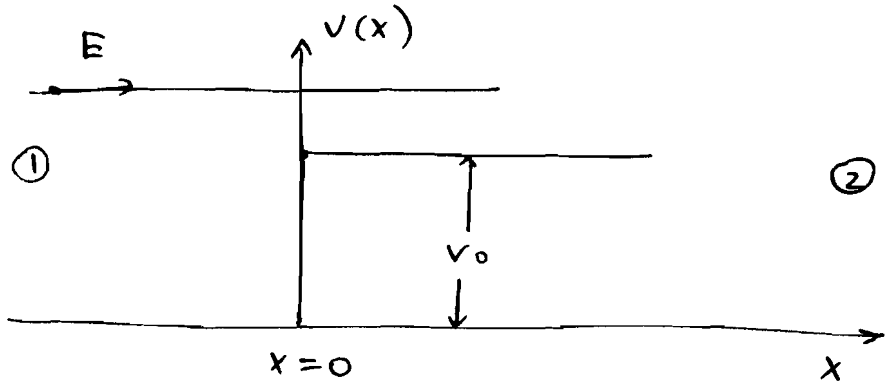
4-1. Potential step



A particle is moving with the energy E above the potential step V_0:

$$E > V_0$$

The question we are asking is what is the probability for the particle in region ① to appear in region ②.

Classical answer: $P = 1$ (because $E > V_0$)

Quantum answer: $P < 1$ (reflection of a wave from the barrier)

Formalizing the problem:

$$\frac{2mE}{\hbar^2} = k^2, \qquad \frac{2m(E-V_0)}{\hbar^2} = q^2 > 0$$

SE: $$\frac{d^2u}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right] u(x) = 0$$

Step 1: separate the solution for the wave function into two regions

$x<0$: $$u(x) = e^{ikx} + R\,e^{-ikx}$$

wave vector

amplitude of the reflected wave

$$\hat{p}\,Re^{-ikx} = \frac{\hbar}{i}\frac{\partial}{\partial x} Re^{-ikx} = -\hbar k\, Re^{-ikx}$$

negative projection on the x-axis, wave going backwards

$x>0$: $$u(x) = T e^{iqx}$$

wave vector in region 2

amplitude of the transmitted wave

Flux at $x<0$:

$$j = \frac{\hbar}{2im}\left(u^*\frac{\partial u}{\partial x} - u\frac{\partial u^*}{\partial x}\right) = \frac{\hbar}{2im}\Big[\left(e^{-ikx} + Re^{ikx}\right)\times$$

$$\times\left(ike^{ikx} - Rike^{-ikx}\right) - \left(e^{ikx} + Re^{-ikx}\right)\times\left(-ike^{-ikx} + Rike^{ikx}\right)\Big]$$

$$= \frac{\hbar k}{2m}\left[\left(1 + Re^{2ikx} - Re^{-2ikx} - R^2\right) + c.c.\right] =$$

$$= \frac{\hbar k}{2m}\left(1 - R^2\right) = \underbrace{\frac{\hbar k}{2m}}_{\text{incoming flux}} - \underbrace{R^2\frac{\hbar k}{2m}}_{\text{reflected flux}}$$

$x>0$:

$$j = \frac{\hbar q}{m}|T|^2$$

Concervation of flux:

$$\frac{\hbar k}{m}\left(1 - R^2\right) = \frac{\hbar q}{m}T^2$$

Continuity of the wave function at $x=0$

$$\Psi(x-0) = \Psi(x+0)$$

$$1 + R = T$$

Continuity of the derivative (finite potential jump)

$$\frac{d^2u}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right]u(x) = 0$$

$$\int_{-\varepsilon}^{\varepsilon} \frac{d^2u}{dx^2}\,dx = \frac{2m}{\hbar^2}\int_{-\varepsilon}^{\varepsilon}(E - V(x))\,u(x)\,dx = 0$$

$$\left(\frac{du}{dx}\right)_{\varepsilon} = \left(\frac{du}{dx}\right)_{-\varepsilon} \leftarrow \text{derivative is continuous}$$

$$\left.\frac{du}{dx}\right|_{x=0+\varepsilon} = \left.\frac{du}{dx}\right|_{x=0-\varepsilon}, \quad \varepsilon \to 0$$

$$ik(1-R) = iq\,T$$

$$ik\,\frac{1-R}{1+R} = iq, \qquad 1 - R = \frac{q}{k}(1+R)$$

$$\boxed{\begin{aligned} R &= \frac{1 - q/k}{1 + q/k} = \frac{k-q}{k+q} \\ T &= \frac{2k}{k+q} \end{aligned}}$$

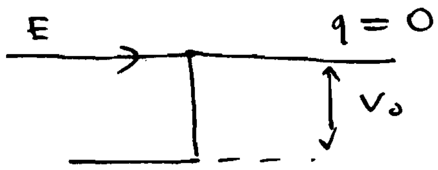
Testing the flux concervation:

$$k(1 - R^2) = k\left(1 - \frac{(k-q)^2}{(k+q)^2}\right) = \frac{4k^2q}{(k+q)^2} = q\,T^2 =$$

$$= \frac{4k^2q}{(k+q)^2}$$

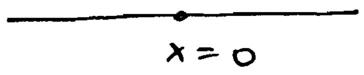
Properties of the solution

① . $R < 1$ except at $q = 0$ (full reflection)



$T < 1$ except at $q = k$

$k = q, \quad V_0 = 0$



Particle reflection from a barrier below E is a quantum phenomenon

② . $E < V_0, \qquad u(x) = T e^{-|q| x}, \quad x > 0$

$$|R|^2 = \frac{(k - i|q|)(k + i|q|)}{(k + i|q|)(k - i|q|)} = 1 \leftarrow \text{full reflection}$$

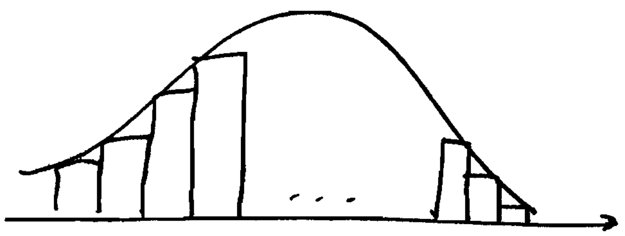
$$T = \frac{2k}{k + i|q|} \leftarrow \text{complex transmission corresponds to } \underline{\underline{\text{tunneling}}}$$

For $E < V_0$, the probability to find a particle with negative kinetic energy inside the barrier

$$P(x) = c\, e^{-2|q|x}$$

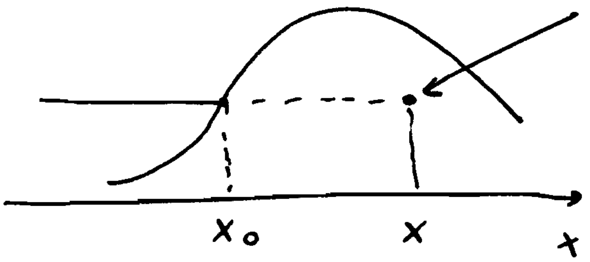
$$q = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}$$

A continuous barrier can be represented by a sequence of square barriers



The above formula then generalizes to an integral

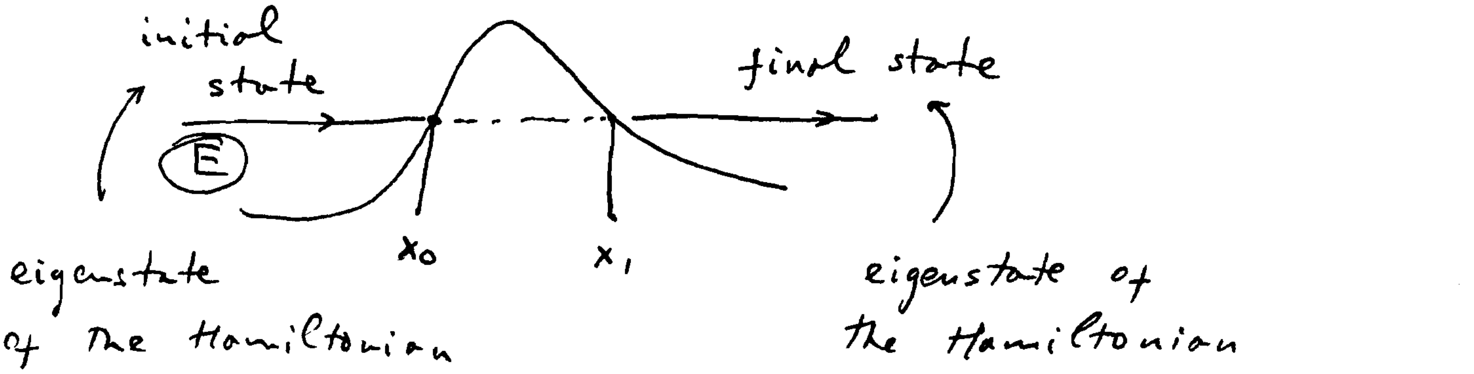
$$\ln P(x) = \text{Const} - 2\int_{x_0}^{x} dz \sqrt{2m(V(z)-E)/\hbar^2}$$



probability to find a particle

Does it make any sense?

Asking about the probability to find a particle with negative kinetic energy is a "forbidden question" in quantum mechanics. It make sense to ask about the probability of observing the eigenstates of an operator, e.g. the Hamiltonian. There are no states within the barrier and the question about the corresponding probability does not make any sense. Asking about the probability to be transmitted is a legitimate question: there are energy states before and after the barrier.

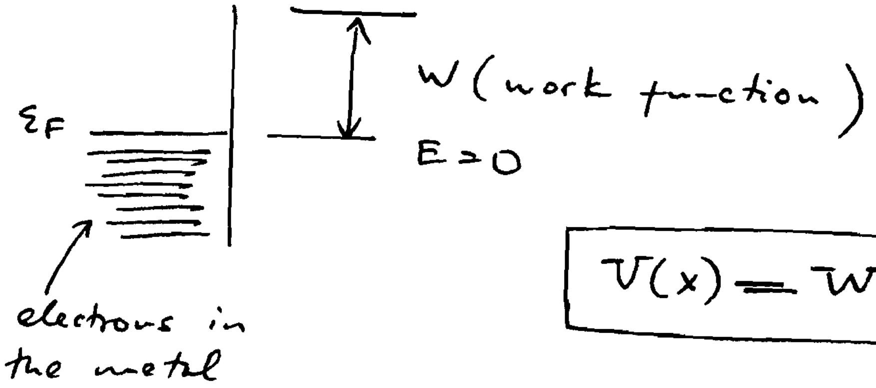


Transmission probability:

$$|T|^2 = \exp\left[-2\int_{x_0}^{x_1} dx\,\sqrt{2m(V(x)-E)/\hbar^2}\,\right]$$

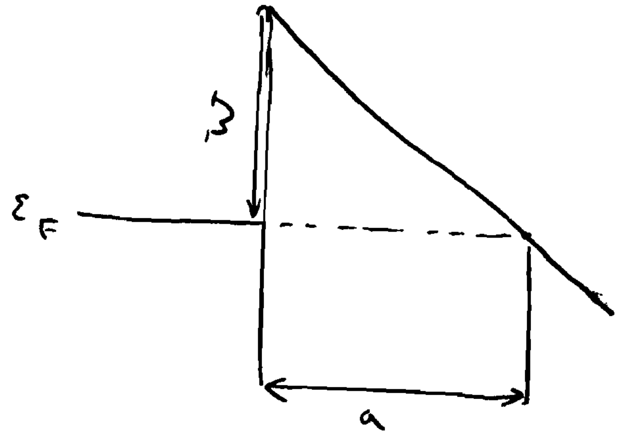
4-4 Cold emission as tunneling

<u>Cold emission</u>: releasing electrons from a metal by applying an external electric field



$$\boxed{V(x) = W - e\mathcal{E}x}$$

electric field



$$W - e\mathcal{E}a = 0$$

$$a = \frac{W}{e\mathcal{E}}$$

$$2\int_0^a dx\,\sqrt{\frac{2m}{\hbar^2}(W - e\mathcal{E}x)} = \frac{2\sqrt{2m}}{\hbar e\mathcal{E}}\int_0^W dt\,\sqrt{t} =$$

$t = W - e\mathcal{E}x$

$$= \frac{4\sqrt{2m}}{3\hbar e\mathcal{E}}\,W^{3/2}$$

$$\boxed{|T|^2 = C\exp\left[-\frac{4\sqrt{2m}}{3\hbar e\mathcal{E}}\,W^{3/2}\right]}$$

Chapter 5 : The general structure of QM

Postulate : The state of a system is completely described by its wavefunction

SE : $$i\hbar \underbrace{\frac{\partial \psi(x,t)}{\partial t}}_{\text{change of the wave function with time}} = \hat{H}\, \psi(x,t)$$

acts to the right

Hamiltonian operator, operates to change $\psi(x,t)$

$$H = \frac{\hat{p}^2}{2m} + V(x), \qquad \hat{p} = -i\hbar \frac{\partial}{\partial x} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

If $V(x)$ does not change with t,

$$\psi(x,t) = u_E(x)\, e^{-iEt/\hbar}$$

$$\hat{H}\, u_E(x) = E\, u_E(x) \leftarrow \text{eigenvalue problem}$$

eigenfunction ($u_E(x)$), eigenvalue (Energy) (E)

Properties of the solution:

① $$\int_{-\infty}^{\infty} u^*_{E_1}(x)\, u_{E_2}(x)\, dx = \begin{cases} \delta_{1,2} & \text{descrete} \\ \underset{\text{constant}}{C}\,\delta(E_1 - E_2) & \text{continuous} \end{cases}$$

② Complete set of $u_E(x)$:

$$\underset{\substack{\text{arbitrary wave}\\ \text{function satisfying the boundary conditions}}}{\psi(x)} = \sum_E C_E\, u_E(x) = \sum_n \underset{\text{descrete}}{C_n\, u_n(x)} + \underset{\text{continuous}}{\int dE\, C(E)\, u_E(x)}$$

③ $$\psi(x,t) = \sum C_E\, u_E(x)\, e^{-iEt/\hbar}$$

separation of time and space variables for $V(x)$ independent of time

④ Momentum: $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$,

Eigenvalue problem: $\hat{p}\, u_p(x) = p\, u_p(x)$

$$u_p = \frac{1}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar}$$

$$\int_{-\infty}^{\infty} u^*_{p_1}(x)\, u_{p_2}(x)\, dx = \delta(p_1 - p_2)$$

$$\psi(x) = \int dp\, \underset{\text{wave function in the momentum space}}{\underline{\underline{\Phi(p)}}}\, u_p(x)$$ ← Complete set of $u_p(x)$ wave functions

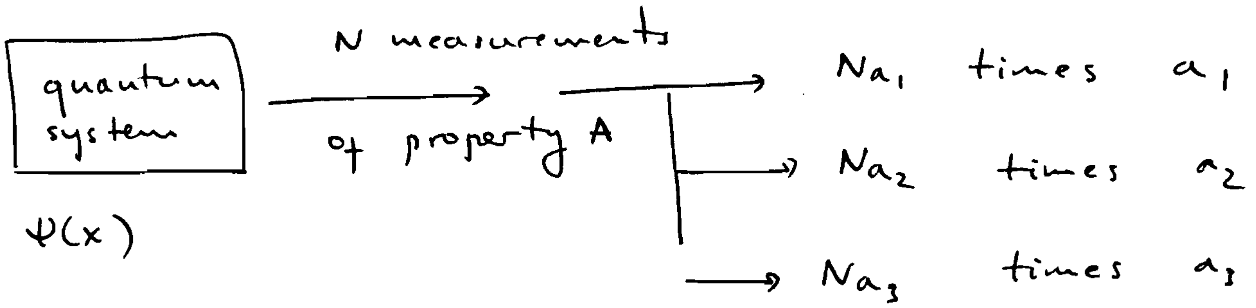
⑤. All observables are represented by Hermitian operators, they have real eigenvalues

$$\hat{A}\, u_a(x) = \underset{\text{real}}{a}\, u_a(x)$$

$$\psi(x) = \sum_a C_a u_a(x), \qquad C_a = \int_{-\infty}^{\infty} \psi(x)\, u_a^*(x)\, dx$$

any square-integrable function ($\int |\psi|^2 dx$ exists) can be represented by an expansion in terms of all eigenfunctions of some Hermitian operator (observable)

⑥. The interpretation of the expansion coefficients



Probability of getting a_1 is:

$$P_{a_1} = \frac{N_{a_1}}{N} = |C_{a_1}|^2$$

$$C_{a_1} = \int dx\, u_{a_1}^*(x)\, \psi(x)$$

⑦. Completeness relation

$$\sum_a P_a = \sum_a |c_a|^2 = 1$$

$$\sum_a |c_a|^2 = \sum_a \int_{-\infty}^{\infty} dx\, u_a^*(x)\psi(x)\, dx \int_{-\infty}^{\infty} dy\, u_a(y)\,\psi^*(y)$$

$$= \iint_{-\infty}^{\infty} dx\, dy\, \psi^*(y)\,\psi(x) \sum_a u_a(y)\, u_a^*(x) = 1$$

One has to require:

$$\sum_a u_a(y)\, u_a^*(x) = \delta(x-y)$$

and then

$$\sum P_a = \iint_{-\infty}^{\infty} dx\, dy\, \psi^*(y)\,\psi(x)\,\delta(x-y) =$$

$$= \int_{-\infty}^{\infty} dx\, |\psi(x)|^2 = 1$$

normalization of the probability density

Example: 1D Box

$$u_n(x) = \sqrt{\frac{2}{a}} \sin \frac{\pi n x}{a}$$

$$\sum_{n=1}^{\infty} \frac{2}{a} \sin \frac{\pi n x}{a} \sin \frac{\pi n y}{a} = \delta(x-y)$$

$$\frac{x}{a} = X, \quad \frac{y}{a} = Y, \quad a\,\delta(x-y) = \delta(X-Y)$$

$$2\sum_{n=1}^{\infty} \sin n\pi X \sin n\pi Y = \delta(X-Y) = \sum_{n=-\infty}^{\infty} \sin n\pi X \sin n\pi Y$$