

On the symmetry of four particles in a one-dimensional box with harmonic interaction

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Received: 9 January 2017 / Accepted: 28 August 2017
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Abstract We show that a system of four particles in a one-dimensional box with a two-particle harmonic interaction can be described by means of the symmetry point group O_h . Group theory proves useful for the discussion of both the small-box and large-box regimes. We apply perturbation theory and obtain the corrections of first order for the lowest states. We carry out a simple Rayleigh–Ritz variational calculation with basis sets adapted to the symmetries of the system. We also obtain alternative variational results for the first three lowest energy levels that are more suitable for larger box sizes.

Keywords Four particles in a box · Symmetry group · Perturbation theory · Variational approach · Small box · Large box

1 Introduction

During the last decades there has been great interest in the model of a harmonic oscillator confined to boxes of different shapes, sizes and dimensions. Such model has been suitable for the study of several physical problems ranging from dynamical friction in star clusters to magnetic properties of solids and impurities in quantum dots (see [1,2] for a review of the relevant literature on the subject). In addition to it, systems of few identical particles in one dimension have proved to exhibit a rich phenomenological structure resembling that of realistic systems [3–6]. In two recent papers Amore and Fernández discussed the problems posed by two [1] and three

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[2] particles confined in a one-dimensional box with impenetrable walls that interact through harmonic forces. They found that a straightforward application of group theory considerably facilitates the analysis of the solutions to the Schrödinger equation. In particular, an accurate Rayleigh–Ritz variational calculation revealed that the energies of the three-particle model as functions of the box length exhibit a most interesting pattern of avoided crossings between pairs of states of the same symmetry [2].

The purpose of this paper is to discuss the case of four particles in a one dimensional box that also interact through harmonic forces. The reason for choosing such interaction is that it has proved quite useful in the past (see the references in [2]) and because the calculation of the matrix elements of the resulting potential is quite simple. In Sect. 2 we introduce the model, Sect. 3 shows a perturbation approach to the small-box regime and a Rayleigh–Ritz calculation with symmetry-adapted basis sets, Sect. 4 describes the large-box limit, in Sect. 5 we discuss a simple variational calculation that is more suitable for larger box sizes and in Sect. 6 we draw conclusions. There is also an “Appendix” outlining the construction of the projection operators used in all the calculations just described.

2 Four particles in a one-dimensional box

We first consider N interacting point particles of mass m in a one-dimensional box of length $L = 2a$ with Hamiltonian

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^N \frac{\partial^2}{\partial x_i^2} + \sum_{i=1}^{N-1} \sum_{j=i+1}^N W(|x_i - x_j|), \quad (1)$$

where x_i is the coordinate of the i -th particle. The boundary conditions are determined by the impenetrable walls of the box

$$\Psi(x_1, x_2, \dots, x_i = \pm a, \dots, x_N) = 0, \quad i = 1, 2, \dots, N. \quad (2)$$

The Hamiltonian operator is invariant under the $N!$ permutations of the particle coordinates as well as under parity inversion $\mathbf{x} \rightarrow -\mathbf{x}$. The $2N! N \times N$ matrices that produce all the permutations of the sets $\{x_1, x_2, \dots, x_N\}$ and $\{-x_1, -x_2, \dots, -x_N\}$ form a group given by the product $S_N \otimes O(1)$ [7, 8]. When $N = 2$ the group is also called C_{2h} (in principle we can also use D_2 or C_{2v} that are isomorphic to C_{2h}) and when $N = 3$ we can resort to either D_{3d} or D_{3h} [9]. Both cases have already been treated by group theory in earlier papers [1, 2].

In order to solve the Schrödinger equation it is convenient to define the dimensionless particle coordinates $q_i = x_i/a$ and the dimensionless Hamiltonian

$$H_d = \frac{2ma^2}{\hbar^2} H = -\sum_{i=1}^N \frac{\partial^2}{\partial q_i^2} + \lambda \sum_{i=1}^{N-1} \sum_{j=i+1}^N w(|q_i - q_j|), \quad (3)$$

where $\lambda w(|q_i - q_j|) = 2ma^2 W(a|q_i - q_j|)/\hbar^2$. The boundary conditions for the eigenfunctions ψ of this operator now become

$$\psi(q_1, q_2, \dots, q_i = \pm 1, \dots, q_N) = 0, \quad i = 1, 2, \dots, N. \tag{4}$$

From now on we only consider the dimensionless Hamiltonian (3) and omit the subscript d . In order to facilitate the numerical calculations we choose a harmonic interaction of the form $W(|x_i - x_j|) = \frac{k}{2}(x_i - x_j)^2$ that leads to $\lambda = ma^2k/\hbar^2$ and $w(|q_i - q_j|) = (q_i - q_j)^2$.

For $N = 4$ our problem just reduces to solving the Schrödinger equation for the operator

$$\begin{aligned} H = & - \left(\frac{\partial^2}{\partial q_1^2} + \frac{\partial^2}{\partial q_2^2} + \frac{\partial^2}{\partial q_3^2} + \frac{\partial^2}{\partial q_4^2} \right) \\ & + \lambda \left[(q_1 - q_2)^2 + (q_1 - q_3)^2 + (q_1 - q_4)^2 + (q_2 - q_3)^2 \right. \\ & \left. + (q_2 - q_4)^2 + (q_3 - q_4)^2 \right], \end{aligned} \tag{5}$$

with the boundary conditions

$$\psi(\pm 1, q_2, q_3, q_4) = \psi(q_1, \pm 1, q_3, q_4) = \psi(q_1, q_2, \pm 1, q_4) = \psi(q_1, q_2, q_3, \pm 1) = 0. \tag{6}$$

In this case the group $S_4 \otimes O(1)$ is isomorphic to O_h and in this paper we resort to the character table of the latter group [9].

3 Small-box-regime

When λ is sufficiently small (sufficiently small box size L) we can estimate the energy levels by means of perturbation theory. The Schrödinger equation is exactly solvable when $\lambda = 0$ and the eigenvalues and eigenfunctions of $H_0 = H(\lambda = 0)$ are

$$\begin{aligned} E_{n_1 n_2 n_3 n_4}^{(0)} &= \frac{\pi^2}{4} \left(n_1^2 + n_2^2 + n_3^2 + n_4^2 \right), \quad n_1, n_2, n_3, n_4 = 1, 2, \dots \\ \psi_{n_1 n_2 n_3 n_4}^{(0)}(q_1, q_2, q_3, q_4) &= \phi_{n_1}(q_1) \phi_{n_2}(q_2) \phi_{n_3}(q_3) \phi_{n_4}(q_4) \\ \phi_n(q) &= \sin \frac{n\pi(q + 1)}{2}. \end{aligned} \tag{7}$$

Note that $\phi_n(-q) = (-1)^{n-1} \phi_n(q)$.

In order to facilitate the discussion of the results we introduce the notation $\{a, b, c, d\}_P$ to indicate the set of all distinct permutations of four elements that may be either coordinates or quantum numbers. For example, each 4-tuple of quantum numbers in the set $\{n_1, n_2, n_3, n_4\}_P$ leads to the same unperturbed energy $E_{n_1 n_2 n_3 n_4}^{(0)}$. We may eventually add accidental *Pythagorean* degeneracies of the form $m_1^2 + m_2^2 + m_3^2 + m_4^2 = n_1^2 + n_2^2 + n_3^2 + n_4^2$, where $(m_1, m_2, m_3, m_4) \notin \{n_1, n_2, n_3, n_4\}_P$ [10]. If such energy level is g -fold degenerate then the perturbation corrections of first order to the eigenfunctions will be of the form

$$\psi^{(1)} = \sum_{j=1}^g c_j^{(1)} \psi_j^{(0)}, \quad (8)$$

where j denotes a 4-tuple (n_1, n_2, n_3, n_4) . The coefficients $c_j^{(1)}$ are solutions to the secular equation

$$\left(\mathbf{H}' - E^{(1)}\mathbf{I}\right)\mathbf{c}^{(1)} = 0, \quad (9)$$

where \mathbf{H}' is the $g \times g$ matrix of the perturbation $H' = H - H_0$ in the set of degenerate eigenfunctions $\{\psi_j^{(0)}, j = 1, 2, \dots, g\}$, \mathbf{I} is the $g \times g$ identity matrix, $\mathbf{c}^{(1)}$ is a column vector with elements $c_j^{(1)}$ and $E^{(1)}$ is one of the g roots of the secular determinant $|\mathbf{H}' - E^{(1)}\mathbf{I}| = 0$.

In order to determine the symmetry of the solution $\psi^{(1)}$, which provides a suitable label for the corresponding root $E^{(1)}$, we apply the projection operators P_S associated to the irreducible representations (irreps) S of the group O_h [9]. The result is well known to be $P_S\psi^{(1)} = \psi^{(1)}$ if $\psi^{(1)}$ is a basis for the irrep S or $P_S\psi^{(1)} = 0$ otherwise. The construction of the projection operators is outlined in the ‘‘Appendix’’. In this way we obtain the following results for the first energy levels:

$$E_{1A_{1g}} = \pi^2 + \frac{4(\pi^2 - 6)}{\pi^2}\lambda + \dots, \quad (10)$$

$$E_{1A_{1u}} = \frac{7\pi^2}{4} + \frac{216\pi^4 - 1053\pi^2 - 4096}{54\pi^4}\lambda + \dots, \quad (11)$$

$$E_{1T_{2u}} = \frac{7\pi^2}{4} + \frac{648\pi^4 - 3159\pi^2 + 4096}{162\pi^4}\lambda + \dots, \quad (11)$$

$$E_{2A_{1g}} = \frac{5\pi^2}{2} + \frac{324\pi^4 - 1215\pi^2 - 8192}{81\pi^4}\lambda + \dots,$$

$$E_{1T_{2g}} = \frac{5\pi^2}{2} + \frac{4\pi^2 - 15}{\pi^2}\lambda + \dots, \quad (12)$$

$$E_{1E_g} = \frac{5\pi^2}{2} + \frac{324\pi^4 - 1215\pi^2 + 4096}{81\pi^4}\lambda + \dots, \quad (12)$$

$$E_{3A_{1g}} = 3\pi^2 + \frac{4(3\pi^2 - 14)}{3\pi^2}\lambda + \dots,$$

$$E_{2T_{2g}} = 3\pi^2 + \frac{4(3\pi^2 - 14)}{3\pi^2}\lambda + \dots, \quad (13)$$

$$E_{2A_{1u}} = \frac{13\pi^2}{4} + \frac{216\pi^4 - 567\pi^2 - 4096}{54\pi^4}\lambda + \dots,$$

$$E_{2T_{2u}} = \frac{13\pi^2}{4} + \frac{648\pi^4 - 1701\pi^2 + 4096}{162\pi^4}\lambda + \dots, \quad (14)$$

$$E_{3A_{1u}} = \frac{15\pi^2}{4} + \frac{405000\pi^4 - 1434375\pi^2 - 8105984}{101250\pi^4}\lambda + \dots,$$

$$\begin{aligned}
 E_{3T_{2u}} &= \frac{15\pi^2}{4} + \frac{405000\pi^4 - 1434375\pi^2 - 6144\sqrt{424321} - 1280000}{101250\pi^4} \lambda + \dots, \\
 E_{1E_u} &= \frac{15\pi^2}{4} + \frac{405000\pi^4 - 1434375\pi^2 - 425984}{101250\pi^4} \lambda + \dots, \\
 E_{4T_{2u}} &= \frac{15\pi^2}{4} + \frac{405000\pi^4 - 1434375\pi^2 + 6144\sqrt{424321} - 1280000}{101250\pi^4} \lambda + \dots, \\
 E_{1T_{1u}} &= \frac{15\pi^2}{4} + \frac{405000\pi^4 - 1434375\pi^2 + 5545984}{101250\pi^4} \lambda + \dots, \tag{15}
 \end{aligned}$$

$$E_{4A_{1g}} = 4\pi^2 + \frac{2(2\pi^2 - 3)}{\pi^2} \lambda + \dots, \tag{16}$$

$$\begin{aligned}
 E_{5A_{1g}} &= \frac{9\pi^2}{2} + \frac{202500\pi^4 - 489375\pi^2 - 5545984}{50625\pi^4} \lambda + \dots, \\
 E_{3T_{2g}} &= \frac{9\pi^2}{2} + \frac{202500\pi^4 - 489375\pi^2 - 6144\sqrt{53329} - 1386496}{50625\pi^4} \lambda + \dots, \\
 E_{4T_{2g}} &= \frac{9\pi^2}{2} + \frac{202500\pi^4 - 489375\pi^2 + 6144\sqrt{53329} - 1386496}{50625\pi^4} \lambda + \dots, \\
 E_{1T_{1g}} &= \frac{9\pi^2}{2} + \frac{202500\pi^4 - 489375\pi^2 + 2772992}{50625\pi^4} \lambda + \dots, \\
 E_{2E_g} &= \frac{9\pi^2}{2} + \frac{202500\pi^4 - 489375\pi^2 + 2772992}{50625\pi^4} \lambda + \dots, \tag{17}
 \end{aligned}$$

where A_{1g} , A_{2g} , A_{1u} , and A_{2u} are nondegenerate, E_g and E_u are two-fold degenerate, and T_{1g} , T_{2g} , T_{1u} and T_{2u} are three-fold degenerate.

We appreciate that the degeneracy of the unperturbed states is partially removed by the perturbation. The remaining degeneracies are expected to be broken at higher perturbation orders. One does not expect that such remaining degeneracies are due to an unknown hidden symmetry [10] because they are rather inconsistent. For example, in the case $\{1, 1, 1, 3\}_P$ we have $E_{3A_{1g}} = E_{2T_{2g}}$; however, $\{1, 2, 2, 3\}_P$ leads to $E_{5A_{1g}} < E_{3T_{2g}} < E_{4T_{2g}} < E_{2E_g} = E_{1T_{1g}}$ where the state A_{1g} and the three states T_{2g} are not degenerate as in the preceding case.

Figure 1 shows the lowest energy levels in the interval $0 \leq \lambda \leq 1$ where perturbation theory is expected to yield sufficiently accurate results. We also carried out a simple Rayleigh–Ritz variational calculation with symmetry-adapted basis sets for A_{1g} and T_{2g} choosing only those functions coming from $\{1, 1, 1, 1\}$, $\{1, 1, 2, 2\}_P$ and $\{1, 1, 1, 3\}_P$ in order to show the splitting of the levels $E_{3A_{1g}}$ and $E_{2T_{2g}}$. These levels appear to be degenerate in the upper subfigure but the finer scale of the lower one clearly reveals the splitting that takes place at the second order of perturbation theory ($E_{3A_{1g}} > E_{2T_{2g}}$). The symmetry-adapted basis set was constructed by straightforward application of the projection operators $P_{A_{1g}}$ and $P_{T_{2g}}$ to the zeroth-order eigenfunctions (7) (see [1, 2] for more details).

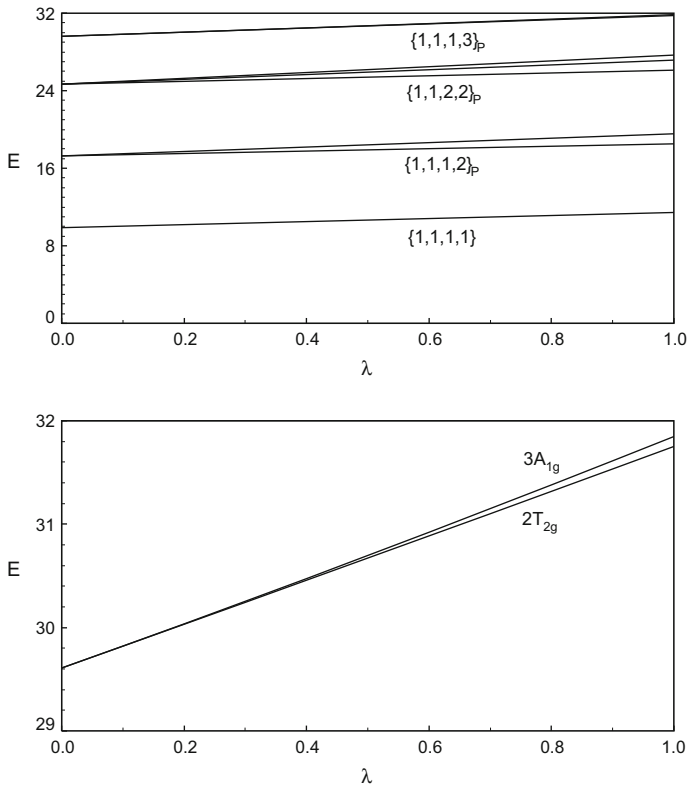


Fig. 1 Lowest eigenvalues calculated by means of perturbation theory and the Rayleigh–Ritz variational method

4 Large-box-regime

When $L \rightarrow \infty$ ($\lambda \rightarrow \infty$) we have a system of four unconfined particles with harmonic-pair interaction. In order to discuss this case it is convenient to define the new coordinates

$$\begin{aligned}
 \xi_1 &= \frac{\sqrt{2}q_2}{2} - \frac{\sqrt{2}q_1}{2} \\
 \xi_2 &= -\frac{\sqrt{6}q_1}{6} - \frac{\sqrt{6}q_2}{6} + \frac{\sqrt{6}q_3}{3} \\
 \xi_3 &= -\frac{\sqrt{3}q_1}{6} - \frac{\sqrt{3}q_2}{6} - \frac{\sqrt{3}q_3}{6} + \frac{\sqrt{3}q_4}{2} \\
 \xi_4 &= \frac{q_1 + q_2 + q_3 + q_4}{2}
 \end{aligned} \tag{18}$$

because the Hamiltonian operator becomes

$$H = - \left(\frac{\partial^2}{\partial \xi_1^2} + \frac{\partial^2}{\partial \xi_2^2} + \frac{\partial^2}{\partial \xi_3^2} + \frac{\partial^2}{\partial \xi_4^2} \right) + 4\lambda \left(\xi_1^2 + \xi_2^2 + \xi_3^2 \right). \tag{19}$$

We appreciate that the center of mass described by the coordinate ξ_4 moves freely while there is harmonic oscillation along the 3 remaining coordinates. The eigenvalues and eigenfunctions are expected to be

$$\begin{aligned} E_{K,n_1,n_2,n_3} &= K^2 + 2\sqrt{\lambda} (2n_1 + 2n_2 + 2n_3 + 3), \\ \psi_{K,n_1,n_2,n_3}(\xi_1, \xi_2, \xi_3, \xi_4) &= \exp(iK\xi_4) \chi_{n_1}(\xi_1)\chi_{n_2}(\xi_2)\chi_{n_3}(\xi_3), \\ n_1, n_2, n_3 &= 0, 1, \dots, \quad -\infty < K < \infty, \end{aligned} \tag{20}$$

where $\chi_n(\xi)$ is a harmonic-oscillator eigenfunction.

The connection between the small and large box regimes is given by

$$\lim_{\lambda \rightarrow \infty} \lambda^{-1/2} E_{m_1,m_2,m_3,m_4}(\lambda) = 2(2n_1 + 2n_2 + 2n_3 + 3). \tag{21}$$

When carrying out this limit we should take into account that the symmetry of the eigenfunction should be conserved as $\lambda \rightarrow \infty$ and that $\exp(iK\xi_4)$ does not exhibit a definite symmetry. Therefore, in order to make a connection between both regimes the eigenfunctions in the large-box case should be of the form

$$\begin{aligned} \psi_{K,n_1,n_2,n_3}^c(\xi_1, \xi_2, \xi_3, \xi_4) &= \cos(K\xi_4) \chi_{n_1}(\xi_1)\chi_{n_2}(\xi_2)\chi_{n_3}(\xi_3), \\ \psi_{K,n_1,n_2,n_3}^s(\xi_1, \xi_2, \xi_3, \xi_4) &= \sin(K\xi_4) \chi_{n_1}(\xi_1)\chi_{n_2}(\xi_2)\chi_{n_3}(\xi_3). \end{aligned} \tag{22}$$

In order to determine the symmetry of a given eigenfunction in the large-box limit we take into account that ξ_4 is basis for the irrep A_{1u} while the set $\{\xi_1, \xi_2, \xi_3\}$ is a basis for the irrep T_{2u} . Therefore, $\cos(K\xi_4)$ and $\sin(K\xi_4)$ are basis for the irreps A_{1g} and A_{1u} , respectively. By means of the direct product of irreps we obtain the symmetry of any eigenfunction of the form (22). For example, when $\{n_1, n_2, n_3\}_P = \{0, 0, 1\}_P$ the three possible products $\chi_{n_1}(\xi_1)\chi_{n_2}(\xi_2)\chi_{n_3}(\xi_3)$ are basis for T_{2u} and the resulting functions $\psi_{K,n_1,n_2,n_3}^c(\xi_1, \xi_2, \xi_3, \xi_4)$ and $\psi_{K,n_1,n_2,n_3}^s(\xi_1, \xi_2, \xi_3, \xi_4)$ are basis for T_{2u} and T_{2g} , respectively.

5 Simple variational method

In order to obtain accurate variational results for large values of λ as was done in the case of two particles [1] we should try variational functions of the form

$$F(q_1, q_2, q_3, q_4) = G(q_1, q_2, q_3, q_4) \exp \left[-a \left(\xi_1^2 + \xi_2^2 + \xi_3^2 \right) \right], \tag{23}$$

where $G(q_1, q_2, q_3, q_4)$ satisfies the boundary conditions at the box walls and $\exp \left[-a \left(\xi_1^2 + \xi_2^2 + \xi_3^2 \right) \right]$ provides the correct asymptotic behaviour of the wavefunc-

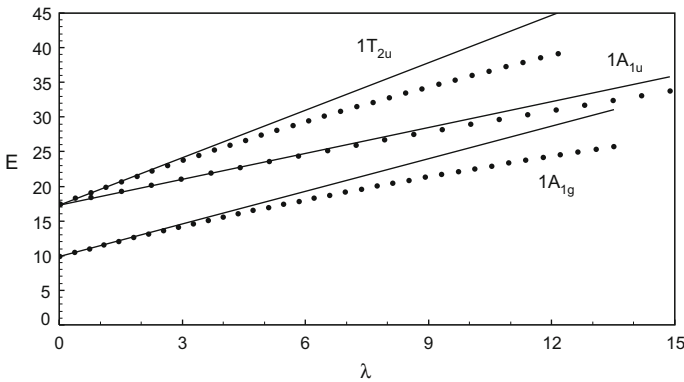


Fig. 2 Lowest three eigenvalues calculated by means of perturbation theory (*solid line*) and the variational method (*circles*)

tion of the free oscillator. The variational parameter a will increase from a_0 to infinity as λ increases from zero to infinity.

However, since this calculation is rather cumbersome here we try a much simpler one with a variational function of the form

$$F(q_1, q_2, q_3, q_4) = G(q_1, q_2, q_3, q_4) \exp \left[-a \left(q_1^2 + q_2^2 + q_3^2 + q_4^2 \right) \right], \quad (24)$$

where we clearly sacrifice the correct description of the asymptotic behaviour when $\lambda \rightarrow \infty$. For example,

$$F_{A_{1g}}(q_1, q_2, q_3, q_4) = N \left(q_1^2 - 1 \right) \left(q_2^2 - 1 \right) \left(q_3^2 - 1 \right) \left(q_4^2 - 1 \right) \times \exp \left[-a \left(q_1^2 + q_2^2 + q_3^2 + q_4^2 \right) \right], \quad (25)$$

$$F_{A_{1u}}(q_1, q_2, q_3, q_4) = N \xi_4 \left(q_1^2 - 1 \right) \left(q_2^2 - 1 \right) \left(q_3^2 - 1 \right) \left(q_4^2 - 1 \right) \times \exp \left[-a \left(q_1^2 + q_2^2 + q_3^2 + q_4^2 \right) \right], \quad (26)$$

and

$$F_{T_{2u}}(q_1, q_2, q_3, q_4) = N \left(q_1^2 - 1 \right) \left(q_2^2 - 1 \right) \left(q_3^2 - 1 \right) \left(q_4^2 - 1 \right) \times \exp \left[-a \left(q_1^2 + q_2^2 + q_3^2 + q_4^2 \right) \right] \begin{cases} \xi_1 \\ \xi_2 \\ \xi_3 \end{cases} \quad (27)$$

are expected to yield approximations to the first energy levels $E_{1A_{1g}} < E_{1A_{1u}} < E_{1T_{2u}}$.

Figure 2 shows the perturbation and variational results for those three states. Both the perturbation corrections of first order and the variational approaches are upper bounds to the corresponding energies because the variational principle applies to the lowest state of each symmetry. Since the perturbation expressions shown in Sect. 3

(E_{PT} from now on) yield the exact result when $\lambda = 0$ they are expected to be more accurate than the variational results (E_{var}) for sufficiently small λ . Figure 2 reveals that $E_{var} < E_{PT}$ for $\lambda > \lambda_c$ that tells us that E_{var} is more accurate for sufficiently large values of λ . As expected, the perturbation expressions exhibit a wrong behaviour for large values of λ . On the other hand, E_{var} increases correctly as $\sqrt{\lambda}$ but the choice of an incorrect exponential factor in the trial function leads to a wrong coefficient of the leading term of the energy; for example a numerical calculation suggests that

$$\lim_{\lambda \rightarrow \infty} \lambda^{-1/2} E_{1A_{1g}} = \sqrt{48} > 6. \quad (28)$$

6 Conclusions

Throughout this paper, as well as in the two earlier ones [1,2], we have shown that group theory is useful for the analysis of systems of particles in a one-dimensional box. In the present case we can label the states of the system of four particles by means of the irreps of the point group O_h . The knowledge of the symmetry of the states for finite λ and for $\lambda \rightarrow \infty$ facilitates the analysis of the connection between the states of the confined and free systems, respectively. In addition to it, point group proves suitable for the construction of simple variational trial functions like those in Sect. 5 as well as for the construction of symmetry-adapted basis sets for more accurate calculations like the Rayleigh–Ritz method used in Sect. 3.

Appendix: Construction of projection operators

In this appendix we outline the procedure for the construction of the projection operators that enabled us to determine the symmetry of the corrections of first order to the eigenfunctions as well as to construct symmetry-adapted basis sets and the variational trial functions.

First, we build a set of 48 matrices $G_M = \{\mathbf{M}_j, j = 1, 2, \dots, 48\}$ given by the 24 permutations of the rows of the 4×4 identity matrix \mathbf{I} and the 24 permutations of the rows of $-\mathbf{I}$. This set of matrices is a group with respect to the matrix product $\mathbf{M}_i \cdot \mathbf{M}_j$. Second, we define a set $G_O = \{O_j, j = 1, 2, \dots, 48\}$ of linear invertible operators according to the rule

$$O_j f(\mathbf{q}) = f(\mathbf{M}_j^{-1} \mathbf{q}), \quad (29)$$

where \mathbf{q} is a column vector with elements q_i (the four dimensionless particle coordinates) and $f(\mathbf{q})$ is an arbitrary function of them. These operators form a group with respect to the composition $O_i \circ O_j$. If \mathbf{M}_i and \mathbf{M}_j are the matrix representations of O_i and O_j , respectively, then $\mathbf{M}_i \cdot \mathbf{M}_j$ is the matrix representation of $O_i \circ O_j$. In other words, the groups G_M and G_O are isomorphic.

Third, we determine the classes for the group of matrices G_M in the usual way. Two matrices \mathbf{M}_i and \mathbf{M}_j belong to the same class if $\mathbf{M}_k \cdot \mathbf{M}_i \cdot \mathbf{M}_k^{-1} = \mathbf{M}_j$ for some $\mathbf{M}_k \in G_M$. Fourth, we calculate the traces, determinants and orders of the matrices in

every class. In this way we connect each class of matrices \mathbf{M}_j (or operators O_j) with the corresponding class of symmetry operations that appear in the character table of the group O_h [9].

Finally, we obtain the projection operators by means of the well known expression [7–9]

$$P_S = \frac{n_S}{h} \sum_{j=1}^h \chi_j(S) O_j, \quad (30)$$

where $h = 48$ is the order of the group, n_S is the dimension of the irreducible representation S and $\chi_j(S)$ is the character of the operation O_j for S that appears in the character table. Since the matrices in a class share the same trace it is sufficient to obtain a one-to-one correspondence between the classes of matrices and the classes of symmetry operations.

The application of the projection operators to the eigenfunctions of order zero given by some of the sets of quantum numbers $\{n_1, n_2, n_3, n_4\}_P$ yields the following irreps:

Quantum numbers	Number of states	E_0	Symmetry
$\{1, 1, 1, 1\}$	1	π^2	$1A_{1g}$
$\{1, 1, 1, 2\}_P$	3	$7\pi^2/4$	$1A_{1u}, 1T_{2u}$
$\{1, 1, 2, 2\}_P$	6	$5\pi^2/2$	$2A_{1g}, 1T_{2g}, 1E_g$
$\{1, 1, 1, 3\}_P$	4	$3\pi^2$	$3A_{1g}, 2T_{2g}$
$\{1, 2, 2, 2\}_P$	4	$13\pi^2/4$	$2A_{1u}, 2T_{2u}$
$\{1, 1, 2, 3\}_P$	12	$15\pi^2/4$	$3A_{1u}, 3T_{2u}, 1E_u, 4T_{2u}, 1T_{1u}$
$\{2, 2, 2, 2\}_P$	1	$4\pi^2$	$4A_{1g}$
$\{1, 2, 2, 3\}_P$	12	$9\pi^2/2$	$5A_{1g}, 3T_{2g}, 4T_{2g}, 2E_g, 1T_{1g}$
$\{1, 1, 1, 4\}_P$	4	$19\pi^2/4$	$4A_{1u}, 5T_{2u}$
$\{1, 1, 3, 3\}_P$	6	$5\pi^2$	$6A_{1g}, 3E_g, 5T_{2g}$
$\{2, 2, 2, 3\}_P$	4	$21\pi^2/4$	$5A_{1u}, 6T_{2u}$
$\{1, 1, 2, 4\}_P$	12	$11\pi^2/2$	$7A_{1g}, 2T_{1g}, 6T_{2g}, 4E_g, 2T_{1g}$

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