

Qualitative Features of the Spectrum of One-Dimensional Three-Body Systems

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Abstract General qualitative features of the bound-spectrum of a one-dimensional system of three identical particles are deduced in the case of Bose-Einstein, Fermi-Dirac and Boltzmann statistics. Using the symmetry properties of one-dimensional hyperspherical harmonics components, it is shown how to construct eigenfunctions having definite parity and definite transformation properties under permutation of any particle pair.

1. INTRODUCTION

The N -body problem is well known to be unsolvable in both classical and quantum theory. In particular, the three-body problem already possesses the intractability of the general N -body problem.

This intractability however should be carefully qualified. When a mathematician says that the classical two-body problem can be solved he means that *all* possible motions of a generic two-body problem are known. When he says that the classical potential system with two degrees of freedom is "hors des possibilités de la science contemporaine" (reference 1, pg.28) he means that he cannot describe all possible motions of such a system. In the three-body problem this is so because Bruns' theorem² says that there are not sufficient first integrals of motion in involution.

Nevertheless, for a specific classical three-body system, a computer code can be written to integrate the equations of motion and determine the position of the system known at any time. It is just a question of patience and money to pay to the computer owner.

What about quantum systems? In this paper we select the simplest example of a many-body system: a quantum system with two degrees of freedom, namely, three identical interacting particles moving on a line. We concentrate on the bound-state spectrum of the system and show

that computer Integration of the time-independent Schrödinger equation cannot be attempted blindly: it is necessary to separate first the eigenfunctions according to the symmetry invariances of the system. We thus illustrate, in a simple context, how symmetry techniques can be applied and completely worked out with moderate ease.

For solving the problem we have chosen the hyperspherical harmonics (or K-harmonics) method^{3,4}, which has been extensively used^{5,7}, as it allows, in principle, for a systematic treatment of the few body problem. However, it has the drawback that the high dimensionality of the hyperangle makes its visualisation rather difficult. In order to gain a better insight of the method, Amado and Coelho⁶ considered the case of one-dimensional three-body system, interacting via a general two-body potential, and obtained an infinite set of coupled ordinary differential equations (see equations (9) and (10) of Amado and Coelho⁸) which were then solved in the particular case of three identical particles interacting via an attractive δ -potential.

In this paper we investigate the symmetry properties, under the permutation group, of the K-harmonics (bound-state) solutions for the one-dimensional system of identical particles interacting via an attractive two-body potential $V(|x_1-x_2|)$. As the one-dimensional problem of N identical particles interacting via an attractive δ -potential has a single³ bound-state solution which is totally symmetric under the permutation of any pair of particles, this particular case will not be considered here. The three-dimensional problem of three interacting particles is considerably more involved^{4,5} and we believe that the solution given here is of considerable pedagogical value.

In Section 2 we make a brief exposition of the hyperspherical harmonics method for the case of three identical particles; the time independent Schrödinger equation is reduced to an infinite set of coupled ordinary differential equations. In Section 3 we discuss the effect of the action of the permutation group on the K-harmonics components and construct functions, of definite parity, which provide a basis for irreducible representations^{10,11} of the S_3 symmetry group. In Section 4 these functions are used for constructing eigenfunctions of definite parity and permutation properties. Concluding the paper, we present some very general properties exhibited by the bound-state spec-

trum of a one-dimensional system of three identical interacting particles obeying Bose-Einstein, Fermi-Dirac and Boltzmann statistics.

2. THE HYPERSPHERICAL METHOD FOR ONE-DIMENSIONAL THREE-BODY SYSTEM

The Schrödinger equation for a system of three identical particles moving in one dimension, interacting via an attractive two-body potential $V(|x_i - x_j|)$, is

$$\left[- \sum_{i=1}^3 \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_i^2} + V(x_1, x_2, x_3) \right] \psi(x_1, x_2, x_3) = E' \psi(x_1, x_2, x_3) \quad (1)$$

where $E' = E + E_{CM}$ and

$$V(x_1, x_2, x_3) = V(|x_1 - x_2|) + V(|x_2 - x_3|) + V(|x_1 - x_3|) \quad (2)$$

In terms of the Jacobi coordinates

$$\eta = \frac{1}{\sqrt{2}} (x_1 - x_2) \quad (3a)$$

$$\xi = \sqrt{2/3} \left[\frac{x_1 + x_2}{2} - x_3 \right] \quad (3b)$$

$$R = \frac{x_1 + x_2 + x_3}{\sqrt{3}} \quad (3c)$$

the Schrödinger equation (1), with the center of mass removed, can be written as

$$\left[- \frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial \eta^2} \right) + V(\xi, \eta) \right] \psi(\xi, \eta) = E \psi(\xi, \eta) \quad (4)$$

where

$$V(\xi, \eta) = V(\sqrt{2} |\eta|) + V\left(\left|\sqrt{3/2} \xi + \frac{1}{\sqrt{2}} \eta\right|\right) + V\left(\left|\sqrt{3/2} \xi - \frac{1}{2} \eta\right|\right) \quad (5)$$

Introducing the "hyperspherical coordinates", the hyper-radius ρ and the hyperangle θ

$$\eta = \rho \cos \theta, \quad \xi = \rho \sin \theta, \quad 0 \leq \theta \leq 2\pi \quad (6)$$

Schrödinger equation (4) can be written as

$$-\frac{\hbar^2}{2m} \left[\frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \theta^2} \right] \psi(\rho, \theta) + V(\rho, \theta) \psi(\rho, \theta) = E \psi(\rho, \theta) \quad (7)$$

where

$$V(\rho, \theta) = V(\sqrt{2} \rho |\cos \theta|) + V(\sqrt{2} \rho \left| \frac{\sqrt{3}}{2} \sin \theta + \frac{1}{2} \cos \theta \right|) \\ + V(\sqrt{2} \rho \left| \frac{\sqrt{3}}{2} \sin \theta - \frac{1}{2} \cos \theta \right|) \quad (8)$$

The hyperspherical (or K-harmonics) method for solving the equation (7) consists of expanding $\psi(\rho, \theta)$ in terms of a complete set of angular eigenfunctions. Following Amado and Coelho⁸, we use the set $e^{iK\theta}/(2\pi)^{1/2}$, K Integer, so that

$$\psi(\rho, \theta) = \sum_{K=-\infty}^{\infty} R_K(\rho) \frac{e^{iK\theta}}{(2\pi)^{1/2}} \quad (9)$$

Substitution of the expansion given by equation (9) in the time independent Schrödinger equation (7), leads to the following infinite set of coupled ordinary differential equations

$$-\frac{\hbar^2}{2m} \left(\frac{1}{\rho} \frac{d}{d\rho} \rho \frac{d}{d\rho} - \frac{K^2}{\rho^2} \right) R_K(\rho) + \sum_{K'=-\infty}^{\infty} \langle K|V|K' \rangle_{R_{K'}}(\rho) = E R_K(\rho) \quad (10)$$

where

$$\langle K|V|K' \rangle = \frac{1}{2\pi} \int_0^{2\pi} e^{i(K'-K)\theta} V(\rho, \theta) d\theta \quad (11)$$

One may now feel tempted to enter eq.(10) in a computer, truncating the expansion at some K_{\max} ¹². However, simply truncating eq.(10) at some K_{\max} will not work, because, as we shall see in the next section, eigenfunctions of different symmetry are mixed in eq.(10), although in fact uncoupled. The separation of eigenfunctions of different symmetry will be done in an elementary way in the next section. The method we use is simple but cannot be easily extended to higher dimension or larger number of particles. The reader may find in the series of articles by Efros¹³ how the separation is done in three-dimensions for an arbitrary number of particles. In another paper we intend to present a pedagogical introduction to these methods for

the case of four (and N) particles moving in **one-dimension**¹⁴.

Finally we should mention that in the three-dimensional case, even after the separation of the different symmetry functions has been achieved, there still remain formidable computational problems. These are aggravated if three-body forces are included. A way of dealing with the situation is presented in *reference 6*.

3. SYMMETRY PROPERTIES OF THE K-HARMONICS SOLUTIONS

As is well known^{10,11}, the invariance of the hamiltonian under any symmetry group implies the existence of eigenfunctions exhibiting the group transformation properties. We shall then explore the symmetry invariances of the three-body hamiltonian H for obtaining eigenfunctions with definite symmetry properties labelled by the K-harmonics components (eq. (9)). Under the action of the parity operator, (x_1, x_2, x_3) go onto $(-x_1, -x_2, -x_3)$, (ξ, η) go onto $(-\xi, -\eta)$ (see eqs. (3a) and (3b)) and (ρ, θ) go onto $(\rho, \pi + \theta)$ (see eq. (6)) so that the potential V of the three-body system is invariant under parity transformation (see eqs. (2), (5) and (8)). Thus, there exist eigenfunctions of H that have definite parity and we shall now determine the set of K-values that enter the hyperspherical harmonic expansion (eq. (9)) for an eigenfunction with definite parity.

Due to parity invariance of the potential, the matrix elements $\langle K | V | K' \rangle$, given in eq. (11), have the following properties

$$\langle K | V | K' \rangle \equiv 0 \quad \text{for} \quad (K' - K) \text{ odd} \quad (12a)$$

$$\langle K | V | K' \rangle \equiv \langle K' | V | K \rangle \equiv \langle -K | V | -K' \rangle \quad (12b)$$

Selection rule (12a) decouples K -even and K -odd equations in the system (10) and we are left with two infinite sets of coupled ordinary differential equations: one for even K and one for odd K . So, the eigenfunctions of H having positive (negative) parity will contain only even (odd) K components when expanded in terms of the hyperspherical harmonics (eq. (9)).

Now, using property (12b), the differential equations for components $R_{-K}(\rho)$ and $R_K(\rho)$ (eq. (10)) are

$$-\frac{\hbar^2}{2m} \left(\frac{1}{\rho} \frac{d}{d\rho} \rho \frac{d}{d\rho} - \frac{K^2}{\rho^2} \right) R_K(\rho) + \sum_{K'=-\infty}^{\infty} \langle K|V|K'\rangle R_{K'}(\rho) = E R_K(\rho)$$

$$-\frac{\hbar^2}{2m} \left(\frac{1}{\rho} \frac{d}{d\rho} \rho \frac{d}{d\rho} - \frac{K^2}{\rho^2} \right) R_{-K}(\rho) + \sum_{K'=-\infty}^{\infty} \langle K|V|K'\rangle R_{-K'}(\rho) = E R_{-K}(\rho)$$

so that,

$$R_{-K}(\rho) = \pm R_K(\rho) \quad (13)$$

The invariance of the potential V under the group S_3 (group of all permutations of three objects) is evident from expression (2). We shall now obtain the transformation properties of variables (ρ, θ) and (ξ, η) under the group S_3 .

The permutation of any pair (i, j) of particles leaves ρ invariant. As for the angle θ , under the action of the permutation operator P_{ij} , it transforms as follows

$$P_{12} : \quad \theta \rightarrow \pi - \theta \quad (14a)$$

$$P_{13} : \quad \theta \rightarrow 5\pi/3 - \theta \quad (14b)$$

$$P_{23} : \quad \theta \rightarrow \pi/3 - \theta \quad (14c)$$

Using eqs. (14a), (14b) and (14c) in eq. (6) we obtain the well known⁴ transformation properties of ξ and η

$$P_{12} \begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix} \quad (15a)$$

$$P_{13} \begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix} \quad (15b)$$

and

$$P_{23} \begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix} \quad (15c)$$

In terms of the variables ρ and θ , the invariance of the potential V under the action of the permutation operator P_{ij} is expressed as

$$V(\rho, \theta) = V(\rho, 5\pi/3 - \theta) = V(\rho, \pi/3 - \theta) = V(\rho, \pi - \theta) \quad (16)$$

(Relation (16) is obtained by using eqs. (14a), (14b) and (14c) in expression (8) for $V(\rho, \theta)$).

Using the invariance property (16), the matrix elements $\langle K|V|K'\rangle$, given by eq.(11), can be rewritten as

$$\begin{aligned} \langle K|V|K'\rangle &= \frac{1}{2\pi} \int_0^{\pi/3} d\theta e^{i(K'-K)\theta} V(\rho, \theta) \left[1 + e^{-i(K'-K)\pi} \right] \\ &\times \left[1 + e^{-i(K'-K)\pi/3} + e^{-i(K'-K)2\pi/3} \right] \end{aligned}$$

from which it follows that (remember that parity invariance requires $K-K$ even)

$$\langle K|V|K'\rangle = \begin{cases} \frac{6}{2\pi} \int_0^{\pi/3} d\theta e^{i(K'-K)\theta} V(\rho, \theta) & \text{for } K'-K=6n, \quad n \text{ integer} \\ & \text{from } -\infty \text{ to } +\infty \\ 0 & \text{otherwise} \end{cases} \quad (17)$$

Therefore each of the two infinite sets (K even and K odd) of coupled ordinary differential equations (10) splits into three infinite sets of K values

$$K \text{ even} : 6n, \quad 2+6n, \quad 4+6n \quad (18)$$

$$K \text{ odd} : 1+6n, \quad 3+6n, \quad 5+6n$$

with n , integer, running from $-\infty$ to $+\infty$.

Notice that

$$2 + 6n \equiv -4 + 6(n+1)$$

and

$$1 + 6n \equiv -5 + 6(n+1)$$

(18a)

i.e., the elements belonging to the sets $(4+6n)$ and $(5+6n)$ are minus the elements of the sets $(2+6n)$ and $(1+6n)$ respectively.

The invariance of the potential V under the action of the permutation group S_3 implies the invariance of the hamiltonian H under S_3 , so that there are eigenfunctions of H that have definite transformation properties under permutation of particles, besides having definite parity, We shall show that these eigenfunctions can be obtained by including in the K-harmonics expansion (11) the appropriate set of K-values (eq. (18)).

Eqs. (15a), (15b) and (15c) show that the vectors ξ and η provide a basis for the two dimensional irreducible (mixed) representation of the permutation group S_3 . An object that transforms as ξ will carry the index MS (mixed symmetric) as it is symmetric under the permutation of particles 1 and 2 (see eq. (15a)) and mixes with the corresponding η under permutation of particles 1 and 3 or 2 and 3 (see eqs. (15b) and (15c)). Analogously, an object that transforms like η will carry the index MA (mixed antisymmetric) as it is antisymmetric under the permutation of particles 1 and 2 (see eq. (15a)) and mixes with the corresponding ξ under permutation of any other pair of particles (see eqs. (15b) and (15c)). An object totally symmetric (antisymmetric) will carry the index S(A).

Using eqs. (14a), (14b) and (14c), the transformation properties, under S_3 , of $\cos(K\theta)$ and $\sin(K\theta)$ are easily obtained. We find that for each set of K-values given in eq. (18) the functions $\cos(K\theta)$ and $\sin(K\theta)$ exhibit definite symmetry properties under permutations of particle pairs. Thus, $\cos(6n\theta)$ ($\sin(6n\theta)$) is totally symmetric (antisymmetric), providing a one-dimensional symmetric (antisymmetric) irreducible representation of S_3 , with positive parity. The function $\cos[(2+6n)\theta]$ is MS and $\sin[(2+6n)\theta]$ is MA thus providing a basis for the two-dimensional mixed irreducible representation of S_3 (also with the positive parity). Another positive parity mixed irreducible representation is provided by $\cos[(4+6n)\theta]$ (MS) and $\sin[(4+6n)\theta]$ (MA). As for the negative parity irreducible representations, $\sin[(3+6n)\theta]$ ($\cos[(3+6n)\theta]$) provide the one-dimensional totally symmetric (antisymmetric) irreducible representation. The odd parity two-dimensional mixed irreducible representations of S_3 are provided by $\sin[(1+6n)\theta]$ (MS) and $\cos[(1+6n)\theta]$ (MA) and also by $\sin[(5+6n)\theta]$ (MS) and $\cos[(5+6n)\theta]$ (MA). These properties of $\sin(K\theta)$ and $\cos(K\theta)$ will be used in the next

section for constructing eigenfunctions of positive and negative parity that are symmetric, antisymmetric and mixed symmetric under permutation of particles.

We conclude this section with a comment about the usefulness of mixed symmetry eigenfunctions. Systems of identical fermions (bosons) must be described by totally antisymmetric (symmetric) wavefunctions. If the particles have only one degree of freedom then only the totally symmetric (for bosons) or totally antisymmetric (for fermions) eigenfunctions are admissible. However, if the particles have an extra degree of freedom, for instance, spin, using the well known^{11,12} prescription of multiplying mixed representations, we can obtain total eigenfunctions that are totally symmetric or antisymmetric.

4. CONSTRUCTION OF EIGENFUNCTIONS WITH DEFINITE PARITY AND PERMUTATION PROPERTIES

We shall first construct the eigenfunctions that are totally symmetric or totally antisymmetric. As we have seen, these eigenfunctions are associated with the sets $K=6n$ ($\cos(6n\theta)$) and $\text{sen}(6n\theta)$, and $K=3+6n$ ($\sin[(3+6n)\theta]$ and $\cos[(3+6n)\theta]$) (positive and negative parity respectively). For these K sets, expansion (10) can be written as

$$\psi^{(+)}(\rho, \theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=1}^{\infty} \left[R_{6n}(\rho) e^{i6n\theta} + R_{-6n}(\rho) e^{-i6n\theta} \right] + \frac{R_0(\rho)}{(2\pi)^{1/2}} \quad (19)$$

and

$$\psi^{(-)}(\rho, \theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=0}^{\infty} \left[R_{3+6n}(\rho) e^{i(3+6n)\theta} + R_{-3-6n}(\rho) e^{-i(3+6n)\theta} \right] \quad (20)$$

respectively.

Introducing the notation

$$\begin{aligned} R_{6n}(\rho) &= R_{6n}^E(\rho) & \text{if} & & R_{6n}(\rho) &= R_{-6n}(\rho) \\ R_{6n}(\rho) &= R_{6n}^O(\rho) & \text{if} & & R_{6n}(\rho) &= -R_{-6n}(\rho), \quad n \neq 0 \end{aligned} \quad (21)$$

the eigenfunctions $\psi_S^{(+)}(\rho, \theta)$ and $\psi_A^{(+)}(\rho, \theta)$ are immediately obtained from eq. (19)

$$\begin{aligned} \psi_S^{(+)}(\rho, \theta) &= \frac{2}{(2\pi)^{1/2}} \sum_{n=1}^{\infty} R_{6n}^E(\rho) \cos(6n\theta) + \frac{1}{(2\pi)^{1/2}} R_0^E(\rho) \\ &\equiv \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} R_{6n}^E(\rho) \cos(6n\theta) \end{aligned} \quad (22)$$

$$\psi_A^{(+)}(\rho, \theta) = \frac{2i}{(2\pi)} \sum_{n \neq 1}^{\infty} R_{6n}^O(\rho) \sin(6n\theta) \equiv \frac{i}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} R_{6n}^O(\rho) \sin(6n\theta) \quad (23)$$

Analogously, introducing the eigenvectors $R_{3+6n}^E(\rho)$ and $R_{3+6n}^O(\rho)$

$$\begin{aligned} R_{3+6n}^E(\rho) &= R_{-3-6n}^E(\rho) \\ R_{3+6n}^O(\rho) &= -R_{-3-6n}^O(\rho) \end{aligned} \quad (24)$$

the eigenfunctions $\psi_S^{(-)}(\rho, \theta)$ and $\psi_A^{(-)}(\rho, \theta)$ are immediately obtained from eq. (20)

$$\psi_S^{(-)}(\rho, \theta) = \frac{i}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} R_{3+6n}^O(\rho) \sin[(3+6n)\theta] \quad (25)$$

$$\psi_A^{(-)}(\rho, \theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} R_{3+6n}^E(\rho) \cos[(3+6n)\theta] \quad (26)$$

As we have seen, the mixed symmetry eigenfunctions are associated with $K=2+6n$ and $K=4+6n$ sets, for positive parity, and with $K=1+6n$ and $K=5+6n$ sets, for negative parity. Expansion (11) for the K sets are, respectively

$$\psi_M^{(+)}(\rho, \theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} R_{2+6n}(\rho) \{\cos[(2+6n)\theta] + i \sin[(2+6n)\theta]\} \quad (27)$$

$$\psi_{M'}^{(+)}(\rho, \theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} R_{4+6n}(\rho) \{\cos[(4+6n)\theta] + i \sin[(4+6n)\theta]\} \quad (27a)$$

and

$$\psi_M^{(-)}(\rho, \theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} R_{1+6n}(\rho) \{\cos[(1+6n)\theta] + i \sin[(1+6n)\theta]\} \quad (28)$$

$$\psi_{M'}^{(-)}(\rho, \theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} R_{5+6n}(\rho) \{ \cos[(5+6n)\theta] + i \sin[(5+6n)\theta] \} \quad (28a)$$

Using eqs.(13) and (18a) it can be easily verified that

$$\psi_{M'}^{(\pm)}(\rho, \theta) = \pm (\psi_M^{(\pm)}(\rho, \theta))^* \quad (29)$$

therefore we shall consider only the eigenfunctions $\psi_M^{(\pm)}(\rho, \theta)$.

† In order to exhibit the mixed symmetry character of the eigenfunctions (27) to (28a), the simple and elegant method devised by Simonov' will be used. The following complex conjugate vectors are introduced

$$Z = \sin \theta + i \cos \theta \quad \text{and} \quad Z^* = \sin \theta - i \cos \theta \quad (30)$$

Their transformation properties under P_{ij} can be obtained from those of ξ and η (eqs. (15a), (15b), (15c) since $Z = (\xi + i\eta)/\rho$ (eq.(6)). The transformations are

$$P_{12}Z = Z^*, \quad P_{13}Z = e^{-i2\pi/3} Z^*, \quad P_{23}Z = e^{i2\pi/3} Z^* \quad (31a)$$

and

$$P_{12}Z^* = Z, \quad P_{13}Z^* = e^{i2\pi/3} Z, \quad P_{23}Z^* = e^{-i2\pi/3} Z \quad (31b)$$

Likewise, for any given mixed symmetry basis (MS, MA), complex conjugate vectors of the form in eq. (30)

$$M_Z = MS + iMA \quad \text{and} \quad M_{Z^*} = MS - iMA \quad (30a)$$

can be introduced (they transform, of course, like Z and Z^* , thus the indexes).

As discussed in the previous section $\cos[(2+6n)\theta]$ ($\sin[(1+6n)\theta]$) is a MS function and $\sin[(2+6n)\theta]$ ($\cos[(1+6n)\theta]$) is a MA function of positive (negative) parity. Therefore, $\psi_M^{(+)}(\rho, \theta)$ in eq. (27) can be written as

$$\psi_M^{(+)}(\rho, \theta) = \psi_{MS}^{(+)}(\rho, \theta) + i \psi_{MA}^{(+)}(\rho, \theta) \quad (32)$$

where

$$\psi_{MS}^{(+)}(\rho, \theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} R_{2+6n}(\rho) \cos [(2+6n)\theta] \quad (33a)$$

and

$$\psi_{MA}^{(+)}(\rho, \theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} R_{2+6n}(\rho) \sin [(2+6n)\theta] \quad (33b)$$

Analogously, $\psi_M^{(-)}(\rho, \theta)$ in eq. (28) can be written as

$$\psi_M^{(-)}(\rho, \theta) = i (\psi_{MS}^{(-)}(\rho, \theta) - i \psi_{MA}^{(-)}(\rho, \theta)) \quad (34)$$

where

$$\psi_{MS}^{(-)}(\rho, \theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} R_{1+6n}(\rho) \sin [(1+6n)\theta] \quad (35a)$$

and

$$\psi_{MA}^{(-)}(\rho, \theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} R_{1+6n}(\rho) \cos [(1+6n)\theta] \quad (35b)$$

Thus, $\psi_M^{(+)}(\rho, \theta)$ in eq. (27), and its complex conjugate, transform under S_3 as Z and Z^* , respectively (eqs. (31a) and (31b)). As for the eigenfunction $-i \psi_M^{(-)}(\rho, \theta)$ (eq. (28)), and its complex conjugate, they transform like Z^* and Z respectively (eqs. (31b) and (31a)).

We now show how the eigenfunctions $\psi_M^{(\pm)}(\rho, \theta)$ and $(\psi_M^{(\pm)}(\rho, \theta))^*$ can be used to obtain totally symmetric or totally antisymmetric functions. As mentioned in the end of section 3, the particles must have an extra degree of freedom. We shall assume that the particles have spin 1/2 and the eigenvector corresponding to spin up (down) will be denoted by $u(d)$. Spin eigenfunctions of the three-particle system that under the permutation group S_3 transform as Z and Z^* , will be obtained through that procedure of combining the MS and MA spin functions as in eq. (30a). The three-particle mixed symmetry functions¹⁵ have total spin 1/2 and superscript $\pm 1/2$ will be used to indicate the Z -component of the total spin. The spin up functions are

$$\chi_{MS}^{1/2} = \frac{1}{\sqrt{6}} [udu + duu - 2uud]$$

$$\chi_{MA}^{1/2} = \frac{1}{\sqrt{2}} [udu - duu]$$

and the spin down are

$$\psi_{MS}^{-1/2} = \frac{1}{\sqrt{6}} [\overline{dud} + u\overline{dd} - 2\overline{d}d\overline{u}]$$

$$\psi_{MA}^{-1/2} = \frac{1}{\sqrt{2}} [\overline{dud} - u\overline{d}\overline{d}]$$

The corresponding complex conjugate vectors, which transform as Z and Z^* (eqs.(31a), (31b)), are

$$\chi_Z^{1/2} = \chi_{MS}^{1/2} + i \chi_{MA}^{1/2} \quad , \quad \chi_{Z^*}^{1/2} = \chi_{MS}^{1/2} - i \chi_{MA}^{1/2} \quad (36)$$

and

$$\chi_Z^{-1/2} = \chi_{MS}^{-1/2} + i \chi_{MA}^{-1/2} \quad , \quad \chi_{Z^*}^{-1/2} = \chi_{MS}^{-1/2} - i \chi_{MA}^{-1/2} \quad (37)$$

The totally symmetric and totally antisymmetric wavefunctions are now obtained from the appropriate combination of $\psi_M^{(\pm)}(\rho, \theta)$ (eqs. (27) and (28)), and their complex conjugates, with $\psi_Z^{\pm 1/2}(\rho, \theta)$, and their complex conjugates, (eqs. (36) and (37)). The positive parity functions are

$$\psi_S^{(+)}(\rho, \theta; \pm \frac{1}{2}) = \frac{1}{\sqrt{2}} \left[\psi_M^{(+)}(\rho, \theta) \chi_{Z^*}^{\pm 1/2} + \left(\psi_M^{(+)}(\rho, \theta) \right)^* \chi_Z^{\pm 1/2} \right] \quad (38)$$

$$\psi_A^{(+)}(\rho, \theta; \pm \frac{1}{2}) = \frac{1}{\sqrt{2}} \left[\psi_M^{(+)}(\rho, \theta) \chi_{Z^*}^{\pm 1/2} - \left(\psi_M^{(+)}(\rho, \theta) \right)^* \chi_Z^{\pm 1/2} \right] \quad (39)$$

and the negative parity are

$$\psi_S^{(-)}(\rho, \theta; \pm \frac{1}{2}) = \frac{1}{\sqrt{2}} \left[\left(\psi_M^{(-)}(\rho, \theta) \right)^* \chi_{Z^*}^{\pm 1/2} + \psi_M^{(-)}(\rho, \theta) \chi_Z^{\pm 1/2} \right] \quad (40)$$

$$\psi_A^{(-)}(\rho, \theta; \pm \frac{1}{2}) = \frac{1}{\sqrt{2}} \left[\left(\psi_M^{(-)}(\rho, \theta) \right)^* \chi_{Z^*}^{\pm 1/2} - \psi_M^{(-)}(\rho, \theta) \chi_Z^{\pm 1/2} \right] \quad (41)$$

Of course, if the three-fermion system has no other degree of freedom besides spin, only the above totally antisymmetric eigenfunctions $\psi_A^{(\pm)}(\rho, \theta; \pm \frac{1}{2})$ (eqs. (39) and (41)) are admissible.

5. CONCLUSIONS

We now analyse some qualitative features of the bound-state spectrum of one-dimensional three-particle system described by a hamiltonian invariant under parity and under the group S_3 . We shall consider the cases of bosons of spin zero, fermions of spin $1/2$ and also the case of distinguishable particles (Boltzmann statistics).

For a system of bosons of zero spin, the only admissible eigenfunctions are the totally symmetric ones, $\psi_S^{(\pm)}(\rho, \theta)$ (eqs. (22) and (25)). Due to the absence of centrifugal barrier for $K=0$, the ground-state eigenfunctions will be $\psi_S^{(+)}(\rho, \theta)$. There may be an excited state described by $\psi_S^{(-)}(\rho, \theta)$, for which the lowest component is $K=3$, thus having a considerable centrifugal barrier. Depending on the potential depth, there may be a whole family of states of type $\psi_S^{(+)}(\rho, 0)$ and $\psi_S^{(-)}(\rho, \theta)$, but no mixed symmetry type is allowed. In the case of the 6-potential, there is only one bound-state, $\psi_S^{(+)}(\rho, \theta)$.

Now for a system of spin $1/2$ fermions, the eigenfunction in spin-space will have mixed symmetry character due to Pauli principle (two states for accommodating three particles). Thus the spatial eigenfunction will be either $\psi_M^{(+)}(\rho, \theta)$ or $\psi_M^{(-)}(\rho, \theta)$ (eqs. (27) and (28)), the corresponding total eigenfunction being, respectively, $\psi_A^{(+)}(\rho, \theta; \pm \frac{1}{2})$ or $\psi_A^{(-)}(\rho, \theta; \pm \frac{1}{2})$ (eqs. (39) and (41)). Due to the centrifugal barrier we expect the eigenfunctions $\psi_M^{(-)}(\rho, \theta)$ (which contains $K = -1, 5$ components) to have an eigenvalue smaller than that of the eigenfunction $\psi_M^{(+)}(\rho, \theta)$ (which contains $K = 2, -4$ components).

Finally, for a system of distinguishable particles, (Boltzmann statistics), all symmetry type states are allowed. The ground-state will be described by $\psi_S^{(+)}(\rho, \theta)$ (eq. (22)) due to the absence of centrifugal barrier for $K=0$. The other symmetry states, due to the centrifugal barrier, should occur in the following order: $\psi_M^{(-)}(\rho, \theta)$ (eq. (28)), $\psi_M^{(+)}(\rho, \theta)$ (eq. (27)), $\psi_{S,A}^{(-)}(\rho, \theta)$ (apparently degenerate) (eqs. (25), (26)) and $\psi_A^{(+)}(\rho, \theta)$ (eq. (23)).

The degeneracy of $\psi_{S,A}^{(-)}(\rho, \theta)$ is shown to be false by examining the system of differential eqs. (10) for the radial vectors $R_{3+6n}^E(\rho)$ and $R_{3+6n}^O(\rho)$ eq. (24) which enter in $\psi_A^{(-)}(\rho, \theta)$ eq. (26), and $\psi_S^{(-)}(\rho, \theta)$, eq. (25), respectively. For $R_{3+6n}^E(\rho)$ the system in eq. (10) can be cast into the form

$$\begin{aligned}
& - \frac{\hbar^2}{2m} \left[\frac{1}{\rho} \frac{d}{d\rho} \rho \frac{d}{d\rho} - \frac{(3+6n)^2}{\rho^2} \right] R_{3+6n}^E(\rho) + \sum_{n'=0}^{\infty} \left[\langle 3+6n | V | 3+6n' \rangle \right. \\
& \left. + \langle 3+6n | V | -3-6n' \rangle \right] R_{3+6n'}^E(\rho) = E R_{3+6n}^E(\rho)
\end{aligned} \tag{42}$$

and for $R_{3+6n}^O(\rho)$ it becomes

$$\begin{aligned}
& - \frac{\hbar^2}{2m} \left[\frac{1}{\rho} \frac{d}{d\rho} \rho \frac{d}{d\rho} - \frac{(3+6n)^2}{\rho^2} \right] R_{3+6n}^O(\rho) + \sum_{n'=0}^{\infty} \left[\langle 3+6n | V | 3+6n' \rangle \right. \\
& \left. - \langle 3+6n | V | -3-6n' \rangle \right] R_{3+6n'}^O(\rho) = E R_{3+6n}^O(\rho)
\end{aligned} \tag{43}$$

For an interparticle potential monotonically increasing in the interparticle distance, the potential is more attractive for $R_{3+6n}^O(\rho)$ than for $R_{3+6n}^E(\rho)$ and the state $\psi_S^{(-)}(\rho, \theta)$ will be lower than $\psi_A^{(-)}(\rho, \theta)$. Therefore, assuming that the potential is attractive enough to bind all the states, the band of states with parity and permutation symmetry will occur in the order

$$\psi_S^{(+)}(\rho, \theta) \quad , \quad \psi_M^{(-)}(\rho, \theta) \quad , \quad \psi_M^{(+)}(\rho, \theta)$$

$$\psi_S^{(-)}(\rho, \theta) \quad , \quad \psi_A^{(-)}(\rho, \theta) \quad , \quad \psi_A^{(+)}(\rho, \theta)$$

(of course $(\psi_M^{(-)}(\rho, \theta))^*$ and $(\psi_M^{(+)}(\rho, \theta))^*$ are degenerate with $\psi_M^{(-)}(\rho, \theta)$ and $\psi_M^{(+)}(\rho, \theta)$ respectively).

Depending on the potential depth, there may be whole families of excited states for each type of symmetry state and the above order of occurrence of states refers to the lowest lying state of each symmetry family.

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12. One should mention that for making a computer calculation it is better to define $R_K = \phi_K(\rho)/\rho^{1/2}$ obtaining from eq.(10) the following equation for $\phi_K(\rho)$

$$-\frac{\hbar^2}{2m} \left[\frac{d^2}{d\rho^2} - \left(K^2 - \frac{1}{4} \right) \right] \phi_K(\rho) + \sum_{K'} \langle K|V|K' \rangle \phi_{K'}(\rho) = E \phi_K(\rho)$$
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Resumo

Aspectos qualitativos do espectro pontual de um sistema de três partículas idênticas movendo-se em uma dimensão são analisados. Usando-se o método dos harmônicos-K mostra-se como construir funções de onda com paridade e propriedades de transformação bem definidas sob permutação de qualquer par de partículas.