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# Classical system underlying a diffracting quantum billiard

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**Abstract.** For a point scatterer placed slightly off the centre of a circular enclosure, rays are found which vividly exhibit the effect of diffraction. The Schrödinger equation was mapped in the complex plane by employing a fractional linear transformation which brings the point scatterer to the centre. But the mass of the particle becomes a function of space coordinates, bearing anisotropy. For the transformed problem, the corresponding classical Hamiltonian is written and solved with Snell's laws on the boundary. The solutions of the Hamilton's equations thus found constitute, in fact, the ray-manifold underlying the diffraction at the level of the wave description.

**Keywords.** Wave equation; rays; quantum chaos.

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## 1. Introduction

Diffraction [1] is a complex wave phenomenon which manifests classically and quantum mechanically. Among a wide range of systems where diffraction becomes important, there is an interesting situation of a point scatterer present in an enclosure where a wave propagates. Quantum mechanically, there is a de Broglie wave propagating in a box with Dirichlet boundary condition on the boundaries, and, at a point [2]. The wave scatters off the point scatterer, and upon diffraction it spreads and reflects from the walls, interferes, and eventually appears as a standing wave. A rigorous mathematical theory of diffraction was developed by Sommerfeld and advanced significantly by Keller and others [3–6].

In the earlier work by Seba [7], it was reported that the quantum operator ceases to be self-adjoint, and a self-adjoint extension has to be constructed. In a related work, the point scatterer was replaced by a statistical flux line by Date *et al* [8], and the dynamical system so obtained was shown to be classically non-integrable (pseudointegrable). The breakdown of integrability results in this case as the vector fields become singular at the position where the flux line pierces the rectangle. It is known that there exists an intimate connection between the presence of diffraction and non-integrability, as discussed in generous detail by Sutherland [9].

We consider a circular billiard with a point scatterer placed off its centre. This breaks the circular symmetry and makes the energy level sequence more complicated [2]. By employing a conformal transformation, the unsymmetric problem can be mapped to a symmetric problem [10] where the scatterer is placed at the centre of the circle but the mass of the particle becomes position-dependent. The breakdown of symmetry appears in the anisotropy of mass. In this article, we study the classical dynamics underlying this quantum problem with position-dependent mass. The results of this classical system correspond to the classical ray-manifold orthogonal to the Huygens wavefronts. The interesting and important point is that our discussion takes the treatment beyond the eikonal approximation.

## 2. Mapping asymmetry to anisotropy

Quantum mechanically, we have the Schrödinger equation with Dirichlet boundary conditions. Let us place the point scatterer at a distance $a_0$ from the centre of the circle. We may choose the $x$-axis to pass through this point. Thus, in polar coordinates, the shift of the scatterer is given by a radial distance $\rho_0$ from the centre which is, of course, numerically equal to $a_0$. To treat this asymmetric problem, we use the powerful machinery of the theory of complex variables. To do so, we first need to express the Schrödinger equation in complex variables by transforming $x \pm iy$ to $z, z^*$. The equation is

$$\left(4\frac{\partial^2}{\partial z \partial z^*} + k^2\right)\psi(z, z^*) = 0 \quad (1)$$

with $k^2 = (2mE/\hbar^2)$. The fractional linear transformations (FLT) [11] which brings the scatterer to the centre of the circle are

$$z' = \frac{z - a_0}{1 - a_0^* z}, \qquad z'^* = \frac{z^* - a_0^*}{1 - a_0 z^*}. \quad (2)$$

After some manipulations, and on employing the inverse of FLT, we get

$$4\frac{|a_0^* z' + 1|^4}{|1 - a_0^2|^2}\frac{\partial^2 \psi(z', z'^*)}{\partial z' \partial z'^*} + k^2\psi(z', z'^*) = 0. \quad (3)$$

Now we return to the Cartesian coordinates by identifying $z'$ with $(\xi, \eta)$, $a_0 = (\xi_0, \eta_0)$. We denote $\sqrt{\xi^2 + \eta^2}$ by $\rho$; thus, $z' = \rho e^{i\theta}$. The angular coordinate of the scatterer is zero as the $x$-axis passes through it. Casting now the Schrödinger equation in polar coordinates, $(\rho, \theta)$, we have

$$\nabla^2_{\rho,\theta}\psi(\rho, \theta) + \frac{k^2(1 - \rho_0^2)^2}{[(\rho\rho_0)^2 + (2\rho\rho_0\cos\theta) + 1]^2}\psi(\rho, \theta) = 0. \quad (4)$$

It can be rewritten as

$$\frac{-\hbar^2}{2m}\nabla^2_{\rho,\theta}\psi(\rho, \theta) - \frac{(1 - \rho_0^2)^2}{[(\rho\rho_0)^2 + (2\rho\rho_0\cos\theta) + 1]^2}E\psi(\rho, \theta) = 0. \quad (5)$$

## 3. Classical solutions

Let $p_\theta$ and $p_\rho$ be the angular and radial components of momentum. Hamiltonian of this system can be written as

$$H = \frac{1}{2M(\rho, \theta)}\left[p_\rho^2 + \left(\frac{p_\theta}{\rho}\right)^2\right], \quad (6)$$

where

$$M(\rho, \theta) = m\frac{(1 - \rho_0^2)^2}{[(\rho\rho_0)^2 + (2\rho\rho_0\cos\theta) + 1]^2}. \quad (7)$$

Although the scatterer has been mapped to the geometrical centre, the mass shows anisotropy, as seen in figure 1.

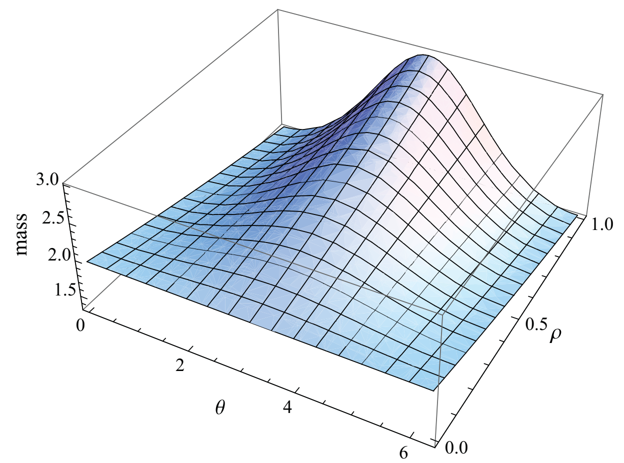


**Figure 1.** The anisotropy of mass is vividly seen here. With respect to angle, the mass increases as we go anticlockwise from zero to $pi$, and then decreases symmetrically. So the circular symmetry is replaced by a reflection symmetry in the mass about $\theta = \pi$. It is interesting to note that the quantum states found in were also anisotropic. Radius of the circle is taken as unity.

Four canonical equations of motion for the variables $p_\theta$ and $p_\rho$ are

$$\dot\rho = \frac{\partial H}{\partial p_\rho}, \qquad \dot\theta = \frac{\partial H}{\partial p_\theta},$$
$$\dot p_\rho = -\frac{\partial H}{\partial \rho}, \qquad \dot p_\theta = -\frac{\partial H}{\partial \theta}. \quad (8)$$

Using the equations for $\dot\rho$ and $\dot\theta$,

$$\dot\rho = \frac{p_\rho}{m}\frac{1}{(1 - \rho_0^2)^2}[((\rho\rho_0)^2 + 2\rho\rho_0\cos\theta + 1)^2]$$
$$\dot\theta = \frac{p_\theta}{m\rho^2}\frac{1}{(1 - \rho_0^2)^2}[((\rho\rho_0)^2 + 2\rho\rho_0\cos\theta + 1)^2]. \quad (9)$$

Dividing the above two equations, we get an equation connecting four variables $p_\theta, p_\rho, \dot\rho, \dot\theta$,

$$\dot\rho p_\theta - \rho^2\dot\theta p_\rho = 0. \quad (10)$$

Using the equations for $\dot p_\theta$ and $\dot p_\rho$,

$$\dot p_\rho = -\frac{[(\rho\rho_0)^2 + (2\rho\rho_0\cos\theta) + 1]}{2m(1 - \rho_0^2)^2} \times \left[4\rho_0(\rho\rho_0 + \cos\theta)(p_\rho^2 + (p_\theta/\rho)^2) - 2\frac{(p_\theta)^2}{\rho^3}(\rho\rho_0)^2 + ((2\rho\rho_0\cos\theta) + 1)\right],$$
$$\dot p_\theta = \frac{(p_\rho^2 + (p_\theta/\rho)^2)}{2m(1 - \rho_0^2)^2} \times [4\rho\rho_0\sin\theta((\rho\rho_0)^2 + 2\rho\rho_0\cos\theta + 1))]. \quad (11)$$

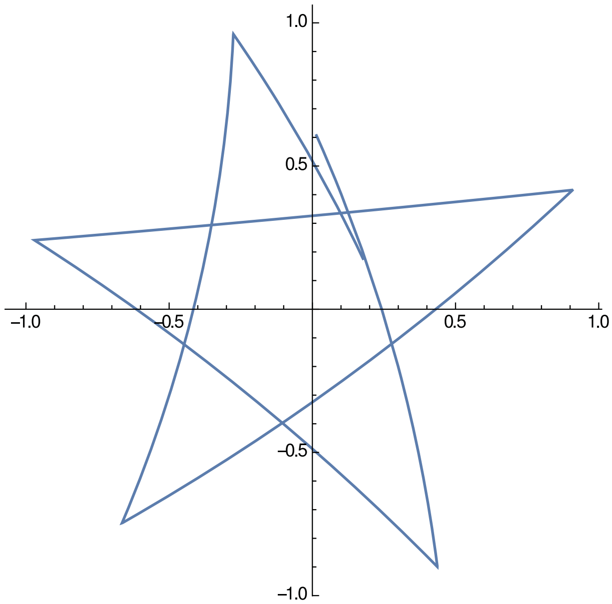


**Figure 2.** We plot the trajectory in the $xy$-plane. The initial angle is $\pi/4$ with initial value of $\rho$ as 0.25. The orbit is close to the classical five-pointed star but the orbit does not close.

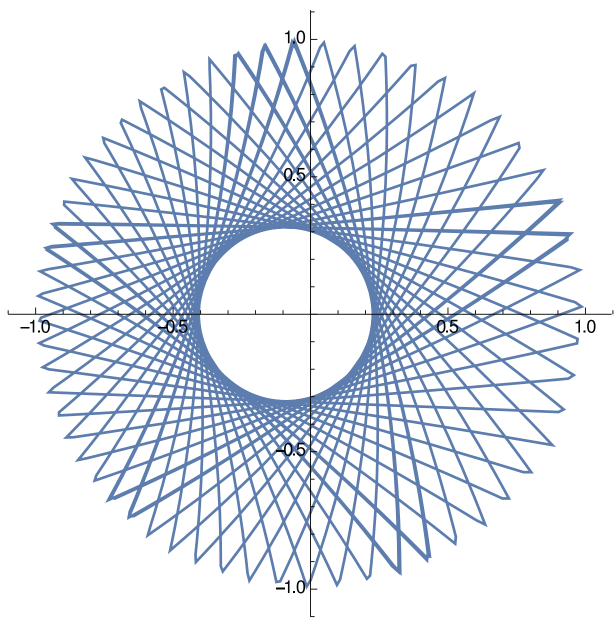


**Figure 3.** Same orbit as in figure 2, but even after many reflections the orbit does not close.

The coupled nonlinear, ordinary differential equations are solved using MATHEMATICA for various initial conditions. The results are shown in figures 3 and 4. For the case of a circular billiard, with initial conditions such that the initial angle is $\pi/4$, the orbit is a five-pointed star. Due to free Hamiltonian in that case, all the chords are straight line segments. In our case where there is anisotropy, and diffraction, the 'rectilinear star' modifies to a new star with curved segments (figure 2). The same orbit makes many rounds and arranges itself as in figure 3.

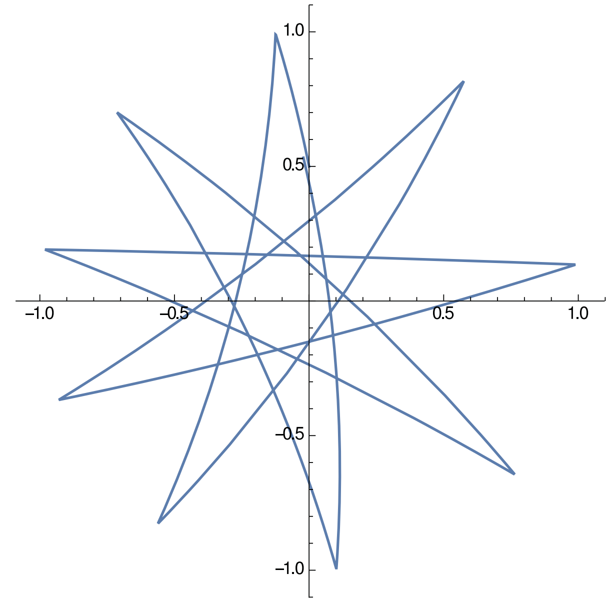


**Figure 4.** The initial angle is $\pi/2$ with initial value of $\rho$ as 0.5. The nature of trajectories is evident, there is a curving of all the segments, reminiscent of what is expected of diffracted rays.

## 4. Concluding remarks

The results we see are a remarkable depiction of the rays that underlie the wavefronts after diffraction from a point scatterer. A study of the equations of motion reveals that the critical point is at $\theta = 0$ and $\rho = -0.1$. In the figures shown, the scatterer is at 0.1 where the radius of the circle is unity. The scatterer is kept at 0.1 as we intend to show the breaking of symmetry. We notice that even though the angular momentum is not conserved, the circular caustic remains. This might be because of eq. (10) which presents an 'effective' invariant.

It is usually stated that waves bend around the corners due to diffraction from edges. Here, we see vividly how the rays bend due to diffraction from the point scatterer. The direction of propagation of the wavefront is along the grad of action, $\nabla S$. Since $\nabla S$ and ray $(\mathrm{d}q/\mathrm{d}t)$ are Legendre duals [5], and trajectories and rays are parallel, it follows that $\nabla S$ must also bend. Thus, the bending of the trajectories seen is accompanied by the corresponding distortion of the wavefronts.

The classical mechanical-optical analogy championed by Hamilton [12] is seen here once again in a beautiful manner.

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