BOUND AND RESONANCE STATES FOR ISOCHRONOUS POTENTIALS ☆

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The bound and resonance states for a family of piecewise linear potentials are obtained by the complex coordinate method. The complex spectra were found to be weakly affected by isochronous transformations of the potential, i.e. transformations which keep the classical periods of bound trajectories and the classical delay times of scattering trajectories invariant.

1. Introduction

Given a one-dimensional classical potential $V(x)$ which supports oscillatory ("bound") trajectories over some energy range $E_0 \leqslant E \leqslant E_{max}$ it is well known that a simple class of distortions of this potential exists such that the period of oscillation $T(E)$ remains unaffected over the entire range of energies specified above. In particular, assume that $V(x)$ is continuous, monotonically decreasing for $x \leqslant x_0$ and monotonically increasing for $x > x_0$, and obtains its minimum at x_0; $V(x_0) = E_0$. If $U(x)$ is related to $V(x)$ in such a way that $x_+(E) - x_-(E)$, the distance between the right and left classical turning points, remains invariant at all the energies in the range of the oscillatory trajectories, then these two potentials are isoperiodic. Two such potentials can be shown to support the same WKB spectrum.

Two aspects of the quantum-mechanical properties of classically isoperiodic potentials have recently been discussed. It was shown that the classical ($\hbar \to 0$) limits of quantal isospectral potentials (specifically, potentials satisfying the Korteweg–de Vries hierarchy of evolution equations) are classically isoperiodic potentials [1]. This result, as well as the fact that within the WKB approximation classically isoperiodic potentials are isospectral, suggest that these potentials will be approximately isospectral in quantum mechanics as well. This expectation is supported by some numerical evidence [1].

On the other hand, Subramanian and Bhagwat [2] have recently shown that in a family of isoperiodic potentials the member with the lowest quantal ground state energy is the symmetric potential, satisfying $V(x-x_0) = V(x_0-x)$. While the same statement does not hold for the excited states, the approach presented in ref. [3] to the variational treatment of excited state energies suggests that $\sum_{i=0}^{k} E_i$, where E_0, E_1, ..., E_k are the ground and the k lowest excited states, is minimal for the symmetric potential.

For classically non-binding potentials the notion of isoperiodic trajectories can be extended into the idea of equal time delay of scattering trajectories. Thus, the time delays, relative to free particle motion, affected by two potentials $U(x)$ and $V(x)$ can be shown to be equal, at all energies $E \geqslant E_{max}$ if the two potentials are related to one another in the manner specified above for $E_0 \leqslant E \leqslant E_{max}$, and obtain the values E_{max} either at two finite points (vanishing

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thereafter) or asymptotically as $x \to \pm\infty$. We shall refer to such potentials, which have the same periods for the bound trajectories and the same delay times for the scattering trajectories, as isochronous potentials.

Yet another possibility is the case where the potential exhibits a finite barrier. Classically, such a potential is impenetrable by particles with energies below the top of the barrier. However, it can be shown by a slight modification of the argument presented in ref. [1] that two potentials which have equal non-classical widths at all energies below the barrier, possess the same WKB tunneling probabilities. Both the classical delay time above the top of the barrier and the WKB tunneling probability below it are closely related to the properties of quantal resonance states.

The purpose of the present study is to explore by means of a simple example the extent to which classically isochronous potentials with finite barriers support similar resonance states. It will be interesting to observe the change in the resonance energy and width resulting from isochronous distortions, and the validity of the Subramanian and Bhagwat theorem [2] or its extension suggested above, concerning the minimal property of the energy for the symmetric potential, within a family of isochronous potentials.

2. A piecewise linear isochronous family of potentials

The family of potentials (shown in fig. 1) given by

$$V(x)=0 \quad \text{for } x<-C+U, \tag{1a}$$

$$V(x)=\frac{(x+C-U)V_0(B-A)}{U(B-A)/A(C-B)} \quad \text{for } -C+U<x<-B+UB/A, \tag{1b}$$

$$V(x)=-V_0[1+x/(A-U)] \quad \text{for } -B+UB/A<x<0, \tag{1c}$$

$$V(x)=V_0[x/(A+U)-1] \quad \text{for } 0<x<B+UB/A, \tag{1d}$$

$$V(x)=\frac{(x-C-U)V_0(B-A)}{U(B-A)-A(C-B)} \quad \text{for } B+UB/A<x<C+U, \tag{1e}$$

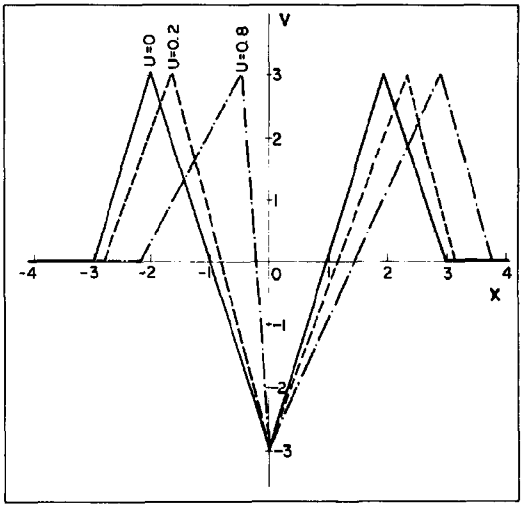

Fig. 1. The piecewise linear potentials given in eq. (1) in the text. The symmetric potential is obtained for $U=0$ and the most distorted potential studied is that for $U=0.8$.

$$V(x)=0 \quad \text{for } x>C+U, \tag{1f}$$

is a one-parameter family satisfying the following properties:

(a) For a particular choice of the parameter U, $U=0$, the potential is even.

(b) The horizontal distances between any two classical turning points, at the whole range of energies for which they exist, are independent of the parameter U.

(c) It follows from (b) that all integrals of the form

$$\int_{a(E)}^{b(E)} F(E-V(x))\,\mathrm{d}x \tag{2}$$

between two classical turning points at the same energy E are independent of $U^{(1)}$. Here, F is an arbitrary function of its argument.

If $a(E)$ and $b(E)$ are two classical turning points across a well, the above integral is related to the classical period of oscillation for one choice of F and to the WKB quantization condition for another. If $a(E)$ and $b(E)$ are classical turning points on two sides of a barrier, the above integral, for a particular choice of F, is related to the WKB tunneling probability.

A comprehensive derivation of the semiclassical expressions for the energies and widths of the resonance states in one-dimensional double-humped potentials was presented by Connor [4]. Inspection of eqs. (2.2), (2.8), (3.3) and (3.4) in ref. [4] indicates that the resonance position and width depend on three integrals of the type presented in our eq. (2). It follows that within the semiclassical approximation the bound state energies as well as the resonance energies and widths are independent of U. In the following sections we examine this prediction by means of an accurate quantum-mechanical computation.

The bound and resonance states for the potential presented in eq. (1) can be obtained by using free-particle and Airy functions in the appropriate ranges, matching the logarithmic derivative at each one of the five points of discontinuity. The system of transcendental equations obtained can only be solved numerically, requiring an accurate evaluation of the Airy function. The approach chosen in the present work, i.e. the complex coordinate method applying an appropriate basis set, has the advantage of being applicable to a wide class of potentials with only minor modification to the formalism.

3. Bound and resonance states of piecewise linear continuous potentials by the complex coordinate method

The resonances of a physical system are associated with the complex eigenvalues $E-\frac{1}{2}i\Gamma$ of the Hamiltonian $H(x)$. The probability of finding a particle in the element dx of configuration space is proportional to $\exp(-\Gamma t/\hbar)$ and decays with time. The eigenfunctions, $\psi(x)$, associated with *complex* eigenvalues do not belong to the Hermitian domain of H and diverge as $x\to\infty$. Therefore, the number of particles in the coordinate space is not conserved at any given time [5]. By complex scaling the internal coordinates of the Hamiltonian, i.e. $x\to x\exp(i\theta)$, we "correct" the asymptotic behavior of the resonance eigenfunctions such that $\psi(x\exp(i\theta))\to 0$ as $x\to\infty$ if θ becomes large enough [6]. The complex coordinate method (CCM) enables one to isolate the resonance states from the other states in the continuum. The scattering states are rotated into the complex plane,

$$E(\text{continua})=|E-E_{\text{threshold}}|\exp(-2i\theta),$$

whereas the bound and resonance states are unaffected by $\theta>\theta_c$ (for bound states $\theta_c=0$ and for resonances

$$\theta_c=\arctan[2(E-E_{\text{threshold}})/\Gamma]).$$

On the CCM and its application to different types of physical systems, see refs. [7-9] and references therein.

The spectrum of $\hat{H}(x)$ including its resonance lifetimes (i.e. inverse of the width Γ) can be obtained for piecewise continuous potentials by selecting a path in the complex coordinate plane which avoids the intrinsic non-analyticities of the potential. Simon's extension of the scaling method provides such a path in the complex coordinate plane [10]. Another possibility is to expand $\psi(x)$ to the desired degree of accuracy, $\psi(x)=\sum_{i=1}^{N}c_i\phi_i(x)$ where $\boldsymbol{c}$ is an eigenvector of the $N\times N$ Hamiltonian matrix obtained by carrying out analytical continuation of the *Hamiltonian matrix element* into the complex plane,

$$\begin{aligned}\mathcal{H}_{ij}&=\langle\phi_i(x)|\hat{H}(x\eta)|\phi_j(x)\rangle\\&=\langle\phi_i(x/\eta)|\hat{H}(x)|\phi_j(x/\eta)\rangle\\&=f(\eta)|_{\eta=\exp(i\theta)}\,.\end{aligned}\tag{3}$$

For example, this method (i.e. scale the basis set and not the Hamiltonian) has been used previously in the application of the CCM to molecular autoionization resonances [7,11]. For a more detailed discussion of this method, see ref. [12]. Recently, it has been shown that these two computational methods are only two out of many possible different types of similarity transformations which conserve probability for $\psi(x)$ [13]. In the case studied here we used particle-in-a-box functions as a basis set, $\phi_n(x)=\sqrt{2/a}\sin[n\pi((x+\frac{1}{2}a)/a]$, where $-\frac{1}{2}a\leqslant x\leqslant\frac{1}{2}a$. The piecewise linear potential matrix elements for the potential

$$V(x)=\sum_{i=0}^{L+1}\Theta(x-x_{i-1})\,\Theta(x_i-x)(\alpha_i+\beta_i x),\tag{4}$$

where

$$\begin{aligned}\Theta(x)&=1\,,\quad x\geqslant 0\,,\\&=0\,,\quad x<0\,,\end{aligned}$$

$$x_{-1}=-\tfrac{1}{2}a\,,$$

$$x_i=\gamma_i\,,\quad i=0,...,L\,,$$

$$x_{L+1}=\tfrac{1}{2}a\,,$$

can be analytically obtained as functions of a:

$$V_{n,m}(a)=\int_{-\frac{1}{2}a}^{\gamma_0}\phi_n(x)(\alpha_0+\beta_0 x)\,\phi_m(x)\,dx$$

$$+\sum_{k=1}^{L-1}\int_{\gamma_{k-1}}^{\gamma_{k+1}}\phi_n(x)(\alpha_k+\beta_k x)\,\phi_m(x)\,dx$$

$$+\int_{\gamma_L}^{\frac{1}{2}a}\phi_n(x)(\alpha_L+\beta_L x)\,\phi_m(x)\,dx\,. \qquad (5)$$

By substituting $a=|a|\exp(i\theta)$ into eq. (4) a complex symmetric non-Hermitian Hamiltonian matrix is obtained. For a given basis set (fixed $|a|$ and N) the resonances are associated with the stationary solutions in the complex variational plane that are associated with the cusps [14] in the θ-trajectory calculations and satisfy the complex virial theorem [15–17].

4. Results and discussion

The bound and resonance states for the series of model potentials given in section 2 were obtained by using $N=70$ particle-in-a-box basis functions where $A=1$, $B=2$, $C=3$, $V_0=3$, $|a|=15$ and U is varied from zero (for the symmetric potential) to $U=0.8$. (The case where $N=150$ and $|a|=25$ was also studied.)

The spectrum of the complex rotated Hamiltonian matrix shows typical Balslev–Combes behavior. The results obtained for $\theta=0.15$ varying $|a|$ from 12 to 24 are shown in fig. 2. From fig. 2 one can see that – as is expected on the basis of Balslev–Combes theorem [6] – the continuum is rotated into the complex plane by the angle $2\theta=0.3$. The bound state remains on the real axis (zero width) as $|a|$ is varied whereas the resonances are stable in the complex energy plane.

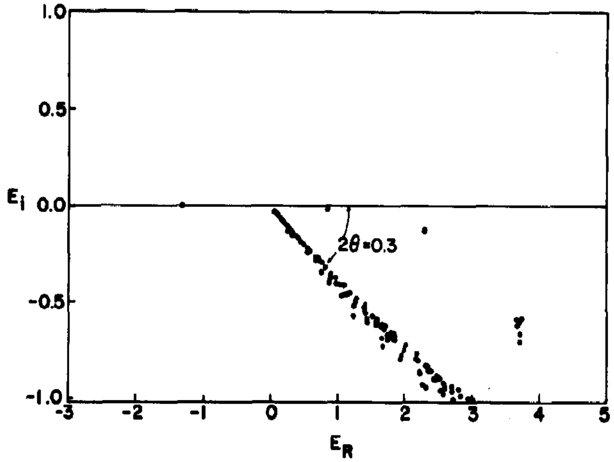

Fig. 2. Complex eigenvalues of the Hamiltonian given in eq. (1) where $A=1$, $B=2$, $C=3$, $V_0=3$ and $U=0$ as the size of the "box" is increased from 12 to 24. The complex rotation angle is $\theta=0.15$. The bound state ($E_i=0$) and the resonance states ($E_i\neq 0$) converge as a increases. The continuum is rotated into the complex plane by the angle 2θ.

By carrying out θ-trajectory calculations stationary solutions for which $\partial E_r/\partial\theta=0$ and $\partial E_i/\partial\theta=0$ were obtained. These stationary solutions are associated with the resonance states and $E_r=E$(position), $-2E_i=\Gamma$(width) [14]. The results presented in table 1 show clearly that the range of variation of the

Table 1
Complex eigenvalues of the Hamiltonian given in eq. (1) as function of the symmetry-breaking parameter U. The semiclassical results, which are independent of U, were obtained (for states below the barrier) using Connor's [4] expressions

	$E=-\frac{1}{2}i\Gamma$					
	$U=0$	$U=0.2$	$U=0.4$	$U=0.6$	$U=0.8$	semi-classical
bound state	−1.3182	−1.3108	−1.2870	−1.2421	−1.1656	−1.1781
first resonance	0.846 −0.0078i	0.830 −0.0072i	0.788 −0.0062i	0.744 −0.0060i	0.714 −0.0052i	0.791 −0.0044i
second resonance	2.295 −0.126i	2.308 −0.129i	2.312 −0.144i	2.30 −0.136i	2.21 −0.17i	2.320 −0.092i
third resonance	3.695 −0.626i	3.672 −0.622i	3.67 −0.70i	3.763 −0.755i	3.79 −0.87i	–

positions and widths of the resonances as functions of U are narrow relative to the separation among these resonances in the complex energy plane.

In view of the fact that the transformation was formulated on the basis of a classical argument, it is remarkable that even the resonance widths, *which are "pure" quantum phenomena, are only mildly affected by varying U.*

As the energy of the system increases, the quantum and classical behavior should become more similar. Indeed, the resonance position and width of the third resonance in table 1, which is located above the potential barrier, are the most stable and are least affected by the distortion of the potential. The tendency for the ground state energy to be higher as U is increased making the potential less symmetrical, follows from the theorem of Subramanian and Bhagwat [2]. The dependence of the resonance position and width on the isochronous distortion of the potential is beyond the scope of the above theorem, but the regularity of the results suggests a possible extension, which has yet to be investigated.

In conclusion, it is found that classically isochronous potentials give rise to almost invariant quantal complex spectra.

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