Conduction bands in classical periodic potentials

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Abstract. The energy of a quantum particle cannot be determined exactly unless there is an infinite amount of time to perform the measurement. This paper considers the possibility that $\Delta E$, the uncertainty in the energy, may be complex. To understand the effect of a particle having a complex energy, the behaviour of a classical particle in a one-dimensional periodic potential $V(x) = -\cos(x)$ is studied. On the basis of detailed numerical simulations it is shown that if the energy of such a particle is allowed to be complex, the classical motion of the particle can exhibit two qualitatively different behaviours: (i) The particle may hop from classically allowed site to nearest-neighbour classically allowed site in the potential, behaving as if it were a quantum particle in an energy gap and undergoing repeated tunnelling processes or (ii) the particle may behave as a quantum particle in a conduction band and drift at a constant average velocity through the potential as if it were undergoing resonant tunnelling. The classical conduction bands for this potential are determined numerically with high precision.

Keywords. $\mathcal{PT}$ symmetry; complex trajectories; complex classical mechanics; conduction bands.

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1. Introduction

The theme of $\mathcal{PT}$ quantum mechanics is that it is possible to extend the Hamiltonian for a quantum system into the complex domain while retaining the fundamental properties of a quantum theory [1,2]. Complex quantum mechanics has proved to be so interesting that the research activity on $\mathcal{PT}$ quantum mechanics has motivated studies of complex classical mechanics. Early work on the particle trajectories in complex classical mechanics is reported in refs [3,4]. Subsequently, detailed studies of the complex extensions of conventional classical-mechanical systems were undertaken: The remarkable properties of complex classical trajectories were examined in refs [5–9]; the complex behaviour of the pendulum, the Lotka–Volterra equations for population dynamics and the Euler equations for rigid body rotation were studied in refs [10,11]; the complex Korteweg–de Vries equation was examined in refs [12–15]; the complex Riemann equation was examined in ref. [16]; complex Calogero models were examined in ref. [17]; the complex extension of chaotic behaviour was recently discussed in ref. [18].
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Figure 1. Classical trajectories \( x(t) \) in the complex-\( x \) plane for the anharmonic-oscillator Hamiltonian \( H = \frac{1}{2}p^2 + x^4 \). All trajectories represent a particle of energy \( E = 1 \). There is one real trajectory that oscillates between the turning points at \( x = \pm 1 \) and an infinite family of nested complex trajectories that enclose the real turning points but lie inside the imaginary turning points at \( \pm i \). (The turning points are indicated by dots.) Two other trajectories begin at the imaginary turning points and drift off to infinity along the imaginary \( x \)-axis. Apart from the trajectories beginning at \( \pm i \), all trajectories are closed and periodic. All orbits in this figure have the same period \( \sqrt{\frac{\pi}{2}} \Gamma \left( \frac{1}{4} \right) / \Gamma \left( \frac{3}{4} \right) = 3.70815 \ldots \).

This paper explores more deeply a newly discovered aspect of complex classical mechanics, namely, that there are remarkable similarities between complex classical mechanics and quantum mechanics: Bender et al [19] performed numerical studies to show that standard quantum effects such as tunnelling could be displayed by classical systems having complex energy [19]. The work in ref. [19] relies on the observation that when the energy is real, the classical trajectories in the complex plane are closed and periodic but when the energy is complex, the classical trajectories are open and nonperiodic [11].

In ref. [19] these features are illustrated by using the simple example of the classical anharmonic oscillator, whose Hamiltonian is \( H = \frac{1}{2}p^2 + x^4 \). When the classical energy is real, the classical orbits in the complex plane are all closed and periodic (see figure 1), but if the energy is complex, the classical orbits are no longer closed and they spiral outward to infinity (see figure 2).

The Bohr–Sommerfeld quantization formula provides a heuristic way to understand the association between real energy and closed orbits versus complex energy and open orbits. The quantization formula

\[
\oint p \, dx \sim \left( n + \frac{1}{2} \right) \pi, \quad n \gg 1,
\]

where the integral is performed along a closed classical orbit, gives a semiclassical approximation to the energies of a Hamiltonian for large quantum number; that is, it takes advantage of particle–wave duality and assumes that there are an integral number of wavelengths along the classical orbit. For the anharmonic-oscillator Hamiltonian considered in figures 1 and 2 this formula gives the (real) spectrum of this Hamiltonian, whether or not the classical orbit lies on the real axis in the
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Figure 2. A single classical trajectory in the complex-$x$ plane for a particle governed by the anharmonic-oscillator Hamiltonian $H = \frac{1}{2}p^2 + x^4$. This trajectory begins at $x = 1$ and represents the complex path of a particle whose energy $E = 1 + 0.1i$ is complex. The trajectory is not closed or periodic. The four turning points are indicated by dots. The trajectory does not cross itself.

Figure 3. Six classical trajectories in the complex-$x$ plane representing a particle of energy $E = -1$ in the potential $x^4 - 5x^2$. The turning points are located at $x = \pm 2.19$ and $x = \pm 0.46$ and are indicated by dots. Because the energy is real, the trajectories are all closed. The classical particle stays in either the right-half or the left-half plane and cannot cross the imaginary axis. Thus, when the energy is real, there is no effect analogous to tunnelling.

Complex-$x$ plane. However, the formula cannot be applied if the orbit is open and the energy is complex.

In ref. [19] it was seen that it is possible to observe tunnelling-like behaviour in classical mechanics when the classical energy of a particle is taken to be complex. The double-well anharmonic oscillator $H = p^2 + x^4 - 5x^2$ was used to illustrate this observation. If the energy of a classical particle is taken to be real, the classical motion is periodic and the orbits lie either on the left side or on the right side of the imaginary axis, which separates the two wells (see figure 3).

However, if the energy of a classical particle whose motion is determined by the Hamiltonian $H = p^2 + x^4 - 5x^2$ is taken to be complex, it was found that the classical trajectory is no longer closed. Rather, the trajectory spirals outward, crosses the imaginary axis, and then spirals inward into the companion well. It then repeats this process, alternately visiting one well and then the other. This motion is shown in figure 4. Note that the trajectory never crosses itself. This
Figure 4. Classical trajectory of a particle moving in the complex-$x$ plane under the influence of a double-well $x^4 - 5x^2$ potential. The particle has complex energy $E = -1 - i$ and thus its trajectory does not close. The trajectory spirals outward around one pair of turning points, crosses the imaginary axis, and then spirals inward around the other pair of turning points. It then spirals outward again, crosses the imaginary axis, and goes back to the original pair of turning points. The particle repeats this behaviour endlessly but at no point does the trajectory cross itself. This classical-particle motion is analogous to the behaviour of a quantum particle that repeatedly tunnels between two classically allowed regions. Here, the particle does not disappear into the classically forbidden region during the tunnelling process; rather, it moves along a well-defined path in the complex-$x$ plane from one well to the other.

Strange-attractor-like behaviour resembles quantum-mechanical tunnelling. Moreover, it provides a heuristic answer to the question, How did the particle get from one well to the other? In a tunnelling experiment the particle disappears from one well and then appears in the other well; what path did the particle follow to get from one well to the other? Figure 4 shows that the particle can travel smoothly from one well to the other if the trajectory lies in the complex plane.

The heuristic picture proposed in ref. [19] is that there is some quantum uncertainty in the measurement of the energy of a particle, $(\Delta E)(\Delta t) \sim \hbar$, because an energy measurement is performed in a finite, rather than an infinite, amount of time. If this uncertainty in the energy has an imaginary component, then the classical picture of particle motion and the quantum picture of particle motion come closer to one another.

The question that is investigated in this paper is how a classical particle whose energy is allowed to be complex behaves in a periodic potential. In ref. [19] some numerical experiments were performed for the potential $V(x) = -\cos(x)$ which suggested that depending on the real and the imaginary parts of the energy of a particle one can observe two kinds of classical motion:
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• Localized tunnelling behaviour – The particle tunnels from one well to the adjacent well, either to the right or to the left. This hopping behaviour resembles a deterministic random walk, and is what is usually observed for an arbitrary choice of complex energy. This motion is like that of a quantum particle in a crystal, where the energy of the particle is not in a conduction band.

• Delocalized conduction – The particle drifts through the potential in one direction. This classical motion resembles the behaviour of a quantum particle in a crystal, where the energy of the particle lies in a conduction band.

These two kinds of behaviours were conjectured in ref. [19] on the basis of limited numerical experiments. We have now performed an extremely detailed numerical study of the behaviour of a classical particle in a periodic potential well. Our study shows that the types of behaviour that were conjectured in ref. [19] do indeed occur. More importantly, there are well-defined and narrow energy bands with precise edges in which ‘conduction’ takes place.

2. Complex motion in a periodic potential

We consider here the Hamiltonian

\[ H(x, p) = \frac{1}{2}p^2 - \cos(x) \] (2)

and solve the associated Hamilton’s equations of motion,

\[ \frac{dx}{dt} = p \quad \text{and} \quad \frac{dp}{dt} = -\sin(x), \] (3)

to determine the kinds of classical behaviours that arise. If we choose a value of the classical energy at random, say \( E = 0.1 - 0.15i \), we find that the classical particle usually tunnels from well to well following a deterministic random walk (see figure 5). On the other hand, if we search carefully for a conduction band, we see the classical particle drift through the lattice in one direction only (see figure 6).

We have run continuously on a computer for several months to determine which complex energies give rise to tunnelling (hopping) behaviour and which complex energies produce conduction-like behaviour. We have been able to determine that conduction behaviour is found when the energy lies in narrow bands with crisp well-defined edges (see figure 7). To distinguish between hopping behaviour and conduction behaviour we allowed the particle to undergo 10 tunnelling incidents, and if the particle always tunnelled in the same direction we classified the energy as lying in a conduction band. (In ref. [19], seven tunnelling incidents were used.) Figure 7 reports the major result in this paper.

Two detailed blow-up views of the complex-energy plane shown in figure 7 are given in figures 8 and 9. In figure 8 a region of the complex-\( E \) plane is shown for which \( 0.28 < \Re E < 0.31 \) and \(-0.72 < \Im E < -0.71 \), and in figure 9 a portion of the complex-\( E \) plane is shown for which \( 0.69 < \Re E < 0.72 \) and \(-0.26 < \Im E < -0.25 \). These figures indicate that the border between hopping behaviour and conduction behaviour is clean and crisp.
Figure 5. A tunnelling trajectory for the Hamiltonian (2) with $E = 0.1 - 0.15i$. The classical particle hops at random from well to well in a random-walk fashion. The particle starts at the origin and then hops left, right, left, right, left, left, right, right. This is the sort of behaviour normally associated with a particle in a crystal at an energy that is not in a conduction band. At the end of this simulation the particle is situated to the left of its initial position. The trajectory never crosses itself.

Figure 6. A classical particle exhibiting a behaviour analogous to that of a quantum particle in a conduction band that is undergoing resonant tunnelling. Unlike the particle in figure 5, this classical particle tunnels in one direction only and drifts at a constant average velocity through the potential.

3. Concluding remarks

We know that quantum-mechanical amplitudes are determined by performing infinite sums over classical configurations. However, tunnelling is not thought of as
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Figure 7. Complex-energy plane showing those energies that lead to tunnelling (hopping) behaviour and those energies that give rise to conduction. Hopping behaviour is indicated by a hyphen - and conduction is indicated by an X. The symbol & indicates that no tunnelling takes place; tunnelling does not occur for energies whose imaginary part is close to 0. In some regions of the energy plane we have done very intensive studies and the X’s and -’s are densely packed. This picture suggests the features of band theory: If the imaginary part of the energy is taken to be $-0.9$, then as the real part of the energy increases from $-1$ to $+1$, five narrow conduction bands are encountered. These bands are located near $\text{Re} E = -0.95, -0.7, -0.25, 0.15, 0.7$. This picture is symmetric about $\text{Im} E = 0$ and the bands get thicker as $|\text{Im} E|$ increases. A total of 68689 points were classified to make this plot. In most places the resolution (distance between points) is 0.01, but in several regions the distance between points is shortened to 0.001. The regions indicated by arrows are blown up in figures 8 and 9.

Figure 8. Detailed portion of the complex energy plane shown in figure 8 containing a conduction band. Note that the edge of the conduction band, where tunnelling (hopping) behaviour changes over to conducting behaviour, is very sharp.
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Figure 9. Like figure 8, a detailed portion of the complex energy plane in figure 8 containing a conduction band. Note that the edges of the conduction band are sharp.

Figure 10. Tunnelling time as a function of the imaginary part of the energy. The curve is a hyperbola; that is, the product of the imaginary part of the energy and the tunnelling time is a constant. This result is strongly reminiscent of the time–energy uncertainty principle.

a possible classical behaviour. Thus, the usual view is that quantum phenomena can appear only when an infinite sum over classical behaviours is performed. However, in this paper we have argued that some aspects of quantum behaviour (such as bands and gaps in periodic potentials) can already be seen in the context of classical mechanics. As an example, we can already see in classical mechanics a version of the time–energy uncertainty principle. In figure 10 we have plotted the tunnelling time vs. the size of the imaginary part of the energy. The graph is a hyperbola, and thus the product of these two quantities is a constant.

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