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Some specific solutions to the translation-invariant N-body harmonic oscillator Hamiltonian

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Abstract

The resolution of the Schrödinger equation for the translation-invariant N-body harmonic oscillator Hamiltonian in D dimensions with one-body and two-body interactions is performed by diagonalizing a matrix $\mathbb{J}$ of order $N - 1$. It has been previously established that the diagonalization can be analytically performed in specific situations, such as for $N \leqslant 5$ or for N identical particles. We show that the matrix $\mathbb{J}$ is diagonal, and thus the problem can be analytically solved, for any number of arbitrary masses provided some specific relations exist between the coupling constants and the masses. We present analytical expressions for the energies under those constraints.

1. Introduction

The general translation-invariant N-body harmonic oscillator Hamiltonian in D dimensions with one-body and two-body forces is given by [1–3]

$$H_{\text{ho}} = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m_i} - \frac{\boldsymbol{P}^2}{2M} + \sum_{i=1}^{N} k_i\,(\boldsymbol{r}_i - \boldsymbol{R})^2 + \sum_{i<j=2}^{N} g_{ij}\,(\boldsymbol{r}_i - \boldsymbol{r}_j)^2, \quad (1)$$

where in the last term the double sum runs over all pairs $\{i, j\}$ with $i < j$. According to their module and sign, the coupling constants k_i and g_{ij} determine the strength and the attractive or repulsive character of the interactions. The momentum $\boldsymbol{p}_i$ of the ith particle of mass m_i is the conjugate variable of its position $\boldsymbol{r}_i$. The center of mass coordinate is noted $\boldsymbol{R} = \sum_{i=1}^{N} m_i\, \boldsymbol{r}_i / M$ where $M = \sum_{i=1}^{N} m_i$, and the total momentum is noted $\boldsymbol{P} = \sum_{i=1}^{N} \boldsymbol{p}_i$.

This Hamiltonian is particularly interesting since analytical eigensolutions are available for some special values of the parameters $\{m_i, k_i, g_{ij}\}$. Indeed, many approximation methods rely on analytical solutions of simpler Hamiltonians, such as expansions in oscillator basis [4] or in Gaussian states [5]. Furthermore, the existence of analytical solutions for the Hamiltonian H_{ho} is at the heart of the envelope theory [6] used to solve general translation-invariant N-body Hamiltonians [7, 8]. So, it is particularly relevant to study and expand the availability of analytical solutions of H_{ho}.

The general procedures already existing in the literature to formally compute the eigensolutions of H_{ho} are recalled in section 2. New analytical solutions are given in section 3. Some concluding remarks and perspectives are presented in section 4.

2. General procedures

The Schrödinger equation for H_{ho} can be solved because the Hamiltonian can be rewritten as a sum of $N - 1$ decoupled harmonic oscillators

$$H_{\rm ho}=\sum_{i=1}^{N-1}\left[\frac{\boldsymbol{\sigma}_i^2}{2m}+\frac{1}{2}m\,\omega_i^2\boldsymbol{z}_i^2\right],\tag{2}$$

where m is an arbitrary mass scale (m can be one of the masses of the system or M, for instance), $m_i = m\,\alpha_i$ for $i = 1, 2,\ldots,N$, and ω_i are frequencies of the relative oscillations (see below). The $\boldsymbol{z}_i$ and $\boldsymbol{\sigma}_i$ are new conjugate variables resulting from a change of variables defined in [3] where the center of mass reference frame has been adopted.

All the eigenvalues of the system are then given by ($\hbar = 1$)

$$E_{\rm ho}=\sum_{i=1}^{N-1}\omega_i\,Q_i,\tag{3}$$

where $Q_i = n_i + 1/2$ for $D = 1$ and $Q_i = 2n_i + l_i + D/2$ for $D \geqslant 2$ [9]. The n_i, l_i are the quantum numbers associated with the coordinates of the harmonic oscillators in equation (2). Let us note that degeneracies can occur if some frequencies ω_i are commensurable. These frequencies ω_i are given by $d_i = m\,\omega_i^2/2$ where d_i are the eigenvalues of a symmetrical matrix of order $N-1$, let us say $\mathbb{J}$. This matrix can be written as $\mathbb{J}=\mathbb{F}+\mathbb{G}$ where each term corresponds to the contributions from the one-body and two-body interactions respectively. The matrix elements of $\mathbb{F}$ are given in [3] and those of $\mathbb{G}$ in [2, 3], and they can be written as follows ($1 \leqslant l, m \leqslant N-1$),

$$\mathbb{F}_{lm}=\lambda_l\lambda_m\sum_{i=1}^{N}k_i\mathbb{B}_{il}\mathbb{B}_{im},\qquad \mathbb{G}_{lm}=\lambda_l\lambda_m\sum_{i<j=2}^{N}g_{ij}(\mathbb{B}_{il}-\mathbb{B}_{jl})(\mathbb{B}_{im}-\mathbb{B}_{jm}),\tag{4}$$

where $\lambda_j \equiv \sqrt{\frac{\alpha_{1,\ldots,j+1}}{\alpha_{1,\ldots,j}\,\alpha_{j+1}}}$ with $\alpha_{1,\ldots,j}=\alpha_1+\ldots+\alpha_j$ and where $\mathbb{B}$ is an invertible matrix whose elements can be found on equation (24) of [3]. The matrix $\mathbb{B}$ is built with ratios of the masses of the system and establishes the relation between the individual momenta and the relative ones plus the total momentum. Let us note that some parameters k_i or g_{ij} can be null or negative, provided all values found for ω_i^2 are strictly positive. In this case only, bound states can exist with well defined eigenvalues $E_{\rm ho}$.

When $N \leqslant 5$, finding the eigenvalues d_i comes down to solving a polynomial of order $\mathcal{O} \leqslant 4$, thus analytical expressions for the ω_i can be obtained. For instance, the complete solution for 3 different particles is given in [3]. Analytical expressions for the ω_i can also be found when all particles are identical ($m_i = m, k_i = k, g_{ij} = g, \forall\, i, j$), and the eigenvalues are given by [3]

$$E_{\rm ho}=\sqrt{\frac{2}{m}(k+N\,g)}\sum_{i=1}^{N-1}Q_i.\tag{5}$$

In this case, the degeneracy is maximal. When the system contains N_s sets of identical particles which interact via two-body forces, another very elegant way to compute the N-body problem is presented in [1]. In that case, $H_{\rm ho}$ can be expressed as a sum of Hamiltonians, a term H_s for each set s of identical particles and one term $H_{\rm cm}$ which describes the motion of the centers of mass of the sets of identical particles. All Hamiltonians H_s are completely solvable, and the solutions of $H_{\rm cm}$ are given by equation (3), meaning that analytical solutions can be found in specific cases such as when $N_s \leqslant 5$ or when the total mass of every set is equal. This procedure is generalized in [8] for one-body and two-body forces, where an explicit example is calculated for $N_s = 2$.

3. New analytical solutions

In the following, we show that the matrix $\mathbb{J}$ is diagonal, and thus $H_{\rm ho}$ completely solved, for any number of arbitrary masses provided some specific relations exist between the coupling constants and the masses.

After some tedious calculations, from equation (4) one can deduce the matrix elements of the symmetrical matrices $\mathbb{F}$ and $\mathbb{G}$,

$$\mathbb{F}_{ii}=\frac{[k_{i+1}\,\alpha_{1,\ldots,i}^2+(k_1+\ldots+k_i)\alpha_{i+1}^2]}{\alpha_{1,\ldots,i}\,\alpha_{1,\ldots,i+1}\,\alpha_{i+1}}\tag{6}$$

$$\mathbb{F}_{ij<i}=\Gamma_F(\alpha)\quad\frac{(k_1+\ldots+k_j)\alpha_{j+1}-k_{j+1}\,\alpha_{1,\ldots,j}}{\alpha_{1,\ldots,j+1}\,\alpha_{1,\ldots,i}}\tag{7}$$

$$\mathbb{G}_{ii}=\frac{\sum_{m=i+1}^{N}\sum_{l=1}^{i}g_{l\,m}}{\alpha_{1,\ldots,i}}-\frac{\sum_{m=i+2}^{N}\sum_{l=1}^{i+1}g_{l\,m}}{\alpha_{1,\ldots,i+1}}+\frac{\sum_{l=1}^{i}g_{l\,i+1}}{\alpha_{i+1}}+\frac{\sum_{l=i+1}^{N}g_{i+1\,l}}{\alpha_{i+1}}\tag{8}$$

$$\mathbb{G}_{ij<i} = \Gamma_G(\alpha)\left[\alpha_{j+1}\alpha_{1,\ldots,i}\left(\sum_{l=1}^{j} g_{l\ i+1}\right) - \alpha_{i+1}\alpha_{1,\ldots,j}\left(\sum_{l=i+2}^{N} g_{j+1\ l}\right)\right.$$
$$\left. + \alpha_{i+1}\alpha_{j+1}\left(\sum_{m=i+1}^{N}\sum_{l=1}^{j} g_{l\ m}\right) - \alpha_{1,\ldots,i+1}\alpha_{1,\ldots,j}\, g_{j+1\ i+1}\right] \tag{9}$$

where $\Gamma_F(\alpha) = \sqrt{\frac{\alpha_{1,\ldots,j+1}\ \alpha_{1,\ldots,j}\ \alpha_{i+1}}{\alpha_{1,\ldots,i+1}\ \alpha_{1,\ldots,j}\ \alpha_{j+1}}}$ and $\Gamma_G(\alpha) = \frac{\sqrt{\frac{1}{\alpha_{1,\ldots,j}} + \frac{1}{\alpha_{j+1}}}\sqrt{\frac{1}{\alpha_{1,\ldots,i}} + \frac{1}{\alpha_{i+1}}}}{\alpha_{1,\ldots,i+1}\alpha_{1,\ldots,j+1}}$. Notice that $\Gamma_F(\alpha)$ and $\Gamma_G(\alpha)$ are strictly positive numbers. We must note at this point that g_{ij} with $i > N$ or $j > N$ are in principle not defined, however in these equations and later in this paper they should be considered as zero.

From equations (7) and (9) one can notice that the off-diagonal matrix elements of both $\mathbb{F}$ and $\mathbb{G}$ will vanish under certain conditions. In particular, it is easy to see that if $k_i = \rho\ m_i\ \forall\, i$, where ρ is a real constant, then $\mathbb{F}$ becomes diagonal, and its eigenvalues are all given by $\rho\ m$. For $\mathbb{G}$, if $g_{ij} = g_{1j}\frac{\alpha_i}{\alpha_1}$ then $\mathbb{G}$ becomes diagonal, and its eigenvalues are given by $\frac{(g_{1\ i+2} + g_{1\ i+3} + \ \ldots\ + g_{1\ N})\alpha_{i+1} + g_{1\ i+1}\ \alpha_{1,\ldots,i+1}}{\alpha_1\alpha_{i+1}}$ with $i = 1,\ldots,N - 1$. The condition $g_{ij} = g_{1j}\frac{\alpha_i}{\alpha_1}$ should not be mistaken for a special requirement on a given particle as the choice of the assignment of particle 1 is completely free. With this choice of numbering j ($>i$) can take any value from 2 to N.

Under these very specific conditions over the nature of the one-body and two-body forces and the masses of the system, we find analytical solutions to H_{ho} given by

$$E_{\text{ho}}|_{k_i=\rho\ m_i, g_{ij}=g_{1j}\frac{\alpha_i}{\alpha_1}} = \sqrt{2}\sum_{i=1}^{N-1}\sqrt{\rho + \frac{[(g_{1\ i+2} + g_{1\ i+3} + \ldots + g_{1\ N})\alpha_{i+1} + g_{1\ i+1}\ \alpha_{1,\ldots,i+1}]}{m\ \alpha_1\ \alpha_{i+1}}}\ Q_i. \tag{10}$$

One can check that formula (5) is recovered when all particles are identical. The parameters ρ and g_{1j} can be positive, null or negative numbers provided all expressions under the square roots are strictly positive. When $N = 3$, we have $k_i = \rho\ m_i$, $g_{23} = g_{13}\ m_2/m_1$, and g_{12} and g_{13} arbitrary. Formula (10) reduces then to

$$E_{\text{ho}}|_{k_i=\rho\ m_i, g_{ij}=g_{1j}\frac{\alpha_i}{\alpha_1}} = \sqrt{2\ \rho + 2\ \frac{g_{13}\ m_2 + g_{12}(m_1 + m_2)}{m_1\ m_2}}\ Q_1$$
$$+ \sqrt{2\ \rho + 2\ \frac{g_{13}(m_1 + m_2 + m_3)}{m_1\ m_3}}\ Q_2. \tag{11}$$

When only one-body or two-body forces are present, equation (10) gives eigenvalues of

$$E_{\text{ho}}^{1B}|_{k_i=\rho\ m_i} = \sqrt{2\rho}\sum_{i=1}^{N-1} Q_i, \tag{12}$$

$$E_{\text{ho}}^{2B}|_{g_{ij}=g_{1j}\frac{\alpha_i}{\alpha_1}} = \sum_{i=1}^{N-1}\sqrt{\frac{2[(g_{1\ i+2} + g_{1\ i+3} + \ \ldots\ + g_{1\ N})\alpha_{i+1} + g_{1\ i+1}\alpha_{1,\ldots,i+1}]}{m\ \alpha_1\ \alpha_{i+1}}}\ Q_i. \tag{13}$$

When only one-body forces are present, ρ must be strictly positive. Since $k_i = \rho\ m_i$, this implies that all relative oscillations associated with E_{ho}^{1B} are characterized by the same frequency $\omega = \sqrt{2\rho}$.

A simpler expression for E_{ho}^{2B} can be found under more restrictive conditions: if $g_{ij} = \beta\ m_i m_j$ where β is a strictly positive constant, then

$$E_{\text{ho}}^{2B}|_{g_{ij}=\beta\ m_i m_j} = \sqrt{2\beta M}\sum_{i=1}^{N-1} Q_i. \tag{14}$$

4. Concluding remarks

As mentioned in the introduction, finding analytical solutions to specific Hamiltonians can be crucial to some approximation methods. In particular, the envelope theory [6] is a simple and powerful method to obtain approximate but reliable eigensolutions of quite general N-body Hamiltonians [7, 8]. As this method relies on the existence of analytical solutions of the translation-invariant N-body harmonic oscillator Hamiltonian, it is particularly relevant to study and expand the availability of these analytical solutions. For instance, relation (14) has been used to study the possible existence of a quasi Kepler's third law for quantum many-body systems [10].

The results presented here are obtained by imposing that matrices $\mathbb{F}$ and $\mathbb{G}$ are both diagonal. However, it is possible that off-diagonal elements of these two matrices cancel out each other in particular situations resulting in a diagonal matrix $\mathbb{J}$. This is an interesting study case that might be considered in a future work.

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Data availability statement

No new data were created or analysed in this study.

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References

[1] Hall R L and Schwesinger B 1979 The complete exact solution to the translation-invariant N-body harmonic oscillator problem *J. Math. Phys.* **20** 2481
[2] Ma Z-Q 2000 Exact Solutions to the N-Body Schrödinger Equation for the Harmonic Oscillator *Found. Phys. Lett.* **13** 167
[3] Silvestre-Brac B, Semay C, Buisseret F and Brau F 2010 The quantum $\mathcal{N}$-body problem and the auxiliary field method *J. Math. Phys.* **51** 032104
[4] Stancu F 1997 *Group Theory in Subnuclear Physics* (Oxford: Clarendon)
[5] Suzuki Y and Varga K 1998 *Stochastic Variational Approach to Quantum-Mechanical Few-Body Problems* (Berlin: Springer)
[6] Hall R L 1980 Energy trajectories for the N-boson problem by the method of potential envelopes *Phys. Rev.* D **22** 2062
[7] Semay C 2015 Numerical tests of the envelope theory for few-boson systems *Few-Body Syst.* **56** 149
[8] Semay C, Cimino L and Willemyns C 2020 Envelope theory for systems with different particles *Few-Body Syst.* **61** 19
[9] Yáñez R J, Van Assche W and Dehesa J S 1994 Position and momentum information entropies of the D-dimensional harmonic oscillator and hydrogen atom *Phys. Rev.* A **50** 3065
[10] Semay C and Willemyns C T 2021 Quasi Kepler's third law for quantum many-body systems *Eur. Phys. J. Plus* **136** 342