymbol{\nabla}_1+i\boldsymbol{\nabla}\Lambda(1)]^2\}G(1,1';\Lambda)$$

$$-\int\Sigma(1,\bar{1};G(\Lambda))G(\bar{1},1';\Lambda)=\delta(1-1'). \quad (7)$$

The following argument is familiar from discussions of gauge invariance in quantum electrodynamics. The equation for $G_0(1,1';\Lambda)$ in the presence of Λ is

$$\{i\partial/\partial t_1-\partial\Lambda(1)/\partial t_1+(1/2m)[\boldsymbol{\nabla}_1+i\boldsymbol{\nabla}\Lambda(1)]^2\}$$
$$\times G_0(1,1';\Lambda)=\delta(1-1'), \quad (8)$$

which has the solution

$$G_0(1,1';\Lambda)=e^{-i\Lambda(1)}G_0(1-1')e^{i\Lambda(1')}, \quad (9)$$

where $G_0(1-1')$ satisfies Eq. (8) with $\Lambda=0$. This solution obeys the boundary condition if we assume

$$\Lambda(\mathbf{r},0)=\Lambda(\mathbf{r},-i\beta). \quad (10)$$

The crucial point in the argument now is that the effect of Λ is to transform G as it transforms G_0, that is,

$$G(1,1';\Lambda)=e^{-i\Lambda(1)}G(1-1';\Lambda=0)e^{i\Lambda(1')}. \quad (11)$$

To be convinced of this it is only necessary to see that under the transformation

$$G(2,2';\Lambda)\rightarrow e^{-i\Lambda(2)}\bar{G}(2,2';\Lambda)e^{i\Lambda(2')},$$

Σ transforms as

$$\Sigma(1,\bar{1};G(\Lambda))=e^{-i\Lambda(1)}\Sigma(1,\bar{1};\bar{G})e^{i\Lambda(\bar{1})}. \quad (12)$$

This follows directly from the conservation of particles at the vertices. Under the transformation

$$G(2,2')\rightarrow e^{-i\Lambda(2)}\bar{G}(2,2')e^{i\Lambda(2')}$$

the exponential factors cancel at the internal vertices in Σ because the factors from the particles entering the vertex cancel the factors from the particles leaving the vertex. Only the factors at the external vertices remain. Thus, $\bar{G}$ obeys the equation of motion (7) with $\Lambda=0$, and, therefore, $\bar{G}(\Lambda)=G(\Lambda=0)$.

We may now expand both sides of (11) to first order in Λ. Because L, by definition, gives the linear change in G, we find

$$\pm\int_0^{-i\beta}d2\left\{L(12,1'2')\partial\Lambda(2)/\partial t_2\right.$$

$$\left.+\left[\left(\frac{\boldsymbol{\nabla}_2-\boldsymbol{\nabla}_{2'}}{2im}\right)L(12,1'2')\right]_{2'=2}\cdot\boldsymbol{\nabla}_2\Lambda(2)\right\}$$

$$=-i[\Lambda(1)-\Lambda(1')]G(1-1').$$

Integrating by parts on the left-hand side, using (10) and setting the coefficient of $\Lambda(2)$ in this equation equal to zero yields the number conservation law for L:

$$(\partial/\partial t_2)L(12,1'2)+\boldsymbol{\nabla}_2\cdot\left(\frac{\boldsymbol{\nabla}_2-\boldsymbol{\nabla}_{2'}}{2im}L(12,1'2')\right)_{2'=2}$$

$$=\pm i[\delta(1-2)-\delta(1'-2)]G(1-1'). \quad (13)$$

Compare this with (I,35). The number conservation law in the 2, 2′ variables thus follows from L being of the form $\pm\delta G/\delta U$ and having each G that occurs in Σ depend on U. This latter requirement is what is responsible for Σ transforming as in (11). The conservation laws in 1, 1′ will follow when we demand that L be symmetrical under 1, 1′ $\leftrightarrow$ 2, 2′.

The total momentum conservation law follows as simply. Because of its connection to the translational invariance of the system, over-all momentum conservation for L can be demonstrated by choosing a U that corresponds to the system being described by an observer whose origin of coordinates is at the time-varying point $\mathbf{R}(t)$. Then this observer would describe the system with the extra term (to first order in $\mathbf{R}$)

$$-\frac{d\mathbf{R}(t)}{dt}\cdot\int d\mathbf{r}\,m\mathbf{j}(\mathbf{r},t)=-\frac{d\mathbf{R}(t)}{dt}\cdot\mathbf{P}(t) \qquad (14)$$

added to the Hamiltonian. Here $\mathbf{P}(t)$ is the total momentum operator. With this external disturbance G obeys

$$\{i\partial/\partial t_1+\nabla_1^2/2m-i[d\mathbf{R}(t_1)/dt_1]\cdot\nabla_1\}G(1,1';\mathbf{R})$$

$$-\int\Sigma(1,\bar{1};G(\mathbf{R}))G(\bar{1},1';\mathbf{R})=\delta(1-1'). \qquad (15)$$

The argument now parallels the number conservation argument. In the variable coordinate system, G_0 obeys

$$\{i\partial/\partial t_1+\nabla_1^2/2m-i[d\mathbf{R}(t_1)/dt_1]\cdot\nabla_1\}$$
$$\times G_0(1,1';\mathbf{R})=\delta(1-1'),$$

and hence

$$G_0(\mathbf{r}t,\mathbf{r}'t';\mathbf{R})=G_0(\mathbf{r}+\mathbf{R}(t),t;\mathbf{r}'+\mathbf{R}(t'),t';\mathbf{R}=0), \qquad (16)$$

as may be checked by direct differentiation. With no loss of generality we may assume $\mathbf{R}(0)=\mathbf{R}(-i\beta)$. Then the solution (16) also obeys the boundary condition.

Again Σ and G are transformed by $\mathbf{R}$ exactly as G_0. Under the substitution

$$G(\mathbf{r}t,\mathbf{r}'t';\mathbf{R})\to\bar{G}(\mathbf{r}+\mathbf{R}(t),t;\mathbf{r}'+\mathbf{R}(t'),t';\mathbf{R}),$$

Σ becomes

$$\Sigma(\mathbf{r}t,\mathbf{r}'t';G(\mathbf{R}))$$
$$=\Sigma(\mathbf{r}+\mathbf{R}(t),t;\mathbf{r}'+\mathbf{R}(t'),t';\bar{G}(\mathbf{R})). \qquad (17a)$$

This follows because at each internal vertex in Σ, the two-particle potential V is local in time and depends on the difference of the spatial coordinates, and the spatial integrations are over all space, so that the spatial integrations are invariant under a shift in the origin. Thus, $\bar{G}(1,1')$ obeys Eq. (15) with $\mathbf{R}=0$ so that $\bar{G}(\mathbf{R})=G(\mathbf{R}=0)$ and

$$G(\mathbf{r}t,\mathbf{r}'t';\mathbf{R})=G(\mathbf{r}+\mathbf{R}(t),t;\mathbf{r}'+\mathbf{R}(t'),t';\mathbf{R}=0). \qquad (17b)$$

Clearly the Green's function as "seen" by an observer with a variable origin of coordinates is obtained by just

shifting the coordinates in the equilibrium $(\mathbf{R}=0)$ Green's function.

The proof of momentum conservation would break down at this point if V were nonlocal in time, as it would be if it represented, say, the effective interaction between electrons due to phonons in a metal. In this case one would not, of course, expect the electrons alone to conserve momentum, since they can transfer momentum to the phonons.

We now expand both sides of (17b) to first order in $\mathbf{R}$. Since L, by definition, gives the linear response of G, we have

$$\mp\int_0^{-i\beta}d2\left[\frac{\nabla_2-\nabla_2'}{2i}L(12,1'2')\right]_{2'=2}\cdot\frac{d\mathbf{R}(t_2)}{dt_2}$$

$$=\nabla_1 G(1-1')\cdot[\mathbf{R}(t_1)-\mathbf{R}(t_1')].$$

Since this is true for arbitrary $\mathbf{R}(t)$, the coefficient of $\mathbf{R}$ must vanish at each time. Integrating the left side by parts and picking out the coefficient of $\mathbf{R}(t_2)$, we have

$$\frac{\partial}{\partial t_2}\int d\mathbf{r}_2\left[\frac{\nabla_2-\nabla_2'}{2i}L(12,1'2')\right]_{2'=2}$$

$$=\pm\nabla_1 G(1-1')[\delta(t_1-t_2)-\delta(t_1'-t_2)]. \qquad (18)$$

This is the momentum conservation law for L in the 2, 2′ variables. Compare it with (I,37a).

It is from the momentum conservation argument that we can most clearly see the connection between the conservation laws at the vertices and the statement of over-all momentum conservation. The conservation of momentum at a vertex is equivalent to the statement that the vertex is invariant if the origins in the spatial integrations are both shifted by the same amount. Because of this invariance Σ transforms by (17a), G by (17b), and from this it follows that L is over-all momentum-conserving in the 2, 2′ variables. This is the extent to which conservation at the vertices influences over-all conservation. Conservation at the vertices is necessary, but not sufficient. The other necessary point is that each line in Σ transforms when one uses a shifting coordinate system. Suppose that we had decided to let some internal line in Σ be a $G(U=0)$ instead of a $G(U)$. Then when we formed L as

$$L=\pm\delta G/\delta U=\mp G(\delta G^{-1}/\delta U)G$$
$$=\mp GG\mp G(\delta\Sigma/\delta U)G, \qquad (19)$$

the $G(U=0)$ line in Σ would not be differentiated with respect to U. This would correspond to leaving a certain term out of the equation for L. Though momentum would be conserved at each vertex in the L equation, L would not in general be momentum conserving because, with a $G(U=0)$ line, Σ and thus G would not transform as in (17).

To prove the energy conservation law for the 2, 2′ variables in L, we consider the system as described by an

observer who uses a rubbery clock, i.e., his "flexible" time t would be measured by us as $\theta(t)$, where $\theta(t)$ is some imaginary function of the imaginary time variable t, chosen such that $d\theta/dt$ is never zero and such that $\theta(0)=0$ and $\theta(-i\beta)=-i\beta$. Such an observer would, because of the irregularity of his clock, describe the system with the additional term

$$[(d\theta/dt)-1]H(t) \qquad (20)$$

added to the Hamiltonian of the system. However, because H is not a two-particle operator, the linear effects of (20) on G are not given in terms of L. To derive the energy conservation law for L we therefore simulate the external disturbance (20) by the two-particle operator

$$\left(\frac{d\theta}{dt}-1\right)\frac{1}{4}\int d\mathbf{r}\left[\left(i\frac{\partial}{\partial t}-i\frac{\partial}{\partial t'}+\frac{\nabla\cdot\nabla'}{m}\right)\right.$$
$$\left.\times\psi^\dagger(\mathbf{r}'t')\psi(\mathbf{r}t)\right]_{\mathbf{r}'=\mathbf{r},\,t'=t}, \qquad (21)$$

which to linear order in $d\theta/dt-1$ will produce essentially the same effect on G as (20). By using the equations of motion of ψ and $\psi^\dagger$ one can see that (20) and (21) agree to linear order in $d\theta/dt-1$. The disturbance (21) corresponds to a U given by

$$U(1',1)=\left[\frac{1}{2}\left(\frac{d\theta(t_1)}{dt_1}-1\right)\left(i\frac{\partial}{\partial t_1}-\frac{\nabla_1^2}{2m}\right)\right.$$
$$\left.+\tfrac{1}{4}id^2\theta(t_1)/dt_1^2\right]\delta(1-1'). \qquad (22)$$

Then G, to linear order in $d\theta/dt-1$, obeys the equation of motion

$$\left[\left(\frac{d\theta_1}{dt_1}\right)^{-1/2}i\frac{\partial}{\partial t_1}+\left(\frac{d\theta_1}{dt_1}\right)^{1/2}\frac{\nabla_1^2}{2m}-\frac{i}{4}\frac{d^2\theta_1}{dt_1^2}\right]G(1,1';\theta)$$
$$-\int\Sigma(1,\bar{1};G(\theta))G(\bar{1},1';\theta)=\delta(\mathbf{r}_1-\mathbf{r}_1')\delta(t_1-t_1'), \qquad (23)$$

where θ_1 stands for $\theta(t_1)$. To see the relation between $G(1,1',\theta)$ and the equilibrium Green's function, we multiply both sides by $(d\theta_1/dt_1)^{-3/4}(d\theta_1'/dt_1')^{-1/4}$:

$$\left(i\frac{dt_1}{d\theta_1}\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}\right)\left[\left(\frac{d\theta_1}{dt_1}\right)^{-1/4}G(1,1';\theta)\left(\frac{d\theta_1'}{dt_1'}\right)^{-1/4}\right]$$
$$-\left(\frac{d\theta_1}{dt_1}\right)^{-3/4}\int\Sigma(1,\bar{1};G(\theta))G(\bar{1},1';\theta)\left(\frac{d\theta_1'}{dt_1'}\right)^{-1/4}$$
$$=\frac{dt_1}{d\theta_1}\delta(t_1-t_1')\delta(\mathbf{r}_1-\mathbf{r}_1'). \qquad (24)$$

The free-particle Green's function in the presence of θ

therefore obeys the equation

$$\left(i\frac{\partial}{\partial\theta_1}+\frac{\nabla_1^2}{2m}\right)\left[\left(\frac{d\theta_1}{dt_1}\right)^{-1/4}G_0(\mathbf{r}_1t_1,\mathbf{r}_1't_1';\theta)\left(\frac{d\theta_1'}{dt_1'}\right)^{-1/4}\right]$$
$$=\delta(\theta_1-\theta_1')\delta(\mathbf{r}_1-\mathbf{r}_1'), \qquad (25)$$

and consequently $G_0(1,1',\theta)$ is given by

$$G_0(\mathbf{r}_1t_1,\mathbf{r}_1't_1';\theta)$$
$$=\left(\frac{d\theta_1}{dt_1}\right)^{1/4}G_0(\mathbf{r}_1,\theta(t_1);\mathbf{r}_1',\theta(t_1'))\left(\frac{d\theta_1'}{dt_1'}\right)^{1/4}, \qquad (26)$$

where the G_0 on the right is the equilibrium free-particle Green's function.

We may now easily verify that G in the presence of the disturbance (21) is also related to the equilibrium G by

$$G(\mathbf{r}_1t_1,\mathbf{r}_1't_1';\theta)$$
$$=\left(\frac{d\theta_1}{dt_1}\right)^{1/4}G(\mathbf{r}_1,\theta(t_1);\mathbf{r}_1',\theta(t_1'))\left(\frac{d\theta_1'}{dt_1'}\right)^{1/4}. \qquad (27)$$

To do this we must notice that

$$\left(\frac{d\theta_1}{dt_1}\right)^{-1/4}G(\mathbf{r}_1t_1,\mathbf{r}_1't_1';\theta)\left(\frac{d\theta_1'}{dt_1'}\right)^{-1/4} \qquad (28)$$

obeys the equilibrium Green's function equation, written with $\theta(t)$ as the time variable. Now at each internal vertex in Σ, the four factors of $(d\theta/dt)^{1/4}$, from writing Σ in terms of (28), convert dt into $d\theta$. The excess three such factors at the $\mathbf{r}_1t_1$ external vertex in Σ are explicitly canceled by the $(d\theta_1/dt_1)^{-3/4}$ factor in Eq. (24), and at the $\bar{\mathbf{r}}_1\bar{t}_1$ vertex they contribute towards converting $d\bar{t}_1$ into $d\bar{\theta}_1$. The net result is that the quantity (28) obeys the equilibrium equation, and hence G in the presence of the disturbance (21) is given by Eq. (27). That $\theta(t)$ is the natural time variable is clear from the physical interpretation of the external disturbance.

We now expand Eq. (27) to linear order in $\theta-t$. This gives

$$\pm\int d2d2'L(12,1'2')\left[\frac{1}{2}\left(\frac{d\theta_2}{dt_2}-1\right)\left(i\frac{\partial}{\partial t_2}-\frac{\nabla_2^2}{2m}\right)\right.$$
$$\left.+\tfrac{1}{4}i\frac{d^2\theta_2}{dt_2^2}\right]\delta(2-2')$$
$$=\frac{\partial}{\partial t_1}G(1-1')[(\theta_1-t_1)-(\theta_1'-t_1')]$$
$$+\tfrac{1}{4}G(1-1')\left[\frac{d\theta_1}{dt_1}-1+\frac{d\theta_1'}{dt_1'}-1\right].$$

Integrating by parts on the left side and picking out the

coefficient of $\theta - t$ we find

$$\mp \frac{d}{dt_2} \int d\mathbf{r}_2 \frac{1}{4}\left[\left(i\frac{\partial}{\partial t_2} - i\frac{\partial}{\partial t_2'} + \frac{\nabla_2 \cdot \nabla_2'}{m}\right)L(12,1'2')\right]_{2'=2}$$

$$= \frac{\partial G(1-1')}{\partial t_1}[\delta(t_1-t_2) - \delta(t_1'-t_2)]$$

$$- \tfrac{1}{4}G(1-1')\frac{d}{dt_2}[\delta(t_1-t_2) + \delta(t_1'-t_2)]. \quad (29)$$

This is the energy conservation law obeyed by L in the 2, 2' variables. Compare this with Eq. (I,37c).

In the above proofs of the conservation laws we need not have required all the internal lines in Σ to be $G(U)$'s. They could also have been $G_0(U)$'s. The conservation laws are obeyed by L in the 2, 2' variables because $L(12,1'2')$ is in the form of a derivative of $G(1,1')$—which has the proper transformation properties—with respect to a function U of 2, 2'. Because L is such a derivative, all the effects of U are taken into account in the linear order. It is the inclusion of all the effects of $U(2,2')$ on the system that guarantees that $L(12,1'2')$ obeys the conservation laws in 2, 2'. If L were not in the form of a derivative, because certain terms were omitted in the integral equation determining L, then L would not in general obey the conservation laws in 2, 2'.

In a perturbation expansion of L in terms of V, each order will obey the conservation laws in both the 1, 1' and 2, 2' variables. The reason why we must pay attention to the conservation laws is that we want to have terms to arbitrarily high order of V in L in order to use L to describe transport phenomena, and yet at the same time we want to have an approximate equation for L which we can solve. This requires picking some subset of terms in each order in perturbation theory. It is the correct way of choosing the subsets in each order that is the difficulty. Generating L as a derivative with respect to U is a correct way of choosing the subsets of terms and, as we have seen, it is physically the correct way.

The conservation laws for the 1, 1' variables in L are guaranteed by requiring condition C of I, i.e., that any approximation for L be symmetric under the interchange 1, 1' $\leftrightarrow$ 2, 2'. This is, of course, obeyed by the exact L. We shall therefore impose this one requirement of symmetry on any approximation. If L is symmetric, then, since $L = \pm\delta G/\delta U$, we have

$$\delta G(1,1')/\delta U(2',2) = \delta G(2,2')/\delta U(1',1). \quad (30)$$

This statement is essentially one of a vanishing "curl." Thus (barring possible pathological counter-examples), there exists a W such that

$$G(1,1') = \delta W/\delta U(1',1). \quad (31)$$

We know that this statement is true for the exact G, since, except for a possible term independent of U, the exact W is

$$W = \pm\ln \text{Tr}\left\{e^{-\beta(H-\mu N)}\right.$$

$$\left. \times T\left[\exp\left(-i\int_0^{-i\beta} \psi^\dagger(1)U(1,1')\psi(1')\right)\right]\right\}. \quad (32)$$

If an approximation maintains the 1, 1' $\leftrightarrow$ 2, 2' symmetry of L, then the approximate G is derivable from some approximate W.

We see that the W in (32) is closely related to the partition function of the system. In equilibrium, that is, when $U(1,1') = \delta(t_1-t_1')U(\mathbf{r}_1,\mathbf{r}_1')$, W is the logarithm of the partition function. In fact, in the general case, if the partition function is evaluated as a path integral from 0 to $-i\beta$, as Feynman[4] did for He[4], then W is just this same path integral only with the nonlocal potential $U(1,1')$ acting along the paths from 0 to $-i\beta$.

The 1, 1' conservation laws for L may be stated as a condition on Σ. We consider only approximations in which Σ is a functional of only $G(U)$ and V and not of $G_0(U)$ also. Then, since Σ depends on U only through its dependence on $G(U)$, we may write $\delta\Sigma/\delta U$ in Eq. (19) for L as

$$\frac{\delta\Sigma(1,1')}{\delta U(3',3)} = \int d2d2' \frac{\delta\Sigma(1,1')}{\delta G(2',2)} \frac{\delta G(2',2)}{\delta U(3',3)}. \quad (33)$$

Then Eq. (19) may be written as

$$\int [G^{-1}(1-\bar{2}')G^{-1}(\bar{2}-1') - \delta\Sigma(1,1')/\delta G(\bar{2}',\bar{2})]L(\bar{2}'3,\bar{2}3')$$

$$= \pm\delta(1-2')\delta(2-1'). \quad (34)$$

Now L will be symmetric under 1, 1' $\leftrightarrow$ 2, 2' if L^{-1} has this symmetry, and this will be so if and only if

$$\delta\Sigma(1,1')/\delta G(2',2) = \delta\Sigma(2,2')/\delta G(1',1). \quad (35)$$

This is a vanishing curl condition on Σ, and thus it follows that there exists a functional Φ of G and V such that

$$\Sigma(1,1') = \delta\Phi/\delta G(1',1). \quad (36)$$

The effective "particle-hole" interaction, $\delta\Sigma(1,1')/\delta G(2',2)$, is therefore

$$\delta^2\Phi/[\delta G(1',1)\delta G(2',2)].$$

(Since differentiation with respect to G means just plucking out a line from a diagram, two such derivatives commute.) Conversely, if Σ is of this form, then L will be symmetric and obey the conservation laws in the 1, 1' and 2, 2' variables. This is the one condition that must be imposed on any approximation for Σ as a functional of G and V. There must exist a "closed" functional Φ of G and V such that $\Sigma = \delta\Phi/\delta G$.
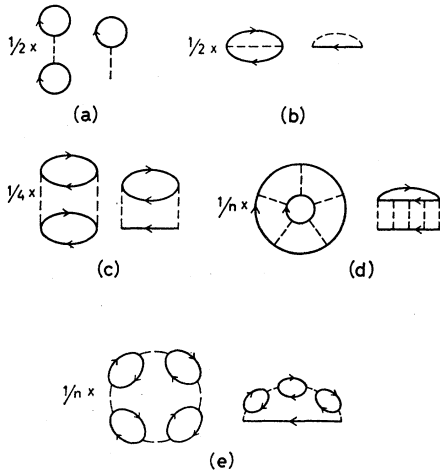
[4] R. P. Feynman, Phys. Rev. 91, 1291 (1953).

FIG. 1. Diagrams for Σ and the corresponding Φ's. On the left of each set is the Φ diagram, and on the right the corresponding term in Σ. The direction of time is not associated with any direction in these diagrams. (a) is the Hartree approximation, (b) the exchange term in the Hartree-Fock approximation, and (c) is one term involving V explicitly to second order. (d) shows a typical term in the T-matrix approximation described in I, and (e) is a typical term in the shielded potential approximation described in I. The factors $1/n$ refer to the number of G's occurring in the particular term in Φ.

In the figure we give several examples of Σ's and the associated Φ's.

For the Hartree approximation, Φ is given by

$$\Phi = \pm \frac{i}{2} \int_0^{-i\beta} d1 d2 \; G(1,1^+) V(1-2) G(2,2^+), \quad (37)$$

and for the exchange term in the Hartree-Fock approximation,

$$\Phi = \frac{i}{2} \int_0^{-i\beta} d1 d2 \; G(1,2^+) V(1-2) G(2,1^+). \quad (38)$$

The diagrams for Φ bear a strong resemblance to ground-state energy diagrams, but with the zero-order Green's functions replaced by the self-consistent G's.

Suppose that G is changed by the amount δG. Then Φ as a functional of G will change by the amount

$$\delta \Phi = \int_0^{-i\beta} d1 d1' \; \frac{\delta \Phi}{\delta G(1,1')} \delta G(1',1^+). \quad (39)$$

The way in which the t_1' limit is to be taken in δG is significant only in the Hartree-Fock terms in Φ, and it is clear from (37) and (38) that this t_1' must approach the t_1' in $\delta \Phi / \delta G(1,1')$ from "larger" values, i.e., from lower on the imaginary axis.

We will frequently use a four-dimensional matrix notation, and by the trace of a quantity we mean

$$\mathrm{tr} X = \int_0^{-i\beta} dt \int d\mathbf{r} \; X(\mathbf{r}t, \mathbf{r}t^+). \quad (40)$$

In this notation (39) becomes

$$\delta \Phi = \mathrm{tr} \Sigma \delta G.$$

III. CONSERVATION LAWS FOR $G(U)$

The reason for imposing condition (36) on an approximation was to guarantee that the conservation laws be obeyed by L in the 1, 1' variables. These laws are special cases of the conservation laws obeyed by the nonequilibrium function $G(U)$. Now when Σ is derivable from a Φ, we can give simple proofs of these more general conservation laws as well.

First, consider transforming G by

$$G(1,1';U) \to e^{i\Lambda(1)} G(1,1';U) e^{-i\Lambda(1')}. \quad (41)$$

The first-order change in Φ induced by this change in G is, from (39),

$$\delta \Phi = \int d1 d1' \; \Sigma(1,1') i [\Lambda(1') - \Lambda(1)] G(1',1)$$

$$= -i \int d1 d1' [\Sigma(1,1') G(1',1)$$
$$- G(1,1') \Sigma(1',1)] \Lambda(1). \quad (42)$$

On the other hand, from the number conservation at each vertex in Φ, i.e., one line leaves wherever one line enters, the transformation (41) must be an invariance of Φ. Thus the coefficient of $\Lambda(1)$ in (42) must vanish identically. Hence[5]

$$\int d1' [\Sigma(1,1';U) G(1',1;U)$$
$$- G(1,1';U) \Sigma(1',1;U)] = 0. \quad (43)$$

Subtracting Eq. (5b) from (5a), setting $1'=1^+$, and using (41) we find the number conservation law (I,22) obeyed by $G(U)$.

A similar consideration of the invariance

$$G(\mathbf{r},t;\mathbf{r}',t';U) \to G(\mathbf{r}+\mathbf{R}(t), t; \mathbf{r}'+\mathbf{R}(t'), t'; U) \quad (44)$$

of Φ leads to the momentum conservation law (I,25). The energy conservation law follows from an only slightly more complicated argument. The appropriate invariance of Φ is

$$G(\mathbf{r},t;\mathbf{r}',t';U) \to$$
$$(d\theta/dt)^{1/4} G(\mathbf{r},\theta(t);\mathbf{r}',\theta(t');U)(d\theta'/dt')^{1/4}. \quad (45)$$

This is an invariance since four G's entering each vertex supply a net factor $d\theta(t)/dt$ which changes dt into $d\theta$. Then

$$0 = \delta \Phi = \int d1 d2 \; \Sigma(1,2) \delta \left[\left(\frac{d\theta_2}{dt_2} \right)^{1/4} G(\mathbf{r}_2,\theta_2;\mathbf{r}_1,\theta_1) \left(\frac{d\theta_1}{dt_1} \right)^{1/4} \right],$$

---

[5] The reader may convince himself from Eq. (43), written in terms of the original approximation to G_2, that "Φ-derivable" approximations obey condition A, Eq. (I,29).

and taking the coefficient of term linear in $\theta_1 - t_1$ we have

$$0 = -\frac{1}{4} \int \frac{\partial}{\partial t_1} [\Sigma(1,2)G(2,1) + G(1,2)\Sigma(2,1)] d2$$

$$+ \int \left[\frac{\partial}{\partial t_1} G(1,2) \cdot \Sigma(2,1) + \Sigma(1,2) \frac{\partial}{\partial t_1} G(2,1) \right] d2. \quad (46)$$

An argument similar to that given in the appendix to I, in which Eq. (44) plays the role of Eq. (I,A1), leads to the energy conservation law (I,28).

To summarize, if one starts with an approximation for Σ as a functional of $G(U)$ and V such that Σ is of the form $\delta\Phi/\delta G$, then the nonequilibrium function $G(U)$ obeys the differential number conservation law, and the total momentum (angular momentum) and energy conservation laws. In addition, the effective "particle-hole" interaction, in Eq. (34) for L, is given by $\delta^2\Phi/\delta G \delta G$.

The results up to now can be formulated for superconductors. Φ is composed of the matrix Green's functions defined by Nambu.[6] For the BCS theory, Φ is just the Hartree-Fock Φ, Fig. 1(a), (b), but with the lines standing for matrices rather than single functions.

IV. CONSISTENCY OF APPROXIMATIONS TO THE PARTITION FUNCTION

The one-particle Green's function, in addition to giving the single-particle excitations of a many-body system, contains information about the equilibrium statistical mechanics of the system. This information is found from the grand partition function, which can be constructed from the one-particle Green's function by a variety of means. The more common methods include integrating the expectation value of the potential energy with respect to a coupling constant—this is the linked cluster expansion, integrating the expectation value of the number with respect to the chemical potential μ, and integrating $\langle (H - \mu N) \rangle$ with respect to the inverse temperature β. It is often desirable, when making an approximation to the one-particle Green's function, to have these various methods lead to the same result, so that one has a consistent picture of the equilibrium properties. This requirement, at the same time that it places great restrictions on an approximation to G, provides us, when perturbation theory is no longer valid, with a possible guide in truncating the infinite hierarchy of coupled Green's function equations.

Also, by requiring that the solution to a given approximation obey certain general theorems we provide ourselves with additional criteria to decide whether the approximation is good. An important example of such a theorem is the Hugenholtz-Van Hove theorem for zero-temperature normal fermions, a theorem which should

be obeyed, for example, by a satisfactory theory of nuclear matter.

The self-consistent Φ-derivable approximations, described by Eqs. (5) and (36), which lead to a fully-conserving transport theory, have the further property that when specialized to the equilibrium case, they satisfy all the requirements set forth above. The remainder of this paper shall be given to a discussion of these equilibrium properties.

We begin by pointing out the relation between Φ and the quantity W in Eq. (31). This shall lead to a very useful formula from which all the equilibrium properties of Φ-derivable approximations follow. Consider a small variation in U. This induces a change in Φ given by $\delta\Phi = \mathrm{tr}\Sigma\delta G$, whereas from Eq. (31) the change induced in W is $\delta W = \mathrm{tr}(\delta U)G$. Thus,

$$\delta W = \delta\Phi - \delta \, \mathrm{tr}\Sigma G - \mathrm{tr}[\delta(G_0^{-1} - U - \Sigma)]G.$$

But the last term is[7] $-\mathrm{tr}(\delta G^{-1})G = \delta \, \mathrm{tr} \ln(-G)$, so that to within a possible added term independent of U,

$$W = \Phi - \mathrm{tr}\Sigma G - \mathrm{tr} \ln(-G). \quad (47)$$

We shall now show that formula (47) for W, with no added term, is equivalent to the linked cluster expansion for the expectation value (32) and, in the equilibrium case, (47) becomes an expression for the logarithm of the partition function.

To do this we let the potential V become λV, where λ is a numerical coupling constant, and then differentiate Eq. (47) with respect to λ. Now Φ depends on λ in two ways; first, through its explicit dependence on V, and second, through its dependence on G. Therefore (denoting the λ dependence by a subscript),

$$(d\Phi_\lambda/d\lambda) = (\partial\Phi_\lambda/\partial\lambda)_G + \mathrm{tr}\Sigma_\lambda(dG_\lambda/d\lambda). \quad (48)$$

Thus the derivative of (47) is

$$dW_\lambda/d\lambda = (\partial\Phi_\lambda/\partial\lambda)_G. \quad (49)$$

We can find the derivative of Φ at constant G by noticing a simple invariance of Φ. Suppose we let each explicit V in Φ become αV, and let each G become $\alpha^{-1/2}G$. Then, because each G in Φ joins two vertices, and each V is joined to four G's, the α transformation is an invariance of Φ. Thus, under this transformation

$$\frac{d\Phi_\lambda}{d\alpha} = \frac{\lambda}{\alpha} \left(\frac{\partial\Phi_\lambda}{\partial\lambda} \right)_G + \mathrm{tr} \frac{\delta\Phi_\lambda}{\delta G_\lambda} \frac{d}{d\alpha} (\alpha^{-1/2}G_\lambda)$$

$$= \frac{\lambda}{\alpha} \left(\frac{\partial\Phi_\lambda}{\partial\lambda} \right)_G - \tfrac{1}{2}\alpha^{-3/2} \, \mathrm{tr}\Sigma_\lambda G_\lambda.$$

Evaluating the above at $\alpha = 1$ yields

$$(\partial\Phi_\lambda/\partial\lambda)_G = (1/2\lambda) \, \mathrm{tr}\Sigma_\lambda G_\lambda. \quad (50)$$

Thus, integrating (49) with respect to λ from zero to

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

[7] We choose the branch of the logarithm so that the cut is along the negative axis and $\ln 1 = 0$.

one:

$$W = -\operatorname{tr}\ln[-G_0(U)] + \int_0^1 \frac{d\lambda}{2\lambda}\,\operatorname{tr}\Sigma_\lambda G_\lambda. \qquad (51)$$

We have used the fact that $\Phi_{\lambda=0}=0$ and $\Sigma_{\lambda=0}=0$ in evaluating $W_{\lambda=0}$ from Eq. (47). Equation (51) for W, when Σ_λ and G_λ are expanded in series in λ, becomes the linked cluster expansion[8] with $G_0(U)$'s instead of equilibrium G_0's.

From now on we assume $U(1,1')$ to be of the form $\delta(t_1-t_1')U(\mathbf{r}_1,\mathbf{r}_1')$, so that the system is in equilibrium, possibly in a static external field. Then W becomes equal to $\pm \ln Z$ evaluated as an integral of the potential energy with respect to the coupling constant λ. We see this as follows. In equilibrium, with the interaction λV, Z is given by

$$Z = \operatorname{Tr}\exp\left[-\beta\left(H_0 + \lambda\mathcal{V} - \mu N \right.\right.$$
$$\left.\left. + \int d\mathbf{r}\,d\mathbf{r}'\,\psi^\dagger(\mathbf{r}')U(\mathbf{r}',\mathbf{r})\psi(\mathbf{r}) \right)\right]. \quad (52)$$

Thus,

$$(\partial \ln Z/\partial\lambda)_{\beta,\mu,\Omega} = -(\beta/\lambda)\langle\lambda\mathcal{V}\rangle. \qquad (53)$$

(Ω is the volume of the system.) Now the interaction energy is

$$\langle\lambda\mathcal{V}\rangle_\lambda = \tfrac{1}{2}\lambda\int V(1-3)\langle\psi^\dagger(1)\psi^\dagger(3)\psi(3)\psi(1)\rangle_\lambda\,d\mathbf{r}_1 d3$$

$$= -\tfrac{1}{2}\lambda\int d\mathbf{r}_1\left[\int d3\,V(1-3)G_{2,\lambda}(13,1'3^+)\right]_{1'=1^+}, \quad (54)$$

which is expressible in terms of Σ_λ and G_λ by means of (4):

$$(1/2\lambda)\,\operatorname{tr}\Sigma_\lambda G_\lambda = \mp(\beta/\lambda)\langle\lambda\mathcal{V}\rangle = \pm(\partial \ln Z/\partial\lambda). \quad (55)$$

This equation together with the formula for a non-interacting system

$$\ln Z_0 = \pm\operatorname{tr}\ln(-G_0) \qquad (56)$$

proves that the right side of (51) is an evaluation of $\pm\ln Z$. Because Σ_λ and G_λ are approximate, this is an approximation to $\ln Z$. In the equilibrium case we have then shown that in the approximation

$$\ln Z = \pm[\Phi - \operatorname{tr}\Sigma G + \operatorname{tr}\ln(-G)], \qquad (57)$$

where $\ln Z$ is determined by integrating the potential energy with respect to the coupling constant λ. The relevant properties of self-consistent equilibrium approximations all follow from Eq. (57).[9]

For instance, the statistical mechanical relations that arise from varying a parameter in the grand partition function are preserved when Σ is Φ-derivable. As a first example, we consider evaluating the number of particles as a function of β and μ. It is clear from (52) that

$$\partial \ln Z/\partial\mu = \beta\langle N\rangle.$$

Thus we can evaluate $\langle N\rangle$ in terms of β and μ by differentiating the $\ln Z$ in Eq. (57) with respect to μ. On the other hand, we can also evaluate $\langle N\rangle$ in terms of G by

$$\langle N\rangle = \pm i\int G(\mathbf{r}t,\mathbf{r}t^+)\,d\mathbf{r}. \qquad (58)$$

The $\ln Z$ in (57) was found from a coupling constant integration. There is no reason why, for any arbitrary approximation, these two ways of evaluating $\langle N\rangle$ should agree. However, for Φ-derivable approximations they do agree. To show this it is best to use the Hamiltonian $\tilde{H} = H - \mu N$. Then G_0^{-1} will be given by

$$G_0^{-1}(\mathbf{r}t,\mathbf{r}'t') = (i\partial/\partial t + \mu - \nabla^2/2m)\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'),$$

and μ will not occur explicitly in the boundary condition on G.

If we now vary the chemical potential, Φ will change only as G changes. Therefore, from Eq. (57),

$$\frac{\partial \ln Z}{\partial\mu} = \pm\left(\operatorname{tr}\Sigma\frac{\partial G}{\partial\mu} - \frac{\partial}{\partial\mu}\operatorname{tr}\Sigma G - \operatorname{tr}\frac{\partial G^{-1}}{\partial\mu}G \right).$$

But

$$(\partial G^{-1}/\partial\mu) = (\partial G_0^{-1}/\partial\mu) - (\partial\Sigma/\partial\mu) = 1 - (\partial\Sigma/\partial\mu).$$

Thus

$$\frac{\partial \ln Z}{\partial\mu} = \mp\int_0^{-i\beta} dt\,d\mathbf{r}\,G(\mathbf{r}t,\mathbf{r}t^+) = \pm i\beta\int d\mathbf{r}\,G(\mathbf{r}t,\mathbf{r}t^+), \quad (59)$$

since $G(t,t^+)$ is independent of t. Equation (59) proves that the two evaluations of N agree.

As a consequence the approximation to the partition function determined by integrating Eq. (59) with respect to μ is identical to that which results from a coupling constant integration.

Consider next the derivative of the $\ln Z$ in Eq. (57) with respect to β. This gives an approximate evaluation of $-\langle(\tilde{H}-\mu N)\rangle$. We can also write an expression for $\langle(\tilde{H}-\mu N)\rangle$ in terms of the one-particle Green's function:

$$\langle(\tilde{H}-\mu N)\rangle = \pm i\int d\mathbf{r}\left[\frac{1}{2}\left(i\frac{\partial}{\partial t} - \frac{\nabla^2}{2m} - 2\mu\right)G(\mathbf{r}t,\mathbf{r}'t')\right]_{\mathbf{r}'=\mathbf{r},\,t'=t}$$

$$= \pm i\int d\mathbf{r}\left(-\frac{\nabla^2}{2m}G(\mathbf{r}t,\mathbf{r}'t^+)\right)_{\mathbf{r}'=\mathbf{r}}$$

$$\pm\frac{i}{2}\int d\mathbf{r}_1 d2\,\Sigma(1,2)G(2,1^+)$$

$$\mp i\mu\int d\mathbf{r}_1\,G(1,1^+). \qquad (60)$$

[8] C. Bloch and C. DeDominicis, Nuclear Phys. 7, 459 (1958).
[9] This formula was first given by J. M. Luttinger and J. C. Ward, Phys. Rev. 118, 1417 (1960).

The first term is the kinetic energy and the second, as we have seen, is the potential energy. Once again, when $\Sigma = \delta\Phi/\delta G$, these two approximate evaluations of $\langle(H-\mu N)\rangle$ agree.

To show this equality, we must differentiate Eq. (57) with respect to β. This is complicated by the fact that the inverse temperature occurs explicitly in the limits of the time integrations (0 to $-i\beta$). We shall therefore proceed in a somewhat roundabout fashion.

We first differentiate Eq. (57) with respect to m^{-1}, the inverse of the particle mass. The calculation is identical to the μ differentiation that we just carried out, only now

$$(\partial/\partial m^{-1})G_0^{-1}(\mathbf{r}t,\mathbf{r}'t') = \tfrac{1}{2}\nabla^2\delta(\mathbf{r}-\mathbf{r}')\delta(t-t').$$

Hence

$$m^{-1}\frac{\partial \ln Z}{\partial m^{-1}} = \mp \int_0^{-i\beta} dt d\mathbf{r}\left[\frac{\nabla^2}{2m}G(\mathbf{r}t,\mathbf{r}'t^+)\right]_{\mathbf{r}'=\mathbf{r}}. \quad (61)$$

The right side is exactly $-\beta$ times the kinetic energy evaluated from G. (This is another exact relation preserved by Φ-derivable approximations.)

We now notice that the entire β, m, μ, and λV dependence of $\ln Z$ in Eq. (57) enters through the combinations βm^{-1}, $\beta\mu$, and $\beta\lambda V$. This is obvious for the exact partition function from its definition. It must only be seen that the approximation maintains this structure.

Let us write the exact G equation in terms of the time variable $\tau = t/\beta$ which ranges from 0 to $-i$. Also, we include μN in the Hamiltonian. Let $\mathcal{G}(\tau,\tau') = G(\beta\tau,\beta\tau')$. Then the boundary condition obeyed by $\mathcal{G}(\tau,\tau')$ contains no reference to β or μ, and it obeys the exact equation of motion

$$\left(i\frac{\partial}{\partial\tau}+\beta\frac{\nabla^2}{2m}+\beta\mu\right)\mathcal{G}(\tau,\tau')$$

$$= \delta(\tau-\tau')\pm i\int \beta\lambda V\mathcal{G}_2(\tau,\tau;\tau',\tau^+).$$

Here $\mathcal{G}_2(\tau,\tau';\tau'',\tau''') = G_2(\beta\tau,\beta\tau';\beta\tau'',\beta\tau''')$. The m and μ dependence is in the combinations $\beta\mu$ and βm^{-1}. The remaining β dependence is in the $\beta\lambda V\mathcal{G}_2$ term. When $V G_2$ is approximated by ΣG, and Σ depends on G and V, it is clear that $\beta\lambda V\mathcal{G}_2$ will be approximated by the corresponding functional of $\mathcal{G}$ and $\beta\lambda V$. Thus the remaining β dependence as well as the entire λV dependence is in the combination $\beta\lambda V$. It follows then that the $\ln Z$, constructed by Eq. (57) in terms of $\mathcal{G}$, will depend only on $\beta\mu$, βm^{-1}, and $\beta\lambda V$. We may therefore evaluate $\partial \ln Z/\partial\beta$ as

$$-\frac{\partial \ln Z}{\partial\beta} = -\frac{m^{-1}}{\beta}\frac{\partial \ln Z}{\partial m^{-1}}-\frac{\lambda}{\beta}\frac{\partial \ln Z}{\partial\lambda}-\frac{\mu}{\beta}\frac{\partial \ln Z}{\partial\mu}. \quad (62)$$

But we have already established that the three terms on the right are, respectively, the kinetic energy, the potential energy, and minus μ times the number of particles, each calculated in terms of the one-particle

Green's function. Thus the two methods of evaluating $\langle(H-\mu N)\rangle$ lead to the same result.

Consequently the partition function determined by integrating $\langle(H-\mu N)\rangle$, as found from G, with respect to β is identical to that which appears in Eq. (57).

Another important quantity obtained from the grand partition function is the pressure. This is determined by

$$P = (1/\beta)(\partial \ln Z/\partial\Omega), \quad (63)$$

where Ω is the volume of the system. (We assume now that $U=0$, and employ the translational invariance of the system.) The pressure is alternatively evaluated as one third the trace of the stress tensor. In the limit of large volume, this formula is[10]

$$P = \mp i[(\nabla^2/3m)G(\mathbf{r}t,\mathbf{r}'t^+)]_{\mathbf{r}'=\mathbf{r}}$$

$$-\frac{1}{6}\int d\mathbf{r}'(\mathbf{r}-\mathbf{r}')\cdot\boldsymbol{\nabla}v(\mathbf{r}-\mathbf{r}')$$

$$\times\langle\psi^\dagger(\mathbf{r}t)\psi^\dagger(\mathbf{r}'t)\psi(\mathbf{r}'t)\psi(\mathbf{r}t)\rangle. \quad (64)$$

We shall now show that evaluating P from (63) using the $\ln Z$ in Eq. (57) leads to the same result as does Eq. (64), where $\langle\psi^\dagger\psi^\dagger\psi\psi\rangle$ is evaluated in terms of the G_2 approximation in the G equation. A change in the volume of the system can be simulated by a change in the scale of lengths in the system. Besides the volume (or the density), the only lengths in the system are the potential range and the thermal wavelength of the particles, $\hbar(\beta/2m)^{1/2}$. Thus, if we let $m \to \sigma^2 m$ and $v(\mathbf{r}) \to v(\sigma\mathbf{r})$, we effectively change the volume of the system by a factor σ^3. Hence,

$$\frac{1}{\beta}\frac{\partial \ln Z}{\partial\Omega} = \frac{1}{3\beta\Omega}\left[\frac{\partial}{\partial\sigma}\ln Z[\sigma^2 m,v(\sigma\mathbf{r})]\right]_{\sigma=1}$$

$$= \frac{2m}{3\beta\Omega}\frac{\partial \ln Z}{\partial m}+\frac{1}{3\beta\Omega}\left[\frac{\partial}{\partial\sigma}\ln Z[m,v(\sigma\mathbf{r})]\right]_{\sigma=1}. \quad (65)$$

We have already shown in Eq. (61) that the first term on the right is $\mp[i(\nabla^2/3m)G(\mathbf{r}t,\mathbf{r}'t^+)]_{\mathbf{r}'=\mathbf{r}}$. To evaluate the second term, let $v(\mathbf{r}) \to v(\sigma\mathbf{r})$ in Eq. (57). Then Φ depends on σ through both its explicit V dependence and its dependence on G. Thus

$$\frac{\partial \ln Z}{\partial\sigma} = \pm\left[\left(\frac{\partial\Phi}{\partial\sigma}\right)_G+\text{tr}\Sigma\frac{\partial G}{\partial\sigma}-\frac{\partial}{\partial\sigma}\text{tr}\Sigma G-\text{tr}\frac{\partial G^{-1}}{\partial\sigma}G\right].$$

But $\partial G^{-1}/\partial\sigma = -\partial\Sigma/\partial\sigma$, so that

$$\frac{\partial \ln Z}{\partial\sigma} = \pm\left(\frac{\partial\Phi}{\partial\sigma}\right)_G$$

$$= \pm\int d1d2(\mathbf{r}_1-\mathbf{r}_2)\cdot\boldsymbol{\nabla}_1 V(1-2)\frac{\delta\Phi}{\delta V(1-2)}.$$

[10] See, for example, P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959), Eq. (2.34).

Here the variation of Φ with respect to V is understood to be the variation with respect to the explicit occurrences of V in Φ. But from Eqs. (50) and (54) it is clear that[11]

$$\delta\Phi/\delta V(1-2)=\pm(i/2)G_2(\mathbf{r}_1 t_1,\mathbf{r}_2 t_1;\mathbf{r}_1 t_1^{++},\mathbf{r}_2 t_1^{+}), \quad (66)$$

so that

$$\frac{1}{3\beta\Omega}\frac{\partial\ln Z}{\partial\sigma}=\frac{1}{6}\int d\mathbf{r}_2(\mathbf{r}_1-\mathbf{r}_2)$$

$$\cdot\nabla v(\mathbf{r}_1-\mathbf{r}_2)G_2(\mathbf{r}_1 t_1,\mathbf{r}_2 t_1;\mathbf{r}_1 t_1^{++},\mathbf{r}_2 t_1^{+}). \quad (67)$$

This is precisely the final term in Eq. (64) for the pressure. Therefore we see that Eqs. (63) and (64) both lead to the same approximate evaluation of the pressure.

Thus, we have shown that the common methods for obtaining the partition function from the equilibrium one-particle Green's function all lead to the same results when the self-energy is derivable from a Φ. These methods consist in integrating the potential energy, expressed in terms of ΣG, with respect to a coupling constant λ, integrating the number with respect to μ, integrating $\langle(H-\mu N)\rangle$ with respect to β, and finding the pressure directly in terms of the stress tensor. Because of this self-consistency, all thermodynamic relations derived from the partition function must remain true in the approximation.

One can expect the results of the above methods to agree exactly only when the approximate equation $(G_0^{-1}-\Sigma)G=1$ has been solved exactly. This is possible only in a few special cases. But the various evaluations of the partition function should agree more and more precisely as the approximate Green's function equation is solved with increasing accuracy.

Equation (57), because it is true in the exact theory, presents yet another method of calculating $\ln Z$ in the approximate theory. If one interprets the self-energy Σ in this formula to be $G_0^{-1}-G^{-1}$, then, as initially shown by Luttinger and Ward,[9] this evaluation of the partition function is stationary under variations of G arising from variations in the self-energy, at the point

$$\Sigma=G_0^{-1}-G^{-1}=\delta\Phi/\delta G. \quad (68)$$

This variational principle is true for W in the presence of any external disturbance $U(1,1')$. The evaluation of $\ln Z$ from (57) agrees with the other methods when (68) holds. But none of the other means of calculating $\ln Z$ have this stationary property, unless the variations preserve the relation (68); for we had to use this relation in order to introduce Σ into Eq. (47) relating Φ and W. The variations of Σ that preserve (68) are those arising from a variation of an explicit parameter in the theory, such as β, λ, μ, etc. (This does not mean that Z is stationary under variations of these parameters; only

that it is stationary under the variation of Σ due to variation of these parameters.)

The second variation of $\ln Z$, defined by Eq. (57) (where Σ means $G_0^{-1}-G^{-1}$), with respect to changes in G arising from changes in Σ has an interesting relation to the two-particle correlation function L. The first variation of (57) is

$$\delta\ln Z=\pm\mathrm{tr}(\delta\Phi/\delta G-\Sigma)\delta G, \quad (69)$$

which vanishes when we enforce (68). The second variation yields

$$\delta^2\ln Z=\pm\mathrm{tr}[\delta^2\Phi/\delta G^2-\delta\Sigma/\delta G]\delta G\delta G\pm\mathrm{tr}[\delta\Phi/\delta G-\Sigma]\delta^2 G.$$

But $\delta\Sigma=G^{-1}(\delta G)G^{-1}$, so that on setting $\delta\Phi/\delta G$ equal to Σ, we find

$$\frac{\delta^2\ln Z}{\delta G(1',1)\delta G(2',2)}$$

$$=\pm\left[\frac{\delta^2\Phi}{\delta G(1',1)\delta G(2',2)}-G^{-1}(1,2')G^{-1}(2,1')\right], \quad (70)$$

which, from Eq. (34), is just $-L^{-1}$. Thus

$$\delta^2\ln Z=-\int\delta G(1',1)L^{-1}(12,1'2')\delta G(2',2). \quad (71)$$

This equation is possibly a point from which to investigate, for a given approximation, the relation between the collective behavior described by L, and the extremum properties of the partition function calculated from (57) with $\Sigma=G_0^{-1}-G^{-1}$.[12]

V. ZERO-TEMPERATURE NORMAL FERMION SYSTEMS

There are several exact theorems, proven by perturbation theory for zero-temperature many-fermion systems, which remain true in Φ-derivable approximations. The Hugenholtz-Van Hove[13] theorem is one. This theorem may be regarded as having two parts, the first part, the simple one in this formalism, says that

$$\partial E/\partial N=\mu, \quad (72)$$

where E is the ground-state energy. If E is calculated from

$$E-\mu N=-\lim_{\beta\to\infty}\beta^{-1}\ln Z,$$

where

$$N=\lim_{\beta\to\infty}\beta^{-1}\partial\ln Z/\partial\mu,$$

then (72) is a trivial statement, since

$$\lim_{\beta\to\infty}\frac{\partial}{\partial\mu}\left(\frac{\ln Z}{\beta}-\frac{\partial\ln Z}{\partial\beta}\right)=0=N-\frac{\partial}{\partial\mu}(E-\mu N).$$

[11] From this equation and the symmetry of V in 1 and 2, one may show that condition B of I, the symmetry of $G_2(12,1^+2^+)$ in 1 and 2, must hold if Σ can be derived from a Φ.

[12] One example of such a connection, that between the stability of the zero-temperature random phase approximation and the minimization of the expectation value of the Hamiltonian in the Hartree-Fock approximation, has been shown by D. J. Thouless, Nuclear Phys. 21, 225 (1960).

[13] N. M. Hugenholtz and L. Van Hove, Physica 24, 363 (1958).

What is not trivial is that for Φ-derivable approximations, $\partial E / \partial N$ equals μ regardless of whether E or N is calculated from $\ln Z$ or from the one-particle Green's function. This is seen from the fact that

$$\lim_{\beta \to \infty} \left(\frac{\ln Z}{\beta} - \frac{\partial \ln Z}{\partial \beta} \right) = 0,$$

so that in the zero-temperature limit, $-\beta^{-1} \ln Z$ equals the right side of (60).

The second part of the Hugenholtz-Van Hove theorem, in its weaker form, states that the volume of the Fermi sea of the interacting system is equal to the volume of the Fermi sea of a non-interacting system with the same expectation value of the number of particles as the interacting system.

Luttinger[14] has given a proof of this theorem for the exact theory, which works for Φ-derivable approximations with no trouble. His proof makes use of the structure of the perturbation expansion in two ways. First, the proof depends on the fact that, for all $\mathbf{k}$, the single-particle lifetime function $\Gamma(\mathbf{k}, \omega)$, which is the discontinuity in the self-energy $\Sigma(\mathbf{k}, z)$ as z crosses the real axis at ω, is proportional to $(\omega - \mu)^2$, for ω very close to μ. This behavior of Γ follows from phase-space arguments,[15] and must therefore survive in a Φ-derivable approximation. The remainder of the structure of the exact theory in the proof is embodied in the existence of the exact Φ, which is expressed in terms of the Fourier series for G. As long as the approximate Σ can be derived from a Φ, this structure is fully maintained, and the proof goes through without modification.

The Brueckner theory of nuclear matter, carried out using the self-consistent T-matrix approximation [Eqs, (I, 53–56) with $U = 0$] is a Φ-derivable approximation.

and hence it must obey the Hugenholtz-Van Hove theorem. The failure of present nuclear matter calculations to obey this theorem must lie ultimately in their lack of self-consistency in determining the one-particle Green's function (or the equivalent).

In addition, the other results that Luttinger[11] has shown for zero-temperature normal fermions, such as the fact that the specific heat is linear in T, continue to hold for Φ-derivable approximations. This is because the proofs of those results rely only on the structure of Φ, expressed in terms of Fourier series for G, and the relation (57) of Φ to the partition function.

In conclusion, we remark that the requirement that an approximation be Φ-derivable is a useful criterion to apply in terminating the infinite hierarchy of coupled Green's function equations. Such an approximation leads to a completely self-consistent description of the equilibrium statistical mechanics, and furthermore it leads to a nonequilibrium theory in which the over-all conservation laws are included and which takes into account the same correlations as are considered in the equilibrium theory. One reason underlying the fact that these approximations have such a remarkable structure has been discovered by Kraichnan,[16] who has shown that in a certain sense they are exact solutions to model Hamiltonians containing an infinite number of stochastic parameters.

[14] J. M. Luttinger, Phys. Rev. 119, 1153 (1960).
[15] J. M. Luttinger, Phys. Rev. 121, 942 (1961).

[16] R. H. Kraichnan, Report HT-9, Division of Electromagnetic Research, Institute of Mathematical Sciences, New York University, 1961 (unpublished).