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Renormalised perturbation theory of normal systems

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Abstract. Employing an infinite hierarchy of equations for the Green functions of a many particle system in its ground state $|\psi_N\rangle$, the well known non-relativistic, time-dependent, ground-state perturbation theory of a normal system of interacting fermions is derived, without introducing the hypothesis that $|\psi_N\rangle$ is the adiabatic transform of a non-interacting state. This new formulation of the problem allows us to renormalise conventional perturbation theory by introducing an effective interaction Γ and the final result is a highly summed and manifestly self-consistent perturbation expansion in powers of Γ. We calculate Γ to second order and demonstrate that many of the well known results of time-dependent perturbation theory may be obtained by choosing the simplest approximations for Γ. The results are readily generalised to finite temperatures and the formalism provides a generalised form of Hartree–Fock theory which may have important applications in many areas of physics.

1. Introduction

A combination of time-dependent perturbation theory and the theory of Green functions has been particularly successful in describing the equilibrium properties of non-relativistic many particle systems (Abrikosov *et al* 1963, Fetter and Walecka 1971). An essential feature of the above formalism is the use of diagrams as an aid to evaluating the various terms which appear in the perturbation series and any practical calculation consists of summing an infinite subset of these diagrams, selected on the basis of physical arguments.

The theory may be modified by replacing the bare (i.e. non-interacting) propagators $g(1;2)$ which appear in the perturbation series by the exact propagator $G(1;2)$ of the interacting system (Mattuck and Johansson 1968); the improved convergence which results from this renormalisation is evidenced by the fact that many practical calculations are reduced to the task of evaluating only the zero- and first-order (i.e. Hartree–Fock (HF)) terms in the resulting series. The success enjoyed by this approximation in a wide range of physical situations is arguably a consequence of the self-consistency introduced by the above renormalisation.

The HF approximation is the first-order approximation to a 'once renormalised' perturbation series, but when this approximation fails, the theory is not usually improved by summing a finite number of the remaining diagrams for the self-energy Σ. The random phase approximation (which sums ring diagrams) and the ladder approximation are two well known examples which have met with success in situations in which the bare interaction lines and not the bare propagator lines need to be renormalised

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(Hubbard 1957, Galitskii 1958). However, unlike the renormalisation of bare propagators in terms of the exact propagators which proceeds almost by inspection, the problem of the renormalisation of bare interaction lines has not been solved in general. A solution to this problem is highly desirable, because in view of the success enjoyed by the first-order approximation to the 'once renormalised' perturbation series, it is to be anticipated that the first-order approximation to the resulting 'twice renormalised' perturbation series will be applicable to a wide range of many-body problems.

In the present paper, we provide a solution to this problem by introducing an effective interaction Γ which may be computed to any degree of accuracy. The result is a highly summed and manifestly self-consistent version of conventional perturbation theory whose superior convergence properties are evidenced by the fact that all perturbation theoretic calculations known to the authors are contained in zeroth- or first-order approximations to Γ. An interesting feature which emerges from the present analysis is that the HF approximation can be rendered exact by replacing the bare interaction by an effective interaction involving Γ. Thus the HF approximation may be improved by solving simultaneously the usual HF equations together with the self-consistent equation for Γ.

In the present paper, we consider the perturbation theory of normal systems and defer a discussion of systems exhibiting long-range order, characterised by the appearance of anomalous propagators, to a subsequent publication.

2. Conventional perturbation theory

In order to define notation and to introduce a hierarchy of equations for the Green functions of an interacting system, we begin by deriving some well known results of conventional ground-state (i.e. $T = 0$ K) perturbation theory in a rather unconventional manner.

We consider the ground state $|\Psi_N\rangle$ of a uniform system of N spinless particles (any spin is trivially included in the Feynman rules which apply later) enclosed in a volume V, and suppose N and V to become infinite while the particle density $n = N/V$ remains finite. Employing standard notation (Fetter and Walecka 1971), we write the Hamiltonian of the system in the form

$$H = H_0 + H_1 \tag{2.1}$$

where

$$H_0 = \int \mathrm{d}^3x\, \psi^+(\boldsymbol{x})\left(\frac{-\nabla^2(\boldsymbol{x})}{2m}\right)\psi(\boldsymbol{x}) = \sum_k \hbar\omega_k a_k^+ a_k \tag{2.2}$$

and

$$H_1 = \frac{1}{2}\int \mathrm{d}^3x\, \mathrm{d}^3x'\, \psi^+(\boldsymbol{x})\psi^+(\boldsymbol{x}')U(\boldsymbol{x}-\boldsymbol{x}')\psi(\boldsymbol{x}')\psi(\boldsymbol{x}). \tag{2.3}$$

$U(\boldsymbol{x}-\boldsymbol{x}') \equiv U(|\boldsymbol{x}-\boldsymbol{x}'|)$ is an instantaneous two-body potential and the field operators satisfy the usual anticommutation rules

$$[\psi(\boldsymbol{x}), \psi^+(\boldsymbol{x}')]_+ = \delta(\boldsymbol{x}-\boldsymbol{x}'); \qquad [\psi(\boldsymbol{x}), \psi(\boldsymbol{x}')]_+ = 0.$$

We take $|\Psi_N\rangle$ to be normalised and define an m-particle Green function of the

interacting system by

$$(\mathrm{i})^m G^{(m)}(1\ldots m;1'\ldots m') = \langle \Psi_N | T[\psi_H(1)\ldots\psi_H(m)\psi_H^+(1')\ldots\psi_H^+(m')] | \Psi_N \rangle \tag{2.4}$$

where all labels which appear after (before) the semicolon in the argument of $G^{(m)}$ refer to creation (annihilation) operators. In equation (2.4), T is the Wick time-ordering operator,

$$\psi_H(j) \equiv \psi_H(\boldsymbol{x}_j, t_j) = \exp(\mathrm{i}Ht_j/\hbar)\psi(\boldsymbol{x}_j)\exp(-\mathrm{i}Ht_j/\hbar) \tag{2.5}$$

is a field operator in the Heisenberg picture and we have employed the notation

$$j \equiv \boldsymbol{x}_j, t_j \qquad \text{and} \qquad j' \equiv \boldsymbol{x}_j', t_j'.$$

The operator H_0 defines a non-interacting system whose chemical potential is of the form $\hbar\omega_{\boldsymbol{K}'}$. For a Fermi system, $\boldsymbol{K}'$ is the Fermi wavevector. A single particle Green function of the non-interacting system is written

$$\begin{aligned} \mathrm{i}g(j;j') = V^{-1}\sum_{\boldsymbol{K}} \{\exp[\mathrm{i}\boldsymbol{K}\cdot(\boldsymbol{x}_j - \boldsymbol{x}_j')]\exp[-\mathrm{i}\omega_{\boldsymbol{K}}(t_j - t_j')][\theta(t_j - t_j')\theta(|\boldsymbol{K}| - |\boldsymbol{K}'|) \\ - \theta(t_j' - t_j)\theta(|\boldsymbol{K}'| - |\boldsymbol{K}|)]\}. \end{aligned} \tag{2.6}$$

The hierarchy of equations which we now introduce is defined by the equation

$$\begin{aligned} G^{(m)}(1\ldots m;1'\ldots m') = \sum_{j=1}^{m}(-1)^{m+j} g(1;j')G^{(m-1)}(2\ldots m;1'\ldots j'-1, j'+1\ldots m') \\ + \frac{\mathrm{i}}{\hbar}\int \mathrm{d}_{m+1}\int \mathrm{d}_{m+2}\, U((m+1)-(m+2)) \\ \times g(1;m+1)G^{(m+1)}(2\ldots m, m+1, m+2;1'\ldots m', m+2) \end{aligned} \tag{2.7a}$$

and its 'conjugate'

$$\begin{aligned} G^{(m)}(m'\ldots 1';m\ldots 1) = \sum_{j=1}^{m}(-1)^{m+j} g(j';1)G^{(m-1)}(m'\ldots j+1', j-1',\ldots 1';m\ldots 2) \\ + \frac{\mathrm{i}}{\hbar}\int \mathrm{d}_{m+1}\int \mathrm{d}_{m+2}\, U((m+1)-(m+2))g(1;m+1) \\ \times G^{(m+1)}(m+2, m'\ldots 1';m+2, m+1, m\ldots 2). \end{aligned} \tag{2.7b}$$

Here we define $G^{(0)} \equiv 1$. We have employed the notation

$$\int \mathrm{d}_j \equiv \int_{-\infty}^{\infty} \mathrm{d}t_j \int_V \mathrm{d}^3 x_j \tag{2.8}$$

and

$$U(i-j) \equiv U(\boldsymbol{x}_i - \boldsymbol{x}_j)\delta(t_i - t_j)\exp(-\varepsilon|t_i|). \tag{2.9}$$

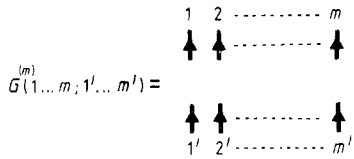
A detailed derivation and discussion of equations (2.7) forms part of a previous publication (Lambert and Hagston 1981) and here we merely note that the limit $\varepsilon \to 0^+$ is to be taken *after* the time integrations have been carried out.

Equations (2.1) to (2.9) define our notation and we now demonstrate how equations (2.7) may be employed to yield a well known perturbation expansion for $G^{(1)}$. To this end we introduce the following rules which allow us to write (2.7) in terms of diagrams.

(i) Denote $G^{(m)}(1 \ldots m; 1' \ldots m')$ by m thick full lines with free ends entering (leaving) the points $1 \ldots m$ $(1' \ldots m')$.

(ii) The lines which correspond to primed (unprimed) labels are to be arranged in the order in which they appear in the argument of $G^{(m)}(1 \ldots m; 1' \ldots m')$. The line corresponding to $1'$ (1) is to be placed furthest to the left while that corresponding to m' (m) is to be placed furthest to the right.

The above rules identify two sets of lines; one set refers to labels which appear after the semicolon in the argument of $G^{(m)}$ and the other refers to those which do not. Although the relative order of lines within a given set is significant, the positions of the lines of one set relative to those of the other is irrelevant. However, when convenient, we shall arrange for the lines which refer to labels appearing before the semicolon of $G^{(m)}$ to lie above those which refer to labels appearing after the semicolon. In this way, rules (i) and (ii) allow us to write the left-hand side (LHS) of equation (2.7a) in the form:



(2.7a')

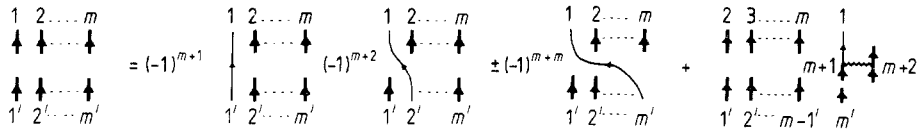
Diagrammatic analysis of the right-hand side (RHS) of (2.7) requires further rules.

(iii) Denote $g(j; j')$ by a thin full line running from j' to j.

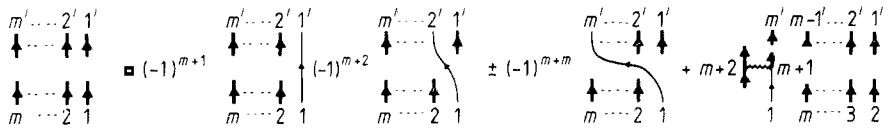
(iv) Denote the 'potential' $(\mathrm{i}/h)U(j, j')$ by a wavy line joining the points j and j'.

(v) Integrate over all internal coordinates, (i.e. $m+1$ and $m+2$ of equations (2.7)).

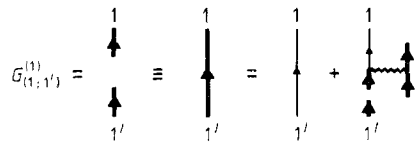
Employing the above rules, we find that equations (2.7) take the form:



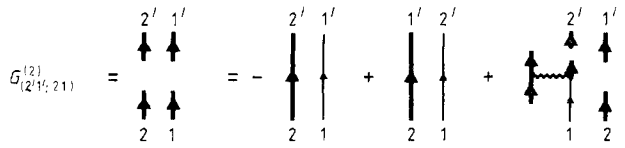
(2.10a)



As a special case of rule (i), it is convenient to denote $G^{(1)}(1; 1')$ by a thick full line running from $1'$ to 1. In this way, the $m = 1$ $(m = 2)$ version of equation (2.10a) (equation (2.10b)) takes the form of equation (2.11) (equation (2.12))



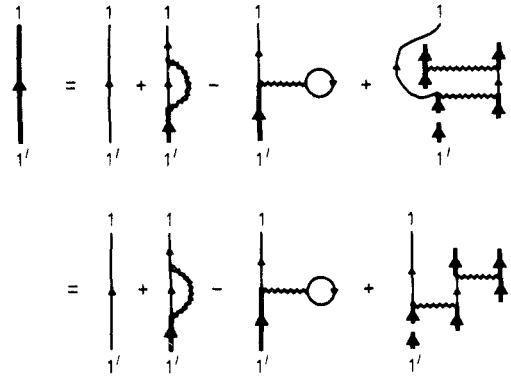
(2.11)



(2.12)

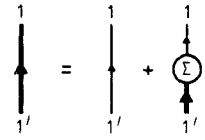
where we have omitted (and shall henceforth omit) the dummy variables $m+1$ and $m+2$.

It is now easy to see how conventional perturbation theory arises from the hierarchy of equations. To this end we substitute equation (2.12) into (2.11) to yield equation (2.13)



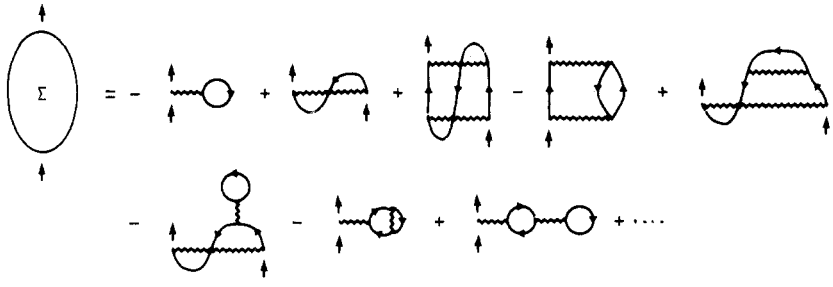
(2.13)

(The last line follows from the fact that operators (anti-) commute under the T operator.) The last term on the RHS of (2.13) is evaluated by substituting equation (2.10*b*) for the three particle Green function. The result contains terms involving $G^{(2)}$ and $G^{(4)}$ which may be expanded by employing equations (2.12) and (2.10*b*). Repeating this iterative procedure to infinity and assuming convergence yields:



(2.14)

where to second order, the contributions to the proper self-energy Σ are shown explicitly in equation (2.15).



(2.15)

The perturbation expansion of equation (2.14) is well known from the theory of interacting Fermi systems (see e.g. Fetter and Walecka 1971) where it is known that the factors $(-1)^i$ appearing in (2.15) may be omitted providing the following rule is employed.

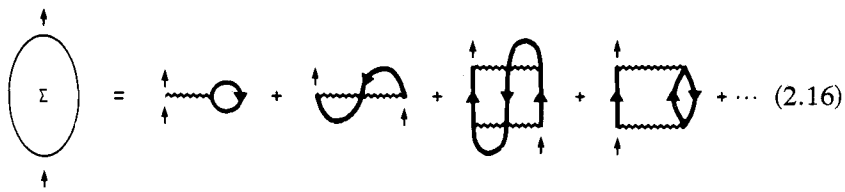
Associate a factor $(-1)^i$ with each diagram containing i fermion loops. Henceforth we adopt this rule.

The present section serves to illustrate the connection between the hierarchy of equations and perturbation theory and in what follows, we utilise this feature to perform a renormalisation of interaction lines. However, before proceeding we make a few remarks concerning the expansion represented by (2.14).

In conventional fermion perturbation theory, equation (2.14) is derived by introducing the adiabatic hypothesis, demonstrating the cancellation of disconnected diagrams and finally summing an infinite class of diagrams to remove 'improper' self-energies. The last operation has the effect of introducing the thick full line to the RHS of (2.14) and as such may be regarded as a first step towards the 'first renormalisation' of the perturbation series.

The derivation of equation (2.14) presented above has many advantages over the conventional method. The hierarchy of equations (2.7) is obtained (Lambert and Hagston 1981) without recourse to the adiabatic hypothesis, by employing an equation of motion method. Disconnected diagrams are avoided from the outset and by solving the equation for $G^{(1)}$ in the manner discussed above, Dyson's equation appears automatically at each stage of iteration.

The RHS of equation (2.15) represents the first- and second-order terms of the unrenormalised expansion for Σ. The first- and second-order terms in the 'once renormalised' expansion for Σ are given in equation (2.16) which, unlike equation (2.15), contains only thick full lines corresponding to exact propagators.



(2.16)

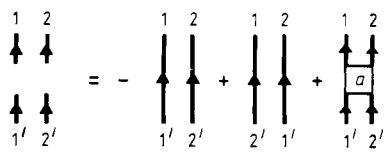
The equivalence of these two expressions is readily demonstrated (to second order) by substituting (2.14) for the exact propagators of (2.16) and repeating this substitution to remove thick full lines from all resulting second-order diagrams; the proof that this renormalisation may be carried out in all orders of perturbation theory proceeds along similar lines (Mattuck and Johansson 1968).

Finally, we remark that the first two terms on the RHS of equation (2.16) constitute the lowest-order approximation to the once renormalised expansion for Σ and when coupled with equation (2.14) yield the Hartree–Fock approximation.

3. The effective interaction Γ

As a first step towards obtaining a 'twice renormalised' perturbation expansion, we consider how vertex functions enter the theory.

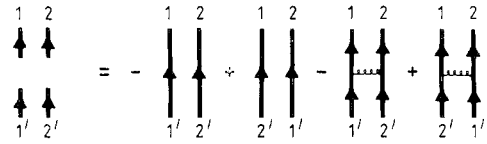
It is well known from conventional fermion perturbation theory that the exact expansion for the two particle Green function is of the form



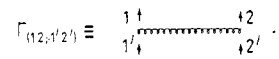
(3.1)

which serves to define a four-point vertex function α. This expression is also readily obtained from the hierarchy of equations, by solving equation (2.7*a*) for $m = 2$. The solution is obtained after employing the iterative technique which led to equation (2.14), followed by the renormalisation which led to equation (2.16).

Examination of the RHS of equation (3.1) reveals that it may be written in the more symmetrised form:

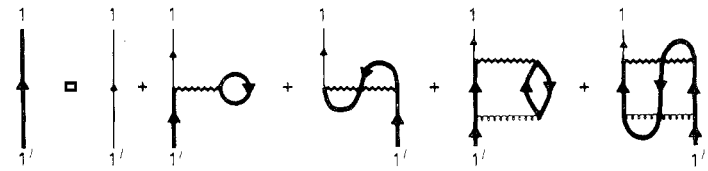


(3.2)



The latter defines a four-point vertex function $\Gamma(12, 1'2')$ which, under certain circumstances, is expected to play the role of an effective interaction (see e.g. Nozieres 1964). In equation (3.2), the 'spring' denotes an infinite series and the diagram rules developed earlier apply to this well known perturbation expansion for Γ. (Note that in view of the renormalisation of propagators, implicitly carried out, the expression for Γ contains exact propagators and bare interactions only.)

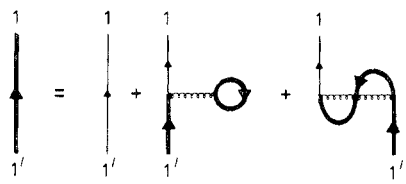
We are now in a position to carry out the second renormalisation, but before proceeding we pause to consider some consequences of equation (3.2). Substituting this expression into the RHS of equation (2.11) yields



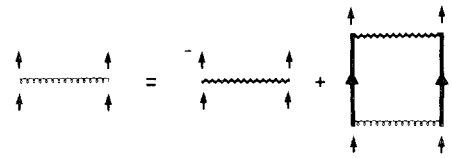
(3.3)

This equation forms an exact expression for the single particle Green function and possesses several interesting features.

For example, the zeroth-order solution to this equation, obtained by equating Γ to zero, is the celebrated Hartree–Fock approximation. Furthermore, the simplest *self-consistent* solution to (3.3)

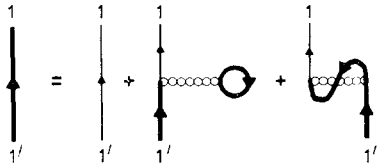


(3.4)

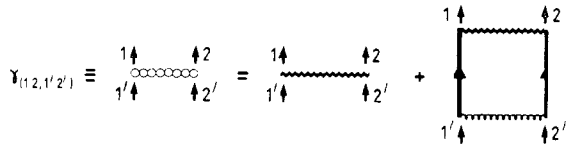


(3.5)

is the well known ladder approximation (Galitskii 1958, Fetter and Walecka 1971). Finally, we note that the exact solution to (3.3) is of the form



(3.6)



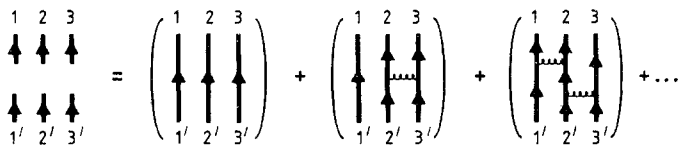
(3.7)

which define a further 'effective interaction' γ. Equation (3.6) is exact and proves our initial assertion concerning the exactness of the HF approximation after substituting an effective interaction for the bare interaction. This is useful because it provides some justification for employing, in HF-type calculations, effective interactions arrived at via physical arguments. Furthermore, the expression for Γ which we obtain in the following section provides a means of checking the self-consistency of such calculations.

4. An expression for the effective interaction Γ

We now proceed to the task of obtaining a twice renormalised perturbation theory. To this end we seek a self-consistent expression for the vertex function Γ.

The RHS of equation (2.12) involves $G^{(3)}$ and the latter may be expressed in terms of Γ in an analogous manner to that which led to equation (3.2). The result

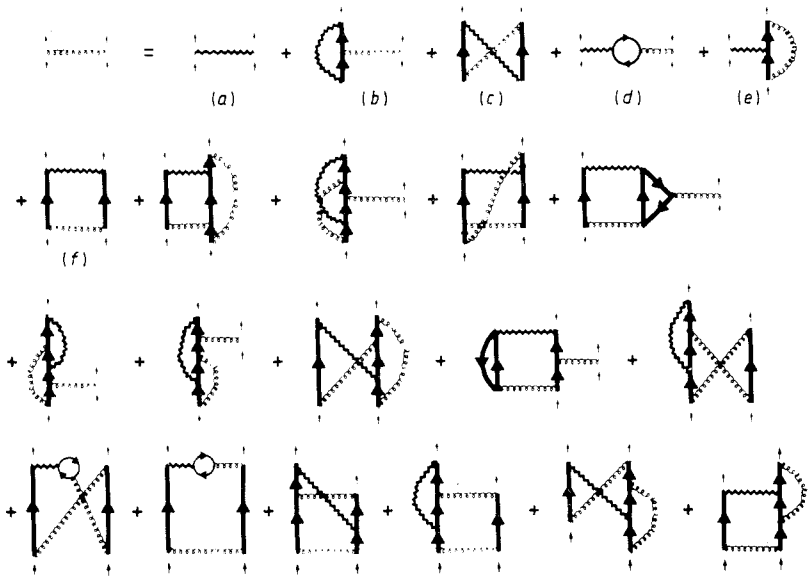


(4.1)

is a highly renormalised perturbation series in powers of Γ. In equation (4.1) the parentheses around a given term indicate that a sum over all possible distinct permutations of the labels $1, 2, 3; 1', 2', 3'$ is to be carried out. Each set of parentheses encompasses a term of a given topology. The rapid convergence of the series on the RHS of this equation will become self-evident as we proceed. Anticipating this feature we restrict ourselves to a self-consistent evaluation of Γ, correct to second order in Γ.

After substituting equation (4.1) into the RHS of (2.12), the resulting equation may be compared with (3.2) to yield a self-consistent expression for Γ. The result is a 'twice renormalised' perturbation series involving the exact propagator $G^{(1)}$ and the vertex function Γ. Retaining terms up to second order in Γ, the expression takes the form

(Lambert 1979):



(4.2)

This completes our renormalisation of conventional perturbation theory and we note that these results apply equally well at finite temperatures, provided the finite temperature Green functions are substituted for their $T = 0$ K counterparts, and a Wick rotation carried out on the time variables.

Before leaving this section, we note some interesting conclusions that can be drawn from consultation of (4.2), which must be solved self-consistently with equation (3.3). For example, the zeroth-order solution to these simultaneous equations is obtained by ignoring all terms involving Γ on the right-hand sides of these equations, thus giving the Hartree–Fock approximation. If we retain terms up to first order in Γ, we are left with (3.3) and the terms (*a*) to (*f*) of (4.2). The ladder approximation is obtained by inserting the terms (*a*) and (*f*) only into the RHS of (3.3). Similarly, to obtain what is essentially the ring approximation (Nozieres and Pines 1958), we substitute terms (*a*) and (*d*) of (4.2) into the fourth term on the RHS of (3.3).

5. Discussion

An important feature of the present analysis is that it provides a link between the equation of motion method (which is the basis of the hierarchy of equations) and diagrammatic perturbation theory. The former proceeds by making an approximation on the higher-order Green functions (ter Haar 1977, Stolz 1977), while the latter performs a summation of a selected subset of diagrams and the present analysis renders the relationship between these two approaches more transparent.

The connection between the hierarchy of integral equations and perturbation theory is illustrated in § 2, where it is shown that Dyson's equation may be obtained without the introduction of disconnected diagrams and improper self-energies.

In § 3 we recall a well known equation (3.1) which results after employing fermion perturbation theory to evaluate $G^{(2)}$. This result, when coupled with the first-order

equation of the hierarchy, is shown to yield the exact expression for $G^{(1)}$ given in equations (3.6) and (3.7).

The above expression for $G^{(1)}$ involves the vertex function Γ, which is determined self-consistently in § 4. The first step in the evaluation of Γ consists of recognising that $G^{(3)}$, when expressed in terms of Γ, takes the form of equation (4.1). Unlike the corresponding expression for $G^{(2)}$ (equation (3.2)) the result for $G^{(3)}$ is of the form of an infinite series in powers of Γ. (This result readily follows after employing standard fermion perturbation theory (or the method of § 2) to evaluate $G^{(3)}$, 'once renormalising' and then expressing the result in terms of Γ.)

Equations (4.1), (2.12) and (3.2) form the basis of our self-consistent evaluation of Γ. It is clear that when (4.1) is substituted into the RHS of (2.12), the result is an infinite series and we compare this with equation (3.2) to obtain the desired expression. The manipulations involved are lengthy, but straightforward and we have restricted our evaluation to second order in Γ. The result is given in equation (4.2) where it is evident that several well known approximations, currently employed in many-body theory, are contained in the first-order approximation for Γ.

The above theory also provides a useful framework for treating the general question of effective interactions between the particles in a system in terms of a self-consistent formalism. For example, by simply making an initial guess for the effective interaction Γ and solving simultaneously equations (3.6) and (3.7) by a process of iteration, one obtains a Hartree–Fock theory together with a self-consistent determination of Γ. The system of equations should be readily soluble, i.e. within the capacity of modern high-speed computers, and since they represent a generalisation of ordinary Hartree–Fock theory their range of application in various areas, such as atomic and nuclear physics, should be extensive. Indeed this could turn out to be one of the most powerful attributes of the present theory as applied to normal fermion systems.

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