ON THE RE-ARRANGEMENT ENERGY
OF THE NUCLEAR MANY-BODY PROBLEM

M. E. GRYPEOS

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M.E. Grypeos

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Mittelstaedt's definition of the re-arrangement energy, which is related to many-body calculations for the separation energy of a particle by means of model wave functions, is extended in a straightforward manner to the case in which a trial many-body wave function is used. The "trial re-arrangement energy" so defined is studied in the case of the separation of a particle s from a system of A + 1 particles in which the A particles (nucleons) are not identical to the s. In this treatment a Jastrow-like trial wave function is used. Some general properties of this trial re-arrangement energy are derived and the first term of its cluster expansion is given in the case in which the A nucleons form an infinite nuclear matter of density \( \rho \). Numerical estimates of this first order term are performed for a case of physical interest.
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1. INTRODUCTION

The re-arrangement energy enters as a contribution, in addition to the kinetic and potential energy, to the corresponding energy expressions of various processes in nuclear physics as, for example, the separation of a particle from a system of particles. Other such processes are the excitation of a particle or the scattering of a particle by a system. The re-arrangement energy is usually discussed in connection with Brueckner's theory in which perturbation many-body techniques are used \(^1,2\).

A comprehensive definition of the concept of re-arrangement energy has been given by Mittelstaedt (see ref. 3). Mittelstaedt's definition is independent of perturbation theory and refers to calculations in which model nuclear many-body wave functions \(\Phi\) are used, in which case the energy quantities are not expressed as expectation values but by means of the model wave functions \(\Phi\) and the actual wave functions \(\Psi\). In the next section we briefly review Mittelstaedt's definition, employing this approach, which is very suitable as a starting point for perturbation calculations.

Perturbation techniques are not the only means of treating many-body problems. Variational techniques have proved quite useful in a variety of many-body problems. In particular, short-range correlations of the nuclear many-body problem have been treated in a promising way by applying cluster expansion-variational techniques. The basic quantity in these techniques is a trial many-body wave function. In Sec. 3 Mittelstaedt's definition of the re-arrangement energy (connected to the process of the separation of a particle from a system) is extended to the case in which a trial many-body wave function is employed. Using this definition and a JASTROW-like \(^4,5\) many-body trial wave function, we investigate the properties of the "trial re-arrangement energy" \(\Delta[\Psi^{tr}]\) which corresponds to the separation of a particle \(s\) from a system of \(A+1\) particles, in which the rest \(A\) particles (nucleons) are not identical to the \(s\). Namely, we show that this trial re-arrangement energy is
positive (or zero, if there were no correlations between the particle and the nucleons) and also that it does not depend explicitly upon the interparticle potentials. Finally, in the last section, we consider the case in which the \( A \) nucleons form an infinite nuclear matter of density \( \rho \) and we give the first-order term of the cluster expansion of \( \Delta \Psi \). This term, which is proportional to \( \rho \), is estimated in the case where the separated particle is a \( \Lambda \) particle in its ground state in nuclear matter. A variation calculation connected with this problem has been performed during the last few years\(^6\).

2. **THE MODEL RE-ARRANGEMENT ENERGY**

Let us consider a many-body system consisting of \( A \) particles (nucleons). The Hamiltonian of this system is taken to be

\[
H_A = T_A + V_A = \sum_{i=1}^{A} t_i + \frac{1}{2} \sum_{i,j}^{A} V_{ij}
\]

(1)

The actual ground state wave function of the system satisfies the Schrödinger equation

\[
H_A \Psi_A = E_A \Psi_A
\]

(2)

In order to calculate the energy \( E_A \), it has been shown convenient in many cases to introduce a model wave function \( \Phi_A \) of such a kind that \( \Psi_A \) can be normalized by \( \langle \Phi_A \mid \Psi_A \rangle = 1 \). Then the energy can be written\(^3\)

\[
E_A = \langle \Phi_A \mid H_A \mid \Psi_A \rangle
\]

(3)

Consider now the process of the separation of a particle from a system of \( A + 1 \) particles. We shall indicate by \( s \) that particle among the \( A + 1 \) particles which is separated. In the present paper we shall concern ourselves with separation processes.
The Hamiltonian operator for particle \( s \) is:

\[
H_s = t_s + \sum_{i=1}^{A} v_{si}
\]

its separation energy is \( -E(s) \) , where

\[
E(s) = E_{A+1} - E_A
\]

\( E_{A+1} \) and \( E_A \) are the energies of the systems of \( A + 1 \) particles and \( A \) particles, respectively. We can write eq. (5) as follows:

\[
E(s) = \langle \Phi_{A+1} | H_A + H_s | \Psi_{A+1} \rangle - \langle \Phi_A | H_A | \Psi_A \rangle \Omega_{A+1}
\]

where \( \Omega_{A+1} \) and \( \Omega_A \) are the corresponding normalization volumes. For simplicity we shall omit these in the following.

\( E(s) \) can be written

\[
E(s) = \langle \Phi_{A+1} | H_s | \Psi_{A+1} \rangle + \Delta
\]

where

\[
\Delta = \langle \Phi_{A+1} | H_A | \Psi_{A+1} \rangle - \langle \Phi_A | H_A | \Psi_A \rangle
\]

The quantity \( \Delta \) defined above, which depends on the model wave functions \( \Phi \) : \( \Delta = \Delta[\Phi] \), is the model re-arrangement energy.

Mittelstaedt has separated \( \Delta \) into a kinetic and potential re-arrangement energy part:

\[
\Delta = \Delta_k + \Delta_p
\]
where

$$\Delta_k = \sum_{i=1}^{A} [\langle \Phi_{A+i} | t_i | \Psi_{A+i} \rangle - \langle \Phi_{A} | t_i | \Psi_{A} \rangle]$$

(10)

and

$$\Delta_p = \frac{1}{2} \sum_{i,j}^{A} [\langle \Phi_{A+i} | v_{ij} | \Psi_{A+i} \rangle - \langle \Phi_{A} | v_{ij} | \Psi_{A} \rangle]$$

(11)

In the special case of infinite nuclear matter ($A \rightarrow \infty$ and $\Omega_{A} \rightarrow 0$ such that the density $\rho = \frac{A}{\Omega_{A}}$ is constant) one can express $\Delta$ as follows:

$$\Delta = \sum_{i=1}^{A} \frac{2}{\beta A} \langle \Phi_{A} | t_i | \Psi_{A} \rangle + \frac{1}{2} \sum_{i,j}^{A} \frac{2}{\beta A} \langle \Phi_{A} | v_{ij} | \Psi_{A} \rangle$$

(12)

3. THE TRIAL RE-ARRANGEMENT ENERGY

As we have pointed out in the introduction, one can in many cases apply the variational principle in calculating energy quantities and, for this purpose, matrix elements with respect to a trial many-body wave function are used. Considering again the process of the separation of a particle $s$ from a system of $A + 1$ particles, we can write* for the trial expression of the separation energy

$$E_{(s)}^{tr} = \frac{\langle \Psi_{A+1}^{tr} | H_A + H_s | \Psi_{A+1}^{tr} \rangle}{\langle \Psi_{A+1}^{tr} | \Psi_{A+1}^{tr} \rangle} - \frac{\langle \Psi_{A} | H_A | \Psi_{A} \rangle}{\langle \Psi_{A} | \Psi_{A} \rangle}$$

(13)

or

$$E_{(s)}^{tr} = \frac{\langle \Psi_{A+1}^{tr} | H_s | \Psi_{A+1}^{tr} \rangle}{\langle \Psi_{A+1}^{tr} | \Psi_{A+1}^{tr} \rangle} + \Delta [\Psi_{s}^{tr}]$$

(14)

where the "trial re-arrangement energy" is defined by

* We have added the superscript tr to indicate that we are considering a trial many-body function in the calculation.
We must emphasize that $\Delta[\psi^{tr}]$ depends on the particular trial wave function we consider. In calculating the trial re-arrangement energy, a trial many-body wave function of the Jastrow type, which allows for correlations between pairs of particles, may be used.

In the following we shall consider the trial re-arrangement energy in the case in which the separated particle $s$ is not identical to the rest $A$ particles (nucleons). The trial wave function of the system of $A + 1$ particles, one of which is the $s$, will be taken to be

$$
\psi^{tr}_{A+1} = \psi^A \prod_{i=1}^{A} f(r_{si}) \varphi(s)
$$

(16)

$\varphi(s)$ is the single-particle wave function for the $s$. The functions $f(r_{si})$ which allow for correlations between the $s$ and the nucleons, must be such that they tend to unity if the distances between the $s$ and each nucleon tend to infinity. Also they must be equal to zero inside and at the hard core radius if a hard core exists in the potential between the $s$ and each nucleon. In the following when we write $\Delta[\psi^{tr}]$ we shall mean the trial re-arrangement energy with respect to the trial wave function (16). With this wave function we can easily calculate the numerator in the first term of the r.h.s. of (15).

The internucleon potential $V_A$ "does not couple" the particle $s$ and the nucleons (we assume that $\prod_{i=1}^{A} f(r_{si})$ commutes with $V_A$):

$$
\langle \psi^{tr}_{A+1} | V_A | \psi^{tr}_{A+1} \rangle = \int |\varphi(s)|^2 \prod_{i=1}^{A} f(r_{si}) \psi^A_V \psi^A d\vec{r}_s d\vec{r}_1 \ldots d\vec{r}_A
$$

(17)

On the other hand $T_A$ does couple. If we put
we can write

$$X_s = \frac{A}{\prod_{i=4}^{\text{ }} f(r_{i3})}$$

(18)

$$\left< \Psi_{A+4}^{t_r} \right| T_A \left| \Psi_{A+4}^{t_r} \right> = (-\frac{1}{2m_N}) \int |\phi(s)|^2 \left\{ \sum_{i=4}^{A} \left[ |\Psi_A|^2 X_s \nabla_i^2 X_s + X_s^2 \Psi_A^* \nabla^2 \Psi_A + \frac{1}{2} \nabla_i X_s \cdot \nabla_i |\Psi_A|^2 \right] \right\} \, d\vec{r}_S \, d\vec{r}_i \cdots d\vec{r}_A$$

(19)

where \( m_N \) is the nucleon mass.

From (17) and (19) we obtain

$$\left< \Psi_{A+4}^{t_r} \right| H_A \left| \Psi_{A+4}^{t_r} \right> = \int |\phi(s)|^2 \left\{ X_s \Psi_A^* \left[ T_A + V_A \right] \Psi_A \, d\vec{r}_S \, d\vec{r}_i \cdots d\vec{r}_A + \right.$$  

$$+ (-\frac{1}{2m_N}) \int |\phi(s)|^2 \left\{ \sum_{i=4}^{A} \left[ |\Psi_A|^2 X_s \nabla_i^2 X_s + \frac{1}{2} \nabla_i X_s \cdot \nabla_i |\Psi_A|^2 \right] \right\} \, d\vec{r}_i \, d\vec{r}_i \cdots d\vec{r}_A$$

(20)

Taking into account that

$$\nabla_i^2 X_s = \left[ \nabla_i^2 f(r_{i3}) \right] \cdot \prod_{k=1}^{A} f(r_{sk})$$

(21)

and introducing the function

$$B(r_S, r_i) = \left| \phi(s) \right| \int |\Psi_A|^2 \left( \prod_{i=4}^{A} f(r_{i3}) \right) \, d\vec{r}_i \cdots d\vec{r}_A$$

(22)
we can write expression (20) as follows:

$$\langle \Psi_{A^t}^{tr} | H_A | \Psi_{A^t}^{tr} \rangle = E_A \langle \Psi_{A^t}^{tr} | \Psi_{A^t}^{tr} \rangle + \left( -\frac{\hbar^2}{2m_n} \right) A \left[ \int_1 f_{(r_{s_i})} \nabla_i^2 f_{(r_{s_i})} \right] .$$

Substituting this into expression (15) and applying Green's theorem we find:

$$\Delta [\Psi^{tr}] = \left( -\frac{\hbar^2}{2m_n} \right) \frac{A}{\langle \Psi_{A^t}^{tr} | \Psi_{A^t}^{tr} \rangle} \left[ \int_1 \nabla_i^2 f_{(r_{s_i})} - \frac{1}{2} \nabla_i^2 f_{A} \right] B_{r_{s_i}, r_{s_i}'} d_{r_{s_i}}^2 d_{r_{s_i}'} d_{r_{A}}^2 \quad (24)$$

Using the identity

$$\frac{1}{2} \nabla_i^2 f^2 = \nabla_i (f \nabla_i f) = (\nabla_i f)^2 + f \nabla_i^2 f \quad (25)$$

we easily obtain the following expression for $\Delta [\Psi^{tr}]$:

$$\Delta [\Psi^{tr}] = \left( -\frac{\hbar^2}{2m_n} \right) \frac{A}{\langle \Psi_{A^t}^{tr} | \Psi_{A^t}^{tr} \rangle} \left[ \int_1 \nabla_i^2 f_{(r_{s_i})} \Psi_A^2 \left( \nabla_i f(r_{s_i}) \right)^2 \prod_{i=2}^A f_{(r_{n_i})} d_{r_{s_i}}^2 d_{r_{s_i}'} d_{r_{A}}^2 \quad (26)$$

We can therefore conclude the following:

i) $\Delta [\Psi^{tr}] \equiv 0$. The equality holds if there were no correlations between the particle $s$ and the nucleons in the trial wave function.

ii) The trial re-arrangement energy $\Delta [\Psi^{tr}]$ does not depend explicitly upon the interparticle potential. However, there is an implicit
dependence since the form of the correlation functions depends upon the interparticle potential.

From these properties we see that $\Delta\{\psi^{+}\}$ is of correlation nature. It is a contribution to $E^{\nu}_s$ due to the action of the kinetic energy operator of the $A$ particle system on the correlation functions $f_{r_{k}}$.

In view of these remarks it would perhaps be appropriate to characterize $\Delta\{\psi^{+}\}$ as "additional kinetic correlation energy". The other kinetic energy contributing to $E^{\nu}_s$ comes from the kinetic energy operator of the separated particle.

4. INFINITE NUCLEAR MATTER

Expression (26) for $\Delta\{\psi^{+}\}$ can be expanded as a power series of the constant density $\rho$ of the infinite nuclear matter in the case in which the $A$ nucleons form such a medium. The first term of this expansion can be easily obtained, while the others are more complicated and additional approximations seem necessary.

If we use the cluster expansion

$$\prod_{i=1}^{A} f_{r_{i}}^{2} \equiv \prod_{i=1}^{A} (1 + F_{r_{i}}) = 1 + \sum_{i=1}^{A} F_{r_{i}} + \sum_{i<j}^{A} F_{r_{i}} F_{r_{j}} + \cdots$$

in the nominator and denominator of (26) and introduce the so-called (configurational) "generic distribution functions"

$$\eta_{h}(\vec{r}_{1}, \ldots, \vec{r}_{h}) = \frac{A!}{(A-h)!} \frac{\int |\Psi_{A}|^{2} d^{3}r_{h+1} \cdots d^{3}r_{A}}{\int |\Psi_{A}|^{2} d^{3}r_{1} \cdots d^{3}r_{A}}$$

that is, in our case,

$$\eta_{1}(\vec{r}_{1}) = A \frac{\int |\Psi_{A}|^{2} d^{3}r_{2} \cdots d^{3}r_{A}}{\int |\Psi_{A}|^{2} d^{3}r_{1} \cdots d^{3}r_{A}} = e$$
we obtain for the "first-order trial re-arrangement energy":

\[
\Delta^{(1)}_{\Lambda^+} = \rho \left( \frac{\hbar^2}{2m_\rho} \right) \int (\nabla f(r_{\Lambda^+}))^2 \, d\tau_{\Lambda^+} \tag{30}
\]

A numerical estimate of this can be given in the case of a \( \Lambda \) particle in its ground state in nuclear matter. A variational calculation of the first-order term of \( E_{(\Lambda)}^{(1)} \) has been performed\(^6\). Using for the \( \Lambda \)-nucleon interaction the DOWNS-WARE potential\(^8\),

\[
\mathcal{V}_{\Lambda N}(r_{\Lambda^+}) = \begin{cases} 
\infty, & r_{\Lambda^+} \leq \xi = 0.4 \, fm \\
(-334 \, MeV) e^{-3.219(r_{\Lambda^+} - \xi)} , & r_{\Lambda^+} > \xi 
\end{cases} \tag{31}
\]

and for the \( f \)

\[
\{f(r_{\Lambda^+}) = \begin{cases} 
0, & r_{\Lambda^+} \leq \xi \\
1 - e^{-\alpha(r_{\Lambda^+} - \xi)}, & r_{\Lambda^+} > \xi \tag{32}
\end{cases}
\]

we find

\[
\Delta^{(1)}_{\Lambda^+} = 30.6 \, MeV \tag{33}
\]

This value corresponds to \( \rho = 0.172 \) nucleon/(fermi)\(^3\) and \( \alpha = 2.18 \)

which minimizes the first-order term in the expression for \( E_{(\Lambda)}^{(1)} \) of DOWNS and CHYFEOS\(^6\)

\[
E_{(\Lambda)}^{(1)} = \rho \int [f(r_{\Lambda^+}) H_{\Lambda^+} f(r_{\Lambda^+})] \, d\tau_{\Lambda^+} \tag{34}
\]

If we use for the \( f \)

\[
-10-
\]
\[
\begin{align*}
\mathcal{f}(x) &= \begin{cases} 
0 & r_n < c \\
\left[1 - e^{-\alpha(r_n - c)} \right] \left[1 + \xi e^{-\alpha(r_n - c)} \right], & r_n > c
\end{cases} 
\end{align*}
\] (35)

in which \( \xi \) is determined by the condition

\[
e \int F(x) \, dF(x) = 0
\] (36)

which is a possible way of achieving reasonably rapid convergence of the cluster expansion\(^6\), we find

\[
\Delta^{(f)}_{\Lambda} = 32.4 \text{ MeV}
\] (37)

This corresponds to the same value of \( \xi \) and to \( \alpha = 0.92 \), which minimizes (34) with expression (35) for the \( f \).

In the variational calculation of the binding energy of a \( \Lambda \)-particle in nuclear matter\(^6\), \( \Delta[\psi^{\Lambda}] \) enters as an additional contribution but it was not calculated separately. In particular, its first-order part \( \Delta^{(f)}_{\Lambda} \) was combined with the corresponding first-order terms coming from the Hamiltonian operator of the \( \Lambda \)-particle in order to derive expression (34) which shows that \( F^{(f)}_{\Lambda} \) depends on the relative motion of a \( \Lambda \)-nucleon pair.

Investigations of the \( \Lambda \)-nuclear matter problem by methods different from the cluster expansion-variational one have been done and in the early version of these investigations, which were based on Brueckner's independent pair approximation, and in particular on a solution of the Bethe-Goldstone equation, the corresponding re-arrangement energy correction was neglected\(^{10,8} \). These were considered by DABROWSKI and KÖHLER\(^11\). The re-arrangement energy which enters in this approach was studied by means of Brueckner's reaction matrix \( K \) and was calculated separately as an additional correction. In particular, it was split into two terms, the "particle" and the "hole re-arrangement energy", of which the last one contributes mostly.\(^{14} \)

* This is appropriate to the central density in heavy nuclei\(^9\).
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