On the symmetry of three identical interacting particles in a one-dimensional box

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Abstract

We study a quantum-mechanical system of three particles in a one-dimensional box with two-particle harmonic interactions. The symmetry of the system is described by the point group D_{3d}. Group theory greatly facilitates the application of perturbation theory and the Rayleigh-Ritz variational method. A great advantage is that every irreducible representation can be treated separately. Group theory enables us to predict the connection between the states for the small box length and large box length regimes of the system. We discuss the crossings and avoided crossings of the energy levels as well as other interesting features of the spectrum of the system.

Keywords: identical particles, box trap, point-group symmetry, perturbation theory, variational method

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1. Introduction

During the last decades there has been great interest in the model of a harmonic oscillator confined to boxes of different shapes and sizes[1–23]. Such model has been suitable for the study of several physical problems ranging from dynamical friction in star clusters[4] to magnetic properties of solids[6] and impurities in quantum dots[23].

One of the most widely studied models is given by a particle confined to a box with impenetrable walls at $-L/2$ and $L/2$ bound by a linear force that produces a parabolic potential-energy function $V(x) = k(x - x_0)^2/2$, where $|x_0| < L/2$. When $x_0 = 0$ the problem is symmetric and the eigenfunctions are either even or odd; such symmetry is broken when $x_0 \neq 0$. Although interesting in itself, this model is rather artificial since the cause of the force is not specified. It may, for example, arise from an infinitely heavy particle clamped at x_0. For this reason we have recently studied the somewhat more interesting and realistic case in which the other particle also moves within the box[24]. Such a problem is conveniently discussed in terms of its symmetry point-group; for example: it is C_i when the two particles are different and C_{2h} for identical ones.

It follows from what was just said that the case of identical particles is of greater interest from the point of view of symmetry. For this reason in this paper we analyse the model of three interacting particles confined to a one–dimensional box with impenetrable walls. In Section 2 we consider three particles in a general one-dimensional trap with two-particle interactions and discuss its symmetry as well as suitable coordinates for its treatment. In Section 3 we focus on the case that the trap is given by a box with impenetrable walls and apply perturbation theory based on the exact results for infinitely small box length. In Section 4 we discuss the limit of infinite box length as well as the connection between both regimes. In Section 5 we construct a symmetry-adapted basis set for the application of the Rayleigh-Ritz variational method and discuss the main features of the spectrum. Finally, in Section 6 we provide further comments on the main results of the paper and draw conclusions.

2. Three particles in a one-dimensional trap

We consider three structureless particles in a one-dimensional trap with a Hamiltonian of the form

$$\begin{aligned} H &= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial x_3^2}\right)+V(x_1)+V(x_2)+V(x_3) \\ &\quad +W(|x_1-x_2|)+W(|x_2-x_3|)+W(|x_3-x_1|), \end{aligned} \tag{1}$$

where $V(x_i)$ confines each particle in a given space region (trap) and $W(|x_i - x_j|)$ are two-body interactions that couple the particles. It is convenient to define dimensionless coordinates $(x,y,z)=(x_1/L,x_2/L,x_3/L)$, where L is a suitable length unit. The resulting dimensionless Hamiltonian is

$$\begin{aligned} H' &= \frac{2mL^2}{\hbar^2}H=-\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+v(x)+v(y)+v(z) \\ &\quad +\lambda\left[w(|x-y|)+w(|y-z|)+w(|z-x|)\right], \end{aligned} \tag{2}$$

where $v(x)=2mL^2V(Lx)/\hbar^2$ and $\lambda w(|x-y|)=2mL^2W(L|x_1-x_2|)/\hbar^2$, etc. In this equation λ is a dimensionless parameter that measures the strength of the coupling interaction.

From now on we omit the prime and simply write H instead of H'. In addition to it, we assume that the trap is symmetric: $v(-q) = v(q)$. The Hamiltonian $H_0 = H(\lambda = 0)$ is invariant under the following transformations

$$
\begin{aligned}
(x,y,z) &\rightarrow \{x,y,z\}_P \\
(x,y,z) &\rightarrow \{-x,y,z\}_P \\
(x,y,z) &\rightarrow \{x,-y,z\}_P \\
(x,y,z) &\rightarrow \{x,y,-z\}_P \\
(x,y,z) &\rightarrow \{-x,-y,z\}_P \\
(x,y,z) &\rightarrow \{-x,y,-z\}_P \\
(x,y,z) &\rightarrow \{x,-y,-z\}_P \\
(x,y,z) &\rightarrow \{-x,-y,-z\}_P,
\end{aligned} \tag{3}
$$

where $\{a,b,c\}_P$ denotes the different permutations of the three real numbers a, b and c[25]. Note that the 48 coordinate transformations (3) form a group that is commonly named O_h[26, 27]. In the particular case that $v(q) = q^2$ the symmetry of H_0 is given by the full rotation group $O(3)$[26].

When $\lambda \neq 0$ the Hamiltonian is invariant under the 12 coordinate transformations

$$
\begin{aligned}
(x,y,z) &\rightarrow \{x,y,z\}_P \\
(x,y,z) &\rightarrow \{-x,-y,-z\}_P,
\end{aligned} \tag{4}
$$

and we can describe the symmetry of the system in configuration space by means of the point group D_{3d}[26, 27]. However, if $v(q) = q^2$ the symmetry increases because the trapping potential is invariant under arbitrary rotations about any axis in configuration space. The coordinate transformation

$(x, y, z) = (q_1, q_2, q_3) \cdot \mathbf{J}$, where[28]

$$\mathbf{J} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix}, \tag{5}$$

makes the coupling term independent of q_3 because

$$(x - y, y - z, z - x) = \left(\sqrt{2} q_1, \frac{\sqrt{6}}{2} q_2 - \frac{\sqrt{2}}{2} q_1, -\frac{\sqrt{2}}{2} q_1 - \frac{\sqrt{6}}{2} q_2 \right). \tag{6}$$

Since the coupling term is therefore invariant under rotations about the q_3 axis by angles of $\frac{2\pi j}{6}$, $j = 1, 2, 3, 4, 5$ the resulting Hamiltonian operator

$$\begin{aligned} H &= -\left(\frac{\partial^2}{\partial {q_1}^2} + \frac{\partial^2}{\partial {q_2}^2} + \frac{\partial^2}{\partial {q_3}^2} \right) + {q_1}^2 + {q_2}^2 + {q_3}^2 \\ &\quad + \lambda \left[w\left(\sqrt{2} \left| q_1 \right| \right) + w\left(\left| \frac{\sqrt{6}}{2} q_2 - \frac{\sqrt{2}}{2} q_1 \right| \right) + w\left(\left| \frac{\sqrt{2}}{2} q_1 + \frac{\sqrt{6}}{2} q_2 \right| \right) \right], \end{aligned} \tag{7}$$

is separable into its (q_1, q_2) and q_3 parts and exhibits symmetry D_{6h}.

If $w(|s - t|) = (s - t)^2$ the resulting Hamiltonian

$$H = -\left(\frac{\partial^2}{\partial {q_1}^2} + \frac{\partial^2}{\partial {q_2}^2} + \frac{\partial^2}{\partial {q_3}^2} \right) + {q_1}^2 + {q_2}^2 + {q_3}^2 + 3\lambda \left(q_1^2 + q_2^2 \right) \tag{8}$$

is fully separable and exhibits symmetry $D_{\infty h}$[27].

3. One-dimensional box

As stated in the introduction we are interested in a system of three identical particles in a one-dimensional box. To this end we resort to the Hamiltonian (2) and choose the trapping potential

$$v(q) = \begin{cases} 0 \text{ if } |q| < 1 \\ \infty \text{ elsewhere} \end{cases}. \tag{9}$$

Therefore, the boundary conditions for the solutions to the Schrödinger equation $H\psi = E\psi$ become

$$\psi(\pm 1, y, z) = \psi(x, \pm 1, z) = \psi(x, y, \pm 1) = 0. \tag{10}$$

For concreteness we focus the discussion on the Hamiltonian

$$H = -\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + \lambda\left[(x-y)^2 + (y-z)^2 + (z-x)^2\right], \tag{11}$$

that is an extension of the two-particle model discussed earlier[24].

This problem is exactly solvable when $\lambda = 0$ and the eigenvalues and eigenfunctions of H_0 are

$$\begin{aligned} E_{n_1n_2n_3} &= \frac{\pi^2}{4}(n_1^2 + n_2^2 + n_3^2),\ n_1, n_2, n_3 = 1, 2, \ldots \\ \varphi_{n_1n_2n_3}(x, y, z) &= \phi_{n_1}(x)\phi_{n_2}(y)\phi_{n_3}(z) \\ \phi_n(q) &= \sin\frac{n\pi(q+1)}{2}. \end{aligned} \tag{12}$$

All the sets of quantum numbers produced by the distinct permutations $\{n_1, n_2, n_3\}_P$ lead to the same energy (degenerate eigenstates). In addition to it, there is a Pythagorean degeneracy[25] that we do not discuss here. Each of the functions $\phi_n(q)$ is even (e) or odd (o) when n is either odd or even, respectively. A straightforward analysis based on group theory shows that[25]

$$\begin{aligned} \{e, e, e\}_P &\rightarrow A_{1g} \\ \{e', e, e\}_P &\rightarrow A_{1g} \oplus E_g \\ \{e', e'', e'''\}_P &\rightarrow A_{1g} \oplus A_{2g} \oplus E_g \oplus E_g \\ \{o, e, e\}_P &\rightarrow A_{2u} \oplus E_u \end{aligned}$$

$$
\begin{aligned}
\{o,e',e''\}_P &\rightarrow A_{1u}\oplus A_{2u}\oplus E_u\oplus E_u \\
\{e,o,o\}_P &\rightarrow A_{1g}\oplus E_g \\
\{o,o',e\}_P &\rightarrow A_{1g}\oplus A_{2g}\oplus E_g\oplus E_g \\
\{o,o,o\}_P &\rightarrow A_{2u} \\
\{o',o,o\}_P &\rightarrow A_{2u}\oplus E_u \\
\{o,o',o''\}_P &\rightarrow A_{1u}\oplus A_{2u}\oplus E_u\oplus E_u, \qquad (13)
\end{aligned}
$$

where $\{s',s'',s'''\}_P$ denotes a set of distinct permutations of products of functions $\phi_n(q)$ with the indicated symmetry. The characters for every irrep, as well as some of the basis functions for them, are given in Table 1.

It is instructive to carry out a straightforward calculation based on perturbation theory of first order. For the first energy levels we have

$$
\begin{aligned}
E_{1A_{1g}} &= \frac{3\pi^2}{4}+\frac{2\left(\pi^2-6\right)}{\pi^2}\lambda+O(\lambda^2) \\
E_{1A_{2u}} &= \frac{3\pi^2}{2}+\frac{162\pi^4-729\pi^2-4096}{81\pi^4}\lambda+O(\lambda^2) \\
E_{1E_u} &= \frac{3\pi^2}{2}+\frac{162\pi^4-729\pi^2+2048}{81\pi^4}\lambda+O(\lambda^2) \\
E_{2A_{1g}} &= \frac{9\pi^2}{4}+\frac{2\left(81\pi^4-243\pi^2-2048\right)}{81\pi^4}\lambda+O(\lambda^2) \\
E_{1E_g} &= \frac{9\pi^2}{4}+\frac{2\left(81\pi^4-243\pi^2+1024\right)}{81\pi^4}\lambda+O(\lambda^2) \\
E_{3A_{1g}} &= \frac{11\pi^2}{4}+\frac{2\left(9\pi^2-38\right)}{9\pi^2}\lambda+O(\lambda^2) \\
E_{2E_g} &= \frac{11\pi^2}{4}+\frac{2\left(9\pi^2-38\right)}{9\pi^2}\lambda+O(\lambda^2) \\
E_{2A_{2u}} &= 3\pi^2+\frac{2\pi^2-3}{\pi^2}\lambda+O(\lambda^2) \\
E_{3A_{2u}} &= \frac{7\pi^2}{2}+\frac{101250\pi^4-275625\pi^2-2772992}{50625\pi^4}\lambda+O(\lambda^2)
\end{aligned}
$$

$$
\begin{aligned}
E_{2E_u} &= \frac{7\pi^2}{2} + \frac{101250\pi^4 - 275625\pi^2 - 2048\sqrt{466441}}{50625\pi^4}\lambda + O(\lambda^2) \\
E_{3E_u} &= \frac{7\pi^2}{2} + \frac{101250\pi^4 - 275625\pi^2 + 2048\sqrt{466441}}{50625\pi^4}\lambda + O(\lambda^2) \\
E_{1A_{1u}} &= \frac{7\pi^2}{2} + \frac{101250\pi^4 - 275625\pi^2 + 2772992}{50625\pi^4}\lambda + O(\lambda^2) \qquad (14)
\end{aligned}
$$

The eigenvalues that are degenerate at $\lambda = 0$ exhibit the same parity u or g. Note that the energy levels $E_{3A_{1g}}$ and E_{2E_g} (stemming from the set of quantum numbers $\{3,1,1\}_P$) remain degenerate at first order. We will discuss them in Section 5.

4. Infinite box

The parameter λ introduced in Section 2 is proportional to the square of an arbitrary length L. In the particular case discussed in Section 3 the three particles are confined into a box of length $2L$ as shown by the boundary conditions (10). Therefore, the infinite-box limit $L \to \infty$ corresponds to $\lambda \to \infty$. We appreciate that when $\lambda \to \infty$ the motion of the system center of mass is unbounded and the eigenfunctions of the Hamiltonian operator are of the form

$$
f_{n_1\,n_2\,k}(q_1, q_2, q_3) = g_{n_1}(q_1) g_{n_2}(q_2) e^{ikq_3}, \qquad (15)
$$

where $g_n(q)$ is a harmonic-oscillator eigenfunction, $n_1, n_2 = 0, 1, \ldots$, and $-\infty < k < \infty$. The eigenvalues behave asymptotically as

$$
\lim_{\lambda\to\infty} \lambda^{-1/2} E_{n_1,n_2,k} = 2\sqrt{3}(n_1 + n_2 + 1). \qquad (16)
$$

Since the symmetry of the eigenfunction is conserved as λ increases we expect that the small-λ eigenfunctions are connected with

$$\begin{cases} \cos(kq_3)g_{n_1}(q_1)g_{n_2}(q_2) \\ \sin(kq_3)g_{n_1}(q_1)g_{n_2}(q_2) \end{cases} \tag{17}$$

instead of (15). The symmetry of these functions is also given by equation (13). For example, we expect that

$$\begin{aligned} \lim_{\lambda\to\infty} \lambda^{-1/2}E_{1A_{1g}} &= \lim_{\lambda\to\infty} \lambda^{-1/2}E_{1A_{2u}} = 2\sqrt{3} \\ \lim_{\lambda\to\infty} \lambda^{-1/2}E_{1E_u} &= \lim_{\lambda\to\infty} \lambda^{-1/2}E_{1E_g} = 4\sqrt{3} \\ \lim_{\lambda\to\infty} \lambda^{-1/2}E_{1A_{2g}} &= \lim_{\lambda\to\infty} \lambda^{-1/2}E_{1A_{1u}} = 8\sqrt{3}. \end{aligned} \tag{18}$$

It is worth noting that (q_1, q_2) and q_3 are bases for the irreps E_u and A_{2u}, respectively.

5. Rayleigh-Ritz variational method with a symmetry-adapted basis set

As indicated in earlier papers on the application of group theory to a variety of problems[24, 25, 29–35], we can obtain approximate eigenvalues and eigenfunctions of H from the eigenvalues and eigenvectors of the matrix representation $\mathbf{H}^S$ of the Hamiltonian operator for every irrep S that we can treat separate from the other irreps. In the present case the linear combinations of eigenfunctions of H_0 (12) adapted to the symmetry species are

A_{1g} :

$$\varphi_{2n-1\,2n-1\,2n-1}$$

$$\frac{1}{\sqrt{3}}\left(\varphi_{2m-1\,2n-1\,2n-1}+\varphi_{2n-1\,2m-1\,2n-1}+\varphi_{2n-1\,2n-1\,2m-1}\right)$$
$$\frac{1}{\sqrt{6}}\left(\varphi_{2k-1\,2m-1\,2n-1}+\varphi_{2n-1\,2k-1\,2m-1}+\varphi_{2m-1\,2n-1\,2k-1}\right.$$
$$\left.+\varphi_{2m-1\,2k-1\,2n-1}+\varphi_{2n-1\,2m-1\,2k-1}+\varphi_{2k-1\,2n-1\,2m-1}\right)$$
$$\frac{1}{\sqrt{3}}\left(\varphi_{2m-1\,2n\,2n}+\varphi_{2n\,2m-1\,2n}+\varphi_{2n\,2n\,2m-1}\right)$$
$$\frac{1}{\sqrt{6}}\left(\varphi_{2k\,2m\,2n-1}+\varphi_{2n-1\,2k\,2m}+\varphi_{2m\,2n-1\,2k}\right.$$
$$\left.+\varphi_{2m\,2k\,2n-1}+\varphi_{2n-1\,2m\,2k}+\varphi_{2k\,2n-1\,2m}\right), \qquad (19)$$

A_{2g} :

$$\frac{1}{\sqrt{6}}\left(\varphi_{2k-1\,2m-1\,2n-1}+\varphi_{2n-1\,2k-1\,2m-1}+\varphi_{2m-1\,2n-1\,2k-1}\right.$$
$$\left.-\varphi_{2m-1\,2k-1\,2n-1}-\varphi_{2n-1\,2m-1\,2k-1}-\varphi_{2k-1\,2n-1\,2m-1}\right)$$
$$\frac{1}{\sqrt{6}}\left(\varphi_{2k\,2m\,2n-1}+\varphi_{2n-1\,2k\,2m}+\varphi_{2m\,2n-1\,2k}\right.$$
$$\left.-\varphi_{2m\,2k\,2n-1}-\varphi_{2n-1\,2m\,2k}-\varphi_{2k\,2n-1\,2m}\right), \qquad (20)$$

E_g :

$$\left\{\frac{1}{\sqrt{6}}\left(2\varphi_{2m-1\,2n-1\,2n-1}-\varphi_{2n-1\,2m-1\,2n-1}-\varphi_{2n-1\,2n-1\,2m-1}\right),\right.$$
$$\left.\frac{1}{\sqrt{2}}\left(\varphi_{2n-1\,2m-1\,2n-1}-\varphi_{2n-1\,2n-1\,2m-1}\right)\right\}$$
$$\left\{\frac{1}{\sqrt{6}}\left(2\varphi_{2k-1\,2m-1\,2n-1}-\varphi_{2n-1\,2k-1\,2m-1}-\varphi_{2m-1\,2n-1\,2k-1}\right),\right.$$
$$\left.\frac{1}{\sqrt{2}}\left(\varphi_{2n-1\,2k-1\,2m-1}-\varphi_{2m-1\,2n-1\,2k-1}\right)\right\}$$
$$\left\{\frac{1}{\sqrt{6}}\left(2\varphi_{2m-1\,2k-1\,2n-1}-\varphi_{2n-1\,2m-1\,2k-1}-\varphi_{2k-1\,2n-1\,2m-1}\right),\right.$$

$$\frac{1}{\sqrt{2}}\left(\varphi_{2n-1\,2m-1\,2k-1}-\varphi_{2k-1\,2n-1\,2m-1}\right)\Big\}$$

$$\left\{\frac{1}{\sqrt{6}}\left(2\varphi_{2m-1\,2n\,2n}-\varphi_{2n\,2m-1\,2n}-\varphi_{2n\,2n\,2m-1}\right),\frac{1}{\sqrt{2}}\left(\varphi_{2n\,2m-1\,2n}-\varphi_{2n\,2n\,2m-1}\right)\right\}$$

$$\left\{\frac{1}{\sqrt{6}}\left(2\varphi_{2k\,2m\,2n-1}-\varphi_{2n-1\,2k\,2m}-\varphi_{2m\,2n-1\,2k}\right),\left(\varphi_{2n-1\,2k\,2m}-\varphi_{2m\,2n-1\,2k}\right)\right\}$$

$$\left\{\frac{1}{\sqrt{6}}\left(2\varphi_{2m\,2k\,2n-1}-\varphi_{2n-1\,2m\,2k}-\varphi_{2k\,2n-1\,2m}\right),\frac{1}{\sqrt{2}}\left(\varphi_{2n-1\,2m\,2k}-\varphi_{2k\,2n-1\,2m}\right)\right\}, \tag{21}$$

A_{1u} :

$$\begin{aligned}&\frac{1}{\sqrt{6}}\left(\varphi_{2k\,2m-1\,2n-1}+\varphi_{2n-1\,2k\,2m-1}+\varphi_{2m-1\,2n-1\,2k}\right.\\&\left.-\varphi_{2m-1\,2k\,2n-1}-\varphi_{2n-1\,2m-1\,2k}-\varphi_{2k\,2n-1\,2m-1}\right)\\&\frac{1}{\sqrt{6}}\left(\varphi_{2k\,2m\,2n}+\varphi_{2n\,2k\,2m}+\varphi_{2m\,2n\,2k}\right.\\&\left.-\varphi_{2m\,2k\,2n}-\varphi_{2n\,2m\,2k}-\varphi_{2k\,2n\,2m}\right),\end{aligned} \tag{22}$$

A_{2u} :

$$\begin{aligned}&\varphi_{2n\,2n\,2n}\\&\frac{1}{\sqrt{3}}\left(\varphi_{2m\,2n\,2n}+\varphi_{2n\,2m\,2n}+\varphi_{2n\,2n\,2m}\right)\\&\frac{1}{\sqrt{6}}\left(\varphi_{2k\,2m\,2n}+\varphi_{2n\,2k\,2m}+\varphi_{2m\,2n\,2k}\right.\\&\left.+\varphi_{2m\,2k\,2n}+\varphi_{2n\,2m\,2k}+\varphi_{2k\,2n\,2m}\right)\\&\frac{1}{\sqrt{3}}\left(\varphi_{2m\,2n-1\,2n-1}+\varphi_{2n-1\,2m\,2n-1}+\varphi_{2n-1\,2n-1\,2m}\right)\\&\frac{1}{\sqrt{6}}\left(\varphi_{2k\,2m-1\,2n-1}+\varphi_{2n-1\,2k\,2m-1}+\varphi_{2m-1\,2n-1\,2k}\right.\\&\left.+\varphi_{2m-1\,2k\,2n-1}+\varphi_{2n-1\,2m-1\,2k}+\varphi_{2k\,2n-1\,2m-1}\right),\end{aligned} \tag{23}$$

$$
\begin{aligned}
E_u \quad : \quad & \\
& \left\{ \frac{1}{\sqrt{6}} \left(2\varphi_{2m\,2n-1\,2n-1} - \varphi_{2n-1\,2m\,2n-1} - \varphi_{2n-1\,2n-1\,2m} \right), \right. \\
& \left. \frac{1}{\sqrt{2}} \left(\varphi_{2n-1\,2m\,2n-1} - \varphi_{2n-1\,2n-1\,2m} \right) \right\} \\
& \left\{ \frac{1}{\sqrt{6}} \left(2\varphi_{2k\,2m-1\,2n-1} - \varphi_{2n-1\,2k\,2m-1} - \varphi_{2m-1\,2n-1\,2k} \right), \right. \\
& \left. \frac{1}{\sqrt{2}} \left(\varphi_{2n-1\,2k\,2m-1} - \varphi_{2m-1\,2n-1\,2k} \right) \right\} \\
& \left\{ \frac{1}{\sqrt{6}} \left(2\varphi_{2m-1\,2k\,2n-1} - \varphi_{2n-1\,2m-1\,2k} - \varphi_{2k\,2n-1\,2m-1} \right), \right. \\
& \left. \frac{1}{\sqrt{2}} \left(\varphi_{2n-1\,2m-1\,2k} - \varphi_{2k\,2n-1\,2m-1} \right) \right\} \\
& \left\{ \frac{1}{\sqrt{6}} \left(2\varphi_{2m\,2n\,2n} - \varphi_{2n\,2m\,2n} - \varphi_{2n\,2n\,2m} \right), \right. \\
& \left. \frac{1}{\sqrt{2}} \left(\varphi_{2n\,2m\,2n} - \varphi_{2n\,2n\,2m} \right) \right\} \\
& \left\{ \frac{1}{\sqrt{6}} \left(2\varphi_{2k\,2m\,2n} - \varphi_{2n\,2k\,2m} - \varphi_{2m\,2n\,2k} \right), \right. \\
& \left. \frac{1}{\sqrt{2}} \left(\varphi_{2n\,2k\,2m} - \varphi_{2m\,2n\,2k} \right) \right\} \\
& \left\{ \frac{1}{\sqrt{6}} \left(2\varphi_{2m\,2k\,2n} - \varphi_{2n\,2m\,2k} - \varphi_{2k\,2n\,2m} \right), \right. \\
& \left. \frac{1}{\sqrt{2}} \left(\varphi_{2n\,2m\,2k} - \varphi_{2k\,2n\,2m} \right) \right\}, \qquad (24)
\end{aligned}
$$

where $k, m, n = 1, 2, \ldots$. It is understood that $\varphi_{i\,j\,k}$ means that the three subscripts are different; equal subscripts are indicated explicitly as in $\varphi_{i\,i\,i}$ or $\varphi_{i\,j\,j}$.

In this paper we have carried out a diagonalization of the matrix representation of the Hamiltonian operator with 1000 basis functions of each symmetry species. Figs. 1-6 show $E(\lambda)$ and $\lambda^{-1/2}E(\lambda)$ for the first eigenvalues of each irrep. The latter illustrate the conclusions drawn in Section 4 and in particular equations (18). To facilitate the analysis we have drawn horizontal dashed lines that mark the limits (16).

It is well known that eigenvalues of the same symmetry do not cross but exhibit what is commonly known as avoided crossings[36]. Figs. 1-6 exhibit some clear avoided crossings and others that appear to be actual crossings because of the scale of the figures. As an example in Fig. 7 we show the third and fourth states of symmetry A_{1g} on a finer scale to make it clear that they in fact undergo an avoided crossing.

Fig. 8 shows a most interesting feature of the spectrum of this system of identical particles. The eigenvalues E_{2E_g} and $E_{3A_{1g}}$ are almost degenerate for small λ (in Section 5 we have seen that they share the same energy of order zero and first order correction). However, the slope of the energy level $E_{3A_{1g}}$ changes dramatically at the avoided crossing λ_c with the level $E_{4A_{1g}}$ but the slope of E_{2E_g} does not change and the latter level approaches and remains close to $E_{4A_{1g}}$ for $\lambda > \lambda_c$.

6. Conclusions

It is interesting that a simple one-dimensional model exhibits such a rich symmetry. We have shown that group theory is remarkably useful for the interpretation of the results produced by approximate methods like perturbation theory and the variational method. The treatment of each irrep separately from the others renders the analysis of the spectrum considerably simpler. For example, the avoided crossings between levels of equal symmetry can be studied separate from the crossings between levels of different symmetry. The interplay among the energy levels $E_{3A_{1g}}$, $E_{4A_{1g}}$ and E_{2E_g} is most interesting and one wonders if such behaviour also takes place in more realistic models of quantum-mechanical problems.

Since the symmetry of the problem does not change with λ we can resort to group theory to predict the connection of the states in the small-λ and large-λ regimes embodied in Eq. 18. These results were confirmed by the accurate Rayleigh-Ritz variational calculation in Section 5.

Group theory is also useful for the calculation of matrix elements of observables because we already know beforehand which of them vanish. This is the reason why we can treat each irrep separate from the others in the Rayleigh-Ritz calculation. The prediction of zero matrix elements is also the basis, for example, of the well known selection rules in spectroscopic transitions[26, 27].

In closing we mention that the combination of group theory and perturbation theory has recently led us to the conclusion that the well known parity-time symmetry is less easily broken that other forms of the more general space-time symmetry[33]. This result is of great relevance for the study of non-Hermitian Hamiltonians.

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References

[1] F. C. Auluck and D. S. Kothari, Energy-levels of an artificially bounded linear oscillator, Science and Culture 7 (1940) 370-371.

[2] F. C. Auluck, Energy levels of an artificially bounded linear oscillator, Proc. Nat. Inst. India 7 (1941) 133-140.

[3] F. C. Auluck, White dwarf and harmonic oscillator, Proc. Nat. Inst. India 8 (1942) 147-156.

[4] S. Chandrasekhar, Dynamical friction II. The rate of escape of stars from clusters and the evidence for the operation of dynamical friction, Astrophys. J. 97 (1943) 263-273.

[5] F. C. Auluck and D. S. Kothari, The quantum mechanics of a bounded linear harmonic oscillator, Proc. Camb. Phil. Soc. 41 (1945) 175-179.

[6] R. B. Dingle, Some magnetic properties of metals IV. Properties of small systems of electrons, Proc. Roy. Soc. London Ser. A 212 (1952) 47-65.

[7] J. S. Baijal and K. K. Singh, The energy -levels and transition probabilities for a bounded linear harmonic oscillator, Prog. Theor. Phys. 14 (1955) 214-224.

[8] P. Dean, The constrained quantum mechanical harmonic oscillator, Proc. Camb. Phil. Soc. 62 (1966) 277-286.

[9] R. Vawter, Effects of finite boundaries on a one-dimensional harmonic oscillator, Phys. Rev. 174 (1968) 749-757.

[10] R. Vawter, Energy eigenvalues of a bounded centrally located harmonic oscillator, J. Math. Phys. 14 (1973) 1864-1870.

[11] A. Consortini and B. R. Frieden, Quantum-mechanical solution for the simple harmonic oscillator in a box, Nuovo Cim. B 35 (1976) 153-163.

[12] J. E. Adams and W. H. Miller, Semiclassical eigenvalues for potential functions defined on a finite interval, J. Chem. Phys. 67 (1977) 5775-5778.

[13] F. C. Rotbar, Quantum symmetrical quadratic potential in a box, J. Phys. A 11 (1978) 2363-2368.

[14] V. C. Aguilera-Navarro, E. Ley Koo, and A. H. Zimerman, Perturbative, asymptotic and Pade-approximant solutions for harmonic and inverted oscillators in a box, J. Phys. A 13 (1980) 3585-3598.

[15] V. C. Aguilera-Navarro, H. Iwamoto, E. Ley Koo, and A. H. Zimerman, Quantum-mechanical solution of the double oscillator in a box, Nuovo Cim. B 62 (1981) 91-128.

[16] R. Barakat and R. Rosner, The bounded quartic oscillator, Phys. Lett. A 83 (1981) 149-150.

[17] F. M. Fernández and E. A. Castro, Hypervirial treatment of multidimensional isotropic bounded oscillators, Phys. Rev. A 24 (1981) 2883-2888.

[18] F. M. Fernández and E. A. Castro, Hypervirial calculation of energy eigenvalues of a bounded centrally located harmonic oscillator, J. Math. Phys. 22 (1981) 1669-1671.

[19] V. C. Aguilera-Navarro, J. F. Gomes, A. H. Zimerman, and E. Ley Koo, On the radius of convergence of Rayleigh-Schrödinger perturbative solutions for quantum oscillators in circular and spherical boxes, J. Phys. A 16 (1983) 2943-2952.

[20] R. N. Chaudhuri and B. Mukherjee, The eigenvalues of the bounded λx^{2m} oscillators, J. Phys. A 16 (1983) 3193-3196.

[21] W. N. Mei and Y. C. Lee, Harmonic oscillator with potential barriers-exact solutions and perturbative treatments, J. Phys. A 16 (1983) 1623-1632.

[22] N. Aquino, The isotropic bounded oscillators, J. Phys. A 30 (1997) 2403-2415.

[23] Y. P. Varshni, Simple wavefunction for an impurity in a parabolic quantum dot, Superlattice Microst 23 (1998) 145-149.

[24] P. Amore and F. M. Fernández, Two-particle harmonic oscillator in a one-dimensional box, Acta Polytech. 50 (2010) 17-24. arXiv:0908.0006 [quant-ph]

[25] F. M. Fernández, On the symmetry of the quantum-mechanical particle in a cubic box, arXiv:1310.5136 [quant-ph].

[26] M. Hammermesh, Group Theory and its Application to Physical Problems, (Addison-Wesley, Reading, Massachussets, 1962).

[27] F. A. Cotton, Chemical Applications of Group Theory, (John Wiley & Sons, New York, 1990).

[28] N. L. Harshman, Symmetries of three harmonically trapped particles in one dimension, Phys. Rev. A 86 (2012) 052122.

[29] F. M. Fernández, Perturbation theory by the moment method and point-group symmetry, J. Math. Chem. 53 (2015)998-1009. arXiv:1409.4120 [quant-ph]

[30] F. M. Fernandez and J. Garcia, Eigenvalues and eigenfunctions of the anharmonic oscillator $V(x,y) = x^2y^2$, Cent. Eur. J. Phys. 12 (2014) 499-502. arXiv:1310.5229v1 [quant-ph]

[31] F. M. Fernández and J. Garcia, Non-Hermitian Hamiltonians with unitary and antiunitary symmetries, Ann. Phys. 342 (2014) 195-204. arXiv:1309.0808 [quant-ph]

[32] F. M. Fernández and J. Garcia, PT-symmetry broken by point-group symmetry, J. Math. Phys. 55 (2014) 042107. arXiv:1308.6179v2 [quant-ph].

[33] P. Amore, F. M. Fernández, and J. Garcia, Is space-time symmetry a

suitable generalization of parity-time symmetry?, Ann. Phys. 350 (2014) 533-548. arXiv:1405.5234 [quant-ph]

[34] P. Amore, F. M. Fernández, and J. Garcia, Non-Hermitian oscillators with Td symmetry, Ann. Phys. 353 (2015) 238-251. arXiv:1409.2672 [quant-ph]

[35] F. M. Fernandez, Group theoretical analysis of a quantum-mechanical three-dimensional quartic anharmonic oscillator, Ann. Phys. 356 (2015) 149-157. arXiv:1501.00975 [quant-ph]

[36] F. M. Fernandez, On the crossing of the energy levels of a parameter-dependent quantum-mechanical Hamiltonian, J. Math. Chem. 52 (2014) 2322-2329.

[37] Till Tantau, The TikZ and PGF Packages, Manual for version 3.0.0, http://sourceforge.net/projects/pgf/, 2013-12-20

[38] International Derive User Group. http://www.austromath.at/dug/index.htm. International Derive User Group, http://www.austromath.at/dug/.

Table 1: Character table for D_{3d} point group

	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$		
A_{1g}	1	1	1	1	1	1		$x^2+y^2+z^2$ $xy+yz+zx$
A_{2g}	1	1	-1	1	1	-1		
E_g	2	-1	0	2	-1	0		$(2z^2-x^2-y^2, x^2-y^2)$, $(2yz-xy-xz, xy-xz)$
A_{1u}	1	1	1	-1	-1	-1		
A_{2u}	1	1	-1	-1	-1	1	$x+y+z$	
E_u	2	-1	0	-2	1	0	$(2z-x-y, x-y)$	

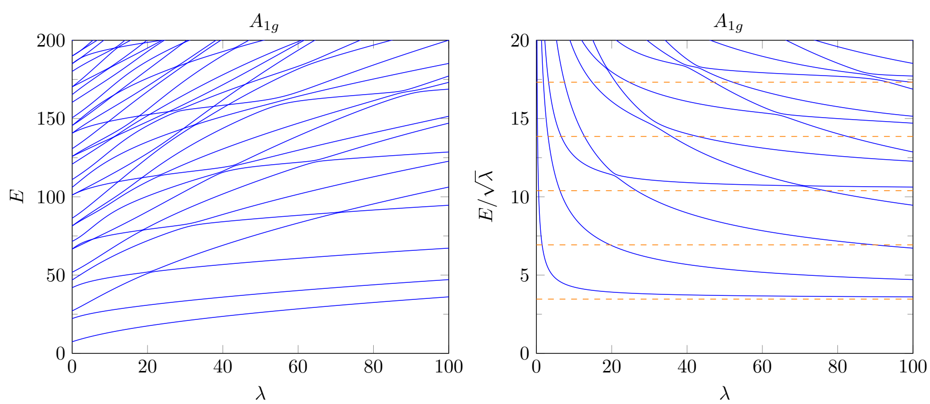

Figure 1: Eigenvalues for the irrep A_{1g}

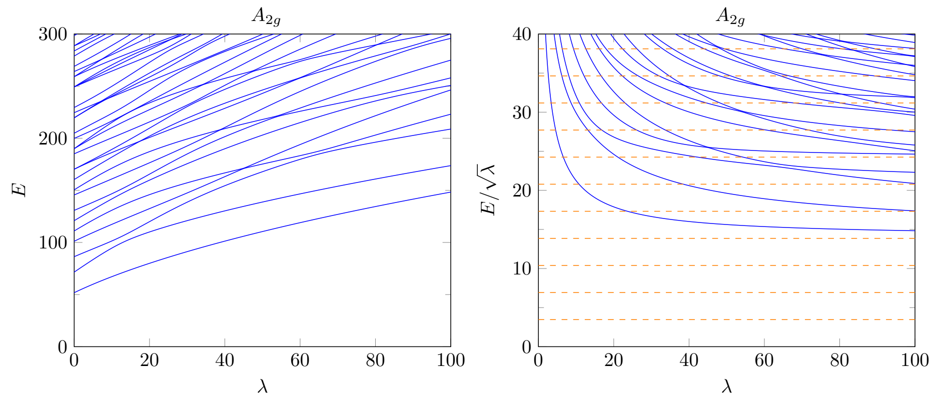

Figure 2: Eigenvalues for the irrep A_{2g}

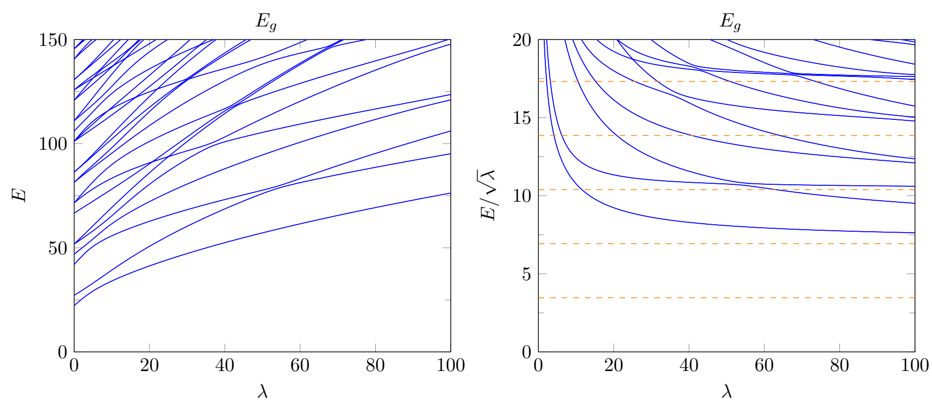

Figure 3: Eigenvalues for the irrep E_g

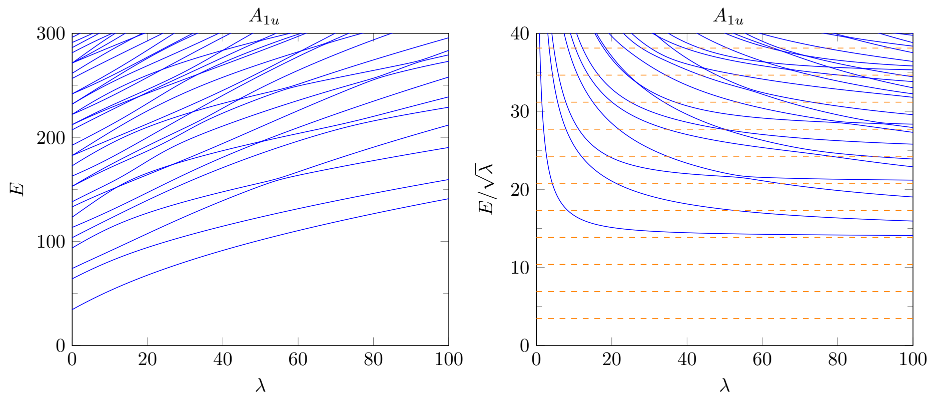

Figure 4: Eigenvalues for the irrep A_{1u}

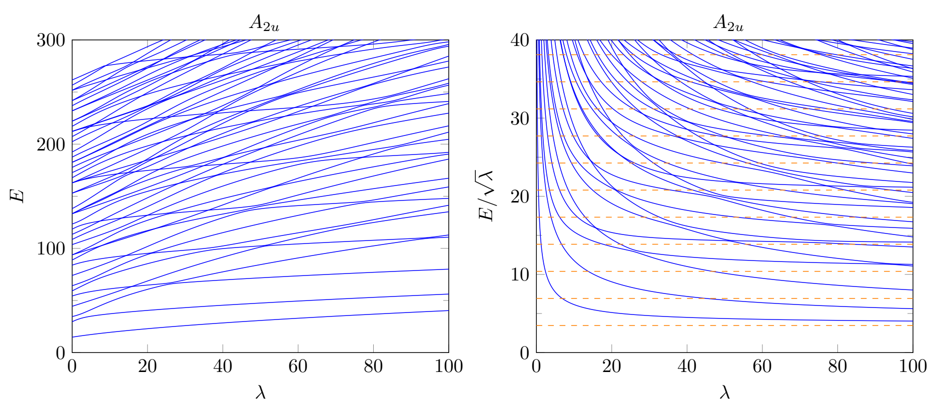

Figure 5: Eigenvalues for the irrep A_{2u}

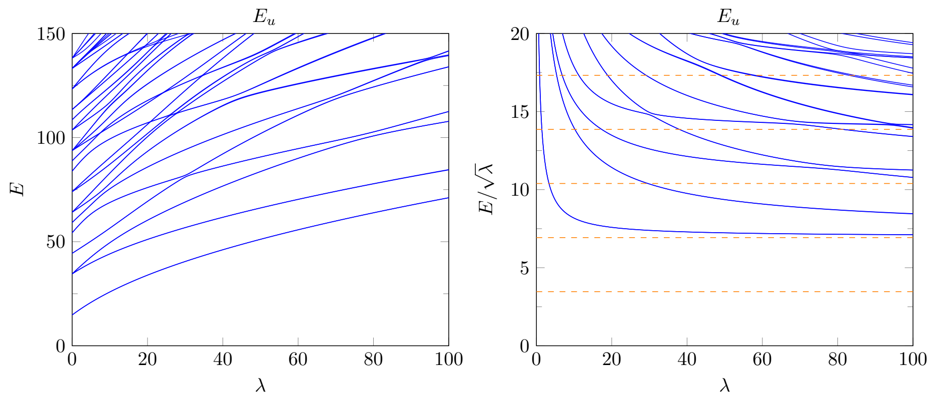

Figure 6: Eigenvalues for the irrep E_U

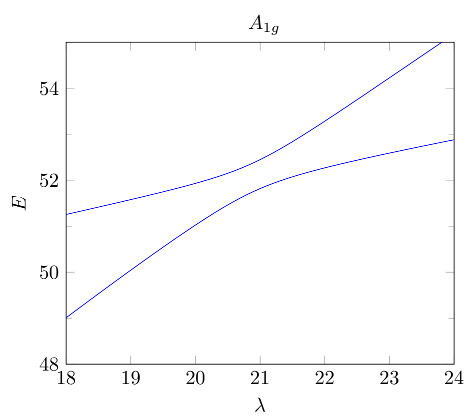

Figure 7: Third and fourth eigenvalues of symmetry A_{1g}

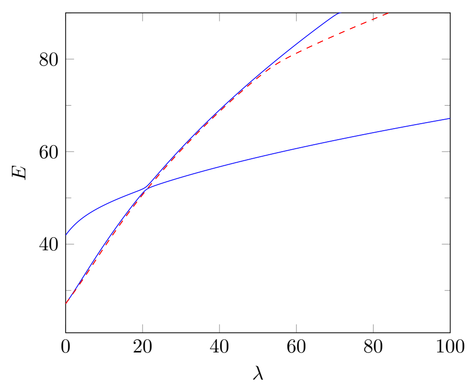

Figure 8: Third and fourth eigenvalues of symmetry A_{1g} (blue, solid line) and second pair of eigenvalues of symmetry E_g (red, dashed line)