Quantum tunneling as a classical anomaly

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Abstract. Classical mechanics is a singular theory in that real-energy classical particles can never enter classically forbidden regions. However, if one regulates classical mechanics by allowing the energy \(E\) of a particle to be complex, the particle exhibits quantum-like behavior: Complex-energy classical particles can travel between classically allowed regions separated by potential barriers. When \(\text{Im} \ E \to 0\), the classical tunneling probabilities persist. Hence, one can interpret quantum tunneling as an anomaly. A numerical comparison of complex classical tunneling probabilities with quantum tunneling probabilities leads to the conjecture that as \(\text{Re} \ E\) increases, complex classical tunneling probabilities approach the corresponding quantum probabilities. Thus, this work attempts to generalize the Bohr correspondence principle from classically allowed to classically forbidden regions.

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Classical mechanics is a singular limit of quantum mechanics. (The limit \(\epsilon \to 0\) is singular if an abrupt change occurs at \(\epsilon = 0\). For example, \(\lim_{\epsilon \to 0} \epsilon x^5 + x = 1\) is singular because four of its five roots abruptly disappear at \(\epsilon = 0\).) The classical limit \(\hbar \to 0\) of the time-independent Schrödinger equation \(\hbar^2 \psi''(x) = [V(x) - E] \psi(x)\) is singular because at \(\hbar = 0\) it is no longer possible to impose initial or boundary conditions on the wave function \(\psi(x)\). Moreover, while quantum particles are able to enter classically forbidden regions, these particles abruptly lose this ability at \(\hbar = 0\). Thus, the phenomenon of tunneling seems to be entirely quantum mechanical, and one may not ask such classical questions as, Which path does the particle follow while tunneling?

It may be possible to recover some features of a theory that were abruptly lost in a singular limit, like the ability of a particle to enter a classically forbidden region. To do so, one introduces a regulator, which is then removed in a careful limiting process. The features that remain after the regulator is removed are referred to as anomalies. (The axial anomaly in quantum field theory can be obtained by using dimensional regulation.)

Particle trajectories in conventional classical mechanics are real functions of time, but recent studies of the complex solutions to the classical equations of motion...
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Hamilton’s equations have shown that real-energy classical particles may leave the real axis and travel through complexified coordinate space \([1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]\). While these complex classical trajectories may pass through classically forbidden regions on the real axis, complex classical mechanics is still a singular theory because there is no tunneling; that is, no complex path runs from one classically allowed region on the real axis to another.

Complex classical mechanics may be regulated by taking the energy of a particle to be complex. Surprisingly, a complex-energy classical particle exhibits qualitative features normally associated with a quantum particle: Such a classical particle can exhibit tunneling-like behavior in which it travels from one classically allowed region to another classically allowed region even though these two regions are separated on the real axis by a classically forbidden region \([13, 14]\). Furthermore, a complex-energy classical particle in a periodic potential exhibits quantum-like behavior; there are sharply defined energy bands separated by gaps. In these energy bands the classical particle exhibits a kind of resonant tunneling \([13]\). The time-energy uncertainty principle supports our choice of regulator. This uncertainty principle implies that a precise measurement of the energy of a particle in a finite time interval is impossible; some uncertainty \(\Delta E\) is associated with such a measurement. In this paper we allow \(\Delta E\) to be complex.

This paper explores the connection between standard quantum mechanics and complex-energy classical mechanics at a quantitative level. We show that as the regulator is removed (\(\text{Im} \ E \to 0\)), the tunneling behavior of complex-energy classical mechanics persists. Thus, we recover tunneling as a kind of anomaly.

To compare the behavior of quantum particles and complex classical particles, we use quartic and sextic asymmetric double-well potentials and compute numerically the relative probabilities of finding these particles in each well. We find that as the number of nodes in the quantum-mechanical eigenfunction increases, the quantum and classical probabilities approach one another. Thus, we demonstrate that the Bohr correspondence principle, which has recently been generalized to the complex domain \([15, 16]\), actually applies to tunneling phenomena.

The quartic double-well potential

\[
V^{(4)}(x) = \frac{7}{2}x(x-1) \left( x + \frac{191}{100} \right) \left( x - \frac{49}{20} \right)
\]  

(1)

is shown in the upper panel in Fig. 1. The first six quantum energy levels of \(H = p^2 + V^{(4)}(x)\), where we have set \(\hbar = 1\), are \(E_0 = -18.0182\) (below the bottom of the right well), \(E_1 = -7.1879\), \(E_2 = -6.8595\), \(E_3 = 1.6806\), and \(E_4 = 2.8845\) (above the bottom of the right well and below the peak of the barrier), and \(E_5 = 8.3312\) (above the barrier).

We plot the sextic potential

\[
V^{(6)}(x) = x^6 - 2x^5 - 4x^4 + 11x^3 - \frac{11}{4}x^2 - 13x
\]  

(2)

in the lower panel in Fig. 1. The exact ground-state energy for \(H = p^2 + V^{(6)}(x)\) with \(\hbar = 1\) is \(E_0 = -23/2\). (This exact value of \(E_0\) provides a benchmark confirming that our
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Figure 1. Upper panel: Quartic asymmetric double-well potential $V^{(4)}(x)$ in (1) and the first six quantum energy levels. There are minima at $x = -1.2499$, where $V^{(4)} = -24.0384$, and at $x = 1.9165$, where $V^{(4)} = -12.5501$. The peak of the barrier is at $x = 0.4884$, where $V^{(4)} = 4.1144$. The ground-state energy $E_0$ lies below the bottom of the right potential well. The next four energy levels lie between the bottom of the right potential well and the top of the barrier. The sixth energy level $E_5$ lies above the barrier. Lower panel: Sextic asymmetric double-well potential $V^{(6)}(x)$ in (2). The minima of the wells are at $x = -1.7083$, where $V^{(6)} = -20.7710$, and at $x = 1.8215$, where $V^{(6)} = -13.9373$. The peak of the barrier is located at $x = -0.5184$, where $V^{(6)} = 4.2731$. 
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Figure 2. Quantum probability density for a particle in the $n$th eigenstate in the quartic potential $V^{(4)}(x)$ in (1). The probability $P_{\text{right},n}^{\text{quant}}$ in (3) of finding a particle in the $n$th eigenstate to the right of the barrier is determined by integrating the $n$th probability density.

Numerical calculations are accurate to better than 13 decimal places.) The first three excited quantum states have energies $E_1 = -9.9690$, $E_2 = -3.9819$, and $E_3 = 1.8095$.

The eigenfunction $\psi_n(x)$ corresponding to the energy $E_n$ has $n$ nodes. In Fig. 2 we plot the probability density $|\psi_n(x)|^2$ for a particle in $V^{(4)}(x)$ for $n = 0, 1, \ldots, 5$. We integrate $|\psi_n(x)|^2$ to determine the probability $P_{\text{right},n}^{\text{quant}}$ of finding the particle to the right of the barrier [13]:

$$P_{\text{right},1}^{\text{quant}} = 99.5933\%, \quad P_{\text{right},2}^{\text{quant}} = 0.4316\%,$$

$$P_{\text{right},3}^{\text{quant}} = 59.7584\%, \quad P_{\text{right},4}^{\text{quant}} = 40.7689\%. \quad (3)$$
For the sextic potential $V^6(x)$ in (2) we find that for the first four quantum states the probabilities of finding the particle to the right of the top of the barrier are

\[ P_{\text{quant right},0} = 0.0391\%, \quad P_{\text{quant right},1} = 99.9986\%, \]
\[ P_{\text{quant right},2} = 99.8651\%, \quad P_{\text{quant right},3} = 78.7223\%. \]  

(4)

We now describe the behavior of a classical particle in the quartic potential (1) for the case in which $x$ is complex. Such a particle may have either real or complex energy, and we begin by considering the complex trajectories of a real-energy classical particle. Let us take the energy of a classical particle in $V^{(4)}$ to be $E_4 = 2.8845$. There are two real turning points at $x = -1.9428$ and 0.2234, which bound the classically allowed region to the left of the barrier and two turning points at $x = 0.7596$ and 2.4998, which bound the classically allowed region to the right of the barrier. If the initial position of the particle is real and in the classically allowed region in the right (or left) well, the trajectory of the particle oscillates on the real axis between the right (or left) pair of turning points. However, if the particle is initially in a classically forbidden region on the real axis, the particle leaves the real axis and travels in a closed periodic orbit in the complex-$x$ plane [see Fig. 3 (upper panel)]. The orbits in the complex-$x$ plane enclose the classically allowed regions on the real axis and never cross the vertical line $\text{Re} \, x = 0.4884$, which passes through the peak of the barrier. The periods $T$ of all closed orbits, both on the left and right side of Fig. 3, are the same and are given by

\[ T = \int_{x_{\text{left}}}^{x_{\text{right}}} \frac{dx}{\sqrt{E - V^{(4)}(x)}}, \]

where $x_{\text{left}}$ and $x_{\text{right}}$ are the left and right turning points in either well and $E$ is the (real) classical energy of the particle. For the case in which the energy $E = E_4 = 2.8845$, the period $T = 0.8464$. The particle in the upper panel of Fig. 3 cannot travel from one classically allowed region to the other classically allowed region, so there is no tunneling effect when the classical energy is exactly real.

We now explain how deterministic classical systems can produce results that are numerically comparable to the quantum results in (3) and (4). If the energy $E$ of the classical particle is complex, the classical trajectory of such a particle is not in general closed [13]. In Fig. 4 we plot the complex path of a classical particle of energy $E = 2.8845 + 0.25i$ for the time interval from $t = 0$ to $t = T = 0.8464$. Observe that while the particle executes a loop of nearly $360^\circ$ around the two turning points, the trajectory of the particle is no longer closed. If this particle is initially in a classically allowed region, it spirals outward around the pair of turning points that bound the region. However, the particle does not drift off to infinity. Rather, it crosses the vertical line that passes through the top of the barrier and spirals into the other well. This behavior is shown in Fig. 3 (lower panel), where a particle of energy $E = 2.8845 + 0.5i$ alternately visits both potential wells. This classical particle executes deterministic tunneling from well to well.

There is an unexpected subtlety in the behavior of complex-energy classical particles that should not be overlooked. While the spiral motion shown in the lower panel in Fig. 3...
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Figure 3. Upper panel: Periodic trajectories in the complex-$x$ plane of a classical particle of real energy $E_4 = 2.8845$ in the quartic potential. The dots indicate the four turning points. There is no tunneling-like behavior; no trajectory runs from one classically allowed region to the other. Lower panel: Classical trajectory in the complex-$x$ plane of a particle of complex energy $E = 2.8845 + 0.5i$ in the same potential. Unlike the closed trajectories in the upper panel, this classical trajectory is open. The particle begins at $x = 1$ and traces an outward anticlockwise spiral around the right pair of turning points. It then crosses to the left of the peak of the barrier and spirals inward and clockwise around the left pair of turning points. Next, it crosses the real axis between the left turning points and spirals outward and anticlockwise around the left pair of turning points. The time for the displayed trajectory is $t = 8$. For $t > 8$, the particle continues to spiral inward and outward as it oscillates from well to well. The particle exhibits this deterministic tunneling-like behavior for all time, but the trajectory never crosses itself. This trajectory behaves as if it were controlled by a pair of strange attractors.
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Figure 4. Complex path of a particle of complex energy $E = 2.8845 + 0.25i$. The time of this path is taken to be $t = T = 0.8464$, which is the same as the period of a classical particle of real energy $E = 2.8845$. Note that the particle in this figure makes an approximately full angular revolution around the two turning points, which are denoted by dots. However, the path is not closed.

is typical of complex-energy classical particles, it has recently been discovered that for a dense set of measure zero of complex classical energies the classical paths are periodic [14]. The complex energies for which the classical motion remains closed and periodic lie on an infinite number of nearly straight lines that emanate from the origin in the complex-energy plane. A schematic representation of these lines is shown in Fig. 5.

The key advance in this paper is the numerical observation that the probabilities associated with the tunneling of a classical particle having complex energy persist as the regulator $\text{Im} \Delta E$ tends to zero even though there is no classical tunneling when $\text{Im} E = 0$. The upper panel in Fig. 3 shows that a classical particle having real energy does not exhibit tunneling behavior. Yet, a classical particle having $\text{Im} E \neq 0$ typically does exhibit tunneling behavior, and the corresponding probabilities can be compared in the limit as $\text{Im} E \to 0$ with the quantum tunneling probabilities in (3) and (4).

To demonstrate the persistence of classical tunneling in the limit $\text{Im} E \to 0$, we compute the classical trajectory for long times [17] and determine the fraction of time...
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Figure 5. Schematic drawing of the special complex energies for which the particle motion in the quartic potential \(E\) is periodic for any choice of initial condition. These energies lie on asymptotically straight dashed curves that approach the origin in the complex-\(E\) plane. The energies form a set of measure zero; there are an infinite number of such curves and these curves are dense in the complex-\(E\) plane. The regulation procedure used in this paper establishes a connection between complex classical mechanics and quantum mechanics by taking a sequence of complex classical energies in which the imaginary part tends to 0. This sequence is indicated by dots on the solid vertical line. Although this line intersects the dashed lines infinitely many times, the numerical procedure remains unaffected.

that the classical particle spends to the left and to the right of the line \(\text{Re } x = 0.4884\) (the location of the peak of the potential barrier). As \(\text{Im } E\) gets smaller, the fraction of time spent to the right (and to the left) of the barrier approaches a constant.\(^\dagger\) Take the real part of the classical energy to be the fourth excited quantum energy \(\text{Re } E = E_4 = 2.8845\) and take \(\text{Im } E = 2^{-k}\). For \(k = 0, 1, 2, 3, 4, 5\) the chance of finding the classical particle to the right of the barrier is 50.4\%, 53.9\%, 55.0\%, 53.1\%, 52.8\%, 53.3\%. This sequence approaches a limiting anomalous value of about 53\%, which exceeds 50\% in accordance with the heuristic semiclassical argument in Ref. [18]. A classical version of the time-

\(^\dagger\) Figure 4 shows that each angular revolution in the complex-energy spiral takes approximately the same time regardless of whether the spiral encircles the left or the right pair of turning points. The left-right asymmetry in the well gives rise to different left and right winding numbers in the spiral path.
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...energy uncertainty principle applies here: As the imaginary part of the energy gets smaller, it takes more time for the particle to oscillate between the wells [13], and thus this extrapolation procedure for determining the classical tunneling probabilities requires more computer time.

Classical tunneling persists in the limit as $\text{Im} E \to 0$ even though there is no classical tunneling at $\text{Im} E = 0$; Fourier series exhibit strongly analogous behavior.

Take the function $f(x) = 1$ on $[0, \pi]$. Although $f(0) \neq 0$ and $f(\pi) \neq 0$, we can represent $f(x)$ as the Fourier sine series

$$4\pi \sum_{k=0}^{\infty} \frac{1}{2k+1} \sin[(2k+1)x].$$

The partial sum $S_K(x) = \sum_{k=0}^{K} a_k \sin(kx)$ converges to $f(x)$ as $K \to \infty$ on the open interval $(0, \pi)$ because $f(x)$ is continuous. All terms in $S_K(x)$ vanish at 0 and $\pi$, but we can still recover the nonzero value of $f(0)$ and $f(\pi)$ from $S_K(x)$. The extrapolation procedure used above for classical tunneling probability can be applied to Fourier series to determine $f(0)$. We take twice as many terms in $S_K(x)$ as $x$ is halved and thereby circumvent the problem of nonuniform convergence (the Gibbs phenomenon): We evaluate $S_{100}(x)$ at $K = 100 \times 2^k$ and $x = 2^{-k}$ for $k = 0, \ldots, 5$. The numerical values of $S_K(x)$ are $S_{100} = 0.997\,776$, $S_{200} = 0.996\,704$, $S_{400} = 0.997\,293$, $S_{800} = 0.997\,818$, $S_{1600} = 0.998\,128$, $S_{3200} = 0.998\,292$. We infer that $f(0) = 1$.

In analogy with the extrapolation scheme used for Fourier series, we determine the classical probability of finding the particle to the right of the peak of the barrier for a sequence of energies in which the real part of the energy is held fixed and the imaginary part of the energy tends to zero. For a small but fixed imaginary classical energy, the classical probability approaches the quantum probability as the real part of the energy increases. For example, when $\text{Im} E = 1/4$ and $\text{Re} E = E_n$, where $E_n$ is the $n$th quantum eigenenergy for the quartic potential $V^{(4)}(x)$ in (1), we obtain the following classical probabilities for finding the classical particle in the right well:

$$
P_{\text{class right,1}} = 55.4\%, \quad P_{\text{class right,2}} = 55.0\%,$$

$$
P_{\text{class right,3}} = 54.3\%, \quad P_{\text{class right,4}} = 55.0\%. 
$$

The quantum probabilities $P_{\text{quant right,n}}$ in (3) oscillate about these classical probabilities and are in good agreement when $n = 3$ and $n = 4$. For deeper double-well potentials, the classical probabilities continue to approach the quantum probabilities as $n$ increases.

For the sextic potential $V^{(6)}(x)$ in (2) there are six turning points. When the classical energy is real and between the minimum of the lower well and the top of the barrier, the turning points group into three pairs, one pair on the real axis to the left of the barrier, a second pair on the real axis to the right of the barrier, and a complex-conjugate pair that is associated with the complex extension of the barrier. If we take the classical energy to be real, say $E_n$, we cannot observe tunneling because the classical orbits are closed and periodic and just encircle the pairs of turning points, as shown in the upper panel of Fig. [6].

When the classical energy $E$ is complex, the classical path is no longer closed. A particle trajectory beginning at $x = 1$ in the right well spirals outward and eventually circles around the barrier turning points. The trajectory does not always penetrate
Figure 6. Complex classical trajectories for a particle subject to the sextic potential \([2]\). The energy of the particle in the upper panel is real and three closed nonintersecting trajectories for this particle are shown. The energy of the particle in the lower panel is complex and a single open trajectory is plotted.

to the left well; sometimes the particle is ejected and falls back into the right well. However, after sufficiently many tunneling attempts the particle spirals inward around the left pair of turning points, as shown in the lower panel of Fig. 6. Taking \(\text{Im } E = 1/16\) and \(\text{Re } E = E_n\) \((n = 0, 1, 2, 3)\), we find that as the real part of the energy increases, the classical tunneling probabilities \(P_{\text{class}, n}^{\text{right}}\) listed below approach the quantum probabilities \(P_{\text{quant}, n}^{\text{right}}\) in (4):

\[
\begin{align*}
P_{\text{class}, 0}^{\text{right}} &= 91.7\%, & P_{\text{class}, 1}^{\text{right}} &= 87.1\%, \\
P_{\text{class}, 2}^{\text{right}} &= 32.4\%, & P_{\text{class}, 3}^{\text{right}} &= 72.3\%. 
\end{align*}
\]
The agreement between (4) and (6) is better than that for the quartic case, possibly because the mixture of successful and failed tunneling attempts through the central barrier region leads to a more accurate analog of quantum tunneling. We conclude that complex classical mechanics provides a good approximation to quantum tunneling for the higher-energy states, as one would expect of a generalized Bohr correspondence principle.

Of course, the agreements between (3) and (5), and (4) and (6) are not very precise. To obtain better agreement, it is necessary to take deeper asymmetric double wells having more quantum eigenenergies below the top of the central barrier and above the bottom of the shallower well. This can also be achieved by taking $\hbar$ to have a smaller numerical value. (The coefficient of $-d^2/dx^2$ in the Schrödinger equation is $\hbar^2$.) Until now, we have taken $\hbar = 1$ but we have repeated our numerical work for the quartic potential (1) with $\hbar = 1/2$. Now, the highest eigenvalue below the top of the barrier is $E_8 = 3.7239$. The corresponding probability density $|\psi_8(x)|^2$ is shown in Fig. 7. For this eigenfunction, the quantum probability of finding the particle to the right of the peak of the barrier is $60.29\%$ and the corresponding classical probability using the complex energy $E = E_8 + i/4$ is $55.2\%$. (These numbers compare favorably with $P_{\text{quant}}^{\text{right},4} = 40.7689\%$ and $P_{\text{class}}^{\text{right},4} = 55.0\%$ for the highest eigenvalue in the double well with $\hbar = 1$.) Doing further calculations for successively smaller values of $\hbar$ would require a considerable increase in computer time. The purpose of this paper is only to demonstrate, in principle, our conjectured connection between complex classical and quantum tunneling, and not to carry out an extensive and detailed numerical investigation.

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Figure 7. Quantum probability density for a particle in the $\psi_8(x)$ eigenstate in the quartic potential [1] with $\hbar = 1/2$. The energy of the particle is $E_8 = 3.7239$. The probability density has eight nodes. Note that the particle is most likely to be found inside or near the classically forbidden region associated with the barrier; this shows that the particle does not have a high enough quantum number for its behavior to resemble that of a classical particle.

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[17] To determine the long-time behavior we calculate numerically the characteristic time required for a particle to spiral into and away from a pair of turning points. The characteristic time, which is different for each well, is almost constant and approaches a constant for very long times.
[18] The data in [3] can be used to contrast quantum and classical mechanics. One might argue heuristically (but wrongly!) as follows: A classical particle of energy $E$ in the deep left well has more kinetic energy than the same particle in the shallow right well. Thus, in the left well the particle would make more frequent tunneling attempts than the same particle in the right well. Hence, it is more likely to find the particle in the right well. From [3] we see that $P_{\text{quant right,1}} = 99.5933\%$, so a quantum particle of energy $E_1$ is almost always in the right well, which seems to support this heuristic argument. However, the quantum probability alternates with increasing $n$: $P_{\text{quant right,2}} = 0.4316\%$, so the particle is almost never in the right well. The heuristic argument is invalid because it treats the quantum particle in the classically allowed region as a localized classical particle that repeatedly collides with the barrier. According to the correspondence principle, such semiclassical reasoning only works for larger quantum numbers. Indeed, $P_{\text{quant right,3}} = 59.7584\%$ and $P_{\text{quant right,4}} = 40.7689\%$, which is more consistent with the heuristic argument.