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Exact separation of a three-body problem in one dimension

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Abstract. It is shown that the problem of three equal-mass particles moving in one dimension, and interacting through anharmonic two-body forces, is exactly separable in hyperspherical coordinates. It is further proved, under mild conditions, that this is the most general 'well behaved' two-body force for which separation is possible. Some typical spectra are calculated numerically, and compared with analytic expressions based upon the semiclassical approximation.

1. Introduction

It is well known that, in general, the three-body problem in classical and quantum mechanics cannot be solved exactly by any currently known technique. Indeed, even the two-body problem can only be solved exactly because the introduction of centre-of-mass and relative coordinates allows it to be rewritten in the form of two one-body problems. However, there are a few special cases, involving simplified interactions and restrictions to one-dimensional motion, for which exact solutions of the three-body problem may be determined. McGuire (1964) has shown that the problem of N equal-mass particles moving in one dimension and interacting through equal and finite strength pairwise delta function potentials is susceptible to exact solution. The three-body problem is also exactly soluble for the one-dimensional motion of equal-mass particles interacting through two-body harmonic forces. In this connection, the introduction of hyperspherical coordinates provides a particularly elegant and convenient tool to effect the solution (Amado and Coelho 1978, Ballot and Fabre de la Ripelle 1980).

In this paper, we show that the problem of three equal-mass particles moving in one dimension, and interacting through *anharmonic* two-body forces, is also exactly separable in hyperspherical coordinates. Furthermore, we prove that this anharmonic form is the most general two-body force for which separation is possible. Finally, we present some typical spectra (calculated numerically) and, in the case of a pure r^4 potential, compare them with some approximate analytic expressions for the energy levels of the system derived from the semiclassical WKB method.

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2. One-dimensional three-body problem with anharmonic forces

Consider three particles of equal mass, m, moving in a single spatial dimension, and interacting through two-body potentials of the form

$$V(x_i, x_j) = \alpha(x_i - x_j)^2 + \beta(x_i - x_j)^4 \tag{2.1}$$

where the x_i label the positions of the particles with respect to some arbitrary origin. The strength α of the quadratic potential may be either positive or negative, but we only allow the strength β of the quartic potential to be positive, so as to ensure confinement. We wish to solve the time-independent Schrödinger equation for the wavefunction ψ of the three-particle system:

$$\frac{-\hbar^2}{2m}\nabla^2\psi + \left(\sum_{i\leqslant j=1}^{3} \alpha(x_i - x_j)^2 + \beta(x_i - x_j)^4\right)\psi = E\psi. \tag{2.2}$$

It is convenient to rewrite the particle coordinates with explicit reference to the centre of mass of the system, $X = (x_1 + x_2 + x_3)/3$, in terms of the hyperspherical radius and angle, ρ and θ respectively. Thus

$$r_1 = x_1 - X = \sqrt{\tfrac{2}{3}}\rho\cos(\theta - 2\pi/3) \tag{2.3}$$

$$r_2 = x_2 - X = \sqrt{\tfrac{2}{3}}\rho\cos(\theta + 2\pi/3) \tag{2.4}$$

$$r_3 = x_3 - X = \sqrt{\tfrac{2}{3}}\rho\cos(\theta). \tag{2.5}$$

These relations give equally convenient forms for the relative coordinates of any two particles:

$$r_1 - r_2 = x_1 - x_2 = \sqrt{2}\rho\sin(\theta) \tag{2.6}$$

$$r_2 - r_3 = x_2 - x_3 = \sqrt{2}\rho\sin(\theta - 2\pi/3) \tag{2.7}$$

$$r_3 - r_1 = x_3 - x_1 = \sqrt{2}\rho\sin(\theta + 2\pi/3). \tag{2.8}$$

By construction, we know that $\Sigma_{i=1}^{3} r_i = 0$. It is also easy to confirm that $\Sigma_{i=1}^{3} r_i^2 = \rho^2$, which is what motivated our choice of hyperspherical coordinates. However, a rather more curious identity, which was not foreseen but is at the heart of our ability to separate the Schrödinger equation in this case, is

$$\sum_{i=1}^{3} r_i^4 = \tfrac{1}{2}\rho^4. \tag{2.9}$$

With this information, we can return to (2.2) and simplify the potential by writing

$$\begin{aligned}\sum_{i\leqslant j=1}^{3}(x_i - x_j)^2 &= \tfrac{1}{2}\sum_{i,j=1}^{3}(r_i - r_j)^2 = \tfrac{1}{2}\sum_{i,j=1}^{3}(r_i^2 + r_j^2 - 2r_i r_j) \\ &= 3\sum_{i=1}^{3} r_i^2 = 3\rho^2\end{aligned} \tag{2.10}$$

and similarly

$$\begin{aligned}\sum_{i\leqslant j=1}^{3}(x_i - x_j)^4 &= \tfrac{1}{2}\sum_{i,j=1}^{3}(r_i - r_j)^4 = \tfrac{1}{2}\sum_{i,j=1}^{3}(r_i^4 + r_j^4 - 4r_i^3 r_j - 4r_i r_j^3 + 6r_i^2 r_j^2) \\ &= 3\sum_{i=1}^{3} r_i^4 + 3\left(\sum_{i=1}^{3} r_i^2\right)^2 = \tfrac{9}{2}\rho^4.\end{aligned} \tag{2.11}$$

Equations (2.3)-(2.5) make it clear that we can write the differential element, ds, as

$$(\mathrm{d}s)^2=(\mathrm{d}x_1)^2+(\mathrm{d}x_2)^2+(\mathrm{d}x_3)^2=3(\mathrm{d}X)^2+(\mathrm{d}\rho)^2+\rho^2(\mathrm{d}\theta)^2. \tag{2.12}$$

The corresponding Laplacians are

$$\begin{aligned}\nabla^2&=\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial x_3^2}\\&=\frac{1}{3}\frac{\partial^2}{\partial X^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}\end{aligned} \tag{2.13}$$

and (2.2) is clearly separable, since the potential only depends on the single coordinate ρ. If we write our wavefunction $\psi(\rho,\theta,X)$ as

$$\psi(\rho,\theta,X)=U(\rho)W(\theta)Y(X) \tag{2.14}$$

the standard separation procedure leads immediately to the following three second-order ordinary differential equations. Firstly

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2Y}{\mathrm{d}X^2}=E_{\mathrm{CM}}Y \tag{2.15}$$

describes the motion of the centre of mass of the system, with the separation constant labelled as E_{CM}. Secondly

$$\frac{-\hbar^2}{2m}\frac{\mathrm{d}^2W}{\mathrm{d}\theta^2}=\alpha W \tag{2.16}$$

describes the behaviour of the hyperspherical angular motion. If our particles have equal masses but are not identical, such as would be the case for three quarks of the same flavour but different colour, then the requirement that a 'rotation' of 2π should leave our system in the same physical state leads to the constraint

$$\alpha=\hbar^2l^2/2m \tag{2.17}$$

where $l=0,\pm1,\pm2,\ldots$. If, on the other hand, the particles are identical, then the state of the system must remain unchanged by a 'rotation' of $2\pi/3$ and we would have the alternative condition $\alpha'=9\hbar^2l^2/2m$. Throughout the rest of this paper we shall use the relation of (2.17) since it generates a richer spectrum of states while at the same time encompassing the more symmetric case of three identical particles. Finally

$$\frac{-\hbar^2}{2m}\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\rho\frac{\mathrm{d}U}{\mathrm{d}\rho}\right)+[\tfrac{9}{2}\beta\rho^4+3\alpha\rho^2-(E-E_{\mathrm{CM}})+\hbar^2l^2/2m\rho^2]U=0 \tag{2.18}$$

describes the 'radial' motion of the three-body system.

We have thus shown that the problem of three equal-mass particles moving in one dimension, and interacting through anharmonic two-body forces, is exactly separable in hyperspherical coordinates.

3. Functional equations for the three-body problem in one dimension

In this section we seek to find the most general form of the two-body potential for which the equal-mass three-body problem in one dimension is separable. We shall use the technique of functional equations, and in so doing require that the first- and

second-order derivatives of our desired functions exist. We shall therefore not be able to say anything about delta function or other 'badly behaved' potentials which do not possess such derivatives, but may nevertheless also conceivably lead to separable problems.

To guarantee separation we wish to find the most general two-body potential such that $\Sigma_{i<j=1}^{3} u(r_i - r_j) = v(\rho)$. In this case, when we write the equations of the three-body problem in terms of the hyperspherical coordinates ρ and θ they will decouple, enabling us to obtain an exact solution. Using the relations of equations (2.6)-(2.8) this is equivalent to trying to find functions f and g such that

$$\sum_{\kappa=1}^{3} f[\rho \sin(\theta - 2\pi\kappa/3)] = g(\rho). \tag{3.1}$$

Let us begin by setting $\theta = 0$ in (3.1). Then

$$f(0) + f(\sqrt{3}\rho/2) + f(-\sqrt{3}\rho/2) = g(\rho) \tag{3.2}$$

which leads to the conclusion that g must be an even function of ρ:

$$g(\rho) = g(-\rho). \tag{3.3}$$

Now, separate the function f into symmetric and antisymmetric parts S and A respectively:

$$f(x) = S(x) + A(x) \tag{3.4}$$

where $S(x) = S(-x)$ and $A(x) = -A(-x)$. Conversely

$$S(x) = \tfrac{1}{2}[f(x) + f(-x)] \tag{3.5}$$

and

$$A(x) = \tfrac{1}{2}[f(x) - f(-x)]. \tag{3.6}$$

Substitution of these relations into (3.1) leads to

$$\sum_{\kappa=1}^{3} S[\rho \sin(\theta - 2\pi\kappa/3)] + \sum_{\kappa=1}^{3} A[\rho \sin(\theta - 2\pi\kappa/3)] = g(\rho). \tag{3.7}$$

However, since we already know that g must be an even function of ρ we can write separately

$$\sum_{\kappa=1}^{3} A[\rho \sin(\theta - 2\pi\kappa/3)] = 0 \tag{3.8}$$

$$\sum_{\kappa=1}^{3} S[\rho \sin(\theta - 2\pi\kappa/3)] = g(\rho). \tag{3.9}$$

To begin with, we concentrate on the antisymmetric function A. Setting $\theta = \pi/2$ in (3.8) and writing the terms of the sum explicitly gives

$$A(\rho) + 2A(-\rho/2) = 0. \tag{3.10}$$

This, in turn, implies that $A(\rho) = 2A(\rho/2)$, which has the linear solution

$$A(\rho) = a\rho \tag{3.11}$$

where a is an arbitrary constant.

The symmetric function, S, may be found by taking first and second derivatives of (3.9) with respect to ρ and θ, respectively, as follows;

$$\sum_{\kappa=1}^{3} \sin(\theta - 2\pi\kappa/3) S'[\rho \sin(\theta - 2\pi\kappa/3)] = g'(\rho) \tag{3.12}$$

$$\sum_{\kappa=1}^{3} \sin^2(\theta - 2\pi\kappa/3) S''[\rho \sin(\theta - 2\pi\kappa/3)] = g''(\rho) \tag{3.13}$$

$$\sum_{\kappa=1}^{3} \rho \cos(\theta - 2\pi\kappa/3) S'[\rho \sin(\theta - 2\pi\kappa/3)] = 0 \tag{3.14}$$

$$\sum_{\kappa=1}^{3} \{\rho^2 \cos^2(\theta - 2\pi\kappa/3) S''[\rho \sin(\theta - 2\pi\kappa/3)]$$

$$- \rho \sin(\theta - 2\pi\kappa/3) S'[\rho \sin(\theta - 2\pi\kappa/3)]\} = 0 \tag{3.15}$$

where the primes denote successive derivatives of the functions. Multiplying (3.12) by ρ, (3.13) by ρ^2 and then adding the two resultants to (3.15) leads to

$$\rho^2 \sum_{\kappa=1}^{3} S''[\rho \sin(\theta - 2\pi\kappa/3)] = \rho^2 g''(\rho) + \rho g'(\rho). \tag{3.16}$$

Writing out the terms in the above sum explicitly for $\theta = 0$, and using the symmetric nature of S,

$$S''(0) + 2S''(\sqrt{3}\rho/2) = g''(\rho) + g'(\rho)/\rho. \tag{3.17}$$

Let us return momentarily to (3.9) and there also write out the terms of the sum explicitly when $\theta = 0$:

$$S(0) + 2S(\sqrt{3}\rho/2) = g(\rho). \tag{3.18}$$

Differentiating this with respect to ρ yields

$$g'(\rho) = \sqrt{3} S'(\sqrt{3}\rho/2) \tag{3.19}$$

and

$$g''(\rho) = 3S''(\sqrt{3}\rho/2)/2 \tag{3.20}$$

which may be substituted in (3.17). Thus

$$S''(0) + 2S''(\sqrt{3}\rho/2) = 3S''(\sqrt{3}\rho/2)/2 + \sqrt{3} S'(\sqrt{3}\rho/2)/\rho. \tag{3.21}$$

For convenience, let us write $x = \sqrt{3}\rho/2$, so that

$$S''(x) - 3S'(x)/x + 2S''(0) = 0 \tag{3.22}$$

for which an integrating factor of $1/x^3$ is readily found. This leads to

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{S'(x)}{x^3}\right) + \frac{2}{x^3} S''(0) = 0 \tag{3.23}$$

which may be straightforwardly integrated twice to obtain $S(x)$. Therefore

$$\frac{S'(x)}{x^3} + \frac{S''(0)}{x^2} = b \tag{3.24}$$

where b is a constant of integration, and finally

$$S(x)=\frac{bx^4}{4}+\frac{S''(0)x^2}{2}+c \tag{3.25}$$

where c is a second constant of integration.

Bearing in mind that our antisymmetric function, $A(x)=ax$, will not contribute to the total potential when summed over all particles, we can claim to have shown that the most general form of two-body potential, f, possessing first and second derivatives, which can lead to a separable three-body problem in one dimension, has the anharmonic form

$$f(x)=C_0+C_2x^2+C_4x^4. \tag{3.26}$$

This peculiar result does not appear to generalise to more than three particles or to motion in two or three dimensions.

4. Some examples of the associated spectra

To calculate the energy levels of our one-dimensional three-body system we must solve the 'radial' equation given by (2.18). To simplify the appearance of this equation, let us define a new radial function, $\chi=u/\sqrt{\rho}$, which will allow us to eliminate the first derivative and so write

$$\frac{d^2\chi}{d\rho^2}+\left(\varepsilon-A\rho^4-B\rho^2-\frac{(l^2-\frac{1}{4})}{\rho^2}\right)\chi=0 \tag{4.1}$$

where $\varepsilon=2m(E-E_{CM})/\hbar^2$, $A=9m\beta/\hbar^2$ and $B=6m\alpha/\hbar^2$. In general, no analytic solutions of this equation are known and the eigenvalue, ε, must be found numerically. The requirement that the wavefunction remain finite at the origin and approach zero as ρ approaches infinity allows us to identify the limiting behaviour of χ at small and large ρ. Near the origin $\chi\sim\rho^{l+1/2}$, and at the other extremity, $\chi\sim\exp(-\sqrt{A}\rho^3/3)$ as $\rho\to\infty$. If, however, $A=0$ but $B>0$ then the asymptotic behaviour is $\chi\sim\exp(-\sqrt{B}\rho^2/2)$. With these boundary conditions, numerical solutions of (2.18) may be found by standard techniques (a shooting method based on a Pruefer transformation).

To get some feeling for the spectra generated by the anharmonic potential we shall investigate some particular cases. They are (i) $A=0$, $B>0$ (which is the equation describing the two-dimensional simple harmonic oscillator), (ii) $A>0$, $B=0$ (for which approximate analytic expressions for the energy levels have been obtained within the semiclassical approximation) and (iii) $A>0$, $B\neq 0$.

4.1. $A=0$, $B>0$

In this case (4.1) reduces to the well known form

$$\frac{d^2\chi}{d\rho^2}+\left(\varepsilon-B\rho^2-\frac{(l^2-\frac{1}{4})}{\rho^2}\right)\chi=0 \tag{4.2}$$

which describes a two-dimensional simple harmonic oscillator and has analytic solutions. It is actually identical in form to the equation describing a three-dimensional simple harmonic oscillator except that here the centrifugal potential takes the form

$(l^2-\frac{1}{4})/\rho^2$ instead of $l(l+1)/\rho^2=[(l+\frac{1}{2})^2-\frac{1}{4}]/\rho^2$. Hence, the well known results for the three-dimensional case can be converted to this problem by simply making the substitution $l+\frac{1}{2}\to l$. In particular, the energy levels are given by $E(n, l)$ where

$$E(n, l)=2\sqrt{B}(2n+l+1) \tag{4.3}$$

and n is the number of interior nodes in the radial wavefunction. This analytic result also allows us to check our numerical methods against a known spectrum, and so confirm their correct functioning.

All levels of non-zero l are doubly degenerate because (4.1) depends only on l^2 and so is not sensitive to the difference between $\pm l$. Clearly, in this special case, states with the same value of $N=2n+l$ are 'accidentally' degenerate.

4.2. $A>B$, $B=0$

We now consider a pure ρ^4 power-law potential. Although no analytic solutions of the radial wave equation are known in this case, several approximate analytic expressions for the energy levels, based on the WKB method, have been proposed. In table 1 we compare our numerical results with two such approximate formulae.

The Quigg and Rosner (1979) formula for a general ρ^s potential is

$$\varepsilon(\nu, \lambda)\simeq\left(\sqrt{\pi}\,\frac{\Gamma(1/s+\frac{3}{2})}{\Gamma(1/s+1)}(2\nu+\lambda)\right)^{2s/(s+2)} \tag{4.4}$$

where, in our case, $s=4$, $\nu=n+\frac{1}{2}$ and $\lambda=l$, giving explicitly

$$\varepsilon(n, l)=\left(\sqrt{\pi}\,\frac{\Gamma(\frac{7}{4})}{\Gamma(\frac{5}{4})}(2n+l+1)\right)^{4/3}. \tag{4.5}$$

This expression has the same 'accidental' degeneracies as the two-dimensional simple harmonic oscillator, since it only depends on the single quantum number $N=2n+l$, and cannot therefore give a completely adequate description of the true spectrum, in which these degeneracies are lifted. Nevertheless, table 1 shows that it does give a good approximation to the energies of all of the low-lying states of the spectrum considered here.

Another approximate formula has been derived by Buck and Spiers (1979) within the framework of the WKB approximation. For a ρ^s potential their result is

$$\varepsilon(\nu, \lambda)=\frac{s+2}{s}\left(\frac{s}{2}\right)^{2/(s+2)}[\lambda+\nu(s+2)^{1/2}]^{2s/(s+2)} \tag{4.6}$$

which in our case becomes

$$\varepsilon(n, l)=\tfrac{3}{2}2^{1/3}[l+\sqrt{6}(n+\tfrac{1}{2})]^{4/3}. \tag{4.7}$$

This expression does not retain the harmonic oscillator degeneracies and is expected to be particularly accurate for states having large l and small n, which is borne out by table 1.

Figure 1 shows the numerically calculated spectrum for the parameter value $A=1$ so that the radial equation now takes the simple form

$$\frac{d^2\chi}{d\rho^2}+\left(\varepsilon-\rho^4-\frac{(l^2-\frac{1}{4})}{\rho^2}\right)\chi=0. \tag{4.8}$$

Table 1. A comparison of the numerically calculated energies of the low-lying states in the potential $V(x) = x^4$ with the analytic approximations of Quigg and Rosner (1979) (QR) and Buck and Spiers (1979) (BS).

l	n	QR	BS	Numerical
0	0	2.185	2.476	2.345
	1	9.454	10.71	9.528
	2	18.68	21.17	18.74
	3	29.26	33.16	29.30
	4	40.91	46.36	40.94
1	0	5.506	5.489	5.394
	1	13.87	14.77	13.81
	2	23.82	25.90	23.78
	3	34.96	38.42	34.92
	4	47.08	52.05	47.04
2	0	9.454	9.004	8.928
	1	18.68	19.13	18.31
	2	29.26	30.83	28.96
	3	40.91	43.86	40.66
3	0	13.87	12.91	12.84
	1	23.82	23.75	23.03
	2	34.96	36.03	34.30
	3	47.08	49.47	46.51
4	0	18.68	17.13	17.08
	1	29.26	28.61	27.96
	2	40.91	41.39	39.81
5	0	23.82	21.64	21.59
	1	34.96	33.68	33.10
	2	47.08	46.93	45.46
6	0	29.26	26.40	26.35
	1	40.91	38.96	38.42
7	0	34.96	31.38	31.34
	1	47.08	44.42	43.91
8	0	40.91	36.56	36.52
9	0	47.08	41.94	41.91

We see that the simple harmonic oscillator degeneracies are broken in such a way that, for a given value of $N = 2n + l$, the states of higher l have lower energies. This is essentially due to the curvature of the potential. Baumgartner *et al* (1984, 1985) have shown that, if $(\mathrm{d}/\mathrm{d}\rho^2)^2 V(\rho) > 0$, for all ρ, then $E_{n,l} > E_{n-1,l+2}$. Our results are certainly in line with these two inequalities, since we have $(\mathrm{d}/\mathrm{d}\rho^2)^2\rho^4 = 2$ and the energy level ordering in figure 1 is clearly in agreement with the consequences predicted.

4.3. $A > 0$, $B \neq 0$

Figures 2 and 3 show our numerical determinations of the energies of the low-lying states generated by the potentials $V(\rho) = A\rho^4 \pm B\rho^2$. We have chosen the constants so that $A = 1$ and $B = \pm 4$ for convenience. The spectra display similar patterns to those of the pure ρ^4 potential, but exhibit a little more spread in energy when $B = 4$ and

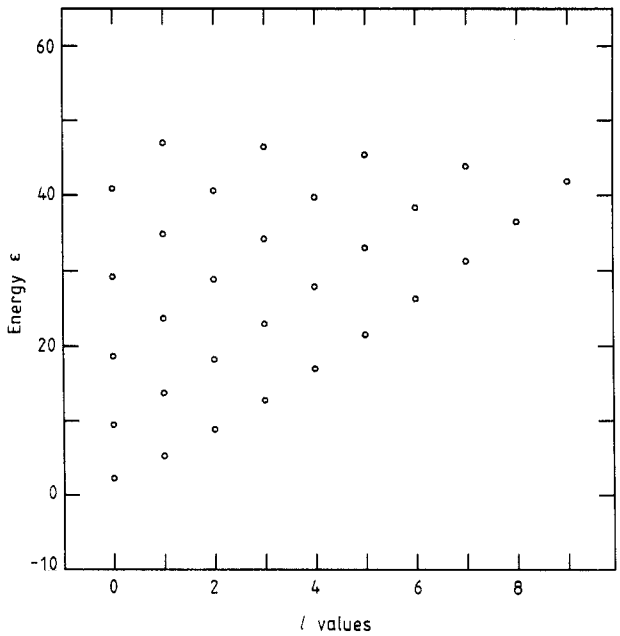

Figure 1. The energies of the low-lying states generated by the potential $V(x) = x^4$. The states having $l = 0$ are unique, whilst those having $l \neq 0$ are doubly degenerate. Note that the 'accidental' degeneracy between states having the same values of $N = 2n + l$ associated with the simple harmonic oscillator is only lightly lifted.

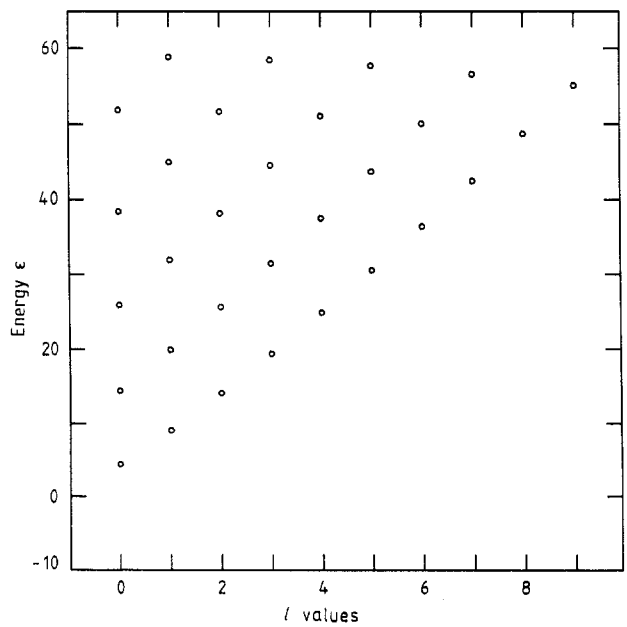

Figure 2. The energies of the low-lying states generated by the potential $V(x) = x^4 + 4x^2$.

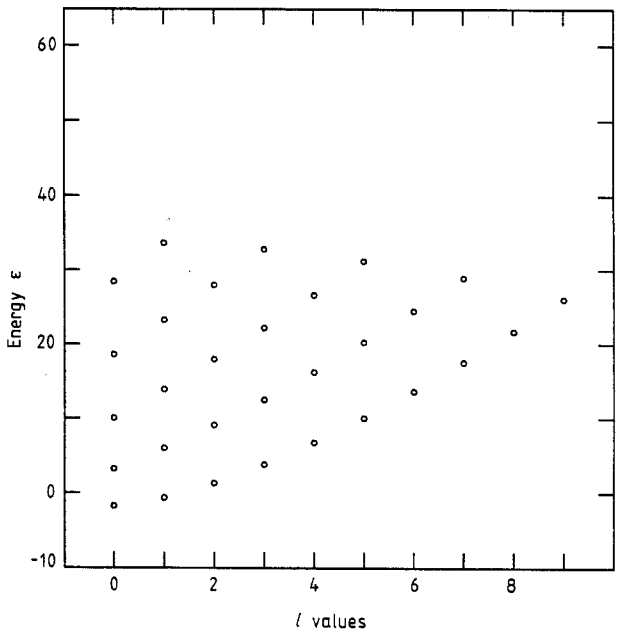

Figure 3. The energies of the low-lying states generated by the potential $V(x) = x^4 - 4x^2$. Note that it is possible to generate states with $\varepsilon \leqslant 0$ in this case.

slightly more compression when $B = -4$. We also note that when $B = -4$, it is possible to generate states with negative energy; i.e. bound in the local minimum of the potential near the origin.

5. Conclusions

We have shown that the equations governing the one-dimensional motion of three equal-mass particles interacting through anharmonic forces are separable, and hence exactly soluble, in hyperspherical coordinates. We have further shown by functional equations that the anharmonic potential $V(x) = C_0 + C_2x^2 + C_4x^4$ is the most general one for which such a separation occurs. Finally, we have numerically calculated the spectra generated in some typical cases and compared these energies with the predictions of some analytic approximations in the special case of a pure, $V(x) = x^4$, power-law potential.

Tables of the exact energies of the low-lying states generated by the potentials $V(x) = x^4 \pm 4x^2$ may be of use to other authors in checking the accuracy of alternative methods of solution of the three-body problem and are available on request.

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