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Complement to the Rayleigh-Ritz principle for the energy spectrum of a system composed of identical particles

Richard L. Hall
Department of Mathematics, Concordia University, Montreal, Quebec, Canada
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A theorem is proved which states that the energies E_i of a general translation-invariant system of N identical particles interacting by pair potentials and obeying nonrelativistic quantum mechanics are bounded *below* one by one by the energies E_i^L of a related model system consisting of $(N\text{-}1)$ noninteracting particles of the same symmetry type bound to a fixed center. The theorem is applied to a three-fermion harmonic oscillator test system whose exact eigenvalues are found. The ratios E_i^L/E_i for this problem satisfy $E_i^L/E_i \geq E_0^L/E_0 = \sqrt{3}/4$ for at least the first twenty three-body states.

[NUCLEAR STRUCTURE Lower energy bounds provided by exactly soluble atom-like model. Justification for shell theory. Application to harmonic oscillator test system.]

I. INTRODUCTION

We shall be concerned with a system of N identical particles which interact by pair potentials and obey nonrelativistic quantum mechanics. The translation-invariant Hamiltonian H for the system is as follows

$$H = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} - \frac{1}{2Nm}\left(\sum_{i=1}^{N} \vec{p}_i\right)^2 + \sum_{i<j} v_{ij}\,, \tag{1}$$

where v_{ij} depends on the pair distance $|\vec{r}_i - \vec{r}_j|$, the spins, and the isotopic spins of the particles i and j. For clarity of presentation we shall assume throughout that the particles are identical *fermions* although an exactly similar treatment is also possible for bosons.

A great deal of physics is encompassed by Hamiltonians with the form H. Our purpose here is to exploit the necessary permutation symmetry of the eigenstates to relate the energies E_i of H to those of specially constructed two-body problems. The methods we establish yield energy lower bounds $E_i^L \leq E_i$ which complement the upper bounds available by variational calculations.

Method I (Ref. 1) which can be regarded as a rigorous formulation of Wigner's equivalent two-body method[2] gives some excellent results for a wide variety of nonsaturating boson systems [e.g., $(E_0^L - E_0)E_0^{-1} \downarrow 0$ as $N \uparrow \infty$ for the square-well potential]. For N-fermion systems our Method II (Ref. 3) is sensitive to the choice of relative coordinates: with a suboptimal set of $(N-1)$ pair-distance coordinates [with "coefficient of orthogonality" $\lambda = 2(N-1)/N$] this method yields a bound E_0^L which is equal to the lowest energy of an atom-like Hamiltonian $\mathcal{H}$ corresponding to $(N-1)$ noninteracting identical particles bound to a fixed center [see Eq. (4) below]. We shall prove in Sec. II that the exact energies E_i of H are bounded one by one by the energies E_i^L of $\mathcal{H}$; that is to say, we can immediately extend method II to the excited N-body states.

In an earlier brief outline[4] of this approach to the excited-states problem, we gave no estimate of the quality of the bounds. If the bounds are good, then the theorem provides, for example, a very general justification for the success of nuclear shell theory [the total relative angular momentum operator is *exactly* the sum of the angular momenta of the $(N-1)$ particles of the model $\mathcal{H}$]. While the success of method I can be understood *a posteriori* on physical grounds, we have as yet no such intuitive understanding of method II or its present generalization. Instead we offer an example, the exact solution of a three-fermion harmonic oscillator problem. For this test system the lower-bound method gives as good results for the energies of the first twenty many-body states as for the ground state; the ground-state bound itself improves with increasing N for we have[3]

$$E_0^L/E_0 = \sqrt{3}\,(N-1)/2(N+1)\,.$$

II. LOWER-BOUND SPECTRAL THEOREM

We denote by A_N the Hilbert space of translation-invariant wave functions which are antisymmetric in the indices 1 to N and by A_{N-1} the corresponding Hilbert space of wave functions antisymmetric only in the indices 2 to N: Thus A_N is a subspace of A_{N-1}.

Throughout this section of the paper we use a set of relative coordinates $\vec{\rho}_i$ which are proportional to $(N-1)$ pair distances, thus

$$\vec{\rho}_i = \frac{1}{\sqrt{2}}(\vec{r}_i - \vec{r}_1), \quad i = 2, 3, \ldots, N. \tag{2}$$

For these coordinates the coefficient of orthogonality[3] λ has the value $\lambda = 2(N-1)/N$. By the argument of Hall[3] we can write

$$\langle H \rangle = \langle \mathcal{H} \rangle, \tag{3}$$

where

$$\mathcal{H} = (N-1)^{-1}(\mathcal{H}_2 + \mathcal{H}_3 + \cdots + \mathcal{H}_N), \tag{4}$$

$$\mathcal{H}_i = (N-1)\left(-\frac{\hbar^2}{2m\lambda}\Delta_{\vec{\rho}_i} + \tfrac{1}{2}Nv_{1i}\right), \tag{5}$$

and the wave function for the expectation values is chosen in the Hilbert space A_N. We note that $\mathcal{H}_2$ is just the reduced Hamiltonian of our method II.[3]

We now consider the finite dimensional subspace U_n of A_N spanned by the first n eigenfunctions of the full N-particle Hamiltonian H, i.e.,

$$\psi \in U_n, \quad \psi = \sum_{i=1}^{N} C_i \psi_i, \tag{6}$$

where the C_i are constants. Since $U_n \subset A_N \subset A_{N-1}$, we may consider ψ given by Eq. (6) as a "trial function" for the problem $\mathcal{H}$ in A_{N-1}. Thus we are using the (unknown) exact N-particle wave functions to construct a trial function for the model system $\mathcal{H}$ in A_{N-1}. The Rayleigh-Ritz theorem (e.g., Weinstein and Stenger (Ref. 5, p. 13); other accounts of the general theorem, including the excited states, may be found in Refs. 16, 17, 18, and 19) tells us that the n (not necessarily distinct) minima of $(\psi, \mathcal{H}\psi)/(\psi, \psi)$ are one by one *upper* bounds to the first n energies E_i^L, $i = 1, 2, \ldots, N$, of our model $\mathcal{H}$ in A_{N-1}. Since $\psi \in U_n \subset A_N$, $(\psi, \mathcal{H}\psi) = (\psi, H\psi)$, and we see that the minima of $(\psi, \mathcal{H}\psi)/(\psi, \psi)$ are just the first n energies E_i, $i = 1, 2, \ldots, n$, of H in A_N. Therefore, since n is limited only by the number of bound states of H in A_N, we have proved the *lower bound spectral theorem:*

$$E_i^L \leq E_i. \tag{7}$$

The model energies E_i^L can be found as in zeroth approximation atomic physics (noninteracting electrons) by considering all linearly independent $(N-1)\times(N-1)$ Slater determinants of eigenfunctions of the Hamiltonians $\mathcal{H}_i$ [Eq. (5)]. The proof of the corresponding theorem for bosons is obtained by replacing antisymmetry by symmetry in all the above steps.

If one uses instead of $\mathcal{H}$ the *two-body* reduced Hamiltonian $\mathcal{H}_2$ of method I,[1] or that of method II,[3] then the above proof of the lower bound spectral theorem will not go through because the Hilbert space spanned by the eigenfunctions of $\mathcal{H}_2$ does not contain A_N as a subspace and the Rayleigh-Ritz theorem is therefore not applicable in the sense required. Furthermore, the conjecture that the spectrum of $\mathcal{H}_2$ (as in either method I or II) provides lower bounds to the spectrum of H is easily falsified by the harmonic oscillator.

III. THE EXACT SPECTRUM OF A THREE-FERMION PROBLEM

It is difficult, even for the harmonic oscillator interaction, to find *exact* many-body solutions which satisfy both the translation invariance and the permutation symmetry requirements. Moreover, in order to test the theorem of Sec. II we must find the correct degeneracies for the eigenvalues. The simplest system which has the features of an N-fermion problem consists of three scalar particles interacting in one spatial dimension and restricted to spatially antisymmetric states, i.e., a system of "scalar fermions."[6] In this section of the paper we use only Jacobi orthogonal relative coordinates (x, y) which are given by

$$x = (1/\sqrt{2})(x_1 - x_2)$$

and

$$y = (1/\sqrt{6})(x_1 + x_2 - 2x_3), \tag{8}$$

where (x_1, x_2, x_3) are the individual-particle coordinates. In terms of Jacobi coordinates the Hamiltonian H [Eq. (1)] separates for the harmonic oscillator[6] so that we may write

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}\right) + \frac{\hbar^2}{6m}\left(\frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} + \frac{\partial}{\partial x_3}\right)^2 + k^2[(x_1 - x_2)^2 + (x_1 - x_3)^2 + (x_2 - x_3)^2] \tag{9}$$

and

$$H = \tfrac{1}{2}(\mathcal{H}_x + \mathcal{H}_y), \tag{10}$$

where

$$\mathcal{H}_x = -\frac{\hbar^2}{m}\frac{\partial^2}{\partial x^2} + 6k^2x^2, \tag{11}$$

and similarly for $\mathcal{H}_y$. We see that $\mathcal{H}_x$ is just the reduced Hamiltonian of method I.[1] In the present problem the eigenfunctions ϕ_i of $\mathcal{H}_x$ are Hermite functions with corresponding nondegenerate eigenvalues given by

$$\epsilon_i = (2i+1)\epsilon_0, \tag{12}$$

where i is a positive or zero integer and

$$\epsilon_0 = 2\sqrt{3}\,(\hbar^2 k^2/2m)^{1/2}\,. \tag{13}$$

In view of Eqs. (10) and (12) we see that *every* eigenfunction of H is either a single product of the form

$$\phi_{ij}(x, y) = \phi_i(x)\phi_j(y) \tag{14}$$

or a linear combination of such products with constant total order $n = (i+j)$. A single product can never be antisymmetric[7,8] but suitable linear combinations may so be. Thus, for example, the ground state of H in A_3 is given[3] by

$$\psi_0 = (\sqrt{3}/2)\phi_{12} - \tfrac{1}{2}\phi_{30}\,, \tag{15}$$

and consequently

$$E_0 = 4\epsilon_0\,. \tag{16}$$

Our problem at present is to determine the higher eigenfunctions and eigenvalues of H in A_3. The analysis of Post[9] tells us how to arrange the correct permutation symmetry for certain "suspect" excited states but does not guarantee their translation invariance. For example, if $(i+j) = 4$, Post's "suspect" state has the factor $\det|\phi_0(x_1)\ \phi_1(x_2)\ \phi_3(x_3)|$ but this Slater determinant turns out *not* to be translation invariant. Our approach therefore will be to work initially with translation-invariant functions and project them into A_3.

Since the coordinate y is invariant under the permutation (12), a single product ϕ_{ij} will be antisymmetric under the operator P corresponding to (12) if and only if i is odd; we shall now therefore only consider single-products with first index odd, i.e., single products in A_2. If the three cycle (123) has corresponding operator Q (see the Appendix), then the projector A onto A_3 may be written

$$A = \tfrac{1}{6}(1 - QP - Q^2P)(1 - P)\,. \tag{17}$$

Since $P\phi = -\phi$ for $\phi \in A_2$, the projector from A_2 to A_3 becomes

$$A = \tfrac{1}{3}(1 + Q + Q^2) = \tfrac{1}{3}(1 + 2T)\,, \tag{18}$$

where

$$T = \tfrac{1}{2}(Q + Q^2) = \tfrac{1}{2}(Q + Q^\dagger) = T^\dagger\,. \tag{19}$$

We have studied inner products of the form $(\phi_{ij}, T\phi_{km})$ and we find (in the Appendix) that they vanish unless $i+j = k+m$. Hence $A\phi_{ij}$ yields a linear combination of single products with the same total order $(i+j)$ (of Hermite polynomials in x and y). We have found [Eq. (A5)] an explicit expression for the elements

$$T^{(n)}_{ik} = (\phi_{i(n-i)}, T\phi_{k(n-k)})\,, \tag{20}$$

and we denote by $T^{(n)}$ the corresponding matrix (note that i and k are *odd* because we *only* consider single products which lie in A_2). Thus A_3 is divided into subspaces (of fixed total order) by projectors with matrix representations $A^{(n)} = \frac{1}{3}(I + 2T^{(n)})$. The dimensions of the subspace (n) is given by $\mathrm{tr}A^{(n)}$ which is also the degeneracy of the corresponding eigenvalues $(n+1)\epsilon_0$ of H: the dimensions of the subspaces are at least 1 unless $n = 0, 1, 2$, or 4 for which values the dimensions are zero (see the Appendix).

Since $A^{(n)}A^{(n)} = A^{(n)}$ we have

$$\sum_k A^{(n)}_{ik}A^{(n)}_{kj} = A^{(n)}_{ij} \tag{21}$$

and the normalized eigenstates of H in A_3 are therefore given by

$$\frac{A\phi_{i(n-i)}}{\|A\phi_{i(n-i)}\|} = \left(\sum_k A^{(n)}_{ki}\phi_{k(n-k)}\right)(A^{(n)}_{ii})^{-1/2}\,, \tag{22}$$

The number of linearly independent functions for a given value of n is just the dimension $\mathrm{tr}A^{(n)}$ of the subspace defined by $A^{(n)}$. From Eq. (22) we find, for example, the following first three eigenfunctions of H in A_3 which correspond, respectively, to the nondegenerate eigenvalues $E_0 = 4\epsilon_0$, $E_1 = 6\epsilon_0$, and $E_2 = 7\epsilon_0$:

$$\begin{aligned}
\psi_0 &= (\sqrt{3}/2)\phi_{12} - \tfrac{1}{2}\phi_{30}\,,\\
\psi_1 &= \tfrac{3}{4}\phi_{14} + (\sqrt{2}/4)\phi_{32} - (\sqrt{5}/4)\phi_{50}\,,\\
\psi_2 &= (\sqrt{3}/4)\phi_{15} - (\sqrt{10}/4)\phi_{33} + (\sqrt{3}/4)\phi_{51}\,.
\end{aligned} \tag{23}$$

The degeneracies of the first few eigenvalues $(n+1)\epsilon_0$ of H in A_3 which occur (i.e., $n \neq 0, 1, 2$, or 4) are shown in Table I. Hence we have in Table I the first 20 exact eigenvalues of the translation-invariant three fermion problem with Hamiltonian H [Eq. (9)].

TABLE I. The exact eigenvalues of H and their degeneracies for the three-fermion harmonic-oscillator problem: the units are $\epsilon_0 = 2\sqrt{3}(\hbar^2k^2/2m)^{1/2}$; the positive integer n is the total order of Hermite polynomials in x and y in the corresponding eigenfunctions, and $n \neq 0$, 1, 2, or 4.

$E/\epsilon_0 = (n+1)$	4	6	7	8	9	10	11	12	13	14	15	16
Degeneracy	1	1	1	1	1	2	2	2	2	2	2	3

An arduous part of this work has been to find the explicit recipe [Eq. (A5)] for the matrices $T^{(n)}_{ik}$: with this formula all the eigenfunctions and eigenvalues of H for the three-fermion harmonic oscillator can readily be obtained. The author feels that there must be an easier route to these results, perhaps via the properties which matrix representations of $T=\frac{1}{2}(Q+Q^{\dagger})$ must necessarily have. The three-body harmonic oscillator functions which are doubly orthogonal[10] are also useful as *trial functions* for other interaction potentials. For example, if we use ψ_1 [Eq. (23)] we have

$$E_0 \leq (\psi_1, H\psi_1) = (\psi_1, \mathcal{H}_x\psi_1)$$
$$= \tfrac{9}{16}(\phi_1, \mathcal{H}_x\phi_1) + \tfrac{1}{8}(\phi_3, \mathcal{H}_x\phi_3)$$
$$+ \tfrac{5}{16}(\phi_5, \mathcal{H}_x\phi_5),$$

and the integrations required for this variational upper bound are only with respect to the single variable x. If linear combinations of the ψ_i are used, $\mathcal{H}_x$ will in general connect different ϕ_i; however, the double orthogonality will eliminate many terms and the remaining integrals will again all be over a single variable.

IV. AN EXPLICIT LOWER BOUND SPECTRUM

We now apply the theorem of Sec. II to the three-fermion problem which we have solved exactly in Sec. III. For the lower bound spectrum we must find the eigenvalues of $\mathcal{H}=\frac{1}{2}(\mathcal{H}_2+\mathcal{H}_3)$ [Eq. (4)] in the space A_2 of translation-invariant wave functions which are antisymmetric under the permutation (23). We use (x,z) to represent the pair-distance coordinates (ρ_2,ρ_3) for the three-particle problem in one dimension, i.e.,

$$x=(1/\sqrt{2})(x_1-x_2),$$
$$z=(1/\sqrt{2})(x_1-x_3). \tag{24}$$

The eigenvalues ϵ_i' of the operator $\mathcal{H}_2$ [see Eq. (5), $\lambda=\frac{4}{3}$], i.e.,

$$\mathcal{H}_2=-\frac{3\hbar^2}{4m}\frac{\partial^2}{\partial x^2}+6k^2x^2 \tag{25}$$

are given by

$$\epsilon_i'=(2i+1)(\sqrt{3}/2)\epsilon_0, \tag{26}$$

where ϵ_0 is the same as in Eq. (13) and i is a positive or zero integer. The eigenfunctions of $\mathcal{H}$ in A_2 are therefore 2×2 Slater determinants of eigenfunctions of $\mathcal{H}_2$ and $\mathcal{H}_3$, and the corresponding eigenvalues E^L have the form $E^L=(n+1)(\sqrt{3}/2)\epsilon_0$ where $n\geq 1$ is a positive integer. The first few of these eigenvalues along with their degeneracies are presented in Table II. In Table III we give

TABLE II. The eigenvalues of the model $\mathcal{H}$ and their degeneracies for the three-fermion harmonic oscillator problem: ϵ_0 is the same as in Table I; the positive integer n is the total order of Hermite polynomials in x and z in the corresponding eigenfunctions, and $n\geq 1$.

$2E^L/\sqrt{3}\epsilon_0=(n+1)$	2	3	4	5	6	7	8	9
Degeneracy	1	1	2	2	3	3	4	4

the ratio E_i^L/E_i (determined from Tables I and II) in terms of the ratio $E_0^L/E_0=\sqrt{3}/4$, i.e., the ratio we get by applying method II[3] to estimate the *ground-state* energy of the three-fermion problem. Thus, as far as we have calculated (the 20th three-body state), the lower bound spectral theorem of Sec. II gives results for the excited state energies of the harmonic oscillator test problem which are at least as good as method II[3] applied to the ground state energy, i.e., $E_i^L/E_i\geq\sqrt{3}/4 = 0.433$. The degeneracies for the model eigenvalues (Table II) appear to increase faster than the degeneracies for the exact eigenvalues (Table I) so that the quality of the lower bound may deteriorate as we go to even higher excited states of the system.

V. CONCLUSION

We have proved that the spectrum E_i of a translation invariant nuclear or molecular physics type of N-particle Hamiltonian H is bounded below by the spectrum E_i^L of an atomic physics type of $(N-1)$ particle Hamiltonian

$$\mathcal{H}=\frac{1}{N-1}\sum_{i=2}^{N}\mathcal{H}_i,$$

i.e., $E_i^L\leq E_i$. The theorem we have proved requires a model Hamiltonian which, for fermions, satisfies $\langle\mathcal{H}\rangle=\langle H\rangle$ in A_N, and whose eigenfunctions span a Hilbert space which includes A_N as a subspace (for bosons A_N is replaced by S_N). The quality of the lower bounds in the case of our fermion harmonic oscillator test problem is as good as was method II[3] for the lowest eigenvalue E_0 alone.

It is both surprising and interesting that a nuclear (or molecular) type of Hamiltonian H should be so closely related to a simple atomlike Hamiltonian $\mathcal{H}$ (i.e., with noninteracting "electrons"), whereas the corresponding lower-bound results[10-12] for general atomlike Hamiltonians *themselves* appear to be less impressive. For atomlike systems we have the following comparisons with the results of this paper: (a) the "reduction" of the $(N+1)$-body problem[12] is only to a three-body problem so that the many-body difficulty has not

TABLE III. The ratio of the lower bound E_i^L to the exact energy E_i for the first 20 states of the three-fermion harmonic oscillator problem.

i = eigenvalue index	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
$(E_i^L/E_i)\times 4/\sqrt{3}$	1	1	$\frac{8}{7}$	1	$\frac{10}{9}$	1	$\frac{6}{5}$	$\frac{12}{11}$	$\frac{12}{11}$	$\frac{7}{6}$	$\frac{7}{6}$	$\frac{14}{13}$	$\frac{16}{13}$	$\frac{8}{7}$	$\frac{8}{7}$	$\frac{16}{15}$	$\frac{6}{5}$	$\frac{9}{8}$	$\frac{9}{8}$	$\frac{9}{8}$

been removed; (b) the exact results[6] for the ground-state energies of appropriate harmonic-oscillator test systems show that the lower bound may become arbitrarily bad as N increases[12]; (c) an extension of the ground-state energy bound for atomlike systems to the excited states does not appear to follow immediately[11] from the theorems of Coleman,[10] Calogero,[11] or Hall[12]; in fact, the natural analog of the main result of the present paper is falsified for atomlike systems by the exact harmonic oscillator solutions.[6] Therefore, although it runs counter to our usual expectations, we are tempted to ask the general question whether "shells" may not be a more fundamental feature of nuclear type systems than they are of atomlike systems. If this were really the case, we should expect that method II[3] could be sequentially improved so that the exact solutions were approached without losing the shell structure of the model. Improvements to method II to date, however, are still rather modest[13]: for the ground-state of the N-fermion harmonic oscillator test system we still obtain at best about 86% of the exact energy for large N.[3,13]

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APPENDIX

The operator Q corresponding to the 3 cycle (123) acting on the individual-particle indices is defined for functions of Jacobi coordinates (x, y) by

$$(Q\psi)\left(-\tfrac{1}{2}x-\frac{\sqrt{3}}{2}y,\frac{\sqrt{3}}{2}x-\tfrac{1}{2}y\right)=\psi(x,y)\,. \tag{A1}$$

The matrix elements we need are

$$T_{ijkm}=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\phi_i(x)\phi_j(y)T\phi_k(x)\phi_m(y)dxdy\,, \tag{A2}$$

where $T=\frac{1}{2}(Q+Q^2)=T^\dagger$, and $\phi_i(x)$ is an ith-order Hermite function. Now from Jahnke, Emde, and Lösch[14] (p. 102) we have

$$\frac{(a^2+b^2)^{n/2}}{n!}H_n\left(\frac{ax+by}{(a^2+b^2)^{1/2}}\right)=\sum_{i+j=n}\frac{a^ib^i}{i!j!}H_i(x)H_j(y)\,, \tag{A3}$$

where a and b are constants and $H_n(x)$ is an nth-order Hermite polynomial. Meanwhile by adapting from Erdélyi[15] (p. 290, No. 15) we have

$$\int_{-\infty}^{\infty}e^{-x^2}H_k(x)H_m(x)H_n(x)dx=\frac{\pi^{1/2}k!m!n!2^{(m+n+k)/2}}{(s-k)!(s-m)!(s-n)!}\,, \tag{A4}$$

provided $k+m+n=2s$ is an even integer, and $s\geq k,m,n$; otherwise the integral vanishes. By applying (A3) and (A4) in (A2) we find after a very lengthy calculation that T_{ijkm} is zero unless $i+j=k+m$ and, in this case, assuming i and k are odd and $i\geq k$,

$$T_{i(n-i)k(n-k)}\equiv T_{ik}^{(n)}=T_{ki}^{(n)}$$

is given by the following expression:

$$T_{ik}^{(n)}=\left(-\frac{1}{2}\right)^n\left(\frac{k!(n-k)!}{i!(n-i)!}\right)^{1/2}3^{(i-k)/2}\times\sum_{w=0}^{\min(k,n-i)}\binom{i}{k-w}\binom{n-i}{w}(-3)^w\,, \tag{A5}$$

where $\binom{n}{m}$ is the binomial coefficient $n!/m!(n-m)!$. The matrix representation $A^{(n)}$ of the Hermitian projector from A_2 to A_3 is given by

$$A^{(n)}=\tfrac{1}{3}(2T^{(n)}+I)\,. \tag{A6}$$

We have used (A5) and (A6) to find the antisymmetric wave functions with total order n of Hermite polynomials in x and y and also the degeneracies $\mathrm{tr}A^{(n)}$ of the corresponding eigenvalues $(n+1)\epsilon_0$ of H. The diagonal elements $T_{ii}^{(n)}$ can be expressed as the values of certain Jacobi polynomials but we have not found this relationship to be very helpful.

In order that $\mathrm{tr}A^{(n)}=0$ it is *necessary* in particular that $A\phi_{1(n-1)}=0$ and therefore also that $T_{11}^{(n)}=-\frac{1}{2}$. Now from (A5) we find

$$T_{11}^{(n)}=(-\tfrac{1}{2})^n(4-3n)\,. \tag{A7}$$

Therefore $T_{11}^{(n)}=-\frac{1}{2}$ for $n=1,2$, and 4 *only*, and consequently the subspace defined by $A^{(n)}$ is nonempty for *all other* positive integer values of n. By direct computation we find $\mathrm{tr}A^{(n)}=0$ for $n=0,1,2$, and 4.

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