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Theory of mean removal energies for single particles in nuclei*

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A useful way to characterize the hole-energy spectrum excited in a direct particle-removal reaction like $(p, 2p)$ or $(e, e'p)$ is through the centroid or mean removal energy. We derive the rules for computing this quantity in a linked-cluster expansion, and give some examples. We demonstrate the close relation of the mean removal energy to Brandow's self-consistent orbital energy, and discuss briefly the connection with Green's function theory.

[NUCLEAR STRUCTURE Linked-cluster theory of mean or centroid removal energies measured in $(p,2p)$ or $(e,e'p)$; applications and relation to other hole energies.]

1. INTRODUCTION

The subject of this paper is the single-particle removal energy, or hole energy, in nuclei. Hole-energy spectra are measured by a variety of direct reactions in which one particle is removed from the nuclear target, such as the $(p, 2p)$ or $(e, e'p)$ reactions. The hole energy also plays a role in the theory of the ground state of nuclei; the most familiar example is the self-consistent orbital energy in Hartree-Fock theory. The theoretical problem is how to make a proper comparison between the experimentally measured hole spectra, and the theoretical hole energies from nuclear structure theory.

The hole spectrum for a given target nucleus A (with A nucleons) may be characterized by a spectral function $P(\lambda, E)$ which gives the probability that the final nucleus B (with $A-1$ nucleons) is left with excitation energy E, if a nucleon in a single-particle orbit λ is removed from the ground state of A. Extraction of this function from $(p, 2p)$ or $(e, e'p)$ experiments requires the use of the plane-wave or distorted-wave impulse approximations.[1-3] A number of experiments have been analyzed[2,4-7] assuming the validity of these approximations. For the purposes of this paper, we shall assume that $P(\lambda, E)$ is a measurable quantity.

The spectral function is a complicated theoretical quantity, which contains considerable information about the structure and spectrum of the nucleus B. There has been little attempt to produce the function directly from nuclear-structure theory, except for recent work of Lipperheide and co-workers.[8] Theorists have generally tried to characterize the spectrum in terms of a "hole energy" whose definition is to be related to an appropriate theoretical orbital energy. There are a number of possible choices, which have been discussed and compared by several authors,[9-11] and which will not be reviewed here.

We choose to characterize the spectrum by the *mean removal energy* (mre) which we define (2.8) in terms of the centroid or first energy moment of $P(\lambda, E)$ for a given orbit, λ. This is a much simpler theoretical quantity than the spectral function itself, as will be shown in Sec. 2. French[12] has stressed the connection of the centroid energies for low-energy single-particle transfer reactions to nuclear spectroscopy. Baranger[13] has made the particle-transfer centroid energies a basis for defining a single-nucleon potential, although he requires information from particle *addition* experiments as well as from particle removal.

The mean removal energy may be related directly to properties of the target-nucleus ground state. This close connection appears, for example, in the sum rule which relates the mre to the binding energy of the target, which has been presented elsewhere.[14,15] We shall stress this relationship heavily in our development of a theory of the mre.

Our first goal will be to derive a linked-cluster expansion for the mre. This will follow closely along the lines of the usual linked-cluster perturbation theory[16,17] of the nuclear ground-state energy. By this development one shows explicitly how to define and calculate the mre given any approximate theory (of the linked-cluster form) of the target ground state. We begin with definitions and some formal matters in Sec. 2. The linked-cluster expansion is developed in Sec. 3, and explicit examples are worked out in Sec. 4, for some well-known approximations for the ground-state energy (e.g. Brueckner theory).

Our second goal in this paper is to connect the theory of the mre with Brandow's treatment of

particle energies in his "compact-cluster" theory.[18,19] We shall demonstrate that Brandow's definition of a self-consistent orbital energy is identical with the mre, to any order of approximation. This discussion appears in Sec. 5. We shall also compare these results with some features of the Green's function theory, in Sec. 6.

2. SPECTRAL FUNCTION AND MEAN REMOVAL ENERGY

For an orbital description, we need a complete set of single-particle states, labeled by λ, which denotes the set of quantum numbers (e.g. $\{\lambda\} = \{nljmt_3\}$. We need not specify the choice of the complete set $\{\lambda\}$ at this point. We require the operators $a^\dagger(\lambda)$ and $a(\lambda)$ which create or annihilate a particle in the state λ.

The spectral function is defined by

$$P(\lambda, E) \equiv \langle A | a^\dagger(\lambda)\delta(E + E_A - H)a(\lambda) | A\rangle = \sum_f |\langle f | a(\lambda) | A\rangle|^2 \delta(E - E_f), \quad (2.1)$$

where A labels the target ground state (an A-particle nucleus), and f the final state of the nucleus B (with $A-1$ particles). The nuclear Hamiltonian is denoted by H. The energy of the final state, E_f, is measured relative to the ground state of A: that is, $E_f = E^* + E_B - E_A$ where E^* is the excitation energy of f relative to the ground state of B, and E_A, E_B are ground-state energies. Note that since H in (2.1) is evaluated in the target rest frame, the recoil energy of B must be included in the excitation energy E^*

Analysis of the $(p, 2p)$ or $(e, e'p)$ measurements under the assumptions of the plane-wave impulse approximation[1-3] yields the spectral function for proton removal $P(\vec{k}, E)$, as defined by (2.1) with plane-wave orbits $\lambda = \vec{k}$, where $\vec{k}$ is the initial momentum of the struck nucleon. In the distorted-wave impulse approximation, one finds[3] that the measured spectral quantity is off diagonal in momentum:

$$P(\vec{k}, \vec{k}', E) = \langle A | a^\dagger(\vec{k})\delta(E + E_A - H)a(\vec{k}') | A\rangle \quad (2.2)$$

such that $P(\vec{k}, \vec{k}, E) = P(\vec{k}, E)$. One could obtain (2.1) from (2.2) by integration

$$P(\lambda, E) = \int d^3k d^3k' \phi_\lambda^*(\vec{k}) P(\vec{k}, \vec{k}', E)\phi_\lambda(\vec{k}'), \quad (2.3)$$

where $\phi_\lambda(\vec{k})$ is the orbital wave function in momentum space. With less information than the complete function (2.2), one might expand the experimental spectral function in terms of a finite number of orbits $\{\lambda\}$, e.g.

$$P(\vec{k}, E) = \sum_\lambda |\phi_\lambda(\vec{k})|^2 P(\lambda, E) \quad (2.4)$$

to determine $P(\lambda, E)$ approximately. This fitting procedure was used by the Liverpool group in the analysis of their $(p, 2p)$ experiments[4,5]: They chose the $\{\lambda\}$ to be the harmonic-oscillator orbits normally occupied in a shell-model description of the target nuclei (see Fig. 10 of Ref. 5).

The energy integral or zeroth moment of $P(\lambda, E)$ gives the occupation number or summed spectroscopic strength for the orbit λ

$$n(\lambda) \equiv \int_{-\infty}^{\infty} P(\lambda, E)dE = \langle A | a^\dagger(\lambda)a(\lambda) | A\rangle, \quad (2.5)$$

which is simply the (target) ground-state expectation value of the particle number operator $N(\lambda) \equiv a^\dagger(\lambda)a(\lambda)$.

The first energy moment of (2.1)

$$\epsilon(\lambda) \equiv -\int_{-\infty}^{\infty} EP(\lambda, E)dE = \langle A | a^\dagger(\lambda)[a(\lambda), H] | A\rangle \quad (2.6)$$

is the ground-state expectation of the operator

$$H(\lambda) \equiv a^\dagger(\lambda)[a(\lambda), H]. \quad (2.7)$$

The mean removal energy is defined by

$$E_\lambda^{(-)} = \epsilon(\lambda)/n(\lambda), \quad (2.8)$$

which is the centroid of the hole-energy spectrum.

We assume that the nuclear Hamiltonian is of the form $H = T + V$ where T is the kinetic energy operator

$$T = \sum_{\lambda,\mu} \langle \lambda | T | \mu \rangle a^\dagger(\lambda)a(\mu) \quad (2.9)$$

and V is a two-body interaction operator

$$V = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle_a a^\dagger(\alpha)a^\dagger(\beta)a(\delta)a(\gamma) \quad (2.10)$$

with antisymmetrized matrix elements given by

$$\langle \alpha\beta | V | \gamma\delta \rangle_a = \langle \alpha\beta | V | \gamma\delta \rangle - \langle \alpha\beta | V | \delta\gamma \rangle. \quad (2.11)$$

It follows that $H(\lambda)$ may also be written as a one-plus two-body operator $H(\lambda) = T(\lambda) + V(\lambda)$ with

$$T(\lambda) = \sum_\mu \langle \lambda | T | \mu \rangle a^\dagger(\lambda)a(\mu), \quad (2.12)$$

$$V(\lambda) = \frac{1}{2} \sum_{\beta\gamma\delta} \langle \lambda\beta | V | \gamma\delta \rangle_a a^\dagger(\lambda)a^\dagger(\beta)a(\delta)a(\gamma). \quad (2.13)$$

So $\epsilon(\lambda)$ may be written as the expectation value of an operator whose highest particle rank (as a many-body operator) is two. This makes it rather

easy to evaluate, as we shall see in the next section. By contrast, the spectral function $P(\lambda, E)$ is the ground-state expectation value of an exceedingly complicated operator [see (2.1)] whose maximum particle rank must equal the number of particles, A. Similarly, the second energy moment

$$\begin{aligned}\int_{-\infty}^{\infty} E^2 P(\lambda, E)dE &= \langle A|\, a^\dagger(\lambda)(E_A - H)^2 a(\lambda)|\, A\rangle \\ &= \langle A|\, a^\dagger(\lambda)[H,[H, a(\lambda)]\,]\,|A\rangle \\ &= \langle A|\,[a^\dagger(\lambda), H][H, a(\lambda)]\,|A\rangle\end{aligned} \tag{2.14}$$

involves the ground-state expectation value of an operator whose maximum rank is *three*. The width (or dispersion) of the spectrum is then given by

$$\sigma^2 = \int_{-\infty}^{\infty} E^2 P(\lambda, E)/n(\lambda) - (E_\lambda^{(-)})^2 . \tag{2.15}$$

The operator $H(\lambda)$ is also simply related to the original Hamiltonian, through

$$H = \tfrac{1}{2}T + \frac{1}{2}\sum_\lambda H(\lambda), \tag{2.16}$$

which is obtained by comparing (2.9) and (2.10) with (2.12) and (2.13). Taking the ground-state expectation value we obtain a sum rule for[14,15] the total energy E_A of the target ground state:

$$E_A = \tfrac{1}{2}\langle A|\, T\,|A\rangle + \frac{1}{2}\sum_\lambda \epsilon(\lambda). \tag{2.17}$$

This has been applied to $(p, 2p)$ reactions[15] in the plane-wave representation ($\lambda = \vec{k}$).

3. LINKED-CLUSTER THEORY

In the linked-cluster theory one expresses ground-state properties in a perturbation series, the terms of which may be represented by diagrams. In this section we outline the linked-cluster evaluation of the mean removal energy (2.8), and its relation to the usual linked-cluster evaluation of the ground-state energy. If we have an approximate theory of the ground-state energy, which is given in terms of the linked-cluster series, then we shall also be able to evaluate the mean removal energy to the same order of approximation.

For the perturbation expansion, one partitions the Hamiltonian

$$\begin{aligned} H &= H_0 + H', \\ H_0 &= T + U, \\ H' &= V - U, \end{aligned} \tag{3.1}$$

where we have introduced an auxilliary one-body potential

$$U = \sum_{\lambda,\mu} \langle \lambda|\, U\,|\mu\rangle a^\dagger(\lambda) a(\mu). \tag{3.2}$$

The unperturbed Hamiltonian H_0 has a set of single-particle eigenstates $|\lambda\rangle$ with energies W_λ:

$$H_0|\lambda\rangle = W_\lambda|\lambda\rangle \tag{3.3}$$

or

$$\langle\lambda|\, T\,|\mu\rangle + \langle\lambda|\, U\,|\mu\rangle = W_\lambda \delta_{\lambda\mu}.$$

The potential U is arbitrary, but it is convenient if we choose it so that the orbital states $|\lambda\rangle$ are the same set of states $\{\lambda\}$ as defined for the particle removal, in Sec. 2, that is

$$|\lambda\rangle = a^\dagger(\lambda)|\rangle, \tag{3.4}$$

where $|\rangle$ is the vacuum state. In analogy with (2.12), we shall also need

$$U(\lambda) = \sum_\mu \langle\lambda|\, U\,|\mu\rangle\, a^\dagger(\lambda) a(\mu). \tag{3.5}$$

The ground-state energy may be written

$$\begin{aligned} E_A &= E_0 + \Delta E_A \\ E_0 &= \sum_{\lambda \le F} W_\lambda, \end{aligned} \tag{3.6}$$

where the unperturbed ground state $|0\rangle$ has all orbits filled up to some (Fermi) level F, and

$$H_0|0\rangle = E_0|0\rangle.$$

We assume this state is nondegenerate, for example: a spherical closed-shell state.

The linked-cluster expansion for the energy shift E_A is given by

$$\Delta E_A = \sum_{n=0}^{\infty} \left\langle 0 \left| H' \left(\frac{Q_0}{E_0 - H_0} H' \right)^n \right| 0 \right\rangle_{\text{l.c.}}, \tag{3.7}$$

where $Q_0 = 1 - |0\rangle\langle 0|$ projects out of the unperturbed ground state. The (l.c.) refers to the restriction of (3.7) to include only *linked-cluster* terms[16,17] (or diagrams).

It is also possible to expand the ground-state expectation value of any operator M in a linked-cluster series[17,20]:

$$\begin{aligned}\langle A|M|A\rangle = \sum_{l=0}^{\infty}\sum_{m=0}^{\infty} &\times \left\langle 0 \left| \left(H' \frac{Q_0}{E_0 - H_0} \right)^l M \left(\frac{Q_0}{E_0 - H_0} H' \right)^m \right| 0 \right\rangle_{\text{l.c.}} .\end{aligned} \tag{3.8}$$

The first energy moment $\epsilon(\lambda)$ may be expressed as the ground-state expectation value (2.7) of $H(\lambda)$. If we partition $H(\lambda) = [T(\lambda) + U(\lambda)] + [V(\lambda) - U(\lambda)]$,

we find

$$\langle A \mid T(\lambda) + U(\lambda) \mid A \rangle = W_\lambda n(\lambda), \tag{3.9}$$

using (2.5) and (3.3), so that

$$\epsilon(\lambda) = W_\lambda n(\lambda) + \Delta E(\lambda), \tag{3.10}$$

where we define the removal energy shift

$$\Delta E(\lambda) \equiv \langle A \mid V(\lambda) - U(\lambda) \mid A \rangle . \tag{3.11}$$

Then $\Delta E(\lambda)$ may be expanded in linked-cluster form, using (3.8), where $M = V(\lambda) - U(\lambda)$. Similarly, the expansion of $n(\lambda)$ is obtained from (3.8) with $M = a^\dagger(\lambda)a(\lambda)$.

The mean removal energy is given by

$$E_\lambda^{(-)} = W_\lambda + \frac{\Delta E(\lambda)}{n(\lambda)} . \tag{3.12}$$

In order to evaluate the terms of the expansions (3.7) and (3.8) in terms of the one- and two-body matrix elements of H' (and M), it is useful to consider perturbation (e.g., Feynman or Goldstone) diagrams. For the present discussion we do not require the rules for explicit evaluation of diagrams (for which, see Refs. 17, 21, and 22) but will need some of the general structural features.

Consider first the series (3.7) for ΔE_A. The diagrams are closed connected figures made up of vertical directed line segments representing hole or particle states, and horizontal segments representing interaction matrix elements. A simple example is shown in Fig. 1(a). Upward directed lines represent particles ($\lambda > F$); downward lines represent holes. We include "inert" lines which return to the point of origin with the holes (e.g., α_1, of Fig. 1.) The wiggly lines denote antisymmetrized two-body matrix elements of V (2.11), and dashed lines one-body matrix elements of $(-U)$ from (3.2). The value of each diagram is an expression containing these interaction matrix elements, and the unperturbed energies W_λ for the particle and hole line states.

Consider a diagram which has ρ hole lines and σ particle lines. (If the diagram is pth order in V and qth order in U, then $2p + q = \rho + \sigma$.) We label the hole lines, in some order, by the orbital quantum numbers $\alpha_1, \alpha_2, \ldots, \alpha_\rho$ ($\alpha \leq F$) and the particle lines by $\beta_1, \ldots, \beta_\sigma$ ($\beta > F$). We denote the value of this diagram by

$$D^x(\alpha_1 \cdots \alpha_\rho; \beta_1 \cdots \beta_\sigma), \tag{3.13}$$

where x distinguishes different diagrams with the same ρ and σ. Figure 1(a) illustrates a specific diagram whose value is $D^x(\alpha_1, \alpha_2, \alpha_3, \alpha_4; \beta_1, \beta_2, \beta_3)$.

To obtain the contribution of all the different labelings of D^x to ΔE_A, we sum (3.13) over all particle and hole states. [Any factors for "equivalent" lines may be absorbed into the definition of (3.13).]

$$D^x_{\rho\sigma} = \sum_{\alpha_1 \cdots \alpha_\rho \leq F} \; \sum_{\beta_1 \cdots \beta_\sigma > F} D^x(\alpha_1 \cdots \beta_\sigma). \tag{3.14}$$

Then ΔE_A is simply the sum of all diagrams

$$\Delta E_A = \sum_{\sigma=0}^{\infty} \sum_{\rho=1}^{\infty} \sum_{x} D^x_{\rho\sigma} . \tag{3.15}$$

Now consider the linked-cluster diagrammatic series (3.8) and (3.11) for $\Delta E(\lambda)$, the removal energy shift. The diagrams will also be closed figures with ρ hole lines and σ particle lines. In addition to the (horizontal) interaction lines for V or $(-U)$, each diagram will have one horizontal interaction line representing a matrix element of either $V(\lambda)$ or $[-U(\lambda)]$. In Fig. 1(b) we have illustrated a set of diagrams contributing to $\Delta E(\lambda)$, for the hole case ($\lambda \leq F$), whose configurations are most similar to that of Fig. 1(a). The horizontal double bar stands for an antisymmetrized two-body matrix element of $V(\lambda)$, and the dotted line for one-body matrix element of $[-U(\lambda)]$.

We see from (2.13) and (3.5) that at least one line emerging from a $V(\lambda)$ or $U(\lambda)$ interaction must carry the λ label. We may construct all the diagrams of $\Delta E(\lambda)$ by first selecting those diagrams (3.15) for which some line is labeled λ. Then we replace the interaction line from which the λ line emerges, V or $(-U)$, by $V(\lambda)$ or $-U(\lambda)$, respectively. If we do this in Fig. 1(a), for $\lambda \leq F$, we ob-

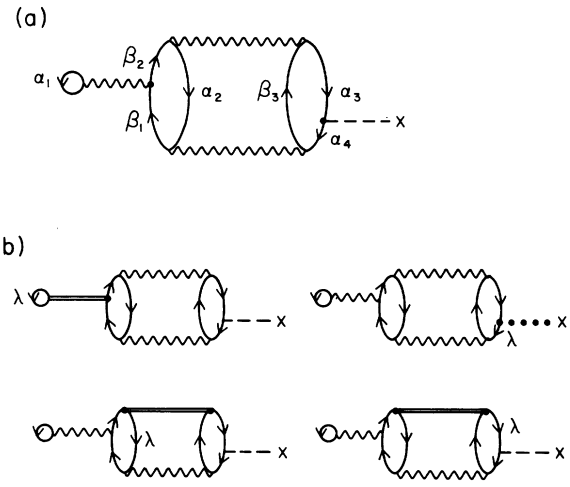

FIG. 1. (a) An example of a Goldstone diagram for ΔE_A, with hole lines labeled by α, particle lines by β. Matrix elements of V are denoted by wiggly lines, and of $-U$ by the dashed line. (b) Diagrams for contributions to $\Delta E(\lambda)$, obtained from diagram (a); the doubled line denotes a matrix element of $V(\lambda)$, and the dotted line a matrix element of $-U(\lambda)$.

tain the diagrams of Fig. 1(b): one for each of the four hole lines in 1(a).

In changing one interaction V to $V(\lambda)$ in a diagram, one changes an antisymmetrized two-body matrix element (2.11) of V to the same two-body matrix element of $V(\lambda)$. But these two matrix elements are identical, as one can verify by comparing (2.10) with (2.13). Remember that one particle must carry the quantum number λ for this matrix element. Similarly, changing an interaction U to $U(\lambda)$, replaces a one-body matrix element of U by one of $U(\lambda)$. These two matrix elements are also identical, as one can see from (3.2) and (3.5). Therefore, the numerical value of the original diagram, which was part of the original linked-cluster series for ΔE_A, is not altered when it is converted into a diagram of the linked-cluster series for $\Delta E(\lambda)$.

It follows that each diagram of the $\Delta E(\lambda)$ series has the value of some diagrams of the ΔE_A series

$$D^x(\alpha_1\cdots\lambda\cdots\beta_\sigma) \tag{3.16}$$

in which some hole line (if $\lambda \leq F$) or particle line (if $\lambda > F$) takes the label λ. For example the diagrams of Fig. 1(b) take the values

$$D^x(\alpha_1\alpha_2\alpha_3\alpha_4;\beta_1\beta_2\beta_3)$$

with $\alpha_1=\lambda$, $\alpha_2=\lambda$, $\alpha_3=\lambda$, $\alpha_4=\lambda$ in succession.

We may sum over the free particle and hole lines, defining

$$D^x_{\rho\sigma}(\lambda) \equiv \sum_{\alpha_1\cdots\alpha_\rho\leq F}\ \sum_{\beta_1\cdots\beta_\sigma>F} \times D^x(\alpha_1\cdots\beta_\sigma)\left(\sum_{i=1}^{\rho}\delta_{\lambda,\alpha_i}+\sum_{j=1}^{\sigma}\delta_{\lambda,\beta_j}\right). \tag{3.17}$$

Then we may sum the entire series

$$\Delta E(\lambda)=\sum_{\rho=1}^{\infty}\sum_{\sigma=0}^{\infty}\sum_{x} D^x_{\rho\sigma}(\lambda). \tag{3.18}$$

Note that

$$\sum_{\lambda\leq F} D^x_{\rho\sigma}(\lambda)=\rho D^x_{\rho\sigma} \quad \text{for} \quad \lambda\leq F,$$
$$\sum_{\lambda>F} D^x_{\rho\sigma}(\lambda)=\sigma D^x_{\rho\sigma} \quad \text{for} \quad \lambda>F, \tag{3.19}$$

so that, for example, if $\lambda \leq F$, we can reexpress (3.15) as

$$\Delta E_A=\sum_{\rho=1}^{\infty}\frac{1}{\rho}\sum_{\sigma=0}^{\infty}\sum_{\lambda\leq F}\sum_{x} D^x_{\rho\sigma}(\lambda). \tag{3.20}$$

For the calculation of the mean removal energy Eq. (3.12) we also need a linked-cluster expansion for $n(\lambda)$. This may be obtained directly from Eq. (3.8) by taking M to be number operator $N(\lambda) \equiv a^\dagger(\lambda)a(\lambda)$. The expansion (3.8) may be treated as an extension of (3.7), as if one had added to the perturbing interaction H', an external one-body potential $N(\lambda)$ (diagonal in λ), which is to be kept to first order only.

The diagrams corresponding to the series for $n(\lambda)$ can be obtained from these of the ΔE_A series (3.13)–(3.15) as follows. First consider the hole case ($\lambda \leq F$). There is contribution of unity from the zeroth-order term (in H') $\langle 0|a^\dagger(\lambda)a(\lambda)|0\rangle = 1$. To obtain the rest of the series, we start with the expression (3.16) for a diagram with some fixed hole line λ. However, λ may not be an inert loop [as in the first diagram of Fig. 1(b)]. As an example, consider Fig. 2(a).

Now we create new diagrams by inserting the number operator into the λ-hole line. If the diagram (3.16) has r interaction vertices (V or $-U$) spanned by the λ-hole line (that is, occurring on other particular or hole lines, at positions between the beginning and end of the λ-hole line), then there are $r+1$ distinct positions for inserting $N(\lambda)$ (between other interactions). Thus $r+1$ distinct diagrams are created, which include $N(\lambda)$ to first order. For the example of Fig. 2(a), three distinct diagrams contribute to $n(\lambda)$; they are shown in Fig. 2(b).

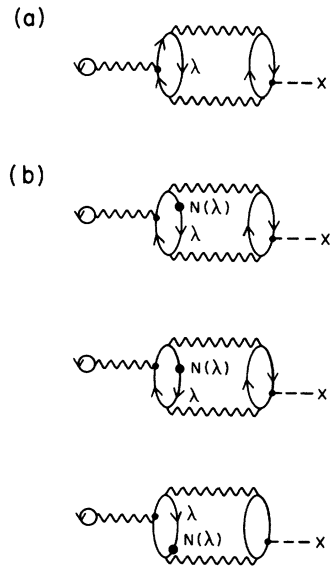

FIG. 2. (a) A ΔE_A diagram, as in Fig. 1(a), with one hole line specified to be λ. (b) The three diagrams contributing to $n(\lambda)$, which can be made by inserting the number operator $N(\lambda)$ into the λ line.

The effect of inserting the operator $N(\lambda)$ into a λ-hole line, on the value of the original diagram, is to replace the energy denominator $(E_0 - H_0)$ appropriate at the point of the insertion by $(E_0 - H_0)^2$, and multiply by (-1). This (-1) is the linked-cluster contribution of $N(\lambda) = a^\dagger(\lambda)a(\lambda) = 1 - a(\lambda)a^\dagger(\lambda)$. The denominator $(E_0 - H_0)$ takes the value

$$d_q = \sum W_\alpha - \sum W_\beta , \tag{3.21}$$

where the sum is over all hole or particle lines which appear at the same level (horizontally: same "time") as the insertion denoted by q. So for each diagram of the form (3.16), with λ as a hole line, we obtain a contribution to $n(\lambda)$

$$F^x(\alpha_1 \cdots \lambda \cdots ; \cdot \beta_\sigma) = -\sum_{q=1}^{r+1} \frac{D^x(\alpha_1 \cdots \lambda \cdot ; \cdot \beta_\sigma)}{d_q} ,$$

$$\lambda \leq F . \tag{3.22a}$$

Similarly, for a particle line λ

$$F^{-x}(\alpha_1 \cdot ; \cdot \cdot \lambda \cdot \cdot \beta_\sigma) = \sum_{q=1}^{r+1} \frac{D^x(\alpha_1 \cdots \lambda \cdots \beta_\sigma)}{d_q} ,$$

$$\lambda > F . \tag{3.22b}$$

To obtain the complete linked-cluster series for $n(\lambda)$ we sum (3.22) over all particle and hole states, and permutations of λ:

$$F^x_{\rho\sigma}(\lambda) = \sum_{\alpha_1 \cdots \alpha_\rho \leq F} \sum_{\beta_1 \cdots \beta_\sigma > F} F^x(\alpha_1 \cdots \beta_\sigma) \times \left(\sum_{i=1}^{\rho} \delta_{\lambda, \alpha_1} + \sum_{j=1}^{\sigma} \delta_{\lambda, \beta_j} \right) \tag{3.23}$$

and over all diagrams

$$n(\lambda) = 1 + \sum_{\rho=1}^{\infty} \sum_{\sigma=0}^{\infty} \sum_{x} F^x_{\rho\sigma}(\lambda), \quad \lambda \leq F \tag{3.24a}$$

$$= \sum_{\rho=1}^{\infty} \sum_{\sigma=0}^{\infty} \sum_{x} F^x_{\rho\sigma}(\lambda), \quad \lambda > F. \tag{3.24b}$$

By combining the linked-cluster expansions (3.18) for $\Delta E(\lambda)$ and (3.24) for $n(\lambda)$, we may evaluate the mean removal energy (3.12). As we have noted, both $\Delta E(\lambda)$ and $n(\lambda)$ are expressed in terms of diagrams (3.16), which also appear in the expression for the ground-state energy shift ΔE_A, through (3.20). This means that if we are considering a particular approximation to the ground-state energy which can be expressed by specifying which diagrams (3.13) are to be included in ΔE_A, we can immediately generate $E_\lambda^{(-)}$ to the same approximation by including the subset of diagrams (3.16) of the chosen set (3.13), in the calculation of (3.18), (3.24), and (3.12).

In fact, the values of $E_\lambda^{(-)}$, $n(\lambda)$, and E_A given in such a diagrammatic approximation, are interrelated through the sum rule (2.17) for the ground-state energy. Using (3.3) and (3.12), the sum rule may be written

$$E_A = \sum_\lambda [W_\lambda n(\lambda) + \tfrac{1}{2}\Delta E(\lambda)] - \tfrac{1}{2}\langle A|U|A\rangle . \tag{3.25}$$

It can be shown (see Appendix) that if $n(\lambda)$, $\Delta E(\lambda)$, and $\langle U \rangle$ are all calculated from a given set of diagrams (3.16), the value of E_A obtained in (3.25) is identical with that calculated directly from (3.6) using the same set of diagrams (summed over λ). Note that this is not a trivial application of (2.17) to an approximate state since (3.25) is not, in any given diagrammatic approximation, equivalent to an expectation value.

If the unperturbed target ground state is degenerate, the linked-cluster treatment must be modified. There are several possible procedures; see, e.g. Ref. 17.

4. APPLICATIONS

We now outline the calculation of the mean removal energies for several familiar examples of approximation to the ground-state energy. We consider the contributions to ΔE_A in the linked-cluster expansion, including the terms represented by the various diagrams of Fig. 3. The contribution of each diagram will be denoted by $C(i)$, where i = a, b, ... in the index of the diagram (or subset of diagrams) in the figure. For a given approximation we write $\Delta E_A = \sum_i C(i)$, specifying the set $\{i\}$, where the ground-state energy is $E_A = E_0 + \Delta E_A$.

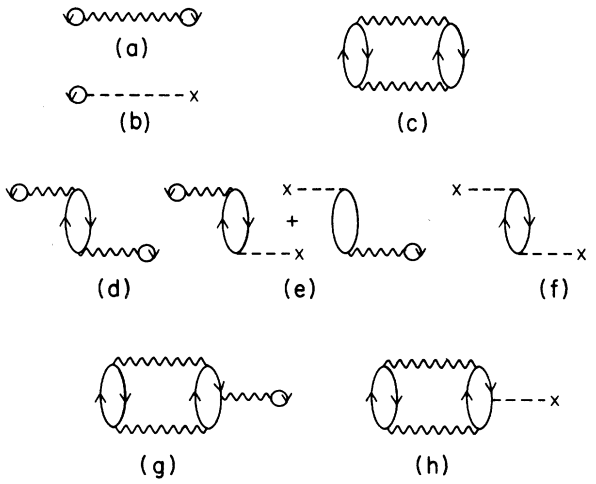

FIG. 3. Diagrams representing the linked-cluster expansion for ΔE_A through second order in $(V-U)$, with two selected diagrams of third order (g) and (h).

In the Hartree-Fock approximation (HF),

$$E_A = C(\mathrm{a}) + C(\mathrm{b}) = \frac{1}{2}\sum_{\lambda,\mu\le F}\langle\lambda\mu|V|\lambda\mu\rangle_a - \sum_{\lambda\le F}\langle\lambda|U|\lambda\rangle. \quad (4.1)$$

The usual Hartree-Fock self-consistency condition gives

$$\langle\lambda|U|\nu\rangle = \sum_{\mu\le F}\langle\lambda\mu|V|\nu\mu\rangle_a \quad (4.2)$$

from which it follows that

$$E_A(\mathrm{HF}) = E_0 - \frac{1}{2}\sum_{\lambda\le F}\langle\lambda|U|\lambda\rangle = \frac{1}{2}\sum_{\lambda\le F}(\langle\lambda|T|\lambda\rangle + W_\lambda). \quad (4.3)$$

To include all terms of second order in $(V-U)$, we add the diagrams c, d, e, f (of Fig. 3). However the HF condition (4.2) makes the sum $C(\mathrm{d})+C(\mathrm{e})+C(\mathrm{f})=0$, so that

$$E_A(2) = \frac{1}{2}\sum_{\lambda\le F}(\langle\lambda|T|\lambda\rangle + W_\lambda) + C(\mathrm{c}),$$

$$C(\mathrm{c}) = \frac{1}{4}\sum_{\lambda,\mu\le F}\sum_{\alpha,\beta>F}\frac{\langle\lambda\mu|V|\alpha\beta\rangle_a^2}{W_\lambda + W_\mu - W_\alpha - W_\beta}. \quad (4.4)$$

If we also include the two third-order terms g and h, we get no change in (4.4), since $C(\mathrm{g})+C(\mathrm{h})=0$, due to (4.2).

We may also include the Brueckner-Hartree-Fock (BHF) approximation, if we now understand the wiggly horizontal lines of Fig. 3 to denote the antisymmetrized two-body matrix elements $\langle\alpha\beta|G|\gamma\delta\rangle_a$ of the Brueckner reaction (G) matrix, rather than of the interaction V(2.11). Denoting the contributions by $C'(i)$, we have

$$C'(\mathrm{a}) = \frac{1}{2}\sum_{\lambda,\mu\le F}\langle\lambda\mu|G|\lambda\mu\rangle_a. \quad (4.5)$$

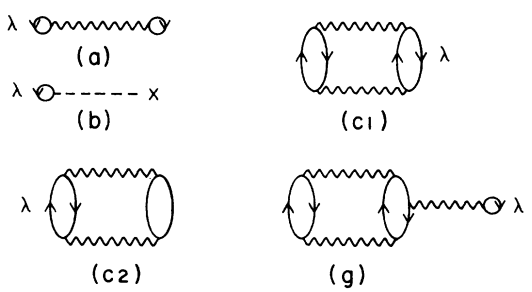

FIG. 4. Diagrams contributing to $\Delta E(\lambda)$, corresponding to those of Fig. 3, omitting those which cancel because of Eq. (4.2).

We must now exclude $C'(\mathrm{c})$, whose contribution is already included in (4.5). We also replace V by G in (4.2) to get BHF self-consistency, and obtain

$$E_A(\mathrm{BHF}) = C'(\mathrm{a}) + C'(\mathrm{b}) = \frac{1}{2}\sum_{\lambda\le F}(\langle\lambda|T|\lambda\rangle + W_\lambda). \quad (4.6)$$

As discussed in the previous section, the linked-cluster diagrams for $\Delta E(\lambda)$ (3.11) are obtained from those for ΔE_A by fixing in turn, each hole line (for $\lambda\le F$, or particle line, for $\lambda>F$) in the orbital λ, summing all other lines, as in (3.17). Starting with Fig. 3, the resulting diagrams are shown in Fig. 4, where diagram 4(a) comes from Fig. 3(a), and so on. We denote the contributions to ΔE_λ by $C_\lambda(i)$. We have omitted diagrams which cancel because of (4.2): $C_\lambda(\mathrm{d})+C_\lambda(\mathrm{e})+C_\lambda(\mathrm{f})=0$, and $C_\lambda(\mathrm{g})+C_\lambda(\mathrm{h})$ has only the nonvanishing term shown in Fig. 4(g).

In Fig. 5 we give the diagrams which contribute to $n(\lambda)$, and which we obtain from Fig. 3 through (3.22) (see Fig. 2). We denote the contributions by $N_\lambda(i)$; again we have omitted canceling diagrams: $N_\lambda(\mathrm{d})+N_\lambda(\mathrm{e})+N_\lambda(\mathrm{f})=0$, $N_\lambda(\mathrm{g})+N_\lambda(\mathrm{h})=0$.

In HF (or BHF) we have, for $\lambda\le F$

$$\Delta E_\lambda = C_\lambda(\mathrm{a}) + C_\lambda(\mathrm{b}) = \sum_{\mu\le F}\langle\lambda\mu|V|\lambda\mu\rangle_a - \langle\lambda|U|\lambda\rangle \quad (4.7)$$

which vanishes under condition (4.2). The mean removal energy is obtained from (3.12), which is in this case

$$E_\lambda^{(-)}(\mathrm{HF\ or\ BHF}) = W_\lambda, \quad \lambda\le F. \quad (4.8)$$

That is, the mean removal energy for holes is the HF orbital energy, as is usually assumed. Note that since in HF,

$$n(\lambda) = 1, \quad \lambda\le F, \quad = 0, \quad \lambda>F, \quad (4.9)$$

$E_\lambda^{(-)}$ is not defined for $\lambda>F$.

If we calculate to second order in $(V-U)$, we obtain

$$\Delta E_\lambda = C_\lambda(\mathrm{a}) + C_\lambda(\mathrm{b}) + C_\lambda(\mathrm{c1}), \quad \lambda\le F, \quad (4.10)$$
$$\Delta E_\lambda = C_\lambda(\mathrm{c2}), \quad \lambda>F,$$

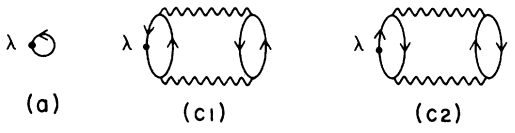

FIG. 5. Diagrams contributing to $n(\lambda)$, corresponding to those of Fig. 3, omitting those which cancel because of Eq. (4.2).

where

$$C_\lambda(\mathrm{c1}) = \frac{1}{2}\sum_{\mu\le F}\sum_{\alpha,\beta>F}\frac{\langle\lambda\mu|V|\alpha\beta\rangle_a{}^2}{W_\lambda + W_\mu - W_\alpha - W_\beta}, \quad \lambda \le F, \tag{4.11a}$$

$$C_\lambda(\mathrm{c2}) = \frac{1}{2}\sum_{\mu,\nu\le F}\sum_{\beta>F}\frac{\langle\mu\nu|V|\lambda\beta\rangle_a{}^2}{W_\mu + W_\nu - W_\lambda - W_\beta}, \quad \lambda > F. \tag{4.11b}$$

To this order, following (3.22) we obtain

$$n(\lambda) = N_\lambda(\mathrm{a}) + N_\lambda(\mathrm{c1}) = 1 - \frac{1}{2}\sum_{\mu\le F}\sum_{\alpha\beta>F}\frac{\langle\lambda\mu|V|\alpha\beta\rangle_a{}^2}{(W_\lambda + W_\mu - W_\alpha - W_\beta)^2}, \quad \lambda \le F, \tag{4.12a}$$

$$n(\lambda) = N_\lambda(\mathrm{c2}) = \frac{1}{2}\sum_{\mu\nu\le F}\sum_{\beta>F}\frac{\langle\mu\nu|V|\lambda\beta\rangle_a{}^2}{(W_\mu + W_\nu - W_\lambda - W_\beta)^2}, \quad \lambda > F. \tag{4.12b}$$

The mean removal energy to second order is given by

$$E_\lambda^{(-)} = W_\lambda + C_\lambda(\mathrm{c1})[1 + N_\lambda(\mathrm{c1})]^{-1} \simeq W_\lambda + C_\lambda(\mathrm{c1}), \quad \lambda \le F, \tag{4.13a}$$

$$E_\lambda^{(-)} = W_\lambda + C_\lambda(\mathrm{c2})N_\lambda{}^{-1}(\mathrm{c2}), \quad \lambda > F, \tag{4.13b}$$

where we may drop the second-order correction $N_\lambda(\mathrm{c1})$ for $\lambda \le F$. However, we must retain $N_\lambda(\mathrm{c2})$ for $\lambda > F$, since there is no zeroth-order term in the denominator $n(\lambda)$ in (4.13b).

Comparing (4.4) and (4.11), we see that

$$C(\mathrm{c}) = \frac{1}{2}\sum_{\lambda\le F} C_\lambda(\mathrm{c1}).$$

Then, using (4.13a) we may express the second-order ground-state energy (4.4) in the form

$$E_A(2) = \frac{1}{2}\sum_{\lambda\le F}(\langle\lambda|T|\lambda\rangle + E_\lambda^{(-)}). \tag{4.14}$$

This relation also holds for the HF and BHF approximations, as can be seen from (4.3) and (4.8). It can be extended to include any linked-cluster diagram with two hole lines (as in the BHF series for G)

However (4.14) differs from the exact sum rule (2.11), which involves a sum over all orbits λ. As discussed in Sec. 3, the sum rule in its linked-cluster form (3.25) holds to any order of approximation. (This is proved in the Appendix.) In particular then, to second order in $(V - U)$, (3.25) must give the same value of E_A as does (4.14). To this order, (3.25) can be written

$$E_A(2) = \sum_{\lambda\le F}\{W_\lambda[1 + N_\lambda(\mathrm{c1})] + \tfrac{1}{2}C_\lambda(\mathrm{c1}) - \tfrac{1}{2}\langle\lambda|U|\lambda\rangle\} + \sum_{\lambda>F}[W_\lambda N_\lambda(\mathrm{c2}) + \tfrac{1}{2}C_\lambda(\mathrm{c2})]. \tag{4.15}$$

Consider a very simple case in which, for $\lambda \le F$, all orbits have $W_\lambda = W_1$, and for $\lambda > F$, $W_\lambda = W_2$ with $W_1 > W_2$. Then it is easy to show from (4.4) and (4.10)–(4.12) that

$$\sum_{\lambda\le F} W_\lambda N_\lambda(\mathrm{c1}) + \sum_{\lambda>F}[W_\lambda N_\lambda(\mathrm{c2}) + \tfrac{1}{2}C_\lambda(\mathrm{c2})] = (W_2 - W_1)\left[\frac{2C(\mathrm{c})}{2(W_1 - W_2)}\right] + C(\mathrm{c}) = 0. \tag{4.16}$$

Therefore (4.15) becomes

$$E_A(2) = \sum_{\lambda\le F}[W_\lambda + \tfrac{1}{2}C_\lambda(\mathrm{c1}) - \tfrac{1}{2}\langle\lambda|U|\lambda\rangle] \tag{4.17}$$

which agrees with (4.13)–(4.14). It also follows from (4.13b) for this simplified case, that for $\lambda > F$,

$$E_\lambda^{(-)} = W_2 + 2(W_1 - W_2) = W_1 + (W_1 - W_2) < W_1. \tag{4.18}$$

That is, the mean removal energy for a normally unoccupied orbit is shifted downward from the unperturbed value W_2, by twice the average excitation energy $(W_1 - W_2)$, so that it falls below the occupied (unperturbed) orbital energy W_1. It is this extra binding energy of the unoccupied orbitals which makes it possible for the sum rule (3.25) to agree with (4.14). This downward shift of $E_\lambda^{(-)}$ for unoccupied relative to occupied orbitals is in fact, more general than the simple example of (4.18).

If we now include the third-order term of Fig. 4(g) in ΔE_λ, we obtain

$$\Delta E_\lambda = C_\lambda(\mathrm{c1}) + C_\lambda(\mathrm{g}), \quad \lambda \le F, \qquad \Delta E_\lambda = C_\lambda(\mathrm{c2}), \quad \lambda > F, \tag{4.19}$$

where

$$C_\lambda(\mathrm{g}) = \sum_{\mu\le F}\langle\lambda\mu|V|\lambda\mu\rangle_a[n(\mu) - 1], \tag{4.20}$$

and $n(\lambda)$ is still given by (4.12). Then, to this order

$$E_\lambda^{(-)}(3) \cong W_\lambda + C_\lambda(\mathrm{c1}) + C_\lambda(\mathrm{g}), \quad \lambda \le F, \tag{4.21a}$$

$$E_\lambda^{(-)}(3) = W_\lambda + C_\lambda(\mathrm{c2})N_\lambda{}^{-1}(\mathrm{c2}), \quad \lambda > F. \tag{4.21b}$$

Combining (4.20) and (4.21a) with (4.2), we find

that $E_\lambda^{(-)}$ for $\lambda \leq F$ is modified from its second-order value (4.13a) to

$$E_\lambda^{(-)}(3) = \langle \lambda | T | \lambda \rangle + \sum_{\mu \leq F} \langle \lambda\mu | V | \lambda\mu \rangle_a n(\mu) + C_\lambda(\mathrm{c1}). \tag{4.22}$$

So the effect of the insertion of Fig. 4(g) is to reduce the potential term in $W = T + U$, since $n(\lambda) \leq 1$.

In the BHF expansion we would have the third-order term

$$C'_\lambda(\mathrm{g}) = \sum_{\mu \leq F} \langle \lambda\mu | G | \lambda\mu \rangle_a [n(\mu) - 1], \tag{4.23}$$

and the mean removal energies are

$$E_\lambda^{(-)}[\mathrm{BHF(g)}] = \langle \lambda | T | \lambda \rangle + \sum_{\mu \leq F} \langle \lambda\mu | G | \lambda\mu \rangle_a n(\mu), \quad \lambda \leq F, \tag{4.24a}$$

$$E_\lambda^{(-)}[\mathrm{BHF(g)}] = W_\lambda + C'_\lambda(\mathrm{c2}) N'^{-1}_\lambda(\mathrm{c2}), \quad \lambda > F. \tag{4.24b}$$

The quantity in (4.24a) has been called the "renormalized" BHF single-particle energy (for $\lambda \leq F$). Its inclusion in the Brueckner theory has been suggested by Brandow[18, 19] and has been used in recent calculations[23, 24] of the ground-state energy E_A. The equality of this single-particle energy with the mre (to the same order) has been obtained previously[9, 25] and is a special case of a more general result (5.7) obtained in the following section.

We noted below Eq. (4.4) that the insertions $C(\mathrm{g})$ and $C(\mathrm{h})$ give no net contribution to the binding energy E_A, because of the HF condition (4.2). However, as is seen from in (4.19) and (4.24), $C_\lambda(\mathrm{g})$ does modify the mre $E_\lambda^{(-)}$ for $\lambda \leq F$. It follows that the HF relation (4.14) between E_A and $E_\lambda^{(-)}$ no longer holds, although the general sum rule is still valid.

5. SELF-CONSISTENT ORBITAL ENERGIES

Self-consistent orbital energies for particles in bound systems appear naturally in the shell theories of atoms and nuclei. The ideas which first appeared in the Hartree-Fock approximation have been incorporated into the development of linked-cluster theory. We saw in the examples of the previous section, that for some approximations, like HF and BHF, the self-consistent orbital energy may also be the mre for that orbit. In this section we show that this equality may be generalized if we use a suitable definition of self-consistency. For this we shall follow the definitions of Brandow,[18, 26] who has also reviewed other generalizations of self-consistency.[17-19]

In the linked-cluster theory, the development is in terms of "insertions" into particle or hole lines in the diagrams, e.g. for binding energy. An insertion is part of a diagram, connected to the rest by two line segments. Some examples of insertions are shown schematically in Fig. 6, where we use shaded blocks to stand for the diagrammatic form of the insertion itself. The blocks contain connected particle and hole line segments, and interaction lines, as in the diagrams of Figs. 1–5. The value of an insertion has the dimension of energy. Insertions may be summed. We denote the sum of a specified set of insertions by $M_{\lambda\mu}(E)$, where E is an energy parameter, which may depend on the diagram in which the insertion appears. The idea of a self-consistent theory is to sum large classes of these insertions in such a way that the effect of $M_{\lambda\mu}(E)$ may be given by a single-particle potential. Finding the potential is a self-consistent problem, since the potential is defined in terms of insertions diagrams which in turn depend on the potential, through further insertions.

Brandow's approach is to separate the insertions into two classes, denoted by M^{on} and M^{off}, referring to on- and off-energy shell insertions. The distinction is given in terms of diagrams: Inser-

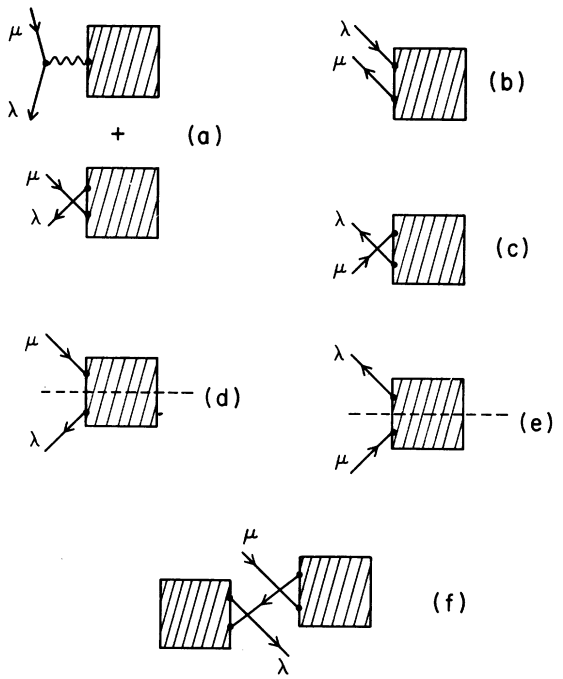

FIG. 6. Examples of insertion diagrams, where the blocks may contain connected particle, hole, and interaction lines, as in Figs. 1–5. (a), (b), and (c) are of type M^{on}, (d) and (e) are of type M^{off}, (f) is of M^{on}, and is reducible to two M^{on} insertions.

tions for which the external lines overlap in "time," that is, can both be cut by some horizontal line, as in Figs. 6(a)–(c), are contributions to M^{on}. If the external lines do not overlap, so that for some "time" [horizontal dashed line in Figs. 6(d) and (e)] neither external line is cut, the diagram contributes to M^{off}. Brandow has shown[18] that the $M^{on}(E)$ insertions are on energy shell in the sense that the value of E is determined only by the energies external $(\lambda - \mu)$ line segments, and not by the rest of the larger diagram. This leads to a definition of the self-consistent potential.

First, consider those insertion diagrams which can be made into two diagrams by cutting one internal particle or hole line, as in Fig. 6(f). We define those M^{on} diagrams which can be so cut to produce two (or more) M^{on} diagrams as *reducible*. Those which cannot be so cut are *irreducible*, and the sum of all irreducible insertions in a set $M^{on}_{\lambda\mu}(E)$ will be denoted by $Q^{on}_{\lambda\mu}(E)$. [Note that this is not the same irreducibility as required for the self-energy diagrams for causal Green's functions: Q^{on} may contain diagrams which can be cut to produce one M^{on} and one (or more) M^{off} insertions, which would be reducible in the Green's function theory.]

Now, following Brandow,[18,26] we may define a self-consistent energy $\mathcal{E}_\alpha$, and its orbital wave function ψ_α, in terms of an implicit eigenvalue equation

$$(\mathcal{E}_\alpha - W_\lambda)q^\alpha_\lambda = \sum_\mu Q^{on}_{\lambda\mu}(\mathcal{E}_\alpha)q^\alpha_\mu , \tag{5.1}$$

$$\psi_\alpha = \sum_\lambda q^\alpha_\lambda \phi_\lambda . \tag{5.2}$$

A self-consistent single-particle potential U can be chosen so that

$$Q^{on}_{\lambda\mu}(\mathcal{E}_\alpha) \equiv 0; \quad \mathcal{E}_\alpha \equiv W_\alpha . \tag{5.3}$$

With this choice, the linked-cluster series for the ground-state energy is simplified, and its convergence possibly improved, as discussed by Brandow. In lowest order (5.3) becomes the HF condition (4.2).

To return to the calculation of the mre; we are interested in the value of diagrams of the form of Figs. 7(a) and 7(b), which, as we have seen in Sec. 3, contribute to ΔE_λ. (We now choose $\{\lambda\}$ as the self-consistent basis.) In the Brandow version, these would be "skeleton" diagrams, with no explicit insertions. The diagrams 7(a) and 7(b) are numerically equal (up to a sign) to those of diagrams 7(c) and 7(d), respectively, with the external λ lines assigned the self-consistent energy $\mathcal{E}_\lambda$. [To be consistent with (5.1), there is a sign change between 7(b) and 7(d).]

But diagrams 7(c) and 7(d) contribute to $M^{on}_{\lambda\lambda}(\mathcal{E}_\lambda)$. For $\lambda \leq F$, there is a one-to-one correspondence of the diagrams of 7(a) with 7(c), so that

$$\Delta E(\lambda) = M^{on}_{\lambda\lambda}(\mathcal{E}_\lambda), \quad \lambda \leq F . \tag{5.4}$$

Using Brandow's analysis of insertions[18,26] one finds that (5.4) can be expressed in terms of the irreducible insertion Q^{on} with "dressed propagators"

$$M^{on}_{\lambda\lambda}(\mathcal{E}_\lambda) = \sum_\mu Q^{on}_{\lambda\mu}(\mathcal{E}_\lambda)P_{\mu\lambda} , \tag{5.5}$$

where $P_{\mu\lambda}$ is a weighting factor given by

$$P_{\mu\lambda} = \left[1 - \frac{\partial}{\partial E} Q^{on}(E)_{E=\mathcal{E}_\lambda}\right]^{-1}_{\mu\lambda} , \tag{5.6}$$

where $P_{\lambda\lambda} \equiv n(\lambda)$.

With the self-consistent choice (5.3), we have $\Delta E(\lambda) \equiv 0$ $(\lambda \leq F)$ from (5.4) and (5.5). We then obtain the mre from (3.12)

$$\begin{aligned} E^{(-)}_\lambda &= W_\lambda + \Delta E(\lambda)/n(\lambda) \\ &= W_\lambda = \mathcal{E}_\lambda, \quad \lambda \leq F . \end{aligned} \tag{5.7}$$

So the self-consistent orbital energies defined in (5.1)–(5.3) are identical with the mre for the normally occupied self-consistent orbits, with one restriction to be discussed shortly. It follows that the self-consistent energies for $\lambda \leq F$ are measurable, in the same sense that the mre are.

It may be worth noting that the single-particle potential could also be chosen so that Q^{on} is diagonal, but not zero, in the self-consistent representation:

$$\mathcal{E}_\lambda = W_\lambda + Q^{on}_{\lambda\lambda}(\mathcal{E}_\lambda) \tag{5.8}$$

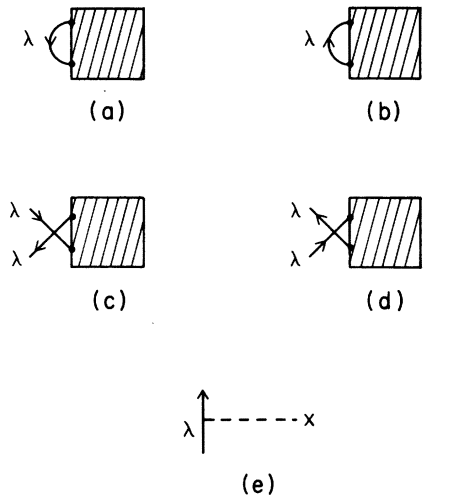

FIG. 7. $\Delta E(\lambda)$ diagrams (a) and (b) and associated M^{on} diagrams (c) and (d). M^{on} diagram (e) is not associated with any diagram of form (b).

in which case (5.4) and (5.5) become

$$\Delta E_\lambda = M^{\rm on}_{\lambda\lambda}(\mathcal{E}_\lambda) = Q^{\rm on}_{\lambda\lambda}(\mathcal{E}_\lambda) n(\lambda), \quad \lambda \leq F, \tag{5.9}$$

and we again obtain

$$E^{(-)}_\lambda = W_\lambda + M^{\rm on}_{\lambda\lambda}(\mathcal{E}_\lambda)/n(\lambda) = \mathcal{E}_\lambda, \quad \lambda \leq F. \tag{5.10}$$

The equality (5.7) or (5.10) holds not only for the exact energies, but also for any approximation which can be expressed in terms of a selection of "skeleton" diagrams, in Brandow's formulation; as always, the same diagrams are used for the binding energy and the mre.

Now there is a difficulty with the result (5.7). It is well known that in general, the orbitals ψ_α in (5.1) and (5.2) will not be orthogonal,[26, 27] and therefore the self-consistent potential U will not be Hermitian. Our formulation of the mre theory has assumed a complete basis of orthogonal orbitals. It is not therefore clear whether the equality (5.5) would also hold for a non-orthogonal basis.

The problem of non-orthogonality does not appear when conserved simple-particle quantum numbers are involved, like momentum for nuclear matter, or angular momentum in spherical nuclei. For principal (radial) quantum numbers, non-orthogonality appears. However, normally occupied orbits ($\lambda \leq F$) are orthogonal to unoccupied orbits ($\lambda > F$). In an approximation to the linked-cluster expansion, one may keep orthogonality by omitting $Q^{\rm on}_{\lambda\mu}$ connecting, e.g. different principal quantum numbers, thereby sacrificing complete radial self-consistency.

For a normally unoccupied orbit ($\lambda > F$) the mre and the self-consistent energy (5.3) differ. There is a one-to-one correspondence between the diagrams of 7(b) and 7(d), except for the potential $(-U_{\lambda\lambda})$ insertion diagram 7(e), which contributes to $M^{\rm on}_{\lambda\lambda}$ but not to $\Delta E(\lambda)$. Therefore [with the sign change between 7(b) and 7(d)]

$$\Delta E(\lambda) = -M^{\rm on}_{\lambda\lambda}(\mathcal{E}_\lambda) - U_{\lambda\lambda}, \quad \lambda > F \tag{5.11}$$

$$= -\sum_\mu Q^{\rm on}_{\lambda\mu}(\mathcal{E}_\lambda)(1 - P_{\mu\lambda}) - U_{\lambda\lambda},$$

$$\lambda > F, \tag{5.12}$$

where we use Brandow's "dressed propagator" in (5.12). For the self-consistent choice (5.3) the mre is found to be

$$E^{(-)}_\lambda = W_\lambda - U_{\lambda\lambda}/n(\lambda), \quad \lambda > F. \tag{5.13}$$

Alternatively, using (5.8) we may express the mre in the form

$$E^{(-)}_\lambda = W_\lambda - U_{\lambda\lambda} - [Q^{\rm on}_{\lambda\lambda}(\mathcal{E}_\lambda) + U_{\lambda\lambda}]\left[\frac{1 - n(\lambda)}{n(\lambda)}\right],$$

$$\lambda > F. \tag{5.14}$$

Clearly $E^{(-)}_\lambda$ is not identical with $\mathcal{E}_\lambda$ for $\lambda > F$. This difference is not unexpected; the mre is bounded above $E^{(-)}_\lambda < E_A - E_B$ (see Sec. 2), while $\mathcal{E}_\lambda$ is not. In general $\mathcal{E}_\lambda > \mathcal{E}_{\lambda'}$ for $\lambda > F$ and $\lambda' < F$. However, the self-consistent potential $U_{\lambda\lambda}$ for $\lambda > F$ is repulsive in general, as noted by Brandow[18]: The second term of (5.13) greatly decreases $E^{(-)}_\lambda$ below W_λ, since $n(\lambda) \ll 1$. A simple example of this effect was given in (4.16)–(4.18).

Finally, although $E^{(-)}_\lambda \neq \mathcal{E}_\lambda$ for $\lambda > F$, we may still consider $\mathcal{E}_\lambda$ to be measurable, since (5.14) may be reexpressed

$$E^{(-)}_\lambda = T_{\lambda\lambda} - (\mathcal{E}_\lambda - T_{\lambda\lambda})\left[\frac{1 - n(\lambda)}{n(\lambda)}\right] \tag{5.15}$$

and $E^{(-)}_\lambda$, $T_{\lambda\lambda}$, and $n(\lambda)$ can all be obtained from $P(\lambda, E)$ or $P(k, E)$.

6. RELATION TO GREEN'S FUNCTION THEORIES

Several authors[3, 9, 10] have approached the problem of removal energies through the theory of the Green's function for the propagation of a single hole in the target nucleus. Gross and Lipperheide[3] have outlined the formalism for calculating the spectral function in a linked-cluster expansion. This has been applied by Lipperheide and co-workers[8] for the hole spectra of ^{12}C and ^{16}O in various shell-model approximations. Dieperink, Brussaard, and Cusson[9] have shown how several differently defined hole energies, including the mre, may be obtained from the Green's function. Engelbrecht and Weidenmüller[10] have used a pole approximation to the Green's function to define a (complex) quasiparticle (or hole) energy for orbits.

The relation of the Green's function theory to the main subject of this paper is obtained by consideration of the self-energy function $\Sigma_{\lambda\mu}(E)$ (see, e.g. Ref. 21 or 28). In the linked-cluster approach one calculates Σ directly from a perturbation series; the Green's function and spectral function are then obtained from Σ. The diagrams for Σ are of the same type as those for *insertions* $M_{\lambda\mu}(E)$, which were discussed in Sec. 5 and illustrated in Fig. 6. However, the diagrams for Σ are irreducible in the sense that no block in Fig. 6 can be further divided into two blocks connected by a single particle or hole line. As remarked above (5.1), the class of diagrams included in $Q^{\rm on}(E)$ may include diagrams which are reducible in this sense. If one defines an on-shell self-energy $\Sigma^{\rm on}$ as in Ref. 10, it is represented by the subset of irreducible (in the Green's function sense) $Q^{\rm on}$ diagrams. (That $Q^{\rm on}$ and $\Sigma^{\rm on}$ are not identical has been noted in Refs. 10 and 18.)

Consider the function $P^{\rm on}(\lambda, E)$, which we take to

be the spectral function calculated (e.g. in the formulation of Ref. 3) with the self-energy function chosen to be

$$\Sigma^{(1)}_{\lambda\mu}(E) = Q^{\rm on}_{\lambda\lambda}(E)\delta_{\lambda\mu} \tag{6.1}$$

in the diagonal representation. It can be shown that (for $\lambda \leq F$)

$$P^{\rm on}(\lambda, E) = n(\lambda)\delta(E - \mathcal{E}_\lambda), \tag{6.2}$$

where $\mathcal{E}_\lambda$ is the self-consistent energy (5.8) or, equivalently, the mre, and $n(\lambda)$ the occupation probability (2.5). Clearly this approximate spectral function (6.2) has the correct centroid (2.6), although it does not have the correct functional dependence on E. However, the approximation

$$\Sigma^{(2)}_{\lambda\mu}(E) = \Sigma^{\rm on}_{\lambda\lambda}(E)\delta_{\lambda\mu} \tag{6.3}$$

leads to a spectral function, similar in form to (6.2), but with the singular points at energies different from $\mathcal{E}_\lambda \equiv E^{(-)}_\lambda$. The difference may be thought of as an induced effect of $\Sigma^{\rm off}$ on the centroids, which enters in the "interference terms" $\Sigma^{(1)} - \Sigma^{(2)} = Q^{\rm on} - \Sigma^{\rm on}$. These interference terms also complicate Brandow's counting of diagrams in his compact cluster theory (see Ref. 26, Appendix D). Since $\Sigma^{\rm off}$ does contribute to $Q^{\rm on}$, it does effect both the mre and the total binding energy E_A of the target.

The spreading of the full spectral function $P(\lambda,E)$ around the centroids is then due to the remainder of the self-energy function

$$\Delta\Sigma_{\lambda\mu}(E) \equiv \Sigma_{\lambda\mu}(E) - Q^{\rm on}_{\lambda\mu}(E). \tag{6.4}$$

This is not identical to $\Sigma^{\rm off}$, since (6.4) contains interference of $\Sigma^{\rm off}$ and $\Sigma^{\rm on}$.

In conclusion, if we divide the self-energy function $\Sigma = \Sigma^{(1)} + \Delta\Sigma$ (6.1) and (6.4) we find that $\Sigma^{(1)}$ contains the information necessary to determine the mre and total binding E_A, basically the ground-state properties of the target nucleus A. On the other hand $\Delta\Sigma$ contains information about the spectrum of the $A-1$ nucleus.

7. CONCLUDING REMARKS

We have tried to show in this paper in what ways the mean removal energy for particles is an interesting theoretical quantity, and how it may be determined within a theory of the target ground-state energy. There remains the large problem of the experimental measurement of this quantity, which lies beyond the scope of this work. Beside the question of the accuracy of the impulse approximation to the reaction theory, there are also the problems of limits of accuracy and of kinematical range of the experiments. One really wants to know more about the spectral function $P(\lambda, E)$ itself, for example: How far in E is the removal strength actually distributed? One recent approach to this question has been given by Dieperink and Brussaard[29] who have examined the second energy moment of $P(\lambda, E)$ (2.14) and (2.15).

Note added: Since the completion of this paper I have received a new work by Dr. L. Schäfer of Heidelberg, on the subject of the single-particle potential, in which he has independently obtained some of the results of Sec. 5. This work will appear in Nuclear Physics.

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APPENDIX

We prove that the sum rule

$$E_A = \sum_\lambda [W_\lambda n(\lambda) + \tfrac{1}{2}\Delta E(\lambda)] - \tfrac{1}{2}\langle A|\, U\,|A\rangle \tag{3.25}$$

holds for any linked-cluster approximation, in which each quantity in (3.25) is obtained from the same set of diagrams (which define the approximation) by the methods of Sec. 3. We first subtract the unperturbed energy $E_0 = \sum_{\lambda\leq F} W_\lambda$ from both sides to obtain

$$\Delta E_A = \sum_{\lambda\leq F} W_\lambda[n(\lambda) - 1] + \sum_{\lambda > F} W_\lambda n(\lambda) + \frac{1}{2}\sum_\lambda \Delta E(\lambda) - \tfrac{1}{2}\langle A|\, U\,|A\rangle. \tag{A1}$$

We shall prove (A1) for a single, general diagram, whose value is denoted by (3.13); the sum follows directly. We label with x the contributions of this diagram to the various terms of (A1). As before, the diagram has ρ hole lines and σ particle lines. If it has n interactions V and m interaction $(-U)$, then $\rho + \sigma = 2n + m$.

For the left side of (A1) we have, from (3.14)

$$\Delta E^x_A = \sum_{\alpha\leq F}\sum_{\beta > F} D^x(\alpha_1 \cdots \beta_\sigma). \tag{A2}$$

For the right side we have, from (3.21)–(3.23)

$$\sum_{\lambda\le F} W_\lambda[n^x(\lambda)-1]+\sum_{\lambda>F} W_\lambda n^x(\lambda)$$
$$=\sum_\lambda W_\lambda \sum_{\alpha\le F}\sum_{\beta>F}\left(-\sum_{i=1}^{\rho}\delta_{\lambda,\alpha_i}+\sum_{j=1}^{\sigma}\delta_{\lambda,\beta_j}\right)\sum_q \frac{D^x(\alpha_1\cdots\beta_\sigma)}{d_q}. \tag{A3}$$

Note that the denominator d_q, and the range of the insertion index q, depend on which line α_i or β_j carries the λ label in the $i-$ or $-j$ sum. We may rewrite (A3) by changing order of summation

$$\sum_\lambda W_\lambda \sum_{\alpha\le F}\sum_{\beta>F}\sum_{p=1}^{m+n-1}\left(-\sum_{i_p}\delta_{\lambda,\alpha_i}+\sum_{j_p}\delta_{\lambda,\beta_j}\right)\frac{D^x(\alpha_1\cdots\beta_\sigma)}{d_p}, \tag{A4}$$

where p specifies the insertion level with respect to the whole diagram D^x, and d_p denotes the denominator (3.21) at that level. Since the diagram has $m+n$ interactions, there are $m+n-1$ denominators [see (3.7)]. The sum on i, j are then restricted to those lines which appear at the level of the insertion [i.e., in (3.21)]. Performing the λ sum in (A4) eliminates the denominators d_p:

$$\sum_{\alpha\le F}\sum_{\beta>F}\sum_{p=1}^{m+n+1}\{-d_p\}\frac{D^x(\alpha_1\cdots\beta_\sigma)}{d_p} \tag{A5}$$

and the p sum yields only a factor of $(m+n-1)$. Comparing this result with (A2) we have

$$\sum_{\lambda\le F} W_\lambda[n^x(\lambda)-1]+\sum_{\lambda>F} W_\lambda n^x(\lambda)=-(m+n-1)\Delta E_A^x. \tag{A6}$$

From (3.15)–(3.19) we have

$$\tfrac{1}{2}\Delta E^x(\lambda)=\tfrac{1}{2}(\rho+\sigma)\Delta E_A^x. \tag{A7}$$

Finally we must evaluate the contribution to the expectation value $\langle U\rangle$ from the diagram D^x. Comparison of (3.8) with $M=U$, with (3.7), leads to

$$-\tfrac{1}{2}\langle A|\,U\,|A\rangle=\tfrac{1}{2}m\Delta E_A^x \tag{A8}$$

since $(-U)$ appears m times in (3.7).

Then the right-hand side of (A1) is obtained by adding (A6)–(A8) to get

$$[-(m+n-1)+(n+\tfrac{1}{2}m)+\tfrac{1}{2}m]\,\Delta E_A^x=\Delta E_A^x \tag{A9}$$

using $\rho+\sigma=2n+m$. This proves (A1) and (3.25).

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