The description of collective motions in terms of many-body perturbation theory

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In this and a succeeding paper it is shown how a theory equivalent to the Bohm & Pines collective motion theory of the electron plasma can be derived directly from a perturbation series which gives in principle an exact solution of the many-body problem. This result is attained by making use of a diagrammatic method of analysis of the perturbation series. By a process analogous to the elimination of photon self-energy parts from the electrodynamic S matrix it is found possible to simplify the perturbation series, introducing a modified interaction between the particles. A useful integral equation for this modified interaction can be set up, and it is shown how the energy of the system can be expressed in terms of the modified interaction. The close connexion between this approach and the dielectric theory of plasma oscillations is indicated.

1. Introduction

Within recent years much attention has been given in the study of the quantum mechanical many-body problem to the collective modes of motion which may be present (Bohm & Pines 1953; Tomonaga 1955; Bohr & Mottelson 1953). Two main theories of collective motion have been developed, that of Tomonaga (1955), and the superfluous co-ordinate type of theory introduced by Bohm & Pines (1953). In the Tomonaga theory a transformation of variables is made in such a way that some of the new co-ordinates are directly related to the collective modes of motion, whilst the remaining new co-ordinates are associated with internal modes of motion. In the superfluous co-ordinate treatment certain auxiliary variables are introduced together with an equal number of subsidiary conditions to preserve the correct number of degrees of freedom, and a transformation is made in such a way that the new auxiliary variables are related to the collective motion, whilst the original co-ordinates when transformed are related to the internal motion. If the collective modes being studied have real physical significance, then it will be found in both these methods that the Hamiltonian is, to a good approximation, separable in the new co-ordinates, and a separation of the collective motion is thereby obtained.

Though these methods are quite successful, they have certain unsatisfactory features. In the Tomonaga method it is generally found that when the Hamiltonian has been separated the problem of finding the eigenvalues of the internal motion part is very difficult. In the superfluous co-ordinate treatment one does not meet with this difficulty but with an equivalent one; this is that it is difficult to find eigenfunctions satisfying the subsidiary conditions. In addition, both theories suffer from the difficulty of not being able to treat very easily the interaction between the collective and internal modes of motion, or the intimately related problem of the damping of the collective motion; where the damping is small this is not a very

serious problem, but in certain cases, e.g. the application of the Bohm & Pines theory to metals, it may be quite serious. We shall see later that this problem of treating the damping is also intimately connected with the problem of the cut-off in the Bohm & Pines theory of the electron plasma (1953).

In the case of the electron plasma an alternative type of theory of a different character from those described above has been developed. In this 'dielectric' theory (Mott 1954; Fröhlich & Pelzer 1955; Hubbard 1955*a*, *b*) one argues along semi-classical lines, regarding the electron gas as a dielectric medium. From this point of view one thinks of the electrons as interacting with one another like particles in the dielectric medium represented by the remaining electrons; their interaction is therefore modified and screened. The plasma oscillations are thought of as being the polarization waves in the dielectric medium. This approach has advantages over the other two approaches in that it can easily treat the damping problem, and does not attempt so complete a separation of the collective and internal modes of motion, the one going smoothly over into the other; it suffers from the disadvantages of being a phenomenological theory and difficult to quantize satisfactorily.

It is the purpose of this and a succeeding paper (Hubbard 1957) to develop yet another approach to the collective motion problem which is applicable to the electron plasma, and to similar systems, and which we hope combines the advantages of the treatments described above and yet is free of their disadvantages. This theory is based upon an (infinite) perturbation series which provides in principle an exact solution to the many-body problem and therefore contains all the physical effects including the collective motion. The various contributions to this perturbation series can be conveniently analyzed making use of diagrams similar to Feynman diagrams (Goldstone 1957). It is now argued that we may be able to simplify our perturbation series by a process exactly analogous to the elimination of photon self-energy parts in the analysis of the S-matrix in quantum electrodynamics (see, for example, Dyson 1949). This is in fact so, and the analysis shows that we need only retain in our perturbation series terms corresponding to diagrams free from these parts, provided everywhere in the perturbation series we replace the ordinary interaction between the particles by a modified interaction.

To establish the connexion between this apparently formal device for simplifying the perturbation series and the collective motion problem let us now consider the physical interpretation of what we shall do. Just as in the electrodynamic case, we can regard the diagrams used in the analysis of the perturbation series as representing the actual physical process which gives rise to the corresponding contribution to the perturbation series. Interpreting the parts of diagrams analogous to photon self-energy parts in this way, we can see that they correspond to the modification of the ordinary interaction between particles by the polarization of the medium represented by the remaining particles; we shall refer to these as polarization parts. Thus, the elimination of these parts and the replacement of the ordinary interaction by the modified interaction in the perturbation series is exactly equivalent to going over to the viewpoint of the dielectric theory described above, so that we may expect our theory to be equivalent to the other theories of collective motion. This expectation is in fact borne out by detailed calculation.

The present paper develops the theory in a general form, and the detailed treatment of the electron plasma is reserved for a succeeding paper. Since the diagrammatic analysis is used in a different (although equivalent) form to that given by Goldstone (1957), it is developed afresh in §§ 2 to 4. In § 5 are discussed certain simplifications which arise when one considers the case of a uniform gas; in the remainder of the paper it is assumed that we are dealing with this case.

Section 6 proceeds with the main programme; the polarization parts are eliminated and the modified interaction introduced. In § 7 an integral equation is derived for the modified interaction which very greatly simplifies its calculation. Finally, in § 8 it is shown how the energy of the system can be expressed exactly in terms of the modified interaction. This result will enable us to calculate correlation energies directly from the modified interaction which in turn can be calculated easily using the integral equation.

2. The diagrammatic analysis of the perturbation series

We shall consider the problem of determining the energy spectrum and wave functions of a gas of Fermi–Dirac particles interacting with one another through an instantaneous two-body potential and moving so slowly that relativistic effects can be neglected; we include also the case in which the particles move in an external potential field. The Hamilton for such a system is

$$H = H_0 + H', \tag{1}$$

where H_0 includes the kinetic energy of the particles and their potential energy in the external field, and H' is the interaction energy of the particles. H' will be treated as a perturbation.

One way in which we may develop the perturbation series for H' is by making use of the adiabatic approximation. We consider the interaction H' to be slowly switched on between $t = -\infty$ and $t = 0$, and to be slowly switched off between $t = 0$ and $t = +\infty$; then a system which at $t = -\infty$ is in an eigenstate Ψ_0 of H_0 will between $t = -\infty$ and $t = 0$ slowly change into an eigenstate of H. This result has been proved by Gell-Mann & Low (1951) in the following form: if Ψ_0 is an eigenstate of H_0 belonging to the energy E_0, then

$$\Psi = \lim_{\alpha \to +0} S_\alpha(0, -\infty)\Psi_0 / (\Psi_0 \mid S_\alpha(0, -\infty) \mid \Psi_0) \tag{2}$$

is an eigenstate of H belonging to the energy

$$E = E_0 + \Delta E = E_0 + \lim_{\alpha \to +0} (\Psi_0 \mid H' S_\alpha(0, -\infty) \mid \Psi_0) / (\Psi_0 \mid S_\alpha(0, -\infty) \mid \Psi_0), \tag{3}$$

where $S_\alpha(t, t')$ is the solution of the equation

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} S_\alpha(t, t') = H_\alpha(t) S_\alpha(t, t'), \tag{4}$$

satisfying the boundary condition $S_\alpha(t', t') = 1$, and

$$H_\alpha(t) = \mathrm{e}^{(i/\hbar)H_0 t} H' \mathrm{e}^{-(i/\hbar)H_0 t} \mathrm{e}^{-\alpha|t|}. \tag{5}$$

The parameter α is seen to govern the rate of switching on and off of the interaction; the limit $\alpha \to +0$ means that the potential is switched on infinitely slowly, the condition for the exactness of the adiabatic approximation.

We can now obtain a perturbation series for Ψ by solving (4) by iteration. To do this we replace (4) by the integral equation

$$S_\alpha(t) = 1 + \frac{1}{i\hbar}\int_{-\infty}^{t} H_\alpha(t')\, S_\alpha(t')\, dt', \tag{6}$$

incorporating the boundary condition at $t = -\infty$ (in future we shall for brevity write $S_\alpha(t, -\infty)$ as $S_\alpha(t)$). Iteration of (6) gives

$$\begin{aligned} S_\alpha(t) &= 1 + \sum_{n=1}^{\infty} \left(\frac{1}{i\hbar}\right)^n \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \dots \int_{-\infty}^{t_{n-1}} dt_n\, H_\alpha(t_1)\, H_\alpha(t_2) \dots H_\alpha(t_n) \\ &= 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{1}{i\hbar}\right)^n \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t} dt_2 \dots \int_{-\infty}^{t} dt_n\, P[H_\alpha(t_1)\, H_\alpha(t_2) \dots H_\alpha(t_n)], \end{aligned} \tag{7}$$

where P is the chronological ordering operator; this is the perturbation series we shall use.

Our interaction Hamilton can be written in the notation of field theory

$$H' = \frac{1}{2}\int \overline{\psi}(\mathbf{x}')\, \psi(\mathbf{x}')\, v(\mathbf{x}-\mathbf{x}')\, \overline{\psi}(\mathbf{x})\, \psi(\mathbf{x})\, d\mathbf{x}\, d\mathbf{x}' - \tfrac{1}{2}Nv(0), \tag{8}$$

where $v(\mathbf{x}-\mathbf{x}')$ is the mutual potential energy of two particles at $\mathbf{x}$ and $\mathbf{x}'$, N is the number of particles in the system, and $\overline{\psi}(\mathbf{x})$, $\psi(\mathbf{x})$ are the particle field operators. These can be written

$$\left.\begin{aligned} \psi(\mathbf{x}) &= \sum_i u_i(\mathbf{x})\, \eta_i, \\ \overline{\psi}(\mathbf{x}) &= \sum_i \overline{u}_i(\mathbf{x})\, \overline{\eta}_i, \end{aligned}\right\} \tag{9}$$

where the $u_i(\mathbf{x})$ are the eigenfunctions of the one-particle Hamiltonian,

$$\left[\frac{p^2}{2m} + U(\mathbf{x})\right] u_i(\mathbf{x}) = E_i\, u_i(\mathbf{x}), \tag{10}$$

in which $\mathbf{p}$ is the momentum and $U(\mathbf{x})$ the external potential. The operators $\overline{\eta}_i$ and η_i are creation and destruction operators for the particle in the state i; since our particles obey Fermi–Dirac statistics they satisfy the anticommutation relations

$$[\eta_i, \eta_j]_+ = [\overline{\eta}_i, \overline{\eta}_j]_+ = 0, \quad [\eta_i, \overline{\eta}_j]_+ = \delta_{ij}. \tag{11}$$

In (8) spinor indices are suppressed since their inclusion only requires a trivial generalization of the theory. The second term in (8) subtracts the self-energies of the particles due to the interaction v, since these are included together with the mutual interactions of the particles in the first term of (8). (If the potential is singular at the origin $v(0)$ is not defined. We can, however, easily introduce a suitable limiting procedure. If we Fourier transform v, $v(\mathbf{x}) = \int v(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}}\, d\mathbf{k}$, then we can work with $v_K(\mathbf{x}) = \int_{k<K} v(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{x}} d\mathbf{k}$, for which $v_K(0)$ is defined, and take the limit $K \to \infty$ at the end of the calculation.)

To obtain our perturbation series in a suitable form for computation we now have to substitute (8) into (5) and (5) into (7). Before doing this it is convenient to include the (constant) second term of (8) in H_0 and to symmetrize the first term; H' then becomes

$$H' = \frac{1}{4}\int v(\mathbf{x}-\mathbf{x}')\,[\overline{\psi}(\mathbf{x}')\,\psi(\mathbf{x}')\,\overline{\psi}(\mathbf{x})\,\psi(\mathbf{x})+\overline{\psi}(\mathbf{x})\,\psi(\mathbf{x})\,\overline{\psi}(\mathbf{x}')\,\psi(\mathbf{x}')]\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}'. \quad (12)$$

Putting (12) into (5) we can easily obtain

$$H_\alpha(t) = \frac{1}{4}\int \mathrm{d}x \int \mathrm{d}x'\, v_\alpha(x-x')\,[\overline{\psi}(x')\,\psi(x')\,\overline{\psi}(x)\,\psi(x)+\overline{\psi}(x)\,\psi(x)\,\overline{\psi}(x')\,\psi(x')], \quad (13)$$

where x stands for $(\mathbf{x}, t)$ and x' for $(\mathbf{x}', t')$,

$$v_\alpha(x-x') = v(\mathbf{x}-\mathbf{x}')\,\delta(t-t')\,\mathrm{e}^{-\alpha|t|}, \quad (14)$$

and

$$\psi(x) = \psi(\mathbf{x}, t) = \sum_i u_i(x)\,\eta_i = \sum_i u_i(\mathbf{x})\,\mathrm{e}^{-(\mathrm{i}/\hbar)E_i t}\eta_i,$$

$$\overline{\psi}(x) = \sum_i \overline{u}_i(x)\,\overline{\eta}_i. \quad (15)$$

Substituting (13) into (7) we obtain

$$\begin{aligned} S_\alpha(t) = 1 + \sum_{n=1}^{\infty}\frac{1}{n!}\left(\frac{1}{4\mathrm{i}\hbar}\right)^n \int^t \mathrm{d}x_1 \int^t \mathrm{d}x_2 \ldots \int^t \mathrm{d}x_n \int^t \mathrm{d}x_1' \ldots \int^t \mathrm{d}x_n' \\ \times v_\alpha(x_1-x_1')\,v_\alpha(x_2-x_2')\ldots v_\alpha(x_n-x_n') \\ \times P[\overline{\psi}(x_1')\,\psi(x_1')\,\overline{\psi}(x_1)\,\psi(x_1)+\overline{\psi}(x_1)\,\psi(x_1)\,\overline{\psi}(x_1')\,\psi(x_1'), \ldots \\ \ldots, \overline{\psi}(x_n')\,\psi(x_n')\,\overline{\psi}(x_n)\,\psi(x_n)+\overline{\psi}(x_n)\,\psi(x_n)\,\overline{\psi}(x_n')\,\psi(x_n')], \end{aligned} \quad (16)$$

where $\int^t \mathrm{d}x$ means the integral over all that part of space-time behind the surface t.

We can conveniently analyze the P product in (16) by making use of Wick's theorem (Wick 1950). This analysis can be simplified if we notice that we are interested only in the operation of S_α on the particular eigenstate Ψ_0 of H_0. We shall, henceforth, assume that Ψ_0 is a non-degenerate eigenstate of H_0 in which certain definite states i are occupied. Then we can conveniently take the state Ψ_0 as a 'redefined vacuum state' (Salam 1953) and resolve $\overline{\psi}$ and ψ according to

$$\psi = \psi^+ + \psi^-, \quad \overline{\psi} = \overline{\psi}^+ + \overline{\psi}^-, \quad (17)$$

where

$$\psi^-(x) = \sum_i^{\text{unocc.}} u_i(x)\,\eta_i \quad \text{(destroys particles)},$$

$$\psi^+(x) = \sum_i^{\text{occ.}} u_i(x)\,\eta_i \quad \text{(creates holes)},$$

$$\overline{\psi}^-(x) = \sum_i^{\text{occ.}} \overline{u}_i(x)\,\overline{\eta}_i \quad \text{(destroys holes)},$$

$$\overline{\psi}^+(x) = \sum_i^{\text{unocc.}} \overline{u}_i(x)\,\overline{\eta}_i \quad \text{(creates particles)}. \quad (18)$$

Here the terms occupied and unoccupied refer to the state of occupation of the state i in Ψ_0. We then have the result

$$\psi^-(x)\Psi_0 = \bar{\psi}^-(x)\Psi_0 = 0. \tag{19}$$

To take advantage of the result (19) we resolve the P product in (16) in such a way as to move all the operators ψ^+, $\bar{\psi}^+$ to the left and all the operators ψ^-, $\bar{\psi}^-$ to the right. This analysis can be performed quite straightforwardly using Wick's theorem. When this analysis has been completed we can reject all terms involving ψ^- and $\bar{\psi}^-$ by virtue of (19). Only one special point arises in this analysis. This is that, whereas in the case dealt with by Wick all operators with the same time argument either commuted or were already arranged as an S product, this is not so in the present case and one has to allow for contractions between operators with the same time argument.

When the analysis has been completed, it is found that the various terms contributing to $S_\alpha(t)\psi_0$ (the terms not involving ψ^- or $\bar{\psi}^-$) can be conveniently classified in terms of certain diagrams similar to Feynmann diagrams, there being a contribution to $S_\alpha(t)\psi_0$ corresponding to each diagram. We proceed at once to the prescription for drawing these diagrams and for calculating the corresponding contribution to $S_\alpha(t)$.

The diagrams will be of orders 1, 2, ..., corresponding to the contributions arising from different order terms of (16). The prescription for drawing an nth order diagram is as follows:

(i) Mark n points on the diagram and label these $x_1, x_2, \ldots, x_n$; mark a further n points and label with $x_1', \ldots, x_n'$; join the pairs of points x_i, x_i' by 'interaction' lines (broken lines in the diagrams of this paper).

(ii) Draw directed 'particle' lines, one entering and one leaving each point; these lines may run between points or from a point to itself or from a point to the edge of the diagram or from the edge of the diagram to a point.

The different nth order diagrams are obtained by drawing in the particle lines in all possible ways. It will be noted that the particle lines form closed polygons and open polygonal arcs, so that to every particle line running inwards from the edge of the diagram there is one running out connected to it by a chain of particle lines.

The contributions to $S_\alpha(t)$ corresponding to a given diagram is a certain integral which can be written down from the following prescription:

(i) For every interaction line $x_i x_i'$ introduce a factor $v(x_i - x_i')$ into the integrand.

(ii) For every particle line running from a point y (= some x_i or x_i') to the edge of the diagram introduce a factor $\bar{\psi}^+(y)$ into the integrand, and for every particle line running from the edge of the diagram to a point y introduce a factor $\psi^+(y)$ into the integrand. The ψ^+ and $\bar{\psi}^+$ are to be arranged so that if $\psi^+(y)$ corresponds to the incoming line of one of the open polygonal arcs and $\bar{\psi}^+(z)$ to the corresponding outgoing line, then $\bar{\psi}^+(z)$ is adjacent to and on the left of $\psi^+(y)$.

(iii) For every particle line running from a point y to a point $z\,(\neq y)$ introduce a factor $S(z, y)$ into the integrand.

(iv) For every particle line running from a point y to itself introduce a factor $\rho(y)$ into the integrand.

(v) Integrate with respect to $dx_1 dx_2 \ldots dx_n dx'_1 \ldots dx'_n$ over the region of space-time behind the surface t.

(vi) Multiply the integral by $(2i\hbar)^{-n}(n!)^{-1}(-1)^p$, where p is the number of closed particle loops in the diagram.

The quantity $\rho(x)$ is just the charge density corresponding to Ψ_0, namely

$$\rho(x) = \sum_{i}^{\text{occ.}} \bar{u}_i(\mathbf{x})\, u_i(\mathbf{x}), \tag{20}$$

whilst the quantity $S(x', x)$ is a propagator given by

$$S(x', x) = \epsilon(t'-t) \sum_{i}^{\text{unocc.}} u_i(x')\, \bar{u}_i(x) - \epsilon(t-t') \sum_{i}^{\text{occ.}} u_i(x')\, \bar{u}_i(x), \tag{21}$$

where

$$\epsilon(t) = 1 \quad \text{if} \quad t > 0$$
$$= 0 \text{ otherwise.}$$

The function $S(x, x')$ is the solution of the equation

$$\left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\nabla^2 - U(\mathbf{x})\right] S(x, x') = \delta(\mathbf{x}-\mathbf{x}')\,\delta(t-t'), \tag{22}$$

which reduces to $\frac{1}{2} - \rho(\mathbf{x}, \mathbf{x}')$ when $t = t'$, where $\rho(\mathbf{x}, \mathbf{x}')$ is the ordinary density matrix corresponding to the state Ψ_0:

$$\rho(\mathbf{x}, \mathbf{x}') = \sum_{i}^{\text{occ.}} u_i(\mathbf{x})\, \bar{u}_i(\mathbf{x}'). \tag{23}$$

As an example of the above prescriptions we give the contribution to $S_a(t)$ corresponding to the diagram shown in figure 1 (*a*); it is

$$-\frac{1}{4!}\left(\frac{1}{2i\hbar}\right)^4 \int dx_1\, dx_2\, dx_3\, dx_4\, dx'_1\, dx'_2\, dx'_3\, dx'_4\; v_a(x_1 - x'_1)\, v_a(x_2 - x'_2)\, v_a(x_3 - x'_3)\, v_a(x_4 - x'_4)$$
$$\times \bar{\psi}^+(x_4)\, \psi^+(x_1)\, \bar{\psi}^+(x'_3)\, \psi^+(x'_1)\, S(x_4, x'_4)\, S(x'_4, x_3)\, S(x_3, x_1)\, S(x'_3, x_2)\, S(x_2, x'_1)\, \rho(x'_2). \tag{24}$$

3. The linked-cluster expansion

The linked-cluster expansion was first suggested by Brueckner (1955) and has been proved by Goldstone (1957) using the diagrammatic method of analysis of the perturbation series. The necessity for this result arises because the ordinary perturbation series for the energy, including that derived above, contain terms which diverge more strongly than N, the number of particles in the system, as $N \to \infty$. Such terms can have no physical significance and must cancel out against each other: we should, therefore, be able to eliminate them from the series, which is done in the linked-cluster expansion. This elimination will be carried out easily and naturally in this section using the diagrammatic analysis.

Before proceeding to develop the linked-cluster expansion it is first convenient to classify the diagrams in a certain way. We shall say that two diagrams belong to the same class if they have the same basic structure, i.e. if they have the same arrangement of vertices, interaction and particle lines and differ only in the labelling of their vertices; for example, the diagrams shown in figures 1 (*a*) and (*b*) belong to the same

class since they have the same basic structure shown in figure 1 (c). It is seen that each class is associated with a certain basic structure.

It can be seen from the prescription of § 2 that if two diagrams G, G' belong to the same class their contributions to $S_\alpha(t)$ are integrals which differ only by a permutation of the variables of integration, and are therefore equal. Thus all the diagrams of the same class give an equal contribution, and the contribution of the whole class is the contribution of a typical member multiplied by the number of diagrams in the class.

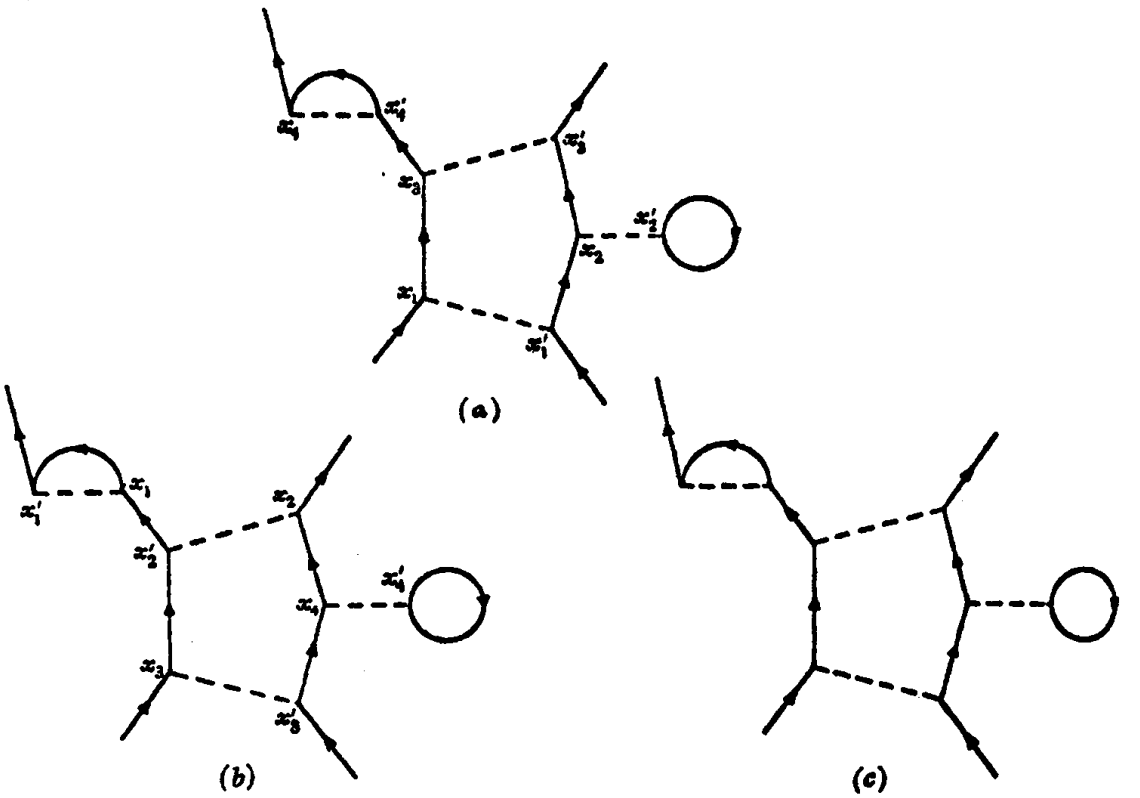

FIGURE 1

Let us consider how many diagrams there are in a given class. Let G be a typical member of a class Γ of order n, i.e. a class whose associated structure has n interaction lines. We can obtain all the other members of the class by performing certain permutations of the labels x_i, x_i' of the vertices of G. The permutations of the labels which lead to diagrams agreeing with the prescriptions of § 2 are those which leave the pairs x_i, x_i' connected by interaction lines in G still connected by interaction lines after the permutation. The only permutations which do this can be built up from the following types of permutation:

(i) simultaneous permutations of the x_i and x_i' in the same way;

(ii) the interchange of any pair x_i, x_i'.

The number of distinct permutations which can be built up from these is $2^n n!$. If the application of every one of these permutations to the labels of G led to a diagram distinct from G, then this would be the number of diagrams in the class. However, it may be that the application of some of these permutations to G leads to diagrams which are not topologically distinct from G; for example, the diagrams shown in

figures 2(*a*) and (*b*) which are obtainable from one another by a permutation of labels are topologically equivalent and must not be counted separately. Suppose the number of permutations which take G into diagrams topologically equivalent to itself is $g(\Gamma)$ (this number is a function of the structure Γ rather than of the particular diagram); then we can easily show that the number of diagrams in the class is in fact $2^n n!/g(\Gamma)$.

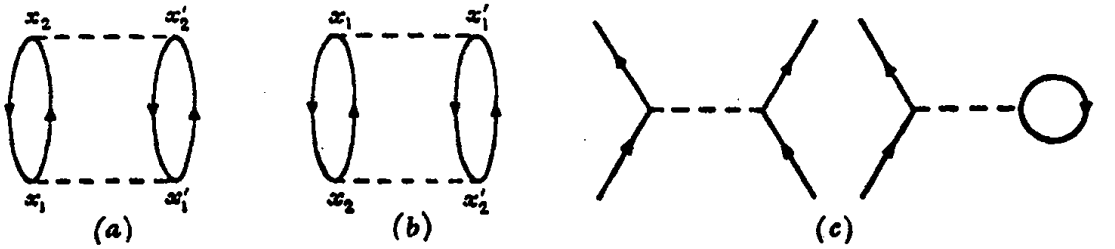

FIGURE 2

If we denote the contribution of a diagram G to $S_\alpha(t)$ by $S_\alpha(t, G)$ and the contribution of the class Γ to which G belongs by $S_\alpha(t, \Gamma)$, then we have

$$S_\alpha(t, \Gamma) = \frac{2^n n!}{g(\Gamma)} S_\alpha(t, G). \tag{25}$$

We can now develop the linked-cluster expansion. A structure Γ may or may not fall into two or more unconnected parts; in the former case we shall say that it is an unlinked, in the latter case linked. For example, the structure shown in figure 1(*c*) is linked whilst that shown in figure 2(*c*) is unlinked. It should be noticed that this definition of linked and unlinked diagrams is not quite the same as that used by Goldstone (1957).

An unlinked structure Γ can be resolved into a set of linked structures; if the unlinked structure Γ is made up of p_1 linked structures Γ_1, p_2 linked structures Γ_2 etc., we shall write

$$\Gamma = p_1 \Gamma_1 + p_2 \Gamma_2 + \ldots.$$

Let G be a typical diagram with the structure Γ. Using the prescription of § 2 we can easily prove that

$$S_\alpha(t, G) = \frac{1}{n!} [n_1! \, S_\alpha(t, G_1)]^{p_1} [n_2! \, S_\alpha(t, G_2)]^{p_2} \ldots,$$

where $G_1, G_2 \ldots$ are typical diagrams with the structures $\Gamma_1, \Gamma_2, \ldots$, n is the order of Γ, and $n_1, n_2 \ldots$ are the orders of Γ_1, Γ_2, etc. Using (25) we obtain

$$S_\alpha(t, \Gamma) = \frac{1}{g(\Gamma)} [g(\Gamma_1) \, S_\alpha(t, \Gamma_1)]^{p_1} [g(\Gamma_2) \, S_\alpha(t, \Gamma_2)]^{p_2} \ldots. \tag{26}$$

Finally it can be seen that

$$g(\Gamma) = p_1! p_2! \ldots [g(\Gamma_1)]^{p_1} [g(\Gamma_2)]^{p_2} \ldots, \tag{27}$$

so that

$$S_\alpha(t, \Gamma) = \frac{1}{p_1! p_2! \ldots} [S_\alpha(t, \Gamma_1)]^{p_1} [S_\alpha(t, \Gamma_2)]^{p_2} \ldots. \tag{28}$$

Let $\Gamma_1, \Gamma_2, \ldots$ be the set of all linked structures; if in (26) we allow $p_1, p_2, \ldots$ to run over all the values $0, 1, 2, \ldots$, then we obtain all possible structures. Since $S_\alpha(t)$ is the sum of the contributions from all possible structures we have

$$\begin{aligned} S_\alpha(t) &= \sum_{p_1=0}^{\infty} \sum_{p_2=0}^{\infty} \ldots \frac{1}{p_1!\, p_2! \ldots} [S_\alpha(t, \Gamma_1)]^{p_1} [S_\alpha(t, \Gamma_2)]^{p_2} \ldots \\ &= \exp\{S_\alpha(t, \Gamma_1)\} \exp\{S_\alpha(t, \Gamma_2)\} \ldots \\ &= \exp\{S_{L\alpha}(t)\}, \end{aligned} \tag{29}$$

where

$$S_{L\alpha}(t) = \sum_{\Gamma}^{\text{linked}} S_\alpha(t, \Gamma), \tag{30}$$

and we have made use of the fact that the various $S_\alpha(t, G)$ commute with each other; this is because all the ψ^+ and $\bar{\psi}^+$ operators anticommute (see equation (18)), and each $S_\alpha(t, G)$ contains an even number of these. Thus we see that $S_\alpha(t)$ can be expressed in terms of $S_{L\alpha}$, the sum of the contributions from linked diagrams.

Let us now resolve $S_{L\alpha}(t)$ into two parts

$$S_{L\alpha}(t) = S^{(0)}_{L\alpha}(t) + S'_{L\alpha}(t), \tag{31}$$

$S^{(0)}_{L\alpha}(t)$ containing the contributions from all linked 'vacuum' diagrams, that is, diagrams with no particle lines running to or from the edge of the diagram, and $S'_{L\alpha}(t)$ the contributions from all linked diagrams with external lines; $S^{(0)}_{L\alpha}(t)$ contains no operators and is a c number.

Substituting (31) into (29) and (29) into (2) and dividing out by the c number $\exp\{S^{(0)}_{L\alpha}(0)\}$, we obtain

$$\Psi = \lim_{\alpha \to +0} \exp\{S'_{L\alpha}(0)\} \Psi_0 / (\Psi_0 \,|\, \exp\{S'_{L\alpha}(0)\} \,|\, \Psi_0). \tag{32}$$

It will be shown in the next section that $S'_{L\alpha}(t)$ is continuous as $\alpha \to +0$ whilst $S^{(0)}_{L\alpha}(t)$ diverges like $1/\alpha$; thus, dropping a normalization factor,

$$\Psi = \exp\{S'_L(0)\} \Psi_0, \tag{33}$$

where

$$S'_L(0) = \lim_{\alpha \to +0} S'_{L\alpha}(0).$$

We shall see in the next section that the energy shift ΔE can be derived from $S^{(0)}_{L\alpha}(t)$, i.e. from a series involving only the linked terms; this series does not contain terms diverging more strongly than N and so is free from the difficulty mentioned at the beginning of this section.

4. The evaluation of integrals

In this section we perform as an illustration the evaluation of the integral representing the contribution of a simple diagram to $S_\alpha(0)$. The result obtained is typical of the general case, and we can deduce from it certain properties of the $S_\alpha(0, G)$: furthermore, these results afford a link between the present formalism and that of Goldstone.

The diagram whose evaluation we shall perform is that shown in figure 3 (*a*). The corresponding contribution to $S_a(0)$ is according to the prescription of § 2

$$\frac{1}{2}\left(\frac{1}{2i\hbar}\right)^2\int_{-\infty}^{0}dt_1\int_{-\infty}^{0}dt_2\int dx_1\,dx_2\,dx_1'\,dx_2'\,v(x_1-x_1')\,v(x_2-x_2')\,e^{\alpha(t_1+t_2)}$$
$$\times S(x_2,t_2;x_1,t_1)\,S(x_2',t_2;x_1',t_1)\,\overline{\psi}^+(x_2,t_2)\,\psi^+(x_1,t_1)\,\overline{\psi}^+(x_2',t_2)\,\psi^+(x_1',t_1), \quad (34)$$

where we have already performed the integrations over t_1' and t_2'. Because of the nature of the function S (equation (21)), it is convenient to divide the integration

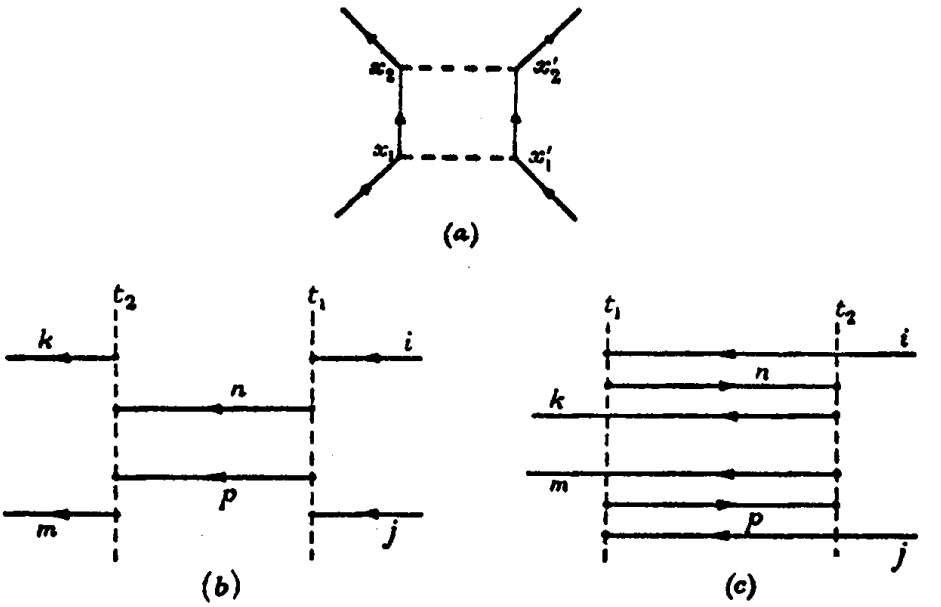

FIGURE 3

over t_1 and t_2 into two parts, one part arising from the region in which $t_2 > t_1$ and the other from the region in which $t_2 < t_1$. Substituting for S from (21) and for $\overline{\psi}^+$, ψ^+, from (18), we have for the first part of the integral

$$\frac{1}{2}\left(\frac{1}{2i\hbar}\right)^2\sum_{i,j}^{\text{occ.}}\sum_{kmnp}^{\text{unocc.}}\int\overline{u}_k(x_2)\,\overline{u}_m(x_2')\,v(x_2-x_2')\,u_n(x_2)\,u_p(x_2')\,dx_2\,dx_2'$$
$$\times\int\overline{u}_n(x_1)\,\overline{u}_p(x_1')\,v(x_1-x_1')\,u_i(x_1)\,u_j(x_1')\,dx_1\,dx_1'\int_{-\infty}^{0}dt_2\int_{-\infty}^{t_2}dt_1$$
$$\times\exp\left\{\alpha(t_1+t_2)+\frac{i}{\hbar}(E_k+E_m-E_n-E_p)\,t_2+\frac{i}{\hbar}(E_n+E_p-E_i-E_j)\,t_1\right\}\overline{\eta}_k\eta_i\overline{\eta}_m\eta_j$$
$$=\frac{1}{8}\sum_{ij}^{\text{occ.}}\sum_{kmnp}^{\text{unocc.}}\frac{(km\,|\,v\,|\,np)\,(np\,|\,v\,|\,ij)}{(E_k+E_m-E_i-E_j+2i\hbar\alpha)\,(E_n+E_p-E_i-E_j+i\hbar\alpha)}\,\overline{\eta}_k\eta_i\overline{\eta}_m\eta_j, \quad (35)$$

where
$$(km\,|\,v\,|\,np)=\int\overline{u}_k(x)\,\overline{u}_m(x')\,v(x-x')\,u_n(x)\,u_p(x')\,dx\,dx'. \quad (36)$$

A similar evaluation of the second part of the integral gives

$$\frac{1}{8}\sum_{ijnp}^{\text{occ.}}\sum_{km}^{\text{unocc.}}\frac{(km\,|\,v\,|\,np)\,(np\,|\,v\,|\,ij)}{(E_k+E_m-E_i-E_j+2i\hbar\alpha)\,(E_k+E_m-E_n-E_p+i\hbar\alpha)}\,\overline{\eta}_k\eta_i\overline{\eta}_m\eta_j. \quad (37)$$

The similarity of these results to the terms of the ordinary perturbation series is at once recognizable.

The two terms (35) and (37) may be represented diagrammatically as in figures 3(*b*), (*c*); these diagrams are obtained from (*a*) by arranging t_1 and t_2 in particular orders and labelling the lines rather than the vertices. Figure 3(*b*) represents a process in which two particles in states i and j interact and scatter into states n and p, and re-interact and scatter into states m and k; thus the whole process is a scattering of particles out of the states i and j into the states k and m via the intermediate state n, p. Similarly, figure 3(*c*) represents a process in which two particles scatter themselves into states k and m leaving holes in the states n and p into which the two particles in states i and j then scatter themselves; thus the final state is the same in both cases but the intermediate state is different. It will be seen that in each case the expressions (35) and (37) contain in their denominators the difference in energy of the final and initial state and the difference in energy of the initial and intermediate state.

These results are quite general. Any of the integrals representing contributions to $S_\alpha(0)$ can be evaluated by the above method, and leads to a series of terms of the form of (35) which can be interpreted as representing certain physical processes with the help of diagrams of the type of figures 3(*b*), (*c*). In each case the denominators of the expression will contain the difference in energy of the final and initial state and the differences in energy between the initial and intermediate states.

We can now make certain deductions from these results. The first thing to notice is that if an expression of the form of (35) arises from a linked diagram, and in view of the results of the preceding section we need only consider such diagrams, then none of the intermediate states can coincide with the initial state. Since the latter has been assumed to be non-degenerate, it follows that the energy of none of the intermediate states can coincide with that of the initial state. If, further, the final state is different from the initial state, as it is in all the terms contributing to $S'_{L\alpha}(0)$, then the energy of the final state will be different from that of the initial state. Thus, in the case of terms contributing to $S'_{L\alpha}(0)$, none of the energy differences in the denominators is zero; it follows at once (see (35)) that each of these terms is continuous as $\alpha \to +0$, and that $S'_{L\alpha}(0)$ is continuous $\alpha \to +0$. Thus $\lim S'_{L\alpha}(0)$ as $\alpha \to +0$ exists, and may be evaluated putting $\alpha = 0$ at the beginning of the calculation.

The situation with $S^{(0)}_{L\alpha}(0)$ is different, however. In the case of terms contributing to $S^{(0)}_{L\alpha}(0)$ the initial and final states coincide (although the intermediate states are different from the initial state), and the corresponding energy difference vanishes giving rise to a factor α in the denominator. Thus $S^{(0)}_{L\alpha}(0)$ diverges like $1/\alpha$ as $\alpha \to +0$.

We should now like to consider the calculation of the energy shift ΔE. This is given by (3). It may, however, be more conveniently calculated using a formula given by Gell-Mann & Low; it is shown in an appendix that it can be derived from $S^{(0)}_{L\alpha}(\infty)$, and is given by the following prescription: *write down the sum of all integrals contributing to* $S^{(0)}_{L\alpha}(\infty)$ *(one from each vacuum diagram); introduce into the integrand of each of these integrals a factor* $i\hbar\delta(t_1)$ *and put* $\alpha = 0$; *the resulting sum gives* ΔE.

In the remainder of this paper we shall devote our attention to the calculation of ΔE.

5. The uniform gas case

The theory of the preceding sections was general in the sense that H_0 was supposed to include not only the kinetic energy of the particles but also their potential energy in an external field. In the remaining sections of this paper we shall for simplicity restrict ourselves to the case in which the external field is constant and the particles form a uniform gas; it is hoped to deal with the general case later.

In the case of a uniform gas it is convenient to resolve the H' of (8) into two parts. Suppose the Fourier transform of v is

$$v(\mathbf{x}) = \sum_{\mathbf{k}} u(\mathbf{k})\, e^{i\mathbf{k}.\mathbf{x}}. \tag{38}$$

Then we split v into two parts according to

$$v(\mathbf{x}) = \sum_{k \neq 0} u(\mathbf{k})\, e^{i\mathbf{k}.\mathbf{x}} + u(0) = v'(\mathbf{x}) + u(0). \tag{39}$$

We can correspondingly write H' in the form

$$H' = \frac{1}{2}\int d\mathbf{x}\, d\mathbf{x}'\, \overline{\psi}(\mathbf{x}')\, \psi(\mathbf{x}')\, v'(\mathbf{x}-\mathbf{x}')\, \overline{\psi}(\mathbf{x})\, \psi(\mathbf{x})\, d\mathbf{x}\, d\mathbf{x}' + \tfrac{1}{2}N^2 u(0) - \tfrac{1}{2}N v(0) \tag{40}$$

and include the last two (constant) terms in H_0. All the above theory then goes through as before except that v is replaced by v' everywhere. The potential v' has the useful property

$$\int v'(\mathbf{x}-\mathbf{x}')\, d\mathbf{x}' = 0. \tag{41}$$

We can now make an important deduction concerning the perturbation series in the case of a uniform gas. This is that *in the case of a uniform gas those diagrams which contain a part which is attached to the rest of the diagram by only a single interaction line give no contribution $S_\alpha(t)$ or any derived quantities.* To prove this let us consider the contribution of a diagram of the type shown in figure 4 (*a*), where the two parts Γ' and Γ'' are connected by only the single interaction line shown. If in the integral representing the contribution of this diagram we perform all the integrations except those over $\mathbf{x}$ and $\mathbf{x}'$, we must obtain an expression of the form

$$\int F(\mathbf{x})\, v'(\mathbf{x}-\mathbf{x}')\, G(\mathbf{x}')\, d\mathbf{x}\, d\mathbf{x}'. \tag{42}$$

However, since the gas is uniform and has no natural origin of co-ordinates, F and G must be independent of $\mathbf{x}$ and $\mathbf{x}'$, so that it reduces to an integral over $v'(\mathbf{x}-\mathbf{x}')$ which must vanish by virtue of (41). Thus we can omit all diagrams of this type.

In future we shall drop the prime on v', it being always understood that we are working with v'.

6. The elimination of polarization parts

As pointed out in the introduction, the main point of introducing the diagrammatic analysis in the present theory is that it enables us easily to recognize those parts of the perturbation series which represent polarization effects. We are now in a position to investigate this.

Let us consider the physical interpretation of the *subdiagram* shown in figure 4 (*b*). The net effect of this subdiagram is that the two incoming particles scatter off each other, not through the ordinary direct interaction but via a closed particle loop. More generally, the subdiagram shown in figure 4 (*c*), where the circle is meant to represent some set of closed particle loops and interaction lines connected to the rest of the diagram by only the two interaction lines shown, represents the scattering of two particles through some more complicated process which, however, returns all the particles involved to their original states. Our hypothesis, which will be borne out by further calculation, is that these subdiagrams represent the polarization effect referred to in the introduction, and that they can be eliminated from the perturbation series by replacing the ordinary interaction by a modified interaction.

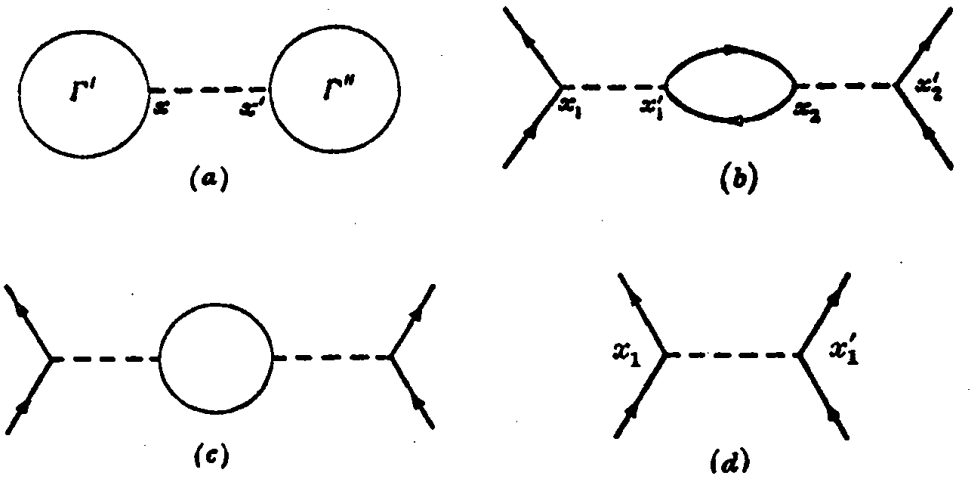

FIGURE 4

The way in which such subdiagrams can be eliminated from the perturbation series is already familiar in quantum electrodynamics, being exactly analogous to the elimination of photon self-energy parts (Dyson 1949). Let Γ be some structure. Then it may or may not be that Γ contains some polarization part, i.e. some connected part without external lines attached to the rest of the structure by only two interaction lines; in the former case we shall say that Γ is (polarization) reducible, in the latter case that Γ is irreducible. It is obvious that we can obtain all reducible structures by inserting polarization parts in place of interaction lines in irreducible structures.

Let us consider as an example the diagram shown in figure 4 (*b*), regarding this now as a complete diagram rather than as a subdiagram of some larger diagram. This is a reducible diagram contributing to $S'_L(t)$, obtainable from the irreducible diagram shown in figure 4 (*d*) by substituting the polarization part shown in figure 6 (*a*) for its interaction line. The contributions to $S'_L(t)$ of the diagrams of figures 4 (*b*), (*d*) are

$$\frac{1}{2!}\left(\frac{1}{2i\hbar}\right)^2\int^t dx_1\int^t dx'_1\int^t dx_2\int^t dx'_2\, v(x_1-x'_1)\,v(x_2-x'_2)$$
$$\times\,\overline{\psi}^+(x_1)\,\psi^+(x_1)\,\overline{\psi}^+(x'_2)\,\psi^+(x'_2)\,S(x'_1,x_2)\,S(x_2,x'_1) \qquad (43)$$

and

$$\frac{1}{1!}\left(\frac{1}{2i\hbar}\right)\int^t dx_1\int^t dx'_1\, v(x_1-x'_1)\,\overline{\psi}^+(x_1)\,\psi^+(x_1)\,\overline{\psi}^+(x'_1)\,\psi^+(x'_1). \qquad (44)$$

It will be seen that (43) is obtainable from (44) (apart from an unimportant change in the integration variable) by:

(i) multiplying by 1!/2!, the ratio of the factorials of the orders of the diagrams;

(ii) by replacing $v(x-x')$ in (44) by the quantity

$$\frac{1}{2i\hbar}\int^t \mathrm{d}x \int^t \mathrm{d}x'\, v(x_1-x)\, v(x_1'-x')\, S(x,x')\, S(x',x) \tag{45}$$

which is just the contribution to (43) of the interaction and particle lines of the polarization part of figure 6 (a) with the integrations at the vertices performed. This result is typical; the contribution of a reducible diagram is the same as that of the corresponding irreducible diagram except that the v's are replaced by functions of the type (45) corresponding to the various polarization parts which have been inserted in place of interaction lines, and the whole integral has been multiplied by the ratio of the factorials of the orders.

We can enunciate this result more precisely as follows. If G is a reducible diagram obtained by substituting the polarization part Γ'_{s_1} for the interaction line x_1x_1', Γ'_{s_2} for x_2x_2', etc., of the irreducible diagram G' (introducing the convention that if the line x_ix_i' of G' is left unchanged we say it has been replaced by the polarization part Γ'_0), then

$$S(t,G) = \frac{n'!}{n!}\, S(t,G';\ W_i'(\Gamma'_{s_1}),\ W_i'(\Gamma'_{s_2}),\ldots), \tag{46}$$

where n and n' are the orders of G and G', $S(t,G';\ W_i'(\Gamma'_{s_1}),\ W_i'(\Gamma'_{s_2}),\ldots)$ means that integral for $S(t,G')$ with the $v(x_i-x_i')$ replaced by the functions $W_i'(x_i',x_i,\Gamma'_{s_i})$, and $W_i'(x',x,\Gamma'')$ is the expression which arises from the polarization part Γ'' in the same way that (45) arises from the polarization part of figure 6 (a), remembering that in the case of the special polarization part Γ_0 this is just $v(x-x')$.

Let Γ be a reducible structure contributing to $S'_L(t)$, i.e. with external lines. Then it can be seen that Γ arises from some unique irreducible structure Γ''. Consider the total contribution to $S'_L(t)$ of all the diagrams with structures which reduce to a given irreducible structure Γ''. A straightforward counting of diagrams shows now that this total contribution is given by the expression

$$\frac{n'!\,2^{n'}}{g(\Gamma'')} \sum_{\Gamma'_{s_1}} \sum_{\Gamma'_{s_2}} \ldots\, S(t,G';\, W_i(\Gamma'_{s_1}),\, W_i(\Gamma'_{s_2}),\ldots), \tag{47}$$

where the sums run over all polarization parts, and

$$W_i(x',x,\Gamma'') = \frac{2^m}{g(\Gamma'')}\, W_i'(x',x,\Gamma''), \tag{48}$$

where $g(\Gamma'')$ is the g factor of the polarization part Γ'', defined to be the number of permutations of the *internal* interaction lines of Γ'' which take it into itself (these g factors are exactly analogous to those of §3), and m is its order, defined to be the number of *internal* interaction lines of Γ'' plus one.

Since $S(t,G';\ W_i(\Gamma'_{s_1}),\ W_i(\Gamma'_{s_2}),\ldots)$ depends linearly upon the $W_i(\Gamma'_s)$ we can write (47) as

$$S(t,\Gamma'';\mathscr{V}_i,\mathscr{V}_i,\ldots), \tag{49}$$

using (25), where

$$\mathscr{V}_i(x',x) = \sum_{\Gamma'} W_i(x',x,\Gamma'_s). \tag{50}$$

Thus, we see that the contribution to $S_L(t)$ of all diagrams reducing to the structure Γ' can be expressed in terms of the contribution of the class Γ' by replacing v everywhere by $\mathscr{V}_t$. Since every diagram contributing to $S_L(t)$ is uniquely reducible, we see that $S_L(t)$ can be expressed as a sum over contributions from irreducible diagrams by replacing v by $\mathscr{V}_t$ in all the integrals. Thus $\mathscr{V}_t$ plays the part of a modified interaction. In order to calculate the perturbed wave function we shall be interested in $\mathscr{V}_0$.

We have shown above how the perturbation series for the perturbed wave function can be contracted by introducing a modified interaction. Let us now consider the perturbation series for the energy shift ΔE. This has been expressed as a sum over vacuum diagrams in §4. We could proceed as above and reduce this to a sum over irreducible vacuum diagrams by replacing v everywhere by $\mathscr{V}_\infty$ (since the time integrations run up to $t = \infty$ in the case of ΔE) except for one feature. Whereas every diagram contributing to $S'_L(t)$ is uniquely reducible, this is not true for vacuum diagrams in general. For example, the diagram shown in figure 5 (*a*) could be reduced to either of the diagrams shown in figures 5 (*b*) or (*c*) by regarding either the right hand or the left hand part as the polarization part.

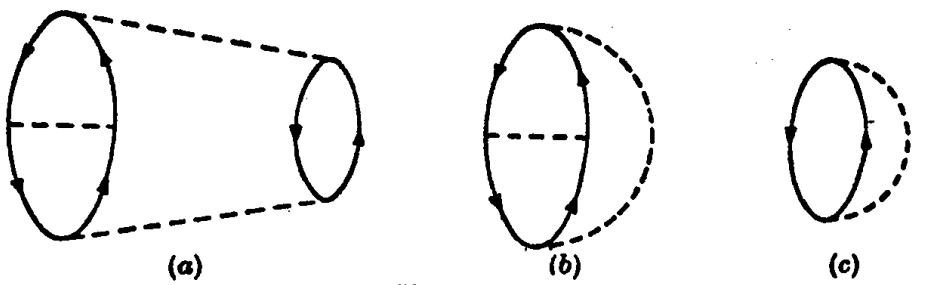

FIGURE 5

The fact that the reduction may not be unique can be overcome by demanding that every vacuum diagram be reduced in such a way that the point x_1 remain in the irreducible residue; any vacuum reducible diagram can always be reduced in this way provided that it contains no part which is connected to the rest of the diagram by only a single interaction line, and we have shown in the preceding section that such diagrams can be omitted. Furthermore, it is necessary to reduce the diagrams contributing to ΔE in this way, otherwise the factor $i\hbar\delta(t_1)$ would appear in some polarization part and spoil the theory.

Taking this point into account, we find by counting diagrams that the total contribution to ΔE of all diagrams which reduce to a given irreducible structure Γ' is

$$\frac{2^{n'}n'!}{g(\Gamma')}\sum_{\Gamma'_{s_1}}\sum_{\Gamma'_{s_2}}\cdots\frac{n'}{n'+n_{s_1}+n_{s_2}+\ldots}\Delta E(G';W_\infty(\Gamma'_{s_1}),W_\infty(\Gamma'_{s_2}),\ldots), \tag{51}$$

where G' is a typical diagram with the structure Γ' and n_s is the order of the polarization part Γ'_s. Because of the factor $(n'+n_{s_1}+n_{s_2}+\ldots)^{-1}$, we cannot perform the sum in the simple way we did in (47). However, we notice that if we regard the interaction v as being linearly proportional to some coupling constant λ, then $\Delta E(G';W_\infty(\Gamma'_{s_1}),W_\infty(\Gamma'_{s_2}),\ldots)$ varies as $\lambda^{n'+n_{s_1}+n_{s_2}+\cdots}$. Thus we can write (51) as

$$\int_0^\lambda\frac{d\lambda}{\lambda}\frac{2^{n'}n'!}{g(\Gamma')}\sum_{\Gamma'_{s_1}}\sum_{\Gamma'_{s_2}}\ldots n'\,\Delta E(G';W_\infty(\Gamma'_{s_1}),W_\infty(\Gamma'_{s_2})\ldots). \tag{52}$$

We can now perform the sum as we did in (47) and obtain

$$\int_0^\lambda \frac{d\lambda}{\lambda} \frac{2^{n'} n'!}{g(\Gamma')} n' \Delta E(G'; \mathscr{V}_\infty, \mathscr{V}_\infty \ldots), \tag{53}$$

enabling us to express ΔE as a sum over irreducible diagrams. In this case we replace v by $\mathscr{V}_\infty$ (which will be written $\mathscr{V}$ for short in future); it is this quantity $\mathscr{V}_\infty$ that we regard as the real modified interaction rather than the more general $\mathscr{V}_t$, since in the calculation of all observable quantities, such as ΔE, $\mathscr{V}_\infty$ will turn up rather than $\mathscr{V}_t$.

7. An integral equation for $\mathscr{V}$

In the preceding section we have introduced the modified interaction and expressed it in terms of an infinite series. In this section we should like to consider some of its properties.

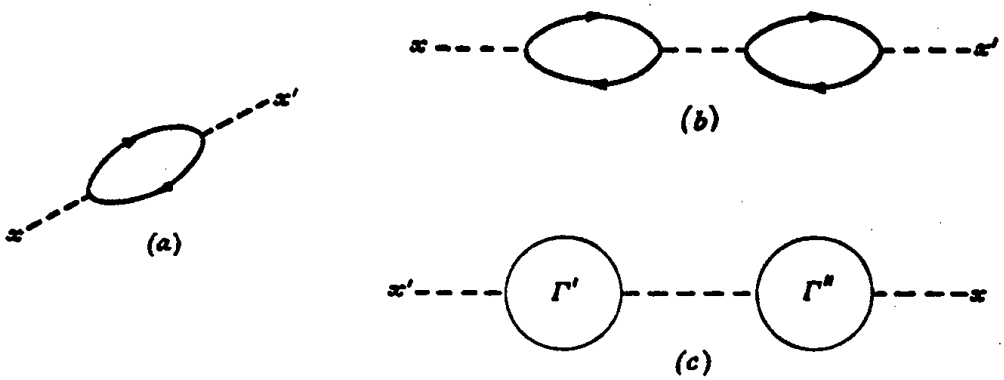

Figure 6

We first notice that in the case of a uniform gas $\mathscr{V}(x', x)$ is a function of $x - x'$ only. For so far as the space co-ordinates are concerned it can only be a function of $\mathbf{x} - \mathbf{x}'$ because of the spatial homogeneity of the system. Also each of the integrals in the series for $\mathscr{V}$ (equation (50) with $t = \infty$) is an integral whose time integrations run from $-\infty$ to $+\infty$ and whose integrands are products of factors each of which depends only upon time differences (see e.g. (45)); consequently $\mathscr{V}(x', x)$ can depend only upon $t' - t$, and is therefore a function of $x' - x$. It should further be noticed that there is no reason why $\mathscr{V}$ should vanish when $t \neq t'$, so that the modified interaction $\mathscr{V}$ will not in general be an instantaneous interaction like v but a sort of retarded interaction.

We shall now see how we can set up an integral equation for $\mathscr{V}$ which will enable us to express it in terms of a series more rapidly convergent than (50). Let Γ be any polarization structure. Then it may or may not be that Γ consists of two or more parts which are only connected by single interaction lines. In the first case we shall say that Γ is an improper polarization structure, in the latter case that it is a proper polarization structure. For example, the polarization structure shown in figure 6 (*a*) is a proper structure whilst that shown in figure 6 (*b*) is an improper one.

Let Γ be some improper polarization structure. Then Γ can be uniquely resolved as shown in figure 6 (*c*) into a proper structure Γ' and some other polarization structure Γ'', proper or improper. Let us introduce as follows the quantity $\overline{W}(x', x, \Gamma)$

related to $W_\infty(\Gamma)$ (to be written $W(\Gamma)$ for brevity in future). It will be seen from the prescription of the previous section for $W(\Gamma)$ that it can be written in the form

$$W(x', x, \Gamma) = \int v(x' - x'')\, \overline{W}(x'', x''', \Gamma)\, v(x''' - x)\, dx''\, dx''', \tag{54}$$

the two v's being those corresponding to the two outgoing lines of the polarization structure, and $\overline{W}$ containing the contribution from all the internal interaction and particle lines with the appropriate integrations performed. For example, in the case of the polarization part shown in figure 6 (*a*) (see (45)) $\overline{W}$ will be

$$\overline{W}(x', x) = \frac{1}{i\hbar} S(x', x)\, S(x, x'). \tag{55}$$

We can now prove that the contribution of the polarization part resolved as in figure 6 (*c*) can be written

$$W(x', x, \Gamma) = \int v(x' - x_1)\, \overline{W}(x_1, x_2, \Gamma')\, v(x_2 - x_3)\, \overline{W}(x_3, x_4, \Gamma'')\, v(x_4 - x)\, dx_1\, dx_2\, dx_3\, dx_4. \tag{56}$$

If we introduce the quantity

$$W^*(x', x, \Gamma') = \int v(x' - x'')\, \overline{W}(x'', x, \Gamma')\, dx'', \tag{57}$$

we can write (56) as

$$W(x', x, \Gamma) = \int W^*(x', x'', \Gamma')\, W(x'', x, \Gamma'')\, dx''. \tag{58}$$

Let us now consider the contribution to $\mathscr{V}$ of all those improper polarization structures which give rise to a given proper structure Γ' when resolved as in figure 6 (*c*). This is evidently obtained by summing over all structures Γ'' apart from Γ_0 on the right-hand side of (58), and is given by

$$\int W^*(x', x'', \Gamma') \sum_{\Gamma'' + \Gamma_0} W(x'', x, \Gamma'')\, dx'' \tag{59}$$

If we add to this the contribution of Γ' itself to $\mathscr{V}$, which from (54) and (57) is given by

$$\int W^*(x', x'', \Gamma')\, v(x'' - x)\, dx, \tag{60}$$

we obtain

$$\int W^*(x', x'', \Gamma') [v(x'' - x') + \sum_{\Gamma'' + \Gamma_0} W(x'', x, \Gamma'')]\, dx'' = \int W^*(x', x'', \Gamma')\, \mathscr{V}(x'', x)\, dx'' \tag{61}$$

for the total contribution to $\mathscr{V}$ of the proper diagram Γ' and all the improper ones which give Γ' on resolution. To obtain $\mathscr{V}$ we now have to sum this expression over all proper polarization parts Γ' and add the contribution of the polarization part Γ_0 which is just $v(x - x')$. Defining

$$\mathscr{V}^*(x', x) = \sum_{\Gamma'' + \Gamma_0}^{\text{proper}} W(x', x, \Gamma''), \tag{62}$$

we have

$$\mathscr{V}(x', x) = v(x' - x) + \int \mathscr{V}^*(x', x'')\, \mathscr{V}(x'', x)\, dx''. \tag{63}$$

Thus we have derived an integral equation which gives $\mathscr{V}$ in terms of $\mathscr{V}^*$. This is desirable because the series (62) is very much more rapidly convergent than (50). The solution of (63) presents no particular difficulty in the uniform gas because all the quantities involved depend upon the differences in their arguments and the equation may be solved by Fourier transformation.

We should like to complete this section with a comment on the physical interpretation of the result (62). The modified interaction between two particles can be regarded as a superposition of their direct interaction and the interaction of each with the polarization field of the other. These two interactions are represented by the first and second terms on the right-hand side of (62). The polarization produced at any point by one of the particles depends, however, not upon the direct field of the particle at that point, but upon the modified field; this is represented in (63) by the dependence of the second term upon $\mathscr{V}$, $\mathscr{V}^*(x', x'')$ representing the field at x' due to the polarization at the point x''.

8. An expression for ΔE in terms of V

We have seen in §6 how ΔE can be expressed as a sum of terms corresponding to irreducible vacuum diagrams. Our result can be written

$$\Delta E = \sum_{G}^{\text{irreducible vacuum}} \int_0^\lambda \frac{\mathrm{d}\lambda}{\lambda} n(G)\, \Delta E_v(G), \tag{64}$$

where $n(G)$ is the order of G and $\Delta E_v(G)$ means the contribution of the diagram G to ΔE with v replaced everywhere by $\mathscr{V}$.

Suppose now that G is some irreducible vacuum diagram. If we break the interaction line $x_1 x_1'$, the diagram may or may not fall into two separate parts. If it does, then it is of the form shown in Figure 4(*a*), and we have seen in §5 that such diagrams give no contribution. If it does not, then breaking this interaction line leads to some proper irreducible polarization part Γ (since G was assumed to be irreducible).

It can now be proved that if on breaking the line $x_1 x_1'$ in the diagram G we obtain the polarization part Γ, then

$$\Delta E_v(G) = \int \mathrm{d}x_1 \int \mathrm{d}x_1'\, i\hbar\delta(t_1)\, \mathscr{V}(x_1 - x_1')\, \overline{W}_v(x_1, x_1', \Gamma) \frac{g(\Gamma)}{n(G)!\, 2^{n(G)}}, \tag{65}$$

where $\overline{W}_v(x', x, \Gamma)$ is the same as $\overline{W}(x', x, \Gamma)$ except that v has been replaced everywhere by $\mathscr{V}$.

If we substitute (65) into (64), our sum over diagrams reduces to a sum over irreducible polarization structures, each structure being counted a certain number of times. Counting of diagrams shows that this sum reduces to

$$\Delta E = \frac{1}{2} \int_0^\lambda \frac{\mathrm{d}\lambda}{\lambda} \int \mathrm{d}x_1 \int \mathrm{d}x_1'\, i\hbar\delta(t_1)\, \mathscr{V}(x_1 - x_1') \sum_{\Gamma + \Gamma_0}^{\text{proper irreducible}} \overline{W}_v(x_1', x_1, \Gamma). \tag{66}$$

Defining the quantity

$$\overline{\mathscr{V}}(x', x) = \sum_{\Gamma + \Gamma_0}^{\text{proper irreducible}} \overline{W}_v(x', x, \Gamma) = \sum_{\Gamma + \Gamma_0}^{\text{proper}} \overline{W}(x', x\Gamma), \tag{67}$$

we see that (66) can be written

$$\Delta E = \frac{1}{2}\int_0^\lambda \frac{\mathrm{d}\lambda}{\lambda}\int \mathrm{d}x_1 \int \mathrm{d}x_1' \, i\hbar\delta(t_1)\,\overline{\mathscr{V}}(x_1, x_1')\,\mathscr{V}(x_1', x_1). \tag{68}$$

The quantity $\overline{\mathscr{V}}$ is closely related to $\mathscr{V}$. We have in fact (57), (62) and (67)

$$\mathscr{V}^*(x', x_1) = \int \overline{\mathscr{V}}(x', x'')\, v(x'' - x)\, \mathrm{d}x, \tag{69}$$

and $\mathscr{V}$ is related to $\mathscr{V}^*$ by (62); thus (68) is in effect an expression for ΔE in terms of $\mathscr{V}$. Using the result (68), we obtain the expression

$$E = \sum_i^{\text{occ.}} E_i - \tfrac{1}{2}Nv(0) + \tfrac{1}{2}N^2 u(0) + \frac{i\hbar}{2}\int_0^\lambda \frac{\mathrm{d}\lambda}{\lambda}\int \mathrm{d}x_1 \int \mathrm{d}x_1' \, \delta(t_1)\,\mathscr{V}(x_1, x_1')\,\overline{\mathscr{V}}(x_1', x_1) \tag{70}$$

for the energy of a uniform interacting gas, where the E_i are those of equation (10). In the case of a uniform gas the first term of (70) is just the kinetic energy of the particles in the occupied states together with their potential energy in any constant background potential which is present.

9. Summary of results

In this paper the following results have been obtained.

(i) It has been shown how the perturbation series for the many-body problem may be expressed as a sum of terms each of which is associated with a certain diagram.

(ii) This has been reduced to a series of terms (linked-cluster expansion) corresponding to linked diagrams.

(iii) A series has been obtained for the energy shift ΔE due to the interaction, each term of which is associated with a certain 'vacuum' diagram.

(iv) In the case of a uniform gas it has been shown that some of the terms of this series give no contribution and may be omitted.

(v) This series has been reduced to one over irreducible vacuum diagrams, i.e. over diagrams containing no polarization parts, by introducing a modified interaction $\mathscr{V}$ in place of the ordinary interaction v. An infinite series has been given for $\mathscr{V}$.

(vi) An integral equation has been obtained for $\mathscr{V}$ in terms of a quantity $\mathscr{V}^*$ which is given by an infinite series much more rapidly convergent than that for $\mathscr{V}$.

(vii) Finally, the energy shift and the energy of the whole system have been expressed in terms of the modified interaction $\mathscr{V}$; the latter is calculated from the integral equation the rapidly convergent series for $\mathscr{V}^*$ replaces the original perturbation series.

In a later paper these results will be applied to calculate the correlation energy of a free-electron gas, and it will be shown that essentially the same results as those of Bohm & Pines (1953) can be obtained by taking only the first term of the series for $\mathscr{V}^*$ and making allowance for certain exchange terms.

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Appendix. The calculation of ΔE

To calculate ΔE we start from a formula given by Gell-Mann & Low (1951), namely

$$\Delta E = \lim_{\alpha \to +0} i\hbar\alpha\lambda \frac{\partial}{\partial\lambda} \ln (\Psi_0 \,|\, S_\alpha(0, -\infty) \,|\, \Psi_0), \tag{A 1}$$

where λ is the coupling constant of the interaction. Using the same method as Gell-Mann & Low we can also derive the formula

$$\Delta E = -\lim_{\alpha \to +0} i\hbar\alpha\lambda \frac{\partial}{\partial\lambda} \ln (\Psi_0 \,|\, S_\alpha^{-1}(\infty, 0) \,|\, \Psi_0). \tag{A 2}$$

Furthermore, we have

$$S_\alpha(\infty, -\infty) = S_\alpha(\infty, 0)\, S_\alpha(0, -\infty), \tag{A 3}$$

from which

$$S_\alpha^{-1}(\infty, 0) = S_\alpha(0, -\infty)\, S_\alpha^{-1}(\infty, -\infty) \tag{A 4}$$

It was shown in § 3 that

$$S_\alpha(\infty, -\infty)\, \Psi_0 = \exp\{S^{(0)}_{La}(\infty) + S'_{La}(\infty)\}\, \Psi_0. \tag{A 5}$$

Since Ψ_0 is non-degenerate and $S_\alpha(\infty, -\infty)$ connects only states with the same energy in the limit as $\alpha \to +0$, we see that $S'_{La}(\infty, -\infty) \to 0$ as $\alpha \to +0$. From (A 1), (A 2), (A 4) and (A 5) we have

$$\begin{aligned}
\Delta E &= \lim_{\alpha \to +0} -i\hbar\alpha\lambda \frac{\partial}{\partial\lambda} \ln (\Psi_0 \,|\, S_\alpha(0)\, [\exp\{S'_{La}(\infty)\}]^{-1} \exp\{-S^{(0)}_{La}(\infty)\} \,|\, \Psi_0) \\
&= \lim_{\alpha \to +0} -i\hbar\alpha\lambda \frac{\partial}{\partial\lambda} [\ln (\Psi_0 \,|\, S_\alpha(0) \,|\, \Psi_0) - S^{(0)}_{La}(\infty)] \\
&= -\Delta E + \lim_{\alpha \to +0} i\hbar\alpha\lambda \frac{\partial}{\partial\lambda} S^{(0)}_{La}(\infty).
\end{aligned} \tag{A 6}$$

Thus

$$\Delta E = \tfrac{1}{2} \lim_{\alpha \to +0} i\hbar\alpha\lambda \frac{\partial}{\partial\lambda} S^{(0)}_{La}(\infty). \tag{A 7}$$

Now $S^{(0)}_{\mathcal{L}_\alpha}(\infty)$ is a sum of terms corresponding to vacuum diagrams. When all the integrations in an nth order diagram except those over $t_1, t_2, \ldots, t_n$ have been performed, we shall have an expression of the form

$$\int \mathrm{d}t_1 \ldots \int \mathrm{d}t_n \, U_\alpha(t_1, t_2, \ldots, t_n). \tag{A 8}$$

We can split this up into $n!$ terms by making different time orderings. In each of these terms we can perform the time integrations in any particular order; let us agree to always perform the integration over t_1 last. When we have performed all the integrations apart from that over t_1 in any term we end up with an expression of the form

$$\int_{-\infty}^{\infty} \mathrm{d}t_1 \, \mathrm{e}^{-\alpha|t_1| + \mathrm{i}Et_1} \, M \, \mathrm{e}^{-(n-1)\alpha|t_1| - \mathrm{i}Et_1} + O(1), \tag{A 9}$$

where the factor $\exp\{-\alpha|t_1| + \mathrm{i}Et_1\}$ arises from the corresponding factor in U_α and the term $\exp\{-(n-1)\alpha|t_1| - \mathrm{i}Et_1\}$ arises from the performance of the remaining integrations. Performing the integration in (A 9) gives $2M/n\alpha + O(1)$. The operation $\lambda(\mathrm{d}/\mathrm{d}\lambda)$ on the contribution to $S^{(0)}_{\mathcal{L}_\alpha}(\infty)$ of an nth order term just multiplies it by n. Thus the contribution of the term (A 9) to ΔE is just

$$\lim_{\alpha \to +0} \tfrac{1}{2}\mathrm{i}\hbar\alpha n \left\{ \frac{2M}{n\alpha} + O(1) \right\} = \mathrm{i}\hbar M. \tag{A 10}$$

Let us now compare this result with

$$\int_{-\infty}^{\infty} \mathrm{d}t_1 \ldots \int_{-\infty}^{\infty} \mathrm{d}t_n \, \mathrm{i}\hbar\delta(t_1) \, U_0(t_1, t_2, \ldots, t_n), \tag{A 11}$$

which arises from (A 8) by inserting a factor $\mathrm{i}\hbar\delta(t_1)$ into the integrand and putting $\alpha = 0$. If we evaluate this by splitting it into terms with different time orderings and perform the integration over t_1 last, we find that the term which corresponds to (A 9) is when all the integrations except that over t_1 have been performed

$$\int_{-\infty}^{\infty} \mathrm{d}t_1 \, \mathrm{i}\hbar\delta(t_1) \, M \, \mathrm{e}^{\mathrm{i}Et_1 - \mathrm{i}Et_1} = \mathrm{i}\hbar M, \tag{A 12}$$

which agrees with (A 11), the terms written $O(1)$ in (A 9) disappearing when $\alpha = 0$. Thus the insertion of a factor $\mathrm{i}\hbar\delta(t_1)$ into the integrand of (A 8) and putting $\alpha = 0$ has the same effect as operating with $\mathrm{i}\hbar\lambda(\mathrm{d}/\mathrm{d}\lambda)\alpha$ and taking the limit as $\alpha \to +0$. Thus we obtain the prescription of § 4.