Quantum tunneling is a phenomenon where particles may "tunnel through" a barrier which they have insufficient kinetic energy to overcome according to classical mechanics. Tunneling is a result of the wavelike nature of quantum particles, and cannot be predicted by any classical system.

Introduction

Tunneling was first directly observed in the early 1900's when researchers were studying the electrical behavior of closely spaced electrodes in gases. An unexplained component of current was observed, even through high vacuum, though no explanation was found. Within a few years, physicists began to find solutions to the new Schrödinger equation. When solving for a double potential well, it was found that the particle could traverse two wells if the barrier separating them was sufficiently small and narrow.

The researchers were observing a phenomenon now called "field emission," where at high potentials electrons may tunnel through the potential barrier at the metal-vacuum interface, where they would then fall through the potential to the counter-electrode. Electron tunneling is exploited in technologies through Esaki diodes, Zener diodes, field emission-based electron guns, and scanning tunneling microscopy. For phenomena more germane to the study of chemistry, tunneling is responsible for the rate of alpha decay, since the alpha particles can escape from the atom even though the reaction that generates them would not produce enough energy to allow them to escape.

Basic description

As previously stated, quantum tunneling is a result of the wave nature of quantum particles. A traveling or standing wave function incident on a non-infinite potential decays in the potential as a function of $A_0 e^{-\alpha x}$, where $A_0$ is the amplitude at the boundary, $\alpha$ is proportional to the potential, and $x$ is the distance into the potential. If a second well exists at infinite distance from the first well, the probability goes to zero, so the probability of a particle existing in the second well is zero. If a second well is brought closer to the first well, the amplitude of the wave function at this boundary is not zero, so the particle may tunnel into that well from the first well. It would appear that the particles are 'leaking' through the barrier; they can travel through it without having to surmount it.

An important point to keep in mind is that tunneling conserves energy. The final sum of the kinetic and potential energy of the system cannot exceed the initial sum. Therefore, the potential on both sides of the barrier does not need to be the same, but the sum of the ground state energy and the potential on the opposite side of the barrier may not be larger than the initial particle energy and potential.

Advanced description

Tunneling is found from the Schrödinger equation, so we will start there. To simplify the calculations, the time-independent, one-dimensional Schrödinger equation is used (Equation \ref{eq1}).

\[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x) \psi = E \psi \]

To find solutions to a particular system, the potential $V(x)$ must be defined. In this case, we will set the potential to
zero for all space, except for the region between 0 and \((a)\), which we will set as \((V_0)\). This is represented by the piecewise function in Equation \ref{eq2}.

\[
V =
\begin{cases}
    0 & \text{if } -\infty<x\leq 0 \\
    V_0 & \text{if } 0<x<a \\
    0 & \text{if } a\leq x<\infty
\end{cases}
\tag{\ref{eq2}}
\]

To solve this, the equation must be solved separately for each region. However, the boundary conditions at 0 and \((a)\) for each region must be consistent such that \(|\psi(x)|\) is continuous for all \(|x|\), so that \(|\psi(x)|\) is a valid wavefunction. The general solution for each region, before applying the boundary conditions, is then

\[
\psi =
\begin{cases}
    A\sin kx + B\cos kx & \text{if } -\infty<x\leq 0 \\
    Ce^{-\alpha x} + De^{\alpha x} & \text{if } 0<x<a \\
    E\sin kx + F\cos kx & \text{if } a\leq x<\infty
\end{cases}
\]

where \(k = \frac{\sqrt{2mE}}{\hbar}\) and \(\alpha = \frac{\sqrt{2m(V_o -E)}}{\hbar}\). To enforce continuity, the boundaries of each region are set equal. This is expressed as \(|\psi_1(0) = \psi_2(0)|\) and \(|\psi_1(a) = \psi_2(a)|\).

\[
[A\sin 0 + B\cos 0 = Ce^{0} + De^{0}]
\]

which implies that \(|A=0\)\), and \(|B=C+D\)\). At the opposite boundary,

\[
[A\sin ka + B\cos ka = Ce^{-\alpha a} + De^{\alpha a}]
\]

It may be observed that, as \(|a\) goes to infinity, the right hand side of this equation goes to infinity, which does not make physical sense. To reconcile this, \(|D\) is set to zero. For the final region, \(|E\) and \(|F\), present a potentially intractable problem. However, if one realizes that the value at the boundary \(|a\) is driving the wave in the region \(|a\) to \(|\infty\)\), it may also be realized that the wavefunction could be rewritten as \(|Ce^{-\alpha a}\cos(k(x-a))|\), phase shifting the wavefunction by the value of \(|a\) and setting the amplitude to the boundary value. The wavefunction is then

\[
\psi =
\begin{cases}
    B\cos kx & \text{if } -\infty<x\leq 0
\end{cases}
\]
The amplitude of the wavefunction is attenuated by the barrier as \( e^{-a\frac{\sqrt{2m(V_o -E)}}{\hbar}} \), where \( a \) represents the width of the barrier and \( (V_o -E) \) is the difference between the potential energy of the barrier and the current energy of the particle. Since the square of the wavefunction is the probability distribution, the probability of transmission through a barrier is \( e^{-2a\frac{\sqrt{2m(V_o -E)}}{\hbar}} \). As the barrier width or height approaches zero, the probability of a particle traveling through the barrier becomes 1. Also of note is that \( k \) is unchanged on the other side of the barrier. This implies that the energy of the particles are exactly the same as it was before they tunneled through the barrier, as stated earlier, the only thing that changes is the quantity of particles going in that direction. The rest are reflected off the barrier, and go back the way they came.

Contributors and Attributions

- Ryan Bunk