

A NON-UNITARY MODEL OPERATOR APPROACH TO TWO-PARTICLE CORRELATIONS IN FINITE NUCLEI *

by

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Abstract: *In this paper a model operator-variational approach is considered for the determination of the two-particle correlations in finite nuclei. The essential difference from some other work is that the model operator is not assumed to be (left) unitary. Two different expressions for the two-body part in a cluster expansion of the energy functional $(\Delta E)_2$ are firstly obtained and a variational method with a separation condition is subsequently applied. Finally, a formula is derived, which can be used directly in order to obtain numerical results for the ground state energy of the He^4 nucleus.*

1. INTRODUCTION

It is well known that two basic approaches have been developed for the nuclear many-body problem. The first is the reaction matrix theory developed mainly by Brueckner, Goldstone and others^{1,2}. This approach is the most fully explored and has been simplified with the Moszkowski and Scott separation method³ and the reference spectrum method of Bethe, Brandow and Petschek⁴. The second is the variational approach⁵.

In the present paper we follow the latter approach and we use a model operator, which however is not assumed to be (left) unitary, as it has been done in some other investigations⁶⁻⁹.

In the second section, the factor-cluster expansion¹⁰ for the energy expectation value of a finite nucleus is employed and two general expressions are given for its one body and two-body part. The variational principle is also applied and the «separation condition» is used. In this way coupled Euler equations are obtained for the correlated, relative two-nucleon wave functions. Finally in section 3t he simplest possible case, that is the calculation of the binding energy of the He^4 nucleus, is discussed.

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2. TWO GENERAL EXPRESSIONS FOR $\langle E \rangle$ AND APPLICATION OF THE VARIATIONAL PRINCIPLE

If we denote the model operator, which introduces short-range correlations by F , an eigenstate Φ of the model system corresponds to an eigenstate

$$\Psi = F\Phi \quad (1)$$

of the true system.

We can choose the operator F in such a way that the model eigenfunction Φ may be well approximated by a single Slater determinant (or a linear combination of a few Slater determinants). Short-range correlations are introduced by the model operator F .

Several restrictions are also made on the model operator, as for example that it depends only on the spins, isospins and relative coordinates and momenta of the particles in the system, it is a scalar with respect to rotations e.t.c. ⁷⁾. The (left) unitarity requirement, however, is not made in the present investigation. Because of the various restrictions on F , Ψ is no longer the true wave function of the system, but can only be considered as trial wave function.

The correlation operator will be determined in this paper by varying the energy expectation value:

$$\langle E \rangle = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Phi | F^+ H F | \Phi \rangle}{\langle \Phi | F^+ F | \Phi \rangle} = \frac{\langle \Phi | \tilde{H} | \Phi \rangle}{\langle \Phi | F^+ F | \Phi \rangle} \quad (2)$$

where

$$H = \sum_{i=1}^A t_i + \sum_{i < j}^A v_{ij} \quad (3)$$

$$t_i = \sum_{i=1}^A \left(-\frac{\hbar^2}{2m} \nabla_i^2 \right)$$

v_{ij} is the two body interaction, which is assumed to be central and $\tilde{H} = F^+ H F$ the effective Hamiltonian for the model system.

We shall use a factor-cluster expansion for the energy expectation value $\langle E \rangle$ of a nucleus, consisting of A nucleons and we shall apply the variational principle by keeping in the cluster expansion the one-body and two-body terms. Two general expressions will be obtained, which will be varied.

The first expression is obtained if we consider the generalized normalization integral

$$I(\beta) = \langle \Psi | e^{\beta(\mathbf{H} - \langle \mathbf{T} \rangle)} | \Psi \rangle \quad (4)$$

corresponding to the quantity $(\mathbf{H} - \langle \mathbf{T} \rangle)$ where $\langle \mathbf{T} \rangle$ is the expectation value of the kinetic energy of the ground state in the independent particle model, which is chosen to be the oscillator shell model.

From equations (2) and (4) we obtain the formula

$$\langle E \rangle = \langle \mathbf{T} \rangle + \left. \frac{\partial}{\partial \beta} \ln I(\beta) \right|_{\beta=0} \quad (5)$$

The cluster analysis of (5) begins with the definition of subnormalization integrals, analogous to (4) for the subsystems of the A-nucleon system ¹⁰⁾

$$\begin{aligned} I_i(\beta) &= \langle i | \mathbf{F}_i^+ \exp\{\beta(t_i - \langle t_i \rangle)\} \mathbf{F}_i | i \rangle \\ I_{ij}(\beta) &= \langle ij | \mathbf{F}_{12}^+ \exp\{\beta(t_1 + t_2 + v_{12} - \langle t_i \rangle - \langle t_j \rangle)\} \mathbf{F}_{12} | ij - ji \rangle \\ I_{ijk}(\beta) &= \langle ijk | \mathbf{F}_{123}^+ \exp\{\beta(t_1 + t_2 + t_3 + v_{12} + v_{23} + v_{31} - \langle t_i \rangle - \\ &\quad - \langle t_j \rangle - \langle t_k \rangle)\} \cdot \mathbf{F}_{123} | ijk - ikj + jki - jik + kij - kji \rangle \\ &\cdot \\ &\cdot \\ &\cdot \\ I_{i_1 \dots i_A} &= I(\beta) \end{aligned} \quad (6)$$

Next, a factor-cluster decomposition of the above subnormalization integrals is made ^{10,11)}

$$\begin{aligned} I_i &= Y_i \\ I_{ij} &= Y_i Y_j Y_{ij} \\ I_{ijk} &= Y_i Y_j Y_k Y_{ij} Y_{jk} Y_{ki} Y_{ijk} \\ &\cdot \\ &\cdot \\ &\cdot \\ I_{i_1 \dots i_A} &= I = \prod_i Y_i \cdot \prod_{i < j} Y_{ij} \cdot \prod_{i < j < k} Y_{ijk} \dots Y_{i_1 \dots i_A} \end{aligned} \quad (7)$$

Inserting the last of the relations (7) into (5) we obtain the factor-cluster expansion for the energy expectation value:

$$\langle E \rangle = \langle T \rangle + (\Delta E)_1 + (\Delta E)_2 + \dots + (\Delta E)_A \quad (8)$$

where

$$\begin{aligned} (\Delta E)_1 &= \left. \sum_{i=1}^A \frac{\partial}{\partial \beta} \ln Y_1 \right|_{\beta=0} = \left. \sum_{i=1}^A \frac{\partial}{\partial \beta} \ln I_1(\beta) \right|_{\beta=0} = 0 \\ (\Delta E)_2 &= \left. \sum_{i < j}^A \frac{\partial}{\partial \beta} \ln Y_{ij} \right|_{\beta=0} = \left. \sum_{i < j}^A \left[\frac{1}{I_{ij}} \frac{\partial I_{ij}}{\partial \beta} - \left(\frac{1}{I_i} \frac{\partial I_i}{\partial \beta} + \frac{1}{I_j} \frac{\partial I_j}{\partial \beta} \right) \right] \right|_{\beta=0} = \\ &= \sum_{i < j}^A \frac{\langle ij | \mathbf{F}_{12}^+ (\mathbf{t}_1 + \mathbf{t}_2 + v_{12} - \langle \mathbf{t}_i \rangle - \langle \mathbf{t}_j \rangle) \mathbf{F}_{12} | ij - ji \rangle}{\langle ij | \mathbf{F}_{12}^+ \mathbf{F}_{12} | ij - ji \rangle} \quad (9) \end{aligned}$$

We do not write the expressions of the three-body and many-body terms, because it is assumed that these terms will give small contribution to the energy expectation value. This assumption would be reasonable provided that the correlations introduced by \mathbf{F} are of short range.

Calculations of the two-particle matrix elements of the two-body part $(\Delta E)_2$ of the effective Hamiltonian can be simplified by making a transformation to relative coordinates of the two interacting nucleons. We can write

$$\mathbf{t}_1 + \mathbf{t}_2 = \mathbf{t}_r + \mathbf{t}_R \quad (10)$$

where \mathbf{t}_r , is the relative kinetic energy operator of the two nucleons and \mathbf{t}_R , their centre of mass kinetic energy operator.

Substituting, now, (10) into (9), we get the following expression for $(\Delta E)_2$

$$(\Delta E)_2 = \sum_{i < j}^A \frac{\langle ij | \mathbf{v}'_{\text{eff}} | ij - ji \rangle + \langle ij | \mathbf{F}_{12}^+ \mathbf{t}_R \mathbf{F}_{12} | ij - ji \rangle}{\langle ij | \mathbf{F}_{12}^+ \mathbf{F}_{12} | ij - ji \rangle} \quad (11)$$

where

$$\mathbf{v}'_{\text{eff}} = \mathbf{F}_{12}^+ \left(\mathbf{t}_r + v_{12} - \frac{E_{n1}}{2} - \frac{E_{NL}}{2} \right) \mathbf{F}_{12} \quad (12)$$

Finally, following a procedure similar to that of reference 7, we can write the expression for $(\Delta E)_2$ as follows:

$$(\Delta E)_2 = \sum_{i < j}^A \left[\frac{\sum_{n_1 S} C_{n_1 S}^{ij} \langle n_1 S | v_{eff} | n_1 S \rangle}{\sum_{n_1 S} C_{n_1 S}^{ij} \langle \psi_{n_1 S} | \psi_{n_1 S} \rangle} + \frac{\sum_{n_1 S} \left[C_{(n, n+1)1S}^{ij} \langle \psi_{n_1 S} | \psi_{n+1,1S} \rangle + C_{(n, n-1)1S}^{ij} \langle \psi_{n_1 S} | \psi_{n-1,1S} \rangle \right]}{\sum_{n_1 S} C_{n_1 S}^{ij} \langle \psi_{n_1 S} | \psi_{n_1 S} \rangle} \right] \quad (13)$$

The notation in this formula is mostly as in ref. 7. The coefficients $C_{n_1 S}^{ij}$ are expressed in terms of Clebsch-Gordan and Talmi-Moshinsky-Smirnov coefficients¹²⁻¹⁵ :

$$C_{n_1 S}^{ij} = \sum_{\substack{NLM \\ m, M_s}} \left\langle \begin{matrix} n_1 l_1 m_1 \\ n_2 l_2 m_2 \end{matrix} \middle| \begin{matrix} NLM \\ nlm \end{matrix} \right\rangle \left\langle \frac{1}{2} \sigma_1 \frac{1}{2} \sigma_2 \middle| SM_s \right\rangle \left[\left\langle \begin{matrix} n_1 l_1 m_1 \\ n_2 l_2 m_2 \end{matrix} \middle| \begin{matrix} NLM \\ nlm \end{matrix} \right\rangle - (-1)^{l_1 - s} \left\langle \begin{matrix} n_2 l_2 m_2 \\ n_1 l_1 m_1 \end{matrix} \middle| \begin{matrix} NLM \\ nlm \end{matrix} \right\rangle \delta_{\tau_1 \tau_2} \right] \quad (14)$$

Similar are the expressions for the coefficients $C_{(n, n+1)1S}^{ij}$ and $C_{(n, n-1)1S}^{ij}$. These contain also matrix elements of the centre of mass kinetic energy operator in the oscillator shell model.

The effective potential v_{eff} is given by

$$v_{eff} = F_{12}^+ (\mathbf{t}_r + v_{12} - \frac{E_{n_1}}{2}) F_{12} \quad (15)$$

Before we proceed it is worth-mentioning that the expression for $(\Delta E)_2$ goes over the expression for the expectation value of the two-body part of the effective Hamiltonian used in ref. 7, if the operator F is taken to be (left) unitary.

If we vary $(\Delta E)_2$ with respect to the trial relative wave function $\psi_{n_1 S}$ (which is taken to be real) we find :

$$\delta(\Delta E)_a = \sum_{i < j}^A \left[\frac{C_{nls}^{ij}}{D^{ij}} \delta \langle nls | v_{eff} | nls \rangle + \frac{C_{(n, n+1)ls}^{ij} + C_{(n+1, n)ls}^{ij}}{D^{ij}} \delta \langle \psi_{nls} | \psi_{n+1, ls} \rangle + \frac{C_{(n, n-1)ls}^{ij} + C_{(n-1, n)ls}^{ij}}{D^{ij}} \delta \langle \psi_{nls} | \psi_{n-1, ls} \rangle - \frac{C_{nls}^{ij} N^{ij}}{(D^{ij})^2} \delta \langle \psi_{nls} | \psi_{nls} \rangle \right] \quad (16)$$

where the factors N^{ij} and D^{ij} are the numerator and the denominator in expression (13).

The condition for the stationarity of $(\Delta E)_2$ is therefore the following:

$$\delta[\langle nls | v_{eff} | nls \rangle + B_{n+1, ls} \langle \psi_{nls} | \psi_{n+1, ls} \rangle + B_{n-1, ls} \langle \psi_{nls} | \psi_{n-1, ls} \rangle - \epsilon_{nls} \langle \psi_{nls} | \psi_{nls} \rangle] = 0 \quad (17)$$

where the quantities:

$$B_{n+1, ls} = \frac{\sum_{i < j}^A (C_{(n, n+1)ls}^{ij} + C_{(n+1, n)ls}^{ij}) / D^{ij}}{\sum_{i < j}^A (C_{nls}^{ij} / D^{ij})} \quad (18a)$$

$$B_{n-1, ls} = \frac{\sum_{i < j}^A (C_{(n, n-1)ls}^{ij} + C_{(n-1, n)ls}^{ij}) / D^{ij}}{\sum_{i < j}^A (C_{nls}^{ij} / D^{ij})} \quad (18b)$$

$$\epsilon_{nls} = \frac{\sum_{i < j}^A [C_{nls}^{ij} N^{ij} / (D^{ij})^2]}{\sum_{i < j}^A (C_{nls}^{ij} / D^{ij})} \quad (19)$$

are considered to be constant in the variation.

It should be noted that each of the quantities $B_{n+1, ls}$, $B_{n-1, ls}$ and ϵ_{nls} depend on the correlated wave functions of the other relative states as well. These quantities are assumed to be calculated initially with

given correlated wave functions. Their values should be determined self-consistently.

The first matrix element in equation (17), can be written:

$$\begin{aligned} \langle n1S | v_{eff} | n1S \rangle &= \langle n1S | \mathbf{F}_{12}^+ (t_r + v_{12} - \frac{E_{n1}}{2}) \mathbf{F}_{12} | n1S \rangle = \\ &= \int_0^\infty \left[\frac{\hbar^2}{M} \left\{ \left(\frac{d\psi_{n1S}}{dr} \right)^2 + \frac{l(l+1)}{r^2} \psi_{n1S}^2 \right\} + v_{1S}(r) \psi_{n1S}^2 - \frac{E_{n1}}{2} \psi_{n1S}^2 \right] dr \quad (20) \end{aligned}$$

In the variational method with the separation condition, we assume that there are no correlations beyond a separation distance $d = d_{n1S}$. In other words, we assume

$$\psi_{n1S}(r) = \varphi_{n1}(r) \quad \text{for } r > d_{n1S} \quad (21)$$

Using this restriction and equation (20) we can write the bracket in equation (17) as follows:

$$\begin{aligned} M'_{n1S} &\equiv \langle n1S | v_{eff} | n1S \rangle + B_{n+1,1S} \langle \psi_{n1S} | \psi_{n+1,1S} \rangle + B_{n-1,1S} \langle \psi_{n1S} | \psi_{n-1,1S} \rangle - \\ &- \varepsilon_{n1S} \langle \psi_{n1S} | \psi_{n1S} \rangle = \int_0^{d_{n1S}} \left[\frac{\hbar^2}{M} \left(\left(\frac{d\psi_{n1S}}{dr} \right)^2 + \frac{l(l+1)}{r^2} \psi_{n1S}^2 \right) + \right. \\ &+ v_{1S}(r) \psi_{n1S}^2 - \frac{E_{n1}}{2} \psi_{n1S}^2 + B_{n+1,1S} \psi_{n1S} \psi_{n+1,1S} + B_{n-1,1S} \psi_{n1S} \psi_{n-1,1S} - \\ &- \varepsilon_{n1S} \psi_{n1S}^2 \left. \right] dr + \int_{d_{n1S}}^\infty \left[\frac{\hbar^2}{M} \left(\left(\frac{d\varphi_{n1}}{dr} \right)^2 + \frac{l(l+1)}{r^2} \varphi_{n1}^2 \right) + v_{1S}(r) \varphi_{n1}^2 - \right. \\ &- \frac{E_{n1}}{2} \varphi_{n1}^2 + B_{n+1,1S} \varphi_{n1} \varphi_{n+1,1} + B_{n-1,1S} \varphi_{n1} \varphi_{n-1,1} - \varepsilon_{n1S} \varphi_{n1}^2 \left. \right] dr \quad (22) \end{aligned}$$

We shall find the «stationary value» of $(\Delta E)_2$ by varying the relative two-body wave functions ψ_{n1S} with boundary conditions

$$\psi_{n1S}(c) = 0 \quad \text{and} \quad \psi_{n1S}(d_{n1S}) = \varphi_{n1}(d_{n1S}) \quad (23)$$

The first is due to the existence of the hard core in the internuclear potential while the second is due to restriction (21).

The Euler equation of our variational problem is

$$\begin{aligned}
& -\frac{\hbar^2}{M} \frac{d^2\psi_{n1S}}{dr^2} + \left[\frac{\hbar^2}{M} \frac{l(l+1)}{r^2} + v_{1S}(r) - \frac{E_{n1}}{2} - \epsilon_{n1S} \right] \psi_{n1S} = \\
& -\frac{B_{n+1,1S}}{2} \psi_{n+1,1S} - \frac{B_{n-1,1S}}{2} \psi_{n-1,1S} \quad (24)
\end{aligned}$$

It is clear that in the present approach the Euler equations, for the correlated, relative, wave functions are generally coupled.

Multiplying equation (24) by ψ_{n1S} and integrating from c to d_{n1S} we obtain the following expression for the $M_{n1S} \equiv \langle n1S | v_{eff} | n1S \rangle$, which appears in $(\Delta E)_2$:

$$\begin{aligned}
M_{n1S} = & \frac{\hbar^2}{M} \varphi_{n1}(d_{n1S}) \left[\psi'_{n1S}(d_{n1S}) - \varphi'_{n1}(d_{n1S}) \right] - \frac{E_{n1}}{2} \int_0^{d_{n1S}} \varphi_{n1}^2 dr + \\
& + \frac{\hbar^2}{M} \frac{1}{b^4} \int_0^{d_{n1S}} r^2 \varphi_{n1}^2 dr + \int_{d_{n1S}}^{\infty} v_{1S}(r) \varphi_{n1}^2 dr + \epsilon_{n1S} \int_c^{d_{n1S}} \psi_{n1S}^2 dr - \\
& - \frac{B_{n+1,1S}}{2} \int_c^{d_{n1S}} \psi_{n1S} \psi_{n+1,1S} dr - \frac{B_{n-1,1S}}{2} \int_c^{d_{n1S}} \psi_{n1S} \psi_{n-1,1S} dr \quad (25)
\end{aligned}$$

where $b = (2\hbar/M\omega)^{1/2}$ is the harmonic-oscillator parameter of the relative motion.

The second expression for $\langle E \rangle$, which we mentioned in the introduction is obtained by writing the Hamiltonian of the system in a different form. This is achieved by adding and subtracting the single particle potential $\sum_{i=1}^A v_i$, where

$$v_i = \frac{\hbar^2}{2M} \frac{r_i^2}{b_i^4} \quad \left(b_i = \left(\frac{\hbar}{M\omega} \right)^{1/2} \right) \quad (26)$$

Therefore, we have:

$$\mathbf{H} = \sum_{i=1}^A \mathbf{t}_i + \sum_{i < j} v_{ij} + \sum_{i=1}^A v_i - \sum_{i=1}^A v_i = \sum_{i=1}^A \mathbf{h}_i + \sum_{i < j} v_{ij}^{res} \quad (27)$$

where

$$\mathbf{h}_1 = \sum_{i=1}^A (\mathbf{t}_i + \nu_i) \quad \text{and} \quad \nu_{ij}^{\text{res}} = \nu_{ij} - \frac{1}{(A-1)} (\nu_i + \nu_j) \quad (28)$$

We consider subsequently the generalized normalization integral

$$\tilde{\Gamma}(\beta) = \langle \Psi | e^{\beta(\mathbf{H} - E_0)} | \Psi \rangle \quad (29)$$

corresponding to the quantity $(\mathbf{H} - E_0)$, where E_0 is the ground state energy in the chosen independent particle model:

$$\mathbf{H}_0 \Phi = E_0 \Phi, \quad \mathbf{H}_0 = \sum_i \mathbf{h}_i$$

From equations (2) and (29) we obtain the formula

$$\langle E \rangle = E_0 + \left. \frac{\partial}{\partial \beta} \ln \tilde{\Gamma}(\beta) \right|_{\beta=0} \quad (30)$$

The cluster analysis of (30) begins with the definition of subnormalization integrals, analogous to (29), for subsystems of the A-nucleon system

$$\begin{aligned} \tilde{\Gamma}_i(\beta) &= \langle i | \mathbf{F}_1^+ \exp\{\beta[\mathbf{h}_i - \varepsilon_i]\} \mathbf{F}_1 | i \rangle \\ \tilde{\Gamma}_{ij}(\beta) &= \langle ij | \mathbf{F}_{12}^+ \exp\left\{\beta \left[\mathbf{h}_1 + \mathbf{h}_2 + \nu_{12}^{\text{res}} - \varepsilon_i - \varepsilon_j \right] \right\} \mathbf{F}_{12} | ij - ji \rangle \\ \tilde{\Gamma}_{ijk}(\beta) &= \langle ijk | \mathbf{F}_{123}^+ \exp\left\{\beta \left[\mathbf{h}_1 + \mathbf{h}_2 + \mathbf{h}_3 + \nu_{12}^{\text{res}} + \nu_{23}^{\text{res}} + \nu_{31}^{\text{res}} - \varepsilon_i - \varepsilon_j - \varepsilon_k \right] \right\} \\ &\quad \cdot \mathbf{F}_{123} | ijk - ikj + jki - jik + kij - kji \rangle \\ &\vdots \\ \tilde{\Gamma}_{i_1 \dots i_A} &= \tilde{\Gamma}(\beta) \end{aligned} \quad (31)$$

where ε_i are the single particle energies in the chosen independent particle model.

Following the same steps as before we find

$$\langle E \rangle = E_0 + (\Delta \tilde{E})_1 + (\Delta \tilde{E})_2 + \dots + (\Delta \tilde{E})_A \quad (32)$$

where

$$(\Delta \tilde{E})_1 = 0$$

$$(\Delta \tilde{E})_2 = \sum_{i < j}^A \frac{\langle ij | \mathbf{F}_{12}^+ (\mathbf{h}_1 + \mathbf{h}_2 + \nu_{12}^{\text{res}} - \varepsilon_i - \varepsilon_j) \mathbf{F}_{12} | ij - ji \rangle}{\langle ij | \mathbf{F}_{12}^+ \mathbf{F}_{12} | ij - ji \rangle} \quad (33)$$

Calculations of the two-particle matrix elements of the two-body part $(\Delta \tilde{E})_2$ of the effective Hamiltonian can be simplified by making, as in the previous case, a transformation to relative and centre of mass coordinates of the two interacting nucleons. We can write

$$\mathbf{h}_1 + \mathbf{h}_2 = \mathbf{h}_r + \mathbf{h}_R \quad (34)$$

$$\varepsilon_1 + \varepsilon_j = \varepsilon_{n_1 i_1} + \varepsilon_{n_j j_j} = E_{n1} + E_{NL} \quad (35)$$

where \mathbf{h}_r , E_{n1} are the relative Hamiltonian and energy of the two nucleons while \mathbf{h}_R , E_{NL} their centre of mass Hamiltonian and energy (in the oscillator shell model). Also

$$\nu_r = \frac{\hbar^2}{M} \frac{r^2}{b^4} \text{ with } b = \left(\frac{2\hbar}{M\omega} \right)^{1/2} \quad (36)$$

$$\nu_R = \frac{\hbar^2}{4M} \frac{R^2}{b_R^4} \text{ with } b_R = \left(\frac{\hbar}{2M\omega} \right)^{1/2} \quad (37)$$

If we substitute (34) and (35) into (33), the contribution arising from the centre of mass Hamiltonian cancels with E_{NL} because of the restrictions made on the model operator \mathbf{F} . Therefore the matrix element which is the numerator of $(\Delta \tilde{E})_2$ becomes

$$\begin{aligned} & \langle ij | \mathbf{F}_{12}^+ (\mathbf{h}_1 + \mathbf{h}_2 + \nu_{12}^{\text{res}} - \varepsilon_i - \varepsilon_j) \mathbf{F}_{12} | ij - ji \rangle = \\ & = \langle ij | \mathbf{F}_{12}^+ \left(\mathbf{h}_r + \nu_{12} - \frac{\nu_r}{A-1} - E_{n1} \right) \mathbf{F}_{12} | ij - ji \rangle - \\ & \quad - \langle ij | \mathbf{F}_{12}^+ \frac{\nu_R}{A-1} \mathbf{F}_{12} | ij - ji \rangle \end{aligned} \quad (38)$$

Following a procedure similar to that of reference 7, we arrive at the following expression:

$$\begin{aligned}
 (\Delta \tilde{E})_2 = & \sum_{i < j}^A \left[\frac{\sum_{n1S} C_{n1S}^{ij} \langle n1S | \tilde{v}_{eff} | n1S \rangle}{\sum_{n1S} C_{n1S}^{ij} \langle \psi_{n1S} | \psi_{n1S} \rangle} + \right. \\
 & \left. + \frac{\sum_{n1S} \left[\tilde{C}_{(n,n+1)1S}^{ij} \langle \psi_{n1S} | \psi_{n+1,1S} \rangle + \tilde{C}_{(n,n-1)1S}^{ij} \langle \psi_{n1S} | \psi_{n-1,1S} \rangle \right]}{\sum_{n1S} C_{n1S}^{ij} \langle \psi_{n1S} | \psi_{n1S} \rangle} \right] \quad (39)
 \end{aligned}$$

where

$$\tilde{v}_{eff} = \mathbf{F}_{12}^+ \left(\mathbf{h}_r + v_{12}(r) - \frac{1}{A-1} v_r - \frac{1}{A-1} \frac{E_{NL}}{2} - E_{n1} \right) \mathbf{F}_{12} \quad (40)$$

The coefficients are of similar structure with those in the previous case.

The $\tilde{C}_{(n,n+1)1S}^{ij}$ and $\tilde{C}_{(n,n-1)1S}^{ij}$ contain now a matrix element of the centre of mass potential energy operator in the oscillator shell model.

Finally, following the same procedure as before we get the following condition for the stationarity of $(\Delta \tilde{E})_2$:

$$\begin{aligned}
 \delta [\langle n1S | \tilde{v}_{eff} | n1S \rangle + \tilde{B}_{n+1,1S} \langle \psi_{n1S} | \psi_{n+1,1S} \rangle + \\
 + \tilde{B}_{n-1,1S} \langle \psi_{n1S} | \psi_{n-1,1S} \rangle - \tilde{\epsilon}_{n1S} \langle \psi_{n1S} | \psi_{n1S} \rangle] = 0 \quad (41)
 \end{aligned}$$

where the quantities $\tilde{B}_{n+1,1S}$, $\tilde{B}_{n-1,1S}$ and $\tilde{\epsilon}_{n1S}$ are given by expressions similar to those in the previous case.

Using restriction (21) we can write the bracket of the equation (41) as follows:

$$\begin{aligned}
 \tilde{M}'_{n1S} & \equiv \langle n1S | \tilde{v}_{eff} | n1S \rangle + \tilde{B}_{n+1,1S} \langle \psi_{n1S} | \psi_{n+1,1S} \rangle + \\
 & + \tilde{B}_{n-1,1S} \langle \psi_{n1S} | \psi_{n-1,1S} \rangle - \tilde{\epsilon}_{n1S} \langle \psi_{n1S} | \psi_{n1S} \rangle = \\
 & = \int_0^{d_{n1S}} \left[\frac{\hbar^2}{M} \left(\left(\frac{d\psi_{n1S}}{dr} \right)^2 + \frac{l(l+1)}{r^2} \psi_{n1S}^2 \right) + \frac{A-2}{A-1} v_r \psi_{n1S}^2 + \right. \\
 & \left. + v_{1S}(r) \psi_{n1S}^2 - \left(E_{n1} + \frac{E_{NL}}{2(A-1)} \right) \psi_{n1S}^2 + \tilde{B}_{n+1,1S} \psi_{n1S} \psi_{n+1,1S} + \right.
 \end{aligned}$$

$$\begin{aligned}
& + \left[\widetilde{B}_{n-1,1S} \psi_{n1S} \psi_{n-1,1S} - \widetilde{\varepsilon}_{n1S} \psi_{n1S}^2 \right] dr + \int_{d_{n1S}}^{\infty} \left[\frac{\hbar^2}{M} \left(\left(\frac{d\varphi_{n1}}{dr} \right)^2 + \right. \right. \\
& \left. \left. + \frac{l(l+1)}{r^2} \varphi_{n1}^2 \right) + \frac{A-2}{A-1} v_r \varphi_{n1}^2 + v_{1S}(r) \varphi_{n1}^2 - \left(E_{n1} + \right. \right. \\
& \left. \left. + \frac{E_{NL}}{2(A-1)} \right) \varphi_{n1}^2 + \widetilde{B}_{n+1,1S} \varphi_{n1} \varphi_{n+1,1} + \right. \\
& \left. + \widetilde{B}_{n-1,1S} \varphi_{n1} \varphi_{n-1,1} - \widetilde{\varepsilon}_{n1S} \varphi_{n1}^2 \right] dr \quad (42)
\end{aligned}$$

We shall find the stationary value of $(\Delta E)_2$ by varying the relative two-body wave functions ψ_{n1S} with boundary conditions (23). The Euler equation is

$$\begin{aligned}
& - \frac{\hbar^2}{M} \frac{d^2 \psi_{n1S}}{dr^2} + \left[\frac{\hbar^2}{M} \frac{l(l+1)}{r^2} + \frac{A-2}{A-1} \frac{\hbar^2}{M} \frac{r^2}{b^4} + v_{1S}(r) - \right. \\
& \left. - \left(E_{n1} + \frac{E_{NL}}{2(A-1)} \right) - \widetilde{\varepsilon}_{n1S} \right] \psi_{n1S} = - \frac{\widetilde{B}_{n+1,1S}}{2} \psi_{n+1,1S} - \\
& - \frac{\widetilde{B}_{n-1,1S}}{2} \psi_{n-1,1S} \quad (c < r < d_{n1S}) \quad (43)
\end{aligned}$$

and the expression for the $\widetilde{M}_{n1S} \equiv \langle n1S | \widetilde{v}_{eff} | n1S \rangle$ which appears in $(\Delta \widetilde{E})_2$ is

$$\begin{aligned}
& \widetilde{M}_{n1S} = \frac{\hbar^2}{M} \varphi_{n1}(d_{n1S}) \left[\psi'_{n1S}(d_{n1S}) - \varphi'_{n1}(d_{n1S}) \right] - \\
& - \frac{1}{2(A-1)} (E_{n1} + E_{NL}) + \frac{1}{A-1} \frac{\hbar^2}{M} \frac{1}{b^4} \int_0^{d_{n1S}} r^2 \varphi_{n1}^2 dr + \\
& + \frac{E_{NL}}{2(A-1)} \int_0^{d_{n1S}} \varphi_{n1}^2 dr + \int_{d_{n1S}}^{\infty} v_{1S}(r) \varphi_{n1}^2 dr + \widetilde{\varepsilon}_{n1S} \int_c^{d_{n1S}} \psi_{n1S}^2 dr - \\
& - \frac{\widetilde{B}_{n+1,1S}}{2} \int_c^{d_{n1S}} \psi_{n1S} \psi_{n+1,1S} dr - \frac{\widetilde{B}_{n-1,1S}}{2} \int_c^{d_{n1S}} \psi_{n1S} \psi_{n-1,1S} dr \quad (44)
\end{aligned}$$

3. REMARKS ON THE CALCULATION OF THE ENERGY OF THE He^4 NUCLEUS

In the case of He^4 the energy expression is quite simple. This ex-

pression is the following, if we take also into account the centre of mass correction, which is quite important for a light nucleus like He⁴.

$$E_{(\text{He}^4)} = 3\hbar\omega - \frac{3}{4}\hbar\omega + 2 \left[\frac{1}{\langle \psi_{000} | \psi_{000} \rangle} + \frac{1}{(\langle \psi_{000} | \psi_{000} \rangle + \langle \psi_{001} | \psi_{001} \rangle)} \right] M_{000} + \\ + 2 \left[\frac{1}{\langle \psi_{001} | \psi_{001} \rangle} + \frac{1}{(\langle \psi_{000} | \psi_{000} \rangle + \langle \psi_{001} | \psi_{001} \rangle)} \right] M_{001} \quad (45)$$

In the present case there are only two equations, one for ψ_{000} and another one for ψ_{001} , which are not (directly) coupled and can therefore be solved more easily.

The procedure in computing $E_{(\text{He}^4)}$ is the following:

For a given potential and harmonic oscillator parameter $b_1 = \frac{b}{\sqrt{2}}$,

the Euler equations are solved numerically with arbitrary values of ϵ_{000} and ϵ_{001} and the corresponding values of M_{000} and M_{001} are computed for various values of the separation distance. The appropriate value of d in each case is the «variational Moszkowski and Scott separation distance» at which the wave function has also continuous derivative. This separation distance is named after the corresponding separation distance in the reaction matrix approach³). If the initial values of ϵ_{000} (or ϵ_{001}) are such that there are no $d_{\text{M.S.}}$, another suitable choice is made. Usually more than one $d_{\text{M.S.}}$ appear and in such a case it may be chosen the one at which M becomes minimum with respect to variations of d . This is particularly desirable in view of the variational nature of the present approach, provided, of course, that such a choice is compatible with the requirement that the correlations are of sufficiently «short range». The usual criterion for the fulfillment of this requirement is the smallness of the value of the corresponding «healing» (or «wound») integral:

$$\eta_{\text{NIS}} = \int_0^\infty |\psi_{\text{NIS}} - \varphi_{\text{NI}}|^2 dr \quad (46)$$

The wave functions, which are obtained in the previously described way may be used in calculating new values for ϵ_{000} and ϵ_{001} .

From the detailed variational treatment of the problem, it turns out that the expression for ϵ_{000} is

$$\epsilon_{000} = \frac{\left[\frac{M_{000}}{\langle \psi_{000} | \psi_{000} \rangle^2} + \frac{(M_{000} + M_{001})}{(\langle \psi_{000} | \psi_{000} \rangle + \langle \psi_{001} | \psi_{001} \rangle)^2} \right]}{\left[\frac{1}{\langle \psi_{000} | \psi_{000} \rangle} + \frac{1}{(\langle \psi_{000} | \psi_{000} \rangle + \langle \psi_{001} | \psi_{001} \rangle)} \right]} \quad (47)$$

Analogous is the expression for ϵ_{001} . It results from the above expression of ϵ_{000} by putting for the last quantum number (S) the value 1 wherever it is 0 and the value 0 wherever it is 1.

The dependence of the quantity ϵ_{000} on the correlated wave functions ψ_{000} and ψ_{001} is quite simple in the present case.

The above expression for ϵ_{000} and the corresponding one for ϵ_{001} may be used in obtaining their new values and this procedure is repeated until the values of each of the ϵ do not change. These quantities are therefore determined in the present approach self-consistently.

Computations based on the prescribed approach are in progress. In our computations the Kallio-Koltveit potential¹⁶⁾ is used.

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Π Ε Ρ Ι Λ Η Ψ Ι Σ

ΜΙΑ ΜΕΘΟΔΟΣ ΔΙΑ ΤΑΣ ΑΛΛΗΛΟΣΥΣΧΕΤΙΣΕΙΣ ΔΥΟ ΣΩΜΑΤΙΩΝ ΕΙΣ ΠΕΠΕΡΑΣΜΕΝΟΥΣ ΠΥΡΗΝΑΣ ΤΗ ΒΟΗΘΕΙΑ ΜΗ ΜΟΝΑΔΙΑΙΟΥ ΤΕΛΕΣΤΟΥ ΥΠΟΔΕΙΓΜΑΤΟΣ

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Εἰς τὴν παροῦσαν ἐργασίαν θεωροῦμεν μίαν μέθοδον μεταβολῶν τῆ βο-
θεία «τελεστοῦ ὑποδείγματος» (model operator) πρὸς καθορισμὸν τῶν ἀλ-
ληλοσυσχετίσεων δύο-σωματίων εἰς πεπερασμένους πυρῆνας. Ἡ οὐσιαστικὴ
διαφορὰ ἀπὸ ἄλλας ἐργασίας εἶναι ὅτι ὁ τελεστής ὑποδείγματος δὲν ὑποτίθε-
ται ὅτι εἶναι μοναδιαῖος ἐξ ἀριστερῶν (left unitary). Κατ' ἀρχὴν δίδονται
δύο διαφορετικαὶ ἐκφράσεις διὰ τὸ $(\Delta E)_2$, ἧτοι διὰ τὸν ὄρον δύο σωμάτων εἰς τὸ
κατὰ «clusters» ἀνάπτυγμα τῆς ἐνεργείας, ἐφαρμόζεται δὲ ἐν συνεχείᾳ ἡ
μέθοδος μεταβολῶν με μίαν συνθήκην διαχωρισμοῦ. Τέλος, ἐξάγεται εἰς τύ-
πος ὁ ὅποιος δύναται νὰ χρησιμοποιηθῇ ἀπ' εὐθείας διὰ τὸν ἀριθμητικὸν ὑπο-
λογισμὸν τῆς ἐνεργείας βασικῆς καταστάσεως τοῦ πυρῆνος ἡλίου (He^4).