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Aspects of Green's Function Methods versus Self-Consistent Field Theory

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Abstract

The basic methods of solving fully symmetric, nonlinear theories are stated. These are discussed in terms of Green's function methods and self-consistent field theory methods. The equivalence of many-body theory based on Green's functions with quantum field theory, on which the self-consistent field theory is based, is reviewed. A number of similarities, differences, and cautions involved with these methods are determined. In particular, since very often both methods are based upon use of the adiabatic theorem, which is typically *not* applicable to the models under consideration, a deviation in the self-consistent theory is discussed that avoids this problem. A similar idea is used for solution of models with the functional integral method. Ferromagnetic models are used at various places in illustrating some of the ideas. By contrasting these methods further insight may be gained into solving nonlinear, physical theories.

1. *Introduction*

One of the most important problems in physics today is the solution of fully symmetric, nonlinear theories, with Hamiltonians expressed in terms of original variables (as compared to observed, physical variables). Some of these, for example, are the theories of ferromagnetism, superconductivity, and superfluidity. There appear to be four basic methods of solution that come to mind from the literature: (1) solution of the equations of motion in original variables; (2) perturbation theory, using Feynman diagrams, etc.; (3) functional integral approach; and (4) canonical transformation to the correct set of physical variables. Now (1), (2), and (3) typically involve Green's functions, whereas the fourth is most often handled by a self-consistent selection theory, either of wave functions (Hartree–Fock theory) or of Hilbert spaces (Umezawa's self-consistent field theory). The overall objective of each one is looking for the correct combination of original fields that produces the effects and characteristics that are physically observed and measured. However, the approach to doing this is very different in many

ways, and yet, similar in other ways for the Green's function methods as compared to the self-consistent field theory. In this paper I will discuss some of the aspects of these methods and contrast them for similarities, differences, and a major caution to be aware of in using them. I strongly feel that coordination and unification of the ideas and results of these methods in treating the same or very similar problems may well lead to further insight and understanding of some of our basic physical phenomena.

2. *Green's Function Methods*

In this section the definition of some of the properties of and ways of evaluating Green's functions will be briefly considered. Most of these will be of interest for the discussions in later sections.

The Green's functions describe the response of a system to external disturbances such as a varying external field or a strange particle moving through the system. They allow in a natural way the introduction of matrix elements connecting states differing in the number of particles. For example, a one-particle Green's function describes the motion of one particle added to a many-body system, and a two-particle Green's function describes the motion of two added particles. The physics of the many-particle medium is examined by studying the propagation in it of externally produced excitations. The propagation characteristics are expressed through one- and two-particle Green's functions defined as follows:

$$G_1(1\sigma_1, 2\sigma_2) \equiv -i\langle T\{\Psi_{\sigma_1}(1)\Psi^{\dagger}_{\sigma_2}(2)\}\rangle \tag{2.1}$$

$$G_2(1\sigma_1 2\sigma_2, 3\sigma_3 4\sigma_4) \equiv (-i)^2\langle T\{\Psi_{\sigma_1}(1)\Psi_{\sigma_2}(2)\Psi^{\dagger}_{\sigma_3}(3)\Psi^{\dagger}_{\sigma_4}(4)\}\rangle \tag{2.2}$$

where $\Psi^{\dagger}_{\sigma_1}(1)$ and $\Psi_{\sigma_1}(1)$ are the creation and annihilation operators associated with particles of spin σ_1, position $\mathbf{r}_1$, and time t_1, etc., and T is the Wick time ordering operator (Hugenholtz et al., 1969a).

There are two main methods of determining the Green's functions:

(1) The first method is perturbation series expansion of G in powers of the interaction potential, using the noninteracting system as the zero-order starting point. This diagrammatic technique has many good points. It enables one to make fairly well-defined approximations in which one chooses a certain class of diagrams and sums them, often to all orders in perturbation theory. At times it is also possible to get a rough idea of the importance of the terms that are neglected. However, it is hard to know how far one can trust perturbation theory. A good deal of juggling with the terms in the perturbation expansion is often done, and this should not be done unless one knows that the series is absolutely convergent. Further, for some of the models we are mainly interested in in this paper, such as superconductivity, the series does not converge (Hugenholtz et al., 1969b).

(2) The second method is solving the equations of motion for G. Here one constructs $(\partial G/\partial t)$ from the known time evolution of the field operators. This ordinarily leads to a set (probably infinite) of coupled equations for higher and higher order Green's functions. In certain cases physical arguments can be used to truncate the set and obtain a closed set of differential equa-

tions for G. Because of the difficulties mentioned above with the perturbation methods, it appears that the equations of motion methods are to be preferred ab initio. Here, however, one often has not such a clear idea of the terms one is neglecting in the approximations. Usually, one is making some sort of higher random-phase approximation, and also it seems more difficult to derive exact results from this formulation (Hugenholtz et al., 1969c). Both methods have proven useful in certain problems, but neither is too good for the Kondo effect, although perturbation theory seems a little better (Keiter and Kimball, 1970).

Some of the above-mentioned difficulties led Evenson, Schrieffer, and Wang (1970) in their analysis of the Hubbard and Anderson models for itinerant ferromagnets to a third method using Green's functions, the functional integral approach:

(3) As applied to the Anderson model (Anderson, 1961), the essential steps are as follows: (a) rewriting the two-body exchange interaction as a perfect square, using the properties for fermion occupation number operators:

$$Un_\uparrow n_\downarrow \to -\tfrac{1}{2}U(n_\uparrow - n_\downarrow)^2 + \text{one-body term} \tag{2.3}$$

where U is the Coulomb interaction, n is a number operator, and the arrows refer to spin. (b) Separate the Hamiltonian H into bilinear terms, H_0, and higher-order terms, H_1. Since H_0 and H_1 do not commute, use the Feynman time-ordering trick:

$$\exp\,[A + B] = T \exp \int_0^1 d\tau (A_\tau + B_\tau) \tag{2.4}$$

where τ is a fictitious "time," T is the chronological ordering operator, which orders products like $A_\tau B_{\tau'} A_{\tau''}$ chronologically with larger "times" to the left. Thus, A_τ and B_τ commute if one operates with T at the end. (Remember this step, in particular, when we later discuss alterations in the self-consistent field theory.)

(c) Use the Stratonovich (1958) trick of reducing the partition function with a two-body interaction term to an average over partition functions with one-body interactions in a random-averaged, external "magnetic" field:

$$\exp(\pi a^2) \equiv \int dx \exp[-\pi x^2 + 2ax] \tag{2.5}$$

where for this model,

$$\exp(\pi a^2) \leftrightarrow \exp\left\{-\beta \int_0^1 d\tau \left[-\frac{U}{2}(n_{\uparrow_\tau} - n_{\downarrow_\tau})^2\right]\right\} \tag{2.6}$$

(d) Then the partition function ($Z = \mathrm{Tr}\,[\exp(-\beta H)]$) becomes

$$Z = \int \mathscr{D}\xi(\tau) \exp\left[-\pi \int_0^1 d\tau\, \xi^2(\tau) Z(\xi)\right] \tag{2.7}$$

where $Z(\xi)$ is

$$Z(\xi) = \mathrm{Tr}\left\{T \exp\left[-\int_0^1 d\tau (\beta H_{\sigma_\tau} - c\xi(\tau)(n_{\uparrow_\tau} - n_{\downarrow_\tau}))\right]\right\} \tag{2.8}$$

At this point the partition function for the two-body system has been reduced to an average over partition functions in an external "magnetic field" $\xi(\tau)$. This is an exact transformation—the external field and Gaussian weight factor being arranged to give the precise effect of the true exchange interaction in the original Hamiltonian. The problem now involves (1) finding $Z(\xi)$, and (2) doing the functional integration; and at this point Green's functions are introduced in the calculations. Either or both of these could involve approximations (Evenson et al., 1970). Then physical properties like magnetic susceptibility, etc., can be calculated.

Having explored the three basic methods using Green's functions, let us look briefly at a general model of itinerant ferromagnetism using Green's functions for analysis to see what quantities and results are typically found so these can be compared with those of the self-consistent field theory in a later section. The occurrence of ferromagnetism in a system of fermions of spin $\frac{1}{2}$ has been discussed extensively by Rajogopal et al. (1967). The Hamiltonian of the fermions is given by

$$H = \sum_{\sigma} \int d^3 1 \Psi_\sigma{}^\dagger(1) \left[-\frac{\Delta_1{}^2}{2m} + V(\mathbf{r}_1) \right] \Psi_\sigma(1) + \tfrac{1}{2} \sum_{\sigma_1, \sigma_2} \int d^3 1 d^3 2 \, dt_1 \, dt_2 \; \Psi^\dagger_{\sigma_1}(1) \Psi^\dagger_{\sigma_2}(2) V(1\text{-}2) \Psi_{\sigma_2}(2) \Psi_{\sigma_1}(1) \tag{2.9}$$

where the Ψ's have the same description as those in equations (2.1) and (2.2) and have the usual anticommutation algebra. $V(\mathbf{r}_1)$ is a background potential, and $V(1\text{-}2)$ is a short-ranged, instantaneous interaction potential between the fermions. Time dependence of operators is in the Heisenberg representation, and expectation values $\langle O \rangle$ of an operator O can be considered as being in the grand canonical ensemble. The magnetization operator is given by

$$M = \int d^3 1 \rho_z(1) = \int d^3 1 \left[\Psi_\uparrow{}^\dagger(1) \Psi_\uparrow(1) - \Psi_\downarrow{}^\dagger(1) \Psi_\downarrow(1) \right] \tag{2.10}$$

As discussed above, the physics of the many-fermion medium is studied using Green's functions, through which the propagation of externally produced excitations are expressed. See equations (2.1) and (2.2). Here the sources of the excitations are classical fields $U(1\sigma_1, 2\sigma_2)$, entering through

$$H' \equiv \sum_{\sigma_1 \sigma_2} \int d^3 1 \, d^3 2 \; U(1\sigma_1, 2\sigma_2) \Psi^\dagger_{\sigma_1}(1) \Psi_{\sigma_2}(2) \tag{2.11}$$

and can be interpreted in terms of nonlocal fluctuations in the internal magnetic field or the chemical potential. The effects of the sources are traced through functional derivatives of the Green's functions, such as the two-particle correlation function

$$L(1\sigma_1 2\sigma_2, 3\sigma_3 4\sigma_4) = G_2(1\sigma_1 2\sigma_2, 3\sigma_3 4\sigma_4) - G_1(1\sigma_1, 3\sigma_3) G_1(2\sigma_2, 4\sigma_4) = \frac{\delta G_1(1\sigma_1, 3\sigma_3)}{\delta U(4\sigma_4, 2\sigma_2)} \bigg|_{V=0} = \frac{\delta G_1(2\sigma_2, 4\sigma_4)}{\delta U(3\sigma_3, 1\sigma_1)} \bigg|_{V=0} \tag{2.12}$$

From the Green's functions one can obtain many important physical quantities. The magnetization $\langle M \rangle$ can be expressed in terms of G_1, the average energy $\langle H \rangle$ in terms of G_1 and G_2 or L, and the susceptibilities and the specific heat are closely related to L (Rajagopal et al., 1967). Also, from the Green's functions one can express the manner in which the interaction $V(1\text{-}2)$ affects the propagation of an excitation in the medium, find a measure of the interaction between the excitations in the medium, and find by iteration an expression for scattering of the excitations (Rajagopal et al., 1967 and Baym and Kadanoff, 1961). Notice that this all involves looking for the correct combinations of original fields, the Ψ's, which gives the physical quantities and effects just stated. This is also the objective of the self-consistent field theory, but the approach is much different.

As will be discussed later, one of the basic results of the self-consistent field theory is the *non*-incidental occurrence of Goldstone-type modes in the theories we are discussing. Now is this a basic result in the Green's functions methods? For the model just above, let us write down the quantity giving a measure of the probability of a spin-flip at 1:

$$\langle j_0(1\uparrow, \downarrow) \rangle \equiv \langle \Psi_\downarrow{}^\dagger(1) \rangle = -iG_1(1\uparrow, 1\downarrow) \tag{2.13}$$

Then if the system is uniform, $\langle \rho_Z(1) \rangle$ is independent of position, and one can use the Fourier transform function $\Lambda_i(\mathbf{k}, \omega)$ given by

$$\Lambda_i(\mathbf{k}, \omega) = \int d^4 1 \exp\{i[\omega(t_1 - t_2) - \mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)]\} \langle T\{j_i(1\uparrow, \downarrow) j_0(2\uparrow, \downarrow)\} \rangle \tag{2.14}$$

to obtain, as R. E. Mills (1970) did, the following equation:

$$\omega \Lambda_0(\mathbf{k}, \omega) - \mathbf{k} \cdot \boldsymbol{\Lambda}(\mathbf{k}, \omega) = \langle (\rho_Z) \rangle \tag{2.15}$$

As pointed out by Mills, the arguments of Lange (1965) concerning the Goldstone mode apply, and one concludes that when $\langle \rho_Z \rangle$ does not vanish, i.e., a continuous rotation is no longer an invariant operation, the functions Λ_i must have singular parts when ω and $\mathbf{k}$ vanish if equation (2.15) is to be satisfied. Thus, the implications of Goldstone-type modes are here if looked for hard enough. Next we will briefly review the self-consistent field theory and some of its implications.

3. *Self-Consistent Field Theory*

As previously indicated, we begin the study of our physical system by writing down an appropriate Hamiltonian $H = H_0 + H_{\text{int}}$ for the system in original variables and second-quantizing it. It gives in general nonlinear equations which we then try to solve in order to deduce the results that can be compared with experiments. Umezawa et al. (1965) have formulated this step as a dynamical mapping between the original set of annihilation and creation operators $(a_k, a_k{}^\dagger)$, in terms of which the model is written down, and the

physical annihilation and creation operators (b_k, $b_k^\dagger$), in terms of which the observed stationary states are written (also referred to as quasiparticle operators):

$$a_k = f(b_k) = C + g_k b_k + h_k b_k^\dagger + N_p(b_k) \tag{3.1}$$

where C stands for a constant and $N_p(b_k)$ for higher-order normal products. Equation (3.1) is one representation of the fourth basic method of solution outlined in the introduction of this paper, where the a's here correspond to the Fourier transforms of the Ψ's in Section 2. The expansion coefficients, such as g and h, are to be determined so that when equation (3.1) is inserted into the original Hamiltonian, H takes the form

$$H = \sum_k E_k b_k^\dagger b_k + C + Q_V(b_k) = H_0(b_k) + Q_V(b_k) \tag{3.2}$$

where $Q_V(b_k) \to 0$ when the volume V becomes very large (maybe infinite), and E_k is a c number. The b_k's satisfy the same commutation (anticommutation) rules as the a_k's (spoken of as a canonical transformation).

In most cases the determination of the coefficients in equation (3.1) is carried out in two stages. First we make a canonical Bogoliubov-type transformation T from the a_k's to the intermediate $\bar{b}_k$ fields, and then we look for a matrix S which takes us from the $\bar{b}_k$'s to the b_k's (physical fields) in such a way that

$$\bar{b}_k = (Z)^{1/2} b_k + N_p(b_k) \tag{3.3}$$

where Z is a c number.

Under the Bogoliubov-type transformation T and upon normal-ordering our operators (denoted by $:X:$) and eliminating off-diagonal bilinear terms, our original Hamiltonian becomes

$$H(\bar{b}_k) = H_0(\bar{b}_k) + :H_{\text{int}}(\bar{b}_k): \tag{3.4}$$

Then Umezawa proceeds to eliminate the higher-order (H_{int}) terms by employing the adiabatic theorem. This is done by taking

$$\bar{b}_k = S^{-1} b_k S \tag{3.5}$$

where, to first order in $:H_{\text{int}}(\bar{b}_k):$,

$$S = 1 + (-i) \int_{-\infty}^{0} :H_{\text{int}}(t): \, dt$$

and

$$H_{\text{int}}(t) = \exp(\epsilon t) \, H_{\text{int}}(b_k \exp(-iE_k t))$$

with

$$\epsilon \sim V^p, \; -(1/3) < p < 0 \tag{3.6}$$

for large V. From equation (3.6), equation (3.4) becomes

$$H(\bar{b}_k) \to S^{-1} H(b_k) S = H_0(b_k) + Q_V(b_k) \tag{3.7}$$

where $Q_V(b_k)$ is an operator such that the limit of its matrix elements taken between any two states of the physical Fock representation of the b_k's as V becomes large (maybe infinite) is zero.

The important result of using the adiabatic theorem above [essentially equation (3.6)] is that $Q_V(b_k)$ in equation (3.7) then has energy-conserving matrix elements with respect to the physical Fock-space states. It is this energy-conserving constraint that causes

$$\lim_{V\to\infty} Q_V(b_k) \to 0 \tag{3.8}$$

as will be indicated below.

The motivation for the above technique came from a proposal by Gunnar Källén (1968) showing the credibility of obtaining bilinear Hamiltonians in general when applying the adiabatic theorem. Again, we start with the Hamiltonian, $H = H_0 + H_{\text{int}}$. Then we introduce formally a coupling constant that is weakly time dependent, writing H as

$$H = H_0 + g \exp(\epsilon t) H_{\text{int}} \tag{3.9}$$

where ϵ is a very small positive number and in the final result we let it go to zero. The general idea is that the coupling constant, $g(t) = g[\exp(\epsilon t)]$, should have its physical value for all finite times where the interaction is important but that it should vanish sufficiently rapidly for large absolute values of the time.

Writing down the equation of motion for H, we have

$$i\frac{dH(t)}{dt} = [H, H] + \frac{i\partial H(t)}{\partial t} = i\frac{dg(t)}{\mathrm{dt}}\frac{\partial [H_{\text{int}} g(t)]}{\partial \mathrm{g}} \tag{3.10}$$

Integrating both sides from t_1 to t gives

$$H(t) = H(t_1) + \int_{t_1}^{t} \dot{g}(t') \frac{\partial [H_{\text{int}} g(t')]}{\partial g}\, dt' \tag{3.11}$$

In particular, letting $t_1 \to -\infty$, we have

$$H(t) = H_0 \text{ (incoming fields)} + \int_{-\infty}^{t} \dot{g}(t') \frac{\partial [H_{\text{int}} g(t')]}{\partial g}\, dt' \tag{3.12}$$

Now considering the off-diagonal matrix elements of the second term on the right-hand side of equation (3.12) and putting them in the form of $g(t)$ above, we have

$$\begin{aligned}
&\int_{-\infty}^{t} \left\langle a \left| \frac{\partial [H_{\text{int}} g(t')]}{\partial g} \right| b \right\rangle \dot{g}(t')\, dt' \\
&= \int_{-\infty}^{t} \exp[-i(E_a - E_b)t'] \langle a | H_{\text{int}} | b \rangle \epsilon g \exp(+\epsilon t')\, dt' \\
&= [\epsilon + i(E_a - E_b)]^{-1} \epsilon \langle a | H_{\text{int}} | b \rangle g \exp(\epsilon t)
\end{aligned} \tag{3.13}$$

Then taking the limit as $\epsilon \to 0$, this expression gives zero unless $E_a = E_b$. The conclusion to be drawn is that off-diagonal matrix elements of the last term on the right-hand side of equation (3.12) must have energy-conserving matrix elements in order to give a contribution.

However, the proof is incomplete in one place namely, in the second line of equation (3.13). Since the Hamiltonian is not exactly time independent due to the introduction of the adiabatic switching factor, $\exp(\epsilon t)$, it is expected that

$$\langle a \mid H_{\text{int}}(t') \mid b \rangle = \exp[-i(E_a - E_b)t'] \langle a \mid H_{\text{int}} \mid b \rangle$$

holds only in the limit as $\epsilon \to 0$, assuming that this limit exists. Otherwise, the states are time dependent and equation (3.13) may not follow. Thus, it is assumed that the solutions exist in the adiabatic limit when $\epsilon \to 0$. However, as Källén points out, at present there is no proof of this independent of perturbation theory. Notice that it is precisely off-diagonal elements of this same type which give rise to asymmetry and condensed phases when using Green's functions methods for models such as the ones we are considering (Mattuck and Johansson, 1968). Thus, both the self-consistent field theory and Green's functions methods could break down if the limit taken in equation (3.13) does not exist.

However, as pointed out by Benson (1973) and Benson and Hatch (1973), the adiabatic theorem need not be used to obtain the energy-conserving constraint above. This condition was instead obtained for the Heisenberg ferromagnetic model by finding the condition for $[H_{\text{bi}}(b_k), H_{\text{quad}}(b_k)] = 0$, a possibility alluded to by Umezawa and Leplae (1964) in a footnote of one of their papers, where [,] stands for the commutator, "bi" for bilinear, and "quad" for quadrilinear. For the Heisenberg magnetic-exchange model this places conditions upon the exchange integral of the interaction term, leading to a nearest-neighbor interaction. The self-consistent field theory of Umezawa then involves the following steps: (1) Transform from the original variables to a generalized, parametrized set of variables (dynamical map), [see equation (3.1)]; (2) normal-order the operators in H by using Wick's theorem; (3) eliminate off-diagonal terms so as to determine the coefficients of the dynamical map (these are self-consistent equations); (4) show that the higher-order (higher than second, and thus involved in H_{int}) terms have energy-conserving matrix elements in our physical Fock space *without* using the adiabatic theorem (see Benson, 1973, for an example clearly showing this); (5) take the limit as V becomes large (maybe infinite) in order to eliminate the higher-order terms and leave one with a physical, bilinear Hamiltonian (see Benson, 1973, where this bilinear Hamiltonian obviously expresses a ferromagnetic system, having been derived from the totally rotationally symmetric Heisenberg magnetic-exchange model using the five steps of this self-consistent field theory).

It is very interesting to note the similarity in technique of step (4) for the self-consistent field theory with step (b) of the third approach based upon finding Green's functions, the functional integral approach. Both involve

looking for commutation between H_{bi} and higher-order terms in H, making up H_{int}. It is apparent that in both cases one is looking for a separation of the Hilbert space upon which H_{bi} is based and that upon which $H = H_{bi} + H_{int}$ is based. This allows for a separation of partition functions in the functional integral method and of Hamiltonian terms in the self-consistent field theory method. Notice that in the former method this leads to just a separation into direct products of Hilbert spaces, whereas in the latter method the implications are much farther reaching [when step (5) is carried out], for then we have disjointness of Hilbert spaces, or inequivalent representations (Benson and Hatch, 1975). It would appear, however, that there is a definite connection between writing the partition function, Z, as a direct product and eliminating higher-order terms in the Hamiltonian. This is indeed the case, as will be determined shortly. However, to see this more clearly let us first review some of the results of Benson (1973) and Benson and Hatch (1973) when the self-consistent field theory outlined above is applied to the Heisenberg-exchange model.

The Hamiltonian of the model can be written as

$$H = -\sum_{\mathbf{l}\neq\mathbf{l}'}\sum J_{\mathbf{l}-\mathbf{l}'}\,\mathbf{S}_{\mathbf{l}}\cdot\mathbf{S}_{\mathbf{l}'} \tag{3.14}$$

where $\mathbf{S}_{\mathbf{l}}$ is the spin operator for the fermion at the $\mathbf{l}$th lattice site, and $J_{\mathbf{l}-\mathbf{l}'}$ is the exchange integral, typically taken as large only when $\mathbf{l}-\mathbf{l}'$ is one or two lattice spacings. This is then second-quantized and written in terms of annihilation and creation operators, the a's. We know that the model ($\mathbf{S}\cdot\mathbf{S}$ form) is totally symmetric with respect to spin orientation, and there is no reason a priori to expect H to describe a ferromagnetic configuration (all spins aligned in a particular direction), since this represents asymmetry. When the five steps of the self-consistent field theory above are carried out, one obtains a Hamiltonian in physical variables of the form

$$H = -\sum_{\mathbf{l}} H_{\mathbf{l}}\mathscr{S}_{\mathbf{l}}^{z} \tag{3.15}$$

where $\mathscr{S}$ is the spin component written in terms of physical variables, the b's, and $B_{\mathbf{l}}$ is a constant depending on $J_{\mathbf{l}-\mathbf{l}'}$ and expectation values of the operators. This obviously describes an assembly of independent spin-$\frac{1}{2}$ particles, and $B_{\mathbf{l}}$ can be interpreted as an internal magnetic field produced by the interactions between the fermions, and all spins are aligned in some manner by this field. This then is indeed a ferromagnetic representation for the Heisenberg-exchange model.

Thus, if one compares the general results of the self-consistent field theory applied to the above model [equation (3.14)] with the functional integral approach applied to the Anderson model (see Section 2), one sees that they both lead to bilinearization in an effective, averaged-out magnetic field. Thus, writing the partition function, Z, as a direct product and eliminating higher-order terms in the Hamiltonian appear to be equivalent steps, but formulated in a different context.

Continuing with some of the results obtained when one applies the self-consistent field theory to the Heisenberg-exchange model, one finds explicitly that Goldstone's theorem (Lange, 1965) is satisfied by comparing the spin-rotation symmetry of the system in original variables with that same symmetry when written in terms of physical variables. The symmetry transformations for the original fields were found to take entirely different forms for the physical fields, spoken of as a dynamical rearrangement of symmetry (Leplae et al., 1967), and it was found that the original spin-rotation symmetry transformation is taken up by physical "massless" fields (Goldstone modes) and that the Bose-Einstein condensations of these fields in the physical (ferromagnetic) ground state produce the asymmetry by "printing" the spin quantum number on that state (Benson and Hatch, 1973). These results come from a quite natural flow of thoughts and questions and give a very good explanation for the microscopic mechanism producing observed macroscopic asymmetry. The Goldstone-type modes and results described above appear in many second-order phase transitions where a symmetry is broken, so the equations and ideas above are indicative of a more general problem than the restriction to magnetism might possibly indicate. Next we look briefly at the basic equivalence between many-body theory based on Green's functions with quantum field theory, on which the self-consistent field theory is based.

4. *Many-Body Theory and Field Theory*

We write the Hamiltonian, H, for a system of many particles interacting with each other as $H = H_0 + H_{\text{int}}$ (as done in the previous two sections), and note that when this is written in second-quantized form it has a great analogy with field-theoretical Hamiltonians. For example, let us consider, as did Van Hove (1961), a Fermi gas of N identical particles in a cubic container of volume V, and apply periodic boundary conditions. Then $H = H_0 + H_{\text{int}}$ is given by

$$H_0 = (1/2M) \sum_l l^2 a_1^\dagger a_1$$

$$H_{\text{int}} = \tfrac{1}{2}(8\pi^3/V) \sum_{l_1, l_2, l_3, l_4} v(l_1, l_2, l_3, l_4)\, \delta_{l_1+l_2, l_3+l_4}\, a_{l_1}^\dagger a_{l_2}^\dagger a_{l_3} a_{l_4} \quad (4.1)$$

where we will take the mass, M, to be $\frac{1}{2}$, v is the interaction potential, l refers to momentum, and the a's are annihilation and creation operators.

The unperturbed ground state, $|\phi_0\rangle$, of the Fermi gas is obtained by filling all states of momentum $|l| \leqslant p_f$ with particles, leaving all other states unoccupied, where for spin-$\frac{1}{2}$ particles the density is given by

$$\rho = (p_f^3/3\pi^2) = N/V \quad (4.2)$$

[This Hamiltonian is very similar in form to that used previously in equation (2.9).]

Now note the analogy with quantum field theory: $|\phi_0\rangle$ corresponds to the vacuum state, $a_1^\dagger$ corresponds to creation of a particle with $|l| > p_f$, and a_1 to the creation of an antiparticle $|l| \leqslant p_f$. However, there is a difference since the energy of the ground state (perturbed as well as unperturbed) is a quantity proportional to V, and so for large V and fixed ρ one sees that for the many-body problem one will have to treat the limit $V \to \infty$ more carefully than in field theory, when all quantities usually calculated have finite limits for $V \to \infty$ (Van Hove, 1961). See step (5) of the self-consistent field theory method (Section 3).

Analogous to the ideas of Gell-Mann and Low in field theory, Goldstone postulated a perturbed ground state given by

$$|\Psi_0\rangle = U(0, -\infty)|\phi_0\rangle \tag{4.3}$$

where $U(t, t_0)$ is the solution of

$$\frac{i\partial U(t, t_0)}{\hbar\,\partial t} = H_{\text{int}}U(t, t_0), \qquad U(t_0, t_0) = 1 \tag{4.4}$$

The limit $t_0 \to -\infty$ in $U(0, -\infty)$ is taken by *adiabatic* switching on of the interaction. One finds quite easily that the difference between the perturbed ground state energy, E_0, and the unperturbed ground state energy, ϵ_0, is given by

$$[E_0 - \epsilon_0] = \frac{\langle\phi_0|H_{\text{int}}U(0, -\infty)|\phi_0\rangle}{\langle\phi_0|U(0, -\infty)|\phi_0\rangle} \tag{4.5}$$

where for the fermion gas, $\epsilon_0 = Vp_f^5/10\pi^2$. Then one can carry out a diagrammatic analysis of the two matrix elements using the iterative solution to equation (4.4),

$$U(t, t_0) = 1 + \sum_{n=1}^{\infty} (-i/\hbar)^n (1/n!) \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t} dt_n T[H_{\text{int}}(t_1) \cdots H_{\text{int}}(t_n)] \tag{4.6}$$

where T is the Wick time-ordering operator. Diagrams are constructed by representing each H_{int} by a vertex, with the same left to right ordering of vertices in the diagram as of the corresponding H_{int}'s in equation (4.6).

Assuming all energies are redefined by subtracting ϵ_0, so that H_0 is replaced by $H_0 - \epsilon_0$, and that $\langle\phi_0|\phi_0\rangle = 1$, one then has *as in field theory*,

$$\langle\phi_0|H_{\text{int}}U(0, -\infty)|\phi_0\rangle = \left[\sum_\delta \langle\phi_0|\{H_{\text{int}}U(0, -\infty)\}_\delta|\phi_0\rangle\right]\langle\phi_0|U(0, -\infty)|\phi_0\rangle \tag{4.7}$$

where $\langle|\{\cdots\}_\delta|\rangle$ means the contribution of a specific diagram δ to the matrix element $\langle|\cdots|\rangle$, and where Σ_δ extends over all connected diagrams. Hence,

$$[E_0 - \epsilon_0] = \sum_\delta \langle\phi_0|\{H_{\text{int}}U(0, -\infty)\}_\delta|\phi_0\rangle \tag{4.8}$$

The importance of the expression $E_0 - \epsilon_0$ is that every term in the sum has the form VX finite quantity for large V, which is the correct behavior in V expected on physical grounds for E_0 itself (Van Hove, 1961).

Furthermore, one finds that

$$|\Psi_0\rangle = \frac{U(0, -\infty)\,|\phi_0\rangle}{\langle\phi_0|\,U(0, -\infty)\,|\phi_0\rangle} \tag{4.9}$$

and that the exact one-particle Green's function is given by

$$G(k, t) = -i\,\frac{\langle\phi_0|\,T[a_k(t)a_k^{\dagger}(0)U(+\infty, -\infty)]\,|\phi_0\rangle}{\langle\phi_0|\,U(\infty, -\infty)\,|\phi_0\rangle} \tag{4.10}$$

where all quantities are again in the interaction representation and $U(\infty, -\infty)$ is the S-matrix like that of field theory. It is then useful to combine equation (4.6) with equation (4.10) to determine the Green's function.

Therefore, many-body theory based upon the determination of the Green's functions above (essentially method one in the introduction) is basically equivalent to quantum field theory. However, note that here, as well as in the original formulation of the self-consistent field theory (Section 3), the adiabatic theorem has been used to obtain final results. Problems and cautions with this were discussed following equation (3.13). Also, one sees immediately from equation (4.9) that one is assuming a one-to-one correspondence between the states of the proper H_0 and those of the interacting Hamiltonian, $H = H_0 + H_{\text{int}}$ (see Noziéres, 1968). But for the type of theories we are considering in this paper, this is usually not the case. For example, it is clearly shown by Benson (1973) that for the Heisenberg-exchange model there is not a one-to-one correspondence between paramagnetic states and ferromagnetic states.

Consequently, *when* one is careful and selects a correct H_0, etc., so that the adiabatic theorem *holds*, then many-body theory based on determining Green's functions is essentially equivalent to quantum field theory. However, one needs to be very cautious and may want to give strong consideration to using the altered self-consistent field theory outlined and discussed in Section 3.

5. *Some Similarities and Differences*

After the discussions, reviews, and developments concerning the basic methods of solving nonlinear theories in the preceding four sections, let us contrast the methods involving Green's functions with the method typically involving the self-consistent field theory. First let us consider some of the similarities.

(1) As pointed out in Section 4, one can employ the techniques of quantum field theory to solve nonlinear theories using Green's functions or the self-consistent field theory. However, as emphasized, one must be very careful when the adiabatic theorem, which is typically used, is employed. In the

case of using Green's functions, the problem comes from the fact that for many fully symmetric, nonlinear theories, such as ferromagnetism, superconductivity, superfluidity, and other phase transition phenomena, there is not a one-one correspondence between the states of H_0 and those of $H = H_0 + H_{\text{int}}$, so that expansion of one in terms of the other is meaningless and not applicable. Whereas, for the self-consistent field theory the problem comes from the fact that the energy-conserving constraint necessary for elimination of H_{int} in physical variables in the limit as V becomes large may not hold because of the time dependence introduced into H_{int} through the adiabatic-switching factor. This may be overcome in this case, however, by using the alternative formulation in Section 3.

(2) As already discussed in (1) above and in the preceding sections, both sets of methods are often based on the adiabatic theorem. The basic difficulties and reasons for these are discussed in (1) above and in Sections 3 and 4.

(3) As seen from the ferromagnetic models considered in Sections 2 and 3, both sets of methods can reveal Goldstone-type modes if they exist. However, as pointed out, these come much more naturally as part of the self-consistent field theory, and as will be discussed in the differences, the importance and emphasis of these modes as a fundamental mechanism in physical phenomena is much different in these methods, being very basic in the self-consistent field theory while only incidental in the Green's functions methods.

(4) Both sets of methods look for appropriate arrangements and combinations of original variables, such as equations (2.1), (2.2), (2.7), (2.14), (3.1), and (3.7), in order to explain physical properties, but as can be seen from examining the foregoing equations and as will be discussed further in the differences, the manner in which this is done is very different.

(5) The altered five-step self-consistent field theory in Section 3 and the functional integral approach, one of the methods involving finding Green's functions, of Section 2 both involve looking for commutation of H_0 with H_{int}. This step leads to bilinearization of the Hamiltonian in physical variables in the self-consistent field theory, whereas it leads to separation of the partition function into direct products in the functional integral method. In the case of ferromagnetic models, both of these led to the common ground of bilinearization of the theory in an effective magnetic field which depends upon the interaction potential, as discussed in Section 3.

After looking at some of the similarities, let us now examine some of the differences.

(1) The Goldstone theorem is an essential, necessary consequence in the self-consistent field theory (Umezawa et al., 1967), whereas, as pointed out in the itinerant ferromagnetic model in Section 2, this result for the Green's functions methods is typically an added feature that is often very difficult to determine and is not a part of the natural flow of the theory.

(2) Green's function techniques focus on the original field variables and finding appropriate combinations of these in order to find expressions for

correlation functions, self energies, vertices, etc., whereas the self-consistent field theory focuses on actually finding how the original fields make up the observed, physical fields explicitly. Another way of expressing this is to say that in the usual way of handling many-body problems using the former methods, the given Hamiltonians (original variables) are usually the starting point of an ab initio calculation in the sense that the original Hamiltonians are *directly* responsible for the final results. However, it appears that this is often too restrictive since most Hamiltonians of physical models for many-body problems are not simple enough to yield solutions without some rather drastic approximations or mathematically doubtful operations. Therefore, it is physically interesting, while mathematically not necessarily more difficult, if one considers the initial Hamiltonians as an abstract operator expression capable of being realized by certain operators satisfying simple algebraic relations. If the operators used for a particular realization enable us either to solve the eigenvalue problem of the given Hamiltonian or to derive an effective Hamiltonian of a simple form such that the problem becomes more manageable, then our goal is accomplished, if the operators satisfy commutation or anticommutation relations. If a perfect diagonalization is accomplished, then the particle interpretation of these operators corresponds to the "quasiparticles." These last three statements are then the basis of the self-consistent field theory, as contrasted with the Green's function methods which concentrates usually only on the original Hamiltonian.

(3) As described in Section 3, the self-consistent field theory looks for the precise reason(s) why one sees a different symmetry expressed physically than that carried by the original Hamiltonian. Thus, another difference between the self-consistent field theory and the Green's function methods is that the former looks for the basic microscopic mechanism producing asymmetry, whereas the latter typically accepts this fact and goes from there to calculate physical parameters based upon original variables. The asymmetry seems to always be associated with the condensation of Goldstone-type particles into the physical ground state. One then usually proceeds to calculate physical parameters in the self-consistent field theory.

(4) Due to the development of appropriate techniques using Green's functions (Matsubara, 1955), it seems much more natural to introduce temperature dependence using the Green's function techniques. This can, however, be formulated in the self-consistent field theory (Leplae and Umezawa, 1969), but it has not been concentrated on as yet.

(5) As shown in Section 2, equations (2.9)' and (2.11) in particular, one most often introduces background potentials, asymmetric potentials, etc., into the original Hamiltonian when using the Green's function methods. On the other hand, in the self-consistent field theory one usually deals with the fully symmetric Hamiltonian to start with [see equation (3.14) for example]. Thus, one typically builds the asymmetric observations in when using the former methods, whereas one finds the basis of these observations in the latter method. This difference is directly related to the third difference stated above.

(6) From Section 4 the many-body theory based upon the adiabatic theorem using Green's function techniques encounters the difficulty of incomplete sets of states for expansion when going from one phase to another [see the discussion following equation (4.10)]. This problem is conveniently handled in the self-consistent field theory by making a canonical transformation from one Hilbert space (specifying a given phase of the system) to another Hilbert space (specifying a different phase) (See Benson and Hatch, 1973). In a future paper, this will be further explored.

(7) Last, but surely not least, as pointed out in the Introduction and Sections 2 and 3, they certainly differ in the choice of mathematical methods and "tricks" employed for achieving their goals. As pointed out at various places, however, there is also a lot of common ground here. For example, see numbers (1), (2), and (5) of the similarities above.

Consequently, there are many similarities and differences between the Green's function methods and the self-consistent field theory method, and from our analysis it boils down to the fact that at this point the Green's function methods appear to be best for more *immediate* calculations of various functions from which physical parameters can be determined, whereas the self-consistent field theory method appears to be much better for understanding *why* the physical phenomena occur with these physical parameters and observed characteristics.

6. *Conclusion*

From the preceding sections, many useful ideas and methods have been drawn together and contrasted, in looking for central threads that may lead to a better understanding of the physical phenomena they try to describe. From the reviews, developments, and discussions we have found that there are a number of similarities and differences that exist between the self-consistent field theory and the Green's function methods.

It is good to stop every so often and ask where are all these roads leading us? After all, we are trying to get to the same final goals, understanding the physical phenomena about us; and to try for unification, clarification, and correlation certainly will give further insight into the best road or combination of roads to accomplish our goals, as it has many times in the past.

Further investigations, aided by the preceding developments, will continue as we look for the best technique or best qualities of a number of techniques that may be most superior and productive in further linking together the methods for describing many physical systems.

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