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

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HIGHLIGHTS

- Three identical interacting particles in a one-dimensional box exhibit D_{3d} symmetry.
- Group theory is useful for labelling the quantum-mechanical system states.
- Approximate solutions can be obtained by perturbation theory.
- The Rayleigh–Ritz method yields accurate eigenvalues and eigenfunctions.
- Each irreducible representation can be treated separate from the others.

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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.

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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

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

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

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

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:

$$(x, y, z) \to \{x, y, z\}_P$$
$$(x, y, z) \to \{-x, y, z\}_P$$
$$(x, y, z) \to \{x, -y, z\}_P$$
$$(x, y, z) \to \{x, y, -z\}_P$$
$$(x, y, z) \to \{-x, -y, z\}_P$$