WKBJ Calculation of the Energy Levels of an Anquartic Potential

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A new anquartic potential is proposed. The pattern of its eigenvalues is calculated by using the four-term WKBJ approximation. The results are shown graphically and are compared with those found for another anquartic potential studied in a previous paper.

In a previous paper [1] we have considered the potential

$$V(r) = D[\{(r_e/r)^m - 1\}^4 - 1], \tag{1}$$

where D is the well depth, r_e the equilibrium interparticle distance and m a constant, which for convenience may be taken to be an integer. This potential has the interesting property that its first three derivatives all vanish at $r = r_e$. The leading term in the Taylor expansion in powers of $(r - r_e)$ is the quartic term. We calculated the pattern of the eigenvalues for potential (1) and also the number of bound vibrational states as a function of a dimensionless parameter η, which depends on D and r_e.

In the present note we examine the potential

$$V(r) = D[\{1 - e^{-\alpha(r - r_e)}\}^4 - 1], \tag{2}$$

where D is the well depth and α a constant. The potential (2) belongs to the same class as the potential (1) in that its first three derivatives vanish at $r = r_e$. It was of interest to examine the pattern of energy eigenvalues for potential (2) and to compare the results with those obtained from potential (1). We calculate the energy eigenvalues for potential (2) by the four-term WKBJ approximation. We also determine the number of vibrational levels that potential (2) can support.

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The quantization condition in the four-term WKBJ approximation can be written as [2, 3]

$$n + \tfrac{1}{2} = I_1 + I_2 + I_3 + I_4, \tag{3}$$

where the I_j's are defined in [3].

The integral I_1 with $V(r)$ from (2) is

$$I_1 = \frac{(2\mu)^{1/2}/\hbar}{\pi} \int_{r_1}^{r_2} (E - D[\{1 - e^{-\alpha(r - r_e)}\}^4 - 1])\,\mathrm{d}r.$$

On substituting $\omega = 1 - e^{-\alpha(r - r_e)}$, and setting

$$\omega_0 = (1 + E/D)^{1/4} \quad \text{and} \quad \lambda = (2\mu D)^{1/2}/\alpha\hbar,$$

we obtain

$$\begin{aligned} I_1 &= \frac{\lambda}{\pi} \int_{-\omega_0}^{\omega_0} (\omega_0^4 - \omega^4)^{1/2} (1 - \omega)^{-1}\,\mathrm{d}\omega \\ &= \frac{2\lambda}{\pi} \int_0^{\omega_0} (\omega_0^4 - \omega^4)^{1/2} (1 - \omega^2)^{-1}\,\mathrm{d}\omega \\ &= \frac{2\lambda}{\pi\omega_0} \left[\omega_0^2 \int_0^1 \frac{z^2\,\mathrm{d}z}{(1 - z^4)^{1/2}} + \int_0^1 \frac{\mathrm{d}z}{(1 - z^4)^{1/2}} \right. \\ &\quad \left. - (1 - \omega_0^4) \int_0^1 \frac{\mathrm{d}z}{(1 - \omega_0^2 z)(1 - z^4)^{1/2}} \right]. \end{aligned}$$

The last expression is recognized as consisting of complete elliptic integrals of first, second and third kinds [4].

Thus

$$\begin{aligned} I_1 = \frac{\lambda\sqrt{2}}{\pi} &\left[2\omega_0 E(45°) - \left(\omega_0 - \frac{1}{\omega_0}\right) K(45°) \right. \\ &\left. - \left(\omega_0 + \frac{1}{\omega_0}\right) \Pi\left(- \frac{\omega_0^2}{1 - \omega_0^2} \,;\, 90° \backslash 45° \right) \right], \\ &\text{if} \quad 0 < \omega_0^2 < \tfrac{1}{2} \end{aligned} \tag{4a}$$

and

$$\begin{aligned} I_1 = \frac{\lambda\sqrt{2}}{\pi} &\left[2\omega_0 E(45°) - \omega_0(1 - \omega_0^2) \right. \\ &\left. \cdot \Pi\left(\frac{1 + \omega_0^2}{2} \,;\, 90° \backslash 45° \right) \right], \\ &\text{if} \quad \tfrac{1}{2} \leqq \omega_0^2 < 1. \end{aligned} \tag{4b}$$

In a similar manner, we obtain

$$I_2 = \frac{(4\lambda)^{-1}}{\pi\sqrt{2}\,\omega_0^3} [K(45°) - 2E(45°)], \tag{5}$$

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$$I_3 = \frac{(4\lambda)^{-3}}{6\pi\sqrt{2}\,\omega_0{}^9} \cdot [(57\,\omega_0{}^2 + 11)\,K(45°) - 114\,\omega_0{}^2\,E(45°)], \tag{6}$$

$$I_4 = \frac{(4\lambda)^{-5}}{210\pi\sqrt{2}\,\omega_0{}^{15}} \cdot [(66255\,\omega_0{}^4 + 79350\,\omega_0{}^2 - 32879) \cdot K(45°) - 14(9465\,\omega_0{}^4 - 4697) \cdot E(45°)]. \tag{7}$$

In order to establish a correspondence between the parameters occurring in potentials (1) and (2) we assume that d^4V/dr^4 should be the same at $r = r_e$ for the two potentials. This condition leads to

$$\alpha = m/r_e, \tag{8}$$

which in its turn provides the following relation between the parameters λ and η:

$$\lambda = 2\eta/m. \tag{9}$$

A choice must be made for m. The potential (2), because of the presence of the exponentials, is a short-tailed potential. On the other hand, the extent of the tail of potential (1) depends on m. When m is small, the potential (1) has a long tail and it can support a great many vibrational levels. Thus to compare the two potentials the chosen value of m should not be too small. We take $m = 4$, as for this value of m, results for the potential (1) are already available [1]. Thus

$$\lambda = \eta/2. \tag{10}$$

In [1] we have displayed results for $\eta = 50$, 25 and 15. Correspondingly here we shall take $\lambda = 25$, 12.5, and 7.5.

The energy eigenvalues were calculated by solving (3). The following series expansion for

$$\Pi(\nu;\ 90°\backslash 45°)$$

was used:

$$\Pi(\nu;\ 90°\backslash 45°) = \sum_{n=0}^{\infty} \frac{\Gamma(\frac{1}{2}+n)}{2\,\Gamma(1+n)}\,\nu^n \cdot \left\{ \sum_{s=0}^{n} \frac{\Gamma(\frac{1}{2}+s)}{\Gamma(1+s)}\,(2\nu)^{-s} \right\}. \tag{11}$$

The series expansion from which (3) is obtained is, in general, semiconvergent [5, 6]. Consequently, if in any case $|I_{j+1}/I_j|$ is greater than 1, the series in (3) has to be truncated at I_j. In actual practice, calculations were carried out in stages for one-, two-, three-, and four-term WKBJ approximations. A few cases were encountered at very low quantum numbers for which $|I_4/I_3|$ was greater than one. In such cases, only three terms were used in calculating the eigenvalue.

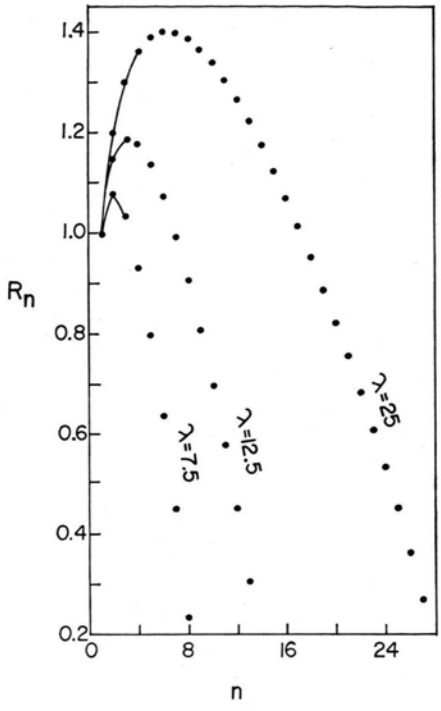

Fig. 1. The ratio R_n as a function of the quantum number n. A few of the points have been joined merely as a guide to the eye.

As before [1], we shall find it convenient to display the pattern of the spacing of the energy levels in terms of the ratio R_n defined by

$$R_n = (E_n - E_{n-1})/(E_1 - E_0). \tag{12}$$

In Fig. 1 we show R_n as a function of the quantum number n for the three chosen values of λ. The general pattern is seen to be quite similar to that found earlier [1] for the potential (1). The ratio R_n at first increases with n, reaches a maximum, and then decreases. The position of the maximum is seen to vary regularly with λ.

It will be noticed from the expressions for I_1, I_2, I_3 and I_4 that each succeeding term in the WKBJ approximation differs in order from the previous one by a factor $1/\lambda^2$. Consequently, for very small values of λ, the accuracy of eigenvalues is expected to diminish.

The potential (2) has one important advantage over potential (1) in that the expressions for I_j's

are much simpler for (2) as compared to those for (1). This means easier computation. On the other hand, the presence of the parameter m in potential (1) makes it more flexible than (2). As noted earlier, potential (1) can permit a considerable variation in the extent of the tail of the potential, while potential (2) is a short-tailed potential.

We have also calculated the number of vibrational states which the potential (2) can support as a function of the parameter λ. It was found that the number of vibrational states is almost a linear function of λ, except when λ is quite small.

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[1] R. N. Kesarwani and Y. P. Varshni, Z. Naturforsch. **33a**, 1581 (1978).
[2] R. N. Kesarwani and Y. P. Varshni, Can. J. Phys. **58**, 363 (1980).
[3] R. N. Kesarwani and Y. P. Varshni, J. Math. Phys. **21**, 90 (1980); **21**, 2852 (1980).
[4] M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions, Dover, New York 1965.
[5] G. D. Birkhoff, Bull. Amer. Math. Soc. **39**, 696 (1933).
[6] E. C. Kemble, The Fundamental Principles of Quantum Mechanics, Dover, New York 1958; this is a reprint of the 1937 edition published by McGraw-Hill.