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Converging upper and lower bounds for ground-state energies of atomic nuclei

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Abstract. By expanding the wave function in terms of the translationally invariant basis of harmonic oscillator functions, we calculate the converging upper (variational) bound for the energy. It is shown that one can construct lower bounds using the reduced density matrix that corresponds to the upper bound. These lower bounds converge to an exact value with the expansion of the basis. We perform the calculations of both bounds with realistic nucleon-nucleon potential for ground states of the triton and the alpha-particle.

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1 Introduction

Matter is invariant with respect to translations in space, therefore the wave functions of the self-bound systems must be translationally invariant. However, the necessity to ensure this invariance significantly complicates the description. As a result, the best-known methods for the description of quantum systems, such as the Shell Model or the Hartree-Fock Self-Consistent Field method, produce wave functions dependent on a set of one-particle variables, thus also on the center of the mass radius-vector of the system. This shortage of mentioned methods is well-known, however, the wave functions dependent on one-particle variables are very attractive because they allow a simple procedure of antisymmetrization. In some cases, such as an atom, molecule or electron gas in solid state, this approximation with the Hamiltonian and the wave functions, both dependent on redundant variables, does not produce any serious problems.

Nuclei, however, are essentially self-bound systems. The translational invariance of the corresponding wave functions appears to be a real problem. Moreover, having in mind serious problems with nucleon-nucleon (NN) potential definition requiring three-nucleon interactions, one can summarize that the Schrödinger problem for atomic nuclei is one of the most complicated tasks even for modern computers. The experience with solving such complex problems clearly demonstrates the value of the variational method. It can be realized either by expanding the wave functions in a complete basis or by constructing a phenomenological ansatz, which is equipped with a sufficient amount of variational parameters. The most attractive point of the variational method is that any approximation for the eigenvalue by definition is an upper bound, converging to the exact value. Unfortunately, the method does not give good enough criteria to estimate how far the obtained value is from the exact one. The obvious advantage of the variational method would be the possibility to determine together with the upper bound also the lower bound for the energy. The possibility to determine both bounds simultaneously as a result of the same calculation enables one to estimate the interval for the exact energy value, *i.e.* in some cases to solve the problem of bound state existence or absence for some exotic systems and make decisions concerning the quality of the obtained wave function.

As will be shown, both bounds for the energy can be obtained while using the Reduced Hamiltonian formalism for the translationally invariant wave-function of the self-bound quantum system [1]. One ensures translational invariance for wave functions taking as arguments the set of translationally invariant spatial variables, the so-called Jacobian variables. As basics for our approach one uses the well-known results that the essential dynamic part of Hamiltonian for a system of identical particles is the Reduced Hamiltonian (RH) operator [2], and that any square-integrable wave function can be present in the basis

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of three-dimensional Harmonic Oscillator functions, enriched by the spin-isospin degrees of freedom and corresponding functions.

2 Expansions in the Reduced Hamiltonian basis

To obtain the mentioned bounds, one has to present the intrinsic Hamiltonian of the self-bound system composed of identical fermions as the sum

$$H = \sum_{i>j=1}^{A} h_{i,j} \tag{1}$$

of the $A(A-1)/2$ identical, but dependent on different variables, two-particle operators

$$h_{i,j} = -\frac{\hbar^2}{2mA}\left(\nabla_i - \nabla_j\right)^2 + V\left(\mathbf{r}_i - \mathbf{r}_j, \sigma_i\sigma_j\tau_i\tau_j\right). \tag{2}$$

For the atomic nucleus, m is the nucleon mass and $V\left(\mathbf{r}_i - \mathbf{r}_j, \sigma_i\sigma_j\tau_i\tau_j\right)$ is the potential of the nucleon-nucleon (NN) interaction [3] depending, as usual, on the difference $\mathbf{r}_i - \mathbf{r}_j$ of the radius-vectors of the nucleons i and j and on a set of spin and isospin degrees of freedom $\sigma_i, \sigma_j, \tau_i$, and τ_j. Since the particles are identical fermions, the Hamiltonian H is symmetric and the wave function is antisymmetric with respect to the permutations of the particles. As a consequence, the expectation values of different operators $\langle h_{i,j}\rangle$ coincide, hence the expectation value of the total Hamiltonian can be expressed in a very simple form:

$$\langle H\rangle = \frac{A(A-1)}{2}\langle h_{A-1,A}\rangle \equiv \langle\mathcal{H}\rangle. \tag{3}$$

Taking the last Jacobi coordinate as

$$\xi_{A-1} = \left(\mathbf{r}_{A-1} - \mathbf{r}_A\right)/\sqrt{2}, \tag{4}$$

one can present the operator $\mathcal{H}$ as

$$\mathcal{H} = \frac{A(A-1)}{2}\left[-\frac{\hbar^2}{mA}\nabla^2_{\xi_{A-1}} + V\left(\sqrt{2}\xi_{A-1}, \sigma_i\sigma_j\tau_i\tau_j\right)\right]. \tag{5}$$

Namely this operator is called the Reduced Hamiltonian (RH) operator. It describes the relative motion of two nucleons therefore the solution of the corresponding Schrödinger equation,

$$\mathcal{H}\psi_{\nu\lambda\mu}\left(A-1, A\right) = \varepsilon_{\nu\lambda}\psi_{\nu\lambda\mu}\left(A-1, A\right), \tag{6}$$

is not more complicated than the Schrödinger problem for the deuteron. Due to dependence of $\mathcal{H}$ on the mass number the corresponding eigenvalues and eigenfunctions all are functions of A.

For $A = 2$ this Hamiltonian describes the two-nucleon system. The binding energy of the deuteron and the phase-shifts of nucleon-nucleon scattering must be reproduced while solving eq. (6) with the realistic nucleon-nucleon (NN) potential. Here the set of exact quantum numbers for two nucleons λ is the same as assignments for states of the lightest atomic nuclei. It consists of angular momentum, parity, isospin and isospin projection quantum numbers, *i.e.* $\lambda \equiv j^\pi t m_t$. The last quantum number, *i.e.* the projection of isospin m_t, is necessary for different two-nucleon pairs (nn, np or pp) characterization, because recent realistic potentials are charge-dependent. For lightest atomic nuclei with the same mass number A it labels the nuclei of charge multiplets. The correspondence between our set of quantum numbers $j^\pi t$ and spectroscopic identifiers of two-nucleon channels is straightforward:

$$0^+1 \sim {}^1S_0, \qquad 0^-1 \sim {}^3P_0, \qquad 1^+0 \sim {}^3S_1 - {}^3D_1, \ldots \tag{7}$$

and so on. μ marks the quantum number of projections of angular momentum j, ν is the number of the eigenvalues with the same λ.

For two nucleons there exists only one bound state of the RH in channel 1^+0 —the deuteron. For $A = 3$, all realistic potentials ensure the appearance of a bound eigenvalue in the state 0^+1. For larger values of mass number the bound eigenvalues of RH begin to appear also in other channels, in which the phase shifts of nucleon-nucleon scattering are positive or change sign. Some of channels in which the phase shifts are negative remain without bound states at any A. This phenomenon is observed and described for the first time in [4].

The Shell Model Hamiltonian has an analogous, but far simpler, structure. It equals a sum of commuting one-particle operators h_i, dependent on one-particle variables:

$$H_0 = \sum_{i=1}^{A} h_i, \tag{8}$$

where

$$h_i = -\frac{\hbar^2}{2m}{\nabla_i}^2 + U\left(\mathbf{r}_i\sigma_i\tau_i\right). \tag{9}$$

The arbitrary eigenvalue of this Hamiltonian can be written as

$$\langle H_0\rangle = A\langle h_A\rangle \equiv \langle\mathcal{H}_0\rangle. \tag{10}$$

The Schrödinger equation for this simple one-particle Reduced Hamiltonian is

$$\mathcal{H}_0\phi_{nljm}\left(A\right) = \varepsilon^{(0)}_{nlj}\phi_{nljm}\left(A\right), \tag{11}$$

where nlj is a set of one-nucleon quantum numbers and m is the projection of angular momentum quantum number. Due to the independence of one-particle variables the eigenfunctions of the entire Hamiltonian

$$\begin{aligned} &H_0\Phi_{\mathcal{N}\Gamma_0\Lambda M}\left(1, 2, \ldots, A-1, A\right) \\ &= \mathcal{E}^{(0)}_{\mathcal{N}\Gamma_0\Lambda}\Phi_{\mathcal{N}\Gamma_0\Lambda M}\left(1, 2, \ldots, A-1, A\right) \end{aligned} \tag{12}$$

can be written in terms of a finite set, defined by configuration, of $\mathcal{H}_0$ eigenfunctions for individual nucleons:

$$\begin{aligned} \Phi_{\mathcal{N}\Gamma_0\Lambda M}\left(1, 2, \ldots, A-1, A\right) = \sum_{\bar\Gamma_0\bar\Lambda_0, nlj}\left\langle\mathcal{N}\Gamma_0\Lambda\|\bar\Gamma_0\bar\Lambda_0; nlj\right\rangle \\ \times\left\{\Phi_{\bar\Gamma_0\bar\Lambda_0}\left(1, 2, \ldots, A-1\right)\otimes\phi_{nlj}\left(A\right)\right\}_{\Lambda M}. \end{aligned} \tag{13}$$

Here Λ marks the set of exact quantum numbers, Γ_0 are all the other quantum numbers (including configuration) necessary for the definition of the state under consideration, and $\mathcal{N}$ is the number of states with the same set of quantum numbers $\Gamma_0\Lambda$. $\bar{\Gamma}_0$ and $\bar{\Lambda}_0$ are the corresponding quantum numbers attributed to the "spectator" functions $\Phi_{\bar{\Gamma}_0\bar{\Lambda}_0}(1,2,\ldots,A-1)$, dependent on variables of remaining $(A-1)$ particles. The functions appearing on the right-hand side of eq. (13) are components of the wave function. The components by definition are products of antisymmetrized only in the first group of nucleons (spectator) wave functions and the RH (actor) eigenfunctions. They are equipped with the same set of exact quantum numbers as the wave function of the system. The coefficients $\langle \mathcal{N}\Gamma_0\Lambda\|\bar{\Gamma}_0\bar{\Lambda}_0; nlj\rangle$ present in expression are the coefficients of fractional parentage, ensuring antisymmetry of the wave function. Taking into account this expression of the wave function, the eigenvalue of the total Hamiltonian equals

$$\mathcal{E}^{(0)}_{\mathcal{N}\Gamma_0\Lambda} = \sum_{nlj} \varepsilon^{(0)}_{nlj} \sum_{\bar{\Gamma}_0\bar{\Lambda}_0} \left|\langle \mathcal{N}\Gamma_0\Lambda\|\bar{\Gamma}_0\bar{\Lambda}_0; nlj\rangle\right|^2 . \qquad (14)$$

In brief this equation can be written as

$$\mathcal{E}^{(0)} = \sum_{\alpha} \varepsilon^{(0)}_{\alpha}\omega^{(0)}_{\alpha} , \qquad (15)$$

where α marks the set nlj, $\varepsilon^{(0)}_{\alpha}$ denote the eigenvalue of the $\mathcal{H}_0$ $(\varepsilon_\alpha \le \varepsilon_{\alpha+1})$, and the coefficients $\omega^{(0)}_{\alpha}$ are diagonal entries of the one-particle reduced density matrix. They satisfy the conditions

$$\sum_{\alpha=1}^{A} \omega^{(0)}_{\alpha} = 1, \quad \text{and} \quad \omega^{(0)}_{\alpha} \ge 0, \qquad (16)$$

caused by normalization of the wave function and can be called the probabilities of the corresponding one-particle states.

To obtain an analogous expression for the eigenvalue of the realistic Hamiltonian, one needs the above-introduced Reduced Hamiltonian, eq. (5), describing the relative movement of two nucleons, and the modified coefficients of fractional parentage [1]. The main problem while realizing this idea is the noncommutation of different operators $h_{i,j}$, present in the translationally invariant expression of the total intrinsic Hamiltonian. Consequently, the RH and the total Hamiltonian cannot have common eigenfunctions, hence none of the eigenfunctions of the total Hamiltonian can be expressed as the product of Reduced Hamiltonian eigenfunctions, as in the Shell Model approximation. The minimal approximation like the one in the Shell Model, does not exist. However, the basis of the RH eigenfunctions is complete, hence any wave function of the self-bound system can be expanded in terms of the basis of eigenfunctions of the operator $\mathcal{H}$. Let us define the above-mentioned expansion of the translationally invariant wave function Ψ in terms of eigenfunctions of RH as follows:

$$\Psi_{\mathcal{E}\Gamma\Lambda M}(1,2,\ldots,A-1,A) = \sum_{\bar{\Gamma}\bar{\Lambda},\nu\lambda} \langle \mathcal{E}\Gamma\Lambda\|\bar{\Gamma}\bar{\Lambda};\nu\lambda\rangle \times \left\{\Phi_{\bar{\Gamma}\bar{\Lambda}}(1,2,\ldots,A-2)\otimes\psi_{\nu\lambda}(A-1,A)\right\}_{\Lambda M} . \qquad (17)$$

Here $\mathcal{E}$ denotes an eigenvalue of the Hamiltonian H of the system, Λ is the set of exact quantum numbers, Γ are all other quantum numbers necessary for the definition of the state under consideration. $\bar{\Gamma}$ and $\bar{\Lambda}$ are the quantum numbers attributed to the "spectator" functions, dependent on all the remaining variables except those appearing in the expression of the RH, eq. (5). Any square-integrable functions of the same set of variables, forming an orthonormalyzed basis, can be taken as the basis of "spectator" functions. The functions appearing in curly brackets on the right-hand side of eq. (17) are components of the wave function. They are unantisymmetrized products of the RH eigenfunctions and the "spectator" wave functions with coupled angular momenta and equipped with the same set of exact quantum numbers as the wave function of the system. The coefficients $\langle \mathcal{E}\Gamma\Lambda\|\bar{\Gamma}\bar{\Lambda};\nu\lambda\rangle$ present in this expression for the wave function are the generalized coefficients of fractional parentage for the translationally invariant function, defined in [1] as entries of the matrix of the spectral decomposition of antisymmetrizer matrix, present in components basis.

By using this expansion one easily obtains that the eigenvalue $\mathcal{E}$ of the total Hamiltonian of the system can be expressed as:

$$\mathcal{E} = \sum_{\nu\lambda} \varepsilon_{\nu\lambda} \sum_{\bar{\Gamma}\bar{\Lambda}} \left|\langle \mathcal{E}\Gamma\Lambda\|\bar{\Gamma}\bar{\Lambda};\nu\lambda\rangle\right|^2 . \qquad (18)$$

In brief this equation can be rewritten as

$$\mathcal{E} = \sum_{\gamma} \varepsilon_{\gamma}\omega_{\gamma} , \qquad (19)$$

where $\gamma = 1,2,...$ marks the set of quantum numbers $\nu\lambda$, and ε_γ denote the eigenvalue of the RH operator $(\varepsilon_\gamma \le \varepsilon_{\gamma+1})$. The coefficients ω_γ, satisfying the conditions

$$\sum_{\gamma} \omega_{\gamma} = 1, \quad \text{and} \quad \omega_{\gamma} \ge 0, \qquad (20)$$

caused by normalization of the wave function, are diagonal elements of the reduced density matrix and can be called the probabilities of corresponding RH states.

Obvious is the complete analogy of both expressions for the eigenvalues —the first given in eq. (15), and the second present in eq. (19). The calculations of the RH eigenvalues in both cases are not more complicated than the solution of the Schrödinger equation for the deuteron. However, while the first expression is for the eigenvalue of the model Hamiltonian, the second one gives a simple expression for the eigenvalue of the intrinsic Hamiltonian of the atomic nucleus with the realistic potential of the NN interaction.

Table 1. The dependence of the upper bounds $\mathcal{E}_{up}$ for the triton and the alpha-particle ground-state energy on a total number of oscillator quanta E. $E = \infty$ corresponds to the exact value. This value for triton (−7.63 MeV) is from [5], for the alpha-particle (−24.56 MeV) from [6].

^{3}H		^{4}He	
E	$\mathcal{E}_{up}$	E	$\mathcal{E}_{up}$
22	−6.38	0	626.82
24	−6.76	2	233.63
26	−7.00	4	93.81
28	−7.20	6	33.70
30	−7.32	8	6.36
32	−7.41	10	−5.77
34	−7.47	12	−13.82
36	−7.52	14	−18.08
38	−7.55	16	−20.84
40	−7.58	∞	−24.56
42	−7.59		
44	−7.60		
∞	−7.63		

3 The bounds for energies

As has been shown, the probabilities of the RH states are diagonal entries of the reduced density matrix. Formerly it was believed, that this density matrix can serve as the main mathematical tool for the description of the A-fermion system because the many-particle wave function tells us more than we need to know. The main task while solving this problem was the formulation of the conditions such a matrix has to fulfill to be derivable from a wave function of the A-particle system. This problem, called the problem of N-representability of the density matrix, is introduced and formulated in the classical works [7]. However, direct construction of acceptable approximations for the reduced density matrix, avoiding the wave function calculation cannot be realized. The only known way is the solution of the Schrödinger equation with the following reconstruction of the probabilities distribution using the obtained wave-function. Obviously, any distribution of probabilities, violating the N-representability of the density matrix, as will be shown later, cannot give an acceptable result. Obvious is only that, for the non antisymmetric wave function, the expectation value of the Hamiltonian always gives the lower bound for the corresponding eigenvalue.

The best known lower bound is the so-called Hall-Post bound [8]. It is obtained by concentrating all the probability on the lowest state of the RH (*i.e.*, taking $\omega_\alpha = \delta_{\alpha,1}$). Obviously, this distribution of probabilities corresponds to one component, therefore cannot be created by the anti-symmetric wave function. As a result, the corresponding estimate for the energy is very inaccurate. Some improvement of this bound can be obtained by taking into account minimal requirements for the density matrix (*i.e.* probabilities), caused by antisymmetry of the wave function [4], but the lower bound anyway stays far from the exact value.

A set of N-representable density matrices can be constructed by applying the basis of translationally invariant three-dimensional harmonic oscillator functions in the expansion for the components of the wave function. This basis can be antisymmetrized in finite subspaces of the Hilbert space, corresponding to the given total number of oscillator quanta E, because such a set of functions forms the complete set for the antisymmetrization operator. Therefore, at any given number of oscillator quanta E the N-representable density matrix can be found, thus the probabilities $\omega_\alpha(E)$, that depend on the maximal number of oscillator quanta E, can be defined. As mentioned, these probabilities correspond to the situation, when all many-particle basic functions whose number of oscillator quanta ranges from E_{min} (minimal value of oscillator quanta, allowed by the Pauli principle) to E are summed up. Due to the condition for parity of the state under consideration $\pi = (-1)^E$, allowed values of the oscillator quanta are of the same parity. Obviously, the eigenvalues of the RH also depend on E because this parameter defines the dimension of the basis for the RH matrix diagonalization [9]. Finally, the eigenvalue of the total Hamiltonian H is

$$\mathcal{E}_{up}(E) = \sum_{\alpha=1}^{N(E)} \varepsilon_\alpha(E)\,\omega_\alpha(E)\ . \tag{21}$$

Here $N(E)$ is the total number of RH states, present in the expansion. Increasing the number E enlarges the basis for the total Hamiltonian matrix, giving the mentioned variational result, converging to the exact value from above, *i.e.*:

$$\mathcal{E}_{up}(E) - \mathcal{E}_{up}(E+2) > 0 \qquad \text{and} \qquad \lim_{E\to\infty} \mathcal{E}_{up}(E) = \mathcal{E}\,. \tag{22}$$

In table 1, we present these upper bounds for the triton and for the alpha-particle as functions of the total number of oscillator quanta E, obtained while using the Reid93 NN potential [10]. In table 1 also are given the values of precise calculations for the ground-states energies of both nuclei.

By applying eq. (21) the convergence condition eq. (22) can be rewritten as

$$\begin{aligned}&\sum_{\alpha=1}^{N(E)} [\varepsilon_\alpha(E) - \varepsilon_\alpha(E+2)]\,\omega_\alpha(E)\\ &+ \sum_{\alpha=1}^{N(E)} \varepsilon_\alpha(E+2)\,[\omega_\alpha(E) - \omega_\alpha(E+2)] >\\ &\sum_{\alpha=N(E)+1}^{N(E+2)} \varepsilon_\alpha(E+2)\,\omega_\alpha(E+2)\ .\end{aligned} \tag{23}$$

In the asymptotic region, *i.e.* for large values of E, this condition can be easily understood and simplified taking

into account the well-known result, that perturbations of the wave functions are of the second order in comparison with the ones for the eigenvalues $\varepsilon_\alpha(E)$. Consequently, the perturbations of the density matrix are even smaller. Thus, the second sum on the left-hand side of the inequality, eq. (23), can be neglected:

$$\sum_{\alpha=1}^{N(E)} \left[\varepsilon_\alpha(E) - \varepsilon_\alpha(E+2)\right] \omega_\alpha(E) > \sum_{\alpha=N(E)+1}^{N(E+2)} \varepsilon_\alpha(E+2)\, \omega_\alpha(E+2)\,. \tag{24}$$

The sums on both sides are positive, because all probabilities are nonnegative and the eigenvalues of the RH, in complete accordance with the behavior of the eigenvalues of the total Hamiltonian, can only decrease when the harmonic oscillator basis increases, *i.e.*

$$\varepsilon_\alpha(E) > \varepsilon_\alpha(E+2)\,. \tag{25}$$

As mentioned above, a very limited number of bound states is characteristic of realistic NN potentials, so all $\varepsilon_\alpha(E+2)$ with $\alpha > N(E)$ at large enough E are positive. Equation (24) illustrates the statement that changes in the eigenvalues of the RH (*i.e.* in $\varepsilon_\alpha(E)$) are large enough, while the probabilities of states corresponding to the expansion tail ($\alpha > N(E)$), present on the right-hand side of the inequality, are small.

As already mentioned, a high-quality lower bound can be obtained when using the N-representable density matrix. The only such construction one has is the density matrix obtained while calculating the upper bound. So, let us apply the following expression for the lower bound:

$$\mathcal{E}_{lw}(E) = \sum_{\alpha=1}^{N(E)} e_\alpha(E)\, \omega_\alpha(E) \tag{26}$$

and consider which $e_\alpha(E)$ values can be used for the definition of these bounds.

Let us summarize the requirements for the lower bounds:

1. Firstly, the lower bound must produce a value for the energy, lower than the value produced by the upper bound at any number of oscillator quanta E, *i.e.* $\mathcal{E}_{lw}(E) \leq \mathcal{E}_{up}(E)$.

2. Secondly, both bounds at growing E must converge to the same value of energy, *i.e.* $\mathcal{E}_{lw}(E) \to \mathcal{E}_{up}(E)$ for $E \to \infty$.

3. Thirdly, the condition

$$\mathcal{E}_{lw}(E) < \mathcal{E}_{lw}(E+2)\,, \tag{27}$$

require the convergence of the lower bound to the exact value from below.

To satisfy the first and the second condition it is necessary to take

$$e_\alpha(E) \leq \varepsilon_\alpha(E) \tag{28}$$

at all values of α and ensure the condition $e_\alpha(E) \to \varepsilon_\alpha(E)$ for $E \to \infty$.

The third condition for the lower bound (27), which can be simplified by neglecting small sums (like simplifying above the conditions for the upper bound), for a given set of $e_\alpha(E)$, can be expressed as

$$\sum_{\alpha=1}^{N(E)} \left[e_\alpha(E+2) - e_\alpha(E)\right] \omega_\alpha(E+2) + \sum_{\alpha=N(E)+1}^{N(E+2)} e_\alpha(E+2)\omega_\alpha(E+2) > 0\,. \tag{29}$$

It is evident that the sums in this inequality have different signs: the first sum is negative and the second positive. Therefore, in some cases this requirement cannot be satisfied.

Let us consider possible alternatives for the definition of $e_\alpha(E)$.

The first one, satisfying all the three mentioned conditions, is based on $e_\alpha(E)$ as *a priori* calculated eigenvalues of the RH at some fixed large value of the oscillator quanta $E_0 \gg E$. The definition for this lower bound (the bound of the first kind) is

$$\mathcal{E}^{(1)}_{lw}(E) = \sum_{\alpha=1}^{N(E)} \varepsilon_\alpha(E_0)\omega_\alpha(E). \tag{30}$$

Obviously, at $E = E_0$ this lower bound equals the upper bound. The condition for the lower bound, eq. (27) requiring the convergence of bound to the exact value from below, can be simplified and presented as

$$\sum_{\alpha=1}^{N(E)} \varepsilon_\alpha(E_0)\left[\omega_\alpha(E+2) - \omega_\alpha(E)\right] + \sum_{\alpha=N(E)+1}^{N(E+2)} \varepsilon_\alpha(E_0)\omega_\alpha(E+2) > 0\,. \tag{31}$$

The first sum here is of an unspecified sign but very small, while the second sum is always positive, hence this condition can be satisfied. In present calculations we choose E_0 equal to 50, 100 and 200. For single NN channels, such as $^1S_0$,$^3P_0$, $^1P_1$, etc., the order of the corresponding matrix of the RH operator equals 26, 51 and 101, correspondingly, while for bound channels, such as $^3SD_1$, $^3PF_2$, etc., the order of the RH operator matrix equals 51, 101 and 201. For triton the lower bound, corresponding to $E_0 = 200$ converges to the value which corresponds to the diagonalization of a total Hamiltonian matrix of order 10^6, while for the alpha-particle the order of the corresponding Hamiltonian matrix equals 10^{10}. It is evident that matrices of such dimensions, hardly attainable even for modern computers, can give the binding energy close enough to the exact one. The results obtained for the mentioned systems are presented in fig. 1.

For comparison, the Hall-Post bound $\mathcal{E}_{\rm HP} = \varepsilon_1$ for triton equals -48.11 MeV and for the alpha-particle -185.68 MeV. The above-mentioned modified

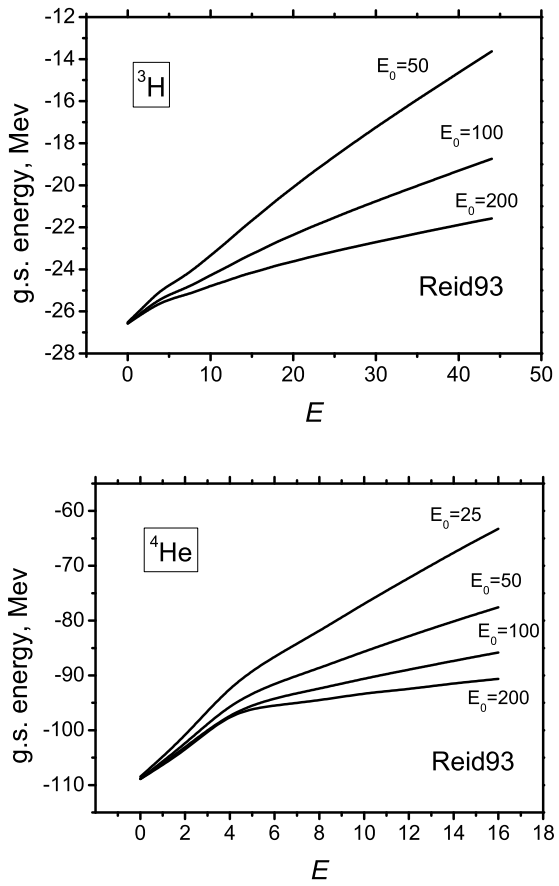

Fig. 1. The dependence of the lower bounds of first kind $\mathcal{E}^{(1)}_{lw}(E)$ for the triton and the alpha-particle on the total number of oscillator quanta E.

bound $\mathcal{E}_{\rm HPM} = (\varepsilon_1 + \varepsilon_2)/2$ give slightly better values -26.98 MeV and -110.96 MeV, respectively. Obviously, all these values for bounds are far from exact energies, hence other alternatives should be searched for.

As one can study from information, present in fig. 1, the lower is the dimension of the RH matrix (E_0), the better is the value of the lower bound. Let us exploit this idea to generate bounds of the second kind taking as eigenvalues of RH the eigenvalues of the maximal order matrix at a given number of oscillator quanta only in two nucleon channels with bound states present, *i.e.*:

$$\begin{aligned} e_{\nu\lambda}(E) &= \varepsilon_{\nu\lambda}(E_0)\,, \qquad \text{when} \qquad \varepsilon_{1\lambda} < 0\,, \\ e_{\nu\lambda}(E) &= \varepsilon_{\nu\lambda}(E)\,, \qquad \text{otherwise}\,. \end{aligned} \tag{32}$$

The lower bounds $\mathcal{E}^{(2)}_{lw}(E)$, obtained in this case in the convergence region, are better than bounds of the first kind. They are given in table 2.

The last alternative (the bounds of third kind) corresponds to a situation when all positive eigenvalues of the RH are taken the same as in the upper-bound expressions, while the eigenvalues of the bound states are taken by solving exactly an appropriate Schrödinger equation,

Table 2. The dependence of the lower bounds $\mathcal{E}^{(2)}_{lw}$ of the second kind for the triton and the alpha-particle on the total number of oscillator quanta E.

^{3}H		^{4}He	
E	$\mathcal{E}^{(2)}_{lw}$	E	$\mathcal{E}^{(2)}_{lw}$
28	-9.19	12	-38.98
32	-9.08	16	-37.81
36	-8.94		
40	-8.82		
44	-8.71		

Table 3. The dependence of the lower bounds $\mathcal{E}^{(3)}_{lw}$ of third kind for the triton and the alpha-particle on the total number of oscillator quanta E.

^{3}H		^{4}He	
E	$\mathcal{E}^{(3)}_{lw}$	E	$\mathcal{E}^{(3)}_{lw}$
28	-7.82	12	-25.114
32	-7.75	16	-25.106
36	-7.72		
40	-7.7198		
44	-7.7174		

i.e. when

$$\begin{aligned} e_{1\lambda}(E) &= \varepsilon_{1\lambda}\,, \qquad \text{when} \qquad \varepsilon_{1\lambda} < 0\,, \\ e_{\beta}(E) &= \varepsilon_{\beta}(E)\,, \qquad \text{when} \qquad \varepsilon_{\beta}(E) > 0\,. \end{aligned} \tag{33}$$

Now the expression for the lower bound is

$$\mathcal{E}^{(3)}_{lw}(E) = \sum_{\alpha=1}^{k} \varepsilon_\alpha \omega_\alpha(E) + \sum_{\alpha=k+1}^{N(E)} \varepsilon_\alpha(E)\omega_\alpha(E)\,, \tag{34}$$

where k is the number of negative eigenvalues of the RH. The results obtained by applying this approximation to the triton and to the alpha-particle in the convergence region are presented in table 3. Obviously, they are the best we can present.

4 Summary

Summarizing, one can conclude that the introduced lower bounds significantly differs from all the lower bounds known earlier.

Firstly, in any approximation, operating with functions of one-particle variables, such as the Shell-Model basis, the construction of these lower bounds is very problematic due to the unavoidable for these calculations transformation from the one-particle density matrix to the reduced two-particle density matrix. The translationally invariant basis is ideal for these bounds definition.

Secondly, all bounds introduced are easily obtainable after the same variational calculation at any dimension of

the basis taken into account. The values for the bounds, converging with the growing dimension of the basis to the same value of energy, define the region, where this "exact" value is situated. This can be useful when solving problems of stability of some exotic systems.

Thirdly, the wave function, associated with every one of the obtained lower bounds is the same, as the variational wave-function for the upper bound, because the density matrices are the same in both cases. The Hall-Post bounds and their known modifications do not have any associated function. In other words, the introduced lower bounds correspond to some "effective interaction", based on the initial bare interaction but with a large basis for Reduced Hamiltonian functions taken into account, hence with some additional dynamic correlations included.

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