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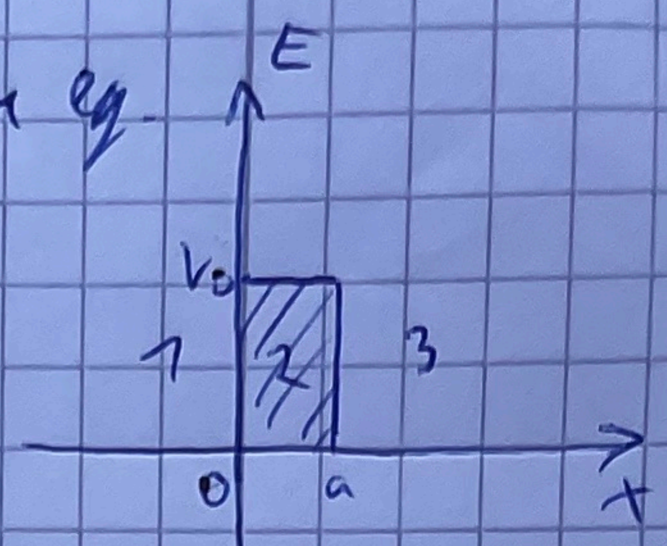
1. Schrödinger eq. for tunnel effect for region I, II, III. Derive eq. 20



We divide space into 3 regions:
- I $V(x) = 0$
- II $V(x) = V_0$
- III $V(x) = 0$

The stationary Schrödinger equation is $-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} + V(x)\phi(x) = E\phi(x)$

We now derive the form of this equation in each region:

Region I $(x<0)$: potential $V(x) = 0$, Schrödinger eq. $-\frac{\hbar^2}{2m}\frac{d^2\phi_1}{dx^2} + 0\cdot\phi_1 = E\phi_1$

$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\phi_1}{dx^2} = E\phi_1 \quad / \cdot -\frac{2m}{\hbar^2} \Rightarrow \frac{d^2\phi_1}{dx^2} + \frac{2mE}{\hbar^2}\phi_1 = 0$

Region II $(0 \le x \le a)$, potential $V(x) = V_0$, Schrödinger eq: $-\frac{\hbar^2}{2m}\frac{d^2\phi_2}{dx^2} = (E-V_0)\phi_2$

$\cdot / \left(-\frac{2m}{\hbar}\right) \Rightarrow \frac{d^2\phi_2}{dx^2} + \frac{2m(V_0-E)}{\hbar^2} = 0$

Region III $(x>a)$, potential $V(x) = 0$ and Schrödinger eq same as for Region I so $-\frac{\hbar^2}{2m}\frac{d^2\phi_3}{dx^2} = E\phi_3 \Rightarrow \frac{d^2\phi_3}{dx^2} + \frac{2mE}{\hbar^2}\phi_3 = 0$

9. Prove that the eigenfunctions for infinite potential are orthonormal 20

The particle is trapped in a 1D box (infinite walls) between $x=0$ and $x=L$. $V(x) = \begin{cases} 0, & 0<x<L \\ \infty, & \text{otherwise} \end{cases} \Rightarrow$ thus $\phi(0) = \phi(L) = 0$

The eigenfunctions are: $\phi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$, for $n = 1, 2, 3 \ldots$

We must show that: $\int_0^L \phi_n(x)\phi_m(x)\,dx = \delta_{nm}$, $\delta_{nm} = \begin{cases} 1, & n=m \\ 0, & n\neq m \end{cases}$

Case 1: $n \neq m$, $\int_0^L \phi_n(x)\phi_m(x)\,dx = \frac{2}{L}\int_0^L \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)dx$

trigonometric identity: $\sin A \sin B = \frac{1}{2}(\cos(A-B) - \cos(A+B))$, thus

$\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right) = \frac{1}{2}\left[\cos\left(\frac{(n-m)\pi x}{L}\right) - \cos\left(\frac{(n+m)\pi x}{L}\right)\right] \Rightarrow$

$\Rightarrow \int_0^L \phi_n(x)\phi_m(x)\,dx = \frac{1}{L}\int_0^L \left[\cos\left(\frac{(n-m)\pi x}{L}\right) - \cos\left(\frac{(n+m)\pi x}{L}\right)\right]dx \Rightarrow$

$\Rightarrow \frac{1}{L}\left(\int_0^L \cos\left(\frac{(n-m)\pi x}{L}\right)dx - \int_0^L \cos\left(\frac{(n+m)\pi x}{L}\right)dx\right)$; $\int \cos(kx)\,dx = \frac{1}{k}\sin(kx)$

$\int_0^L \cos\left(\frac{(n-m)\pi x}{L}\right)dx = \frac{L}{(n-m)\pi}(\sin((n-m)\pi) - \sin(0))$ and $\int_0^L \cos\left(\frac{(n+m)\pi x}{L}\right)dx = \frac{L}{(n+m)\pi}(\sin((n+m)\pi) - \sin(0))$, but $\sin(0) = 0$ and $\sin(k\pi) = 0$ for any k

Thus both sine terms are zero: $\sin((n-m)\pi) = \sin((n+m)\pi) = 0$. Thus both integrals vanish, and $\int_0^L \phi_n(x)\phi_m(x)\,dx = 0$, so when $n \neq m$, functions are orthogonal.

Case 2: $n = m$, now $\int_0^L \phi_n(x)^2 dx$ → we substitute ⇒
$\phi_n(x)^2 = \left(\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)\right)^2 = \frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right)$ thus $\int_0^L \phi_n(x)^2 dx = \frac{2}{L}\int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx$
We again use trigonometric identity: $\sin^2 A = \frac{1}{2}(1-\cos(2A))$ ⇒
⇒ $\sin^2\left(\frac{n\pi x}{L}\right) = \frac{1}{2}\left(1-\cos\left(\frac{2n\pi x}{L}\right)\right)$ ⇒ We substitute ⇒ $\int_0^L \phi_n(x)^2 dx =$
$= \frac{2}{L}\int_0^L \frac{1}{2}\left(1-\cos\left(\frac{2n\pi x}{L}\right)\right)dx = \frac{1}{L}\left(\int_0^L 1\,dx - \int_0^L \cos\left(\frac{2n\pi x}{L}\right)dx\right)$
first integral: $\int_0^L 1\,dx = L$ and second $\int_0^L \cos\left(\frac{2n\pi x}{L}\right)dx = \frac{L}{2n\pi}(\sin(2n\pi)-\sin(0))$
but $\sin(0)=0$ and $\sin(2n\pi)=0$ thus we get $\frac{1}{L}(L-0)=1$ thus ⇒
⇒ $\int_0^L \phi_n(x)^2 dx = 1$, so when $n=m$, the functions are normalized.

Thus we have shown that $\int_0^L \phi_n(x)\phi_m(x)\,dx = \delta_{nm}$ which proves the eigenfunctions are orthonormal.

14. Schrödinger eq. and continuity conditions for a finite potential well, with $E < U_0$

The potential is $V(x) = \begin{cases} 0, & \text{for } |x| \le a \text{ (inside well)} \\ U_0, & \text{for } |x| > a \text{ (outside well)} \end{cases}$ where $U_0 > 0$ and $E < U_0$. Inside well ($|x| \le a$) particle moves freely and outside the well ($|x| > a$) there is a constant potential barrier.

Stationary Schrödinger eq. is $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$ and we split into 3 regions:

Region I: $x < -a$, potential $V(x) = U_0$. Schrödinger eq. $-\frac{\hbar^2}{2m}\frac{d^2\psi_1(x)}{dx^2} + U_0\psi_1(x) = E\psi_1(x)$ → rearranging → $\frac{d^2\psi_1(x)}{dx^2} = \frac{2m}{\hbar^2}(U_0 - E)\psi_1(x)$, lets define $K = \frac{\sqrt{2m(U_0-E)}}{\hbar}$ (positive real, because $E < U_0$) thus $\frac{d^2\psi_1(x)}{dx^2} = K^2\psi_1(x)$
general solution $\psi_1(x) = Ae^{Kx} + De^{-Kx}$, but e^{-Kx} grows exponentially large when $x \to -\infty$, so we must set $D = 0$ so $\psi_1(x) = Ae^{Kx}$

Region II $-a \le x \le a$, potential $V(x) = 0$, Schrödinger eq. $-\frac{\hbar^2}{2m}\frac{d^2\psi_2(x)}{dx^2} = E\psi_2(x)$
⇒ $\frac{d^2\psi_2(x)}{dx^2} = -\frac{2mE}{\hbar^2}\psi_2(x)$, we define $k = \frac{\sqrt{2mE}}{\hbar}$ (real and positive) →
$\frac{d^2\psi_2(x)}{dx^2} + k^2\psi_2(x) = 0$. General solution $\psi_2(x) = B\cos(kx) + C\sin(kx)$

Region III $x > a$, potential $V(x) = U_0$, exactly as region I thus
$\frac{d^2\psi_3(x)}{dx^2} = K^2\psi_3(x)$. General solution $\psi_3(x) = Fe^{-Kx}$, we reject e^{Kx} because it would diverge as $x \to +\infty$

Since the Schrödinger eq. is second-order, both wave function $\psi(x)$ and its derivation $\frac{d\psi}{dx}$ must be continuous at boundaries $x = -a$ and $x = a$.

At $x = -a$, continuity of wavefunction $\psi_1(-a) = \psi_2(-a)$ that is
$Ae^{-kx} = B\cos(-ka) + C\sin(-ka) \Rightarrow Ae^{-ka} = B\cos(ka) - C\sin(ka)$
continuity of derivation $\frac{d}{dx}\psi_1(x) = Ake^{kx}$, $\frac{d}{dx}\psi_2(x) = -Bk\sin(kx) +$
$+ Ck\cos(kx) \Rightarrow Ake^{-ka} = Bk\sin(ka) + Ck\cos(ka)$

At $x = a$, continuity of wave function $\psi_2(a) = \psi_3(a) \Rightarrow$
$B\cos(ka) + C\sin(ka) = Fe^{-ka}$. $\frac{d}{dx}\psi_2(x) = -Bk\sin(kx) + Ck\cos(kx)$,
$\frac{d}{dx}\psi_3(x) = -Fke^{-kx} \Rightarrow -Bk\sin(ka) + Ck\cos(ka) = -Fke^{-ka}$

$\boxed{23}$ 10 Calculate the mean value of square x^2 - coordinate for harmonic oscillator $\int_{-\infty}^{+\infty} \psi_n^* x^2 \psi_n \, dx$. Compare results with the corresponding results for classical harmonic oscillator.

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From the lecture tabular integrals, we get direct result $\langle x^2 \rangle_n = \frac{\hbar}{2m\omega}(2n+1)$, which we can use without having to do full integration manually. Formula tells us the mean value $\langle x^2 \rangle_n$ increases linearly with n; even for $n=0$ (ground state), $\langle x^2 \rangle_0$ is nonzero. Physically, this reflects the zero-point motion: the particle can never be completely at rest, even at the lowest energy level. For $n=0$ $\langle x^2 \rangle_0 = \frac{\hbar}{2m\omega}$, for higher n, $\langle x^2 \rangle_n$ grows with n.

In classical mechanics: total energy $E = \frac{1}{2}m\omega^2 A^2 \rightarrow A = \sqrt{\frac{2E}{m\omega^2}}$
In classical limit, the particle oscillates between $-A$ and $+A$, and x^2 averages ~~to~~ over a cycle to $\langle x^2 \rangle_{classical} = \frac{A^2}{2} \rightarrow \langle x^2 \rangle_{classical} = \frac{E}{m\omega^2}$
In quantum mechanics, the energy levels are $E_n = \hbar\omega(n + \frac{1}{2}) \rightarrow$
$\rightarrow \langle x^2 \rangle_{classical} = \frac{\hbar}{m\omega}(n + \frac{1}{2}) \Rightarrow \langle x^2 \rangle_{quantum,n} = \frac{\hbar}{2m\omega}(2n+1)$
Therefore, the quantum mechanical mean value $\langle x^2 \rangle_n$ exactly equals the classical prediction $\langle x^2 \rangle_{classical}$

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We are dealing with a quantum harmonic oscillator at a finite temperature T. Energy levels: $E_n = \hbar\omega(n+\frac{1}{2})$, $n = 1,2,3\ldots$

At nonzero temperature, different energy ~~states~~ levels are populated according to Boltzmann statistics. The partition function: $Z = \sum_{n=0}^{\infty} e^{-\beta E_n}$, $\beta = \frac{1}{k_B T}$ $\Rightarrow Z = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+\frac{1}{2})} =$

$= Z = e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} e^{-n\beta\hbar\omega}$. Geometric series $\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$ for $|x|<1$. Here $x = e^{-\beta\hbar\omega}$, $\sum_{n=0}^{\infty} e^{-n\beta\hbar\omega} = \frac{1}{1-e^{-\beta\hbar\omega}}$ $\Rightarrow Z = \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}}$

The probability that oscillator is in state n: $P_n = \frac{e^{-\beta E_n}}{Z}$ $\rightarrow$

$\rightarrow P_n = \frac{e^{-\beta\hbar\omega(n+1/2)}}{Z}$.

Average principal quantum number is $\langle n\rangle = \sum_{n=0}^{\infty} n P_n$ $\rightarrow$

$\rightarrow \langle n\rangle = \frac{1}{Z}\sum_{n=0}^{\infty} n e^{-\beta\hbar\omega(n+1/2)} = \frac{e^{-\beta\hbar\omega/2}}{Z}\sum_{n=0}^{\infty} n e^{-n\beta\hbar\omega}$.

We compute $\sum_{n=0}^{\infty} n e^{-n\beta\hbar\omega}$, we know $\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$ for $|x|<1$ $\rightarrow$

$\rightarrow \sum_{n=0}^{\infty} n x^{n-1} = \frac{1}{(1-x)^2}$ $/\cdot x$ $\rightarrow \sum_{n=0}^{\infty} n x^n = \frac{x}{(1-x)^2}$ and substitute

$x = e^{-\beta\hbar\omega}$ $\sum_{n=0}^{\infty} n e^{-n\beta\hbar\omega} = \frac{e^{-\beta\hbar\omega}}{(1-e^{-\beta\hbar\omega})^2}$

now $\langle n\rangle = \frac{e^{-\beta\hbar\omega/2}}{Z}\cdot\frac{e^{-\beta\hbar\omega}}{(1-e^{-\beta\hbar\omega})^2}$, $Z = \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}}$ $\Rightarrow$

$\frac{1}{Z} = (1-e^{-\beta\hbar\omega})e^{\beta\hbar\omega/2}$ $\langle n\rangle = (1-e^{-\beta\hbar\omega})e^{\beta\hbar\omega/2}\cdot\frac{e^{-\beta\hbar\omega/2}e^{-\beta\hbar\omega}}{(1-e^{-\beta\hbar\omega})^2}$.

We simplify: $e^{\beta\hbar\omega/2}e^{-\beta\hbar\omega/2} = 1$ so $\langle n\rangle = \frac{e^{-\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}$ thus $\rightarrow$

$\rightarrow \langle n\rangle = \frac{1}{e^{\beta\hbar\omega}-1}$ (average quantum number)

Behavior at low / high temperatures:

As $T\rightarrow 0$, $\beta\rightarrow\infty$, $e^{\beta\hbar\omega}\rightarrow\infty$ $\Rightarrow \langle n\rangle \rightarrow 0$

At high T $(\beta\rightarrow 0)$, $e^{\beta\hbar\omega} \approx 1+\beta\hbar\omega \Rightarrow e^{\beta\hbar\omega}-1 \approx \beta\hbar\omega$ $\Rightarrow$

$\Rightarrow \langle n\rangle \approx \frac{1}{\beta\hbar\omega} = \frac{k_B T}{\hbar\omega}$