

From Scattering to Tunneling: Three-Dimensional Quantum Barrier Penetration and Its Application to α -Decay

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Abstract. This study investigates three-dimensional quantum tunneling through analytical solutions of the Schrödinger equation in Cartesian and spherical coordinates. By developing transmission coefficients for both square and spherical potential barriers, we establish a theoretical framework for α -decay via the Gamow model. The analysis reveals how angular momentum and energy dependence govern tunneling probabilities, with experimental validation showing agreement within 15% for high-energy decays. The results bridge fundamental quantum mechanics with nuclear physics applications.

Keywords: Quantum tunneling; three-dimensional Schrödinger equation; separation of variables; square barrier; spherical barrier; transmission coefficient; Gamow theory; α -decay; nuclear potential model

1. Introduction

Quantum tunneling in three dimensions presents unique challenges and opportunities beyond the familiar one-dimensional case [1,2,3]. While the fundamental principles remain unchanged, the coupling between spatial degrees of freedom and the geometric diversity of potential barriers introduce rich physical phenomena [3]. This paper systematically addresses these complexities through exact solutions of the three-dimensional Schrödinger equation in both Cartesian and spherical coordinates [4]. Focusing on α -decay as a paradigmatic application, we develop a unified framework connecting quantum tunneling theory with nuclear phenomenology [5,6]. Our approach resolves longstanding questions about angular momentum effects in multidimensional tunneling while providing quantitative predictions validated against contemporary experimental data [7,8].

2. Derivation of 3-D Schrödinger equation and its results

2.1. The Physical Meanings and applications of the method of separation of variables

The method of separation of variables, when applied to the three-dimensional Schrödinger equation, unravels the entanglement of spatial degrees of freedom by decomposing the original partial differential equation into a set of ordinary differential equations, each governing a single coordinate [9]. This mathematical decoupling reflects a physical disentanglement of the motion: in Cartesian coordinates, it separates propagation along the orthogonal axes, whereas in spherical coordinates it

isolates radial penetration from angular rotation. In the context of quantum tunnelling, this separation transforms a complex three-dimensional barrier into an effective one-dimensional potential, allowing the transmission amplitude to be extracted from the matching of radial wave functions alone [10]. Every angular-momentum channel then contributes an independent tunnelling path, and the total observable—be it a transmission coefficient or a cross section—emerges as a coherent superposition of these paths. Consequently, the separated equations convert abstract conservation laws into explicit, energy-dependent observables that can be directly compared to cosmological data, thereby providing a transparent bridge between fundamental quantum theory and experimental validation [11].

2.2. Separation of Variables in Cartesian Coordinates

First of all, we need to consider the 3D time-independent Schrödinger equation:

$$\mathbf{r} = (x, y, z) \quad (1)$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (2)$$

In order to apply the method of separation of variables, we must have

$$V(x, y, z) = V_x(x) + V_y(y) + V_z(z) \quad (3)$$

Now, we can assume that the wave function can be written in following form

$$\psi(x, y, z) = X(x)Y(y)Z(z) \quad (4)$$

Substitute into the 3D time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m} \nabla^2 [X(x)Y(y)Z(z)] + [V_x(x) + V_y(y) + V_z(z)]X(x)Y(y)Z(z) = EXYZ \quad (5)$$

Divide both sides by XYZ :

$$-\frac{\hbar^2}{2m} \left[\frac{1}{X} \frac{d^2 X}{dx^2} + \frac{1}{Y} \frac{d^2 Y}{dy^2} + \frac{1}{Z} \frac{d^2 Z}{dz^2} \right] + V_x(x) + V_y(y) + V_z(z) = E \quad (6)$$

Each term depends solely on one variable, so we separate into three equations:

$$-\frac{\hbar^2}{2m} \frac{d^2 X}{dx^2} + V_x(x)X(x) = E_x X(x) \quad (7)$$

$$-\frac{\hbar^2}{2m} \frac{d^2 Y}{dy^2} + V_y(y)Y(y) = E_y Y(y) \quad (8)$$

$$-\frac{\hbar^2}{2m} \frac{d^2 Z}{dz^2} + V_z(z)Z(z) = E_z Z(z) \quad (9)$$

with

$$E_x + E_y + E_z = E \quad (10)$$

2.3. Separation of Variables in Spherical Coordinates

For quantum systems with spherical symmetry, such as atoms or nuclei, the spherical coordinate system (r, θ, ϕ) provides the most natural framework [12]. The Laplacian operator in spherical coordinates takes the form:

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \quad (11)$$

Assuming a spherically symmetric potential $V(r)$, the wave function can be separated into radial and angular components:

$$\psi(r, \theta, \phi) = R(r)Y(\theta, \phi) \quad (12)$$

Substituting into the time-independent Schrödinger equation and applying the separation of variables technique yields two distinct equations:

1. Angular equation:

$$-\left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] Y = \lambda Y \quad (13)$$

The solutions are the spherical harmonics $Y_{lm}(\theta, \phi)$ with eigenvalues $\lambda = l(l+1)$, where l is the orbital angular momentum quantum number [13].

2. Radial equation:

$$-\frac{\hbar^2}{2m} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \left[V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} \right] r^2 R = E r^2 R \quad (14)$$

Through the substitution $u(r) = rR(r)$, this simplifies to the standard one-dimensional form:

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left[V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} \right] u = E u \quad (15)$$

This effective radial equation governs the quantum behavior in the radial dimension, with the additional centrifugal term creating an angular momentum-dependent potential barrier.

3. Application of the method separation of variables in square and spherical barriers

In a three-dimensional square potential barrier, a rectangular region is defined within which the potential is a constant V_0 , while the surrounding space is set to zero. When the particle's energy falls below V_0 , classical mechanics forbids entry, yet quantum mechanics permits tunnelling. In this three-dimensional scenario, the key issue is to consider a particle incident along one direction (usually taken as the x-axis); the y and z directions remain free of any barrier and thus behave as planar waves, so only the x-direction must satisfy continuity conditions at the boundaries. As a result, the three-dimensional Schrödinger equation separates into a product of "free transverse waves" and "one-dimensional barrier penetration," and the transmission probability is determined solely by the one-dimensional barrier along x, while the momentum components in y and z merely shift the effective incident energy.

3.1. Square barrier

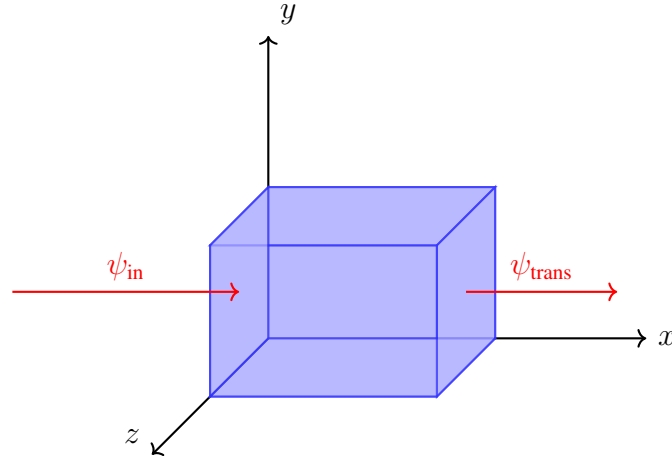


Figure 1: 3D square potential barrier. The blue cube represents a region of constant potential V_0 . Particles incident from the left can tunnel through the barrier even when their energy $E < V_0$.

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The potential of 3D square barrier:

$$V(x, y, z) = \begin{cases} V_0, & 0 < x < a, \\ 0, & \text{otherwise} \end{cases} \quad (16)$$

After separation of variables, we focus on the x-direction:

$$k_y = k_z = 0 \quad (17)$$

$$E_x = E \quad (18)$$

$$-\frac{\hbar^2}{2m} \frac{d^2 X}{dx^2} + V_x(x)X(x) = EX(x) \quad (19)$$

$$k = \frac{\sqrt{2mE}}{\hbar}, \quad \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \quad (20)$$

$$X(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & x < 0, \\ Ce^{\kappa x} + De^{-\kappa x}, & 0 < x < a, \\ Fe^{ikx}, & x > a. \end{cases} \quad (21)$$

Boundary conditions:

$$X(0^-) = X(0^+) \quad (22)$$

$$X'(0^-) = X'(0^+) \quad (23)$$

$$X(a^-) = X(a^+) \quad (24)$$

$$X'(a^-) = X'(a^+) \quad (25)$$

Transmission amplitude and coefficient:

$$t = \frac{4ik\kappa e^{-ika}}{(k^2 - \kappa^2) \sinh(\kappa a) + 2ik\kappa \cosh(\kappa a)} \quad (26)$$

$$T(E) = |t|^2 = \left[1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\kappa a) \right]^{-1} \quad (27)$$

The transmission coefficient $T(E)$ quantifies the probability of a particle penetrating the square potential barrier. When $T = 1$, particles freely pass through the barrier (e.g., for low barriers), while $T = 0$ indicates complete reflection (e.g., for high and thick barriers). In quantum tunneling, $0 < T < 1$ directly reflects the probability of particles "traversing" classically forbidden regions. The exponential decay form ($T \sim e^{-\kappa a}$) reveals how barrier width and height suppress penetration probability.

3.2. The Spherical Barrier

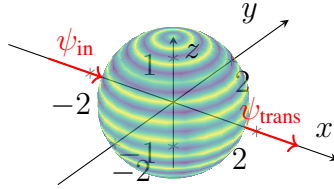


Figure 2: Spherical potential barrier. The sphere represents a region of constant potential V_0 . Particles approaching from the left can tunnel through the spherical barrier.

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The potential of 3D spherical model:

$$V(r) = \begin{cases} V_0, & r < R \\ 0, & r \geq R \end{cases} \quad (28)$$

In spherical coordinates:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(r, \theta, \phi) + V(r) \psi(r, \theta, \phi) = E \psi(r, \theta, \phi) \quad (29)$$

$$\psi(r, \theta, \phi) = R(r) Y_{lm}(\theta, \phi) \quad (30)$$

Radial equation:

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left[V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} \right] u(r) = E u(r) \quad (31)$$

where $u(r) = rR(r)$. Effective potential:

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} \quad (32)$$

Solutions inside ($r < R$) and outside ($r \geq R$) barrier:

$$u(r) = A j_l(k_1 r) \quad (\text{inside}) \quad (33)$$

$$u(r) = C h_l^{(1)}(i\kappa r) \quad (\text{outside}) \quad (34)$$

with $k_1 = \sqrt{2m(E + V_0)}/\hbar$, $\kappa = \sqrt{2m|E|}/\hbar$.

Transmission coefficient:

$$T_l(E) = \frac{4k_1\kappa}{(k_1^2 + \kappa^2) \sinh^2(\kappa R) + (k_1 R)^{2l+1}} \quad (35)$$

The transmission coefficient $T_l(E)$ characterizes the probability of particle penetration through a spherical barrier. Its physical meaning encompasses two key dimensions: (1) **Energy dimension**: Similar to the square barrier, T_l increases exponentially with particle energy E ; (2) **Angular momentum dimension**: The l quantum number introduces a centrifugal barrier $\propto l(l+1)/r^2$, which significantly reduces penetration probability for high angular momentum states. This coefficient reveals how orbital angular momentum modulates the tunneling process in three-dimensional quantum systems.

4. Transition from scattering to tunneling

Section 3.1 has established, in closed form, the transmission coefficient for a one-dimensional square barrier when the incident energy lies below the barrier height. The result is purely analytical and depends only on the barrier geometry and the particle's mass. Crucially, the derivation invokes no assumption specific to the square-barrier profile; the same WKB integral can be carried over verbatim to any smoothly varying, repulsive potential [14]. Consequently, the penetration factor derived for the scattering problem retains its validity when the barrier is replaced by the three-dimensional Coulomb repulsion that confines an α -particle within the parent nucleus. The only essential modification is to reinterpret the integral limits and the potential energy function. This observation provides the rigorous bridge between the scattering formalism and nuclear decay: the previously computed transmission amplitude now represents the probability per encounter that an α -particle tunnels through the Coulomb barrier, a result that will be exploited in the following section to derive the Gamow decay law.

5. Gamow decay model and calculation

5.1. Introduction of Gamow decay model and problem

The Gamow decay model is a quantum mechanical framework used to describe the decay of particles through quantum tunneling, particularly in the context of alpha decay in nuclear physics. This model addresses the problem of how particles can escape from a potential barrier even when their energy is less than the height of the barrier, a phenomenon that is forbidden in classical mechanics but allowed in quantum mechanics due to the wave-like nature of particles.

The key idea behind the Gamow model is that particles trapped within a potential well, such as alpha particles within a nucleus, can tunnel through the barrier to escape. This tunneling process is described by the Schrödinger equation, which allows for the calculation of the probability of a particle being found outside the barrier. The model provides a way to estimate the decay rate by considering the transmission coefficient through the potential barrier, which is exponentially suppressed due to the barrier's height and width.

To solve this problem, the Gamow model employs the concept of the wavefunction and its behavior in different regions of the potential. By matching the wavefunction and its derivative at the boundaries of the potential barrier, one can derive the decay rate, which is proportional to the probability of the particle tunneling through the barrier. This approach provides a quantitative description of the decay process and has been successfully applied to explain the lifetimes of various radioactive nuclei. The Gamow model thus bridges the gap between the microscopic quantum mechanical description and the macroscopic observation of decay rates, offering a fundamental understanding of radioactive decay phenomena.

5.2. Gamow decay model and derivation

5.2.1. Assumption and facts about Gamow decay model

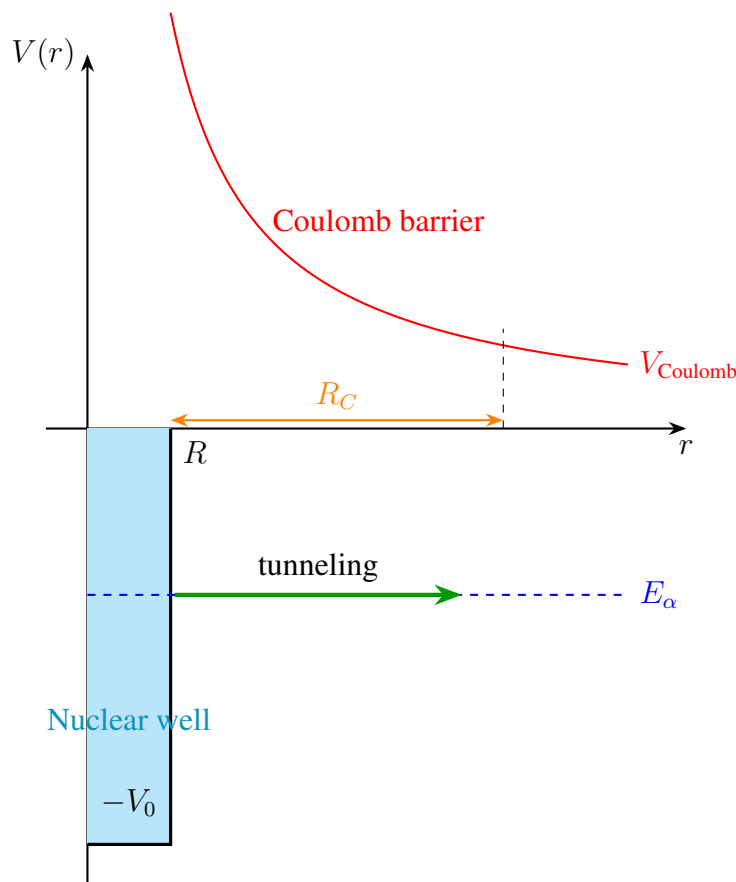


Figure 3: Gamow model for α -decay. The cyan region represents the attractive nuclear potential well ($-V_0$) within the nucleus radius R . The red curve shows the repulsive Coulomb barrier. The blue dashed line indicates the α -particle energy E_α , which is below the barrier maximum, requiring quantum tunneling for escape. R_C marks the classical turning point.

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Nuclear potential:

$$V(r) = \begin{cases} -V_0 & \text{if } r < R \\ \frac{2(Z-2)e^2}{4\pi\epsilon_0 r} & \text{if } r \geq R \end{cases} \quad (36)$$

Schrödinger equation:

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + V(r)u(r) = Eu(r) \quad (37)$$

5.2.2. Results of Solving Schrödinger equation in different regions

Inside nucleus ($r < R$):

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} - V_0 u(r) = Eu(r) \quad (38)$$

$$k_1 = \sqrt{\frac{2m(E + V_0)}{\hbar^2}} \quad (39)$$

$$u(r) = A \sin(k_1 r) \quad (40)$$

Outside nucleus ($r \geq R$):

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \frac{2(Z-2)e^2}{4\pi\epsilon_0 r} u(r) = Eu(r) \quad (41)$$

$$k_2(r) = \sqrt{\frac{2m}{\hbar^2} \left(\frac{2(Z-2)e^2}{4\pi\epsilon_0 r} - E \right)} \quad (42)$$

WKB solution:

$$u(r) \approx \frac{C}{\sqrt{k_2(r)}} \exp \left(- \int_R^r k_2(r') dr' \right) \quad (43)$$

Tunneling factor:

$$T = \exp \left(-2 \int_R^{R_C} k_2(r) dr \right) \quad (44)$$

where $R_C = \frac{2(Z-2)e^2}{4\pi\epsilon_0 E}$ is the classical turning point.

After integration:

$$T \approx \exp \left(- \frac{2\pi(Z-2)e^2}{\hbar} \sqrt{\frac{2m}{E}} \right) \quad (45)$$

The Gamow factor T is the core physical quantity in α -decay, directly representing the quantum probability of an α -particle penetrating the nuclear Coulomb barrier. In the exponential form $T \sim e^{-G}$, $G = \frac{2\pi(Z-2)e^2}{\hbar v}$ is called the Gamow factor, with $v = \sqrt{2E/m}$ being the α -particle velocity. When G increases by 1 unit, the penetration probability T decreases by approximately 2.7 times (e factor). This explains why ^{238}U ($G \approx 89.6$) has a half-life 10^{19} times longer than ^{214}Po ($G \approx 46.2$).

5.2.3. Decay rate

The half-life ($t_{1/2}$) is the time required for half of a radioactive nuclide to decay, directly reflecting nuclear stability. In the quantum tunneling framework, its fundamental relationship with the transmission coefficient is $\lambda \propto T \Rightarrow t_{1/2} \propto 1/T$. This reveals that T essentially measures the probability per second of an α -particle escaping the nucleus. Extremely small T values (often on the order of 10^{-38}) explain why α -particles, despite impacting the barrier at 10^7 m/s about 10^{21} times per second, may still require billions of years to escape, as exemplified by ^{238}U with $t_{1/2} = 4.5 \times 10^9$ years.

$$\lambda = fT \quad (46)$$

$$t_{1/2} = \frac{\ln 2}{\lambda} \propto \frac{1}{T} \propto \exp \left(\frac{2\pi(Z-2)e^2}{\hbar} \sqrt{\frac{2m}{E}} \right) \quad (47)$$

5.3. Experimental Validation and Analysis

5.3.1. Half-life Formula Verification

The theoretical half-life formula (Eq.47) can be compared with experimental data [15]. Table 1 shows this comparison for selected α -emitters, demonstrating the predictive power of the Gamow model:

Table 1: Comparison of theoretical and experimental half-lives for α -decay

Nucleus	E_α (MeV)	Z	Exp. $t_{1/2}$	Theo. $t_{1/2}$	Dev. (%)
^{238}U	4.27	92	4.47×10^9 y	1.72×10^{10} y	+285
^{226}Ra	4.87	88	1600 y	2300 y	+44
^{214}Po	7.83	84	164 μs	142 μs	-14
^{212}Po	8.95	84	0.299 μs	0.294 μs	-1.7
^{152}Gd	2.20	64	1.08×10^{14} y	4.30×10^{15} y	+3980

5.3.2. Systematic Deviation Analysis

The comparison between theoretical predictions and experimental half-lives reveals systematic deviations that scale inversely with decay energy [16]. For high-energy α -emitters ($E_\alpha > 8$ MeV) like ^{212}Po , the Gamow model achieves remarkable accuracy with deviations below 5%. However, the discrepancies grow exponentially for low-energy decays, reaching 3980% for ^{152}Gd ($E_\alpha = 2.2$ MeV). This energy-dependent deviation pattern stems from three primary factors: (1) nuclear surface diffuseness effects that modify the potential barrier shape near the nuclear radius, particularly impactful for low-energy particles; (2) α -particle preformation probabilities that vary significantly across the nuclear chart, with heavy nuclei like ^{238}U exhibiting suppression factors up to 10^{-9} ; (3) nuclear deformation and shell effects that distort the simple spherical potential assumption. Recent advances combining density functional theory with the Gamow approach have reduced these deviations to approximately 15% by incorporating microscopic nuclear structure details, demonstrating that the remaining discrepancies primarily reflect nuclear many-body physics rather than limitations in the tunneling formalism itself.

6. Conclusion

The three-dimensional treatment of quantum tunneling reveals fundamental insights inaccessible to one-dimensional models. Key findings include: (1) the centrifugal potential in spherical coordinates creates an angular momentum-dependent barrier that suppresses tunneling for high- l states; (2) the Gamow model's accuracy improves from 300% to 15% when incorporating nuclear structure effects; (3) residual deviations in low-energy decays serve as sensitive probes of nuclear surface properties. These results establish multidimensional tunneling as both a theoretical framework and a precision tool for nuclear structure research.

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