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Improved energy lower bound for the N -fermion system

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Abstract. The exact analytical solution of inhomogeneous differential equations, resulting from the improvement of the known methods due to Post and Hall, is presented. As an illustration, the energy lower bounds of N -fermion systems with oscillator and gravitational interaction are calculated and the results compared with the earlier data.

1. Introduction

The known energy-lower-bound methods due to Hall and Post for N -fermion systems have recently been modified by Manning (1978) and by Balbutsev and Mikhailov (1977, 1979), in which the original equations were derived and solved using series expansions of limited applicability. The exact solution of these equations is found here. As an illustration, the energy lower bounds of N -fermion systems with oscillator and gravitational interaction are calculated. The results are compared with the earlier data and some mistakes in Manning's (1978) paper are revealed.

2. Hall method

To estimate the energy lower bound of the N -fermion system by the modified Hall method one has to solve the equation

$$(h(\boldsymbol{\rho}) - \epsilon)\psi(\boldsymbol{\rho}) = \beta\delta(\boldsymbol{\rho}) \quad (1)$$

with the constraint $\psi(0) = 0$.

Here $h(\boldsymbol{\rho}) = -(\hbar^2/2\mu)\Delta + (N/2)v(\boldsymbol{\rho})$, $\mu = m\lambda$, m is the mass of a particle, λ is a parameter depending on the definition of relative coordinates $\boldsymbol{\rho}$ (in our case $\lambda = \frac{2}{3}$), v is a two-particle interaction and β is an indefinite multiplier to be found below from the boundary condition. The lower bound is a sum of $N - 1$ lowest energy levels ϵ_i .

To solve the inhomogeneous equation (1) it is natural to use the Green function method. First consider the one-dimensional problem

$$(h(x) - \epsilon)\psi(x) = Q(x). \quad (2)$$

The general solution of this inhomogeneous second-order differential equation is

$$\psi(x) = \alpha_1\varphi_1(x) + \alpha_2\varphi_2(x) + f(x)$$

where $f(x)$ is its particular solution. The functions $\varphi_1(x)$ and $\varphi_2(x)$ are linearly

independent solutions of the homogeneous equation

$$[h(x) - \epsilon]\varphi(x) = 0.$$

The Green function of this equation is (Baz' *et al* 1971)

$$G(x, x') = \begin{cases} \varphi_1(x)\varphi_2(x') & \text{when } x > x' \\ \varphi_2(x)\varphi_1(x') & \text{when } x < x'. \end{cases}$$

Using $G(x, x')$ one can find the particular solution of the inhomogeneous equation (2):

$$f(x) = \int_{-\infty}^{\infty} G(x, x')Q(x') dx'.$$

The factors α_1 and α_2 are defined by normalisation and boundary conditions.

For demonstration purposes we shall solve the problem of N fermions interacting through oscillator forces:

$$\left(-\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + \frac{N}{2} \gamma x^2 - \epsilon\right)\psi(x) = \beta\delta(x). \quad (3)$$

The linearly independent solutions of the corresponding homogeneous equation are the well-known even and odd oscillator functions

$$\varphi_1 = \exp(-\xi^2/2)F\left(\frac{1-e}{4}, \frac{1}{2}; \xi^2\right), \quad \varphi_2 = \xi \exp(-\xi^2/2)F\left(\frac{3-e}{4}, \frac{3}{2}; \xi^2\right)$$

where F is the confluent hypergeometrical function, $\xi = x(\mu\gamma N/\hbar^2)^{1/4}$, $\epsilon = e(\hbar^2\gamma N/4\mu)^{1/2} = e\hbar\omega/2$. The general solution of equation (3) is

$$\psi(x) = \alpha_1\varphi_1(x) + \alpha_2\varphi_2(x) + \beta G(x, 0)$$

where

$$G(x, 0) = \begin{cases} 0 & \text{when } x > 0 \\ \varphi_2(x) & \text{when } x < 0. \end{cases}$$

Using the constraint $\psi(0) = 0$ we have $\alpha_1 = 0$. Putting the wavefunction at $x = \pm\infty$ equal to zero one finds $(3-e)/4 = -n$. This condition gives the energy spectrum:

$$\epsilon = (4n+3)\hbar\omega/2 = [(2n+1) + \frac{1}{2}]\hbar\omega = (k + \frac{1}{2})\hbar\omega, \quad k = 1, 3, 5, \dots \quad (4)$$

Clearly it is this part of the spectrum which corresponds to odd states of the usual oscillator. The Hamiltonian is symmetric under inversion, so the wavefunction must be either odd or even, that is $\psi(-x) = \pm\psi(x)$. Hence β may take two values:

(i) $\beta = 0$ when the wavefunction is odd; then

$$\psi(x) = \alpha_2\varphi_2(x),$$

(ii) $\beta = -2\alpha_2$ when the wavefunction is even; then

$$\psi(x) = \begin{cases} \alpha_2\varphi_2(x), & x > 0 \\ -\alpha_2\varphi_2(x), & x < 0. \end{cases}$$

The coefficient α_2 is defined by the normalisation condition

$$2\alpha_2^2 \int_0^{\infty} \varphi_2^2(x) dx = 1.$$

So we have found that the set of eigenvalues of equation (3) consists of the levels, corresponding to odd states of the usual harmonic oscillator, every level being doubly degenerate.

Manning (1978) came to the same conclusion in quite a different way. He has found odd wavefunctions (together with corresponding energy levels) as solutions of equation (3) with $\beta = 0$. To obtain its eigenvalues at $\beta \neq 0$ he calculated the roots of the equation

$$\sum_{n=0}^{\infty} \frac{|\varphi_{2n}(0)|^2}{e_{2n} - e} = \sum_{n=0}^{\infty} \frac{(2n-1)!!}{(2n)!!} \frac{1}{4n+1-e} = 0$$

where φ_{2n} is an even oscillator wavefunction. This series converges, though very slowly. For the roots of the equation one can deduce analytically the expression

$$e_i = 4i + 3$$

which coincides with equation (4).

The procedure by Manning is useless in the case of the three-dimensional oscillator

$$\left(-\frac{\hbar^2}{2\mu}\Delta + \frac{N}{2}\gamma r^2 - \epsilon\right)\psi(r) = \beta\delta(r) \tag{5}$$

for one must handle the divergent series

$$\sum_{n=0}^{\infty} \frac{(2n+1)!!}{(2n)!!} \frac{1}{4n+3-e} = 0. \tag{6}$$

Let us solve the same problem by the Green function method, although a more simple and obvious solution is possible in this case (see appendix A). The Green function of a three-dimensional Schrödinger equation satisfies the relation (Baz' *et al* 1971)

$$G_E(r, r') = -\frac{2\mu}{\hbar^2} \sum_{l,m} \frac{1}{r \cdot r'} G_{El}(r, r') \cdot Y_{lm}\left(\frac{r}{r}\right) Y_{lm}^*\left(\frac{r'}{r'}\right).$$

Here Y_{lm} is the spherical function, G_{El} is the Green function of the radial Schrödinger equation

$$\left(\frac{d^2}{d\xi^2} - \frac{l(l+1)}{\xi^2} - \xi^2 + 2E\right)R(\xi) = 0$$

where $\xi = r(\mu\omega/\hbar)^{1/2}$, $E = \epsilon/\hbar\omega$, $\omega = (N\gamma/\mu)^{1/2}$. Two of its linearly independent solutions are

$$R_1(\xi) = \xi^{l+1} \exp(-\xi^2/2) F\left(\frac{(3/2)+l-E}{2}, \frac{3}{2}+l; \xi^2\right),$$

$$R_2(\xi) = \xi^{-l} \exp(-\xi^2/2) F\left(\frac{(1/2)-l-E}{2}, \frac{1}{2}-l; \xi^2\right).$$

Hence

$$G_{El}(r, r') = -\frac{1}{2l+1} \begin{cases} R_2(\xi)R_1(\xi') & \text{when } \xi > \xi' \\ R_1(\xi)R_2(\xi') & \text{when } \xi < \xi'. \end{cases}$$

The particular solution of the inhomogeneous equation (5) is

$$f(\mathbf{r}) = -\beta \frac{2\mu}{\hbar^2} \sum_{l,m} \frac{1}{r} Y_{lm}(\theta, \varphi) \iiint \frac{1}{r'} G_{El}(r, r') \delta(r') r'^2 dr' \\ \times Y_{lm}^*(\theta', \varphi') d\Omega' = -\beta \frac{\mu}{\pi \hbar^2} \frac{1}{r} \int_0^\infty \frac{1}{r'} G_{E0}(r, r') \delta(r') dr'$$

The general solution is

$$\psi(\mathbf{r}) = \alpha \frac{R_1(\xi)}{\xi} Y_{lm}(\theta, \varphi) + \frac{R_2(\xi)}{\xi} \left[b Y_{lm}(\theta, \varphi) + \beta \frac{\mu^2 \omega}{2\pi \hbar^3} \delta_{l,0} \right], \quad r > 0.$$

To fulfill the constraint $\psi(0) = 0$ one must put $b = 0, \beta = 0, l \neq 0$. The condition $\psi(\mathbf{r}) \rightarrow 0$ when $r \rightarrow \infty$ determines the eigenvalues

$$E = 2n + l + \frac{3}{2}, \quad l \neq 0.$$

So the required energy spectrum coincides with that of the usual three-dimensional oscillator, but all the s levels must be omitted. This result differs from that of Manning (1978), due to which one has to raise each s level by $1\hbar\omega$, but not to omit it. Apparently, he made a mistake in handling the divergent series (6). The results of calculations are presented in tables 1 (one-dimensional oscillator) and 2 (three-dimensional oscillator).

Table 1. The exact energy of the one-dimensional system of N fermions with the oscillator interaction and its lower bounds calculated by the modified (M) and usual methods by Hall (1967), by the Post (1956) method, and by the modified and usual methods of Carr and Post (1968). The energy is given in units of $(\hbar^2 \gamma N / 2m)^{1/2} = \hbar\omega / \sqrt{3}$.

N	2	3	4	5	6	7	8	9	10
Exact	3	8	15	24	35	48	63	80	99
(M) Hall	2.6	5.2	11.3	17.3	26.9	36.4	49.4	62.4	78.8
Hall	0.9	3.5	7.8	13.9	21.7	31.2	42.4	55.4	70.2
Post	3	6	9	12	15	18	21	24	27
(M) Carr- Post	3	5.2	10.6	15.8	24.0	32.1	43.1	54.0	67.8
Carr-Post	1	3.5	7.4	12.7	19.4	27.5	37.0	48.0	60.4

Table 2. The energy lower bounds of the three-dimensional system of N fermions with the oscillator interaction. The bounds are calculated by the modified (M) and usual methods by Hall (1967), by the Post (1956) method and by the modified and usual methods of Carr and Post (1968). The energy is given in units of $(\hbar^2 \gamma N / 2m)^{1/2} = \hbar\omega / \sqrt{3}$.

N	2	3	4	5	6	7	8	9	10	11	12
(M) Hall	4.3	8.7	13.0	19.1	25.1	31.2	37.2	43.3	51.1	58.9	66.7
Hall	2.6	6.9	11.3	15.6	21.7	27.7	33.8	39.8	45.9	52.0	59.8
Post	5	10	15	20	25	30	35	40	45	50	55
(M) Carr-5 Post		8.7	12.3	17.4	22.5	27.5	32.5	37.5	44.0	50.4	56.9
Carr-Post	3	6.9	10.6	14.2	19.4	24.4	29.5	34.5	39.5	44.5	51.0
Exact	5	10	15	22	29	36	43	50	57	66	75

A further example is the three-dimensional system of N fermions coupled by gravitational forces:

$$\left(-\frac{\hbar^2}{2\mu}\Delta - \frac{N\alpha}{2r} - \epsilon\right)\psi(r) = \beta\delta(r). \quad (7)$$

Here one can use the known results. The Green function of the radial Schrödinger equation

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2}\left(\frac{N\alpha}{2r} + \epsilon\right)\right]R(r) = 0$$

can be expressed (Baz' *et al* 1971) by the Whittaker function $W_{\kappa,\nu}(\xi)$ (Whittaker and Watson 1963) and gamma function

$$G(r, 0) = \frac{\mu}{2\pi\hbar^2} \frac{1}{r} \Gamma(1-\kappa) W_{\kappa,1/2}(-\xi)$$

where $\xi = 2r(-2\mu\epsilon/\hbar^2)^{1/2}$, $\kappa = \alpha N/(-8\epsilon\hbar^2/\mu)^{1/2}$, $\nu = l + \frac{1}{2}$. Only one of two linearly independent solutions of this equation has the required behaviour at the origin:

$$R_1(r) = \exp(-\xi/2)\xi^{l+1}F(l-\kappa+1, 2l+2; \xi).$$

The general solution of the inhomogeneous equation (7) is

$$\psi(r) = \alpha \frac{R_1(r)}{\xi} Y_{lm}(\theta, \varphi) + \frac{\beta}{\pi} \left(\frac{-2\mu^3\epsilon}{\hbar^4}\right)^{1/2} \delta_{l,0} \frac{W_{\kappa,\nu}(\xi)}{\xi}.$$

To fulfill the constraint $\psi(0) = 0$ one has to put $a = 0$ if $l = 0$ and $\beta = 0$ as $W_{\kappa,1/2}(\xi)/\xi \approx \ln \xi$ when $\xi \rightarrow 0$. The wavefunction $\psi(r) \rightarrow 0$ at $r \rightarrow \infty$ only if $\frac{1}{2} + \nu - \kappa = -n$. This equation defines the energy spectrum of the system:

$$\epsilon_{nl} = -\frac{1}{(n+l+1)^2} \frac{\mu N^2 \alpha^2}{8\hbar^2}, \quad l \neq 0.$$

This coincides with the spectrum of the usual Coulomb problem, all the s levels being omitted. This result differs from that of Manning (1978). For the s-level energy he takes the roots of the equation

$$\sum_{n=0}^{\infty} \frac{|R_{n0}(0)|^2}{\epsilon_{n0} - e} = 0 \quad (8)$$

where $R_{n0}(r)$ is the radial Coulomb wavefunction of the s state. Here the mistake is evident: the integral over the continuous spectrum should be added to the sum over the discrete levels in equation (8). This is necessary since the bound states alone do not form the complete basis. The results of the calculation are presented in table 3.

3. Carr-Post method

This method has been improved by Balbutsev and Mikhailov (1977, 1979). To determine the energy lower bound by this method one has to solve the variational problem

$$\delta(\langle\psi|\kappa|\psi\rangle - E\langle\psi|\psi\rangle) = 0$$

Table 3. The energy lower bounds of the system of N fermions coupled by 'gravitational' forces. The bounds are calculated by the modified (M) and usual methods by Hall (1967), by the Post (1956) method, and by the modified and usual methods of Carr and Post (1968). The energy is given in units of $(-mN^2\alpha^2/8\hbar^2)$.

N	2	3	4	5	6	7	8	9	10	11	12	13	14	15
(M) Hall	0.2	0.33	0.5	0.6	0.65	0.72	0.80	0.87	0.94	1.02	1.09	1.13	1.18	1.22
Hall	0.7	0.8	1.0	1.2	1.33	1.41	1.48	1.56	1.63	1.70	1.78	1.85	1.93	2.0
Post	0.1	0.25	0.4	0.5	0.625	0.750	0.875	1.00	1.13	1.25	1.38	1.50	1.63	1.75
(M) Carr- Post	0.1	0.33	0.6	0.7	0.81	0.93	1.05	1.16	1.28	1.39	1.50	1.57	1.64	1.70
Carr-Post	0.5	0.8	1.1	1.4	1.67	1.81	1.94	2.07	2.20	2.32	2.44	2.56	2.68	2.80

where

$$\kappa = \sum_{i=2}^N h(\rho_i) = \sum_{i=2}^N \{-(\hbar^2/2\mu)\Delta_i + (N/2)v(\rho_i)\}, \quad \mu = m(N-1)/N,$$

m is the mass of a particle, $\rho_i = r_i - r_1$, r_i is the i th particle coordinate, $\psi(\rho_2, \rho_3, \dots, \rho_N)$ is the trial wavefunction which is antisymmetric relative to the permutation of its coordinates ρ_i . E is the necessary energy; here it is the Lagrange multiplier by which one takes into account the normalisation condition $\langle \psi | \psi \rangle = 1$.

Balbutsev and Mikhailov (1977, 1979) have proposed the additional constraint on the trial wavefunction:

$$\psi(\rho_2, \dots, \rho_i = 0, \dots, \rho_N) = 0, \quad i = 2, 3, \dots, N.$$

This is natural for the case of the wavefunction of the fermion system, as the equality $\rho_i = 0$ means that the coordinates of the i th and first particles coincide. It is convenient to write this constraint in a form of the orthogonality condition of the ψ and δ functions:

$$\int \delta(\rho_i)\psi(\rho_2, \dots, \rho_N) d\rho_i = 0, \quad i = 2, 3, \dots, N. \tag{9}$$

It should be noted that this equation determines the continuum of conditions, as it must be satisfied at any values of all the coordinates $\rho_k (k \neq i)$. Hence, in order to take into account equation (9) in a variational procedure one needs the continuum of the Lagrange multipliers β , that is, they will be functions of the variables $\rho_k (k \neq i)$:

$$\beta = \beta(\rho_2, \dots, \rho_{i-1}, \rho_{i+1}, \dots, \rho_N).$$

Now the variational problem is

$$\delta \left(\langle \psi | \mathcal{H} | \psi \rangle - E \langle \psi | \psi \rangle - \sum_{i=2}^N \int d\rho_2 \cdots \int d\rho_N \delta(\rho_i) \beta(\rho) \psi(\rho_2, \dots, \rho_N) \right) = 0.$$

From the latter one deduces the basic equation of the modified Carr-Post method:

$$(\mathcal{H} - E)\psi(\rho_2, \dots, \rho_N) = \sum_{i=2}^N \delta(\rho_i) \beta(\rho_2, \dots, \rho_{i-1}, \rho_{i+1}, \dots, \rho_N). \tag{10}$$

How is this equation solved? In the case when all the coordinates $\rho_i \neq 0$, it reduces to the usual Schrödinger equation

$$\sum_{i=2}^N h(\rho_i)\psi(\rho_2, \dots, \rho_N) = E\psi(\rho_2, \dots, \rho_N).$$

Its solution is well known:

$$\psi_\alpha(\rho_2, \dots, \rho_N) = \det \varphi_{\alpha_i}(\rho_i), \quad E_\alpha = \sum_{i=2}^N \epsilon_{\alpha_i} \quad h(\rho_i)\varphi_n(\rho_i) = \epsilon_n\varphi_n(\rho_i). \quad (11)$$

Let us consider the behaviour of ψ_α as a function of, say, the coordinate ρ_k . We have

$$\psi_\alpha(\rho_2, \dots, \rho_N) = \begin{cases} \det(\varphi_{\alpha_2}(\rho_2) \dots \varphi_{\alpha_K}(\rho_K) \dots \varphi_{\alpha_N}(\rho_N)), & \rho_k \neq 0 \\ 0, & \rho_k = 0. \end{cases}$$

It will be seen that $\varphi_{\alpha_k}(0) = 0$ for ψ_α must be supposed continuous. So the expression

$$\psi_\alpha(\rho_2, \dots, \rho_N) = \det(\varphi_{\alpha_2}(\rho_2)\varphi_{\alpha_3}(\rho_3) \dots \varphi_{\alpha_N}(\rho_N)) \quad (12)$$

is true at all values of the coordinates $\rho_i (i = 2, 3, \dots, N)$, the 'one-particle' wavefunction φ_{α_i} vanishing at the origin. Let us now substitute equation (12) into equation (10), the ρ_k being arbitrary and all the other coordinates differing from zero:

$$\begin{aligned} [h(\rho_k) - \epsilon_{\alpha_2}]\varphi_{\alpha_2}(\rho_k)A_{k,2} + [h(\rho_k) - \epsilon_{\alpha_3}]\varphi_{\alpha_3}(\rho_k)A_{k,3} + \dots + [h(\rho_k) - \epsilon_{\alpha_N}]\varphi_{\alpha_N}(\rho_k)A_{k,N} \\ = \delta(\rho_k)\beta(\rho_2, \dots, \rho_{k-1}, \rho_{k+1}, \dots, \rho_N). \end{aligned}$$

Here $A_{k,i}$ are the signed minors of the element $\varphi_{\alpha_i}(\rho_k)$ of the determinant (12). In this equation $\beta(\rho)$ may differ from zero only if

$$[h(\rho_k) - \epsilon_{\alpha_i}]\varphi_{\alpha_i}(\rho_k) = c_{\alpha_i}\delta(\rho_k) \quad (13)$$

and, of course, if $c_{\alpha_i} \neq 0$. Hence, not only solutions of equation (11) but also those of inhomogeneous equation (13) may be used as 'one-particle' wavefunctions. However, it is more convenient to unite these equations. For this one must suppose that in equation (13) c_α may take any value. We have indicated in the previous section how to solve such equations.

The results of the energy lower bound calculations for the one- and three-dimensional systems of N fermions interacting by the oscillator forces and for the three-dimensional system of N fermions interacting by 'gravitational' forces are presented in tables 1, 2, and 3. There one can compare the modified Carr-Post method with the original one and with the methods of Hall.

4. Conclusion

Two modified methods of the lower bound estimates of the N -fermion system ground-state energy were considered. The exact analytical solution of inhomogeneous differential equations of the methods were presented, and illustrative calculations carried out. The results of Manning (1978) and Balbutsev and Mikhailov (1977, 1979) for the one-dimensional harmonic oscillator were confirmed. However, in the case of the three-dimensional harmonic oscillator and of 'gravitational' forces our results differ from those of Manning (1978). Possible mistakes of Manning (1978) were shown.

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Appendix

Let us write equation (5) in Cartesian coordinates:

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{N}{2} \gamma (x^2 + y^2 + z^2) - \epsilon \right] \psi(x, y, z) = \beta \delta(x) \delta(y) \delta(z).$$

This equation is homogeneous everywhere except one point, the origin. This means that it may be treated as the usual Schrödinger equation, its solutions being subjected to some boundary condition at this point. We have

$$\psi(x, y, z) = \varphi(x)\varphi(y)\varphi(z), \quad \epsilon = \epsilon_x + \epsilon_y + \epsilon_z, \quad \left(-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial x^2} + \frac{N}{2} \gamma x^2 - \epsilon_x \right) \varphi(x) = 0.$$

To clear up the role of the inhomogeneity, let us substitute this solution into the initial equation and integrate over some coordinate, for example x , in the (infinitely small) vicinity of zero. Integrals of the type $\int_{-0}^{+0} \varphi(x) dx$ and $\int_{-0}^{+0} x^2 \varphi(x) dx$ must vanish, otherwise one has to suppose $\varphi(x) \sim \delta(x)$, which contradicts the condition $\psi(0, 0, 0) = 0$. So the integration gives

$$-\frac{\hbar^2}{2\mu} [\varphi'(+0) - \varphi'(-0)] \varphi(y)\varphi(z) = \beta \delta(y)\delta(z).$$

If $\varphi'(+0) = \varphi'(-0)$, that is, the derivative $\varphi'(x)$ is continuous at $x = 0$, then $\beta = 0$ automatically. If $\varphi'(+0) \neq \varphi'(-0)$, then one obtains the equality $\varphi(y)\varphi(z) = \text{constant} \delta(y)\delta(z)$ in contradiction of the condition $\psi(0, 0, 0) = 0$. Hence, one must suppose $\beta = 0$.

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