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Visualizing the solutions for the circular infinite well in quantum and classical mechanics

R. W. Robinett
High Energy Physics Division
Argonne National Laboratory
Argonne, IL 60439 USA

and

Department of Physics
The Pennsylvania State University
University Park, PA 16802 USA¹

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Abstract

The classical and quantum mechanical problem of a particle in the infinite circular well has recently surfaced in two quite different manifestations; (i) the observation of 'electron standing waves' in circular 'corrals' of atoms adsorbed on surfaces and (ii) as a benchmark example of an integrable system for comparison to the classical and quantum chaotic behavior of the 'stadium billiards' problem. Motivated by this, we review the quantum and classical probability distributions for both position and momentum for this familiar problem, focusing on the visualization of the quantum wavefunctions and classical trajectories as well as the semi-classical connections between the two.

¹Permanent address

I. Introduction

The problem of a point mass in a one-dimensional infinite well is no doubt the most solved problem in all of introductory quantum mechanics. On the one hand, the quantized energy levels can be easily understood in terms of simple wave mechanics arguments involving ‘fitting deBroglie waves’ into the box, while the position- and momentum-space wavefunctions can be very intuitively connected to the classical behavior of a particle bouncing back-and-forth in the well [1]. The two-dimensional square well ($L_x = L_y$) provides one of the first examples of degeneracy due to a symmetry, while the rectangular well is often the subject of discussions of so-called ‘accidental’ degeneracies (when the $L_x/L_y = p/q$ is the ratio of integers).

The 2D circular infinite well (with its classical wave connection to a circular drum-head) can be used to introduce the quantum description of angular momentum (without the complications of spherical geometry) and also exhibits degeneracies (due to the equivalence of clockwise and counter-clockwise rotations). In the recent past, the two-dimensional circular infinite well has also surfaced (so to speak) in the context of two different problems:

- (i) Surface state electrons have been confined to nanometer length scales in closed structures (called corrals) built from adsorbed iron atoms positioned with a scanning tunneling microscope [2]. The resulting STM images indicate that the local electron density of states on the surface is well approximated by the position-space wavefunctions expected for a particle trapped in a 2D circular box [3].
- (ii) The study of chaotic trajectories in two-dimensional ‘billiards’, i.e., otherwise free particles moving on a surface undergoing elastic collisions with a closed

boundary, has been extensively studied on so-called ‘stadium’ shaped surfaces; these are defined by taking a circular boundary of radius R , cutting it at the top and bottom and inserting straight sections of length a . For $a \neq 0$, the resulting classical trajectories are chaotic for almost all sets of initial conditions [4]. The quantum version of this problem, namely finding the energy eigenvalues and wavefunctions for the particle in an infinite stadium-shaped well (or equivalently, finding the eigenfrequencies of a stadium-shaped drumhead), was one of the first studied [5] with an eye towards analyzing the characteristics of quantum chaos and was very influential in later research [6] on the subject. In each case, the circular infinite well (i.e, $a = 0$) is used as a benchmark against which to compare the classical chaotic motion or quantum wavefunctions. The study of quantum and classical chaos in two dimensional billiards is thus nicely complementary to the more usual discussions of symmetry in such systems; two-dimensional billiard systems are the simplest extensions in which both concepts arise in a physically natural and calculationally straight forward manner.

Because of the renewed interest in this old problem, we illustrate in this note some of the quantum and classical aspects of the circular infinite well. In Sec. II, we focus on the quantum wavefunctions in both position- and momentum-space, illustrating the connections with different types of classical motion and making connection with the notion of a classical probability distribution. Finally, in Sec. III, we review some of the geometry of the classical trajectories.

II. Quantum solutions

The quantum mechanical system of a particle (of mass μ) in the infinite circular well of radius R is defined by the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2\mu}\nabla^2 + V(r) \quad (1)$$

where

$$V(r) = \begin{cases} 0 & \text{for } r < R \\ +\infty & \text{for } r > R \end{cases} \quad (2)$$

This gives the Helmholtz equation

$$(\nabla^2 + k^2)\psi(r, \theta) = 0 \quad (3)$$

where $k^2 = 2\mu E/\hbar^2$ with the boundary condition that $\psi(R, \theta) = 0$. (The strong analogy to other surface wave problems of the same type has been utilized, for example, in an experimental determination of the eigenfrequencies of a stadium-shaped microwave cavity [7].)

Because of the circular symmetry, the solution can be written in the separable form

$$\psi(r, \theta) = R(r)\Theta_m(\theta) \quad \text{where} \quad \Theta_m(\theta) = \frac{1}{\sqrt{2\pi}}e^{im\theta} \quad (4)$$

for $m = 0, \pm 1, \pm 2, \dots$. These solutions are also eigenstates of the angular momentum operator $\hat{L} = (\hbar/i)(\partial/\partial\theta)$ with eigenvalues $L = m\hbar$. The resulting radial equation is

$$\frac{d^2 R(r)}{dr^2} + \frac{1}{r} \frac{dR(r)}{dr} + \left(k^2 - \frac{m^2}{r^2}\right) R(r) = 0 \quad (5)$$

which can be recognized as Bessel's equation in the variable $z = kr$. The solutions which are well-behaved at the origin are the cylindrical Bessel functions $J_{|m|}(kr)$ and the quantized energy eigenvalues are determined by the boundary condition, namely $\psi(R, \theta) = 0 \implies J_{|m|}(kR) = 0$. The n -th zero of the m -th Bessel function can be

labeled as $a_{(m,n_r)}$ where $n = n_r + 1$ and n_r counts the number of radial nodes in the wavefunction; thus $a_{(0,0)} = 2.40483\dots$ is the first zero of $J_0(z)$ and so forth. The solutions are thus simultaneous eigenstates of both energy and angular momentum with eigenvalues given by

$$E = \frac{\hbar^2}{2\mu R^2} [a_{(m,n_r)}]^2 \quad \text{and} \quad L = m\hbar \quad (6)$$

Each state with non-zero m is doubly degenerate due to the two equivalent values of $m = \pm|m|$ corresponding to clockwise and counter-clockwise motion.

As a first step toward visualizing the wavefunctions, we collect all of the values of $a_{(m,n_r)} < 20$ (there are 49 of them), rank order them (not counting degenerate pairs), and present the corresponding ordered energy eigenvalues (in units of $E_0 = \hbar^2/2\mu R^2$) in Fig. 1. For comparison, the same number of the lowest-lying energy states in the square well of side L are shown in the same figure where the areas of the two wells have been made equal, i.e., $\pi R^2 = L^2$. To illustrate the range of wavefunctions corresponding to different classes of classical motion, we choose three relatively closely spaced energy levels (differing by only $\sim 7\%$ in energy) corresponding, as we will discuss below, to different amounts of energy in the radial versus angular motion. (The fact that such sets of closely spaced energy levels can often be found is characteristic of integrable systems where the distribution of the differences in successive energy levels, $\Delta E = E_{N+1} - E_N$, is strongly peaked at $\Delta E = 0$; this is in contrast to the chaotic case where the equivalent distribution is peaked at a finite value of ΔE and is consistent with the distribution of eigenvalues of a random matrix. For a discussion and further references, see Ref. [5].)

The wavefunctions on which we will focus are given by

case	(m, n_r)	$a_{(m, n_r)}$	$E/E_0 = [a_{(m, n_r)}]^2$	ordering	$\langle \hat{T}_\theta \rangle / E$
(a)	(0, 4)	14.9309	222.9318	28th	0.0000
(b)	(4, 2)	14.3725	206.5688	24th	0.3733
(c)	(10, 0)	14.4755	209.5401	25th	0.7721

The fraction of energy which is stored, on average, in the rotational degree of freedom is given in the last column and is defined by

$$\langle \hat{T}_\theta \rangle / E = \left\langle R(r) \left| \frac{\hbar^2 m^2}{2\mu r^2} \right| R(r) \right\rangle / E \quad (7)$$

so that the states (a), (b), and (c) are in order of increasing (decreasing) importance of angular (radial) motion. To illustrate the form of the corresponding position-space wavefunctions, in Figs. 2-4 we plot the properly normalized $|\psi(r, \theta)|^2$; for purposes of visualization, we have used the linear combination $\cos(m\theta) \propto e^{im\theta} + e^{-im\theta}$ as would be appropriate for standing wave solutions and the three cases are plotted on the same scale. (Because of this, the (0, 4) case is somewhat ‘cut-off’ near the origin in order that the other cases can be more easily visualized.) We note that:

- The (0, 4) state, with no angular momentum, would correspond to a classical particle trajectory through the origin and hence purely radial motion. This is consistent with the ‘wiggleness’ of the wavefunction in the radial direction only.
- The (10, 0), with no radial nodes and the radial probability density peaked near the wall, is a model for mostly angular motion, similar to a ball rolling around the inner edge of a roulette wheel; most of the kinetic energy is in the form of ‘angular wiggles’.

The similarity of these pictures to some of the experimentally obtained STM images in Ref. [3] is striking.

The behavior of the wavefunctions can be discussed more concretely by examining the probability density for the radial coordinate, given by

$$P(r) = r|R(r)|^2 \quad \text{with the normalization condition that} \quad \int_0^R P(r)dr = 1 \quad (8)$$

where the additional factor of r comes from the two-dimensional measure for polar coordinates; these are plotted in Fig. 5 for the three cases we consider. We can easily analyze the behavior of two limiting cases:

- For the generic case of $m = 0$ and n_r large, we can make use of asymptotic form (for $z = kr \gg 1$) of the regular Bessel function, namely

$$J_n(z) \sim \sqrt{\frac{2}{\pi z}} \cos\left(z - \frac{n\pi}{2} - \frac{\pi}{4}\right) \quad (9)$$

to note that

$$P_{(0, n_r \gg 1)}(r) \rightarrow r \left[\sqrt{\frac{2}{\pi kr}} \cos\left(kr - \frac{\pi}{4}\right) \right]^2 \propto \cos^2\left(kr - \frac{\pi}{4}\right) \quad (10)$$

This is quite similar to the case of the one-dimensional well where the particle would bounce back-and-forth across a diameter through the origin.

- For the case of almost purely angular motion, $m \gg 1$ and $n_r = 0$, we can make good use of a general variational wavefunction to examine the limiting behavior. We can use

$$R_m(r; \alpha) = r^{|m|} (R^\alpha - r^\alpha) \quad (11)$$

where α is the variational parameter. This form incorporates the appropriate boundary conditions at $r = 0$ (where $R(r) \rightarrow r^{|m|}$ due to the angular momentum barrier) and at $r = R$ and has no radial nodes; it will provide a lower-bound to

the energy of the $n_r = 0$ state for each value of m . The energy functional given by this trial wavefunction is

$$E_m(\alpha) = E[R_m(r, \alpha)] = \left(\frac{\hbar^2}{2\mu R^2} \right) \left[(m+1) \frac{(2m+\alpha+2)(m+\alpha+1)}{(m+\alpha)} \right] \quad (12)$$

which has a minimum for $\alpha = \sqrt{m+2} - m$ for each value of m . This general choice gives an energy for the $n_r = 0$ state which is only 0.78% (4.6%) larger than the exact value for $m = 0$ ($m = 10$) while the overlap (defined via $|\langle R_{exact} | R_{var} \rangle|^2$) with the corresponding true wavefunction is 0.99937 (0.9738). Using this functional form as a guide, we can easily find that in the large m limit we have

$$\langle \hat{T}_\theta \rangle / \langle \hat{H} \rangle \rightarrow 1 - \frac{1}{\sqrt{m}} \quad (13)$$

while

$$\langle r \rangle \rightarrow R \left(1 - \frac{1}{2\sqrt{m}} - \frac{3}{4m} + \dots \right) \quad \text{and} \quad \langle r^2 \rangle \rightarrow R^2 \left(1 - \frac{1}{\sqrt{m}} - \frac{1}{m} + \dots \right) \quad (14)$$

so that

$$\Delta r = \sqrt{\langle r^2 \rangle - \langle r \rangle^2} \rightarrow \frac{R}{2\sqrt{m}} \quad (15)$$

and the limit of purely rotational motion, strongly peaked in radius near the rim, is evident for $m \gg 1$.

The classical probability distribution for position, $P_{CL}(x)$, can be defined by averaging over many measurements of the (precisely known) coordinates along a classical trajectory; examples of comparisons with the classical motion in the infinite well and harmonic oscillator as well as other systems [1] are often discussed and visualized. We can derive a similar quantity for the radial coordinate for comparison with

$P_{QM}(r) = r|R(r)|^2$ by considering the classical expression for the total energy, E , in terms of the radial coordinate and the conserved angular momentum, L

$$E = \frac{1}{2}\mu\dot{r}^2 + \frac{L^2}{2\mu r^2} \quad (16)$$

This gives

$$\frac{dr}{dt} = \sqrt{\frac{2}{\mu}} \left(E - \frac{L^2}{2\mu r^2} \right) \quad (17)$$

or

$$dt = \sqrt{\frac{\mu}{2E}} \frac{r dr}{\sqrt{r^2 - R_{min}^2}} = \frac{1}{v} \frac{r dr}{\sqrt{r^2 - R_{min}^2}} \quad (18)$$

where

$$R_{min} = \sqrt{\frac{L^2}{2\mu E}} \quad (19)$$

is the distance of closest approach to the origin (which can vanish in the case of no angular momentum and is at most R for purely angular motion).

Using the standard argument that the probability of finding the particle in the radial interval $(r, r + dr)$ is proportional to the small time, dt , spent in that region, one makes the association $P_{CL}(r)dr = dt/(\tau/2)$ where τ is the period of motion for the coordinate in question. For the radial variable, we then find that

$$\tau_r = \sqrt{\frac{2\mu}{E}} \sqrt{R^2 - R_{min}^2} \quad (20)$$

and

$$P_{CL}(r) = \frac{r}{\sqrt{R^2 - R_{min}^2} \sqrt{r^2 - R_{min}^2}} \quad (21)$$

The limit of purely radial motion corresponds to $R_{min} = 0$ so that $\tau = \sqrt{2\mu R^2/E} = 2R/v$ as expected while $P_{CL}(r) = 1/R$ corresponding to uniform probability of finding the particle at any point on a given radius, again, similar to the one-dimensional box.

(We urge the reader to evaluate such quantities as $\langle r \rangle$ and Δr and to examine their behavior in the limiting cases of $R_{min} \rightarrow 0$ and $R_{min} \rightarrow R$.)

To make appropriate comparisons with the quantum case, we note that

$$\frac{R_{min}}{R} = \frac{m}{a_{(m,n_r)}} \quad (22)$$

and using this identification, we can compare the classical distributions to their quantum counterparts as included in Fig. 5. For future reference we note that the values of Eqn. 22 for the three cases are

(m, n_r)	$R_{min}/R = m/a_{(m,n_r)}$
(0, 4)	0.0000
(4, 2)	0.2783
(10, 0)	0.6908

It is easy to construct wavepacket solutions for the 2D square or rectangular well (for example, as products of one-dimensional infinite well wavepackets with arbitrary initial central position and velocity) which can illustrate not only the classical ‘bouncing’ trajectories in that simple geometry, but also the eventual spreading. Similar wavepacket solutions for the circular well are more difficult to build and we will not discuss them here; the scattering of free Gaussian wavepackets from cylindrical barriers has been discussed and visualized in Ref. [8].

While the position-space wavefunctions and their classical counterparts are often emphasized in such comparisons, the momentum-space wavefunction, $\phi(\mathbf{p})$, corresponding to any $\psi(\mathbf{r})$ can be obtained via

$$\phi(\mathbf{p}) = \frac{1}{2\pi\hbar} \int dx \int dy e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \psi(\mathbf{r}) \quad (23)$$

We have evaluated this numerically for our three examples and present $|\phi(p_x, p_y)|^2$ versus (p_x, p_y) in Figs. 6-8. The free particle character of the particle in the well, where

one expects $\mathbf{p}^2 = p_x^2 + p_y^2 = 2mE$ being constant in the classical limit, is clear from the figures. The almost common energy of the three states is more clearly indicated when we bin $|\phi(p_x, p_y)|^2$ appropriately in the radial momentum variable $p = |\mathbf{p}|$ to obtain the analog of Eqn. 8 and Fig. 4 for $P(p)$ versus p ; this is plotted in Fig. 9.

III. Classical trajectories

Because of the special nature of the infinite wall boundaries in any ‘billiards’ problem, the classical trajectories are determined more by geometry than by the values of energy and angular momentum individually. As shown in Fig. 10, each ‘leg’ of the trajectory consists of a straight line segment of length $2d < 2R$ which can fit into the circular well; the next ‘leg’ is determined by the equal angle (specular) reflection from the tangent plane at the circular boundary. This means that a given trajectory is determined by the angle ϕ (which is also defined by the initial conditions) and the chord length $2d$; d can also be expressed in terms of either of the two equivalent quantities, R_{min} or Θ , defined by

$$R_{min} = \sqrt{R^2 - d^2} = R \cos\left(\frac{\Theta}{2}\right) \quad (24)$$

(In fact, given ϕ and d , one can even generate the subsequent trajectories by simple compass and ruler manipulations as from high school geometry.) For a given value of $R_{min} = L^2/2\mu E$, the time interval between ‘bounces’ scales as $\tau \propto 1/v \propto 1/\sqrt{E}$ as in Eqn. 20, but the geometric pattern generated by the trajectories depends only on ϕ and Θ .

The connection to the classical probability distribution can also be viewed using the trajectory information for each leg as shown in Fig. 11. Taking the initial time at

the distance of closest approach, the radius $r(t)$ increases as

$$r(t) = \sqrt{(vt)^2 + R_{min}^2} \quad \text{or} \quad t = \frac{1}{v} \sqrt{r^2 - R_{min}^2} \quad (25)$$

so that

$$dt = \frac{1}{v} \frac{r dr}{\sqrt{r^2 - R_{min}^2}} \quad (26)$$

as in Eqn. 18. In this case, one period of the radial motion corresponds to the time between consecutive ‘bounces’ at the wall.

The special values of $\Theta = 2\pi/N$ with integral N correspond to a closed N -sided regular polygon inscribed in the circle, with $N = 2$ corresponding to purely radial motion through the origin and $N \rightarrow \infty$ giving purely rotational motion; any rational value of N will result in a closed star-like curve. We will illustrate examples in Fig. 12 for $N = 3, 10, 2.75$. For irrational values of N , the star-like pattern will ‘precess’ for increasingly large numbers of bounces, n_B . The classical trajectories corresponding to the quantum cases we have considered can be obtained by associating $\cos(\Theta/2) = R/R_{min} = m/a_{(m,n_r)}$ as in Eqn. 22. Given this identification, we note that the $(m, n_r) = (10, 0)$ case correspond to $m/a = 0.6908224...$ which is rather close to the value for the four-sided polygon (i.e. a square) for which $m/a = \cos(\pi/4) = 0.7071....$ We plot the classical trajectories for two values of $n_B = 10, 100$ to show the increasingly ‘filled in’ pattern which arises when the number of ‘bounces’ is made arbitrarily large.

Because of the rotational symmetry in the quantum system, there will no obvious remnants of an individual classical trajectory which can be seen in the quantum wavefunctions as all such paths characterized by any value of ϕ will be equivalent. On the other hand, the reduced symmetry of the stadium problem leads to wavefunctions which have highly enhanced probability amplitudes in the neighborhood of classical periodic orbits (often called ‘scars’ [9]) which are rather simple generalizations of some of the trajectories in Fig. 11.

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Figure Captions

Fig. 1. Ordered energy eigenvalues (in units of $\hbar^2/2\mu R^2$) for the circular well (diamonds) and square well (squares). The areas of the wells are taken equal ($\pi R^2 = L^2$) and degenerate states are only counted once.

Fig. 2. Properly normalized $|\psi(x, y)|^2$ versus (x, y) for an energy eigenstate of the circular well. The case shown here corresponds to (a) $(m, n_r) = (0, 4)$. The same scale is used in Figs. 3 and 4.

Fig. 3. Same as Fig. 2 but for the case (b) $(m, n_r) = (4, 2)$.

Fig. 4. Same as Fig. 2 but for the case (c) $(m, n_r) = (10, 0)$.

Fig. 5. Quantum and classical probability distributions for the radial coordinate for the circular well for the three cases discussed in the text. For the quantum case, $P(r) = r|R(r)|^2$ is plotted (solid curve) while for the classical case $P_{CL}(r)$, as given by Eqn. 21, is used (dashed curve). The classical inner turning point corresponding to $r = R_{min}$ is shown by the vertical dotted line.

Fig. 6. Momentum-space wavefunctions for the circular well given by $|\phi(p_x, p_y)|^2$ versus (p_x, p_y) . This case corresponds to (a) $(m, n_r) = (0, 4)$. The wavefunctions $\phi(p_x, p_y)$ were obtained by numerical integration of the position-space wavefunction in Eqn. 4, but with the standing wave angular dependence given by $\cos(m\theta)$.

Fig. 7. Same as Fig. 6 but for the case (b) $(m, n_r) = (4, 2)$.

Fig. 8. Same as Fig. 6 but for the case (c) $(m, n_r) = (10, 0)$.

- Fig. 9. Quantum probability distribution for the magnitude of the momentum, i.e., $P(p) = p|\phi(p)|^2$ versus p for the three energy-eigenfunctions considered in the text; the vertical lines indicate the location of $\sqrt{\langle p^2 \rangle}$ for each case.
- Fig. 10. Geometry of classical trajectories in circular well.
- Fig. 11. Geometry of classical trajectory in circular well giving $r(t)$ during one ‘leg’ of the path between ‘bounces’ at the walls.
- Fig. 12. Classical trajectories for various values of integral and rational N showing possible closed ‘orbits’.
- Fig. 13. Classical trajectories for values of N or m/a corresponding the three quantum wavefunctions for cases (a), (b), and (c) discussed in the text for numbers of ‘bounces’ given by $n_B = 10, 100$.

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5

Fig. 6

Fig. 7

Fig. 8

Fig. 9

Fig. 10

Fig. 11

$N = 3$

$N = 10$

$N = 2.75$

Fig. 12

(a) $n_B = 10$

(b) $n_B = 10$

(c) $n_B = 10$

(a) $n_B = 100$

(b) $n_B = 100$
Fig. 13

(c) $n_B = 100$