Two-well oscillator

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Very accurate eigenvalues of the two-well oscillator ($H(k,\lambda) = p^2 - kx^2 + \lambda x^4$) are obtained by a nonperturbative method. The splitting between the pairs of lower eigenvalues is found to be remarkably well estimated by the WKB approximation. It is observed that the scaling properties of the exact eigenvalues with respect to the parameters in the Hamiltonian are retained in the WKB approximation.

I. INTRODUCTION

Anharmonic oscillators with nearly degenerate lowest states are receiving a considerable amount of attention.[1,2] The most studied among these is the two-well oscillator described by the Hamiltonian $H(k,\lambda) = p^2 - kx^2 + \lambda x^4$, $p = -id/dx$ $(k, \lambda > 0)$. The feature of its eigenvalue spectrum is that the lower eigenvalues are closely bunched in pairs if the two wells are sufficiently separated. The characteristic quantities to be calculated are the splittings between these pairs of energy levels as a function of the separation distance between the two wells $[\sim (k/\lambda)^{1/2}]$.

This problem does not admit a straightforward perturbative solution. The perturbation expansion of the eigenvalues $E_n(k,\lambda)$ in powers of the parameter λ is divergent for all $\lambda > 0$.[3] This may be seen qualitatively in the fact that the addition of the term λx^4 turns a completely continuous eigenvalue spectrum of $p^2 - kx^2$ into a completely discrete spectrum bounded from below. The alternative perturbation expansion in the parameter k (assuming the spectrum of $p^2 + \lambda x^4$ to be known) is unlikely to be useful since the perturbation becomes too large for small λ, which is the regime of interest. A nonperturbative treatment is therefore necessary. The WKB method is well suited for this purpose. The accuracy of the WKB approximation in thise case[1,2,4] is therefore a matter of considerable interest, especially since it is applied here for the lower eigenvalues. In this work we obtain the energy eigenvalues of the two-well oscillator by a nonperturbative method capable of arbitrarily high accuracy. We also obtain a WKB formula for the splitting between the pairs of lower eigenvalues. A comparison shows that the WKB estimates are remarkably accurate in this case. Finally, we comment on the analytic behavior of the eigenvalues $E_n(k,\lambda)$.

From the scaling $(x \to ax, p \to a^{-1}p)$ properties of the Hamiltonian $H(k,\lambda)$ it follows that $H(k,\lambda)$ and $a^{-2}H(a^4k, a^6\lambda)$ are unitarily equivalent and therefore have the same eigenvalues. Hence $E_n(k,\lambda) = k^{1/2}E_n(1,\lambda')$, $\lambda' = k^{-3/2}\lambda$. It is seen that the effective single parameter in this problem is $k^{-3/2}\lambda$. Thus it is sufficient to consider the eigenvalue problem of the reduced Hamiltonian $H(1,\lambda) = p^2 - x^2 + \lambda x^4$.

II. NONPERTURBATIVE METHOD

A nonperturbative method[5,6] for eigenvalue problems, capable of arbitrarily high accuracy, is applied here. The eigenfunctions are expanded in the form

$$\psi_n(\lambda) = e^{-\alpha x^2} \sum_{m=0}^{\infty} a_m x^m , \quad (1)$$

where $\alpha = \alpha(n,\lambda)$ is a scaling parameter to be set appropriately according to the oscillation properties of the eigenfunction in the required regime of values of the quantum number n and the anharmonicity λ. The expansion (1) on substitution into the Schrödinger equation $H(1,\lambda)\psi_n(\lambda) = E_n\psi_n(\lambda)$ yields a four-term linear recurrence relation in the expansion coefficients $\{a_m\}$:

$$a_{m+2} - \frac{4\alpha m + 2\alpha - E}{(m+1)(m+2)} a_m + \frac{4\alpha^2 + 1}{(m+1)(m+2)} a_{m-2} - \frac{\lambda}{(m+1)(m+2)} a_{m-4} = 0. \quad (2)$$

For the self-consistency of the resulting infinite set of linear homogeneous equations, the characteristic infinite determinant $\Delta(E)$ is set equal to zero. The roots of $\Delta(E) = 0$ are the eigenvalues. It may be shown that the various order truncations of $\Delta(E)$ satisfy an exact four-term recurrence relation,

$$(m+1)(m+2)\Delta_{m+2}(E) + (4\alpha m + 2\alpha - E)\Delta_m(E) + (4\alpha^2 + 1)\Delta_{m-2}(E) + \lambda\Delta_{m-4}(E) = 0, \quad (3)$$

where Δ_{m+2} is the determinant obtained by omitting all rows and columns of $\Delta(E)$ beyond the mth. With

$\Delta_0=1$ normalization the determinants up to any even order may be obtained successively from the recursion (3); for odd orders the initial conditions are $\Delta_0=0$, $\Delta_1=1$. The zeros of $\Delta_m(E)$ are obtained numerically by Newton's method which requires both $\Delta_m(E)$ and $\Delta_m'(E)$; the latter is obtained by differentiating the recursion (3) with respect to E and computing recursively. Both the recursions are numerically stable and the zeros of $\Delta_m(E)$ stabilize for large m to the required eigenvalues.[7] The eigenvalues obtained by Newton's method were checked and in the process upper and lower bounded by computing a sufficiently large-order determinant $\Delta_M(E)$ from the recursion (3) for two neighboring E values. Opposite signs of $\Delta_M(E)$ for the neighboring E values indicates that an eigenvalue lies in between. The appropriate value of the scaling parameter α is $\frac{1}{2}$ in the (small n, small λ) regime since in this regime the eigenvalue spectrum may be understood as the splitting of nearly harmonic levels.[8] The lowest four eigenvalues of $H(1,\lambda)$ for various values of λ are given in Table I. All significant figures quoted are claimed to be accurate. Eigenvalues of such accuracy are computed for the first time in this work.

Eigenvalues in any regime of values of (n,λ), the corresponding eigenfunctions and the transition moments[9] of high accuracy may be obtained by this method. The results will be reported in due course.

III. WKB APPROXIMATION

For any symmetrical two-well oscillator let E_n^0 be an energy level in one of the wells assuming no tunneling. Then for a small probability of tunneling the splitting of this level in the WKB approximation is given by[10]

$$\Delta E^{\rm WKB}=\frac{\omega}{\pi}\exp\left(-\int_{-x_0}^{x_0}|p|\,dx\right),\qquad \omega^{-1}=\frac{1}{2\pi}\int_{x_0}^{x_1}\frac{dx}{p(x)}\,, \tag{4}$$

where $\pm x_0$ and $\pm x_1$ are the four classical turning points. Expressing the above integrals in closed forms in terms of the elliptic integrals[11] we obtain from Eq. (4) the WKB formula

$$\Delta E^{\rm WKB}=\frac{k^{1/2}[2(1+u)]^{1/2}}{K(q)}\times\exp\left(-\frac{\sqrt{2}}{3}\frac{k^{3/2}}{\lambda}(1+u)^{1/2}[E(t)-uK(t)]\right), \tag{5}$$

where $t=[(1-u)/(1+u)]^{1/2}$, $q=[2u/(1+u)]^{1/2}$, $u=[4\lambda\epsilon_n^0(k)]^{1/2}/k$, $\epsilon_n^0(k)=E_n^0+(k^2/4\lambda)$, $K(s)$ and $E(s)$

TABLE I. Eigenvalues of the two-well oscillator in the small-λ regime. $\epsilon_n(\lambda)$ are the computed exact eigenvalues of the energy-shifted operator $H(1,\lambda)+(1/4\lambda)$, which is positive definite.

λ	ϵ_0 / ϵ_1	ϵ_2 / ϵ_3
0.01	1.404 048 605 297 7[a]	4.170 193 605 999 3
	1.404 048 605 297 7	4.170 193 605 999 3
0.02	1.393 527 585 044 2	4.092 028 112 820 5
	1.393 527 587 151 0	4.092 028 608 428 7
0.03	1.382 601 444 053 8	4.006 049 199 465 7
	1.382 605 783 831 4	4.006 655 466 749 5
0.04	1.371 122 236 557 5	3.901 359 951 813 1
	1.371 308 461 612 9	3.918 263 337 997 1
0.05	1.358 422 103 747 8	3.746 917 080 727 9
	1.360 133 597 773 3	3.848 838 300 057 4
0.07	1.323 374 074 208 5	3.342 216 720 258 7
	1.343 365 616 287 4	3.833 129 937 607 9
0.10	1.234 507 162 786 0	3.009 488 545 436 2
	1.346 940 868 922 5	4.043 546 039 767 6
0.15	1.062 499 247 956 5	3.033 667 276 570 6
	1.421 086 890 539 3	4.589 838 495 543 4
0.17	1.007 165 158 778 7	3.118 337 642 119 7
	1.464 225 132 421 2	4.816 923 221 196 9
0.20	0.941 750 342 076 9	3.270 377 801 715 3
	1.535 530 204 085 8	5.148 274 740 096 0

[a] Since near the minima the potentail function $\sim 2x^2+O(\lambda^{1/2}x^3)$, $\epsilon_0\to\sqrt{2}$ (ground-state energy in a potential $2x^2$) as $\lambda\to 0$. We find $\epsilon_0(\lambda=0.001)=1.413\,211\,965\,792$.

TABLE II. Splitting of the $n=0$ level. A comparison between the exact values and the "modified" WKB values.

λ	$\dfrac{(\epsilon_1-\epsilon_0)^{\text{exact}^a}}{(\epsilon_1-\epsilon_0)^{\text{modified WKB}^b}}$
0.02	1.005
0.03	1.006
0.04	1.007
0.05	1.008
0.07	1.006
0.10	0.975
0.15	0.934
0.17[c]	0.940

[a] $(\epsilon_1-\epsilon_0)^{\text{exact}}$ values are obtained from the Table I.
[b] $(\epsilon_1-\epsilon_0)^{\text{modified WKB}}=\Delta E^{\text{WKB}}$ from formula (5) multiplied by $(\pi/e)^{1/2}$.
[c] For $\lambda \gtrsim 0.17$ the number of turning points reduces to two in the $n=0$ case.

are complete elliptic integrals of the first and the second kind, respectively. Equation (5), obtained by using the linear (Airy function) connection formulas, is referred to as the "standard" WKB result. Upon using the more correct quadratic connection formulas the standard WKB result for the $n=0$ case is modified by a factor of $(\pi/e)^{1/2}$ (Refs. 1 and 12); this is referred to as the "modified" WKB result. In Table II the splitting between the lowest pair of eigenvalues for various λ, obtained from the exact values of the previous section, are compared with the corresponding modified WKB estimates. It is seen that the modified WKB values are in closer agreement with the exact values than the corresponding standard WKB estimates. In obtaining the WKB values from Eq. (5) the unperturbed energy E_n^0 is assumed to be the mean of the corresponding split pair of eigenvalues listed in Table I (col. 2). The accuracy of the modified WKB estimates for the splittings is quite impressive.

It is illuminating to examine the WKB formula (5) in the small-λ regime which contains the characteristic features of this eigenvalue spectrum. In this regime the elliptic integrals may be expanded[11] for $u\to 0$, $t\to 1$, $q\to 0$. Since the tunneling probability approaches zero in this limit, the unperturbed energies become harmonic-oscillator-like corresponding to a potential $2x^2$ (Ref. 13): Hence $\epsilon_n^0(k)=\sqrt{k}\,\epsilon_n^0(1)$ and $\epsilon_n^0(1)=\sqrt{2}\,(2n+1)$, and the limit $u\to 0$ implies $k^{-3/2}\lambda\to 0$. Introducing all of this in formula (5) and retaining the highest-order terms, we obtain for the nth unperturbed level

$$\Delta E_n^{\text{WKB}}=\frac{\sqrt{k}}{\pi}\,2^{(14n+13)/4}\left(\frac{k^{3/2}e}{\lambda(2n+1)}\right)^{(2n+1)/2}\times\exp\left(-\frac{\sqrt{2}}{3}\frac{k^{3/2}}{\lambda}\right). \tag{6}$$

The $n=0$ case of Eq. (6) was obtained recently by Gildener and Patrascioiu[1] [their Eq. (5.61)] except for a missed factor of $\hbar\sqrt{\mu}$ in their result. Formula (6) clearly manifests the scaling properties of the WKB eigenvalues. We observe that

$$\Delta E_n^{\text{WKB}}(k,\lambda)=\sqrt{k}\,\Delta E_n^{\text{WKB}}(1,k^{-3/2}\lambda),\quad k^{-3/2}\lambda\to 0 \tag{7}$$

which is precisely the same as the scaling relation satisfied by the *exact* eigenvalues[14]: $E_n(k,\lambda)=\sqrt{k}\,E_n(1,k^{-3/2}\lambda)$. In view of the above it is possible to construct the analytic behavior of $E_n(k,\lambda)$ from the corresponding WKB expression. Thus from (6) it follows that $\Delta E_n(k,\lambda)$ and hence $E_n(k,\lambda)$ have an essential signularity at $\lambda=0$ whenever there are four classical turning points. The possibility of establishing the analytic properties of the eigenvalues from the WKB analysis of the same problem may have more general applications.

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