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ON SOME GENERAL PROPERTIES OF THE POINT SPECTRUM OF THREE PARTICLES MOVING IN ONE-DIMENSION

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ABSTRACT

The eigenstates of three-particles moving in one-dimension are classified according to the S_3 plus parity group. The ordering of the ground state S_3 band is given for a fairly general class of potentials. Sufficient conditions are given both for existence and non-existence of bound states of a given symmetry.

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I. INTRODUCTION

In this paper we investigate some general properties of the bound-state spectrum of three identical particles interacting via two-body potential and moving in one-dimension.

In section II the eigenfunctions are classified according to their transformation properties under parity and the group S_3. Using these criteria the states can be grouped in two bands (positive and negative parity) of four states. As it should, each set of four eigenfunctions of a band provides a basis for the irreducible representations of the group S_3: two one-dimensional (one completely symmetric, one completely antisymmetric) and one two-dimensional (of mixed symmetry).

Sufficient conditions for the existence of the lowest energy state of each symmetry type are given in section III. It results that the totally symmetric state of positive parity is always bound if the two-body potential is attractive. There are sufficient conditions for the existence of the lowest energy state of the other symmetry types and it is possible to give the ordering of ground-state band (of positive parity) for a large class of potentials.

Finally in section IV we give sufficient conditions for the unboundness of the lowest energy, negative parity, totally symmetric and totally antisymmetric states. Sufficient conditions for the unboundness of the first excited totally symmetric state of positive parity are also given.

The tools used are the k-harmonics method[1] (also called hyperspherical-harmonics), the Hall and Post[2] and Post[3] theorems and the comparison theorem[4].

II. THE S_3 BANDS

We consider the time-independent Schrödinger equation for three-identical particle moving in one-dimension and interacting via a two-body attractive potential $V(|x_i - x_j|)$. As it is well known, a three-body (identical particles) problem in one-dimension can be reduced to a one-body problem in two-dimension. Using the "hyperspherical coordinates"[1], the hyperradius ρ and the hyperangle θ, defined by

$$\eta = \rho\cos\theta \quad , \quad \xi = \rho\,\mathrm{sen}\,\theta \quad , \quad 0 \leq \theta < 2\pi \quad , \tag{1}$$

where η and ξ are the Jacobi coordinates

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

$$\xi = \sqrt{\frac{2}{3}}\left(\frac{x_1 - x_2}{2} - x_3\right) \tag{2b}$$

$$R = \frac{x_1 + x_2 + x_3}{\sqrt{3}} = 0 \quad , \tag{2c}$$

the Schrödinger equation becomes (using energy in units of $\hbar^2/2m$)

$$-\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}\right]\psi(\rho,\theta) + V(\rho,\theta)\psi(\rho,\theta) = E\,\psi(\rho,\theta) \quad , \tag{3}$$

where

$$V(\rho,\theta) = V(\sqrt{2}\,\rho|\cos\theta|) + V(\sqrt{2}\,\rho|\cos(\theta + \tfrac{\pi}{3})|) + V(\sqrt{2}\,\rho|\cos(\theta + \tfrac{2\pi}{3})|) . \tag{4}$$

If we now use the (k-harmonics) expansion

$$\psi(\rho,\theta) = \sum_{k=-\infty}^{\infty} \frac{R_k(\rho)}{\rho^{1/2}} \frac{e^{ik\theta}}{(2\pi)^{1/2}} \quad , \tag{5}$$

we get the following infinite set of coupled ordinary differential equation

$$-\left[\frac{d^2}{d\rho^2} - (k^2 - \tfrac{1}{4})\frac{1}{\rho^2}\right]R_k(\rho) + \sum_{k'} V_{k'-k}(\rho)R_{k'}(\rho) = E\,R_k(\rho) \quad , \tag{6}$$

where

$$V_{k'-k}(\rho) = \frac{1}{2\pi}\int_0^{2\pi} e^{i(k'-k)\theta}\,V(\rho,\theta)\,d\theta \quad . \tag{7}$$

Parity operator Π and the permutation operators P_{12}, P_{13} and P_{23} leave ρ invariant and transform θ onto $\pi+\theta$, $\pi-\theta$, $\frac{5\pi}{3}-\theta$ and $\frac{\pi}{3}-\theta$ respectively.

From parity invariance of $V(\rho,\theta)$ (4) it immediately follows that

$$V_{k'-k}(\rho) = 0 \qquad \text{for} \qquad k'-k \ \text{odd} \quad , \tag{8a}$$

$$V_{k'-k}(\rho) = V_{k-k'}(\rho) = V_{-(k'-k)}(\rho) \quad . \tag{8b}$$

Using the invariance of $V(\rho,\theta)$ under P_{12}, P_{13} and P_{23} we get

$$V_{k'-k}(\rho) = \begin{cases} \dfrac{6}{2\pi}\displaystyle\int_0^{\pi/3} e^{i(k'-k)\theta}\,V(\rho,\theta)d\theta & \text{for } k'-k=6n \text{ , n integer from } -\infty \text{ to } +\infty \text{ .} \\ 0 & \text{otherwise .} \end{cases} \tag{9}$$

Due to properties (8a) and (9) the system (6) splits into six infinite sets of k-values

$$\begin{aligned} &k \text{ even}: \quad 6n \;, \quad 2+6n \quad \text{and} \quad -2+6n \\ &k \text{ odd}: \quad 3+6n \;, \quad 1+6n \quad \text{and} \quad -1+6n \;. \end{aligned} \tag{10}$$

Using property (8b) it can be easily verified that the solutions of the system of equations (6) can be chosen such that

$$R_{-k}(\rho) = \pm R_k(\rho) \;. \tag{11}$$

We shall denote by $R_k^E(\rho)$ the solutions such that $R_{-k}(\rho) = R_k(\rho)$ and by $R_k^O(\rho)$ the solutions such that $R_{-k}(\rho) = -R_k(\rho)$.

The eigenfunctions of (3) given by expansion (5) can now be classified. Positive parity corresponds to k even and negative parity to k odd. The totally symmetric eigenfunction of positive parity is given by the set 6n, the totally antisymmetric eigenfunction is given by the set 6n ($n\neq 0$), and the mixed symmetry eigenfunctions are given by the set 2+6n (or −2+6n). Thus, the positive parity ground-state band is given by

$$\psi_S^{(+)}(\rho,\theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} \frac{R_{6n}^E(\rho)}{\rho^{1/2}} \cos 6n\,\theta \tag{12a}$$

$$\psi_A^{(+)}(\rho,\theta) = \frac{i}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} \frac{R_{6n}^O(\rho)}{\rho^{1/2}} \sin 6n\,\theta \tag{12b}$$

$$\psi_M^{(+)}(\rho,\theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} \frac{R_{2+6n}(\rho)}{\rho^{1/2}} \exp i(2+6n)\theta \quad \text{and c.c..} \tag{12c}$$

As the set −2+6n equals minus the set 2+6n, due to property (11) the eigenfunctions given by the set −2+6n differ from (12c) only by a phase factor.

The negative parity totally symmetric and totally antisymmetric eigenfunctions are given by set 3+6n and the mixed symmetry eigenfunctions are given by the set 1+6n (or −1+6n). The negative parity ground-state band is then given by

$$\psi_S^{(-)}(\rho,\theta) = \frac{i}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} \frac{R_{3+6n}^O(\rho)}{\rho^{1/2}} \sin(3+6n)\theta \tag{13a}$$

$$\psi_A^{(-)}(\rho,\theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} \frac{R_{3+6n}^E(\rho)}{\rho^{1/2}} \cos(3+6n)\theta \tag{13b}$$

$$\psi_M^{(-)}(\rho,\theta) = \frac{1}{(2\pi)^{1/2}} \sum_{n=-\infty}^{\infty} \frac{R_{1+6n}(\rho)}{\rho^{1/2}} \exp i(1+6n)\theta \quad \text{and c.c..} \tag{13c}$$

(as in the case of the set −2+6n, the eigenfunctions given by the set −1+6n differ from those given by 1+6n only by a phase factor).

The transformation properties of the mixed symmetry eigenfunctions $\psi_M^{(\pm)}$ and $(\psi_M^{(\pm)})^*$ can be easily verified using the complex two-dimension irreducible representation of the group S_3 introduced by Simonov[1].

Concluding this section we examine the order of the states of the ground-state S_3 band. The lowest state is $\psi_S^{(+)}(\rho,\theta)$ since this state has no centrifugal barrier (k=0). Due to the centrifugal barrier the other symmetry states should occur in the following order (see equation (6)): $\psi_M^{(-)}(\rho,\theta)$, $\psi_M^{(+)}(\rho,\theta)$, $\psi_{S,A}^{(-)}(\rho,\theta)$ (apparently degenerate) and finally $\psi_A^{(+)}(\rho,\theta)$. The degeneracy of $\psi_{S,A}^{(-)}(\rho,\theta)$ is easily shown to be only apparent.

If the potential decreases monotonically with the interparticle distance it is easy to see that $\psi_S^{(-)}$ is lower than $\psi_A^{(-)}$ (See Appendix). Other results concerning the ordering of the states will be presented in section IV.

III. SUFFICIENT CONDITIONS FOR THE EXISTENCE OF THE LOWEST ENERGY STATE OF EACH SYMMETRY TYPE

Truncation of expansion (12) and (13) provides variational functions and consequently an upper-bound for the lowest energy state of each symmetry type. Keeping a single term in the expansions (12) and (13) the corresponding system of differential equations (6) for each symmetry type will be reduced to a single equation. The truncated equation is

$$- \frac{d^2}{d\rho^2} R_k(\rho) - (k^2 - \tfrac{1}{4}) \frac{1}{\rho^2} R_k(\rho) + W_k(\rho) R_k(\rho) = E\, R_k(\rho) \tag{14}$$

where $W_k(\rho) = V_0$ for $k = 1$, 2 and 6 , $W_3(\rho) = V_0 - V_6$ for the $k = 3$ even solution (associated with $\psi_S^{(-)}$) and $W_3(\rho) = V_0 + V_6$ for the $k = 3$ odd solution (associated with $\psi_A^{(-)}$) .

In principle it is not difficult to find sufficient conditions for the existence of a bound-state for equation (14). For this it is necessary to find a trial function $\phi(\rho)$ such that $(\phi, H_k\phi) < -E_{2B}(\phi,\phi)$, where E_{2B} is the two-particle binding energy.

Taking Simon's choice[5], $\phi(\rho) = \rho^\alpha\, e^{-\frac{1}{2}\rho}$, we obtain

$$(\alpha^2 + k^2 - \tfrac{1}{4})\Gamma(2\alpha-1) - \alpha\Gamma(2\alpha) + \tfrac{1}{4}\,\Gamma(2\alpha+1) + \int_0^\infty d\rho\, \rho^{2\alpha}\, e^{-\rho}\, W_k(\rho) < -E_{2B}\Gamma(2\alpha+1) \ , \tag{15}$$

with $\alpha > \frac{1}{2}$ if $k \neq 0$.

For $k = 0$ the limit $\alpha \to \frac{1}{2}$ exists giving the condition

$$\int_0^\infty e^{-\rho}\, \rho\, V_0(\rho)\, d\rho \ < \ - E_{2B} - \frac{1}{4} \ . \tag{16}$$

This result is a weaker version of a previous result obtained by the authors[6] that guarantees the existence of at least one bound state for N-particle system in one- and two-dimension when the two-body interaction is globally attractive. For $k \neq 0$ a simple condition is obtained by taking $\alpha = 1$

$$\int_0^\infty d\rho\, e^{-\rho}\, \rho^2\, e^{-\rho}\, W_k(\rho) < -2E_{2B} - (\tfrac{1}{4} + k^2) \ . \tag{17}$$

Alternatively, taking $\phi(\rho) = \rho^{k+\frac{1}{2}}\, e^{-\sqrt{E_{2B}}\,\rho}$ as trial wave-function, the sufficient condition for the existence of at least one bound state of symmetry k is given by

$$\int_0^\infty \rho^{2k+1}\, e^{-2\sqrt{E_{2B}}\,\rho}\, W_k(\rho)\, d\rho \leq - \frac{(k + \frac{1}{2})}{(4E_{2B})^k}\,(2k)! \ . \tag{18}$$

In reference 7 we show that simple sufficient conditions are obtained by using as trial function the regular and irregular solutions of the modified Helmholtz equation matched at an arbitrary point R (Calogero's sufficient conditions[8] are obtained in this way). In the present case this type of trial wave-function gives the following awkward condition for the existence of a bound state with energy $\leq -\alpha^2$

$$R\int_0^R \left(\frac{\rho}{R}\right)^{2k+1} e^{-2\alpha\rho}\, W_k(\rho)\,d\rho + R\int_R^\infty \left(\frac{R}{\rho}\right)^{2k-1} e^{-2\alpha\rho}\, W_k(\rho)\,d\rho \leq$$

$$\leq -2\alpha\int_0^R \frac{(k+\frac{1}{2})}{R^{2k}}\, e^{-2\alpha\rho}\,\rho^{2k}\,d\rho - 2\alpha\int_R^\infty (k-\tfrac{1}{2})R^{2k}\, e^{-2\alpha\rho}\,\rho^{-2k}\,d\rho\ . \qquad (20)$$

IV. SUFFICIENT CONDITIONS FOR THE NON EXISTENCE OF BOUND-STATES OF A GIVEN SYMMETRY

In the case of totally symmetric or totally anti-symmetric states Hall and Post (HP) theorem[2] provides good lower bounds. Given $V(|x_i-x_j|)$, HP consider the two-body problem

$$H_{HP} = -2\frac{d^2}{d\rho^2} + 3V(\sqrt{2}\rho)\ . \qquad (21)$$

If this hamiltonian H_{HP} has a single bound state then $\psi_A^{(-)}$ is unbound and so is $\psi_A^{(+)}$.

We shall now use Hall (H)[3] theorem. Given $V(|x_i-x_j|)$, the two-body problem

$$H_H = \frac{3}{2}\left[-\frac{1}{2}\frac{d^2}{d\rho^2} + V(\sqrt{2}\rho)\right]\ , \qquad (21)$$

provides lower bounds, state by state, for the three-body bound-state spectrum. If H_H has three bound states with energies $-\varepsilon_1 < -\varepsilon_2 < -\varepsilon_3$ then if $\varepsilon_1+\varepsilon_2-E_{2B} < 0$ the states $\psi_S^{(-)}$, $\psi_A^{(-)}$, $\psi_A^{(+)}$ will be unbound and so will be the first excited totally symmetric state of positive parity; if

$\varepsilon_1+\varepsilon_3-E_{2B} > 0$ and $2\varepsilon_2-E_{2B} < 0$ the states $\psi_S^{(-)}$, $\psi_A^{(-)}$ and $\psi_A^{(+)}$ might be bound but the first excited state of type $\psi_S^{(+)}$ will be unbound and the ground-state bands will not intercept the excited state bands.

Finally, using Hall theorem[3] and the comparison theorem[4], it is easy to see that the three-body problem will have a finite number of bound-states if the potential is such that

$$\lim_{\rho\to\infty} V_0(\rho) \to 0\ . \qquad (22)$$

This condition is satisfied by any finite range potential. This is a particular case of a general result given by Sigal[9].

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APPENDIX

The degeneracy of $\psi_S^{(-)}(\rho,\theta)$ and $\psi_A^{(-)}(\rho,\theta)$ is shown to be false by examining the system of differential equations (6) for the radial vectors $R^E_{3+6n}(\rho)$ and $R^O_{3+6n}(\rho)$ which enter in $\psi_S^{(-)}(\rho,\theta)$ (13a) and $\psi_A^{(-)}(\rho,\theta)$ (13b) respectively. For $R^E_{3+6n}(\rho)$ the system (6) can be cast in the form

$$- \left[\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho} - \frac{(3+6n)^2}{\rho^2}\right] R^E_{3+6n}(\rho) + \sum_{n'=0}^{\infty} \left[V_{6(n'-n)} + \right.$$

$$\left. + V_{6(n'+n+1)}\right] R^E_{3+6n'}(\rho) = E\, R^E_{3+6n'}(\rho)$$

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

$$- \left[\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho} - \frac{(3+6n)^2}{\rho^2}\right] R^O_{3+6n}(\rho) + \sum_{n'=0}^{\infty} \left[V_{6(n'-n)} + \right.$$

$$\left. - V_{6(n+n'+1)}\right] R^O_{3+6n'}(\rho) = E\, R^O_{3+6n}(\rho) \quad .$$

For an interparticle potential monotonically decreasing in the interparticle distance, the potential is more attractive for $R^O_{3+6n}(\rho)$ than for $R^E_{3+6n}(\rho)$ and the state $\psi_S^{(-)}(\rho,\theta)$ will be lower than $\psi_A^{(-)}(\rho,\theta)$.