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The binding energy of three nucleons

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Abstract. A lower bound to the ground-state energy of a system of three nucleons is given in terms of the eigenvalues of a two-particle Hamiltonian. No special assumptions are made about the form of the ground state of the system. For a simple exponential exchange potential we find that the triton energy is $-8{\cdot}1 \pm 3{\cdot}0$ MeV and the tri-neutron energy is greater than $-1{\cdot}35$ MeV. The method is quite generally applicable to current low-energy phenomenological potentials.

1. Introduction

The object of this paper is to provide a simple and effective method for calculating a lower bound on the ground-state energy of a system of three nucleons. We assume that the nucleons are identical fermions interacting by charge-independent pair potentials, and that the motion of the system is governed by non-relativistic quantum mechanics. Earlier work (Hall and Post 1967 (method I), Hall 1967 a (method II), Hall 1967 b, c) provided lower bounds on the ground-state energies of N-nucleon systems for all N. For few-nucleon systems method I gave the best (i.e. the highest) energy bound. This bound is given by the ground-state energy of the two-nucleon problem, in which the potential energy term has been multiplied by the factor 3 and the kinetic energy term has been multiplied by the factor 2. In the case of Wigner forces the energy bound is found to be within a few per cent of the exact energy for wide ranges of the potential parameters. However, if exchange forces are introduced into the potential to 'fit' some of the low-energy scattering data, it is found that the lower bound lies as much as 20% below a variational upper bound where, in the case of pure Wigner forces, the separation of the bounds was only 1% (Hall 1967 c, chap. 6). Intuitively speaking, we might say that, in the case of the exchange potential, the reduced two-particle problem has been loaded with the deepest potential, although in the three-particle system all three pairs cannot simultaneously interact by such a potential. We have now overcome this difficulty, and the new results for exchange forces are as good as those for pure Wigner forces. No restrictions on the pair potential are introduced by the method, and consequently it may be applied to any of the potentials currently used in nuclear phenomenology (e.g. Hamada and Johnston 1962).

Weidemann (1965) tried to overcome the difficulty which we have described above. He made some arbitrary assumptions about the form of the ground state of the system and, moreover, his explicit results apply only to the case of central exchange forces. Great care must be taken with these lower-bound calculations. False assumptions about the form of the ground state of the many-particle system immediately invalidate the derivation of the energy lower bounds. The situation here is very different from the problem of choosing trial functions in a variational calculation.

2. The derivation of the lower-bound method

We consider a system of three identical nucleons interacting by the charge-independent pair potentials V_{ij}. The translation-invariant Hamiltonian for the system is given by

$$H = \frac{1}{6m}\{(\boldsymbol{p}_1-\boldsymbol{p}_2)^2+(\boldsymbol{p}_1-\boldsymbol{p}_3)^2+(\boldsymbol{p}_2-\boldsymbol{p}_3)^2\}+V_{12}+V_{13}+V_{23} \tag{1}$$

where m is the mass of a nucleon and $\boldsymbol{p}_i$ is the momentum operator for the ith nucleon. The energy E_0 which we are studying is the lowest eigenvalue of H with respect to the space spanned by normalized antisymmetric functions of the variables $\boldsymbol{r} = \boldsymbol{r}_1-\boldsymbol{r}_2$,

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$\boldsymbol{\rho} = \boldsymbol{r}_1+\boldsymbol{r}_2-2\boldsymbol{r}_3$, s_1, s_2, s_3, t_1, t_2 and t_3, where $\boldsymbol{r}_i$, s_i and t_i are the position vector and the spin and isospin variables of the ith particle, respectively. The symmetry of the ground state Ψ_0 allows us to write

$$E_0 = (\Psi_0, H\Psi_0) = (\Psi_0, \mathscr{H}\Psi_0)$$

where

$$\begin{aligned}\mathscr{H} &\equiv \frac{1}{2m}(\boldsymbol{p}_1-\boldsymbol{p}_2)^2+3V_{12}\\ &= 2\left(\frac{-\hbar^2}{m}\Delta_r+\tfrac{3}{2}V_{12}\right).\end{aligned} \tag{2}$$

The lower bound to E_0 given by method I is just the lowest eigenvalue ϵ_0 of $\mathscr{H}$ with respect to normalized antisymmetric functions of the variables $\boldsymbol{r}$, s_1, s_2, t_1 and t_2. We shall now exploit the symmetry of Ψ_0 to improve this bound.

We expand Ψ_0 in terms of the complete set of orthonormal isospin functions $|i\rangle$, which are tabulated in appendix 2:

$$\Psi_0 = \sum_{i=1}^{8} \psi_i|i\rangle \tag{3}$$

where the ψ_i only depend on the relative coordinates $\boldsymbol{r}$ and $\boldsymbol{\rho}$ and on the spins. Ψ_0 must satisfy

$$A\Psi_0 = \Psi_0$$

where A is the antisymmetrizing projection operator in the three particle indices. In equation (A10) (appendix 1) we have expressed A in terms of operators acting on the ψ_i (labelled α) and operators acting on the $|i\rangle$ (labelled β). Thus we find

$$\begin{aligned}\Psi_0 = &\sum_{i=1}^{4}(\Lambda^{a\alpha}\psi_i)|i\rangle\\ &+\tfrac{1}{2}\{(\Lambda^{m\alpha}_{22}\psi_5-\Lambda^{m\alpha}_{12}\psi_7)|5\rangle-(\Lambda^{m\alpha}_{21}\psi_5-\Lambda^{m\alpha}_{11}\psi_7)|7\rangle\}\\ &+\tfrac{1}{2}\{(\Lambda^{m\alpha}_{22}\psi_6-\Lambda^{m\alpha}_{12}\psi_8)|6\rangle-(\Lambda^{m\alpha}_{21}\psi_6-\Lambda^{m\alpha}_{11}\psi_8)|8\rangle\}.\end{aligned} \tag{4}$$

Now the operators

$$T_z \equiv (\tau_{1z}+\tau_{2z}+\tau_{3z})$$

and

$$\boldsymbol{T}^2 \equiv (\boldsymbol{\tau}_1+\boldsymbol{\tau}_2+\boldsymbol{\tau}_3)^2$$

are constants of the motion because the pair potentials V_{ij} are charge independent and therefore only depend on the isospin through the products $\boldsymbol{\tau}_i.\boldsymbol{\tau}_j$. For the triton system the eigenvalue M_T of T_z is $\frac{1}{2}$. This means that only the states $|2\rangle$, $|5\rangle$ and $|7\rangle$ contribute to Ψ_0. The states $|5\rangle$ and $|7\rangle$ have equal weights because the norms of their coefficients in equation (4) are equal (this is a consequence of relations (A2) and (A5) in appendix 1). The states $|2\rangle$ and $|5\rangle$ are symmetric in (t_1, t_2), whereas $|7\rangle$ is antisymmetric in these variables. The coefficients of these isospin states, of course, have the opposite symmetries. We have

$$\langle 2|\mathscr{H}|2\rangle = \langle 5|\mathscr{H}|5\rangle \equiv {}_3\mathscr{H}$$

$$\langle 7|\mathscr{H}|7\rangle \equiv {}_1\mathscr{H}$$

and

$$\langle i|\mathscr{H}|j\rangle = 0, \qquad i\neq j.$$

For each of the cases $T = \frac{1}{2}$ and $T = \frac{3}{2}$ we apply a similar argument to the one used for method I.

$T = \frac{3}{2}$: $\quad \Psi_0 = \psi(\widetilde{123})|\widetilde{123}\rangle$ (see appendix 2) therefore

$$E_0 = (\Psi_0, H\Psi_0) = (\Psi_0, \mathscr{H}\Psi_0)$$
$$= \{\psi(\widetilde{123}), {}_3\mathscr{H}\psi(\widetilde{123})\} \geqslant {}_3\epsilon_a. \tag{5}$$

$T = \frac{1}{2}$:
$$\Psi_0 = \frac{1}{\sqrt{2}}\{\psi(\widetilde{12}\,3)|\overline{12}\,3\rangle - \phi(\overline{12}\,3)|\widetilde{12}\,3\rangle\}$$

therefore

$$E_0 = (\Psi_0, H\Psi_0) = (\Psi_0, \mathscr{H}\Psi_0)$$
$$= \tfrac{1}{2}[\{\psi(\widetilde{12}\,3), {}_3\mathscr{H}\psi(\widetilde{12}\,3)\} + \{\phi(\overline{12}\,3), {}_1\mathscr{H}\phi(\overline{12}\,3)\}]$$
$$\geqslant \tfrac{1}{2}({}_3\epsilon_a + {}_1\epsilon_s). \tag{6}$$

The suffixes a and s on the eigenvalues ${}_1\epsilon$ of ${}_1\mathscr{H}$ and ${}_3\epsilon$ of ${}_3\mathscr{H}$ indicate the symmetry (in the indices 1 and 2) of the corresponding eigenstates. If the spin symmetry and the parity of the *two*-nucleon system are constants of the motion (this is the case for the potential of Hamada and Johnston 1962), then a lower bound in E_0 is provided by the lowest of the following six energies:

$$\left.\begin{array}{l} {}^3_3\epsilon^- \\ {}^1_3\epsilon^+ \\ \tfrac{1}{2}({}^3_3\epsilon^- + {}^3_1\epsilon^+) \\ \tfrac{1}{2}({}^3_3\epsilon^- + {}^1_1\epsilon^-) \\ \tfrac{1}{2}({}^1_3\epsilon^+ + {}^3_1\epsilon^+) \\ \tfrac{1}{2}({}^1_3\epsilon^+ + {}^1_1\epsilon^-) \end{array}\right\} \tag{7}$$

and

where the left-hand superscript equals $2S+1$ and the right-hand superscript indicates the parity of the corresponding eigenstate of $\mathscr{H}$. In the next section we shall illustrate this method by applying it to the case of a mixture of central exchange forces.

3. The symmetric exchange potential

We consider the triton problem with the pair potential

$$V_{ij} = -V_0 \exp\left(\frac{-r_{ij}}{a}\right)\{w + mM_{ij} + bB_{ij} + hM_{ij}B_{ij}\} \tag{8}$$

where

$$m = 2b = \tfrac{1}{3}(1+3x)$$
$$h = 2w = \tfrac{1}{3}(1-3x)$$

and

$$x = (w+m-b-h) = {}^1\bar{V}^+/{}^3\bar{V}^+ = 0{\cdot}6.$$

In this example the odd-parity states of $\mathscr{H}$ are unbound, and we have (from equations (7))

$$E_0 \geqslant E_L \equiv \tfrac{1}{2}({}^3_1\epsilon^+ + {}^1_3\epsilon^+). \tag{9}$$

An upper bound E_U to E_0 is easily found by using the spatially symmetric trial function

$$\phi = \left(\frac{12\alpha^2}{\pi^2}\right)^{3/4} \exp\{-\alpha(3\mathbf{r}^2 + \boldsymbol{\rho}^2)\}|a\rangle \tag{10}$$

where $|a\rangle$ is a normalized antisymmetric spin–isospin function. Thus

$$E\{\phi(\alpha)\} = (\phi, H\phi) = (\phi, \mathscr{H}\phi) = \left(\frac{6\alpha}{\pi}\right)^{3/2}\{\exp(-3\alpha\mathbf{r}^2), \langle a|\mathscr{H}|a\rangle \exp(-3\alpha\mathbf{r}^2)\}$$

$$= \left(\frac{6\alpha}{\pi}\right)^{3/2}\{\exp(-3\alpha\mathbf{r}^2), \tfrac{1}{2}({}^3_1\mathscr{H} + {}^1_3\mathscr{H})\exp(-3\alpha\mathbf{r}^2)\} \tag{11}$$

and

$$E_0 \leqslant E_U \equiv \text{the minimum of } E\{\phi(\alpha)\} \text{ with respect to } \alpha. \tag{12}$$

The results of this calculation are shown in figure 1 in terms of the following dimensionless parameters:

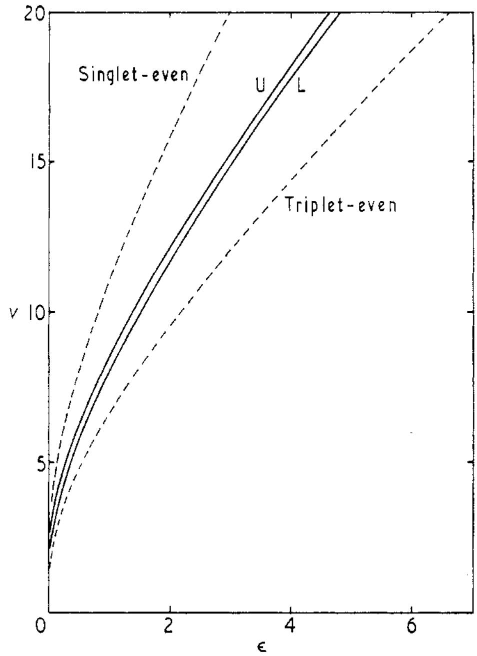

Figure 1. Exponential exchange potential v against ϵ: U, upper bound; L, lower bound.

$$\epsilon \equiv \frac{-E}{N-1}\frac{ma^2}{\hbar^2}$$

$$v \equiv \tfrac{1}{2}NV_0\frac{ma^2}{\hbar^2} \tag{13}$$

and

$$N = 3.$$

The upper bound (U), the lower bound (L), the triplet-even and the singlet-even curves are obtained by setting E in equation (13) equal to E_U, E_L, ${}^3_1\epsilon^+$ and ${}^1_3\epsilon^+$, respectively. The lower bound given by method I is just the triplet-even curve. The new lower bound is therefore a great improvement over method I.

If, in particular, we take the potential (8) with

$$V_0a^2 = 92{\cdot}6 \text{ MeV fm}^2$$

$$a = 0{\cdot}86 \text{ fm} \tag{14}$$

and

$$\hbar^2/m = 41{\cdot}47 \text{ MeV fm}^2$$

we find

$$\left.\begin{aligned} \text{the ground-state energy of the deuteron} &= -2{\cdot}22 \text{ MeV} \\ {}^3_1\epsilon^+ &= -19{\cdot}5 \text{ MeV} \\ {}^1_3\epsilon^+ &= -2{\cdot}7 \text{ MeV} \\ E_L = \tfrac{1}{2}({}^3_1\epsilon^+ + {}^1_3\epsilon^+) &= -11{\cdot}1 \text{ MeV} \\ E_U &= -5{\cdot}13 \text{ MeV} \end{aligned}\right\}. \tag{15}$$

Hence the ground-state energy of the triton system is given by

$$-11{\cdot}1 \leqslant E_0 \leqslant -5{\cdot}13 \text{ MeV}. \tag{16}$$

This result could probably be improved by using a more sophisticated trial function for the upper limit.

It is interesting to mention here the problem of the tri-neutron. For simple interactions where $\boldsymbol{S}^2$ and S_z are constants of the motion, we can go through an analogous argument to that of § 2. The α space is spanned by the normalized functions of $\boldsymbol{r}$ and $\boldsymbol{\rho}$, and the β space is spanned by the spin functions in table 1 (in appendix 2). We find that a lower bound to E_0 is given by the lowest of the energies ${}^3\epsilon^-$ or $\frac{1}{2}({}^3\epsilon^- + {}^1\epsilon^+)$. For the interaction (8), ${}^3\epsilon^- = 0$. Therefore

$$E_0 \geqslant \tfrac{1}{2}({}^1\epsilon^+). \tag{17}$$

Hence from (15) the tri-neutron binding energy satisfies

$$E_0 \geqslant -1{\cdot}35 \text{ MeV}.$$

4. Conclusion

For three-nucleon systems we have greatly improved on the energy lower bounds given by method I. The new bounds for the triton system (equations (7)) are quite general and would apply, for example, to the realistic nucleon–nucleon potential of Hamada and Johnston (1962). In the case of the symmetric exchange potential we have determined the triton binding energy to within a few per cent for wide ranges of the potential parameters (figure 1). In the region of nuclear physics ($v \simeq 3{\cdot}5$) the energy bounds are proportionately more widely separated. We find that the ground-state energy of the triton is $-8{\cdot}1 \pm 3{\cdot}0$ MeV, whilst the ground-state energy of the tri-neutron is greater than $-1{\cdot}35$ MeV.

We are hopeful that a more general analysis of the inner product representations of the symmetric group S_N will enable us to discuss saturation in nuclear physics entirely in terms of the energy spectrum of the reduced two-particle Hamiltonian.

Appendix 1

Hermitian projection operators for the symmetric group

We denote the coordinates and the wave function of an N-particle system by x and $\psi(x)$, respectively. P is a permutation operator acting on x and O_P is an operator defined by the relation

$$O_P\psi(Px) = \psi(x). \tag{A1}$$

The permutation symmetry of ψ can be analysed (Altmann 1962, p. 144) in terms of the symmetrizing operators

$$\Lambda^\mu_{ij} \equiv \sum_P \frac{n_\mu}{g} D^\mu_{ij}(P) O_P = \Lambda^{\mu\dagger}_{ji} \tag{A2}$$

where the matrices $D^\mu(P)$ are a real orthogonal irreducible representation of degree n_μ of the symmetric group S_N ($g = N!$). The elements $D^\mu_{ij}(P)$ obey the orthogonality relation

$$\frac{n_\mu}{g} \sum_P D^\mu_{ij}(P) D^\lambda_{lm}(P) = \delta_{il}\delta_{jm}\delta_{\mu\lambda}. \tag{A3}$$

It follows that

$$O_P\Lambda^\mu_{ij} = \sum_k D^\mu_{ki}(P)\Lambda^\mu_{kj} \tag{A4}$$

and

$$\Lambda^\mu_{ij}\Lambda^\lambda_{lm} = \delta_{jl}\delta_{\mu\lambda}\Lambda^\mu_{im}. \tag{A5}$$

The Hermitian projection operators Λ^μ_{ii} satisfy the completeness relation

$$\sum_{i\mu} \Lambda^\mu_{ii} = \text{the identity operator} \equiv 1. \tag{A6}$$

The associate representation

The matrices $\delta_P D^\mu(P) \equiv D^{\tilde{\mu}}(P)$, where δ_P is -1 if P is odd and $+1$ otherwise, form an irreducible representation which is said to be associate to $D^\mu(P)$.

The construction of an antisymmetric function

We expand the antisymmetrizing projection operator A in terms of the operators $\Lambda_{ij}^{\mu\alpha}$ and $\Lambda_{lm}^{\lambda\beta}$ which act on, say, the coordinate and spin space (α) and the isospin space (β), respectively. The expansion of the identity is given by

$$1 = (\sum_{i\mu} \Lambda_{ii}^{\mu\alpha})(\sum_{l\lambda} \Lambda_{ll}^{\lambda\beta})$$

and the operator

$$A \equiv \frac{1}{g} \sum_{P} \delta_P O_P^{\alpha} O_P^{\beta}.$$

Hence

$$A = \frac{1}{g} \sum_{il\mu\lambda P} \delta_P (O_P^{\alpha} \Lambda_{ii}^{\mu\alpha})(O_P^{\beta} \Lambda_{ll}^{\lambda\beta}). \tag{A7}$$

Substituting (A4) in (A7), we find

$$\begin{aligned} A &= \frac{1}{g} \sum_{\substack{il\mu\lambda P \\ rs}} \delta_P D_{ri}^{\mu}(P) D_{sl}^{\lambda}(P) \Lambda_{ri}^{\mu\alpha} \Lambda_{sl}^{\lambda\beta} \\ &= \frac{1}{g} \sum_{\substack{il\mu\lambda \\ rs}} \{\sum_{P} D_{ri}^{\tilde{\mu}}(P) D_{sl}^{\lambda}(P)\} \Lambda_{ri}^{\mu\alpha} \Lambda_{sl}^{\lambda\beta} \\ &= \sum_{ir\lambda} \frac{1}{n_\lambda} \Lambda_{ri}^{\tilde{\lambda}\alpha} \Lambda_{ri}^{\lambda\beta} \qquad \text{from (A3).} \end{aligned} \tag{A8}$$

The group S_3

Real orthogonal irreducible representations of S_3 are given by Hamermesh (1961, p. 224). We find that the corresponding symmetrizing operators Λ_{ij}^{m} for the two-dimensional representation D^m of S_3 satisfy the relations

$$\Lambda_{12}^{\tilde{m}} = -\Lambda_{21}^{m}$$

and

$$\Lambda_{11}^{\tilde{m}} = \Lambda_{22}^{m}. \tag{A9}$$

The antisymmetrizing projection operator (A8) for three fermions is therefore given by

$$A = \Lambda^{s\alpha}\Lambda^{a\beta} + \Lambda^{a\alpha}\Lambda^{s\beta} + \tfrac{1}{2}(\Lambda_{11}^{m\alpha}\Lambda_{22}^{m\beta} - \Lambda_{21}^{m\alpha}\Lambda_{12}^{m\beta}) + \tfrac{1}{2}(\Lambda_{22}^{m\alpha}\Lambda_{11}^{m\beta} - \Lambda_{12}^{m\alpha}\Lambda_{21}^{m\beta}). \tag{A10}$$

Λ_{11}^{m} and Λ_{21}^{m} generate functions which are symmetric in the indices (12), whilst Λ_{22}^{m} and Λ_{12}^{m} generate functions that are antisymmetric in these indices.

Appendix 2

Functions spanning the spin or isospin space of three fermions

Below we give a table of a complete set of orthonormal spin functions for three fermions (adapted from Schiff 1955, p. 235). The particle indices are ordered 1, 2, 3 in every term.

Table 1

	S or T	M_S or M_T
$\|1\rangle = \uparrow\uparrow\uparrow$	$\frac{3}{2}$	$\frac{3}{2}$
$\|2\rangle = 3^{-1/2}(\uparrow\downarrow\uparrow + \downarrow\uparrow\uparrow + \uparrow\uparrow\downarrow) = \sqrt{3}\Lambda^{s}(\uparrow\uparrow\downarrow)$	$\frac{3}{2}$	$\frac{1}{2}$
$\|3\rangle = 3^{-1/2}(\downarrow\uparrow\downarrow + \uparrow\downarrow\downarrow + \downarrow\downarrow\uparrow)$	$\frac{3}{2}$	$-\frac{1}{2}$
$\|4\rangle = \downarrow\downarrow\downarrow$	$\frac{3}{2}$	$-\frac{3}{2}$
$\|5\rangle = 6^{-1/2}(2\uparrow\uparrow\downarrow - \uparrow\downarrow\uparrow - \downarrow\uparrow\uparrow) = \sqrt{\frac{3}{2}}\Lambda_{11}^{m}(\uparrow\uparrow\downarrow) = \|\overline{12}3\rangle$	$\frac{1}{2}$	$\frac{1}{2}$
$\|6\rangle = 6^{-1/2}(2\downarrow\downarrow\uparrow - \downarrow\uparrow\downarrow - \uparrow\downarrow\downarrow)$	$\frac{1}{2}$	$-\frac{1}{2}$
$\|7\rangle = 2^{-1/2}(\uparrow\downarrow\uparrow - \downarrow\uparrow\uparrow) = \sqrt{\frac{3}{2}}\Lambda_{12}^{m}(\uparrow\uparrow\downarrow) = \|\widetilde{12}3\rangle$	$\frac{1}{2}$	$\frac{1}{2}$
$\|8\rangle = 2^{-1/2}(\downarrow\uparrow\downarrow - \uparrow\downarrow\downarrow)$	$\frac{1}{2}$	$-\frac{1}{2}$

The bar or tilde over two- or more-particle indices indicates symmetry or antisymmetry, respectively, in those indices.

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