Three-body harmonic molecule

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Abstract
In this study, the quantum three-body harmonic system with finite rest length $R$ and zero total angular momentum $L = 0$ is explored. It governs the near-equilibrium $S$-states eigenfunctions $\psi(r_{ij}, r_{i2}, r_{i3})$ of three identical point particles interacting by means of any pairwise confining potential $V(r_{ij}, r_{i2}, r_{i3})$ that entirely depends on the relative distances $r_{ij} = |r_i - r_j|$ between particles. At $R = 0$, the system admits a complete separation of variables in Jacobi-coordinates, it is (maximally) superintegrable and exactly-solvable. The whole spectra of excited states is degenerate, and to analyze it a detailed comparison between two relevant Lie-algebraic representations of the corresponding reduced Hamiltonian is carried out. At $R > 0$, the problem is not even integrable nor exactly-solvable and the degeneration is partially removed. In this case, no exact solutions of the Schrödinger equation have been found so far whilst its classical counterpart turns out to be a chaotic system. For $R > 0$, accurate values for the total energy $E$ of the lowest quantum states are obtained using the Lagrange-mesh method. Concrete explicit results with not less than eleven significant digits for the states $n = 0, 1, 2, 3$ are presented in the range $0 \leq R \leq 4.0$ a.u. In particular, it is shown that (I) the energy curve $E = E(R)$ develops a global minimum as a function of the rest length $R$, and it tends asymptotically to a finite value at large $R$, and (II) the degenerate states split into sub-levels. For the ground state, perturbative (small-$R$) and two-parametric variational results (arbitrary $R$) are displayed as well. An extension of the model with applications in molecular physics is briefly discussed.

Keywords: harmonic molecule, integrability, Lagrange-mesh method, perturbation theory

(Some figures may appear in colour only in the online journal)

1. Introduction
The quantum system of $n$ ($n > 2$) point particles in $\mathbb{R}^3$ with arbitrary masses connected through springs can be considered as a natural $n$-body generalization of the celebrated two-body harmonic oscillator ($n = 2$), the latter being a system of tantamount relevance in theoretical physics [1] and intimately close to the method of second quantization introduced by Dirac in the late 1920s. The corresponding potential $V(r_{ij})$ in classical and quantum mechanics, a linear combination of the squares of the mutual relative distances $r_{ij} = |r_i - r_j|$, is superintegrable and exactly-solvable. However, from a physical point of view a more adequate model is obtained by the replacement $r_{ij}^2 \to (r_{ij} - R_{ij})^2$ where the constants $R_{ij} > 0$ play the role of rest lengths. This model can be called generalized $n$-body harmonic system (GNBHS). Despite of its apparent modesty, in the simplest three-body case $n = 3$ not a single exact solution of the Schrödinger equation is known so far.

In classical mechanics, the three-body generalized harmonic system $n = 3$ possesses a complex rich dynamics. For the case of identical particles, with common rest length $R_{ij} = R > 0$, a chaotic behavior as a function of the energy and the system parameters occurs [2, 3]. At fixed energy $E$, and restricted to the invariant manifold of zero total angular momentum, its dynamics transits between two regular regimes passing through a chaotic one as the parameter $R$ grows. Recently, ¹ These authors contributed equally. * Author to whom any correspondence should be addressed.
an experimental physical realization of this system was built by means of analog electrical components [4]. Therefore, the GNBHS represents a suitable candidate to test theoretical and numerical tools to analyze the nature of the classical-quantum relation in n-body chaotic systems [5].

In quantum mechanics, the solutions of the GNBHS are of great theoretical importance. Moreover, in practice they could be used as a basis for many-body calculations in molecular, nuclear and elementary particle physics just to mention few examples [6].

In the present work, for the three-body generalized harmonic system we now ask how the energies and eigenfunctions of the quantum system behave as the rest length \( R \) increases. We restrict ourselves to the symmetric case of three identical particles \( m_1 = m_2 = m_3 = m \) with zero total angular momentum \( L = 0 \) (S-states). The unfolding of the degenerate states due to a non zero value of \( R \) is of particular interest. It is worth mentioning that different aspects of the three-body potential is of the form:

\[
V_{R}(m) = \frac{1}{2} m \omega^2 \left[ (r_{12} - R)^2 + (r_{13} - R)^2 + (r_{23} - R)^2 \right],
\]

In quantum mechanics, the solutions of the GNBHS are of the form:

\[
|\Psi\rangle = \sum_{n=0}^{\infty} c_n \left| S_n \rightangle \left| \phi_n \right\rangle,
\]

where \( |S_n\rangle \) are the symmetric states due to a non zero value of \( R \) is of particular interest. It is worth mentioning that different aspects of the three-body system in \( \mathbb{R}^d \) with arbitrary masses \( (m_1, m_2, m_3) \) have been presented in [7, 8] (see also [9]). For instance, a reduced Hamiltonian for the S-states which solely depends on the coordinates \( r_{ij} \) was established. Also, at \( R = 0 \) a complete analysis of the one-dimensional case \( d = 1 \) (three masses on a line) can be found in [10]. Here, for three equal masses in \( \mathbb{R}^3 \) and \( R \neq 0 \), using the Lagrange-mesh method (LMM) the solutions of the lowest S-states eigenvalues of the corresponding Schrödinger equation are computed with high accuracy. Specifically, the energies are displayed with not less than eleven significant figures.

The structure of the paper is as follows. In section 2 we define the generalized three-body harmonic system and the concrete setting of the problem is explained. Especially, the relevant reduced Hamiltonian governing the S-states is described. At zero rest length \( R = 0 \), the system becomes superintegrable and solvable. In this case, we review the exact solutions of the corresponding Schrödinger equation in the section 3. This section exposes a detailed comparison between two Lie-algebraic representations of the Hamiltonian as well as the explanation on the degeneracy of the system. The next section 4 treats the ground state solution at \( R > 0 \) within the perturbative and variational formalism. In section 5 we depict the implementation of the LMM in the study of lowest excited states. For \( R \geq 0 \) such a method leads to highly accurate results of the energies. These are displayed and discussed in section 6. Here, the partial splitting of the degenerate states is established. Finally, the section 7 contains the conclusions and future work.

2. Generalities

Let us consider the quantum system of three non-relativistic identical particles with pairwise harmonic interaction. The potential is of the form:

\[
V_R = \frac{3}{2} m \omega^2 \left[ (r_{12} - R)^2 + (r_{13} - R)^2 + (r_{23} - R)^2 \right],
\]

Figure 1. Three-body chain of harmonic oscillators. At the minimum of the potential \( V_R (1) \), the system forms an equilateral triangle with sides \( r_{12} = r_{13} = r_{23} = R \).

\[ r_{ij} \in \mathbb{R}^3, r_{ij} = |r_i - r_j | \] are the relative distances between the \( i \)th and \( j \)th particles, \( m \) is the common mass of each body, \( \omega > 0 \) plays the role of angular frequency and \( R \) denotes the rest length of the system, see figure 1. The minimum of \( V_R (1) \) corresponds to an equilateral triangle with each side equal to \( R \). At \( R = 0 \), the potential \( V_R \) is known under the name of harmonic molecule, see [10] for the case \( d = 1 \) where the particles move on line.

The Hamiltonian of the system is given by:

\[
\mathcal{H} = \frac{1}{2m} \hat{p}_i^2 + \frac{1}{2m} \hat{p}_j^2 + \frac{1}{2m} \hat{p}_k^2 + V_R(r_{ij}),
\]

here \( \hat{p}_j = -i\hbar \nabla_j \) stands for the canonical momentum operator associated with the particle \( j \). Due to translational invariance and rotational symmetry, the center of mass momentum:

\[
\hat{P} = \hat{p}_1 + \hat{p}_2 + \hat{p}_3,
\]

as well as the total angular momentum:

\[
\hat{L} = r_1 \times \hat{p}_1 + r_2 \times \hat{p}_2 + r_3 \times \hat{p}_3,
\]

are conserved quantities, respectively, i.e. they commute with the Hamiltonian (2). The corresponding stationary Schrödinger equation:

\[
\mathcal{H} \Psi(r_1, r_2, r_3) = E \Psi(r_1, r_2, r_3),
\]

is nine-dimensional.

Some remarks are in order:

- At \( R = 0 \), the Hamiltonian \( \mathcal{H} \) (2) admits a complete separation of variables in Jacobi coordinates [11], see below. This separability holds even for the case of non-equal masses. Moreover, when all three masses are equal then the system becomes maximally superintegrable and exactly solvable [12]. It is worth mentioning that for the same solvable model when restricted to a subdomain of the original configuration
space, the supersymmetrization (SUSY realization) immediately encounters subtle difficulties [13].

- For \( R \neq 0 \), not a single exact solution to the Schrödinger equation is known so far. Interestingly, the corresponding classical system exhibits a rich dynamics with mixed regions of regularity and chaos [4].

The integrals of motion (3) and (4) allow us to construct a reduced Hamiltonian which describes all the states of \( \mathcal{H} (2) \) with zero total angular momentum \( L = 0 \) (S-states). It solely depends on the three variables \( r_{ij} \) [7]. Explicitly, such a reduced Hamiltonian reads:

\[
\mathcal{H}_{L=0} = -\frac{1}{2m} \Delta_{\text{rad}} + \frac{3}{2} m \omega^2 \times \left[(r_{12} - R)^2 + (r_{13} - R)^2 + (r_{23} - R)^2\right]
\]

where the kinetic-like term can be written as follows:

\[
\frac{1}{2} \Delta_{\text{rad}} = \frac{1}{r_{12}} \left( \frac{\partial}{\partial r_{12}} \left( r_{12} \frac{\partial}{\partial r_{12}} \right) + \frac{1}{r_{13}} \left( \frac{\partial}{\partial r_{13}} \left( r_{13} \frac{\partial}{\partial r_{13}} \right) \right) \right)
+ \frac{1}{r_{23}} \left( \frac{\partial}{\partial r_{23}} \left( r_{23} \frac{\partial}{\partial r_{23}} \right) \right) + \frac{\alpha_{12}^2 + \alpha_{13}^2 - \alpha_{23}^2}{2 r_{12} r_{23}} \partial^2 + \frac{\alpha_{23}^2 + \alpha_{13}^2 - \alpha_{12}^2}{2 r_{23} r_{13}} \partial^2 - \frac{\alpha_{12}^2 + \alpha_{13}^2 - \alpha_{23}^2}{2 r_{13} r_{12}} \partial^2
\]

with \( h = 1 \), see [8] and references therein. The operator (6) describes a three-dimensional point particle moving in a (curved) space [7]. For the S-states, the relevant spectral problem occurs in the three-dimensional space of radial relative motion \( \mathbb{R}_{\text{rad}} = (r_{12}, r_{13}, r_{23}) \in \mathbb{R}_+^3 \):

\[
\mathcal{H}_{L=0} \psi(r_{12}, r_{13}, r_{23}) = E \psi(r_{12}, r_{13}, r_{23}) \quad \text{(8)}
\]

At \( R = 0 \), the Hamiltonian (6) is \( \mathbb{Z}_2^{\otimes 3} \)-invariant under the reflections:

\[
\begin{align*}
r_{12} &\rightarrow -r_{12} \quad ; \\
r_{13} &\rightarrow -r_{13} \quad ; \\
r_{23} &\rightarrow -r_{23},
\end{align*}
\]

and also under the action of the \( S_3^{\otimes 2} = S_3(r_{12}, r_{13}, r_{13}) \oplus S_3(1, 2, 3) \) symmetry (permutation of the three variables \( r_{12}, r_{13}, r_{13} \), and interchange of any pair of particles). In the case \( R \neq 0 \), the discrete symmetry \( \mathbb{Z}_2^{\otimes 3} \) is absent.

The Hamiltonian (6) is essentially self-adjoint with respect to the measure:

\[
d^3r = 8 \pi^2 r_{12} r_{13} r_{23} dr_{12} dr_{13} dr_{23} \quad \text{(9)}
\]

Accordingly, the configuration space \( \mathbb{R}_{\text{rad}} = (r_{12}, r_{13}, r_{23}) \) is defined by the inequality \( S \geq 0 \) (see figure 2), where \( S \) is the area of the triangle formed by the three masses. Explicitly, using Heron’s formula, the area (squared) \( S^2 \) reads:

\[
S^2 = \frac{1}{16} \left((r_{12} + r_{13} + r_{23})(r_{12} + r_{13} - r_{23})(r_{12} - r_{13} + r_{23}) \times (-r_{12} + r_{13} + r_{23})
\]

\[
\text{Figure 2.} \quad \text{The domain} \quad S \geq 0 \quad \text{(shadow region), in the space of relative motion} \quad \mathbb{R}_{\text{rad}} = (r_{12}, r_{13}, r_{23}) \quad \text{for the harmonic potential} \quad V_R \quad \text{(1)} \quad \text{with} \quad m\omega^2 = 2/3 \quad \text{and unit rest length} \quad R = 1 \quad \text{a.u. The other surfaces (in color) correspond to level surfaces of} \quad V_R \quad \text{(equipotentials).}
\]

2.1. Scaling relation

The three parameters \( (m, \omega, R) \) in (6) define completely the harmonic three-body system. Interestingly, one can relate two different systems \( (m, \omega, R) \) and \( (m', \omega', R') \) by making the scale transformation \( r_{ij} \rightarrow \sqrt{\frac{m}{m'} \frac{\omega'}{\omega}} r_{ij} \). That way, the following simple scaling relation between the two corresponding energies holds:

\[
E[m, \omega, R] = \frac{\omega}{\omega'} E[m', \omega', R'] = \sqrt{\frac{m}{m'} \frac{\omega}{\omega'}} R \quad \text{(10)}
\]

3. Case \( R = 0 \): exact solutions

3.1. Jacobi-representation

Let us consider the original Hamiltonian \( \mathcal{H} \) (2) which, by taking \( R = 0 \), becomes:

\[
\mathcal{H} = \frac{1}{2m} \vec{p}_1^2 + \frac{1}{2m} \vec{p}_2^2 + \frac{1}{2m} \vec{p}_3^2 + \frac{3}{2} m \omega^2 \left[ r_{12}^2 + r_{13}^2 + r_{23}^2 \right] \quad \text{(11)}
\]

This Hamiltonian (11) admits a complete separation of variables in Jacobi coordinates [11, 12, 14]. In the center-of-mass reference frame it takes the form:

\[
\mathcal{H} = -\frac{1}{2} \left[ \frac{\partial^2}{\partial \vec{r}_1^{(j)} \partial \vec{r}_1^{(j)}} + \frac{\partial^2}{\partial \vec{r}_2^{(j)} \partial \vec{r}_2^{(j)}} \right] + \frac{9}{2} \omega^2 \left( \vec{r}_1^{(j)} \cdot \vec{r}_1^{(j)} \right) + \frac{9}{2} \omega^2 \left( \vec{r}_2^{(j)} \cdot \vec{r}_2^{(j)} \right) \quad \text{(12)}
\]
(h = 1 and m = 1) where:

\[ r_1^{(j)} = \sqrt{\frac{1}{2}} (r_1 - r_2), \quad r_2^{(j)} = \sqrt{\frac{2}{3}} \left( r_3 - \frac{r_1 + r_2}{2} \right) \]

are nothing but the two three-dimensional vector Jacobi coordinates. In these variables, the Hamiltonian (11) corresponds to the sum of two identical three-dimensional isotropic harmonic oscillators, more precisely, of two Jacobi harmonic oscillators [12]. Hence, the system is maximally superintegrable and exactly solvable. In particular, in this Jacobi representation the second quantization formalism in terms of creation and annihilation operators, namely:

\[ \mathcal{H} = \sum_{\alpha} a_{\alpha}^\dagger a_{\alpha} + 9 \omega, \quad (13) \]

(\(\alpha\) is an index of a fixed number of quantum numbers) can be introduced immediately. As demonstrated in [15], there exists a connection between the theory of superintegrable two-dimensional systems (on the plane) and the theory of superintegrable systems (on the space of relative motion) of the three-body problem parameterized by Jacobi distances. The spectra of E (11) is the sum of spectra of individual Jacobi oscillators:

\[ E = \Lambda_1 + \Lambda_2 \equiv 3 \omega (2 [n_1 + n_2] + \ell_1 + \ell_2 + 3), \quad (14) \]

and its eigenfunctions are the product:

\[ \Psi \left( r_1^{(j)}, r_2^{(j)} \right) = \Psi_1^{(j)} \left( r_1^{(j)} \right) \times \Psi_2^{(j)} \left( r_2^{(j)} \right), \quad (15) \]

of the well-known individual solutions, see below. In spherical coordinates, \( r_k \equiv (r_k^{(1)}, \rho_k, \phi_k) \), they are given by:

\[ \Psi_k \left( r_k^{(j)}; n_k, \ell_k \right) = \tau_k^{\frac{\ell_k}{2}} e^{-\rho_k \tau_k} L_{\ell_k}^{\ell_k + \frac{1}{2}} (3 \omega \tau_k) Y_{\ell_k,n_k} (\theta_k^{(j)}, \phi_k^{(j)}), \quad k = 1, 2, \quad (16) \]

where \( \tau_k = \left( l_k^{(j)} \right)^2 \), \( L_{\ell_k}^{\ell_k + \frac{1}{2}} (3 \omega \tau_k) \) is a generalized Laguerre polynomial and \( Y_{\ell_k,n_k} \) denotes a spherical harmonic function. In (14)–(16), \( n_k \) and \( \ell_k \) are the individual radial and angular-momentum quantum numbers, respectively, of the \( k \)th Jacobi oscillator. In this representation the eigenfunctions of the Hamiltonian (12) are labeled by six quantum integers numbers \((n_1, \ell_1, s_1; n_2, \ell_2, s_2)\).

In the subspace of fixed \( \ell_1 \) and \( \ell_2 \), the Hamiltonian (12) reduces to:

\[ \mathcal{H} = -\frac{1}{2} \sum_{k = 1}^{2} \left[ \frac{\partial^2}{\partial r_k^{(j)} \partial r_k^{(j)}} + \frac{2}{r_k^{(j)}} \frac{\partial}{\partial r_k^{(j)}} + \frac{\ell_k (\ell_k + 1)}{r_k^{(j)^2}} \right] \]

\[ + \frac{9}{2} \omega^2 \left[ \left( r_1^{(j)} \right)^2 + \left( r_2^{(j)} \right)^2 \right]. \quad (17) \]

It acts on the two-dimensional space \((r_1^{(j)}, r_2^{(j)})\) of radial Jacobi distances alone. Evidently, it possesses a hidden Lie algebra \( sl_2^{\mathbb{R}} \). Moreover, for fixed \( \ell_1 \) and \( \ell_2 \) the zero total angular momentum solutions (S-states) of the system are characterized by \( \ell_1 = \ell_2 = \ell, s_1 = -s_2 \) with \( n_1, n_2 \) arbitrary. Otherwise in (12) the sum of the individual angular momentum of the two Jacobi oscillators is always different from zero. In the case \( \ell_1 = \ell_2 = \ell \) with \( s_1 = s_2 = 0 \) it can be shown that the degeneracy of the Nth-level \( E = 3 \omega \left( 2N + 3 \right) \), with \( N = n_1 + n_2 + \ell \), is \( g = \frac{(N+1)(N+2)}{2} \).

3.2. \( \rho \)-representation

If we now consider the reduced Hamiltonian \( \mathcal{H}_{L=0} \) in (8), it is found that at \( R = 0 \) it admits special solutions in the factored form:

\[ \psi_N^{(q)} = \rho_{N,q} \left( r_{12}^2, r_{13}^2, r_{23}^2 \right) \times e^{-\frac{1}{2} \omega \left( r_{12} + r_{13} + r_{23} \right)}, \quad (18) \]

where \( \rho_{N,q} \) is a multivariate polynomial of degree \( N \) in variables:

\[ \rho_{ij} = r_{ij}^2, \quad i \neq j = 1, 2, 3, \quad (19) \]

and \( g = (N + 1)(N + 2)/2 \) is the degeneracy of the \( N \)th-level \( E_N \):

\[ E_N = 3 \omega \left( 2N + 3 \right), \quad N = 0, 1, 2, 3 \ldots \quad (20) \]

In these variables \( \rho_{ij} = r_{ij}^2 \), the Hamiltonian \( \mathcal{H}_{L=0} \) in (8) possesses a hidden Lie algebra \( sl_4 \), and it can be rewritten (up to a gauge transformation) in terms of \( sl_4 \) algebra generators. The eigenvalues become linear in three quantum numbers [12], namely \( N = n_1 + n_2 + n_3 \). We emphasize that (8) does not separate in the \( \rho \)-variables. In particular, for the normalized ground state \( N = 0 \) eigenfunction we obtain:

\[ \psi_0 = \frac{2 \pi}{3 \sqrt{3} \omega^2} e^{-\frac{1}{2} \omega \left( r_{12} + r_{13} + r_{23} \right)}, \quad (21) \]

with energy \( E_0 = 9 \omega \), whereas for the first excited state \( N = 1 \) there exist three degenerate solutions of the form (18), explicitly they read:

\[ \psi_1^{(0)} = \frac{3 \omega^2}{\sqrt{2 \pi}} (1 - \omega r_{12}) e^{-\frac{1}{2} \omega \left( r_{12} + r_{13} + r_{23} \right)}, \quad \psi_1^{(1)} = \frac{3 \omega^2}{\sqrt{2 \pi}} (1 - \omega r_{13}) e^{-\frac{1}{2} \omega \left( r_{12} + r_{13} + r_{23} \right)}, \quad \psi_1^{(2)} = \frac{3 \omega^2}{\sqrt{2 \pi}} (1 - \omega r_{23}) e^{-\frac{1}{2} \omega \left( r_{12} + r_{13} + r_{23} \right)}, \quad (22) \]

corresponding to the same energy \( E_1 = 15 \omega \). In this way, in the case \( R = 0 \) we arrive to the following results:

- For the \( S \)-states of (12), the subset of the exact eigenfunctions \( \Psi \left( r_1^{(j)}, r_2^{(j)} \right) \) (15) in Jacobi coordinates characterized by \( \ell_1 = \ell_2 = \ell \) and \( s_1 = s_2 = 0 \) can be completely expressed as a linear combination of the \( \rho \)-dependable special solutions (18). To illustrate this point, for the lowest states...
Table 1. S-states: Degeneration of the energy level $E_N = 3\omega (2N + 3)$ in (I) the Jacobi-representation $(N = n_1 + n_2 + \ell)$ with $s_1 = s_2 = 0$ vs (II) the $\rho$-representation $(N = N_1 + N_2 + N_3)$.

| $N$ | $n_1$ | $n_2$ | $\ell$ | $N_1$ | $N_2$ | $N_3$ |
|-----|-------|-------|-------|-------|-------|-------|
| 0   | 0     | 0     | 0     | 0     | 0     | 0     |
| 1   | 1     | 0     | 0     | 1     | 0     | 0     |
| 1   | 1     | 1     | 0     | 1     | 0     | 0     |
| 1   | 0     | 1     | 1     | 0     | 1     | 0     |
| 2   | 0     | 0     | 2     | 0     | 2     | 0     |
| 2   | 2     | 0     | 0     | 2     | 0     | 2     |
| 2   | 1     | 1     | 1     | 0     | 2     | 1     |
| 2   | 1     | 0     | 1     | 1     | 1     | 0     |
| 2   | 0     | 1     | 1     | 0     | 1     | 1     |
| 2   | 0     | 0     | 2     | 0     | 1     | 1     |

In this case, we indicate, see table 1, the degeneration of the system in both representations.

- The ground state eigenfunction of the original Hamiltonian (2) solely depends on the three $\rho$-variables, $\rho_j = \tilde{r}_j^2$, the three relative distances (squared). It is presented in (21).
- For the S-states of (12), the exact eigenfunctions $\psi'^{(j)}(\tilde{r}_1^{(j)}, \tilde{r}_2^{(j)})$ (15) in Jacobi coordinates characterized by $\ell_1 = \ell_2 = \ell$ but $s_1 \neq s_2$ can not be expressed as a polynomial in $\rho$-variables multiplied by the ground state eigenfunction.

It will be shown that for $R > 0$ and fixed $N$, the original degenerate $g$-eigenfunctions with $g = (N(N+1)/2$) split into $g = \ell_{\text{max}} = (N(N+1)/2)$ different energy sub-levels. Here $h^2\ell_{\text{max}}(\ell_{\text{max}} + 1)$ corresponds to the largest eigenvalue associated to the quadratic $so(3)$ Casimir invariant of each of the two individual harmonic oscillators appearing in (12).

4. Case $R > 0$: ground state

In this section, as a first step we study the ground state of the spectral problem (8) as a function of the rest length $R$. To find the corresponding approximate solutions, the perturbative and the variational method (VM) are employed.

4.1. Small $R$: perturbation theory

Taking the $R$-dependent terms in the potential $V_R$ (1) as a perturbation to the exactly solvable problem $V_{R=0}$, one can immediately compute the first correction to the energy within the non-linearization procedure [16]. Putting $m = 1$, the original potential $V_R$ (1) can be written as a sum of three terms:

$$V_R = \frac{3}{2} \omega^2 \left( r_{12}^2 + r_{13}^2 + r_{23}^2 \right) - 3 \omega^2 R (r_{12} + r_{13} + r_{23})$$

$$+ \frac{9}{2} \omega^2 R^2,$$

where the first term corresponds to an exactly solvable potential whereas the last one is just a constant. Let us write the ground state function in exponential form:

$$\psi_0(\tilde{r}_{12}, \tilde{r}_{13}, \tilde{r}_{23}) = e^{i \Phi_0(\tilde{r}_{12}, \tilde{r}_{13}, \tilde{r}_{23})},$$

here $\Phi$ is the phase of the wave function. Next, we develop perturbation theory (PT) in powers of $R$, namely:

$$E_0 = \sum_{n=0}^{\infty} \epsilon_n R^n ; \quad \Phi_0(\tilde{r}_{12}, \tilde{r}_{13}, \tilde{r}_{23}) = \sum_{n=0}^{\infty} a_n(\tilde{r}_{12}, \tilde{r}_{13}, \tilde{r}_{23}) R^n,$$

(24)

with $\epsilon_0 = 9\omega$ and $a_n = \frac{\omega}{2}(r_{12}^2 + r_{13}^2 + r_{23}^2)$ being the exact ground-state solution occurring for $R = 0$. As a result of direct calculations, we obtain the value:

$$E_0(R) = 9\omega + \frac{3\omega^2}{2\pi} \left( 3\pi \omega R^3 - 4R \sqrt{6\pi} \omega \right) + \text{corrections}.$$

(25)

Therefore, taking the zero and first order corrections as well as the constant term appearing in (23), PT predicts the existence of a global minimum in $E_0(R)$, localized at $R = R_{\text{min}} \approx 2\sqrt{\frac{3}{\pi}}$, which would corresponds to an equilateral configuration of equilibrium. Since this phenomenon could be an artifact of the deficiency of PT we will verify it using different approximate methods, see below.

4.2. Arbitrary $R$: variational method

For arbitrary $R$, to evaluate the ground state energy $E_0(R)$ we take the simple two-parametric trial function:

$$\psi_{\text{trial}} = e^{-\alpha \omega^2 \left( (r_{12} - \beta R)^2 + (r_{13} - \beta R)^2 + (r_{23} - \beta R)^2 \right)},$$

(26)

where $\alpha, \beta \in [0, 1]$ are variational parameters. At $\beta = 0$ with $\alpha = 1$, the function (26) degenerates into the exact solution appearing at $R = 0$. Though the value of the minimum in $E_0(R)$ disagrees with that found in PT, the VM also predicts the existence of a global minimum. At fixed $\omega = 1$, a comparison of the values for $E_0(R)$ obtained with the perturbative (25), variational (using the optimal (26)) and LMM (see below), respectively, is displayed in figure 3 within the interval $R \in [0, 3.5]$ a.u. In this case, PT (25) provides reasonable accurate results when $0 \leq R \leq 0.3$ a.u. whereas for the VM the corresponding interval of applicability is larger $0 \leq R \leq 2.3$ a.u., as expected. A quantitative comparison between the variational and Lagrange-mesh results is presented in table 2. In particular, the relative difference increases from $0.003\%$ at $R = 0.2$ a.u. up to $9\%$ at $R = 7/2$ a.u. In table 3 more points are presented in the range $R \in [1.6, 1.95]$ a.u. where the minimum of $E_0(R)$, localized at $R_{\text{min}} \approx 1.763936$ a.u., appears. These values were calculated using the LMM (see below) with not less than 11 significant figures. Using the trial function (26), the probability density $P \propto \psi_0^2(\tilde{r}_{12}, \tilde{r}_{13}, \tilde{r}_{23})$ in the space $(\tilde{r}_1, \tilde{r}_2, \tilde{r}_3)$
satisfy the Lagrange conditions: i.e. correspond to the zeros of Laguerre polynomials of degree domain where a set of this methodology let us consider a one-dimensional problem

\[ 5. \] The Lagrange-mesh method

In order to solve the Schrödinger equation for the Hamiltonian \( \hat{H} \), the LMM is also applied \[ \text{et al.} \]

\[ R \]

\[ 3.202780380949 \]

\[ E_R \]

\[ 0 \]

\[ \alpha \]

\[ \beta \]

\[ LMM \]

\[ E_0 \]

\[ \omega \]

\[ \nu \]

\[ H \]

\[ \psi_\nu \]

\[ \lambda \]

\[ G \]

\[ P \]

\[ f(x) \]

\[ L_M(x) \]

\[ e^{-x/2} \]

\[ \lambda_k \]

\[ G(x_k) \]

\[ \int_0^\infty G(x)dx \approx \sum_{k=1}^M \lambda_k G(x_k) \]

\[ \psi \]

\[ c_i \]

\[ \sum_{i=1}^M c_i f_i(r) \]

\[ 5. \]

\[ \text{The Lagrange-mesh method} \]

In order to solve the Schrödinger equation for the Hamiltonian \( \hat{H} \), the LMM is also applied \[ \text{et al.} \]. To introduce this methodology let us consider a one-dimensional problem where a set of \( M \) Lagrange functions \( f_i(x) \) defined over the domain \( x \in [0, \infty) \) is associated with \( M \) mesh points \( x_i \), which correspond to the zeros of Laguerre polynomials of degree \( M \), i.e., \( L_M(x_i) = 0 \). The Lagrange–Laguerre functions \( f_i(x) \) which satisfy the Lagrange conditions:

\[ f_i(x_j) = \delta_{ij} \]

\[ \text{at the } M \text{ mesh points are given by:} \]

\[ f_i(x) = (-1)^i \frac{1}{x_i^{1/2}} \frac{L_M(x)}{(x-x_i)} e^{-x/2}, \]

\[ \text{and the coefficients } \lambda_i \text{ are the weights associated with a Gauss quadrature:} \]

\[ \int_0^\infty G(x)dx \approx \sum_{k=1}^M \lambda_k G(x_k). \]

In terms of the \( M \) Lagrange functions \( f_i(x) \), the solution of the Schrödinger equation for a particle of mass \( m \) in a potential \( V(x) \) is expressed as:

\[ \psi(r) = \sum_{i=1}^M c_i f_i(r). \]
The function (30), together with the Gauss quadrature (29) and the Lagrange conditions (27) leads to the system of variational equations:

\[ \sum_{j=1}^{M} \left[ \frac{\hbar^2}{2m} T_{ij} + V(x_i) \delta_{ij} \right] c_j = E c_i, \quad (31) \]

where \( T_{ij} \) are the kinetic-energy matrix elements (see for example [18]) and \( V(x) \) is the potential evaluated at the mesh points \( x_i \). By solving the system (31), the energies \( E \) and the eigenvectors \( c_i \) are obtained, from which the approximation to the wave function (30) is obtained.

The present system has three degrees of freedom which are described by the three distances between the particles: \( r_{12} \), \( r_{13} \) and \( r_{23} \). Technically, a considerable simplification results from going over to the so-called perimetric coordinates used by Pekeris in his helium calculations [19]. These perimetric coordinates are defined by the linear relations:

\[ x = r_{12} + r_{13} - r_{23}, \]
\[ y = r_{12} - r_{13} + r_{23}, \]
\[ z = -r_{12} + r_{13} + r_{23}. \]

(32)

The volume element is \( dV \propto (x+y)(x+z)(y+z)dx dy dz \). By the above transformation the limits of the three perimetric coordinates \( x, y \) and \( z \) become independent of each other and they vary from 0 to \( \infty \).

In perimetric coordinates, following the notation presented in [20], the matrix elements of the kinetic energy operator (6) \( \langle F | T | G \rangle \) between functions \( F \) and \( G \) can be written as

\[ \langle F | T | G \rangle = \int_0^{\infty} dx \int_0^{\infty} dy \int_0^{\infty} dz \sum_{i,j=1}^{3} A_{ij}(x,y,z) \frac{\partial F}{\partial x_i} \frac{\partial G}{\partial x_j}, \]

(33)

where \((x_1,x_2,x_3) = (x,y,z)\) and the coefficients \( A_{ij} \) are given by:

\[ A_{1,1} = x + y + z + xz + xy + yz, \]
\[ A_{2,2} = yz + (x+y + xz + xy + yz), \]
\[ A_{3,3} = xy + xz + yz + (x+y + xz + xy + yz), \]
\[ A_{1,2} = A_{2,1} = -xy, \]
\[ A_{1,3} = A_{3,1} = -xz, \]
\[ A_{2,3} = A_{3,2} = -yz. \]

(34)

The generalization of the LMM to the three-dimensional case is as follows [21, 22]. The three-dimensional Lagrange functions \( F_{ijk}(x,y,z) \) are defined as:

\[ F_{ijk}(x,y,z) = \mathcal{N}_{ijk}^{-1/2} f_{ijk}^{M}(x/h_c) f_{ijk}^{M}(y/h_c) f_{ijk}^{M}(z/h_c), \]

(35)

where the functions \( f_{ijk}^{M} \) all have the same structure as (28) with \( M \) replaced by the respective degrees \( M_x, M_y \) and \( M_z \) and the zeros \( x_q \) \((q = 1, \ldots, M_x)\), \( y_q \) \((q = 1, \ldots, M_y)\) and \( z_q \) \((r = 1, \ldots, M_z)\) are the zeros of the respective Laguerre polynomials. The scaling parameters \( h_x, h_y \) and \( h_z \) are incorporated to fit the mesh to the physical system. The normalization factor \( \mathcal{N}_{ijk} \) is defined by:

\[ \mathcal{N}_{ijk} = h_x h_y h_z (h_x x_i + h_y y_i) (h_x x_j + h_z z_i) (h_y y_j + h_z z_i). \]

(36)

This three-dimensional Lagrange functions (35) satisfy:

\[ F_{ijk}(x_i y_i z_i, h_x y_i y_i, h_x z_i, E) = (\mathcal{N}_{ijk} \lambda_i \mu_j \nu_k)^{-1/2} \delta_{ij} \delta_{jk} \delta_{kk}, \]

(37)

where \( \lambda_i, \mu_j \) and \( \nu_k \) are the weights of the Gauss quadratures (29) for the variables \( x, y \) and \( z \), respectively. In terms of the Lagrange functions \( F_{ijk}(x,y,z) \) (35), the wave function is expanded as:

\[ \Psi(x,y,z) = \sum_{i=1}^{M_x} \sum_{j=1}^{M_y} \sum_{k=1}^{M_z} C_{ijk} F_{ijk}(x,y,z), \]

(38)

which makes it possible, together with the Gauss quadratures for each variable and condition (37), to write the Schrödinger equation for the Hamiltonian (6) as a mesh equation:

\[ \sum_{i=1}^{M_x} \sum_{j=1}^{M_y} \sum_{k=1}^{M_z} \left( \langle F_i | \gamma_j k | F_k \rangle \right) + \left[ \langle F_i | \gamma_j k | V | F_k \rangle - E \right] \delta_{ij} \delta_{jk} \delta_{kk} = 0. \]

(39)

The matrix elements of the potential \( \langle F_i | \gamma_j k | V | F_k \rangle \) have a very simple representation:

\[ \langle F_i | \gamma_j k | V | F_k \rangle = V(x_i, x_j, y_i, y_j, z_i, z_j) \delta_{ij} \delta_{jk} \delta_{kk}, \]

(40)

which correspond to the potential \( V_B \) (1) in perimetric coordinates evaluated at the mesh points. In contrast, the matrix elements of the kinetic energy operator \( \langle F_i | \gamma_j k | T | F_k \rangle \) between two elements \( F_{ijk} \) (33) are given by:

\[ \langle F_i | \gamma_j k | T | F_k \rangle = 2N_{ijk}^{-1/2} \left( \sum_{n} \lambda_i h_x^{-2} A_{1,1} \right) \]
\[ \times \left( \frac{h_x x_i + h_y y_i + h_z z_i}{f(x_i) f(y_i) f(z_i)} \right) \]
\[ + \left( \frac{\mu_j}{\nu_k h_y h_z} \right) \sum_{n} A_{2,2} \left( h_x x_i, h_y y_i, h_z z_i \right) \frac{f(y_i)}{f(y_i)} \]
\[ + \left( \frac{\nu_k}{\mu_j h_x h_z} \right) \sum_{n} A_{3,3} \left( h_x x_i, h_y y_i, h_z z_i \right) \frac{f(z_i)}{f(z_i)} \]
\[ + \left( \frac{\delta_{jk}}{\delta_{kk} h_x h_y h_z} \right) \sum_{n} A_{1,2} \left( h_x x_i, h_y y_i, h_z z_i \right) \frac{f(x_i)}{f(x_i)} \]
\[ + \left( \frac{\delta_{jk}}{\delta_{kk} h_x h_y h_z} \right) \sum_{n} A_{1,3} \left( h_x x_i, h_y y_i, h_z z_i \right) \frac{f(x_i)}{f(x_i)} \]
\[ + \left( \frac{\delta_{jk}}{\delta_{kk} h_x h_y h_z} \right) \sum_{n} A_{2,3} \left( h_x x_i, h_y y_i, h_z z_i \right) \frac{f(x_i)}{f(x_i)} \]
\[ + \left( h_x x_i + h_y y_i + h_z z_i \right)^{-1} \left( \lambda_i h_x^{-2} A_{1,1} \right) \]
\[ \langle F_i | \gamma_j k | V | F_k \rangle = V(x_i, x_j, y_i, y_j, z_i, z_j) \delta_{ij} \delta_{jk} \delta_{kk}. \]

(41)
Table 4. Energy \( E_{N,n} \) in a.u. of the three-body system with harmonic interactions for four values of \( N = 0, 1, 2, 3 \). Results for 11 rest lengths \( R \) are presented for \( m = 1 \) and \( \omega = 0.5 \).

\[
\begin{array}{cccccc}
N, n & R = 0.0 & R = 0.5 & R = 1.0 & R = 1.5 & R = 2.0 \\
0.0 & 4.500000000000 & 3.248654270738 & 2.398230647673 & 1.893326994351 & 1.658224669986 \\
1.0 & 7.500000000000 & 5.822579071286 & 4.55679365814 & 3.664836226784 & 3.09742253058 \\
1.0 & 7.500000000000 & 5.822579071286 & 4.55679365814 & 3.664836226784 & 3.09742253058 \\
1.1 & 7.500000000000 & 5.888219366854 & 4.698674842022 & 3.89447971731 & 3.42004994404 \\
2.0 & 10.500000000000 & 8.42599881144 & 6.767207301164 & 5.497092599573 & 4.58573011185 \\
2.1 & 10.500000000000 & 8.47817713040 & 6.87163036857 & 5.662422560165 & 4.80371359194 \\
2.1 & 10.500000000000 & 8.47817713040 & 6.87163036857 & 5.662422560165 & 4.80371359194 \\
2.2 & 10.500000000000 & 8.54520794140 & 7.01948079404 & 5.87230110601 & 5.0804090142 \\
2.2 & 10.500000000000 & 8.54520794140 & 7.01948079404 & 5.87230110601 & 5.0804090142 \\
2.3 & 10.500000000000 & 8.585804667998 & 7.10256453523 & 6.02234772884 & 5.30442611111 \\
2.3 & 10.500000000000 & 8.585804667998 & 7.10256453523 & 6.02234772884 & 5.30442611111 \\
3.0 & 13.500000000000 & 11.17248579552 & 9.151798562159 & 7.58057929596 & 6.37798183868 \\
3.0 & 13.500000000000 & 11.17248579552 & 9.151798562159 & 7.58057929596 & 6.37798183868 \\
3.1 & 13.500000000000 & 11.166486177781 & 9.25682108632 & 7.74945695453 & 6.62164501144 \\
3.2 & 13.500000000000 & 11.182671178672 & 9.28696974298 & 7.88519430823 & 6.65740317017 \\
3.3 & 13.500000000000 & 11.20133020368 & 9.32777238811 & 7.85969484738 & 6.75193120417 \\
3.4 & 13.500000000000 & 11.23740017990 & 9.40182866849 & 7.96194939956 & 6.90779438745 \\
3.5 & 13.500000000000 & 11.299682142132 & 9.52787050754 & 8.15772763021 & 7.15213692085 \\
3.6 & 13.500000000000 & 11.32564849450 & 9.58192910947 & 8.25116413636 & 7.29858551687 \\
\end{array}
\]

6. Results and discussion

In this section the energies \( E = E(R) \) appearing in (8) for the lowest \( S \)-states solutions \( \psi(x,y,z) \) (38) using the LMM are presented. For clarity of the degeneracy as a function of \( R \), the energies are denoted by \( E = E_{N,n} \). At \( R = 0 \) a.u. the label \( N \) corresponds to the quantum number of the exact solution (18). For \( R > 0 \), the degenerate \( N \)th-level splits into sub-levels denoted by \( n = 0, 1, 2, 3, \ldots \).

Table 4 presents the energy values for \( \omega = 0.5 \) and \( R \in [0.0, 4.0] \) a.u. in constant steps of 0.5 a.u. for four different values of \( N: N = 0, 1, 2 \) and 3. In all cases 12 decimal digits are provided. The limit case \( R = 0 \), presented in the second column, is in complete agreement with the analytic solution (20). It can also be noticed that the degeneracy \( g_0 = 1 \), \( g_1 = 3 \), \( g_2 = 6 \) and \( g_3 = 10 \) obtained for \( N = 0, 1, 2 \) and 3 respectively, coincides with the values of the analytic expression \( g_N = (N + 1)(N + 2)/2 \). For \( R \neq 0 \), the degeneracy is partially removed: each \( g_N \)-degenerated energetic level \( E_N \) seems to unfold into \((N+1)(N+2)/2\) different energy levels \( E_{N,n} \), as can be seen in columns 3 through 6 of table 4 (and its continuation) and in figure 5 where the results are depicted.

As pointed out in the previous sections for the case \( \omega = 1 \) (see also below), the ground state \( E_{0,0} \) vs \( R \) presents a minimum. For \( \omega = 0.5 \) the equilibrium length for which the minimum appears is \( R_{\text{min}} \approx 2.494583 \) a.u. and the corresponding
energy value is \( E_{\min}^{\omega} = 1.601390190475 \) a.u. The existence of \( R_{\min} \) defines a distinguished size of the system. If \( R \) is taken as a dynamical variable such that its motion can be neglected (in a first approximation), then the curve in figure 3 would play the role of a Born–Oppenheimer potential curve and the local minimum can be interpreted as a preferential size of the corresponding molecule. A global minimum in energy as a function of \( R \) is present for \( m \) fixed.

Similar calculations were carried out for the case \( \omega = 1.0 \) for \( R \in [0.0, 6.0] \) a.u. in constant steps of 0.5 a.u. for three values of \( N: N = 0, 1 \), and 2. These are depicted in figure 6. The position of the minimum for the ground state \( E_{0,0} \) present in figure 3, appears for a rest length of \( R_{\min} \approx 1.763936 \) a.u. and the energy value is \( E_{\min}^{0,0} = 3.202780380949 \) a.u. (see also table 3).

Results presented in table 4 for the system defined by the parameters \( (m, w, R) = (1, 1.2, R) \) allow us, according to the scaling relation (10), to obtain the spectrum for the system defined by the parameters \( (m', w', R') \) as:

\[
E \left[ m', \omega', R' \right] = \sqrt{\frac{1}{2m' \omega'}} R' = 2 \omega' E \left[ m = 1, \omega = 1/2, R \right].
\]  

(42)

Likewise, for fixed \( m \) and \( \omega \) it can be shown that the energy tends asymptotically to a finite value \( E_{\infty} \) at large \( R \), namely \( E[m, \omega, R \to \infty] \to E_{\infty} \) with \( 0 < E_{\infty} < E[m, \omega, R = 0] \).

For fixed \( m = m' = 1 \) and \( \omega = \omega' \), the expression (42) allows us to relate the critical points of the curve \( E = E(\omega') \). In particular, its minimum value \( E_{\min} \) occurs at:

\[
R_{\min}'(\omega') = \frac{1}{\sqrt{2 \omega'}} R_{\min}^{(\omega=1/2)},
\]  

(43)

where \( R_{\min}^{(\omega=1/2)} \approx 2.494583 \) a.u., with energy:

\[
E_{\min} \left[ m = 1, \omega', R' = \frac{1}{\sqrt{2 \omega'}} R_{\min}^{(\omega=1/2)} \right] = 2 \omega' E \left[ m = 1, \omega = 1/2, R_{\min}^{(\omega=1/2)} \right],
\]  

(44)

here \( E[m = 1, \omega = 1/2, R_{\min}^{(\omega=1/2)}] = 1.6013901904475 \) a.u., in complete agreement with the numerical result obtained for the case \( \omega = 1 \). It is evident that as the value of \( \omega' \) increases, the energy \( E_{\min}(\omega') \) grows and the position of the minimum \( R_{\min}(\omega') \) decreases, see (43) and (44).

Now, in the case of three particles with arbitrary masses and inspired by a phenomenological model of the forces inside a baryon where three quarks are connected by three glue strings and these strings meet at a ‘gluon junction’ (see [23] and references therein), one can also consider a generalization of (1) given by:

\[
\bar{V}_R \equiv \bar{V} \left( \nu_{12} (r_{12} - R_{12})^2 + \nu_{13} (r_{13} - R_{13})^2 + \nu_{23} (r_{23} - R_{23})^2 \right),
\]  

(45)

where \( \nu_{ij} \) are parameters (not all of them necessarily positive) and the rest lengths \( R_{ij} > 0 \) can take different values. Such a model can play an important role in molecular and atomic three-body systems where the configuration of equilibrium

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**Figure 5.** The energy \( E_{N,0} \) vs \( R \) of the three-body harmonic system \( V_R \) (1) for the 14 lowest \( S \)-states. It is a smooth function of \( R \). Numerical values calculated with the LMM are marked by bullets, the lines are a guide to the eye. The values \( m = 1 \) and \( \omega = 1/2 \) were used in the calculations. Energy is presented in Hartrees.
Figure 6. The energy $E_{N,n}$ vs $R$ of the three-body harmonic system $V_R$ (1) for the seven lowest $S$-states with parameters $m = 1$ and $\omega = 1$. It is a smooth function of $R$. Numerical values calculated with the LMM are marked by bullets, the lines are a guide to the eye. Energy is presented in Hartrees.

7. Conclusions

For the generalized three-body harmonic system the energies of the first 14 lowest $S$-states were computed with accuracy of 11 figures in the domain of $R \in [0.0, 4.0]$ a.u. At $R = 0$, the problem becomes maximally superintegrable and exactly solvable. The corresponding degenerate levels were analyzed in two-different Lie-algebraic representations. At $R > 0$, in order to solve the Schrodinger equation for this three-body system (8), three methods were implemented for the ground state: (i) the PT, (ii) the VM and (iii) the LMM. The first two (PT and VM) indicated the presence of a global minimum in the ground state energy for a certain value of $R = R_{\text{min}} > 0$, which was precisely confirmed by the LMM. In all cases the energy $E(R)$ of the lowest states as a function of $R$ displays a smooth behavior (figures 5 and 6). The degeneracy of the system when $R = 0$ is partially removed for $R > 0$, and the quantitative splitting of levels was presented. Making an evident modification of the Hamiltonian (2) the analogue three-body generalized harmonic system can be written for arbitrary masses and different spring constants (45). Such a model can serve as a zero order approximation for the study of three-body Coulomb atomic and molecular systems. In particular, for the traditional triatomic molecule [25], the corresponding Coulomb potential can be expanded around the triangular configuration of equilibrium. That way, by comparing the so obtained quadratic terms with the experimental data, the values of the parameters $\omega$ and $R$ can be fixed. These values will then be used in our three-body harmonic model, and its energies give the rovibrational spectra directly. It is also worth mentioning that within the LMM it is possible and straightforward to consider states with non-zero angular momentum, i.e. states with $L \neq 0$.

Since a distinguished equilibrium distance $R_{\text{min}}$ occurs in the ground state energy, this could suggest that for the corresponding classical system a systematic study of the maximum Lyapunov exponent $\lambda = \lambda(R)$ may reveal a special value at $R = R_{\text{min}} > 0$ or the integrability properties of the system could be modified considerably. We plan to address this subject in future studies.

Data availability statements

All data that support the findings of this study are included within the article (and any supplementary files).

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Conflict of interests

The authors declare no competing interests.

References

[1] Moshinsky M and Smirnov Y 1996 The Harmonic Oscillator in Modern Physics (Contemporary Concepts in Physics) (Amsterdam: Harwood Academic Publishers)

[2] Saporta Katz O and Efrati E 2019 Phys. Rev. Lett. 122 024102

[3] Saporta Katz O and Efrati E 2020 Phys. Rev. E 101 032211

[4] Escobar-Ruiz A M, Quiroz-Juarez M A, Del Rio-Correa J L and Aquino N 2022 Sci. Rep. 12 13346

[5] Gutzwiller M C 1971 J. Math. Phys. 12 343

[6] Richard J-M 1992 Phys. Rep. 212 1

[7] Turbiner A V, Miller W and Escobar-Ruiz A M 2017 J. Phys. A: Math. Theor. 50 215201

[8] Turbiner A V, Miller W and Escobar-Ruiz M A 2018 J. Math. Phys. 59 022108

[9] Gu X-Y, Duan B and Ma Z-Q 2002 J. Math. Phys. 43 2895

[10] Fernández F M 2008 arXiv:0810.2210

[11] de Castro A S and Sugaya M 1993 Eur. J. Phys. 14 259

[12] Turbiner A V, Miller W and Escobar-Ruiz M A 2020 J. Phys. A: Math. Theor. 53 055302

[13] Znojil M 2003 Nucl. Phys. B 662 554

[14] Delves L M 1960 Nucl. Phys. E 20 275

[15] Turbiner A V, Miller W and Escobar-Ruiz M A 2020 J. Phys. A: Math. Theor. 54 015204

[16] Turbiner A V 1984 Sov. Phys. Usp. 27 668

[17] Baye D and Heenen P H 1986 J. Phys. A: Math. Gen. 19 2041

[18] Baye D 2015 Phys. Rep. 32 1–107

[19] Pekeris C L 1958 Phys. Rev. 112 1649

[20] Baye D and Dohet-Eraly J 2015 Phys. Chem. Chem. Phys. 17 31417

[21] Hesse M and Baye D 2001 J. Phys. B: At. Mol. Opt. Phys. 34 1425–42

[22] Hesse M and Baye D 2003 J. Phys. B: At. Mol. Opt. Phys. 36 139–54

[23] Alexandrou C, de Forcrand P and Jahn O 2003 Nucl. Phys. B 119 667

[24] Kutzelnigg W and Jaquet R 2006 Phil. Trans. R. Soc. A 364 2855–76

[25] Wang J and Greene C H 2013 J. Phys. Chem. A 117 9761