Many-Body Perturbation Theory

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The usual perturbation treatment of the many-body problem is modified by eliminating the two-body interaction and introducing in its place a t matrix. The Watson, Brueckner, and Bethe (W.B.B.) treatment of the many-body problem is shown to be a special case of the modified perturbation treatment. The modified perturbation treatment involves no assumption except that of supposing the convergence of the perturbation expansion. Thus to each order in the expansion the results must be meaningful and no unphysical "unlinked cluster" terms can appear. Within the framework of the modified perturbation treatment it is easy to interpret the concepts of the Pauli principle for intermediate states and the self-consistent choice of the comparison potential which play such an important role in the W.B.B. treatment. This work is similar to that of J. Goldstone in that we relate the W.B.B. treatment to a perturbation treatment of the many-body problem. We differ from Goldstone in that we use the usual time-independent perturbation theory instead of the time-dependent one. The time-independent approach permits a direct comparison with the W.B.B. treatment and facilitates discussion of the Pauli principle for intermediate states and of the self-consistent potential.

I. INTRODUCTION

In recent years an approximate method for dealing with the many-body problem has been developed by Watson, Brueckner, Bethe, and their collaborators.[1–7] This method is expected to be valid when the interactions between the particles of the many-body system are strong and short-ranged. For such a system the usual perturbation treatment cannot be applied. Nevertheless it can be shown that this new method for treating the man-body system is a simple modification of the well-known Rayleigh-Schrödinger perturbation theory.

In this article the usual perturbation expansion for the energy of a many-body system is modified by making the expansion in powers of the t matrix rather than in powers of the potentials acting between the particles making up the system. This treatment is then related to the treatment of Watson, Brueckner, and Bethe (W.B.B.). We find that the W.B.B. treatment is a special case of the modified perturbation method.

Comparing the two methods, we find that the W.B.B. treatment contains an unnecessary approximation which causes the appearance of unphysical "unlinked cluster" terms in the expansion. Since the modified perturbation method is based on an exact expression for the level shift, such unphysical terms cannot appear in the expansion.

The modification of the t matrix suggested by Brueckner[3] and by Bethe[6] to include some effects due to the Pauli principle is discussed. We also describe how self-consistent definitions of the comparison potential may be introduced and how they improve the convergence of the perturbation expansion.

Our approach is similar to that of Goldstone[8] but our derivation is based on the usual time-independent form of perturbation theory instead of making use of a time-dependent formulation. This approach permits a direct comparison with W.B.B. theory and facilitates the discussion of the Pauli principle for intermediate states and of the self-consistent potential.

II. MANY-BODY PERTURBATION THEORY

Let the Hamiltonian for the N-body system be

$$H=\sum_{i=1}^{N}-\frac{\hbar^2\nabla_i^2}{2m}+\sum_{i<j}v(|\mathbf{x}_i-\mathbf{x}_j|)$$
$$=\sum_i T_i+\sum_\alpha v_\alpha=T+V, \tag{1}$$

where v is a general two-body potential which may include tensor and exchange terms, and let the eigenstates and eigenvalues of H be represented by Ψ_a and E_a, respectively.

$$(E_a-H)\Psi_a=0. \tag{2}$$

We also introduce a comparison Hamiltonian,

$$H_0=T+U, \tag{3}$$

and define its eigenstates and eigenvalues:

$$(\epsilon_a-H_0)\Phi_a=0. \tag{4}$$

The choice of U should be such that ϵ_a can be determined and the evaluation of the level shift made easier. The level shift is

$$\Delta_a=E_a-\epsilon_a=\frac{\langle\Phi_a|H-H_0|\Psi_a\rangle}{\langle\Phi_a|\Psi_a\rangle}=\langle\Phi_a|(V-U)\Omega_a|\Phi_a\rangle. \tag{5}$$

The wave matrix Ω_a which appears in the above ex-

* Fellow of the National Science Foundation.
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[3] K. A. Brueckner, Phys. Rev. **97**, 1353 (1955).
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[5] K. A. Brueckner and W. W. Wada, Phys. Rev. **103**, 1008 (1956).
[6] H. A. Bethe, Phys. Rev. **103**, 1353 (1956).
[7] R. J. Eden, Proc. Roy. Soc. (London) **A235**, 408 (1956).
[8] J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957).

pression is defined by

$$\Omega_a\Phi_a=\Psi_a/\langle\Phi_a|\Psi_a\rangle. \tag{6}$$

It follows that Ω_a is the solution of the following integral equation.

$$\begin{aligned}\Omega_a&=1+(\epsilon_a-H_0)^{-1}(1-|\Phi_a\rangle\langle\Phi_a|)(V-U-\Delta_a)\Omega_a\\&=1+G_a(V-U-\Delta_a)\Omega_a.\end{aligned} \tag{7}$$

This equation for the wave matrix is simply the integral form of the Schrödinger equation. The exact solution in closed form of this equation is well beyond our reach. What we wish to do here is to consider some perturbation expansions for the wave matrix and the level shift. The customary perturbation expansion is the Rayleigh-Schrödinger expansion in powers of $V-U$. This expansion, however, does not converge rapidly when V is not small, and if V contains a singularity the expansion may not even be defined.

To deal with those cases where V is large or singular, we generalize an approach first suggested by Watson.[1] This generalized approach consists in replacing each two-body potential v by an infinite series in powers of a quantity that we will call the t matrix t. This t matrix will be well-behaved so that any singularity in v will correspond to a lack of convergence of the series expansion of v. We then express the wave matrix and the level shift as perturbation expansions in powers of t. The hope then is that these expansions for Ω_a and Δ_a, which are formally exact, will be rapidly converging even when the expansion of v in powers of t converges poorly or not at all.

We define the t matrix by the following integral equation.

$$t_\alpha=v_\alpha+v_\alpha g_\alpha t_\alpha-\delta_\alpha v_\alpha g_\alpha v_\alpha^{-1}t_\alpha, \tag{8}$$

where the operator g_α and the c number δ_α remain to be defined.[9] Solving Eq. (8) for v_α gives

$$\begin{aligned}v_\alpha&=t_\alpha(1+g_\alpha t_\alpha)^{-1}(1+g_\alpha\delta_\alpha)\\&=(t_\alpha-t_\alpha g_\alpha t_\alpha+t_\alpha g_\alpha t_\alpha g_\alpha t_\alpha-\cdots)(1+g_\alpha\delta_\alpha).\end{aligned} \tag{9}$$

By means of Eq. (9) we can eliminate v from the level shift and wave matrix in favor of t. In this way we get an expansion of the level shift in powers of t and U instead of one in powers of $V-U$.

An alternative method is to eliminate $V-U$ instead of just V. This is done by introducing what we shall call the τ matrix:

$$\tau_\alpha=(v_\alpha-u_\alpha)+(v_\alpha-u_\alpha)g_\alpha(\tau_\alpha-\delta_\alpha[v_\alpha-u_\alpha]^{-1}\tau_\alpha), \tag{10}$$

where $U=\sum u_\alpha$. The τ matrix can thus only be defined when the comparison potential U can be written as a sum of two-body operators. The usual choice for U is a sum of one-body operators which can easily be rewritten as a sum of two-body operators:

$$\begin{aligned}U&=\sum_{i=1}^{N}u_i=\sum_{i<j}u_{ij}=\sum u_\alpha,\\u_{ij}&=\frac{1}{N-1}(u_i+u_j),\end{aligned} \tag{11}$$

where N is the number of particles in the system.

Accordingly, Eq. (5) and (7) can be written

$$\Omega_a=1+G_a(\sum_{n=1}^{\infty}Q_n-\Delta_a)\Omega_a, \tag{12}$$

$$\Delta_a=\langle\Phi_a|\textstyle\sum_n Q_n\Omega_a|\Phi_a\rangle=\langle\sum_n Q_n\Omega_a\rangle, \tag{13}$$

where

$$\begin{aligned}\sum_{n=1}Q_n&=V-U=\sum v_\alpha-U\\&=\sum_\alpha(t_\alpha-t_\alpha g_\alpha t_\alpha+\cdots)(1+g_\alpha\delta_\alpha)-U\\&=\sum_\alpha(\tau_\alpha-\tau_\alpha g\tau_\alpha+\cdots)(1+g_\alpha\delta_\alpha).\end{aligned}$$

Now in the usual way[10] we expand Ω_a and Δ_a in powers Q_n assuming that Q_n is of order $(Q_1)^n$ in smallness. The result for the level shift is

$$\begin{aligned}\Delta_a=&\langle Q_1\rangle+\langle Q_1G_aQ_1\rangle+\langle Q_1G_aQ_1G_aQ_1\rangle\ +\langle Q_1G_aQ_1G_aQ_1G_aQ_1\rangle+\cdots\\&+\langle Q_2\rangle\quad-\langle Q_1\rangle\langle Q_1G_aG_aQ_1\rangle-\langle Q_1\rangle\langle Q_1G_aG_aQ_1G_aQ_1\rangle+\cdots\\&\quad+\langle Q_1G_aQ_2\rangle\quad-\langle Q_1\rangle\langle Q_1G_aQ_1G_aG_aQ_1\rangle+\cdots\\&\quad+\langle Q_2G_aQ_1\rangle\quad-\langle Q_1G_aQ_1\rangle\langle Q_1G_aG_aQ_1\rangle+\cdots\\&\quad+\langle Q_3\rangle\quad+\langle Q_1\rangle^2\langle Q_1G_aG_aG_aQ_1\rangle+\cdots.\\&\quad+\cdots\end{aligned} \tag{14}$$

If we choose $Q_1=(V-U)$, $Q_2=Q_3=\cdots=0$, we get the usual Rayleigh-Schrödinger perturbation expansion.

$$\begin{aligned}\Delta_a=&\{\langle\textstyle\sum v_\alpha-U\rangle+\langle(\sum v_\alpha-U)G_a(\sum v_\alpha-U)\rangle+\cdots\}\\&-\{\langle\textstyle\sum v_\alpha-U\rangle\langle(\sum v_\alpha-U)G_aG_a(\sum v_\alpha-U)\rangle+\cdots\}\\=&A_{RS}-B_{RS}.\end{aligned} \tag{15}$$

By choosing

$$\begin{aligned}Q_1&=\textstyle\sum t_\alpha-U,\\Q_2&=-\sum t_\alpha g_\alpha(t_\alpha-\delta_\alpha),\\Q_3&=\sum t_\alpha g_\alpha t_\alpha g_\alpha(t_\alpha-\delta_\alpha),\end{aligned}$$

etc., we get the t matrix expansion for the level shift:

[9] The operator g_α will in general be chosen to be some sort of propagator. Its definition, of course, will not be complete without a prescription describing how g_α is to be evaluated near its singularities.

[10] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Oxford University Press, New York, 1949), Chap. 7.

$$\Delta_\alpha=\{\langle\sum t_\alpha-U\rangle+\langle(\sum t_\alpha-U)G_\alpha(\sum t_\alpha-U)\rangle+\cdots\}$$
$$-\{\langle\sum t_\alpha-U\rangle\langle(\sum t_\alpha-U)G_\alpha G_\alpha(\sum t_\alpha-U)\rangle+\cdots\}$$
$$-\{\langle\sum t_\alpha g_\alpha t_\alpha\rangle+\cdots\}$$
$$=A_t-B_t-C_t; \tag{16}$$

or finally, by choosing

$$Q_1=\sum_\alpha\tau_\alpha,$$
$$Q_2=-\sum_\alpha\tau_\alpha g_\alpha(\tau_\alpha-\delta_\alpha),$$
$$Q_3=\sum_\alpha\tau_\alpha g_\alpha\tau_\alpha g_\alpha(\tau_\alpha-\delta_\alpha),$$

etc., we get the τ matrix expansion for the level shift:

$$\Delta_\alpha=\{\langle\sum\tau_\alpha\rangle+\langle\sum\tau_\alpha G_\alpha\sum\tau_\alpha\rangle+\cdots\}$$
$$-\{\langle\sum\tau_\alpha\rangle\langle\sum\tau_\alpha G_\alpha G_\alpha\sum\tau_\alpha\rangle+\cdots\} \tag{17}$$
$$-\{\langle\sum\tau_\alpha g_\alpha\tau_\alpha\rangle+\cdots\}$$
$$=A_\tau-B_\tau-C_\tau.$$

Consider first the usual perturbation expansion shown in Eq. (15). We see that it is the difference of two sums which we have denoted by A_{RS} and B_{RS}. If, at each point in a matrix element where the propagator G appears, we introduce a complete set of intermediate states, and if for this purpose we use the eigenstates of H_0, then we get for the level shift a sum of terms, each one of which corresponds to a distinct Feynman diagram with no external lines. One can then show that B_{RS} cancels from A_{RS} all those terms corresponding to Feynman diagrams with two or more disconnected parts. This can be verified to any given order in the way Brueckner[4] has done or one can prove it in general in the way Goldstone[8] has done. These eliminated terms are the so-called unlinked clusters.

The t matrix expansion shown in Eq. (16) and the τ-matrix expansion shown in Eq. (17) are similar in form to the usual perturbation expansion of Eq. (15) except that $\sum v_\alpha-U$ is replaced by $\sum t_\alpha-U$ or $\sum\tau_\alpha$ and there appears a third sum denoted by C. By choosing g_α and δ_α in an appropriate manner, we can cause C to cancel terms which appear in A and B.

If we choose $g_\alpha=G_\alpha$ and $\delta_\alpha=\langle t_\alpha\rangle$ for Eq. (16) [$\delta_\alpha=\langle\tau_\alpha\rangle$ for Eq. (17)], then the terms which are cancelled from A and B are those which correspond to diagrams in which two particles interact with each other twice in succession or more. Thus we can say that with this choice of g_α and δ_α, eliminating v_α in favor of t_α or τ_α causes the first term of the expansion for the level shift to contain the entire effect arising from pure two-body interactions. This last statement requires some qualification which will be provided in Sec. IV.

In most of the literature on this topic the t matrix is defined by Eq. (8) with $\delta_\alpha=0$. But one can verify that having $\delta_\alpha=\langle t_\alpha\rangle$ will cause additional cancellations among the terms of A, B, and C in Eq. (16). To be explicit, this choice for δ_α is necessary in order for C to cancel terms in B corresponding to terms cancelled by C in A. This is necessary to prevent cancellations between C and A from undoing cancellations between B and A. In addition, this choice for δ_α causes $\langle t_\alpha\rangle$ to be the level shift due to the interaction of the αth pair of particles so that the first-order term of the t matrix expansion of the level shift is just the sum of the exact two-body level shifts.

The advantage of the τ matrix expansion is that it is an expansion in powers of quantities of one sort, the τ_α. The t matrix expansion, on the other hand, is an expansion in powers of U as well as powers of t_α.

III. RELATIONSHIP TO THE WATSON, BRUECKNER, AND BETHE TREATMENT

In the W.B.B. treatment of the many-body problem, one breaks the t matrix into two parts:

$$t_\alpha=\bar{t}_\alpha+I_\alpha. \tag{18}$$

The precise definitions of $\bar{t}_\alpha$ and I_α will not concern us at this point. Then the comparison potential is taken to be

$$U=\sum_\alpha\bar{t}_\alpha, \tag{19}$$

and the operators F and F_α are defined.

$$F=1+G_a\sum_\alpha I_\alpha F_\alpha,$$
$$F_\alpha=1+G_\alpha\sum_{\alpha\neq\beta}I_\beta F_\beta. \tag{20}$$

It then follows from simple algebraic manipulation that

$$(\epsilon_a-T-V)F\Phi_a=-WF\Phi_a, \tag{21}$$

where

$$WF=\sum_\alpha\{I_\alpha-(1-|\Phi_a\rangle\langle\Phi_a|)I_\alpha$$
$$-\bar{t}_\alpha GI_\alpha-v_\alpha G\bar{t}_\alpha\}F_\alpha. \tag{22}$$

If $W=0$, then Eq. (21) would imply that $F=\Omega_a$ and $\epsilon_a=E_a$. The claim is made that W is in fact small, and this is made plausible by showing that $\langle\Phi_a|WF|\Phi_a\rangle=\langle WF\rangle$ is small. $\langle WF\rangle$ is evaluated by expanding in powers of $\bar{t}_\alpha$ and I_α.

From Eqs. (21) and (4) it can be shown easily that

$$\langle WF\rangle=\langle(V-U)F\rangle. \tag{23}$$

Thus $\langle WF\rangle$ is an approximation to the level shift, the approximation arising from the substitution of F for the wave matrix Ω_a. Expanding $\langle WF\rangle$ gives

$$\langle WF\rangle=\sum_\alpha\langle I_\alpha\rangle+\sum_{\alpha,\beta}\langle I_\alpha G_a I_\beta\rangle-\sum_\alpha\langle t_\alpha G_a t_\alpha\rangle$$
$$+\sum_{\alpha\beta\gamma}\langle I_\alpha G_a I_\beta G_a I_\gamma\rangle-\sum_{\alpha\beta}\langle I_\alpha G_a I_\beta G_a I_\beta\rangle$$
$$-\sum_{\alpha\beta}\langle t_\alpha G_a t_\alpha G_a I_\beta\rangle+\sum_\alpha\langle t_\alpha G_a t_\alpha G_a t_\alpha\rangle+\cdots. \tag{24}$$

Comparing this to Eq. (16) with U set equal to $\sum\bar{t}_\alpha$,

$\delta_\alpha=0$, and g_α set equal to G_α, we find to third order:

$$\langle WF\rangle-\Delta_a=\sum_{\alpha\beta\gamma}\langle I_\alpha\rangle\langle I_\beta G_a G_a I_\gamma\rangle + \sum_{\alpha\beta}\langle I_\alpha G_a(t_\beta G_a t_\beta - I_\beta G_a I_\beta)\rangle+\cdots. \quad (25)$$

This difference is such as to cause the appearance of "unlinked cluster" terms in $\langle WF\rangle$.

We see that the W.B.B. treatment is the special case of modified perturbation theory where the comparison potential U is chosen to be $\sum\hat{t}_\alpha$ and the wave matrix Ω_a is approximated by F. The W.B.B. choice of U is a source of great complication in the theory. Since the definition of $\hat{t}_\alpha$ involves the eigenfunctions of H_0 and since these eigenfunctions in turn depend on $U=\sum\hat{t}_\alpha$, there is a self-consistency condition to be fulfilled. The self-consistent definition of U is used because among other things it causes the first-order terms in the expansion of the level shift to vanish. This may be desirable if we are trying to prove that the level shift is negligible, but if we are only trying to make the first few terms of the expansion a good approximation to the sum, then the self-consistent definition of U may not have any great advantage. If our purpose is to evaluate the level shift, any convenient choice for the comparison potential can be used subject to the requirement that the choice leads to a sufficiently rapid convergence of the series expansion of the level shift.[11] In the calculation of the level shift, the exact expression $\langle(V-U)\Omega_a\rangle$ should be used in place of $\langle WF\rangle$, since the exact expression when expanded will not contain any "unlinked cluster" terms which in $\langle WF\rangle$ have to be eliminated by special devices.

IV. PAULI PRINCIPLE FOR INTERMEDIATE STATES

We have pointed out that when $g_\alpha=G_\alpha$ and $\delta_\alpha=\langle t_\alpha\rangle$ or $\langle\tau_\alpha\rangle$ in the integral equation for t_α or τ_α, there is a cancellation of the two-body terms in the expansion of the level shift. The terms which then remain in the level shift expansion are those which only involve intermediate states in which a given pair of particles never undergo two successive collisions.[12] However, in subtracting the contributions arising from terms in which a given two particles do undergo successive collisions, we also subtract contributions due to scatterings to states already occupied by other particles. If our system is made up of identical fermions, which for the moment we assume it to be, then these contributions were already missing so that we have in this way subtracted too much.

Brueckner[4,5] and Bethe[6] have suggested an alternate definition of g_α which has the effect of reducing this oversubtraction in the lower order terms. This enhances the cancellations in the terms of low order at the expense of reducing the cancellations in terms of high order. Such a change is certainly desirable since the two-body cancellations are in any case not very important for the terms of high order and since the terms of high order must be negligible anyway if the perturbation method is to be of any use. Thus, by enhancing the cancellations in the terms of low-order, we make the first term in the expansion a better representation of the sum.

The alternate definition of g_α is to set $g_\alpha=G_\alpha P_\alpha$, where P_α is a projection operator which is zero when operating on a wave function in which a particle of the αth pair is in a state which is an occupied one in the initial wave function Φ_a. Thus P_α acts to eliminate intermediate states where particles are scattered into states which are occupied ones in the starting wave function Φ_a. In the lower order terms this tends to eliminate those intermediate states which "violate the Pauli principle." This does not mean that the presence of P_α is a necessary consequence of the exclusion principle. We are free to choose g_α in any way we like. P_α is introduced to make the cancellations between A and C in Eqs. (16) and (17) more complete for the terms of low order and thus to improve the initial convergence of the expansion.

In any perturbation calculation of the energy of a system of fermions, the choice $g_\alpha=G_\alpha P_\alpha$ is to be preferred to $g_\alpha=G_\alpha$. However, if the density of the particles is not too great, or if v_α is short-ranged and very strong, the perturbation expansion might very well converge in a satisfactory manner with $g_\alpha=G_\alpha$. This fact is of interest since it is often possible to calculate the t matrix or τ matrix when $g_\alpha=G_\alpha$ but not when $g_\alpha=G_\alpha P_\alpha$.

V. SELF-CONSISTENT POTENTIAL

The question we consider here is that of making the most advantageous choice of the comparison potential U. We would like to choose U in such a way as to reduce the level shift Δ_a and at the same time increase the rate of convergence of the perturbation expansion for the level shift. As a practical matter, it is also desirable that it be possible to write U as a sum of one-body operators.

$$U=\sum_{i=1}^{N}u(\mathbf{x}_i). \quad (26)$$

When U has this form, our starting wave function Φ_a can be written as a product of one-particle wave functions $\varphi_\beta(\mathbf{x})$. U can be generalized slightly by allowing the addition of terms which are diagonal with respect to the $\varphi_\beta(\mathbf{x})$.

We base our discussion on the usual perturbation expansion given in Eq. (15). Afterwards we will apply the results to the t and τ matrix expansions shown in Eqs. (16) and (17). The operator $V-U$ which appears in Eq. (15) can be rewritten in terms of an occupation

[11] The question of the self-consistent potential is discussed more fully in part V.

[12] The particles are of course indistinguishable. When we speak of two particular particles we mean the occupants of two particular states.

number representation:

$$V-U=\sum_{i<j} v(|\mathbf{x}_i-\mathbf{x}_j|)-\sum_i u(\mathbf{x}_i)$$
$$=\sum_{\alpha,\beta,\gamma,\sigma}(\alpha\beta|\tfrac{1}{2}v|\gamma\sigma)a_\beta^\dagger a_\alpha^\dagger a_\gamma a_\sigma - \sum_{\beta,\sigma}(\beta|u|\sigma)a_\beta^\dagger a_\sigma, \quad (27)$$

where

$$(\alpha\beta|v|\gamma\sigma)$$
$$=\int d\mathbf{x}_i d\mathbf{x}_j \varphi_\alpha^*(\mathbf{x}_i)\varphi_\beta^*(\mathbf{x}_j)v(|\mathbf{x}_i-\mathbf{x}_j|)\varphi_\gamma(\mathbf{x}_i)\varphi_\sigma(\mathbf{x}_j),$$
$$(\beta|u|\sigma)=\int d\mathbf{x}\varphi_\beta^*(\mathbf{x})u(\mathbf{x})\varphi_\sigma(\mathbf{x}),$$
$$[\epsilon_\alpha-T_i-u(\mathbf{x}_i)]\varphi_\alpha(\mathbf{x}_i),$$

and $a^\dagger$ and a are creation and annihilation operators. Let us separate the first sum on the right of Eq. (27) so that the terms that could conceivably be canceled by U are separated from the rest.

$$V-U=\sum_{\substack{\gamma\neq\alpha\\ \beta\neq\sigma}}(\alpha\beta|\tfrac{1}{2}v|\gamma\sigma)a_\beta^\dagger a_\alpha^\dagger a_\gamma a_\sigma-\sum(\beta|u|\sigma)a_\beta^\dagger a_\sigma$$
$$+\sum(\alpha\beta|v(1-\tfrac{1}{2}\delta_{\beta\sigma})|\alpha\sigma)a_\beta^\dagger a_\alpha^\dagger a_\alpha a_\sigma. \quad (28)$$

Clearly, the most desirable choice for the comparison potential U is

$$U=\sum(\alpha\beta|v|\alpha\sigma)a_\beta^\dagger a_\alpha^\dagger a_\alpha a_\sigma$$
$$-\sum\tfrac{1}{2}(\alpha\beta|v|\alpha\beta)a_\beta^\dagger a_\alpha^\dagger a_\alpha a_\beta. \quad (29)$$

Although this operator is diagonal in one pair of indices, it still is a two-body operator. However, we can define a one-body operator which is a good approximation to the U shown in Eq. (29) in the terms of low order in the perturbation expansion. This operator is

$$U=\sum'(\alpha\beta|v(1-\tfrac{1}{2}\delta_{\beta\sigma})|\alpha\sigma)a_\beta^\dagger a_\sigma, \quad (30)$$

where the sum on α is over the chosen configuration, that is to say, over the states occupied in the initial wave function Φ_a.

If the second sum on the right is neglected, Eq. (28) is just the definition of the Hartree potential. The second sum on the right is simply a diagonal operator which causes $\langle\Phi_a|U|\Phi_a\rangle=\langle\Phi_a|V|\Phi_a\rangle$. Its presence does not alter the form of the Hartree wave functions or the value of the energy predicted by the Hartree method, but it does change the definition of the energy from the usual $\langle\Phi_a|T+\frac{1}{2}U|\Phi_a\rangle$ to $\langle\Phi_a|T+U|\Phi_a\rangle$.

Stated somewhat differently: with the comparison potential defined by Eq. (30), the level shift vanishes to first order in $V-U$. With the usual Hartree definition of U,

$$U=\sum'(\alpha\beta|v|\alpha\sigma)a_\beta^\dagger a_\sigma, \quad (31)$$

the level shift is $\Delta_a=\frac{1}{2}\langle\Phi_a|U|\Phi_a\rangle$ to first order in $V-U$. The total energy $\epsilon_a+\Delta_a$, to first order in $V-U$, will be the same in the two cases as will the self-consistent wave functions φ_β.

However, the distinction between the self-consistent potentials defined in Eqs. (30) and (31) is not altogether trivial. If we use the U defined in Eq. (30), more of the higher order terms in the level-shift expansion will be canceled.

We can easily modify the definition of U to include exchange. Separating out the exchange terms in Eq. (28) gives

$$V-U=\sum_{\gamma\neq\alpha,\beta;\,\sigma\neq\alpha,\beta}(\alpha\beta|\tfrac{1}{2}v|\gamma\sigma)a_\beta^\dagger a_\alpha^\dagger a_\gamma a_\sigma$$
$$-\sum(\beta|u|\sigma)a_\beta^\dagger a_\sigma+\sum(\alpha\beta|v(1-\tfrac{1}{2}\delta_{\beta\sigma})|\alpha\sigma)_A$$
$$\times a_\beta^\dagger a_\alpha^\dagger a_\alpha a_\sigma-\sum(\alpha\beta|\tfrac{1}{2}v|\beta\beta)_A a_\beta^\dagger a_\alpha^\dagger a_\beta a_\beta, \quad (32)$$

where

$$(\alpha\beta|v|\gamma\sigma)_A=(\alpha\beta|v|\gamma\sigma)\pm(\alpha\beta|v|\sigma\gamma),$$

the sign depending on whether the particles are bosons or fermions. For a system of identical fermions, a most desirable form for U is

$$U=\sum(\alpha\beta|v[1-\tfrac{1}{2}\delta_{\beta\sigma}]|\alpha\sigma)_A a_\beta^\dagger a_\alpha^\dagger a_\alpha a_\sigma. \quad (33)$$

This operator consists of the diagonal part of V plus the part of V which is diagonal in only two of its indices. But this U is not a one-body operator; we approximate it by

$$U=\sum'(\alpha\beta|v[1-\tfrac{1}{2}\delta_{\beta\sigma}]|\alpha\sigma)_A a_\beta^\dagger a_\sigma, \quad (34)$$

where the prime indicates that the sum over α is restricted to the chosen configuration. Again, if we drop the δ function in Eq. (34), we get the Hartree-Fock self-consistent potential.

The self-consistent potentials defined in Eqs. (30) and (34) are not completely defined for those terms where σ does not belong to the chosen configuration. The sum over α must include all but one of the states making up the chosen configuration. When σ does not belong to the chosen configuration, there is no rule for telling which member of the sum to exclude. For these terms the matter must be settled by making an arbitrary convention.

We have seen how the Hartree and Hartree-Fock self-consistent potentials can be justified for the usual perturbation expansion. Turning now to the t-matrix expansion for the level shift shown in Eq. (16), we see that there also a self-consistent definition of the comparison potential U will speed the initial convergence of the perturbation expansion. The definition of the self-consistent potential is the same as that given above except, of course, that we must replace v by t.

$$U=\sum'(\alpha\beta|t[1-\tfrac{1}{2}\delta_{\beta\sigma}]|\alpha\sigma)_A a_\beta^\dagger a_\sigma, \quad (35)$$

where the prime indicates that the sum over α is restricted to the chosen configuration. This is the self-consistent potential used in the W.B.B. treatment.

In the τ matrix expansion shown in Eq. (17) the comparison potential U no longer appears explicitly, so that the usual self-consistent definition of U will be of no use. But there is a weaker kind of self-consistency condition which can be invoked for the τ matrix expansion. This consists in defining U to be any convenient sum of one-body potentials which have one parameter free. This parameter could be the depth or the range of these potentials. This parameter is then adjusted so that the first-order term of the level shift-expansion, $\langle\sum\tau_\alpha\rangle$, vanishes. While this type of self-consistent potential cannot be expected to be as effective as the Hartree-Fock or W.B.B. types in increasing the initial rate of convergence of the perturbation expansion, it certainly is much easier to implement.

VI. ACKNOWLEDGMENTS

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Appreciation of a Velocity-Dependent Potential to the Nuclear Photoeffect*

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Calculations of the total photonuclear absorption cross sections have been carried out for a number of nuclei throughout the periodic table. The shell model, with a velocity-dependent potential, has been used. This potential is proportional to the kinetic energy of the nucleons, and gives rise to a changed effective nucleon mass. One of the effects of such an effective mass is to change the frequencies of the giant gamma-ray absorption resonances. Previous independent-particle model calculations had resulted in frequencies consistently lower than the observed values.

With an effective nucleon mass inside the nucleus of about 55% of the normal mass, very good agreement with the experimental values is obtained for medium and heavy nuclei. Within the limits of the assumptions made in the calculations, the forms of the observed excitation curves are closely reproduced, and are peaked at roughly the correct energies. Furthermore, the cross sections integrated over excitation energies, which are nearly model-independent quantities in the changed-mass case, are, except for the very light nuclei, consistent with the experimental values.

I. INTRODUCTION

A NUMBER of models have been proposed[1] in order to explain the giant resonance phenomena of the photonuclear effect.[2,3] It has been pointed out by Levinger[1] that there is little difference between the predictions of all reasonable sub-unit models. Recently however, some magic-number phenomena relating to the photoeffect have been observed. In particular, the resonance widths for closed-shell nuclei are smaller than the widths for neighboring nuclei. Since the shell model has been fairly successful in predicting the properties of the ground states,[4] and the low-lying excited states,[5] it is reasonable to attempt an extension of the model to higher levels. Such proposals have been made by Wilkinson,[6] Courant,[7] Burkhardt,[8] and others.[9,10]

If we assume only ordinary (space-dependent) forces to exist between nucleons, photoabsorption is not satisfactorily explained by the independent-particle model. The principal discrepancies are:

1. The calculated transition energies are smaller by about 50% than the observed resonance energies.[6]

2. Photon scattering provides major competition to neutron emission. This is not observed.[8]

3. The resonance frequencies depend too strongly on mass number.[6]

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