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Classical particle in a complex elliptic potential

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Abstract

This paper reports a numerical study of complex classical trajectories of a particle in an elliptic potential. This study of doubly periodic potentials is a natural sequel to earlier work on complex classical trajectories in trigonometric potentials. For elliptic potentials, there is a two-dimensional array of identical cells in the complex plane, and each cell contains a pair of turning points. The particle can travel both horizontally and vertically as it visits these cells, and sometimes the particle is captured temporarily by a pair of turning points. If the particle's energy lies in a conduction band, the particle drifts through the lattice of cells and is never captured by the same pair of turning points more than once. However, if the energy of the particle is not in a conduction band, the particle can return to previously visited cells.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The past decade has seen much research activity devoted to extending quantum mechanics into the complex domain [1]. It has been shown that Dirac Hermiticity may be generalized to include complex non-Dirac-Hermitian Hamiltonians that are $\mathcal{PT}$ symmetric. (A Hamiltonian is *Dirac-Hermitian* if $H = H^\dagger$, where $\dagger$ represents combined complex conjugation and matrix transposition. A Hamiltonian is $\mathcal{PT}$ symmetric if it is invariant under combined spatial reflection $\mathcal{P}$ and time reversal $\mathcal{T}$.) These complex Hamiltonians are physically acceptable because (i) their eigenvalues are all real and (ii) they generate unitary time evolution [2–4]. Research on $\mathcal{PT}$ quantum mechanics has revealed interesting and surprising new phenomena, and in the past year some of these new phenomena have actually been observed in laboratory experiments [5–7].

Motivated by a desire to understand $\mathcal{PT}$ quantum mechanics better, there has been a significant body of research on complex classical mechanics. Conventional classical

mechanics is the study of the real solutions to Hamilton's equations of motion. In the recently established field of *complex classical mechanics*, we expand this study to include *all* solutions, complex as well as real, to Hamilton's equations [8, 9].

Complex classical mechanics has proved to be useful, in part because it provides an intuitive picture of what is happening at the quantum $\mathcal{PT}$ phase transition between a *broken* $\mathcal{PT}$-symmetric phase (where some of the quantum eigenvalues are real and some are complex) and an *unbroken* $\mathcal{PT}$-symmetric phase (where all of the quantum eigenvalues are real). In the broken phase of $\mathcal{PT}$ quantum mechanics, the classical trajectories are open, and in the unbroken phase the classical trajectories are closed and periodic [10]. Bohr–Sommerfeld quantization clarifies the association between complex energy and open classical trajectories versus real energy and closed classical trajectories. This association, which is discussed in detail in [11], arises because the Bohr–Sommerfeld quantization condition contains a path integral along a closed contour: $\oint_C \mathrm{d}x\, p = \left(n + \frac{1}{2}\right)\pi$. Evidently, this quantization condition can only be applied if the classical orbits are closed.

Studies of complex classical trajectories have also led to studies of probability densities in the complex plane, which in turn have given rise to the formulation of a complex correspondence principle [12]. In addition, studies of complex classical mechanics have proved to be useful in their own right and may lead to a deeper understanding of the transition from nonchaotic to chaotic behavior [13].

One particularly interesting area of research concerns the generalization of complex classical mechanics from real to complex energy. It can be argued that because of the time–energy uncertainty principle in quantum mechanics, $\Delta t\,\Delta E \gtrsim \hbar$, one cannot measure an energy with absolute precision unless one has an infinite amount of time in which to perform the measurement. We then suppose that this uncertainty in the value of the energy exists in classical mechanics and further assume that the uncertainty ΔE may be complex. The surprise is that generalizing complex classical mechanics from real to complex energy produces a theory that exhibits many of the qualitative features of quantum mechanics [11, 14, 15].

The principal effect of extending the energy from real to complex values is that particle trajectories $x(t)$, which are curves in the complex-x plane, cease to be closed. For example, while the particle trajectories for the classical anharmonic-oscillator Hamiltonian $H = p^2 + x^4$ are all closed when the energy E is real, the trajectories are open and spiral outward to infinity when $\mathrm{Im}\, E \neq 0$ [11]. More interestingly, while the trajectories $x(t)$ for a double-well anharmonic-oscillator Hamiltonian $H = p^2 - x^2 + x^4$ are closed in the complex-x plane, they are no longer closed when E is complex. However, the remarkable property of these trajectories is that they do not spiral outward to infinity. Rather, they run back and forth endlessly from the vicinity of one well to the vicinity of the other well in a fashion that is reminiscent of quantum tunneling. To be specific, if a particle is initially in the classically allowed region on the real axis in the left well, the particle spirals outward, crosses the imaginary axis and then spirals *inward* into the right well. Then, the particle spirals outward again and visits the left well. Thus, the two wells in the potential act like strange attractors. This oscillatory process continues forever, but the trajectory never crosses itself.

This complex double-well classical system is different from the corresponding quantum-mechanical system in that a trajectory cannot cross itself unless the classical trajectory is periodic, and thus a classical particle on an open trajectory can never revisit any point in the complex plane. However, many features of quantum mechanics are mirrored in the properties of this classical behavior. For example, as the imaginary part of the classical energy increases, the characteristic 'tunneling' time (the time required for the particle to spiral inward and outward around a pair of turning points) decreases inversely, just as one would expect of a quantum particle. As in the case of quantum tunneling, the particle spends a long time in

proximity to a given pair of turning points before crossing the imaginary axis to the other pair of turning points. On average, the classical particle spends equal amounts of time on either side of the imaginary axis. Furthermore, the pattern of trajectories changes qualitatively as the real part of the energy is varied. For some regions of $\mathrm{Re}\, E$, the trajectories form a parity-symmetric pattern and these energy regions interlace with other regions of $\mathrm{Re}\, E$ for which the trajectories form a parity-anti-symmetric pattern.

Having observed the tunneling-like behavior of a classical particle with complex energy in a double well, it is natural to ask what happens to a particle in a periodic potential. An electron in a crystal lattice is described by such a potential. An elementary physical system that also has a periodic potential consists of a simple pendulum in a uniform gravitational field [16]. Without loss of generality we take the pendulum bob to have mass $m = 1$, the string to have length $L = 1$ and the uniform gravitational field to have strength $g = 1$. If the gravitational potential energy of the system is zero at the height of the pivot point of the pendulum and if x represents the angle through which the pendulum bob swings, then the Hamiltonian H for the pendulum is

$$H = \tfrac{1}{2}p^2 - \cos x. \tag{1}$$

The classical equations of motion for this Hamiltonian are

$$\dot{x} = \frac{\partial H}{\partial p} = p, \qquad \dot{p} = -\frac{\partial H}{\partial x} = -\sin x. \tag{2}$$

The energy E for this system is a constant of the motion (it is a time-independent quantity) because the system is Hamiltonian. If we take the energy E to be real, we find that the classical trajectories are confined to cells of horizontal width 2π. This is the periodic analog of the double-well anharmonic oscillator. If the energy of the classical particle in a periodic potential is taken to be complex, the particle hops from well to well in analogy to the behavior of a quantum particle in a double well. This hopping behavior is a deterministic random walk [11, 17].

The most dramatic analogy between complex classical mechanics and quantum mechanics is established by showing that there exist narrow conduction bands in the periodic potential for which the complex classical particle exhibits unidirectional hopping and the quantum particle exhibits resonant tunneling. The behavior of such a classical particle is discussed in detail in [17]. In [17] a lengthy numerical analysis was done that shows that the classical conduction bands have a narrow but finite width (see figure 1). The edges of the conduction bands are sharply defined.

2. Numerical study of elliptic potentials

Having studied the behavior of a particle in a trigonometric periodic potential, it is natural to generalize this analysis by considering the behavior of a particle in an elliptic potential. Elliptic functions are doubly periodic generalizations of trigonometric functions. Also, they are analytic except for simple poles, and this allows us to continue analytically the classical trajectories into the complex plane. The specific Hamiltonian that we have chosen to examine is the obvious generalization of the Hamiltonian in (1):

$$H = \tfrac{1}{2}p^2 - \mathrm{Cn}(x, k). \tag{3}$$

Here $\mathrm{Cn}(x, k)$ is a *cnoidal* function [18, 19]. When the parameter $k = 0$, the cnoidal function reduces to the singly periodic function $\cos x$, and when $k = 1$, the cnoidal function becomes $\tanh x$. When $0 < k < 1$, the cnoidal function is periodic in both the real and imaginary directions and it is meromorphic. (A *meromorphic* function is analytic in the finite-x plane

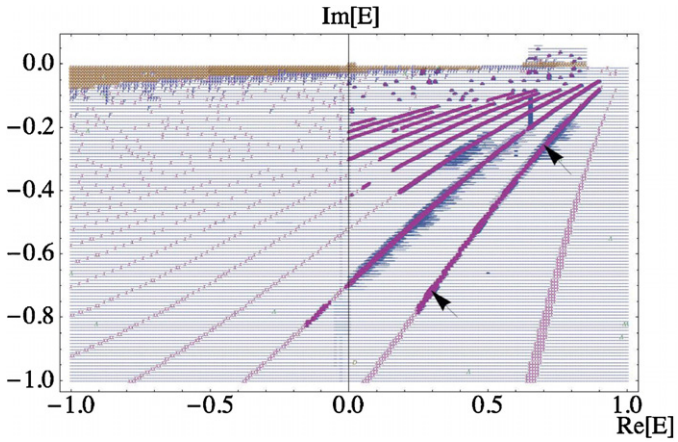

Figure 1. Complex-energy plane showing those energies that lead to tunneling (hopping) behavior and those energies that give rise to conduction for a particle in a $-\cos x$ potential. Hopping behavior is indicated by a hyphen - and conduction is indicated by an X. The symbol & indicates that no tunneling takes place; tunneling does not occur for energies whose imaginary part is close to 0. In some regions of the energy plane very intensive numerical studies were done and the X's and -'s are densely packed. This picture delineates 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 $\mathrm{Re}\,E = -0.95, -0.7, -0.25, 0.15, 0.7$. This picture is symmetric about $\mathrm{Im}\,E = 0$, and the bands get thicker as $|\mathrm{Im}\,E|$ increases. A total of 68 689 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. Note that the band edges are clearly and sharply defined.

except for well-separated pole singularities.) The real part of the cnoidal potential $\mathrm{Cn}(x, k)$ is plotted in figure 2. The classical particle trajectories satisfy Hamilton's equations

$$\dot{x} = \frac{\partial H}{\partial p} = p, \qquad \dot{p} = -\frac{\partial H}{\partial x} = -\mathrm{Sn}(x, k)\,\mathrm{Dn}(x, k). \tag{4}$$

The trajectories for $k > 0$ are elaborate in that the classical particles can move vertically as well as horizontally. Figure 2 shows a typical trajectory of a particle having complex energy. The energy of the particle is $E = 1/2 + i/10$ and $k = 1/10\,000$. We know from [17] that if $k = 0$, the particle will spiral outward from a pair of turning points and then hop horizontally to an adjacent site on the real-x axis. It is remarkable that even though k is very small, the particle moves vertically. Thus, giving the parameter k a nonzero value represents a singular perturbation of the Hamiltonian in (1).

The right panel of figure 2 shows the real part of the cnoidal function $\mathrm{Cn}(x, 1/10\,000)$ plotted as a function of complex x. The poles of the cnoidal function appear as chimneys in both the positive and the negative directions. Note that the path of the particle rolls around the singularities until it is captured by a pair of turning points in another cell. The particle spirals inward around these turning points and then spirals outward again before leaving the cell and heading to another.

The novelty of the cnoidal potential is that complex classical-mechanical particles may hop from cell to cell in both horizontal and vertical directions. While this motion appears to be two dimensional, we emphasize that the Hamiltonian in (3) has only one (complex) degree of freedom.

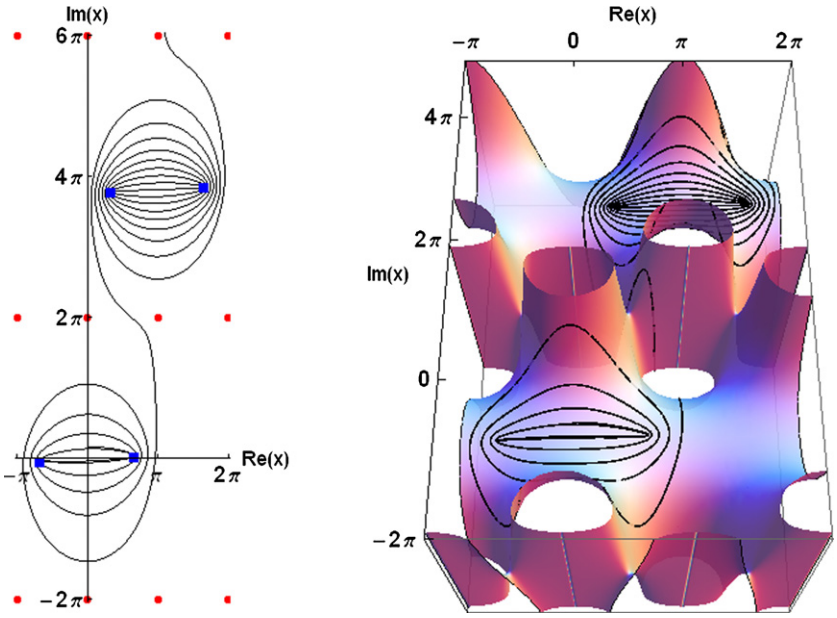

Figure 2. Trajectory of a particle in the complex cnoidal potential $\mathrm{Cn}(x, 1/10\,000)$. The particle is initially at $x(0) = i$ and its path $x(t)$ is plotted in the complex-x plane for $0 \leqslant t \leqslant 124.4$. The energy of the particle is $E = 1/2 + i/10$. In the left panel, the turning points are indicated by small squares and the pole singularities of the cnoidal function are indicated by small circles. In the right panel, the particle trajectory is superimposed on a three-dimensional relief plot of the real part of the cnoidal function.

What happens to the trajectory of the particle in figure 2 if we follow it for a longer period of time? Figure 3 shows the trajectory for $0 \leqslant t \leqslant 1200$. Observe that the particle is temporarily captured by 16 cells in this time period. These cells are numbered in the order in which their turning points capture the particle, where by *capture* we mean that the particle spirals around the turning points in that cell. After the particle leaves cell 1, it is temporarily captured by the turning points in cell 2, which is northeast of and adjacent to cell 1. Similarly, cell 3 is northeast of and adjacent to cell 2. However, the particle then jumps nonadjacently to cell 4, passing briefly through cells 2, 5 and 1, without being captured by the turning points in these cells.

Note that the particle in figure 3 is never captured by the same pair of turning points twice. The behavior of this complex self-avoiding trajectory is typical of a particle whose energy lies in a conduction band. It is not easy to verify this, but a careful examination of figure 1 shows that the energy $E = 1/2 + i/10$ lies in the middle of a conduction band. (Figure 1 was constructed for $k = 0$, but because $k = 1/10\,000$ in figure 3, figure 1 gives an extremely good approximation to the location of the conduction bands.)

To see how the trajectory of a particle behaves when the energy of the particle is not in a conduction band, we change the energy of the particle in figure 3 to $E = 1/2 + 3i/20$. This energy lies outside a conduction band, and consequently the particle can be recaptured by pairs of turning points. In particular, one can see in figure 4 that as t runs from 0 to 1200, the particle is captured twice by the turning points in six cells. This particle appears to be executing a two-dimensional deterministic random walk.

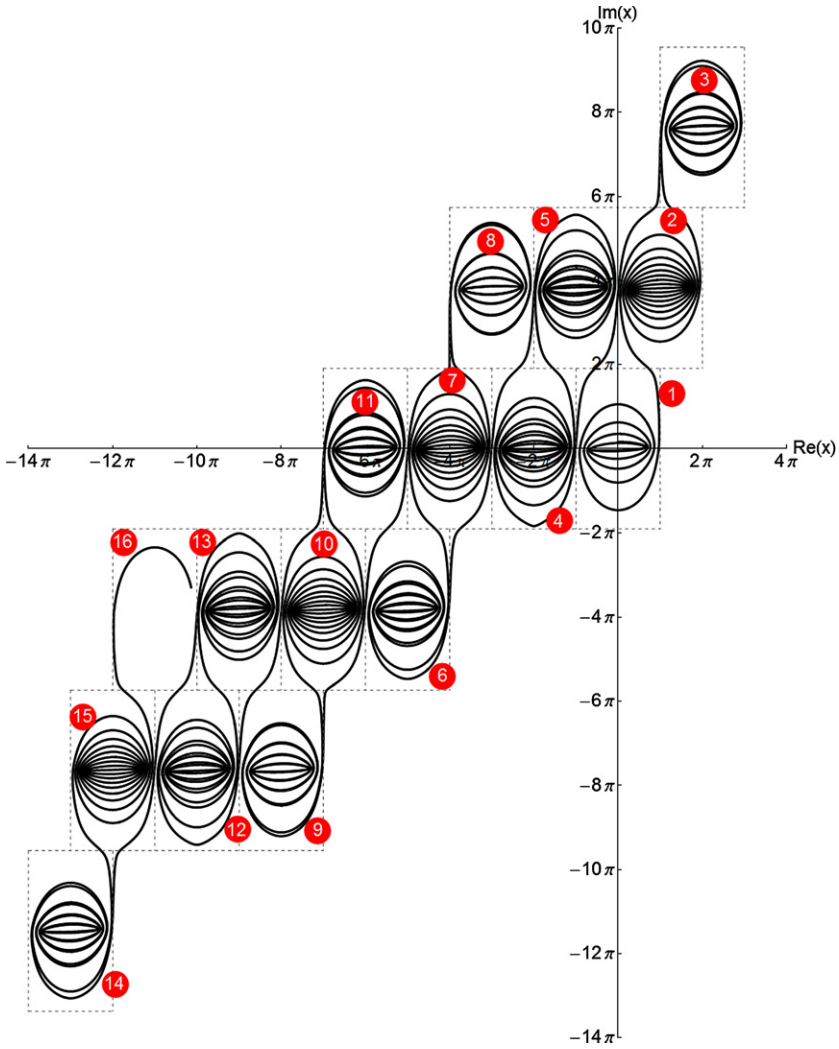

Figure 3. Complex classical trajectory for a particle of energy $E = 1/2 + i/10$ in a cnoidal potential with $k = 1/10\,000$. The trajectory begins at $x(0) = i$ in cell 1. (Cells are delineated by dotted lines and poles lie at the corners of every cell. Each cell contains one pair of turning points.) The particle spirals out of cell 1 and is captured by the turning points in cell 2. It then escapes from these turning points and is captured by the turning points in cell 3, and so on. Note that cell 1 is adjacent to cell 2, and that cell 2 is adjacent to cell 3, but that cell 3 is *not* adjacent to cell 4. The path shown in this figure reaches cell 16 at $t = 1200$. The particle shown in this figure is never captured by the same pair of turning points twice. This is because the energy of the particle lies in a conduction band, as one can see from a careful examination of figure 1.

To compare in greater detail the differences between conduction-band and nonconduction-band trajectories, we investigate two trajectories that arise from the initial point $x(0) = i$ when $k = 1/10$. For the first trajectory, we take the energy to be $E = 0.285 - 0.716i$, and for the second trajectory, we take the energy to be $E = 0.245 - 0.716i$. An examination of figure 1 shows that in the former case, the energy is in a conduction band and in the latter case it is not. In figure 5, we plot both trajectories for $0 \leqslant t \leqslant 200$. The first trajectory moves

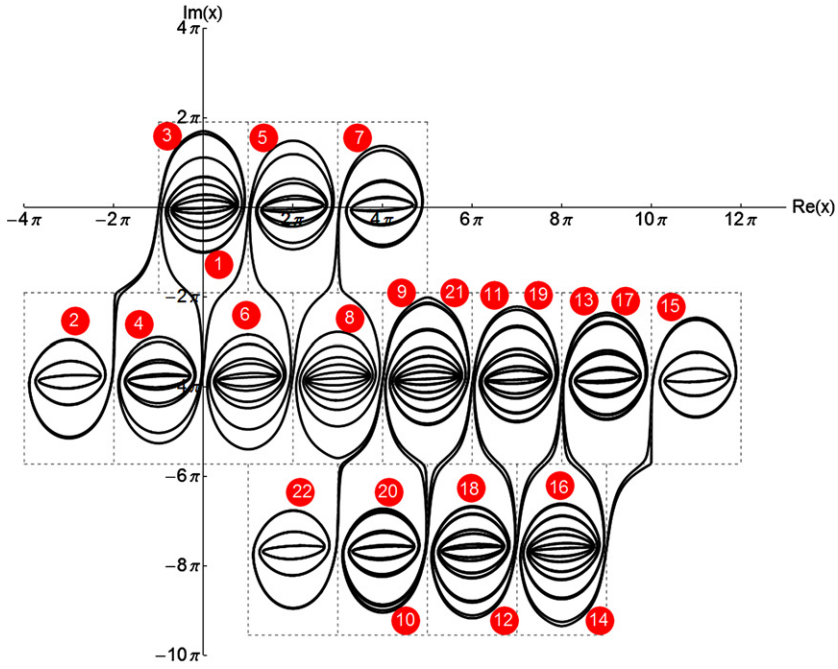

Figure 4. Same as figure 3 except that the energy of the particle is $E = 1/2 + 3i/20$. This energy does not lie in a conduction band, and consequently the particle is captured twice by several pairs of turning points. The turning-point captures are labeled sequentially by the numbers in the circles. As an example of a double capture, when the particle is captured for the sixteenth time, it is in the same cell as it was during its fourteenth capture. Note that complex trajectory never crosses itself.

off in a northwesterly direction and never returns. In the left panel of figure 5, we show the first fourteen captures. The right panel shows the second trajectory. This trajectory begins to revisit cells starting with its seventh capture. We emphasize that the trajectory never crosses itself.

There are two possible ways for a trajectory to turn around when the energy of the particle is not in a conduction band. These are shown in the middle and right panels of figure 6. In all three panels in figure 6, a trajectory begins at the lower end of the figure and moves upward. In the left panel, the trajectory loops around the two turning points and encounters a pole singularity, which deflects the trajectory upward into the next cell. The next two panels show trajectories that are deflected downward by a pole singularity; these trajectories will be recaptured by a previous pair of turning points. The trajectory in the middle panel differs from that in the right panel in that it encircles the lower turning point in an anticlockwise direction and thus it continues downward to the *left* of the original upward trajectory.

To investigate what happens at the edge of a conduction band, we have done a detailed numerical study of trajectories of particles having the same imaginary energy component $\mathrm{Im}\, E = 0.716$ but different real energies for a given value of k and $x(0)$. We have then determined the time required for a particle trajectory to turn around as the real part of the energy nears the edge of a conduction band. One would expect that it takes longer for the particle trajectory to turn around, as it does in the right panel of figure 5, when the real part of the energy approaches the band edge. Measuring the precise turn-around time is difficult, and to do so we must look for turn-around behavior of a consistent type; we have chosen to look

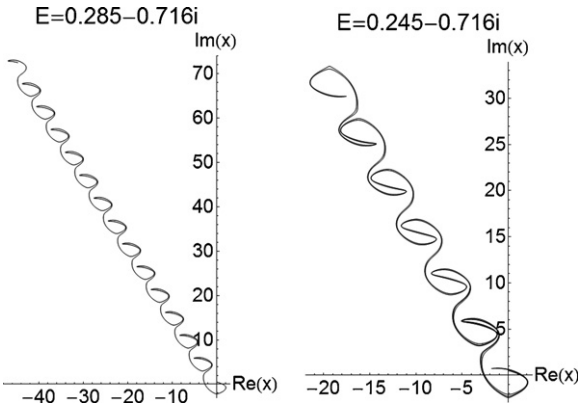

Figure 5. Complex classical trajectories for particles of energy $E = 0.285 - 0.716i$ (left panel) and $E = 0.245 - 0.716i$ (right panel) in a cnoidal potential with $k = 1/10$. Both trajectories begin at $x(0) = i$ and run from $t = 0$ until $t = 200$. In the left panel, the energy is in a conduction band and the trajectory never revisits any cell, but in the right panel the energy is not in a conduction band and the trajectory is recaptured by the previously visited turning points.

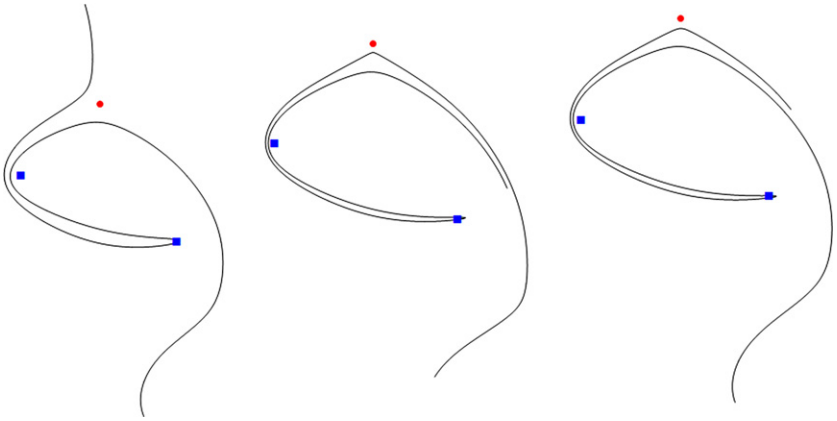

Figure 6. Three classical trajectories similar to those in figure 5. All three trajectories begin at the lower end of the figure. In the left panel, the trajectory loops around a pair of turning points (small squares) and is then deflected by a pole singularity (small circle) upward into the next cell. The other two panels show the different ways for the trajectory to turn back on itself.

for the behavior shown in the *right* panel of figure 6. In figure 7, we plot the turn-around time τ as a function of the real part of the energy while holding the imaginary part of the energy constant. The band edge is located at $\mathrm{Re}\, E = 0.284$. The dotted curve is a fit to the data points of the form

$$\tau(\mathrm{Re}\, E) = \frac{4.872}{(0.284 - \mathrm{Re}\, E)^{8/9}}. \tag{5}$$

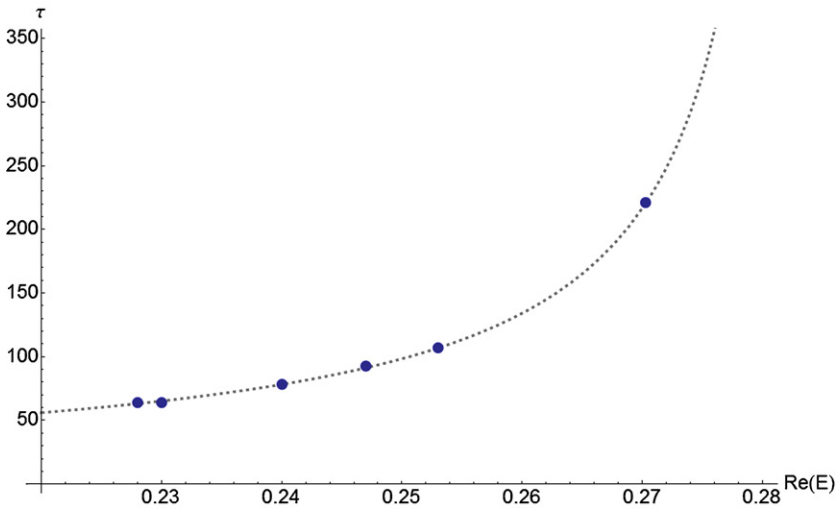

Figure 7. Plot of the turn-around time τ for a complex trajectory near the edge of a conduction band. The complex cnoidal potential has $k = 1/10$ and τ is plotted as a function of the real part of the energy of the particle. The imaginary part of the energy is held constant for all data points at Im $E = 0.716$. The turn-around time becomes infinite at the edge of the conduction band Re $E = 0.284$. The dotted line is the fitting curve in (5).

3. Concluding remarks

There is a deep connection between quantum mechanics and complex classical mechanics. In the complex domain, the classical trajectories exhibit a remarkable behavior that is analogous to quantum tunneling and periodic potentials exhibit a surprising and intricate feature that closely resembles quantum band structure. We have seen in this paper that the classical bands, just like the quantum bands, have finite width and well-defined sharp edges.

The complex trajectories of a particle in a doubly periodic potential can exhibit a wider range of qualitative behaviors than those of a particle in a singly periodic potential partly because there is a two-dimensional array of cells containing pairs of turning points and also because doubly periodic potentials have singularities. We have observed the following features. (i) The path of a particle can go both vertically and horizontally as the particle visits the cells in the complex-x plane (see figure 4). (ii) When a particle is captured by a pair of turning points in a cell, the number of turns in the inward and outward spirals does not change from cell to cell, and thus there is a characteristic capture-and-escape time (see figures 2–4). This time depends on the energy of the particle and on the value of k. (iii) If the energy of the particle does not lie in a conduction band, the particle can be captured by pairs of turning points multiple times (see figure 4). (iv) The particle trajectory is continuous, and therefore each new cell that a particle visits is adjacent to the previous cell. However, the particle is not always captured by the turning points in an adjoining cell; captures may occur nonlocally (see figure 3). (v) Finally, when the energy of a particle lies in a conduction band, the particle is never captured twice by any pair of turning points. However, the trajectory of the particle is not necessarily unidirectional; the particle may exhibit elaborate kinds of zigzag motions as it drifts through the lattice (see figure 3).

A difficult and so far unanswered question is: does a complex classical particle whose energy is not in a conduction band undergo a two-dimensional random walk in a doubly

periodic potential as it visits the cells in the lattice? The answer to this question is not obvious because the trajectory of the particle cannot cross itself. However, this does not mean that the particle must hop from cell to cell in a self-avoiding manner. Numerical studies suggest that it is still possible for the particle to visit cells repeatedly and in any order.

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