Particle in a Box: A Basic Paradigm in Quantum Mechanics - Part 2

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The problem of a particle moving freely inside a region with rigid, perfectly reflecting walls serves as a paradigm to illustrate numerous aspects of quantum mechanics (QM). In Part 1\(^1\) of this two-part article, we discussed several of these aspects using, respectively, a line segment, a ring, and a square as the region concerned. In the present part, we shall consider the cases of a circular region and a surface of constant positive curvature (a sphere). We shall then comment on the general case of a dynamical billiard. Finally, we turn to the inverse problem: given the energy spectrum of a particle moving freely inside a region, what can be deduced about the geometrical properties of the region? Some important results in this regard will be described in brief.

Particle in a Circular Box: Continuous Symmetry

Let us now consider a particle of mass \( m \) moving freely inside a circle of radius \( a \) with its centre at the origin \( O \). The circular wall is a perfect reflector. Classically, this system with two degrees of freedom has two constants of the motion that are in involution (their Poisson bracket vanishes)—namely, the Hamiltonian \( H = (p_x^2 + p_y^2)/(2m) \), and the orbital angular momentum (AM) about \( O \), given by \( xp_y - yp_x \). The conservation of AM arises from the invariance of \( H \) under rotations of the coordinate axes about \( O \), a continuous symmetry. The classical Hamiltonian is therefore integrable, and no chaotic motion can occur. In the QM case, we may once again expect a regular discrete spectrum.


**Keywords**

Quantum mechanics, continuous symmetry, curved surfaces, inverse problem, spectrum, domain, isometry, isospectral domains, eigenvalues.
As before, the time-independent Schrödinger equation for the wave function inside the circle is $-\nabla^2 \Phi = k^2 \Phi$ where $k^2 = 2mE/\hbar^2$. Writing $\nabla^2$ in plane polar coordinates $(\varrho, \varphi)$, we have the following eigenvalue equation for $\Phi(\varrho, \varphi)$:

$$\frac{1}{\varrho} \frac{\partial}{\partial \varrho} \left( \varrho \frac{\partial \Phi}{\partial \varrho} \right) + \frac{1}{\varrho^2} \frac{\partial^2 \Phi}{\partial \varphi^2} + k^2 \Phi = 0. \quad (1)$$

The boundary condition is $\Phi(a, \varphi) = 0$. Note that $k$ can be scaled out, so that $\Phi$ is a function of $k \varrho$ and $\varphi$. Following the standard procedure, we use the method of separation of variables, and set $\Phi(\varrho, \varphi) = R(\varrho)u(\varphi)$. It follows that $u''(\varphi)/u(\varphi)$ must be a constant. In turn, this implies that $u_\ell(\varphi) = e^{i\ell \varphi}$ where $\ell$ is a real number. The requirement that $\Phi$ be single-valued then restricts $\ell$ to integer values. $\ell \hbar$ is the eigenvalue of the angular momentum operator $\hat{\ell} = x\hat{p}_y - y\hat{p}_x = -i\hbar \partial/\partial \varphi$, and $u_\ell$ is the corresponding eigenfunction, where $\ell \in \mathbb{Z}$. For each given value of $\ell$, the radial wave function satisfies the equation

$$\varrho^2 \frac{d^2 R_\ell}{d \varrho^2} + \varrho \frac{d R_\ell}{d \varrho} + (k^2 \varrho^2 - \ell^2)R_\ell = 0. \quad (2)$$

The solution of (2) that is regular (i.e., nonsingular) at the origin $\varrho = 0$ is $J_\ell(k \varrho)$, the Bessel function [1] of the $1^{\text{st}}$ kind of order $\ell$. Since $J_{-\ell}(k \varrho) = (-1)^\ell J_\ell(k \varrho)$ when $\ell$ is an integer, $J_{-\ell}(k \varrho)$ is not linearly independent of $J_\ell(k \varrho)$. It therefore suffices, in this case, to consider only non-negative integer values of $\ell$, as far as the solution of the radial wave equation is concerned. Incorporating the angular part of the wave function, we obtain the pair of linearly independent solutions $J_\ell(k \varrho)e^{i\ell \varphi}$ and $J_\ell(k \varrho)e^{-i\ell \varphi}$ for each positive integer value of $\ell$. An alternative choice would be the linear combinations $J_\ell(k \varrho)(e^{i\ell \varphi} + e^{-i\ell \varphi})$ and $J_\ell(k \varrho)(e^{i\ell \varphi} - e^{-i\ell \varphi})$, or, equivalently, $J_\ell(k \varrho) \cos \ell \varphi$ and $J_\ell(k \varrho) \sin \ell \varphi$. When $\ell = 0$, we have just one solution, namely, $J_0(k \varrho)$ (see below).

The eigenvalues of $H$ are found by imposing the boundary condition $R_\ell(ka) = 0$, that is, $J_\ell(ka) = 0$, to be solved for $k$. For each $\ell = 0, 1, 2, \ldots$, the function $J_\ell(x)$ has an infinite number of zeroes on the positive $x$-axis. For example, the first three zeroes of $J_0(x)$ occur at $x \approx 2.41, 5.52$ and $8.65$, respectively. While $J_0(0) = 1$, all the other functions $J_\ell(x)$ where $\ell \geq 1$ vanish at
$x = 0$, but this zero does not correspond to an eigenvalue of the Hamiltonian of the particle (because the corresponding eigenfunction also vanishes identically). Let $\xi_{\ell n}$ (where $n = 1, 2, \ldots$) denote the numerical values of the zeroes of $J_\ell(x)$ in increasing order (omitting the zero at $x = 0$ for each $\ell \geq 1$). Then $k$ is restricted to the values $k_{\ell n} = \xi_{\ell n}/a$. Hence the energy eigenvalues of a particle moving freely inside a circular stadium of radius $a$ are given by

$$E_{\ell, n} = \frac{\hbar^2 k_{\ell n}^2}{2m} = \frac{\hbar^2 \xi_{\ell n}^2}{2ma^2}. \quad (3)$$

The three lowest energy states correspond to $\xi_{01}^2 \approx 5.78$, $\xi_{11}^2 \approx 14.68$ and $\xi_{21}^2 \approx 26.37$, respectively. The eigenvalues $E_{0, n}$ ($n \geq 1$) are nondegenerate, with eigenfunctions proportional to $J_0(\xi_{\ell n} a)$. The eigenvalues $E_{\ell, n}$ ($\ell \geq 1$, $n \geq 1$) are doubly degenerate, with eigenfunctions proportional to $\propto J_\ell(\xi_{\ell n} a) \cos \ell \varphi$ and $J_\ell(\xi_{\ell n} a) \sin \ell \varphi$.

Unlike the case of a square box, there is no additional numerical degeneracy in this instance, because it can be shown that the positive zeroes of any two Bessel functions $J_\ell(x)$ and $J_{\ell'}(x)$ of different non-negative integer orders never coincide precisely (although they come close to doing so asymptotically as $x \to \infty$). Interestingly, this property of $J_\ell(x)$, although conjectured earlier, was rigorously proved only as late as in 1929, by the mathematician C. L. Siegel [1].

**Particle on the Surface of a Sphere**

The case of a particle on a ring of radius $a$ provided a one-dimensional example of a region without a boundary. The two-dimensional analogue of this is a particle moving freely on the surface of a sphere of radius $a$. A new feature is involved in this case, arising from the intrinsic curvature of the sphere on which the particle moves. Quantization in curved spaces raises several issues. Let us ignore this aspect for the moment, however, and apply standard quantum mechanics to the problem. We take the sphere to be embedded in the usual three-dimensional Euclidean space, with the particle constrained to remain on its surface. This surface is given by the equation $x^2 + y^2 + z^2 = a^2$. It is natural

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to choose spherical polar coordinates \((r, \theta, \varphi)\) to specify the position of the particle, with \(r\) constrained to have the constant value \(a\). The time-independent Schrödinger equation for the position-space eigenfunction \(\Phi\) of \(H\) is, as usual, \((\nabla^2 + k^2) \Phi = 0\) where \(k^2 = 2mE/\hbar^2\). Since \(r\) is fixed at the value \(a\), only the angular part of the Laplacian contributes to \(\nabla^2 \Phi\).

The eigenvalue equation for \(\Phi(\theta, \varphi)\) is then given by

\[
\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Phi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \Phi}{\partial \varphi^2} + k^2 a^2 \Phi = 0. \tag{4}
\]

What follows is standard material, and will therefore be dealt with briefly. Using the method of separation of variables, we assume that \(\Phi(\theta, \varphi)\) is of the form \(u(\theta)w(\varphi)\). We then find that \(w(\varphi) = e^{im\varphi}/\sqrt{2\pi}\) where \(m\) (not to be confused with the mass \(m\) of the particle) must be an integer, in order to ensure the single-valuedness of the wave function. The wave function \(u(\theta)\) then satisfies the associated Legendre equation

\[
\frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{du}{d\theta} \right) - \frac{m^2 u}{\sin^2 \theta} + k^2 a^2 u = 0. \tag{5}
\]

Imposing the requirement that the wave function be single-valued, non-singular and normalisable leads to the condition

\[
k^2 a^2 = \ell(\ell + 1) \quad \text{where} \quad \ell = 0, 1, 2, \ldots, \tag{6}
\]

and further, for a given value of \(\ell\),

\[
m = 0, \pm 1, \pm 2, \ldots, \pm \ell. \tag{7}
\]

The energy levels of the particle are therefore given by

\[
E_\ell = \frac{\hbar^2 \ell(\ell + 1)}{2ma^2}. \tag{8}
\]

There is no dependence on the quantum number \(m\), and the level \(E_\ell\) is \((2\ell + 1)\)-fold degenerate. It is clear that what we have derived here is essentially the quantization of the orbital angular momentum of the particle about the centre of the sphere. The eigenfunction \(u_{\ell m}(\theta)\) is (apart from a normalization constant) the
associated Legendre function $P_{\ell m}(\cos \theta)$. The full eigenfunction $u_{\ell m}(\theta)w_m(\varphi)$ is the spherical harmonic $Y_{\ell m}(\theta, \varphi)$. The ground state is non-degenerate, with energy $E_0 = 0$ and a wave function that is just a constant, namely, $Y_{00}(\theta, \varphi) = 1/\sqrt{4\pi}$. The $(2\ell + 1)$ eigenfunctions corresponding to the energy level $E_\ell$ comprise the set $\{Y_{\ell m}(\theta, \varphi), m = 0, \pm 1, \ldots, \pm \ell\}$.

**Free Particle in the Curved Space $S^2$**

As mentioned in the preceding section, let us now consider a free particle moving in the 2-sphere $S^2$, which is a compact two-dimensional manifold with an intrinsic, constant, positive Gaussian curvature $\kappa$. (This manifold need not be embedded in three-dimensional Euclidean space.) The problem also serves as an example of QM in a curved space, a topic that involves several technicalities. Canonical coordinates and conjugate momenta must be defined properly, and represented by well-defined self-adjoint operators in the transition to quantum mechanics; a consistent quantization procedure must be adopted; the Laplacian must be generalized to the so-called Laplace–Beltrami operator in a curved manifold; and so on. While there are several approaches to the problem at hand, a treatment [2] that uses the curvature $\kappa$ of the two-dimensional manifold as a parameter is both instructive and appealing. It enables one to consider in a unified manner the cases in which $\kappa$ is, respectively, a positive constant (the 2-sphere $S^2$), zero (the Euclidean plane) and a negative constant (the hyperbolic plane $H^2$), to obtain a complete solution. What follows is a brief summary of the result derived in [2] for the energy spectrum in the case of motion in $S^2$.

The starting point is the classical Lagrangian $L$ for geodesic motion of a particle of mass $m$ in $S^2$, which is just the kinetic energy of the particle. Had we assumed the sphere to be embedded in three-dimensional Euclidean space, we could have identified $\kappa$ with $1/a^2$, where $a$ is the radius of the sphere. But we must now use coordinates *intrinsic* to the curved two-dimensional space. A convenient set is provided by the geodesic polar coordinates $(\rho, \phi)$.
in $S^2$, as shown in Figure 1. (To be precise, we are considering points on the northern hemisphere here. For the whole of $S^2$, we need two overlapping ‘charts’ to ensure the uniqueness of the geodesic coordinates of every point.) In terms of these coordinates, the Lagrangian of the particle is given by
\begin{equation}
L = \frac{m}{2} \left( \dot{\rho}^2 + \frac{\sin^2(\sqrt{\kappa} \rho)}{\kappa} \dot{\phi}^2 \right). \tag{9}
\end{equation}

A change of variables from $\rho$ to $r = \sin(\sqrt{\kappa} \rho)/\sqrt{\kappa}$ gives
\begin{equation}
L = \frac{m}{2} \left( \frac{\dot{r}^2}{1 - \kappa r^2} + r^2 \dot{\phi}^2 \right) \quad \text{where} \quad 0 \leq r \leq 1/\sqrt{\kappa}. \tag{10}
\end{equation}

Defining ‘Cartesian’ coordinates $x = r \cos \phi$, $y = r \sin \phi$, the Lagrangian can be written as
\begin{equation}
L = \frac{m}{2(1 - \kappa(x^2 + y^2))} \left\{ \dot{x}^2 + \dot{y}^2 - \kappa(xy - yx)^2 \right\}. \tag{11}
\end{equation}

Note the occurrence of the AM-like last term in the curly brackets in (11). The momenta conjugate to $x$ and $y$ are given by $p_x = \partial L/\partial \dot{x}$, $p_y = \partial L/\partial \dot{y}$. A Legendre transform gives the Hamiltonian $H$ corresponding to the Lagrangian in (11). The momenta $p_x$ and $p_y$ are not constants of the motion (they are not in involution with $H$). However, it can be shown that the so-called Noether momenta
\begin{equation}
P_x = (1 - \kappa r^2)^{1/2} p_x, \quad P_y = (1 - \kappa r^2)^{1/2} p_y, \quad J = xp_y - yp_x \tag{12}
\end{equation}
are in involution with $H$, and are therefore constants of the motion. In terms of these conserved quantities, the Hamiltonian is given by

$$H = \frac{1}{2m}(P_x^2 + P_y^2 + \kappa J^2).$$  \hfill (13)

This Hamiltonian is of the form $H = H_1 + H_2 + H_3$, where each $H_i (i = 1, 2, 3)$ is in involution with the sum of the other two, and hence with $H$. This two-freedom system has two constants of the motion in involution (e.g., $H_1 + H_2$ and $H_3$), and is therefore integrable. Moreover, there are three isolating integrals $H_i (i = 1, 2, 3)$ in the four-dimensional phase space, implying that the classical Hamiltonian $H$ is super-integrable.

In the corresponding quantum mechanical problem, this makes the Schrödinger equation separable in more than one set of coordinates. This equation can be solved to find the normalized eigenfunctions of $H$ explicitly [2]. Two eigenfunction sequences $\Phi^{(1)}_{n,n'}$ and $\Phi^{(2)}_{n,n'}$ occur, labelled by the quantum numbers $n$ and $n'$, each running over the values 0, 1, 2, \ldots. The corresponding eigenvalues are given by

$$E_{n,n'}^{(1)} = \frac{\hbar^2 \kappa}{2m} (2n + n' + 1)(2n + n' + 2) = \frac{\hbar^2 \kappa}{2m} (N + 1)(N + 2)$$ \hfill (14)

and

$$E_{n,n'}^{(2)} = \frac{\hbar^2 \kappa}{2m} (2n + n')(2n + n' + 1) = \frac{\hbar^2 \kappa}{2m} N(N + 1),$$ \hfill (15)

where the integer $N = 2n + n'$ runs over the values 1, 2, \ldots. The compactness of the two-dimensional space $S^2$ leads to a fully discrete energy spectrum. As the energy eigenvalues depend only on the combination $N = 2n + n'$, the levels are degenerate (as we may expect them to be, the classical $H$ being super-integrable).

The ground state however, is non-degenerate, with eigenvalue $E_{0,0}^{(1)} = \frac{\hbar^2 \kappa}{m}$ and eigenfunction $\Phi^{(1)}_{0,0}$. (The energy level $E_{0,1}^{(2)}$ is also equal to $\frac{\hbar^2 \kappa}{m}$, but the eigenfunction $\Phi^{(2)}_{0,1}$ vanishes identically.) The first excited state is doubly degenerate, with energy $E_{0,1}^{(1)} = E_{1,0}^{(1)} = 3\hbar^2 \kappa/m$. The second excited state is three-fold degenerate, with energy $E_{0,2}^{(1)} = E_{1,0}^{(2)} = E_{1,1}^{(2)} = 6\hbar^2 \kappa/m$. In general, the degeneracy of the energy level $N(N + 1)\hbar^2 \kappa/(2m)$ is $N$. 
For completeness, we mention in passing that the energy eigenvalues of a free particle moving in the $n$-sphere $S^n$ ($n \geq 3$) are also known. They comprise a discrete spectrum.

**Dynamical Billiards**

As in the cases of a particle in a square box and a circular box discussed earlier, the energy eigenvalues and eigenfunctions of a particle (a ‘billiard’) moving freely in the interior of other sufficiently symmetric two-dimensional planar regions can be determined, in principle, when the classical Hamiltonian is integrable and the motion sufficiently regular, i.e., non-ergodic [3–5]. Classical integrability in this instance requires a second isolating integral independent of $H$. Other than the square and circle, integrable cases include equilateral triangles, right triangles, rectangles and ellipses. In the case of an ellipse, for instance, the second constant of the motion is the product $L_1L_2$ of the angular momenta of the particle about the two foci of the ellipse. In the corresponding quantum mechanical problem, what is required for integrability is the separability of $\nabla^2$ as well as the boundary conditions in a suitable set of orthogonal coordinates. (In the case of an elliptic stadium, Schrödinger’s equation is separable in elliptic coordinates.) Further, there are close connections between classical superintegrability (which implies some dynamical symmetry over and above the usual geometrical symmetry such as rotational invariance), on the one hand, and the degeneracy of the energy levels, on the other.

If the billiard moves in a stadium in which the classical motion is not integrable, there exist sets of initial conditions of non-zero measure for which dynamical chaos occurs [6, 7]. Of the numerous examples studied, a prototypical one is the Sinai billiard [8]. This is a particle moving inside a square stadium of side length $L$, but with a disc-shaped obstacle or scatterer of radius $a < L/2$ at the centre of the square, as shown in Figure 2. The ‘defocusing’ effect of the convex shape of the scatterer causes a separation of initially close particle trajectories, leading to dynamical chaos.
The origins of chaos in a classical gas can be traced back to this basic situation.

The quantum mechanical counterpart of a classically non-integrable billiard displays ‘quantum chaos’: The energy level patterns appear to be random; the level distribution statistics show features akin to those of random matrices; the positional probability density plots show ‘quantum scars’, i.e., the density is enhanced along classically unstable periodic orbits; and so on. There is a considerable amount of literature on this subject, which continues to be of current interest. Topics of on-going research include the connections between these features and multiparticle entanglement, thermalization of eigenstates, and a variety of related aspects. We shall not go into further detail, as our emphasis in this article is on integrable examples involving a particle moving freely in compact regions with a simple geometry.

The Inverse Problem

In several of the cases discussed in the foregoing, the problem was to find the eigenvalues and eigenfunctions of the Hamiltonian of a particle moving freely inside a two-dimensional planar domain $\mathcal{R}(x, y)$ with a perfectly reflecting boundary. In mathematical terms, this amounted to finding the spectrum of eigenvalues.

Figure 2. The Sinai billiard, showing how the scatterer causes neighboring trajectories to diverge.
**Figure 3.** The first example [10] of two planar domains that are isospectral but non-isometric.

of the operator $-\nabla^2$ with Dirichlet boundary conditions, that is, $\Phi = 0$ on the boundary $\partial \mathcal{R}$. These eigenvalues are $2m/h^2$ times the energy eigenvalues of the particle.

The inverse problem is also of great interest. Suppose one is given the full spectrum of $-\nabla^2$ in $\mathcal{R}$ under Dirichlet boundary conditions. What can be deduced regarding $\mathcal{R}$ from this information? In particular, does the spectrum determine the domain up to an isometry, i.e., up to a translation and rotation? That is, must domains that are isospectral (i.e., have the same spectrum) also be isometric?

This is the question famously posed [9] as “Can you hear the shape of a drum?” The answer depends on the kind of domain involved. For convex domains with an analytic (or everywhere smooth) boundary, it is ‘yes’. For general non-convex polygonal domains, it is ‘no’, as first shown in [10]. Figure 3 shows the pair of isospectral but non-isometric domains presented therein to settle this longstanding question in the case of two-dimensional manifolds.

The areas of the two (non-convex) polygonal domains are equal, as are their perimeter lengths. They also have the same number of sides, corners and corner angles. But they are not congruent. For non-convex domains with analytic (everywhere smooth) boundary, the answer to this question is not known. In any case, the general answer is ‘no’, and there is a systematic procedure to generate distinct non-isometric domains that are isospectral [11]. Figure 4 shows a pair of such domains that are simpler than the original pair in Figure 3.
Isospectral domains and related problems have also been investigated extensively in higher dimensional and curved spaces [12, 13]. In fact, the first example of isospectral but non-isometric domains, presented in [12], involved two 16-dimensional tori. In curved spaces, the Laplacian $\nabla^2$ generalizes to the Laplace–Beltrami operator \((1/\sqrt{|g|}) \partial_i (\sqrt{|g|} g^{ij} \partial_j)\), where $\partial_i = \partial/\partial x^i$, $g^{ij}$ is the metric tensor, and $|g|$ is the modulus of its determinant.

We now turn very briefly to the more general question of the information about the domain that the spectrum of $-\nabla^2$ carries. Under Dirichlet boundary conditions, the self-adjoint operator $-\nabla^2$ has a countably infinite eigenvalue spectrum of the form

$$0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \lambda_4 \leq \cdots \quad \text{(16)}$$

That is, all the eigenvalues (with eigenfunctions $\neq 0$) are real and positive. The links between the set \(\{\lambda_j\}\) and the geometry of the domain concerned are provided by the so-called Weyl formulas and trace formulas [14–18]. They involve advanced mathematical analysis of the ‘heat kernel’ and related topics. We shall merely state a few key results in this regard.

**Weyl Formulas and Trace Formulas**

Consider a planar domain $\mathcal{R}$ of area $A$ and perimeter $P$. Given a positive number $\Lambda$, let $N(\Lambda)$ denote the number of eigenvalues of $-\nabla^2$ on $\mathcal{R}$ with Dirichlet boundary conditions that are less than or equal to $\Lambda$. Owing to the occurrence of rapidly fluctuating number-theoretic functions (like the degeneracy $g(N)$ encountered earlier, in the case of a particle in a square box), $N(\Lambda)$ is also a wildly varying function of $\Lambda$. An averaging procedure softens

**Figure 4.** A simpler example [11] of two isospectral but non-isometric planar domains.
these rapid variations to yield a smooth function \( \langle N(\Lambda) \rangle \). Weyl’s formula is an asymptotic series for this average, given by

\[
\langle N(\Lambda) \rangle = \frac{A}{4\pi} \Lambda - \frac{P}{4\pi} \Lambda^{3/2} + a_1 \Lambda^0 + a_2 \Lambda^{-1/2} + \cdots . \tag{17}
\]

The leading term in \( \langle N(\Lambda) \rangle \) is directly proportional to \( A \), the measure of the domain. The coefficients \( a_1, a_2, \ldots \) specify the number of holes in \( \mathcal{R} \), the number of sharp corners, etc. Thus, \( \langle N(\Lambda) \rangle \) directly yields detailed geometrical information about the domain \( \mathcal{R} \).

The correspondence result for a three-dimensional domain of volume \( V \) was an outstanding problem in the early years of the 20th century, in a different context: to count correctly the number of modes of the radiation field inside a blackbody cavity, and to deduce the intensity \( I(\nu) \) of the radiation as a function of the frequency \( \nu \). (As we know now, Planck’s Law of blackbody radiation was finally derived properly by the application of Bose–Einstein statistics to a gas of non-interacting photons.) The three-dimensional counterpart of Weyl’s formula for a domain of volume \( V \) and surface area \( S \) is given by

\[
\langle N(\Lambda) \rangle = \frac{V}{6\pi^2} \Lambda^{3/2} - \frac{S}{16\pi} \Lambda + b_1 \Lambda^{1/2} + b_2 \Lambda^0 + b_3 \Lambda^{-1/2} + \cdots . \tag{18}
\]

Once again, the leading term in this series is proportional to the measure \( V \) of the domain. The coefficients \( b_i \) depend on more detailed geometrical properties of the domain.

The so-called trace formulas involve what may be viewed as the generating function or ‘partition function’ for the set of eigenvalues \( \{\lambda_1, \lambda_2, \ldots \} \) of \(-\nabla^2\) (or its generalization, the Laplace–Beltrami operator) under Dirichlet boundary conditions. Let \( u \) be a positive variable. Consider the function of \( u \) given by

\[
G(u) = \sum_{j=1}^{\infty} e^{-\lambda_j/u} . \tag{19}
\]

This series converges for all positive values of \( u \), and in fact defines an analytic function of \( u \) in the right half-plane \( \Re u > 0 \).
As \( u \to 0 \) from above, each term in the sum tends to 1, and the series diverges. The analytic function \( G(u) \) may be expected to be singular at \( u = 0 \). The nature of this divergence is seen in the so-called trace formula, an asymptotic expansion for \( G(u) \) as \( u \to 0 \). For a two-dimensional domain of area \( A \) and perimeter \( P \), it can be shown that

\[
G(u) = \frac{A}{2\pi u} - \frac{P}{(32\pi u)^{1/2}} + O(u^0). 
\]  

(20)

Likewise, for a three-dimensional domain of volume \( V \) and surface area \( S \), it is found that

\[
G(u) = \frac{V}{(2\pi u)^{3/2}} - \frac{S}{16\pi u} + \frac{\sigma}{u^{1/2}} + O(u^0),
\]  

(21)

where \( \sigma \) is proportional to the mean curvature of the surface. There are many other such deep results pertaining to the spectrum of the Laplacian on manifolds.

Concluding Remarks

The problem of a particle (both classical and quantum mechanical) moving freely inside a domain with reflecting walls is a paradigm with remarkably wide and diverse ramifications. These range from direct physical applications to nanowires and nanostructures, quantum dots, etc., to studies in semiclassical quantization, quantum chaos, statistical mechanics, and so on, and to problems and results in several areas of mathematics such as functional analysis, variational calculus, group theory, harmonic analysis, differential geometry and ergodic theory, to mention just a few. The particle-in-a-box problem is thus a truly basic paradigm in both classical mechanics and quantum mechanics.

Acknowledgement

I thank Sunethra Ramanan and B. Sharmila for technical assistance. I am deeply grateful to the reviewer for a very thorough reading of the manuscript and for numerous helpful suggestions.
Suggested Reading


[3] Throughout this article, I have tacitly assumed that the reader has some familiarity with the notion of integrability in the context of classical Hamiltonian dynamics. For the aspects of the topic that are relevant to the context and purpose at hand, see, for instance, Refs. [4] and [5] below.


