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Some exact solutions to the translation-invariant N-body problem

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Abstract. It is shown that Schrödinger's equation for a translation-invariant system consisting of N particles with arbitrary masses interacting via Hooke's law pair potentials with the same coupling constant can be solved exactly; explicit solutions are found for the case $N = 3$. Exact solutions are also found explicitly for the translation-invariant problem in which a particle with mass m_0 interacts with N identical particles of mass m_1 via a Hooke's law pair potential with coupling constant k_0^2, and the identical particles interact with each other via Hooke's law pair potentials with coupling constant k_1^2. The latter solution provides a basis problem for an energy lower-bound method for translation-invariant atom-like systems.

1. Introduction

We consider translation-invariant N-body problems in which the particles interact by Hooke's law pair potentials and obey non-relativistic quantum mechanics. For example, the Hamiltonian H for such a system in which the coupling constant k^2 is the same for every pair is given by:

$$H = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m_i} - \frac{1}{2m}\Big(\sum_{i=1}^{N} \boldsymbol{p}_i\Big)^2 + k^2 \sum_{i<j=2}^{N} (\boldsymbol{r}_i - \boldsymbol{r}_j)^2, \tag{1}$$

where $m = \Sigma_{i=1}^{N} m_i$ is the total mass. In the symmetrical case of *equal* masses the exact eigenvalues and eigenfunctions of H have been determined by Post (1953). A more general symmetrical problem including also inverse-square potentials has been solved by Calogero and Marchioro (1969).

The problem is essentially algebraic. One looks for a set of translation-invariant relative coordinates in terms of which both the kinetic and potential energy terms are diagonal quadratic forms. In a *fixed* frame of reference the general problem with arbitrary masses and coupling constants appears to be soluble in principle (Symon 1971, p 467). However, the requirement that the centre-of-mass motion separate is a constraint of this diagonalisation process and the new algebraic problem is consequently more difficult.

In this paper we find exact solutions for two types of system. The first type has the Hamiltonian H in equation (1): we show in § 2 that this system can always be solved exactly and we find in § 3 explicit solutions for the case $N = 3$. In § 4 we consider a particle with mass m_0 interacting with N particles each of mass m_1 via a harmonic

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potential with coupling constant k_0^2; the N identical particles interact with each other via a harmonic potential with constant k_1^2. The exact solution we find to this 'harmonic atom' system generalises the result of Moshinsky and Calles (1970) who solved the problem for $m_0 = \infty$, that is for a system in a fixed frame of reference.

2. The N-body problem

We wish to demonstrate that a transformation of coordinates exists which allows the separation of the centre-of-mass motion and simultaneously diagonalises the kinetic and potential energy terms in the Hamiltonian H (equation (1)). We start with a transformation $\boldsymbol{\rho} = \mathbf{B}\boldsymbol{r}$, where $\boldsymbol{\rho}$ and $\boldsymbol{r}$ are column vectors of the new and old coordinates respectively, and we choose the real $N \times N$ matrix $\mathbf{B}$ so that $\boldsymbol{\rho}_1 = (\sum_{i=1}^{N} m_i \boldsymbol{r}_i)/m$ is the centre-of-mass coordinate, and rows 2 to N of $\mathbf{B}$ are orthonormal row vectors satisfying:

$$\left.\begin{aligned} &\sum_{s=1}^{N} B_{is}B_{js} = \delta_{ij} \\ &\sum_{s=1}^{N} B_{is} = 0 \end{aligned}\right\} \qquad \text{for } i, j > 1. \tag{2}$$

With this choice of coordinates the potential energy term becomes:

$$V = \sum_{i<j=2}^{N} k^2(\boldsymbol{r}_i - \boldsymbol{r}_j)^2 = Nk^2 \sum_{i=2}^{N} \boldsymbol{\rho}_i^2 \tag{3}$$

and the coordinates $(\boldsymbol{\rho}_2, \boldsymbol{\rho}_3, \ldots, \boldsymbol{\rho}_N)$ are translation-invariant relative coordinates.

The new momenta $\boldsymbol{\pi}_i = -\mathrm{i}\hbar\nabla_{\rho_i}$ are related to the old momenta by $\boldsymbol{p} = \mathbf{B}^{\mathrm{T}}\boldsymbol{\pi}$ where $\boldsymbol{\pi}$ and $\boldsymbol{p}$ are column vectors of these momenta respectively. If by $\mathbf{M}$ we denote the diagonal $N \times N$ matrix $[m_i]$, then the *total* kinetic energy K is given by:

$$2K = \boldsymbol{p}^{\mathrm{T}}\mathbf{M}^{-1}\boldsymbol{p} = \boldsymbol{\pi}^{\mathrm{T}}\mathbf{B}\mathbf{M}^{-1}\mathbf{B}^{\mathrm{T}}\boldsymbol{\pi}. \tag{4}$$

In view of the definition of $\boldsymbol{\rho}_1$ and of equations (2) we have

$$K = \boldsymbol{\pi}_1^2/2m + \boldsymbol{\pi}_{\mathrm{R}}^{\mathrm{T}}\mathbf{C}\boldsymbol{\pi}_{\mathrm{R}}, \tag{5}$$

where $\boldsymbol{\pi}_R$ is the column vector of the $(N-1)$ relative momenta and $\mathbf{C}$ is the $(N-1)\times(N-1)$ matrix with elements $(i, j > 1)$:

$$C_{ij} = \tfrac{1}{2}\sum_{s=1}^{N} B_{is}B_{js}/m_s. \tag{6}$$

Now if $\mathbf{T}$ is an orthogonal $(N-1)\times(N-1)$ matrix we may define new relative coordinates by

$$\boldsymbol{\rho}'_{\mathrm{R}} = \mathbf{T}\boldsymbol{\rho}_{\mathrm{R}}$$

and the translation-invariant Hamiltonian H becomes (from equations (3) and (5)):

$$H = (\boldsymbol{\pi}'_{\mathrm{R}})^{\mathrm{T}}\mathbf{T}\mathbf{C}\mathbf{T}^{\mathrm{T}}\boldsymbol{\pi}'_{\mathrm{R}} + Nk^2 \sum_{i=2}^{N} (\boldsymbol{\rho}'_i)^2, \tag{7}$$

where $\boldsymbol{\pi}'_R = \mathbf{T}\boldsymbol{\pi}_R$ are the new relative momenta.

The matrix **C** (equation (6)) is a real symmetric positive definite matrix and therefore **T** may be chosen to diagonalise **C** whose eigenvalues we suppose to be $\{\alpha_i^2\}$, $i = 2, 3, \ldots, N$. The Hamiltonian H now separates completely giving:

$$H = \sum_{i=2}^{N} [\alpha_i^2 (\boldsymbol{\pi}_i')^2 + Nk^2 (\boldsymbol{\rho}_i')^2] \tag{8}$$

whose eigenfunctions are products of $3(N-1)$ Hermite functions. The eigenvalues of H are given by

$$E = \sum_{i=2}^{N} [2(x_i + y_i + z_i) + 3] N^{1/2} \hbar \alpha_i k, \tag{9}$$

where x_i, y_i, and z_i are any positive or zero integers.

Our method of proof in the above argument suggests that we start, for example, with normalised Jacobi relative coordinates and then find the matrix **T** which diagonalises **C**. However, in our explicit discussion of the case $N = 3$, in the next section, we find it more convenient to construct directly the final set of relative coordinates whose existence we have established above.

3. The three-body problem

For $N = 3$, we suppose that the final set of coordinates $\boldsymbol{\rho} = \mathbf{B}\boldsymbol{r}$ are given by

$$\mathbf{B} = \begin{bmatrix} m_1/m & m_2/m & m_3/m \\ a & b & -(a+b) \\ c & d & -(c+d) \end{bmatrix}, \tag{10}$$

where a, b, c, and d are real, and $m = (m_1 + m_2 + m_3)$. If we denote rows 2 and 3 of **B** by the vectors $\boldsymbol{u}^{\mathrm{T}}$ and $\boldsymbol{v}^{\mathrm{T}}$ respectively, then the relative kinetic and potential energy operators become diagonal if the following four conditions hold:

$$\begin{aligned} &\boldsymbol{u}^{\mathrm{T}}\boldsymbol{u} = \boldsymbol{v}^{\mathrm{T}}\boldsymbol{v} = 1 \\ &\boldsymbol{u}^{\mathrm{T}}\boldsymbol{v} = 0 \\ &\boldsymbol{u}^{\mathrm{T}}\boldsymbol{M}^{-1}\boldsymbol{v} = 0. \end{aligned} \tag{11}$$

The eigenvalues α^2 and β^2 of **C** (see § 2) then become

$$\alpha^2 = \tfrac{1}{2}\boldsymbol{u}^{\mathrm{T}}\mathbf{M}^{-1}\boldsymbol{u} \qquad \text{and} \qquad \beta^2 = \tfrac{1}{2}\boldsymbol{v}^{\mathrm{T}}\boldsymbol{M}^{-1}\boldsymbol{v}. \tag{12}$$

3.1. The case $m_2 = m_3$

A solution of equations (11) in this case can be found if we set $a = 0$: we get the Jacobi relative coordinates

$$\boldsymbol{\rho}_2 = \boldsymbol{u}^{\mathrm{T}}\boldsymbol{r} \qquad \text{and} \qquad \boldsymbol{\rho}_3 = \boldsymbol{v}^{\mathrm{T}}\boldsymbol{r},$$

where

$$\boldsymbol{u}^{\mathrm{T}} = (0, 1/\sqrt{2}, -1/\sqrt{2}) \qquad \text{and} \qquad \boldsymbol{v}^{\mathrm{T}} = (2/\sqrt{6}, -1/\sqrt{6}, -1/\sqrt{6}). \tag{13}$$

The parameters α and β become (from equation (12)):

$$\alpha = (2m_2)^{-1/2} \qquad \beta = (1/3m_1 + 1/6m_2)^{1/2}. \tag{14}$$

The eigenvalues of H are given by equation (9) with $\alpha_2 = \alpha$ and $\alpha_3 = \beta$. The ground state ψ_0 and the ground-state energy E_0 are given by:

$$\psi_0(\boldsymbol{\rho}_2, \boldsymbol{\rho}_3) = \left(\frac{\sqrt{3}k}{\alpha\hbar}\right)^{3/2}\left(\frac{\sqrt{3}k}{\beta\hbar}\right)^{3/2} \exp\left(-\frac{\sqrt{3}k}{2\alpha\beta\hbar}(\beta\boldsymbol{\rho}_2^2 + \alpha\boldsymbol{\rho}_3^2)\right)$$

and (15)

$$E_0 = 3\sqrt{3}\hbar k(\alpha+\beta).$$

Since the exchange of $\boldsymbol{r}_2$ with $\boldsymbol{r}_3$ sends $\boldsymbol{\rho}_2$ to $-\boldsymbol{\rho}_2$ and leaves $\boldsymbol{\rho}_3$ invariant, states which are spatially symmetric or antisymmetric in particles 2 and 3 are respectively even and odd functions of $\boldsymbol{\rho}_2$. The system in which particle 1 is fixed at the origin is obtained by the limit $\boldsymbol{r}_1 \to 0$ and $1/m_1 \to 0$; the energies are only affected in this limit by the value of β which becomes $\beta = (6m_2)^{-1/2}$.

3.2. The case $m_1 \geqslant m_2 > m_3$

We have found the following solution to equations (11) in this case:

$$\begin{aligned} w &= \frac{m_1m_3 + m_1m_2 - 2m_2m_3}{m_1m_2 - m_1m_3} \\ a &= [1 - w(3+w^2)^{-1/2}]^{1/2}/\sqrt{3} \\ c &= [1 + w(3+w^2)^{-1/2}]^{1/2}/\sqrt{3} \\ b &= (\sqrt{3}c - a)/2 \\ d &= -(c + \sqrt{3}a)/2. \end{aligned} \tag{16}$$

If $m_1 = m_2$, $w = 1$ and $a = 1/\sqrt{6}$; this agrees with our result in § 3.1 (where $m_2 = m_3$) provided we exchange $\boldsymbol{r}_1$ with $\boldsymbol{r}_3$. If $m_1 > m_2$, then $w > 1$ and $a < 1/\sqrt{6}$. The formulae for α^2 and β^2 (equation (12)) become:

$$\begin{aligned} \alpha^2 &= a^2/2m_1 + [(1-a^2) - a(2-3a^2)^{1/2}]/4m_2 + [(1-a^2) + a(2-3a^2)^{1/2}]/4m_3 \\ \beta^2 &= (2-3a^2)/6m_1 + [1+3a^2+3a(2-3a^2)^{1/2}]/12m_2 \\ &\quad + [1+3a^2-3a(2-3a^2)^{1/2}]/12m_3. \end{aligned} \tag{17}$$

The Hamiltonian in separated form (equation (8)) now reads:

$$H = (\alpha^2\boldsymbol{\pi}_2^2 + 3k^2\boldsymbol{\rho}_2^2) + (\beta^2\boldsymbol{\pi}_3^2 + 3k^2\boldsymbol{\rho}_3^2) \tag{18}$$

and for example, the ground state $\psi_0(\boldsymbol{\rho}_2, \boldsymbol{\rho}_3)$ and the ground-state energy E_0 are given by equations (15) with the values of α and β taken from equations (17).

4. The harmonic atom

The Hamiltonian H for the system of $(N+1)$ particles (labelled $0, 1, 2, \ldots, N$) is as follows:

$$H = \frac{\boldsymbol{p}_0^2}{2m_0} + \frac{1}{2m_1}\sum_{i=1}^{N}\boldsymbol{p}_i^2 - \frac{1}{2m}\left(\sum_{i=0}^{N}\boldsymbol{p}_i\right)^2 + \sum_{i=1}^{N}k_0^2(\boldsymbol{r}_0 - \boldsymbol{r}_i)^2 + \sum_{1=i<j=2}^{N}k_1^2(\boldsymbol{r}_i - \boldsymbol{r}_j)^2 \tag{19}$$

where the total mass $m = m_0 + Nm_1$.

We define new coordinates $\boldsymbol{\rho} = \mathbf{B}\boldsymbol{r}$ for this problem by the following matrix:

$$\mathbf{B} = \begin{bmatrix} m_0/m & m_1/m & m_1/m & . & . & . & m_1/m \\ -Na & a & a & . & . & . & a \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 & . & . & 0 \\ 0 & 1/\sqrt{6} & 1/\sqrt{6} & -2/\sqrt{6} & 0 & . & 0 \\ \vdots & & & \text{etc} & & & \\ 0 & & & & & & \end{bmatrix} \tag{20}$$

where $a = [N(N+1)]^{-1/2}$ and $\{\boldsymbol{\rho}_2, \boldsymbol{\rho}_3, \ldots, \boldsymbol{\rho}_N\}$ are the normalised Jacobi relative coordinates for the N identical particles. In terms of these coordinates we find that the *total* kinetic energy operator K is given by:

$$K = \frac{\boldsymbol{\pi}_0^2}{2m} + \frac{\boldsymbol{\pi}_1^2}{2m'} + \sum_{i=2}^{N} \frac{\boldsymbol{\pi}_i^2}{2m_1} \tag{21}$$

where

$$m' = (N+1)(1/m_1 + N/m_0)^{-1}.$$

Meanwhile, in view of the following identities:

$$\sum_{0=i<j=1}^{N} (\boldsymbol{r}_i - \boldsymbol{r}_j)^2 = (N+1) \sum_{i=1}^{N} \boldsymbol{\rho}_i^2$$

and (22)

$$\sum_{1=i<j=2}^{N} (\boldsymbol{r}_i - \boldsymbol{r}_j)^2 = N \sum_{i=2}^{N} \boldsymbol{\rho}_i^2,$$

we are able to separate the Hamiltonian H giving:

$$H = \left(\frac{\boldsymbol{\pi}_1^2}{2m'} + (N+1)k_0^2\boldsymbol{\rho}_1^2\right) + \sum_{i=2}^{N} \left(\frac{\boldsymbol{\pi}_i^2}{2m_1} + (Nk_1^2 + k_0^2)\boldsymbol{\rho}_i^2\right). \tag{23}$$

The eigenfunctions of H are products of $3N$ Hermite functions in the relative coordinates $\boldsymbol{\rho}_1$ to $\boldsymbol{\rho}_N$, and the eigenvalues are the corresponding sums of single-particle energies. Since $\boldsymbol{\rho}_1$ is symmetric in $\boldsymbol{r}_1$ to $\boldsymbol{r}_N$, the burden of spatial permutation symmetry is carried by the dependence of the eigenstate on the coordinates $\boldsymbol{\rho}_2$ to $\boldsymbol{\rho}_N$. In the case of scalar particles in one dimension we get the following results for the ground-state energies E_0:

bosons

$$E_0 = \frac{\hbar k_0}{(2m_2)^{1/2}} + \hbar(N-1)\left(\frac{Nk_1^2 + k_0^2}{2m_1}\right)^{1/2}; \tag{24}$$

fermions

$$E_0 = \frac{\hbar k_0}{(2m_2)^{1/2}} + \hbar(N^2-1)\left(\frac{Nk_1^2 + k_0^2}{2m_1}\right)^{1/2}, \tag{25}$$

where

$$m_2 = [1/m_1 + N/m_0]^{-1}.$$

Equation (24) agrees with equation (15) of § 3 in which $N=3$ and $k_1=k_0$. If $k_0=0$, the results agree with Post (1953) for N identical particles. Similarly if $k_0=k_1$ and $m_0=m_1$, the boson formula (equation (24)) agrees with Post (1953) for $(N+1)$ identical particles; the fermion formula does not, of course, agree immediately with Post's result (for $(N+1)$ identical fermions) because in deriving equation (25) we have antisymmetrised in only N particles. If we set $1/m_0=0$, i.e. $m_2=m_1$, then the boson formula agrees with Moshinsky and Calles (1970) who considered N identical bosons interacting with each other and with a *fixed* centre by Hooke's law potentials.

From the diagonal form of H (equation (23)) we see that the coupling constant k_1^2 between the identical particles may be chosen to be *negative*, as it is in a Hamiltonian for real atoms. For a bound system, in this case, it would be necessary that $N|k_1^2| \leqslant k_0^2$.

5. Conclusion

We have found some exact solutions to the translation-invariant many-body problem in which the masses are not all equal, and the particles interact by Hooke's law pair potentials. The explicit results for the three-body problem (§ 3) provide solutions suitable for quark models similar to those of Moshinsky (1969, p 60) and Horgan (1976) but allowing for different particle masses. If two masses are equal, the solution of § 4 would apply and two distinct coupling constants would then be admitted. By a similar analysis we can extend these results up to the case of N identical particles with N distinct coupling constants.

The harmonic atom solution of § 4 may be useful for estimating exactly, in a special case, the mass-change effects in the energy lower-bound method of Carr and Post (1971, 1977). This exact solution also provides a basis problem for the design of new energy lower-bound method for translation-invariant *atom-like* systems, just as Post's (1953) exact solution of the 'harmonic nucleus' system provides a basis problem for the lower-bound method I (Post 1956, Hall and Post 1967). By 'basis problem' we mean a specific problem for which the general energy lower-bound method provides the exact energy.

We have proved (Hall 1972a, b) that method I yields the exact energy for (and only for) the boson oscillator system. Thus no systematic improvement in the method seems possible. In this restricted sense we may say that method I is *optimal*. Method II (Hall, 1967) for fermions, on the other hand, is *not* known to be optimal, although for $N>7$ it gives the highest lower bound to-date, when applied to the popular test system consisting of scalar fermions in one dimension interacting by harmonic potentials (Hall 1972c, Carr and Post 1977).

The energy lower-bound methods which are presently available for atom-like systems (Coleman 1963, Calogero and Marchioro 1969) apply only to problems in which there is a central potential which is *fixed*. Also the question of the optimality (with respect to energy) of these methods, in the above sense, has not been discussed.

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