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Analytic WKB energy expressions for three-dimensional anharmonic oscillators

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Abstract. A direct evaluation of the lowest-order WKB integral for three-dimensional quartic ($V(r) = r^4$) and quartic anharmonic ($V(r) = \frac{1}{2}\omega^2 r^2 + \lambda r^4$) oscillators is carried out. The highly implicit relation for the energy defined by the WKB quantisation condition is expressed in terms of complete elliptic integrals. An approximate non-perturbative inversion of the implicit relation provides explicit analytic expressions for the energy which reproduce known energy values quite accurately. This study is believed to be the first to give explicit energy expressions via the WKB method for three-dimensional anharmonic oscillators.

1. Introduction

The study of one- and three-dimensional quantum anharmonic oscillators (AHO) is of considerable interest in view of the importance of these systems in quantum field theory and chemical physics. Very extensive literature is already available on the one-dimensional AHO (Bazley and Fox 1961, Bender and Wu 1969, Biswas *et al* 1971, 1973, Caswell 1979, Halliday and Suranyi 1980, Hioe and Montroll 1975, Hioe *et al* 1976, Loeffel *et al* 1969, Banerjee 1978, Banerjee *et al* 1978, Richardson and Blankenbecler 1979, Blankenbecler *et al* 1980, Killingbeck 1981, Mathews *et al* 1981a, b). In particular Mathews *et al* (1981a, b) have given a simple formula for the energy levels of one-dimensional AHO which works quite well. Hioe and Montroll (1975) and Hioe *et al* (1976) have discussed analytic approximations to the energy values $\mathscr{E}_n(\lambda)$ for large n and/or λ in the case of one-dimensional oscillators characterised by the potential $V(x) = \omega^2 x^2 + \lambda x^{2\alpha}$. More recently, Bender *et al* (1977) have computed WKB expressions for $\mathscr{E}_n(\lambda)$ to high order, while Lakshmanan *et al* (1981) have worked out higher-order phase integrals for computing energies.

In contrast to the one-dimensional case, relatively little information is available in the literature on the physically more interesting three-dimensional AHO. Bell *et al* (1970a, b) have computed the first 50 or so eigenvalues by numerically diagonalising matrices of large dimensions. Mathews *et al* (1982) have presented a very simple analytic formula for the energies of quartic and quartic anharmonic oscillators which reproduces the known energy values quite well with a few parameters. Lakshmanan and Kaliappan (1980) have carried out a Bohr–Sommerfeld quantisation (with the radial quantum number n_r replaced by $n_r + \frac{1}{2}$)†. Their somewhat complicated looking

† A factor of 2 is found to be missing in their implicit relation for the energy.

formula (which could be simplified further) is a highly implicit relation for $\mathscr{E}_n(\lambda)$, and no attempt has been made by them to obtain even approximate explicit expressions for $\mathscr{E}_n(\lambda)$. Pasupathy and Singh (1981) have formulated an exact quantisation condition (generalising the WKB condition) for any central potential, but its applicability is limited to s waves only. Rather surprisingly, there does not seem to be available in the literature any formula for $\mathscr{E}_n(\lambda)$ obtained by evaluating the WKB integral directly for the three-dimensional AHO.

In this paper we evaluate directly the lowest-order WKB integral for the anharmonic oscillator specified by $V(r)=\frac{1}{2}\omega^2r^2+\lambda r^4$ in terms of complete elliptic integrals. (The pure quartic oscillator results follow trivially by setting $\omega^2=0$.) The WKB quantisation condition defines the allowed energies $\mathscr{E}_n(\lambda)$ implicitly through the elliptic integrals. We demonstrate how an explicit analytic inversion can be carried out, and $\mathscr{E}_n(\lambda)$ obtained, by expanding the elliptic integrals about values (of their arguments) which depend on n_r and l. It will be seen that our non-perturbative inversion procedure works very well and gives quite accurate results.

The paper is organised as follows. In the next section the WKB integral for the potential $V(r)=\frac{1}{2}\omega^2r^2+\lambda r^4$, is evaluated. In § 3 the inversion procedure is described first for the simple case of the pure quartic oscillator ($\omega^2=0$), and an accurate analytic formula for the energy from the WKB expression obtained. The formulae for the more involved case of $\omega^2\neq 0$ are then presented. In the final section the results are discussed.

2. Evaluation of the WKB integral

For a particle of unit mass moving in the central potential

$$V(r)=\tfrac{1}{2}\omega^2r^2+\lambda r^4 \tag{1}$$

the WKB quantisation condition for allowed energy values $\mathscr{E}$ is (with $\hbar=1$) (Landau and Lifschitz 1977)

$$(n_r+\tfrac{1}{2})\pi=\int_{r_1}^{r_2}\sqrt{2}\left(\mathscr{E}-\tfrac{1}{2}\omega^2r^2-\lambda r^4-\frac{(l+\frac{1}{2})^2}{2r^2}\right)^{1/2}\mathrm{d}r \tag{2}$$

where $r_1>0$ and $r_2>0$ are the two classical turning points determined by

$$\mathscr{E}-\tfrac{1}{2}\omega^2r^2-\lambda r^4-\frac{(l+\frac{1}{2})^2}{2r^2}=0 \tag{3}$$

and n_r and l are non-negative integers. To solve (3) let us change variables:

$$y=r^2. \tag{4}$$

We then obtain

$$y^3+\frac{\omega^2}{2\lambda}y^2-\frac{\mathscr{E}}{\lambda}y+\frac{(l+\frac{1}{2})^2}{2\lambda}=0. \tag{5}$$

The roots of this cubic equation (denoted a, b, c) are

$$\begin{aligned}
a&=-\omega^2/6\lambda+2\sqrt{\tfrac{1}{3}A}\cos\tfrac{1}{3}\phi\\
b&=-\omega^2/6\lambda+2\sqrt{\tfrac{1}{3}A}\cos(\tfrac{1}{3}\phi+\tfrac{4}{3}\pi)\\
c&=-\omega^2/6\lambda+2\sqrt{\tfrac{1}{3}A}\cos(\tfrac{1}{3}\phi+\tfrac{2}{3}\pi)
\end{aligned} \tag{6}$$

where

$$A=\frac{1}{\lambda}\left(\mathscr{E}+\frac{\omega^4}{12\lambda}\right) \tag{7a}$$

and

$$\cos\phi=-\frac{3\sqrt{3\lambda}}{4}\frac{[(l+\frac{1}{2})^2+\mathscr{E}\omega^2/3\lambda+\omega^6/54\lambda^2]}{(\mathscr{E}+\omega^4/12\lambda)^{3/2}} \tag{7b}$$

with $\frac{1}{2}\pi\leqslant\phi\leqslant\pi$. It is not difficult to verify that the roots are real in the WKB regime and satisfy the relations

$$a>b>0 \tag{8a}$$

$$c<0. \tag{8b}$$

Equation (2) can now be rewritten in terms of a, b, c as

$$(n_r+\tfrac{1}{2})\pi=-\sqrt{\tfrac{1}{2}\lambda}\int_b^a\frac{[y^2+\omega^2y/2\lambda-\mathscr{E}/\lambda+(l+\frac{1}{2})^2/2\lambda y]}{[(a-y)(y-b)(y-c)]^{1/2}}\,\mathrm{d}y.$$

The integral on the RHS of this equation can be expressed in terms of complete elliptic integrals, and we obtain, after some algebra,

$$\begin{aligned}(n_r+\tfrac{1}{2})\pi=(g/\sqrt{2\lambda})\{[\tfrac{2}{3}\mathscr{E}-(l+\tfrac{1}{2})^2/2c-\tfrac{1}{6}\omega^2c]K(k)-\tfrac{1}{6}\omega^2(a-c)E(k)\\+\tfrac{1}{2}(l+\tfrac{1}{2})^2(c^{-1}-b^{-1})\Pi(\alpha^2,k)\}\end{aligned} \tag{9}$$

where K, E and Π are complete elliptic integrals of the first, second and third kinds respectively in the notation of Byrd and Friedman (1971). The quantities k, α^2 and g are defined by

$$\begin{aligned}k^2&=(a-b)/(a-c)\\ \alpha^2&=ck^2/b\\ g&=2/\sqrt{a-c}.\end{aligned} \tag{10}$$

We note that $0<k^2<1$ and $\alpha^2<0$.

Equation (9) defines the energy $\mathscr{E}$ implicitly. Values of $\mathscr{E}$ for given λ, ω, n_r and l can always be evaluated numerically. It is of great interest to investigate whether (9) can be inverted for the energy so that one would write down an explicit formula for $\mathscr{E}$ as a function of λ, ω, n_r and l. Although exact inversion of (9) is impossible, it turns out to be quite possible (as will be shown) to carry out an approximate inversion, which not only reproduces the WKB energies surprisingly well, but also gives values quite close to those obtained by direct diagonalisation of the Hamiltonian.

3. Analytic expression for $\mathscr{E}$

3.1. *Pure quartic oscillator* ($\omega^2=0$)

To illustrate the inversion of equation (9) for $\mathscr{E}$, let us consider the case of a pure quartic oscillator. This means that $\omega^2=0$ in (1). Due to scaling one knows that for this case,

$$\mathscr{E}(\lambda)=\lambda^{1/3}\mathscr{E}(1). \tag{11}$$

Hence we can set $\lambda = 1$ without loss of generality. When $\omega^2 = 0$, the RHS of (9) simplifies and equation (9) becomes

$$(n_r + \tfrac{1}{2})\pi = (g/\sqrt{2})\{[\tfrac{2}{3}\mathscr{E} - (l+\tfrac{1}{2})^2/2c]K(k) + \tfrac{1}{2}(l+\tfrac{1}{2})^2(c^{-1} - b^{-1})\Pi\}. \qquad (9')$$

Also A and $\cos\phi$ in equation (7) become

$$A = \mathscr{E} \qquad \cos\phi = -\tfrac{3}{4}\sqrt{3}(l+\tfrac{1}{2})^2/\mathscr{E}^{3/2}. \qquad (7')$$

Consider first the limit

$$(l+\tfrac{1}{2})^2/\mathscr{E}^{3/2} \equiv \delta \ll 1. \qquad (12)$$

It is easy to see that in this limit

$$\begin{aligned} &a \simeq \sqrt{\mathscr{E}}(1-\tfrac{1}{2}\delta) \qquad b \simeq \sqrt{\mathscr{E}}\delta \qquad c \simeq -\sqrt{\mathscr{E}}(1+\tfrac{1}{2}\delta) \\ &k^2 \simeq \tfrac{1}{2}(1-\tfrac{3}{2}\delta) \qquad \alpha^2 \simeq -1/2\delta \qquad g \simeq \sqrt{2}\mathscr{E}^{1/4} \\ &K(k) \simeq K(\sqrt{\tfrac{1}{2}}) - \tfrac{3}{2}[E(\sqrt{\tfrac{1}{2}}) - \tfrac{1}{2}K(\sqrt{\tfrac{1}{2}})]\delta \qquad \Pi(\alpha^2, k) \simeq \pi\sqrt{\tfrac{1}{2}\delta}. \end{aligned} \qquad (13)$$

Substituting these values in (9′) and simplifying, we obtain

$$(n_r + \tfrac{1}{2})\pi = \mathscr{E}^{3/4}\{\tfrac{2}{3}K(\sqrt{\tfrac{1}{2}}) - \tfrac{1}{2}\pi(l+\tfrac{1}{2})/\mathscr{E}^{3/4} + [\tfrac{3}{4}K(\sqrt{\tfrac{1}{2}}) - \tfrac{1}{2}E(\sqrt{\tfrac{1}{2}})](l+\tfrac{1}{2})^2/\mathscr{E}^{3/2}\}. \qquad (14)$$

Solving this quadratic equation (in $\mathscr{E}^{3/4}$), we readily get

$$\mathscr{E} = \left(\frac{3\pi(n+\tfrac{3}{2})}{4K(\sqrt{\tfrac{1}{2}})}\right)^{4/3}\left(1 - \frac{4K(\sqrt{\tfrac{1}{2}})}{3\pi^2}[\tfrac{3}{2}K(\sqrt{\tfrac{1}{2}}) - E(\sqrt{\tfrac{1}{2}})]\frac{(l+\tfrac{1}{2})^2}{(n+\tfrac{3}{2})^2}\right)^{4/3} \qquad (15)$$

where†

$$n = 2n_r + l. \qquad (16)$$

With regard to the above expression for $\mathscr{E}$, we may observe the following. First of all, it is to be noted that

$$K(\sqrt{\tfrac{1}{2}}) = \frac{\sqrt{\pi}\Gamma(\tfrac{1}{4})}{2\sqrt{2}\Gamma(\tfrac{3}{4})} = 1.854\,075 \qquad (17a)$$

and then by Legendre's relation

$$E(\sqrt{\tfrac{1}{2}}) = \tfrac{1}{2}K(\sqrt{\tfrac{1}{2}}) + \frac{\pi}{4K(\sqrt{\tfrac{1}{2}})} = 1.350\,644. \qquad (17b)$$

Then using (17) the coefficient of the leading term can be written as

$$C \equiv \left(\frac{3\pi}{4K(\sqrt{\tfrac{1}{2}})}\right)^{4/3} = \left(\frac{3\sqrt{\pi}\Gamma(\tfrac{3}{4})}{\sqrt{2}\Gamma(\tfrac{1}{4})}\right)^{4/3} = 1.376\,507. \qquad (18)$$

Our leading term for $\mathscr{E}$ (namely $C(n+\tfrac{3}{2})^{4/3}$) coincides with that given by Quigg and Rosner (1979). They state that in the WKB regime the correct quantisation variable is neither n_r nor l but only $2n_r + l$, since the leading term contains n_r and l only in the combination $2n_r + l$. But when corrections to the leading term are taken into account, $\mathscr{E}$ exhibits a fine structure due to its dependence on l also, as seen from (15). The value of

† The relationship between n and n_r is exactly the same as that obtained in the case of the isotropic harmonic oscillator. We note also that equation (16) shows that for a given n, l can take only the values $n, n-2, \ldots, 1$ or 0 depending on whether n is odd or even.

the constant C given in (18) is exactly the same as that in the one-dimensional case. In fact by setting $l+\frac{1}{2}=0$, and writing $N=n+1=2n_r+1=1, 3, 5, \ldots$, we recover the WKB formula for the one-dimensional quartic oscillator†.

The energy values given by (15) are satisfactory for small l. For instance, for $n=49$, $l=1$, we find $\mathscr{E}=256.833$, which agrees quite well with the value $\mathscr{E}=256.909$ obtained by numerical solution of equation (9′). But as the value of l is increased, $\mathscr{E}$ calculated using (15) deviates more and more from the numerical solution of (9′). For $n=100$, $l=40$, (15) gives $\mathscr{E}=602.16$, whereas the numerical solution of (9′) is $\mathscr{E}=637.17$. Such large discrepancies are not surprising, since the basic condition for the validity of (15) ($\delta \ll 1$) is not satisfied for large values of l such as that in the second example above. It is therefore desirable to devise a better approximation to $\mathscr{E}$ than (15) that will agree well with numerical solutions to $\mathscr{E}$ for large values of l as well as small.

To this end, let us suppose that $\mathscr{E}$ can be written as

$$\mathscr{E}=\mathscr{E}_0(1+x) \qquad |x| \ll 1 \tag{19}$$

where $\mathscr{E}_0$ is the leading approximation to $\mathscr{E}$ in (15):

$$\mathscr{E}_0=C(n+\tfrac{3}{2})^{4/3}. \tag{20}$$

To obtain an explicit expression for x, we expand all quantities on the RHS of equation (9′) to order x and collect terms. Since the LHS is independent of x, we immediately get x on equating the two sides. Substituting (19) and (20) in (7′) we find

$$\cos\phi=-\tfrac{3}{4}\sqrt{3}\mu(1-\tfrac{3}{2}x)$$

where

$$\mu=\frac{1}{C^{3/2}}\left(\frac{l+\frac{1}{2}}{n+\frac{3}{2}}\right)^2. \tag{21}$$

To order x we can then solve for ϕ, and we obtain

$$\phi \simeq \tfrac{1}{2}\pi+\theta-(\tfrac{1}{2}\tan\theta)x \tag{22}$$

with

$$\theta=\sin^{-1}\tfrac{3}{4}\mu\sqrt{3} \tag{23}$$

Using (22) we can evaluate a, b, c:

$$a \simeq a_0+a_1x \equiv 2\sqrt{\tfrac{1}{3}\mathscr{E}_0}\cos(\tfrac{1}{6}\pi+\tfrac{1}{3}\theta)+\sqrt{\tfrac{1}{3}\mathscr{E}_0}\,\frac{\cos(\frac{1}{6}\pi-\frac{2}{3}\theta)}{\cos\theta}x \tag{24a}$$

$$b \simeq b_0+b_1x \equiv 2\sqrt{\tfrac{1}{3}\mathscr{E}_0}\sin\tfrac{1}{3}\theta-\sqrt{\tfrac{1}{3}\mathscr{E}_0}\,\frac{\sin\frac{2}{3}\theta}{\cos\theta}x \tag{24b}$$

$$c \simeq c_0+c_1x \equiv -2\sqrt{\tfrac{1}{3}\mathscr{E}_0}\cos(\tfrac{1}{6}\pi-\tfrac{1}{3}\theta)-\sqrt{\tfrac{1}{3}\mathscr{E}_0}\,\frac{\cos(\frac{1}{6}\pi+\frac{2}{3}\theta)}{\cos\theta}x. \tag{24c}$$

These lead to the following values for k^2, α^2 and g:

$$k^2=\frac{a-b}{a-c} \simeq k_0^2+k_1^2x \cong \frac{\cos(\frac{1}{3}\pi+\frac{1}{3}\theta)}{\cos\frac{1}{3}\theta}+\frac{\sqrt{3}\tan\theta}{4\cos^2\frac{1}{3}\theta}x \tag{25}$$

† This is not surprising in view of the well known result that $l=0$ levels in a spherically symmetric potential are the same as the odd parity (odd N) levels of the one-dimensional system with the same potential.

$$\alpha^2 = \frac{ck^2}{b} \simeq \alpha_0^2 + \alpha_1^2 x \equiv -\frac{\sin(\frac{2}{3}\pi + \frac{2}{3}\theta)}{\sin\frac{2}{3}\theta} - \frac{\sqrt{3}\tan\theta}{2\sin^2\frac{2}{3}\theta}x \tag{26}$$

$$g = \frac{2}{\sqrt{a-c}} \simeq g_0 + g_1 x \equiv \frac{\sqrt{2}}{\mathscr{E}_0^{1/4}(\cos\frac{1}{3}\theta)^{1/2}}\left(1 - \frac{\cos\frac{2}{3}\theta}{4\cos\frac{1}{3}\theta\cos\theta}x\right). \tag{27}$$

We now expand the elliptic integrals around k_0^2 and α_0^2, and obtain

$$\begin{aligned} K(k^2) &\simeq K(k_0^2) + \left.\frac{dK}{dk^2}\right|_{k_0^2} k_1^2 x \\ &= K_0 + \frac{k_1^2[E_0 - (1-k_0^2)K_0]x}{2k_0^2(1-k_0^2)} \\ &\equiv K_0 + K_1 x \end{aligned} \tag{28a}$$

$$\begin{aligned} E(k^2) &\simeq E(k_0^2) + \left.\frac{dE}{dk^2}\right|_{k_0^2} k_1^2 x \\ &= E_0 + \frac{k_1^2(E_0 - K_0)}{2k_0^2}x \\ &\equiv E_0 + E_1 x \end{aligned} \tag{28b}$$

$$\begin{aligned} \Pi(\alpha^2, k) &\simeq \Pi(\alpha_0^2, k_0) + \left(\left.\frac{\partial\Pi}{\partial\alpha^2}\right|_0 \alpha_1^2 + \left.\frac{\partial\Pi}{\partial k^2}\right|_0 k_1^2\right)x \\ &= \Pi_0 + \left(\frac{[\alpha_0^2 E_0 + (k_0^2 - \alpha_0^2)K_0 + (\alpha_0^4 - k_0^2)\Pi_0]\alpha_1^2}{2\alpha_0^2(1-\alpha_0^2)(\alpha_0^2 - k_0^2)} + \frac{[E_0 - (1-k_0^2)\Pi_0]k_1^2}{2(1-k_0^2)(k_0^2-\alpha_0^2)}\right)x \\ &\equiv \Pi_0 + \Pi_1 x \end{aligned} \tag{28c}$$

where

$$K_0 = K(k_0^2) \qquad E_0 = E(k_0^2) \qquad \Pi_0 = \Pi(\alpha_0^2, k_0).$$

Putting the above expressions in equation (9′) and rearranging terms we obtain the following expression for x

$$x = N/D \tag{29}$$

with

$$N = \frac{(n_r + \frac{1}{2})\pi\sqrt{2}}{g_0} - \left(\tfrac{2}{3}\mathscr{E}_0 + \frac{(l+\frac{1}{2})^2}{2c_0}\right)K_0 - \frac{(l+\frac{1}{2})^2}{2b_0c_0}(b_0 - c_0)\Pi_0 \tag{30a}$$

and

$$\begin{aligned} D = {} & \left[\tfrac{2}{3}\mathscr{E}_0\left(1 + \frac{g_1}{g_0}\right) + \frac{(l+\frac{1}{2})^2}{2c_0}\left(\frac{c_1}{c_0} - \frac{g_1}{g_0}\right)\right]K_0 + \left(\tfrac{2}{3}\mathscr{E}_0 - \frac{(l+\frac{1}{2})^2}{2c_0}\right)K_1 \\ & - \frac{(l+\frac{1}{2})^2}{2b_0c_0}\left(\frac{b_0^2c_1 - c_0^2b_1}{b_0c_0} + \frac{g_1}{g_0}(c_0 - b_0)\right)\Pi_0 - \frac{(l+\frac{1}{2})^2}{2b_0c_0}(c_0 - b_0)\Pi_1. \end{aligned} \tag{30b}$$

In terms of μ and θ, N and D are given by

$$N = \frac{\pi}{2}\frac{\sqrt{\cos\frac{1}{3}\theta}}{C^{3/4}}(1 - C^{3/4}\sqrt{\mu}) - \frac{2}{3}\left(1 + \frac{3\sqrt{3}\mu}{8\cos(\frac{1}{6}\pi - \frac{1}{3}\theta)}\right)K_0 + \frac{3\mu\sin(\frac{1}{6}\pi + \frac{1}{3}\theta)}{4\sin\frac{1}{3}\theta\cos(\frac{1}{6}\pi - \frac{1}{3}\theta)}\Pi_0 \tag{31a}$$

and

$$D=\left[\frac{2}{3}\left(1-\frac{\cos\frac{2}{3}\theta}{4\cos\frac{1}{3}\theta\cos\theta}\right)-\frac{\sqrt{3}\mu[\sin(\frac{1}{6}\pi-\frac{1}{3}\theta)+\cos\frac{2}{3}\theta/4\cos\frac{1}{3}\theta]}{4\cos\theta\cos(\frac{1}{6}\pi-\frac{1}{3}\theta)}\right]K_0$$

$$+\frac{2}{3}\left(1+\frac{3\sqrt{3}\mu}{8\cos(\frac{1}{6}\pi-\frac{1}{3}\theta)}\right)K_1-\frac{3\mu}{4\sin\frac{1}{3}\theta\cos(\frac{1}{6}\pi-\frac{1}{3}\theta)}$$

$$\times\left[\frac{1}{2\cos\theta}\left(1-\frac{\sin(\frac{1}{6}\pi+\frac{1}{3}\theta)\cos\frac{2}{3}\theta}{2\cos\frac{1}{3}\theta}\right)\Pi_0+\sin(\tfrac{1}{6}\pi+\tfrac{1}{3}\theta)\Pi_1\right]. \tag{31b}$$

For small $\mu\,(\mu \ll 1)$, $\mathscr{E}_0(1+x)$ obtained from (30) is identical to the $\mathscr{E}$ given by (15).

Our formula for finding $\mathscr{E}$ is defined by equations (29) and (31). We note that once l and n are specified, N and D can be easily evaluated using standard tables of elliptic integrals. (For numerical values of elliptic integrals, see Belyakov *et al* (1965).) Over wide ranges of n and l values we have calculated $\mathscr{E}$ by the above method. We find that these values agree exceedingly well with the numerical solution of equation (9′) obtained by the standard half-interval method (Carnahan *et al* 1969). The results are presented in table 1, where $\mathscr{E}_{\text{WKB}}$ stands for the values obtained by numerically solving (9′), and $\mathscr{E}_{\text{exact}}$ for the very accurate values of Mathews *et al* (1981c).

Table 1. Comparison of $\mathscr{E}_0(1+x)$ with WKB and exact energy eigenvalues for three-dimensional quartic oscillator.

n	l	$\mathscr{E}_0(1+x)$ (equation (29))	$\mathscr{E}_{\text{WKB}}$ (as obtained by numerical solution of equation (9′))	$\mathscr{E}_{\text{exact}}$ (Mathews *et al* 1981c)
100	0	651.718	651.718	651.731
	50	629.105	629.190	629.194
	100	564.405	565.342	565.344
50	0	263.744	263.744	263.751
	20	257.868	257.883	257.890
	50	229.066	229.433	229.437
10	0	35.721	35.721	35.740
	4	34.960	34.963	34.980
	10	31.639	31.679	31.691
0	0	2.327	2.327	2.394

It must be noted that in equation (31) the elliptic integrals and their derivatives are to be computed at values which are explicitly dependent on n and l. It is this feature that accounts for the success of the method.

Special case: One-dimensional pure quartic oscillator. If we set $(l+\frac{1}{2})^2=0$ in (31), we find that $N=0$ but $D\neq 0$. Therefore $x=0$, and

$$\mathscr{E}=\mathscr{E}_0=C(n+\tfrac{3}{2})^{4/3}=C[(2n_r+1)+\tfrac{1}{2}]^{4/3}$$
$$=C(n'+\tfrac{1}{2})^{4/3}.$$

This is in agreement with known results (Hioe and Montroll 1975).

3.2. Anharmonic oscillator

The above analysis can be extended in a straightforward manner to the case $\omega^2 \neq 0$. To save space we shall give only the final expression for x, just indicating the necessary modifications and omitting the details. For this case we should write

$$\mathscr{E} = \mathscr{E}_0(1+x) \qquad |x| \ll 1$$

where

$$\mathscr{E}_0 = C(n+\tfrac{3}{2})^{4/3}\lambda^{1/3}. \tag{32}$$

To order x the roots a, b, c given by (6) are

$$a \simeq a_0 + a_1 x \equiv -\omega^2/6\lambda + 2\sqrt{\tfrac{1}{3}F_0}\cos(\tfrac{1}{6}\pi + \tfrac{1}{3}\theta) + \sqrt{\tfrac{1}{3}F_0}\,\frac{\sigma x}{\cos\psi}\cos(\tfrac{1}{6}\pi + \tfrac{1}{3}\theta - \psi) \tag{33a}$$

$$b \simeq b_0 + b_1 x \equiv -\omega^2/6\lambda + 2\sqrt{\tfrac{1}{3}F_0}\sin\tfrac{1}{3}\theta - \sqrt{\tfrac{1}{3}F_0}\,\frac{\sigma x}{\cos\psi}\sin(\psi - \tfrac{1}{3}\theta) \tag{33b}$$

$$c \simeq c_0 + c_1 x \equiv -\omega^2/6\lambda - 2\sqrt{\tfrac{1}{3}F_0}\cos(\tfrac{1}{6}\pi - \tfrac{1}{3}\theta) - \sqrt{\tfrac{1}{3}F_0}\,\frac{\sigma x}{\cos\psi}\cos(\tfrac{1}{6}\pi - \tfrac{1}{3}\theta + \psi). \tag{33c}$$

Here

$$F_0 = \lambda^{-1}(\mathscr{E}_0 + \omega^4/12\lambda) \qquad \sigma = \mathscr{E}_0/\lambda F_0 \tag{34a}$$

$$\theta = \sin^{-1}\left[\frac{3\sqrt{3}}{4\lambda}F_0^{-3/2}\left((l+\tfrac{1}{2})^2 + \frac{\mathscr{E}_0\omega^2}{3\lambda} + \frac{\omega^6}{54\lambda^2}\right)\right] \tag{34b}$$

and ψ is defined by

$$\tan\psi = (\beta/\sigma)\tan\theta \tag{34c}$$

where

$$\beta = \frac{6\mathscr{E}_0[\mathscr{E}_0\omega^2 + 9\lambda(l+\tfrac{1}{2})^2]}{F_0[54\lambda^2(l+\tfrac{1}{2})^2 + 18\lambda\mathscr{E}_0\omega^2 + \omega^6]}. \tag{34d}$$

Once a, b, c are known, all other required quantities can be calculated (to order x). Proceeding as before we get

$$x = N/D \tag{35}$$

with

$$N = \sqrt{\tfrac{1}{2}\lambda}[(n+\tfrac{3}{2}) - (l+\tfrac{1}{2})]\pi/g_0 - [\tfrac{2}{3}\omega\mathscr{E}_0 - (l+\tfrac{1}{2})^2/2c_0 - \tfrac{1}{6}\omega^2 c_0]K_0 + \tfrac{1}{6}\omega^2(a_0 - c_0)E_0 - \tfrac{1}{2}(l+\tfrac{1}{2})^2(c_0^{-1} - b_0^{-1})\Pi_0 \tag{36a}$$

and

$$\begin{aligned} D = {} & \left[\frac{2}{3}\mathscr{E}_0\left(1 + \frac{g_1}{g_0}\right) + \frac{(l+\frac{1}{2})^2}{2c_0}\left(\frac{c_1}{c_0} - \frac{g_1}{g_0}\right) - \frac{\omega^2}{6}\left(c_1 + \frac{g_1}{g_0}c_0\right)\right]K_0 \\ & + \left(\frac{2}{3}\mathscr{E}_0 - \frac{(l+\frac{1}{2})^2}{2c_0} - \frac{\omega^2 c_0}{6}\right)K_1 - \frac{\omega^2}{6}\left((a_1 - c_1) + \frac{g_1}{g_0}(a_0 - c_0)\right)E_0 \\ & - \frac{\omega^2}{6}(a_0 - c_0)E_1 - \frac{(l+\frac{1}{2})^2}{2c_0 b_0}\left(\frac{(b_0^2 c_1 - c_0^2 b_1)}{b_0 c_0} + (c_0 - b_0)\frac{g_1}{g_0}\right)\Pi_0 \\ & - \frac{(l+\frac{1}{2})^2}{2c_0 b_0}(c_0 - b_0)\Pi_1 \end{aligned} \tag{36b}$$

where K_0, K_1 etc are defined as in (28). It is easily verified that in the pure quartic oscillator ($\omega^2 = 0$) limit, the above expressions reduce to those in (30).

We have evaluated x for several n, l and λ, and find that the energy $\mathscr{E}_0(1+x)$ agrees very well with the values obtained by numerical solution of equation (9) for $\mathscr{E}$. The values given in table 2 for the case $\lambda = 0.5$ are typical of the results obtained.

Table 2. Comparison of $\mathscr{E}_0(1+x)$ with WKB and exact energy eigenvalues for three-dimensional anharmonic oscillator with $\omega^2 = 1$ and $\lambda = 0.5$.

n	l	$\mathscr{E}_0(1+x)$ (equation (35))	$\mathscr{E}_{\mathrm{WKB}}$ (as obtained by numerical solution of equation (9))	$\mathscr{E}_{\mathrm{exact}}$ (Mathews *et al* 1981c)
100	0	524.581	524.594	524.604
	50	507.043	507.065	507.068
	100	456.716	457.284	457.286
50	0	213.973	213.986	213.991
	20	209.477	209.477	209.482
	50	187.340	187.526	187.530
10	0	30.038	30.050	30.065
	4	29.492	29.497	29.510
	10	27.078	27.083	27.092
0	0	2.267	2.275	2.324

Special case. One-dimensional anharmonic oscillator. By setting $(l+\frac{1}{2})^2 = 0$ we can readily obtain the expression for x for the case of one-dimensional AHO. We note that in this limit the term containing the elliptic integral of the third kind drops out. Since our method involves expanding the elliptic integrals about values of the modulus k^2 which are dependent on n, our expression for $\mathscr{E}$ should be better than the ones given in the literature (which arise as a result of expanding around $k^2 = \frac{1}{2}$ which in turn corresponds to the limit $n \to \infty$).

4. Discussion

In this work we have shown that it is straightforward to evaluate the (lowest-order) WKB integral directly for the three-dimensional quartic AHO. The WKB quantisation condition requires that a highly complicated function of $\mathscr{E}$, l and λ (occurring through arguments of elliptic integrals) be equal to $(n_r + \frac{1}{2})\pi$. We have demonstrated how it is possible to carry out an approximate non-perturbative inversion for expressing $\mathscr{E}$ as a function of n, l and λ. The values of $\mathscr{E}$ obtained from the approximate inversion for the pure quartic and quartic anharmonic oscillators are given in tables 1 and 2. For checking the accuracy, we have also numerically solved (9) with $\omega^2 = 0$ and $\omega^2 = 1$ and these values are presented in tables as $\mathscr{E}_{\mathrm{WKB}}$. It is easily checked that the two sets of values are quite close to each other thereby showing that our formula represents an accurate inversion for the energy values. We have in fact tested our formula over wide ranges of values of λ (0.1 to 50), n (10 to 500) and several values of l for each n and found it to be very satisfactory. The percentage error of the energy values calculated from the formula as compared to numerical solution given in tables 1 and 2 is not more than 0.2%. As the lowest-order WKB quantisation itself is an approximation to exact energy levels of the AHO, one may be curious to compare $\mathscr{E}_{\mathrm{WKB}}$ with $\mathscr{E}_{\mathrm{exact}}$. While Bell *et al* (1970b) have calculated a few energy levels exactly, a systematic evaluation of $\mathscr{E}_{\mathrm{exact}}$ to high accuracy (1 part in 10^{15}) for arbitrary values of n and l has been recently carried out by Mathews *et al* (1981c). Their values are also given in tables 1 and 2 as $\mathscr{E}_{\mathrm{exact}}$. A few observations on the numbers given in the tables are in order. We observe that for given n, and λ, $\mathscr{E}$ decreases as l increases. The difference $\mathscr{E}(l=0)-\mathscr{E}(l)$ is roughly proportional to $l(l+1)$ as already noted by Bell *et al.* In analogy with one-dimensional WKB results, one would expect that for fixed l the WKB expression would become more and more accurate as n_r (representing the nodes in the radial wavefunction) increases. Surprisingly even for the smallest values of $n_r=0$ (as happens whenever $n=2n_r+l=l$), the WKB expression yields quite good results. On the other hand, it is as n decreases that the WKB results start deviating from the exact ones. It is amusing that even for the ground state the WKB result is in error only by about 3%. Finally we should like to emphasise that in view of the quite satisfactory results given by our formula, it can be used as a starting point in various types of numerical schemes intended for very accurate evaluation of eigenvalues (particularly for large n, and λ).

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