Quantum Particle in a Ring

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1 Description

Ever wonder what quantum particles really look like? It's certainly hard to imagine: they sometimes are in multiple places at once - unless you measure them. Then, they quickly make up their minds, and are in a specific state.

How do they "decide" where they're measured? As it turns out, when the universe is not looking, a quantum particle shifts back and forth between different possible states. They quickly flit in and out of high-energy states, and they slowly oscillate between low-energy states. The equation that describes this process is the time-dependent Schrodinger equation:

$$\Psi(t) = \exp\left(-\frac{i}{\hbar}Ht\right)\Psi(0).$$

Let's talk about how a particle evolves over time when it isn't being measured. Imagine a particle in a 2D space whose position is not determined. This particle has a certain probability of being measured in each region of the space. If the particle's energy level is determined, meaning it's not mixed between multiple energy levels, then this probability distribution is constant over time.

However, if the particle is mixed between multiple energy levels, then the probability distribution will change over time. This is because each energy level is associated with a specific shape for the distribution. When multiple energy levels are present, and the particle is shifting back and forth between them, the amplitude of each energy level's probability distribution oscillates at its own pace.

This produces wave-like motion as the particle's probability shifts between different shapes. In general, higher energy levels are associated with shorter wavelengths, and as the different probability distributions grow and shrink, they interfere with each other, causing the overall density to shift and morph.

Note that this is not exactly what you'd see if you could look at a quantum particle. When measured, the particle will be in a single location. However, visualizing the particle's evolution without measurements helps us understand how quantum systems evolve and mix between states.

2   Mathematics

2.1   Schrodinger equation

The wavefunction solves $(-\Delta + V(\vec{r}))\psi = E\psi$.

$V(\vec{r})$ defines the boundary conditions for an annulus with infinite walls. In polar coordinates,

$$V(r, \phi) = \begin{cases} \infty, r > a \\ 0, a \geq r \geq b \\ \infty, r < b \end{cases}.$$

Within this region, the Schrodinger equation becomes $-\frac{\hbar^2}{2m}\Delta\psi = E\psi$ with the boundary conditions $\psi(a, \phi) = \psi(b, \phi) = 0$. In polar coordinates,

$$\frac{\hbar^2}{2m}\left(\partial_r^2 + \frac{\partial_r}{r} + \frac{\partial_\phi^2}{r^2}\right)\psi(r, \phi) = E\psi(r, \phi),$$

It can be solved via Separation of Variables,

$$\psi(r, \phi) = P(r)F(\phi).$$

The azimuthal Schrodinger equation is a homogeneous 2nd order equation in ϕ:

$$\partial_\phi^2 F_l(\phi) = L^2 F_l(\phi).$$

The azimuthal part is periodic over $\mathbb{R}_\tau$ and involves no other symmetries. As such, it takes the form $F_l(\phi) = \exp(il\phi)\,\forall\, l \in \mathbb{Z}$. $F_l(\phi)$ is an eigen state of the L^2 operator, so

$$L^2 F_l(\phi) = l^2 F_l(\phi).$$

The kinetic energy operator, Δ, consists of a radial part, $\partial_r^2 + \frac{\partial_r}{r}$, and an azimuthal part, $\frac{\partial_\phi^2}{r^2} = \frac{l^2}{r^2}$.

$P(r)$ solves the radial Schrodinger equation,

$$-\frac{\hbar^2}{2m}\left(\partial_r^2 + \frac{\partial_r}{r} - \frac{l^2}{r^2}\right)P(r) = EP(r).$$

Multiplied by r^2, the radial equation becomes the Bessel equation, and the solutions are related by $P(r) = \gamma_l R_{n|l|}(r)$ with $n \in \mathbb{Z}_{\geq 1}$, $\gamma_l \in \mathbb{R}_{>0}$. So consider the Bessel equation,

$$\left(r^2\partial_r^2 + r\partial_r + k_n^2 r^2 - l^2\right)R_{n|l|}(r) = 0.$$

The radial part is solved by a combination of cylindrical Bessel functions. This is solved in *Loud Speakers Theory: Performance, Testing and Design*↗ on page 81. Some of the process is repeated here.

$$R_{n|l|}(r) = A_{nl}J_{|l|}(k_n r) + B_{nl}Y_{|l|}(k_n r).$$

Appealing to the boundary behavior,

$$R_{n|l|}(a) = R_{n|l|}(b) = 0$$

$$J_{|l|}(k_n a)Y_{|l|}(k_n b) - J_{|l|}(k_n b)Y_{|l|}(k_n a) = 0.$$

Let $r_0 = \frac{a+b}{2}$ and let $R_{n|l|}(r_0) = 1$. This scale factor can be set arbitrarily because it will be accounted for in the wave function's normalization. Then, the radial equation is

$$R_{n|l|}(r) = \frac{J_{|l|}(k_n r)\, Y_{|l|}(k_n a) - J_{|l|}(k_n a)\, Y_{|l|}(k_n r)}{J_{|l|}(k_n r_0)\, Y_{|l|}(k_n a) - J_{|l|}(k_n a)\, Y_{|l|}(k_n r_0)}.$$

Thus, the eigen functions can be separated into radial and azimuthal components with quantum numbers (n, l) :

$$\psi_{nl}(r, \phi) = \gamma_{nl}R_{nl}(r)\exp(il\phi)$$

$$\boxed{\psi_{nl}(r, \phi) = \gamma_{nl}\frac{J_{|l|}(k_n r)\, Y_{|l|}(k_n a) - J_{|l|}(k_n a)\, Y_{|l|}(k_n r)}{J_{|l|}(k_n r_0)\, Y_{|l|}(k_n a) - J_{|l|}(k_n a)\, Y_{|l|}(k_n r_0)}\exp(il\phi)}.$$

We can define the coefficients A_{nl} and B_{nl} accordingly:

$$R_{n|l|}(r) = A_{nl}J_{|l|}(k_n r) + B_{nl}Y_{|l|}(k_n r)$$

$$A_{nl} = \frac{Y_{|l|}(k_n a)}{J_{|l|}(k_n r_0)\, Y_{|l|}(k_n a) - J_{|l|}(k_n a)\, Y_{|l|}(k_n r_0)}$$

$$B_{nl} = \frac{-J_{|l|}(k_n a)}{J_{|l|}(k_n r_0)\, Y_{|l|}(k_n a) - J_{|l|}(k_n a)\, Y_{|l|}(k_n r_0)}$$

$$\boxed{\psi_{nl}(r, \phi) = \gamma_{nl}\left(A_{nl}J_{|l|}(k_n r) + B_{nl}Y_{|l|}(k_n r)\right)\exp(il\phi)}.$$

For each (n, l) pair, the normalization condition for each eigen function is

$$\int_b^a dr \int_0^\tau r d\phi\, \psi_{nl}^\dagger \psi_{nl} = 1.$$

The azimuthal integral result is

$$\int_0^\tau d\phi \exp(il\phi)\exp(-il\phi) = \int_0^\tau d\phi = \tau.$$

(Note on notation: this article uses $\tau = 2\pi$ for the circle constant. *Motivation*↗)

The radial integral is (available at the *Digital Library of Mathematical Functions (DLMF)*↗; these identities hold for linear combinations of Bessel functions):

$$\int_b^a dr\, r \left(R_{n|l|}(r)\right)^2 = \left[r^2 \left(\frac{A_{nl}^2}{2} \left(J_{n|l|}^2 - J_{n\,,|l|-1} J_{n\,,|l|+1} \right) + \frac{B_{nl}^2}{2} \left(Y_{n|l|}^2 - Y_{n\,,|l|-1} Y_{n\,,|l|+1} \right) \cdots \right. \right.$$

$$\left. \left. \cdots + A_{nl} B_{nl} \left(J_{n\,,|l|+1} Y_{n|l|} - J_{n\,,|l|+1} Y_{n|l|} \right) \right) \right] \Bigg|_b^a .$$

The coefficient is the inverse square-root of the entire integral:

$$1 = \tau \gamma_{nl}^2 \int_b^a dr\, r \left(R_{nl}(r)\right)^2$$

$$1 = \frac{\tau \gamma_{nl}^2 r^2}{4} \left(R_{n|l|}^2 - R_{n,\,|l|-1} R_{n,\,|l|+1} \right) \Bigg|_b^a$$

$$\boxed{\gamma_{nl} = \sqrt{\frac{4}{\tau r^2}} \left(R_{n|l|}^2 - R_{n\,,|l|-1} R_{n\,,|l|+1} \right)^{-1/2} \Bigg|_b^a .}$$

2.2   Energy Eigen Value Calculation

For each eigen function ψ_{nl}, the Hamiltonian has one eigen value.

$$\langle \psi_{nl} | H | \psi_{nl} \rangle = E_{nl} = \frac{\hbar^2}{2m} \int_0^\tau d\phi \int_b^a dr\, r \psi_{nl}^\dagger H \psi_{nl}$$

$$H \psi_{nl} = -\frac{\hbar^2}{2m} \gamma_{nl} \left(\partial_r^2 + \frac{\partial_r}{r} - \frac{l^2}{r^2} \right) \left(R_{n|l|}(r) \exp(il\phi) \right)$$

$$E_{nl} = -\frac{\hbar^2}{2m} \gamma_{nl}^2 \int_0^\tau d\phi \int_b^a dr\, r \left(R_{n|l|}(r) \exp(-il\phi) \right) \left(\partial_r^2 + \frac{\partial_r}{r} - \frac{l^2}{r^2} \right) \left(R_{n|l|}(r) \exp(il\phi) \right)$$

$$E_{nl} = \frac{\hbar^2}{2m} l^2 \gamma_{nl}^2 \int_0^\tau d\phi \int_b^a dr\, r \left(R_{n|l|}(r) \right) \left(\partial_r^2 + \frac{\partial_r}{r} - \frac{l^2}{r^2} \right) \left(R_{n|l|}(r) \right)$$

$$I_1 + I_2 + I_3 = \int_b^a dr\, r \left(R_{n|l|} R_{n|l|}'' + \frac{1}{r} R_{n|l|} R_{n|l|}' - \frac{l^2}{r^2} R_{n|l|}^2 \right)$$

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$$I_1 + I_2 + I_3 = \int_b^a dr \left(r R_{n|l|} R''_{n|l|} + R_{n|l|} R'_{n|l|} - \frac{l^2}{r} R^2_{n|l|} \right).$$

$R_{n|l|}$ is a linear combination of Bessel functions of the first and second kind, so the Bessel function derivative recurrence relations hold for $R_{n|l|}$ (available at *The Wolfram Function Site↗*).

$$I_1 = \int_b^a dr\, r R_{n|l|} R''_{n|l|} = \frac{1}{4} \int_b^a dr\, r \left(R_{n,|l|-2}, R_{n|l|} + R_{n,|l|+2}, R_{n|l|} - 2R^2_{n|l|} \right)$$

$$I_1 = I_{11} + I_{12} + I_{13} = \frac{1}{4} \int_b^a dr\, r \left(R_{n,|l|-2}, R_{n|l|} + R_{n,|l|+2}, R_{n|l|} - 2R^2_{n|l|} \right)$$

$$I_2 = I_{21} + I_{22} = \int_b^a dr\, R_{n|l|} R'_{n|l|} = \frac{1}{2} \int_b^a dr \left(r R_{n|l|} R_{n,|l|-1} - |l|\, R^2_{n|l|} \right)$$

$$I_3 = -l^2 \int_b^a \frac{dr}{r} R^2_{n|l|}.$$

I_{13} also appears in "Section 2: Normalization," in the calculation of γ_{nl} (available at the *DLMF↗*):

$$I_{13} = \frac{1}{2} \int_b^a dr\, r R^2_{n|l|} = \frac{1}{2} \int_b^a dr\, r \left(A^2_{nl} J^2_{n|l|} + B^2_{nl} Y^2_{n|l|} + A_{nl} B_{nl} J_{n|l|} Y_{n|l|} \right)$$

$$I_{13} = \frac{r^2}{4} \left(R^2_{n|l|} - R_{n,|l|-1} R_{n,|l|+1} \right) \Big|_b^a.$$

I_3 has an analytic solution when $l \neq 0$ and can be evaluated numerically otherwise:

$$I_3 = -l^2 \int_b^a \frac{dr}{r} R^2_{n|l|} = -|l|\, R^2_{n|l|} \Big|_b^a.$$

The rest of the integrals can be evaluated numerically. In this article, I use Julia's 'QuadGK.jl' package for the integrals, and 'SpecialFunctions.jl' is used for Bessel functions. In Python, 'scipy' contains both tools ('scipy.integrate' and 'scipy.special'). Alternatively, The integral results can be represented with the *Generalized Hypergeometric Function↗*. However, evaluating the function often involves calculating a power series with sufficient precision, which is a performance consideration. Numerically evaluating the integrals also requires significant computation time (in this case, using a quadrature algorithm like 'QuadGK.jl'). Both are viable options with limited computing power, but this article does not compare their performances.

$$\boxed{E_{nl} = \frac{\hbar^2}{2m} l^2 \gamma^2_{nl} \left(I_{11} + I_{12} + I_{13} + I_{21} + I_{22} + I_3 \right).}$$

2.3 Time Evolution of Eigen States

The time-evolution operator is $U(t) = \exp(-\frac{i}{\hbar}Ht)$. Each state has an initial coefficient c_{nl} Applying $U(t)$ it to an initial state,

$$\Psi(t, r, \phi) = U(t)\Psi(0, r, \phi) = U(t)\left(\sum_{nl} c_{nl}\psi_{nl}(r, \phi)\right).$$

Each state has a complex initial coefficient c_{nl}. Assume the initial state coefficients satisfy $1 = \sum_{nl}|c_{nl}|^2$. Then,

$$c_{nl}U(t) = c_{nl}(t) = c_{nl}\exp\left(-\frac{i}{\hbar}tH\right)$$

$$c_{nl}(t)\psi_{nl} = c_{nl}\exp\left(-\frac{i}{\hbar}E_{nl}t\right)\psi_{nl}$$

$$\boxed{\Psi(t, r, \phi) = \sum_{nl} c_{nl}\exp\left(-\frac{i}{\hbar}E_{nl}t\right)\psi_{nl}(r, \phi)}.$$

Thus, the density over time is

$$\rho(t, r, \phi) = |\Psi(t, r, \phi)|^2$$

$$\rho(t, r, \phi) = \left(\sum_{nl} c_{nl}^\dagger\exp\left(\frac{i}{\hbar}E_{nl}t\right)\psi_{nl}^\dagger(r, \phi)\right)\left(\sum_{nl} c_{nl}\exp\left(-\frac{i}{\hbar}E_{nl}t\right)\psi_{nl}(r, \phi)\right)$$

$$\boxed{\rho(t, r, \phi) = \left(\sum_{nl} c_{nl}^\dagger\gamma_{nl}\exp\left(\frac{i}{\hbar}E_{nl}t\right)R_{n|l|}(r)\right)\left(\sum_{nl} c_{nl}\gamma_{nl}\exp\left(-\frac{i}{\hbar}E_{nl}t\right)R_{n|l|}(r)\right)}.$$