for the effect of a nonvanishing value of f to be easily seen.

When population pulsations are taking place there will be a correlated time-dependent excitation of the lower level by cascade. It is possible that more interesting consequences than those obtained would result, and it is hoped to explore this possibility in a later paper.

21. OTHER SOURCES OF BROADENING

For some kinds of line broadening, especially in certain solid-state optical masers, one could adopt the recipe proposed in Sec. 17, and rejected for the case of Doppler broadening. If the effect of environment could be described by a distribution function for the atomic resonance frequencies ω, an averaged nonlinear susceptibility could be used. This could also be done for the case of isotopic mixtures of the active atoms in gaseous masers.

Although γ_a and γ_b were introduced into our equations to describe spontaneous radiative decay of the states a and b, it is plausible that such phenomenological decay constants might also describe certain kinds of collision broadening. In that case, the γ's would be functions of the pressure.[32] A more detailed discussion of collision broadening for a gaseous optical maser will be given in another paper.

[32] Evidence for such a dependence has recently been obtained by Javan and Szöke, Ref. 16.

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Correlation Effects in Many Fermion Systems. II. Linked Clusters*

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In a previous paper a set of coupled equations was derived for the ground-state wave function and energy of a finite system of interacting Fermions. The equations are now modified so as to be more applicable to systems in which the number of particles becomes large. The resulting equations are shown to be equivalent to those obtained from many-body perturbation theory.

I. LINKED CLUSTERS

In a previous paper,[1] a set of coupled equations was derived for the ground-state wave function and energy of a finite system of interacting Fermions. The wave function was expanded in terms of multiple-particle excitations on an uncorrelated zero-order state. The total energy E of the system appeared in the resulting equations and it was pointed out that this restricts the application of these equations to finite systems; in general, the restriction is to systems of small N. In the equations, the amplitudes for one-particle excitations are coupled to those for two-particle and three-particle excitations. The two-particle amplitudes are coupled to those for one-particle, three-particle, and four-particle excitations, and similarly for higher particle excitations. It was mentioned in I that it might be reasonable to approximate four-particle excitation terms, for example, as products of independent two-particle excitations.

It is shown here that four-particle terms involving two independently propagating pairs enter the equations in such a way as to eliminate the dependence of the two-particle excitation equations on the total energy E, and similarly for the other excitations.[2] Explicit inclusion of products of independent excitations yields the equations of the linked cluster expansion. The resulting equations are shown to be the same as those obtained from many-body perturbation theory as formulated by Brueckner[3] and by Goldstone.[4]

In I, the ground-state wave function is expanded as

$$|\psi\rangle=|\Phi_0\rangle+\sum_{\alpha,k}f(k;\alpha)\eta_k{}^+\eta_\alpha|\Phi_0\rangle + \sum_{\alpha,\beta,k,k'}f(kk';\alpha\beta)\eta_k{}^+\eta_{k'}{}^+\eta_\beta\eta_\alpha|\Phi_0\rangle+\cdots. \quad (1)$$

The unperturbed solution $|\Phi_0\rangle$ is a determinant composed of the N single-particle states which are lowest in energy.

Equations are then derived for $f(k;\alpha)$ and $f(kk';\alpha\beta)$ by inserting $|\psi\rangle$ from Eq. (1) into

$$H|\psi\rangle=E|\psi\rangle, \quad (2)$$

where H is written in the usual second-quantized form.[1]

* Work supported in part by the U. S. Atomic Energy Commission.

[1] H. P. Kelly and A. M. Sessler, Phys. Rev. **132**, 2091 (1963), hereafter referred to as I.

[2] I am indebted to Dr. A. M. Sessler for stressing the desirability of including products of independent pair excitations in the four-particle excitations, so as to make the resulting equations more applicable to systems of large N.

[3] K. A. Brueckner, in *The Many Body Problem*, edited by C. DeWitt (John Wiley & Sons, Inc., New York, 1958).

[4] J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957).

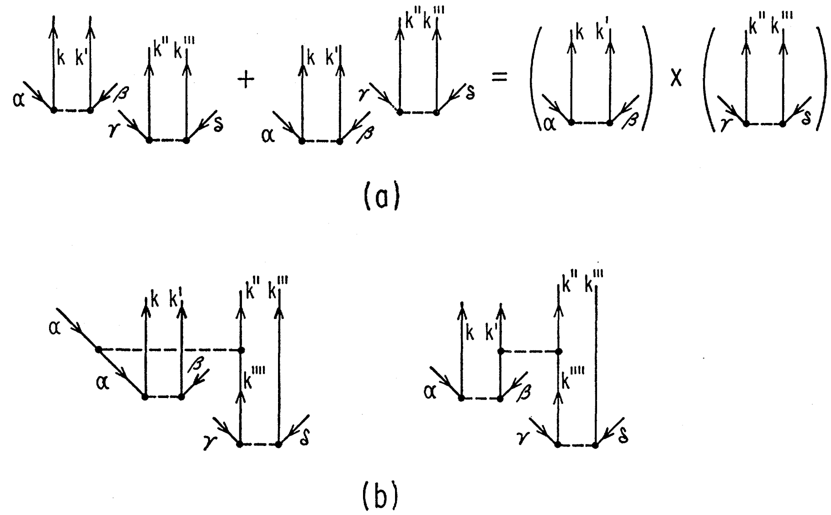

FIG. 1. (a) In perturbation theory two independent pair excitations factor when both time orderings are considered. (b) Typical terms which always link any two excited pairs.

An approximate solution for $f(kk';\alpha\beta)$ is given in Eq. (15) of I, in this paper referred to as Eq. (I.15),

$$f(kk';\alpha\beta)=(\epsilon_\alpha+\epsilon_\beta-\epsilon_k-\epsilon_{k'}-\langle(\alpha\beta)_{ex}|v|\alpha\beta\rangle +E-E_{HF})\langle(kk')_{ex}|v|\alpha\beta\rangle. \quad (3)$$

If we neglect the term $E-E_{HF}$, then this expression is that which is obtained from Rayleigh-Schrödinger perturbation theory when we use a Hartree-Fock basis and include the first-order term and all higher order diagonal hole-hole interaction terms.[5,6] However, for large N the term $E-E_{HF}$ may become so large as to invalidate the equations of I. Such difficulties have been described by Brueckner in his comparison of Rayleigh-Schrödinger and Brillouin-Wigner perturbation theories.[3]

We now show that the term $E-E_{HF}$ may be removed by considering the coupling of four-particle excitations in Eq. (I.11) for $f(kk';\alpha\beta)$. In the equation for $f(kk';\alpha\beta)$, coupling with four-particle excitations adds the term

$$\sum_{\gamma\delta k''k'''}\langle(\gamma\delta)_{ex}|v|k''k'''\rangle f(kk'k''k''';\alpha\beta\gamma\delta) \quad (4)$$

to the left-hand side of Eq. (2) or Eq. (I.11). The coefficients $f(kk'k''k''';\alpha\beta\gamma\delta)$ are composed of parts in which two pairs propagate independently and of remaining parts involving more complicated interactions among the four particles.

The approximation of regarding $f(kk'k''k''';\alpha\beta\gamma\delta)$ solely as a product of two pair excitations has been discussed by Brenig and Sinanoğlu.[7] A justification for this decomposition is found in perturbation theory where the lowest order four-particle excitation is given by the product of two pair excitations when we consider both possible time orderings as in Fig. 1(a). Those parts of $f(kk'k''k''';\alpha\beta\gamma\delta)$ in which two pairs of particles propagate independently should be written as products of $f(kk';\alpha\beta)$. It may be noted that there are always linked terms connecting any two excited pairs, however, as shown in Fig. 1(b).

When product pairs such as $f(kk'';\alpha\gamma)f(k'k''';\beta\delta)$ are inserted into Eq. (4) and used in the equation for $f(kk';\alpha\beta)$, than linked terms result as shown in Fig. 2.

When we consider the products

$$f(kk';\alpha\beta)\sum f(k''k''';\gamma\delta)\,, \quad \begin{matrix}\gamma\neq\alpha,\beta & k''\neq k,k' \\ \delta\neq\alpha,\beta & k'''\neq k,k'\end{matrix}\,, \quad (5)$$

these give us terms

$$f(kk';\alpha\beta)\sum\langle\gamma\delta|v|(k''k''')_{ex}\rangle f(k''k''';\gamma\delta) \quad \begin{matrix}\gamma\neq\alpha,\beta & k''\neq k,k' \\ \delta\neq\alpha,\beta & k'''\neq k,k'\end{matrix} \quad (6)$$

on the left-hand side of Eq. (2).

In Eq. (I.8) it is shown that

$$E-E_{HF}=\sum_{\alpha,\beta,k,k'}\langle\alpha\beta|v|(kk')_{ex}\rangle f(kk';\alpha\beta). \quad (7)$$

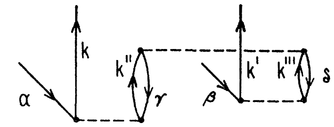

FIG. 2. Diagram illustrating how H may couple two independent pair excitations with a single pair excitation. There is also a diagram in which the time ordering of the first two interactions is reversed. This term enters the equation for $f(kk';\alpha\beta)$.

[5] H. P. Kelly, Phys. Rev. **131** 684 (1963).

[6] Hartree-Fock single-particle states are assumed, although they are not essential for this discussion.

[7] W. Brenig, Nucl. Phys. **4**, 363 (1957); O. Sinanoğlu, J. Chem. Phys. **36**, 706 (1962).

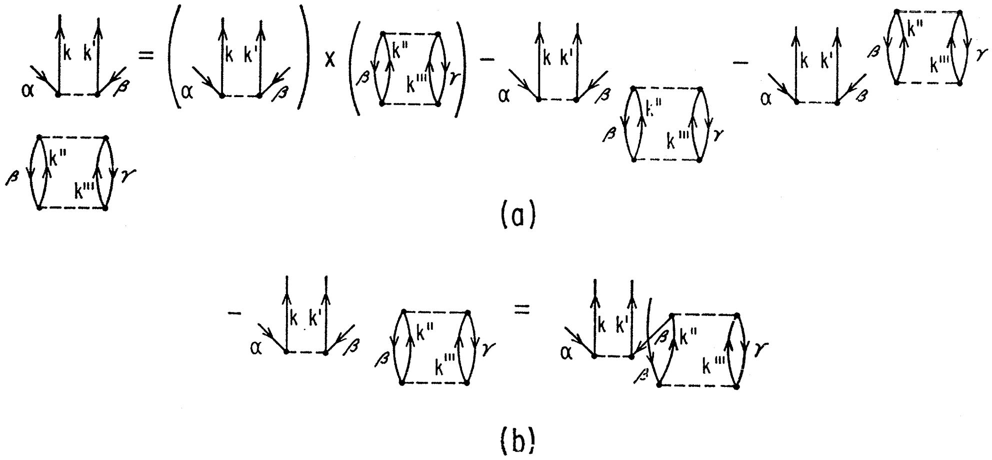

FIG. 3. (a) Diagram factorization when the two disconnected parts have one or more particle or hole lines in common. The two subtracted diagrams are really linked diagrams as shown in (b).

Equation (6) is then rewritten

$$f(kk';\alpha\beta)[E-E_{HF}-\sum_{\delta,k'',k'''}\langle\alpha\delta|v|(k''k''')_{ex}\rangle(k''k''';\alpha\delta)$$
$$-\sum_{\gamma\neq\alpha,k'',k'''}\langle\gamma\beta|v|(k''k''')_{ex}\rangle f(k''k''';\gamma\beta)$$
$$-\sum_{k''';\ \gamma\neq\alpha,\beta;\ \delta\neq\alpha,\beta}\langle\gamma\delta|v|(kk''')_{ex}\rangle f(kk''';\gamma\delta)$$
$$-\sum_{k''\neq k;\ \gamma\neq\alpha,\beta;\ \delta\neq\alpha,\beta}\langle\gamma\delta|v|(k''k')_{ex}\rangle f(k''k';\gamma\delta)]. \quad (8)$$

When the term of Eq. (8) is added to the left-hand side of Eq. (I.11), $f(kk';\alpha\beta)(E-E_{HF})$ cancels on both sides of Eq. (I.11).

At this point we now have the linked cluster expansion for two-particle excitations.[4] Equation (I.11) is also now nonlinear but in many cases this should not cause any difficulty.[5] The remaining terms are not proportional to N like $E-E_{HF}$; they will be given a simple physical interpretation. The denominators in Eqs. (I.15) and (I.16) are now modified by replacing the terms $E-E_{HF}$ by the summations in Eq. (8) with positive signs. For example, Eq. (I.15), an approximate equation for $f(kk';\alpha\beta)$, becomes

$$f(kk';\alpha\beta)$$
$$=[\epsilon_\alpha+\epsilon_\beta-\epsilon_k-\epsilon_{k}'-\langle(\alpha\beta)_{ex}|v|\alpha\beta\rangle$$
$$+\sum_{\delta,k'',k'''}\langle\alpha\delta|v|(k''k''')_{ex}\rangle f(k''k''';\alpha\delta)$$
$$+\sum_{\gamma\neq\alpha,k'',k'''}\langle\gamma\beta|v|(k''k''')_{ex}\rangle f(k''k''';\gamma\beta)$$
$$+\sum_{k''';\ \gamma\neq\alpha,\beta;\ \delta\neq\alpha,\beta}\langle\gamma\delta|v|(kk''')_{ex}\rangle f(kk''';\gamma\delta)$$
$$+\sum_{k''\neq k;\ \gamma\neq\alpha,\beta;\ \delta\neq\alpha,\beta}\langle\gamma\delta|v|(k''k')_{ex}\rangle f(k''k';\gamma\delta)]^{-1}$$
$$\times\langle(kk')_{ex}|v|\alpha\beta\rangle. \quad (9)$$

The new terms appearing in the denominator of Eq. (9) which refer to states $|\alpha\rangle$ and $|\beta\rangle$ combine with the single-particle energies ϵ_α and ϵ_β and with the diagonal hole-hole interaction term $\langle(\alpha\beta)_{ex}|v|\alpha\beta\rangle$ to give an effective two-body energy for $|\alpha\beta\rangle$. When the denominator also includes the particle-particle and exclusion principle violating (EPV) hole-particle terms of Eq. (I.17), then the denominator becomes approximately the difference between the two-body energies of the states $|\alpha\beta\rangle$ and $|kk'\rangle$. However, the two-body energy of $|kk'\rangle$ is not given so accurately as that of $|\alpha\beta\rangle$ because the interaction of the excited particles with unexcited particles is accounted for only in the Hartree-Fock approximation. However, pair-correlation energy terms of a ground-state particle with the other ground-state particles are now included. The last two terms in the denominator of Eq. (9) which refer to states $|\gamma\delta\rangle$ account for the fact that correlation terms for ground-state particles which involve excited states $|k\rangle$ or $|k'\rangle$ will be eliminated by the Pauli principle when there are other particles excited into $|k\rangle$ or $|k'\rangle$.

As a simple example of this result we consider the beryllium atom and let α, β, γ, δ refer to the $2S^+$, $2s^-$, $1s^+$, and $1s^-$ single-particle states, respectively. In Ref. 5 it was shown that the $1s-2s$ interactions are small compared to $1s-1s$ and $2s-2s$ interactions and so $f(kk';1s2s)$ is omitted in the denominators. Also the excited single-particle states used in Ref. 5 were all in the continuum and so the sums in Eq. (9) which do not run over both continuum states vanish because, as shown in Ref. 5, $\Sigma=(R_0/\pi)\int dk$ and continuum states have normalization $(2/R_0)^{1/2}$. Equation (9) becomes

$$f(kk';\alpha\beta)$$
$$=(\epsilon_\alpha+\epsilon_\beta-\langle(\alpha\beta)_{ex}|v|\alpha\beta\rangle+\sum_{k'',k'''}\langle\alpha\beta|v|(k''k''')_{ex}\rangle$$
$$\times f(k''k''';\alpha\beta)-\epsilon_k-\epsilon_{k'})^{-1}\times\langle(kk')_{ex}|v|\alpha\beta\rangle. \quad (10)$$

In the denominator of Eq. (10) we have the effective two-particle energy for the state $|\alpha\beta\rangle$. The term

$-\langle(\alpha\beta)_{ex}|v|\alpha\beta\rangle$ corrects for the inclusion of the Coulomb interaction of $|\alpha\rangle$ and $|\beta\rangle$ in both single-particle energies ϵ_α and ϵ_β. The term $\sum_{k''k'''}\langle\alpha\beta|v|(k''k''')_{ex}\rangle f(k''k''';\alpha\beta)$ accounts for second and higher order interactions among the particles in states $|\alpha\rangle$ and $|\beta\rangle$. In the calculations of Ref. 5 it was found that omission of this term would have resulted in approximately a 10% error in the correlation energy among the two $2s$ electrons When there are bound "excited" states in the complete set of single-particle states then the energy denominators will also include terms from the last two summations in the denominator of Eq. (9). These correlation terms which we have been considering may be related to a type of "rearrangement diagram" considered by Brueckner and Goldman.[8]

The equation for one-particle excitations $f(k;\alpha)$ also has the term $E-E_{HF}$ removed when coupling with the three-particle excitation term is considered. We write

$$f(kk'k'';\alpha\beta\gamma)=f(k;\alpha)\sum_{k',k''\neq k,\beta,\gamma\neq\alpha} f(k'k'';\beta\gamma)+\cdots. \qquad (11)$$

The result is that we replace $(E-E_{HF})$ in Eq. (I.10) by

$$\sum_{\gamma,k',k''}\langle\alpha\gamma|v|(k'k'')_{ex}\rangle f(k'k'';\alpha\gamma)+\sum_{\beta,\gamma\neq\alpha,k''}\langle\beta\gamma|v|(kk'')_{ex}\rangle f(kk'';\beta\gamma). \qquad (12)$$

II. CONNECTION WITH PERTURBATION THEORY

The results which we have just obtained may also be derived by a consideration of the perturbation expansion.[3,4] We begin by examining the factorization of unlinked diagrams as shown in Fig. 3(a). The two apparently disconnected parts of each diagram are assumed to have one or more hole or particle lines in common and the two diagrams on the right of Fig. 3(a) must not be considered as "unlinked." They are really "linked" as is shown in Fig. 3(b). The first term on the right-hand side of Fig. 3(a) is eliminated by the usual cancellation of unlinked clusters.[3,4] Similar factorizations were considered in Ref. 5 where the two diagrams on the right of Fig. 3(a) were called third-class EPV diagrams. These diagrams were summed in an approximate way, although with sufficient accuracy for the numerical calculations of that paper. However, these two diagrams on the right of Fig. 3(a) may be summed exactly by noticing that both possible time orderings appear[9] or by merely writing down the algebraic expressions and adding.[8] For example, in the first subtracted diagram of Fig. 3(a), shown in Fig. 3(b), the product of the energy denominators is $(B(A+B)A)^{-1}$, where B is the denominator of the closed part considered separately and A is the denominator of the other part. The second subtracted diagram of Fig. 3(a) has the same matrix elements and a contribution $(A(A+B)A)^{-1}$ from the denominators. The sum of these expressions is $(A^2B)^{-1}$, so the two subtracted expressions add to give a result which is the first correction term obtained in an expansion of the linked part with a shifted denominator. In other words, it is the second term obtained in an expansion of the denominator of the following expression:

$$(\epsilon_a+\epsilon_b-\epsilon_k-\epsilon_{k'}+\langle bc|v|(k''k''')_{ex}\rangle(\epsilon_b+\epsilon_c-\epsilon_{k''}-\epsilon_{k'''})^{-1}\times\langle k''k'''|v|bc\rangle)^{-1}\langle(kk')_{ex}|v|ab\rangle. \qquad (13)$$

The higher order terms are obtained from a consideration of the factorizations of diagrams of Fig. 4. Such factorizations were shown in more detail in Ref. 5. Correction terms resulting from the factorization of the diagrams in Figs. 4(c) and 4(d) and from the diagrams of 4(e) and 4(f) add to give the second correction term in an expansion of the denominator of Eq. (13) and the first correction term which would result from using the appropriately shifted denominator in the correction term of the denominator of Eq. (13). The result of such factorizations then gives the summation terms in the denominator of Eq. (9) or, in a more simple case, it produces the shift in energy denominators as shown in Eq. (10).

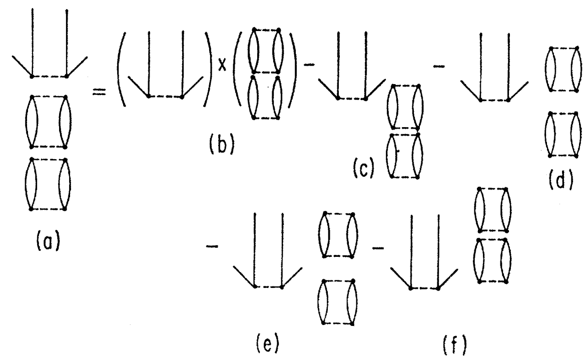

FIG. 4. Factorization of an unlinked diagram. It is assumed that all the disconnected parts have at least one hole or particle line in common so that there are correction terms (c), (d), (e), and (f) to the factorization (b). Diagrams (c) and (d) must be factored further.

ACKNOWLEDGMENTS

I would like to thank Dr. Andrew M. Sessler for his encouragement and for very helpful suggestions and Professor Keith A. Brueckner for his support and for a helpful discussion.

[8] K. A. Brueckner and D. T. Goldman, Phys. Rev. **117**, 207 (1960).

[9] H. A. Bethe, B. H. Brandow, and A. G. Petschek, Phys. Rev. **129**, 225 (1963).