

Derivation of the Brueckner many-body theory

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An exact formal solution is obtained to the problem of a system of fermions in interaction. This solution is expressed in a form which avoids the problem of unlinked clusters in many-body theory. The technique of Feynman graphs is used to derive the series and to define linked terms. The graphs are those appropriate to a system of many fermions and are used to give a new derivation of the Hartree-Fock and Brueckner methods for this problem.

1. INTRODUCTION

The Hartree-Fock approximation for the many-body problem uses a wave function which is a determinant of single-particle wave functions—that is, an independent-particle model. The single-particle states are eigenstates of a particle in a potential V , which is determined from the two-body interaction v by a self-consistent calculation. The Brueckner theory (Brueckner & Levinson 1955; Bethe 1956; Eden 1956) gives an improved method of defining V and shows why the residual effects of v not allowed for by V can be small. In particular, in the nuclear problem the corrections to the energy are small, even though the corrections to the wave function are large. The theory thus gives a reconciliation of the shell model, the strong two-nucleon interactions, and the observed two-body correlations in the nucleus. The smallness of the corrections is due to the operation of the exclusion principle. Bethe (1956) has shown that this same exclusion effect makes even the Hartree-Fock approximation good for quite strong interactions, such as an exponential potential fitted to low-energy nucleon-nucleon scattering.

The first problem on which calculations have been made is that of 'nuclear matter', that is, a very large nucleus with surface effects neglected (Brueckner 1955*a*; Wada & Brueckner 1956). In this problem the aim is to show that at a fixed density the energy is proportional to the number of particles, and that as the density is varied the energy per particle has a minimum at the observed density of large nuclei, and that this minimum value gives the observed volume energy of large nuclei. The single-particle wave functions are plane waves, and the potential V is diagonal in momentum space (in contrast to the ordinary Hartree potential which is diagonal in configuration space). The independent-particle model state is a 'Fermi gas' state with all the one-particle states filled up to the Fermi momentum k_F which depends only on the density.

Brueckner & Levinson's derivation, and that of Eden, is based on the multiple scattering formalism of Watson (Watson 1953). The proportionality of the energy of nuclear matter of a given density to the number of particles follows at once from the theory provided certain terms which represent several interactions occurring

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independently are not present. There is no satisfactory proof of this in the usual presentation of the theory. It has been shown (Brueckner 1955*b*) that the usual perturbation theory for bound states can be recast so that these terms disappear from the first few orders. The present paper proves a new perturbation formula in which these terms are absent and so completely solves this problem of 'unlinked clusters'.

The method of Feynman graphs (Feynman 1949) is used to enumerate the terms of the perturbation series. To derive the 'linked cluster' result it is essential to describe states in a particular way explained later, which is equivalent to treating the independent-particle ground state as a 'vacuum' state. This description then emphasizes the important exclusion effects, and is used to give a derivation of the Hartree-Fock approximation which seems very natural in this context. The ideas of the Brueckner method for dealing with strong potentials are then introduced and are shown to fit naturally into the Feynman graph treatment.

2. TIME-DEPENDENT PERTURBATION THEORY AND FEYNMAN GRAPH ANALYSIS

Consider A particles with the Hamiltonian

$$H = \sum_{i=1}^A T_i + \sum_{i<j} v_{ij}. \quad (2-1)$$

T_i is the kinetic energy of the i th particle and v_{ij} the interaction potential between particles i and j . Introduce the one-body potential V which is to be chosen later to give a reasonable independent-particle model of the system. Let V_i be this potential acting on particle i . Define

$$H_0 = \sum_i (T_i + V_i), \quad (2-2)$$

$$H_1 = \sum_{i<j} v_{ij} - \sum_i V_i, \quad (2-3)$$

so that

$$H = H_0 + H_1. \quad (2-4)$$

Expansions will be in powers of H_1 , but the complete series obtained will finally be rearranged so that higher-order terms represent small effects when V is suitably defined. Let the solutions of the one-particle Schrödinger equation

$$(T + V)\psi = E\psi \quad (2-5)$$

be a series of one-particle eigenstates ψ_n with eigenvalues E_n . V must be a potential which gives a discrete series of bound eigenstates ψ_n . (From now on suffixes m, n , etc., will refer to these states, not to particles.)

The second-quantized formalism will be used. Let η_n^\dagger, η_n be creation and destruction operations for the state ψ_n with the usual anti-commutation relations. Define matrix elements of v and V by

$$\langle rs | v | mn \rangle = \int \psi_r^*(1) \psi_s^*(2) v_{12} \psi_m(1) \psi_n(2) d\tau_1 d\tau_2, \quad (2-6)$$

$$\langle r | V | m \rangle = \int \psi_r^*(1) V_1 \psi_m(1) d\tau_1. \quad (2-7)$$

The matrix element of v defined by (2.6) is not antisymmetrized and corresponds to an interaction in which one particle goes from state ψ_m to state ψ_r , while the other goes from state ψ_n to state ψ_s . With these definitions

$$H_0 = \sum_n E_n \eta_n^\dagger \eta_n \quad (2.8)$$

$$H_1 = \sum \langle rs | v | mn \rangle \eta_r^\dagger \eta_s^\dagger \eta_n \eta_m - \sum \langle r | V | m \rangle \eta_r^\dagger \eta_m \quad (2.9)$$

The first sum in (2.9) is over all distinct matrix elements, a matrix element $\langle rs | v | mn \rangle$ being characterized by the pair of transitions (ψ_m to ψ_r) and (ψ_n to ψ_s). Thus $\langle sr | v | nm \rangle$ is not distinct from $\langle rs | v | mn \rangle$, but $\langle sr | v | mn \rangle$ is distinct. This way of introducing antisymmetry is the most suitable for graphical representation.

An eigenstate Φ of H_0 is a determinant formed from A of the ψ_n and can be described by enumerating these A one-particle states. A different description is necessary to obtain the results of this paper. It is supposed that H_0 has a non-degenerate ground state Φ_0 formed from the lowest A of the ψ_n . The proofs of this paper only apply to this case, that is, only to the ground state of a closed-shell nucleus or the ground state of 'nuclear matter'. The states ψ_n occupied in Φ_0 will be called unexcited states, and all the higher states ψ_n will be called excited states. Thus for 'nuclear matter' with a Fermi momentum k_F , an unexcited state means one with momentum $k < k_F$, an excited state one with $k > k_F$. An eigenstate Φ of H_0 can now be described by enumerating all the excited states which are occupied, and all the unexcited states which are not occupied. An unoccupied unexcited state is regarded as a 'hole', and the theory will deal with particles in excited states and holes in unexcited states. This treatment is analogous to the theory of positrons, with Φ_0 as the 'vacuum' state. An unexcited state is automatically regarded as occupied and so excluded for other particles, unless a hole in that state is introduced explicitly. Thus the chief effect of the exclusion principle is emphasized by this description. This is the essential difference from the theory of positrons, in which there is symmetry between particles and holes. In this theory the asymmetry between particles and holes is emphasized. To introduce this method formally equations (2.8) and (2.9) are retained, but the interpretation of η_n^\dagger, η_n for unexcited ψ_n is altered. η_n will now be the operator creating a hole in state ψ_n , η_n^\dagger , the operator destroying a hole.

The following derivation of the perturbation formula uses time-dependent perturbation theory in the interaction representation. In this way certain of the results needed appear more naturally than in a completely time-independent presentation. Let Φ_0 be the ground state of H_0 as described above, assumed to be non-degenerate, and let Ψ_0 be the lowest eigenstate of H . Ψ_0 will be derived from Φ_0 by adiabatically switching on the interaction H_1 over the time interval $-\infty$ to 0. For this case of a discrete series of eigenstates with a unique ground state the adiabatic theorem can be proved in the following form (Gell-Mann & Low 1951).

Define
$$H_1(t) = e^{iH_0 t} H_1 e^{-iH_0 t} e^{xt}, \quad (2.10)$$

and let
$$U_x = \sum_{n=0}^{\infty} (-i)^n \int_{0 > t_1 > t_2 > \dots > t_n} H_1(t_1) H_1(t_2) \dots H_1(t_n) dt_1 \dots dt_n. \quad (2.11)$$

As $\alpha \rightarrow 0$ the unitary operator U_α describes the adiabatic process.

Let
$$\Psi_0 = \lim_{\alpha \rightarrow 0} \frac{U_\alpha \Phi_0}{\langle \Phi_0 | U_\alpha | \Phi_0 \rangle}. \quad (2.12)$$

By using Feynman graphs this limit will be shown to exist and an explicit expression derived for it. Then the adiabatic theorem states that

$$H\Psi_0 = (E_0 + \Delta E)\Psi_0, \quad (2.13)$$

where
$$H_0 \Phi_0 = E_0 \Phi_0 \quad (2.14)$$

and
$$\Delta E = \langle \Phi_0 | H_1 | \Psi_0 \rangle = \lim_{\alpha \rightarrow 0} \frac{\langle \Phi_0 | H_1 U_\alpha | \Phi_0 \rangle}{\langle \Phi_0 | U_\alpha | \Phi_0 \rangle}. \quad (2.15)$$

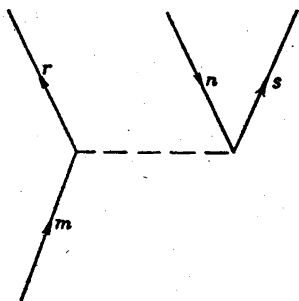


FIGURE 1. In all the graphs the direction of increasing time is upwards.

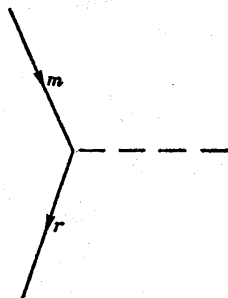


FIGURE 2

The required perturbation formulae for Ψ_0 and ΔE will be obtained on carrying out the time integrations in the expression for the limits in equations (2.12) and (2.15).

$H_1(t)$ is derived from equation (2.9) for H_1 by substituting $\eta_n(t)$ for η_n , where

$$\eta_n(t) = \eta_n e^{-E_n t} \quad (2.16)$$

and then multiplying by $e^{\alpha t}$. The expression (2.11) for U_α then becomes a sum of products of v and V matrix elements, e^{iEt} and $e^{\alpha t}$ factors and operators η^\dagger and η . Analysis of the products of operators by the same algebra as is used in proving Wick's theorem (Wick 1950) leads to the following expression for $U_\alpha \Phi_0$ as a sum of terms represented by Feynman graphs. Each graph represents a series of $H_1(t)$ interactions. A particle in an excited state is represented by a line in the direction of increasing time. A hole in an unexcited state is represented by a line in the opposite direction. A matrix element $\langle rs | v | mn \rangle$ in $H_1(t)$ is represented as in figure 1. This is for the case in which ψ_m, ψ_r, ψ_s are excited states and ψ_n an unexcited state. It represents an interaction between two particles in which one is scattered from ψ_m to ψ_r , while the other jumps from ψ_n into ψ_s leaving a hole in ψ_n . With this graph is associated a time factor $e^{i(E_r + E_s - E_m - E_n)t} e^{\alpha t}$. The other combinations of excited and unexcited states $\psi_m \psi_n \psi_r \psi_s$ are represented similarly.

A matrix element $\langle r | V | m \rangle$ is represented as in figure 2. This shows a particle scattered from state ψ_m to ψ_r by V , both states unexcited. Initially there was a hole in state ψ_r , otherwise the interaction is excluded, and finally there is a hole in state ψ_m .

There are further possibilities which do not occur in positron theory. Here the unexcited states are occupied by real particles not explicitly represented in the graphs, but interacting with each other and with the particles represented in the graphs. These particles will be called passive unexcited particles. Their interactions are the most important ones present, and it is these interactions which must be

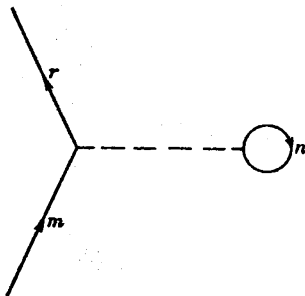


FIGURE 3

allowed for in the choice of V . They are represented as in figure 3. This shows a particle scattered from excited state ψ_m to excited state ψ_r by the particle in the unexcited state ψ_n which remains in the same state after the interaction. (In 'nuclear matter' this is 'forward' scattering.) Figure 3 corresponds to a factor

$$\langle rn | v | mn \rangle e^{i(E_r - E_m)t}.$$

The 'exchange' term corresponding to this contains the matrix element $\langle rn | v | nm \rangle$ and is represented as in figure 4. Finally, figure 5 shows the graphs representing interactions in which only passive unexcited particles take part. The matrix elements are for figure 5 (a), $\langle mn | v | mn \rangle$; for figure 5 (b) $\langle mn | v | nm \rangle$; for figure 5 (c) $\langle n | V | n \rangle$.

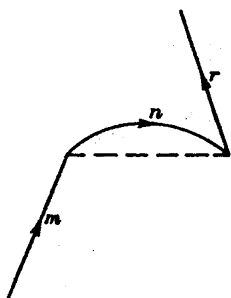


FIGURE 4

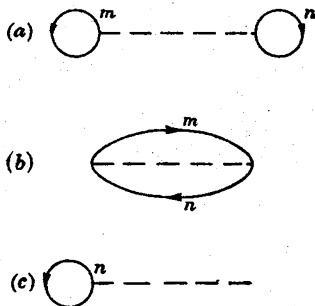


FIGURE 5

The algebra of Wick's theorem now gives the following rule for $U_\alpha \Phi_0$. All distinct graphs starting with no free lines at the bottom, that is, with Φ_0 , are drawn. Each such graph consists of a number of open loops of nucleon lines and a number of closed loops. For example, figure 6 contains one open loop and two closed loops. For each graph multiply the v and V matrix elements and the e^{iEt} and e^{iVt} factors and a factor $(-1)^{h+l}$, where h is the number of internal hole lines (four in figure 6; the line labelled m is an external line) and l the number of closed loops. A passive unexcited particle loop as in figure 5 (c) contributes a plus sign, counting as one

These linked-cluster expansions can be derived without using time-dependent theory. Ψ_0 can be defined to be given by (3.2). It then follows that

$$(E_0 - H_0)\Psi_0 = \sum_L H_1 \left(\frac{1}{E_0 - H_0} H_1 \right)^n \Phi_0 \quad (3.4)$$

and

$$H_1 \Psi_0 = H_1 \sum_L \left(\frac{1}{E_0 - H_0} H_1 \right)^n \Phi_0. \quad (3.5)$$

The right-hand side of (3.5) is given by those graphs which are linked when the last H_1 is removed. Some care is needed to prove this, since Wick's theorem does not immediately apply to the time-integrated expression (3.4). Subtracting (3.4) from (3.5) gives

$$(H - E_0)\Psi_0 = \sum' H_1 \left(\frac{1}{E_0 - H_0} H_1 \right)^n \Phi_0 \quad (3.6)$$

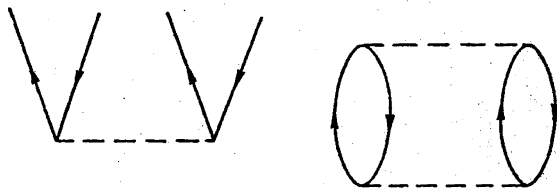


FIGURE 8

where Σ' means summed over all graphs containing an unlinked part but which are linked when the last H_1 line is removed. Such graphs must be of the type shown in figure 8. Now the last H_1 line in the unlinked part may be kept fixed and a sum taken over the different positions of the rest of the unlinked part relative to the rest of the graph. By using algebraic identities on the energy denominators which are equivalent to the separation of the time integrations in the time-dependent proof it can be shown that the right-hand side of (3.6) is equal to the product of Ψ_0 with the sum of all connected closed graphs, that is, with ΔE as defined by (3.3). Then (3.6) gives

$$H\Psi_0 = (E_0 + \Delta E)\Psi_0 \quad (3.7)$$

the required result.

This method of proof has one advantage over the other in that it does not use time-dependent methods to prove a time-independent result. However, the time-dependent proof gives the easiest way of enumerating the terms correctly and of combining the contributions of different positions of unlinked parts. The adiabatic theorem used can be strictly proved under the conditions of this paper. The time-independent method has been used by the author to extend the results to excited and degenerate states.

4. CHOICE OF V : THE HARTREE-FOCK METHOD

The simplest way to choose V is to make it allow for the first-order interaction with passive unexcited particles. This is done by making the graph parts in figure 9 cancel, that is, by defining

$$\langle r | V | m \rangle = \sum_n \{ \langle rn | v | mn \rangle - \langle rn | v | nm \rangle \}. \quad (4.1)$$

The sum is over all unexcited states ψ_n . The states ψ_n are determined by

$$(T + V)\psi_n = E_n\psi_n. \tag{4.2}$$

(4.1) and (4.2) are the Hartree-Fock self-consistent equations.

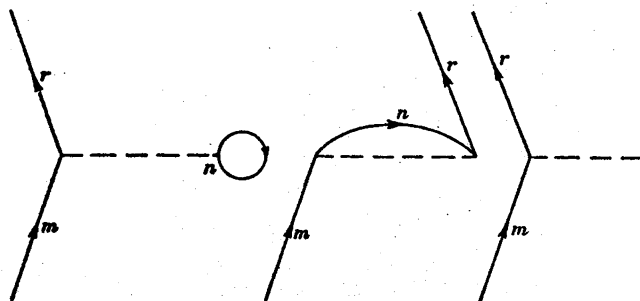


FIGURE 9

This definition ensures the complete disappearance of the V interaction and the interactions with passive unexcited states from all graphs except the connected closed parts in figure 5. These represent the first-order terms in ΔE . Figure 5 (c) contributes $-\sum_n \langle n | V | n \rangle$, while figures 5 (a) and (b) contribute

$$\frac{1}{2} \sum_{m,n} \{ \langle mn | v | mn \rangle - \langle mn | v | nm \rangle \} = \frac{1}{2} \sum_n \langle n | V | n \rangle \tag{4.3}$$

when summed over all distinct possibilities. Also,

$$E_0 = \sum_n \{ \langle n | T | n \rangle + \langle n | V | n \rangle \}. \tag{4.4}$$

Thus, to the first order in v ,

$$E = E_0 + \Delta E = \sum_n \langle n | T | n \rangle + \frac{1}{2} \sum_n \langle n | V | n \rangle. \tag{4.5}$$

This factor of $\frac{1}{2}$ is familiar in the Hartree-Fock method.

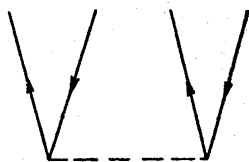


FIGURE 10

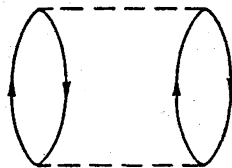


FIGURE 11

The higher-order corrections to E are given by the sum (3.3) over all connected graphs with no external lines and with no V interactions and no interactions with passive unexcited particles. The wave function Ψ_0 is given by the sum (3.2) again without the above interactions. The expression for Ψ_0 contains terms which are the product of many factors represented by graphs like figure 10. The result is that Φ_0 is only a very small component of Ψ_0 . (Note that Ψ_0 is normalized to $\langle \Psi_0 | \Psi_0 \rangle = 1$.) However, the corresponding correction to the energy can contain the factor represented by figure 11 once only. Bethe (1956) has shown that the exclusion principle

which limits the particles in excited states to states with momentum $> k_F$ can make this correction fairly small even for strong potentials for the values of k_F of interest. Thus the Hartree-Fock method can give the energy quite well even for strong potentials. This is a quantitative version of the old argument that strong interactions would be inhibited by the exclusion principle. It applies to the energy but not to the wave function. There are certainly strong correlations between nucleons in a nucleus and the Brueckner theory can be used to explain them (Brueckner, Eden & Francis 1955).

5. THE BRUECKNER THEORY

The nucleon-nucleon potential very probably has a steep repulsive core at small distances. (This will certainly ensure saturation but a proper theory is needed to obtain an energy minimum at the observed nuclear density.) For this v it is clearly impossible to choose V by the Hartree-Fock method, as the matrix elements of

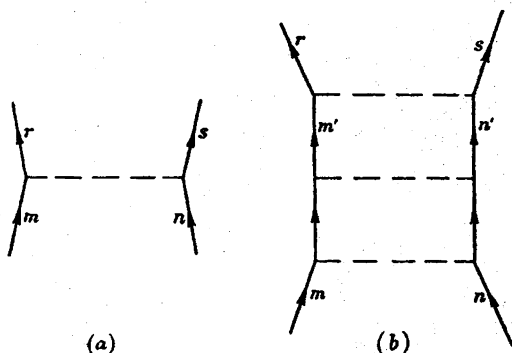


FIGURE 12

v will have a large contribution from the core. The Brueckner theory replaces v by a reaction matrix t calculated from a two-body equation of the type

$$t = v + v \frac{1}{E_0 - H_0} t. \quad (5.1)$$

The idea is to derive V from t instead of from v . Since H_0 contains V , V occurs in the energy denominator so that there is a further self-consistency requirement in addition to the Hartree-Fock condition on the wave functions. In fact, for 'nuclear matter' the Hartree-Fock self-consistency disappears since the wave functions must be plane waves. Brueckner (1955*a*) has shown that this new self-consistency is important.

The procedure in terms of graphs is as follows. Corresponding to any graph with a single v line in a certain position as in figure 12 (a), there are more complicated ones in which figure 12 (a) is replaced by the 'ladder' graph of figure 12 (b). In the intermediate states of figure 12 (b) both particles are in excited states. The sum of all such parts is given by an integral equation of the type (5.1). When figure 12 (b) occurs as part of a larger graph the energy denominator for the intermediate state containing $\psi_m \psi_n$ is

$$-E_{m'} - E_{n'} - E_R = E_m + E_n - E_{m'} - E_{n'} - \delta E, \quad (5.2)$$

where E_R is the excitation energy of the other particles present while the interaction represented in 12 (b) occurs and δE is the excitation energy of the complete intermediate state at the beginning of the interaction. The excitation energy of a state is the sum of the energies E_n of occupied excited states minus the sum of the energies of unexcited states in which there are holes. The integral equation for the sum of the terms represented by figure 12 is then

$$\langle rs | t | mn \rangle = \langle rs | v | mn \rangle + \sum_{m'n'} \frac{\langle rs | v | m'n' \rangle \langle m'n' | t | mn \rangle}{E_m + E_n - E_{m'} - E_{n'} - \delta E}, \quad (5.3)$$

where the sum is over $\psi_{m'}, \psi_{n'}$ excited states only. The solution is a matrix $t(\delta E)$ which can be used to replace v and which is finite even for a repulsive core potential.

A graph will be called irreducible if it contains no 'ladders' of the type of figure 12 (b). A sequence of v interactions as in figure 12 (b) only forms a 'ladder' if all the intermediate states are excited and if there are no other interactions in other

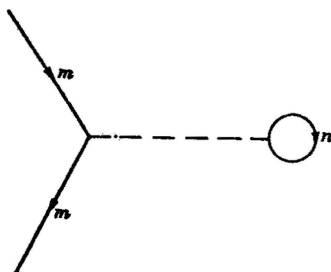


FIGURE 13

parts of the graph between the ends of the ladder. All graphs can be obtained by substituting independently 'ladders' for each v line in the irreducible graphs. The terms of the linked cluster expansion can thus be grouped together so that each v matrix element is replaced by a matrix element of $t(\delta E)$. δE is the excitation energy of the intermediate state to the right of the matrix element in the series (below it in the graph). The sums must now be taken over linked irreducible graphs only.

Figure 7 (b) is an important type of ladder graph and is absorbed into the t matrix element $\langle mn | t | mn \rangle$ represented in figure 13. Note that (5.3) is not antisymmetrized. The ladder graph in which the lines of figure 12 (b) cross over is counted in $\langle sr | t | mn \rangle$.

V can now be defined to cancel the t -interactions with passive unexcited states, that is, by (4.1) with v replaced by t . However, the cancellation cannot be complete because of the dependence of t on δE . (The procedure in this problem contrasts with that in field theory in which the time ordering and the dependence of one part of a graph on another are completely removed by introducing an extra energy variable for each particle. This does not seem appropriate here.) The best that can be done is to choose some average value of δE appropriate to the matrix element of t being evaluated.

Equation (4.5) is replaced by the following expression for the energy to first order in t :

$$E = \sum_n \langle n | T | n \rangle + \frac{1}{2} \sum_{m,n} \{ \langle mn | t(0) | mn \rangle - \langle nm | t(0) | mn \rangle \}. \quad (5.4)$$

The $\langle n | V | n \rangle$ in E_0 is cancelled by the term represented by figure 5 (c) whatever the definition of V . The second term in (5.4) will equal $\frac{1}{2} \sum_n \langle n | V | n \rangle$ only if $\langle n | V | n \rangle$ is derived from t with $\delta E = 0$. This is the most straightforward choice for the diagonal elements of V between unexcited states.

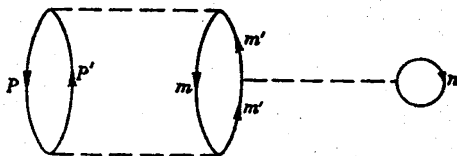


FIGURE 14

Figure 14 represents a term in the energy given by

$$\langle mp | t(\delta E) | m'p' \rangle \left(-\frac{1}{\delta E} \right) \langle m'n | t(\delta E) | m'n \rangle \left(-\frac{1}{\delta E} \right) \langle m'p' | t(0) | mp \rangle, \quad (5.5)$$

where
$$\delta E = E_{p'} - E_p + E_{m'} - E_m. \quad (5.6)$$

An average of this δE used in the definition of $\langle m' | V | m' \rangle$ will ensure as much cancellation of this term as possible. For 'nuclear matter' the conservation of momentum limits the possible values of $\psi_p \psi_{p'}$, and ψ_m given $\psi_{m'}$.

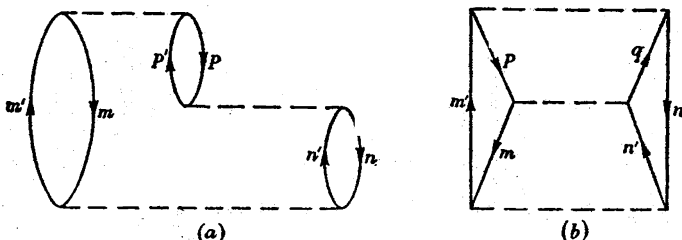


FIGURE 15

Apart from the corrections due to the dependence of t on E the remaining graphs for the energy all represent three or more particle interactions. It is hoped that these are small because of the exclusion-principle limitation of the number of states to be summed over (Brueckner & Levinson 1955; Bethe 1956). Two typical three-particle interactions are shown in figure 15. Figure 15 (a) represents two particles jumping from states $\psi_m \psi_n$ into excited states $\psi_{m'} \psi_{n'}$. Then the particle in $\psi_{n'}$ falls back into ψ_n while another particle jumps from ψ_p into $\psi_{p'}$. Finally the particles in $\psi_{p'}$ and $\psi_{m'}$ interact and fall back. The corresponding matrix elements are

$$\langle pm | t | p'm' \rangle \langle np' | t | n'p \rangle \langle m'n' | t | mn \rangle. \quad (5.7)$$

Figure 15 (b) represents two particles jumping from states $\psi_m \psi_n$ into states $\psi_{m'} \psi_{n'}$. The particle in $\psi_{n'}$ then interacts with the particle in the occupied state ψ_p . The particle in $\psi_{n'}$ is scattered into ψ_q while that in ψ_p jumps into the hole in ψ_m leaving a hole in $\psi_{p'}$. Finally the particles in $\psi_{m'}$, ψ_q fall back into the holes in $\psi_{p'}$, ψ_n . The corresponding matrix elements are

$$\langle np | t | qm' \rangle \langle qm | t | n'p \rangle \langle m'n' | t | mn \rangle. \quad (5.8)$$

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