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LETTER TO THE EDITOR

On the energy levels of an isotropic anharmonic oscillator

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Abstract. An approximate implicit energy level expression is obtained for a spherically symmetric anharmonic oscillator with three degrees of freedom, by using a semi-classical, WKB type Bohr–Sommerfeld quantisation rule.

Quantal anharmonic systems with a single degree of freedom have been extensively studied in the literature (Bender and Wu 1969, Biswas *et al* 1973, Hioe *et al* 1976, Banerjee 1978). In particular, several semi-classical (Mathews and Eswaran 1972, Lakshmanan 1973 and references therein), WKB type (Handelsman and Lew 1969; see also Fröman *et al* 1979) and phase-integral calculations of energy levels exist for these systems. Anharmonic systems with many degrees of freedom, though of much physical relevance, are more complicated and consequently much less is known about them (Lu and Nigam 1969, Bell *et al* 1970, Ehlenberger and Mendelsohn 1972, Hioe 1978, Isaacson and Marshesin 1978). Therefore, any explicit calculation is of much relevance to an understanding of these systems. One particular case for which semi-classical, WKB or phase-integral calculations can be carried out explicitly is the system of a spherically symmetric anharmonic oscillator. The Bohr–Sommerfeld semi-classical quantisation rule in the modified form (in conjunction with the usual angular momentum quantisation rules) applicable to such systems is

$$\oint p \, \mathrm{d}r = (n+\tfrac{1}{2})h, \tag{1a}$$

where r is the radial coordinate and p is the corresponding canonical momentum. The quantisation rule (1a) is also equivalent to the familiar first-order WKB approximation formula

$$\oint \left[2m\left(\mathscr{E} - V(r) - \frac{(l+\frac{1}{2})\hbar^2}{2mr^2}\right)\right]^{1/2} \mathrm{d}r = (n+\tfrac{1}{2})h, \tag{1b}$$

where $V(r)$ corresponds to the potential and $\mathscr{E}$ is the total energy. For a systematic derivation of this result and higher-order corrections, the phase-integral method of Fröman and Fröman (1965, 1974, 1977) could be used.

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In the present paper, we consider the three-dimensional anharmonic oscillator system described by the Hamiltonian

$$H=\boldsymbol{p}^2/2m+\tfrac{1}{2}m\omega^2\boldsymbol{r}^2+\tfrac{1}{4}\lambda(\boldsymbol{r}\cdot\boldsymbol{r})^2, \tag{2}$$

$$\boldsymbol{r}=(r_1, r_2, r_3)$$

and apply the semi-classical, WKB quantisation rule (1) to obtain the approximate energy level expression corresponding to the Schrödinger equation

$$[-(\hbar^2/2m)\boldsymbol{\nabla}^2+\tfrac{1}{2}m\omega^2\boldsymbol{r}^2+\tfrac{1}{4}\lambda(\boldsymbol{r}\cdot\boldsymbol{r})^2]\Psi(\boldsymbol{n})=\mathscr{E}\Psi(\boldsymbol{r}). \tag{2a}$$

The evaluation of the integral (1) (as well as higher-order corrections, which we will report separately) is facilitated by a knowledge of the underlying classical dynamics of the system (which itself is of intrinsic interest). To this end, we consider Newton's equation of motion corresponding to the system (2):

$$m\ddot{\boldsymbol{r}}+m\omega^2\boldsymbol{r}+\lambda(\boldsymbol{r}\cdot\boldsymbol{r})\boldsymbol{r}=0. \tag{3}$$

This could be separated out in spherical polar coordinates (r, θ, ϕ) in the form

$$r^2(\sin^2\theta)\dot{\phi}=C_1=\text{constant}, \tag{4a}$$

$$r^4\dot{\theta}^2+C_1^2/\sin^2\theta=C_2^2=\text{constant} \tag{4b}$$

and

$$m\ddot{r}+m\omega^2 r+\lambda r^3=mC_2^2/r^3. \tag{4c}$$

On integrating equation (4*c*) explicitly, we can show that it admits periodic solutions of the form

$$r(t)=A[1-\beta^2\,\mathrm{sn}^2(\gamma t)]^{1/2} \tag{5a}$$

where

$$\gamma^2=(1/2m)[(m\omega^2+\tfrac{3}{2}\lambda A^2)+(m^2\omega^4+m\omega^2\lambda A^2+\tfrac{1}{4}\lambda^2A^4+2\lambda mC_2^2/A^2)^{1/2}] \tag{5b}$$

and

$$\beta^2=\frac{1}{2}\left[3\left(1+\frac{2}{3}\frac{m\omega^2}{\lambda A^2}\right)-\left(1+\frac{4m\omega^2}{\lambda A^2}+\frac{4m^2\omega^4}{\lambda^2A^4}+\frac{8mC_2^2}{\lambda A^6}\right)^{1/2}\right]. \tag{5c}$$

Here, the square of the modulus of the Jacobian elliptic function is given by

$$k^2=\lambda A^2\beta^2/2m\gamma^2 \qquad (0\leqslant k^2\leqslant\beta^2\leqslant 1). \tag{5d}$$

Then the classical energy $\mathscr{E}_c$ corresponding to the Hamiltonian (2) is obtained by substituting the solution (5) in (2):

$$\mathscr{E}_c=\tfrac{1}{2}m\omega^2A^2\left(1+\frac{\lambda A^2}{2m\omega^2}+\frac{C_2^2}{\omega^2A^4}\right). \tag{6}$$

Now the classical radial momentum is obtained from (5) as

$$p=m\frac{\mathrm{d}r}{\mathrm{d}t}\equiv mA\frac{\mathrm{d}}{\mathrm{d}t}[1-\beta^2\,\mathrm{sn}^2(\gamma t)]^{1/2}$$

$$=-mA\beta^2\gamma\frac{(\mathrm{sn}\,u)(\mathrm{cn}\,u)(\mathrm{dn}\,u)}{(1-\beta^2\,\mathrm{sn}^2\,u)^{1/2}} \qquad (u=\gamma t). \tag{7}$$

Then with the angular momentum quantisation rule

$$m^2C_2^2 = (l+\tfrac{1}{2})^2\hbar^2, \tag{8}$$

the quantisation condition (1) for the radial part becomes

$$m\gamma\beta^4A^2\int_0^{2K}\frac{(\mathrm{sn}^2\,u)(\mathrm{dn}^2\,u)(\mathrm{cn}^2\,u)}{(1-\beta^2\,\mathrm{sn}^2\,u)}\,\mathrm{d}u = (n+\tfrac{1}{2})h. \tag{9}$$

Here K is the complete elliptic integral of the first kind. On evaluation of the integral on the left-hand side of equation (9), by using the formulae of Byrd and Friedman (1969), one obtains

$$\frac{m\gamma A^2}{3k^2}\left[(\beta^2+2\beta^2k^2-3k^2)K-(\beta^2+\beta^2k^2-3k^2)E-3k^2\frac{(\beta^2-k^2)(1-\beta^2)}{\beta^2}(D_1-K)\right]$$
$$= (n+\tfrac{1}{2})h, \tag{10}$$

where

$$D_1 = \frac{1}{2}\left[\Pi(K,\beta^2)+\frac{\beta^2k'^2}{(1-\beta^2)(\beta^2-k^2)}\Pi\left(K,\frac{k^2-\beta^2}{1-\beta^2}\right)-\frac{k^2K}{(\beta^2-k^2)}\right] \qquad (k'^2=1-k^2). \tag{11}$$

E and Π, here, are the complete elliptic integrals of the second and third kinds respectively. Equation (10) implicitly gives the quantised expressions for the amplitude A; this, when substituted in the classical energy expression (6) together with (8), gives the quantised energy levels. Useful approximate formulae may be obtained for small k and for large k, by approximating K, E and Π suitably in terms of series expansions, but we do not consider them here. Equation (10) could be used conveniently for numerical computations.

Finally, we remark that the limiting forms of spherical harmonic and linear anharmonic oscillators are obtained as follows.

(i) *Spherical harmonic oscillator limit*

In this case $k^2 \to 0$. Correspondingly we have

$$K \to \tfrac{1}{2}\pi(1+\tfrac{1}{4}k^2), \qquad E \to \tfrac{1}{2}\pi(1-\tfrac{1}{4}k^2) \tag{12}$$

and

$$\Pi(\tfrac{1}{2}\pi, \alpha^2) \to \tfrac{1}{2}\pi(1-\alpha^2)^{-1/2}. \tag{13}$$

Also we have $\beta^2 \to (1-C_2^2/\omega^2A^4)$. Thus equation (10) becomes

$$\tfrac{1}{2}m\gamma A^2(2-\beta^2) = mC_2+(2n+1)\hbar. \tag{14a}$$

Now substituting the limiting forms for γ and β and making use of equation (6), we finally obtain

$$\mathscr{E} = (2n+l+\tfrac{3}{2})\hbar\omega. \tag{14b}$$

(ii) *Linear anharmonic oscillator limit*

Here $C_2^2 \to 0$, $\beta \to 1$ and, further, the range is twice that of the radial case. Correspondingly, equation (10) gives

$$(4m\gamma A^2/3k^2)[k'^2K-(1-2k^2)E] = (n+\tfrac{1}{2})h, \tag{15}$$

in agreement with the unpublished results of M Lakshmanan, F Karlsson and P O

Fröman (Phase Integral Calculations for the Energy Levels of an Anharmonic Oscillator).

The above results on the spherical anharmonic oscillator could be obtained as the first-order result of the systematic higher-order phase-integral calculations of Fröman and Fröman (1974). In a subsequent paper, we will report the higher-order (up to $2N+1=5$) phase-integral results.

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