Quantum Mechanics

Department of Physics,
Tongji University, Shanghai, 200092, China

Zhi-Guo Wang

Autumn, 2024

- 2.1 Stationary States
- 2.2 The Infinite Square Well
- 2.3 The Harmonic Oscillator
- **2.4 The Free Particle**
- 2.5 The Delta-Function Potential
- 2.6 The Finite Square Well

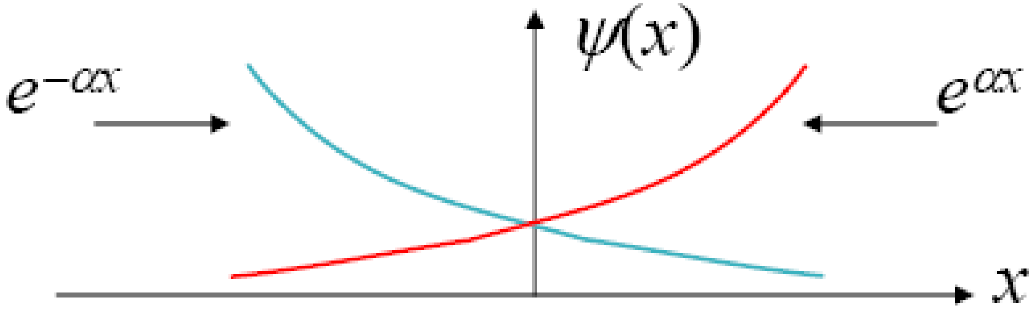
2.4 The Free Particle

For a free particle, V=0 and TISE becomes

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi(x)$$

It have the solutions:

$$\psi(x) = \begin{cases} Ae^{\alpha x} + Be^{-\alpha x}, \alpha = \dfrac{\sqrt{-2mE}}{\hbar} & E < 0 \\ Ax + B & E = 0 \\ Ae^{ikx} + Be^{-ikx}, k = \dfrac{\sqrt{2mE}}{\hbar} & E > 0 \end{cases}$$



- As the particle can be found in the range $-\infty < x < \infty$, for $E < 0$, it is not physically acceptable to have a nonzero A or a nonzero B, otherwise $\psi(x) \to \infty$ as $x \pm \infty$.
- For $E = 0$, $A = 0$ for the same reason and $\psi(x) = B$ which can be regarded as a solution of $E \geq 0$ with $k = 0$.

- For $E \geq 0$, any value of $k \geq 0$ gives an acceptable solution. This means that all energies in the continuous range $0 \leq E < \infty$ are allowed, that is, the energy of a free particle is not quantized.

- Recall $\Psi(x,t) = \psi(x)e^{-i\frac{E}{\hbar}t}$,

$$\Psi(x,t) = Ae^{i(kx-\frac{E}{\hbar}t)} + Be^{-i(kx+\frac{E}{\hbar}t)}$$

is a superposition of two plane waves, one moving in the $+x$-direction (with coefficient A) and the other moving in the $-x$-direction (with coefficient B).

- Thus, $Ae^{i(kx-\frac{E}{\hbar}t)}$ represents a particle with definite momentum k moving in the $+x$-direction and $Be^{-i(kx+\frac{E}{\hbar}t)}$ represents a particle with momentum of the same magnitude k but moving in the $-x$-direction.

- We note the following remarks for $\Psi(x,t) = Ae^{i(kx-\frac{E}{\hbar}t)}$ or $Be^{-i(kx+\frac{E}{\hbar}t)}$:

- $|\Psi(x,t)|^2$ ($=|A|^2$ or $|B|^2$) is uniform, that is, the probability of finding the particle in any interval of the x-axis is the same as that for any other interval of equal length and does not change with time.

例　证明一维自由粒子的速度 v 可以表示为

$$v=\frac{J}{\rho}$$

其中，ρ 和 J 分别是一维自由粒子的概率密度和概率流密度。

证明　一维自由粒子波函数及其共轭式为

$$\Psi(x,t)=A\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(px-Et)},\quad \Psi^*(x,t)=A^*\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(px-Et)}$$

由式(2.1.18)求得自由粒子的概率密度和概率流密度：

$$\rho=|\Psi(x,t)|^2=|A|^2$$

$$J=-\frac{\mathrm{i}\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\frac{\partial\Psi^*}{\partial x}\Psi\right)=\frac{p}{m}|A|^2=v\rho$$

于是式(4.2.8)得证。这是概率密度与概率流密度之间的基本关系。

- Thus the particle's **location** *can be anywhere* and is thus *completely unknown* (because $\Delta x \to \infty$).
- On the other hand, its momentum is known precisely as $p_x = k \Rightarrow \Delta p_x = 0$.
- Ψ is *not* normalizable, that is, the condition $\int_{-\infty}^{+\infty} \Psi^2(x,t)dx = 1$ is not satisfied. (Indeed, $\int_{-\infty}^{+\infty} \Psi^2(x,t)dx$ is infinite.)
- In the case of the free particle, then, the separable solutions do not represent physically realizable states. *A free particle cannot exist in a stationary state*; or, to put it another way, *there is no such thing as a free particle with a definite energy*.

- If we know (by measurement) a particle initially (t = 0) is in some range Δx about x_0, then it is not described by the plane wave $Ae^{i(kx-\frac{E}{\hbar}t)}$ or $Be^{-i(kx+\frac{E}{\hbar}t)}$.
- However, the general solution to the time-dependent Schrodinger equation is a linear combination of separable solutions (only this time it's an integral over the continuous variable k, instead of a sum over the discrete index n).

- Instead, free particle is represented by a wavepacket as an integral of plane waves with different wavenumbers

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{i[kx - i\omega(k)t]} dk$$

And $\varphi(k)$ is given by the initial shape of the wavepacket $\Psi(x,0)$:

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi(k) e^{ikx} dk$$

Recall that because each of the constituents moves at a different phase speed $v_{\mathrm{phase}} = \omega/k$, the wavepacket changes its shape as it moves.

Example: A free particle, initially localized in [-*a*, *a*] is released at time *t* = 0

$$\Psi(x,0) = \begin{cases} A, -a < x < a \\ 0, otherwise \end{cases}$$

A and a are positive real constant. Find $\Psi(x,t)$

Solution: Normalize

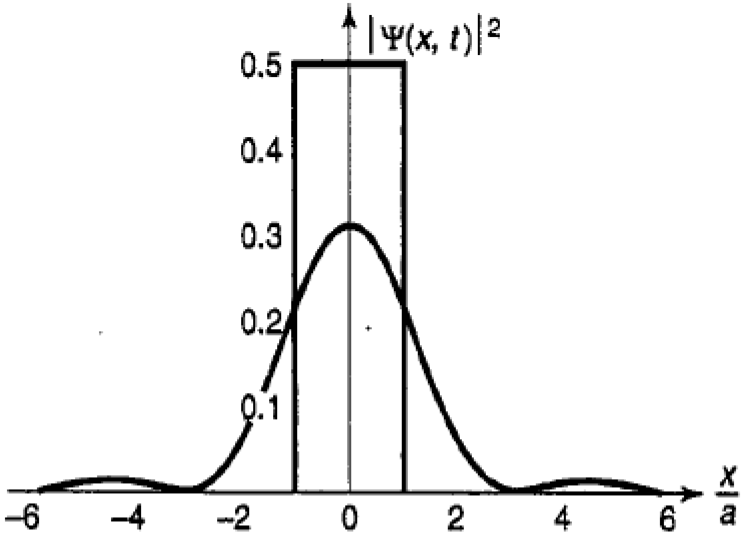
$$\Psi(x,0), A = 1/\sqrt{2a}$$

$$\varphi(k) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2a}}\int_{-a}^{+a} e^{-ikx}dk = \frac{1}{2\sqrt{\pi a}}\frac{e^{-ikx}}{-ik}\Bigg|_{-a}^{a} = \frac{1}{k\sqrt{\pi a}}\frac{e^{ika}-e^{-ika}}{2i}$$

$$= \frac{1}{\sqrt{\pi a}}\frac{\sin(ka)}{k}$$

Finally,

$$\Psi(x,t)=\frac{1}{\pi\sqrt{2a}}\int_{-\infty}^{+\infty}\frac{\sin(ka)}{k}e^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}dk$$



Graph of $|\Psi(x,t)|^2$ at $t=0$ (the rectangle) and at $t=ma^2/\hbar$ (the curve).

In the limiting case $a \to 0$, we use the small angle approximation

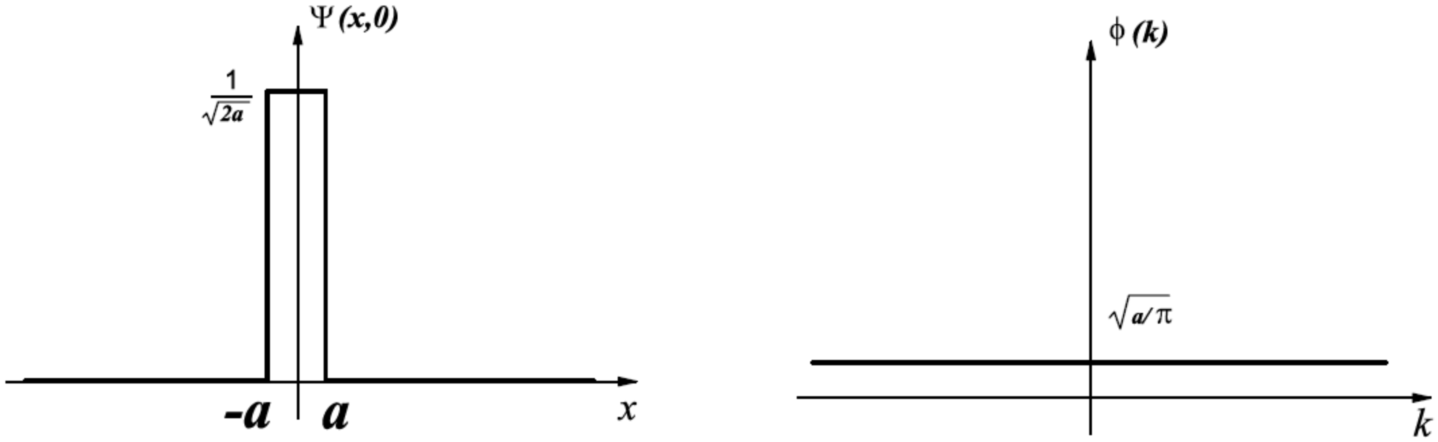
$$\varphi(k) = \frac{1}{\sqrt{\pi a}} \frac{\sin(ka)}{k} \approx \frac{1}{\sqrt{\pi a}} a = \sqrt{\frac{a}{\pi}}$$

it is flat. This is an example of uncertainty principle: if the spread in position is small, the spread in momentum must be large.

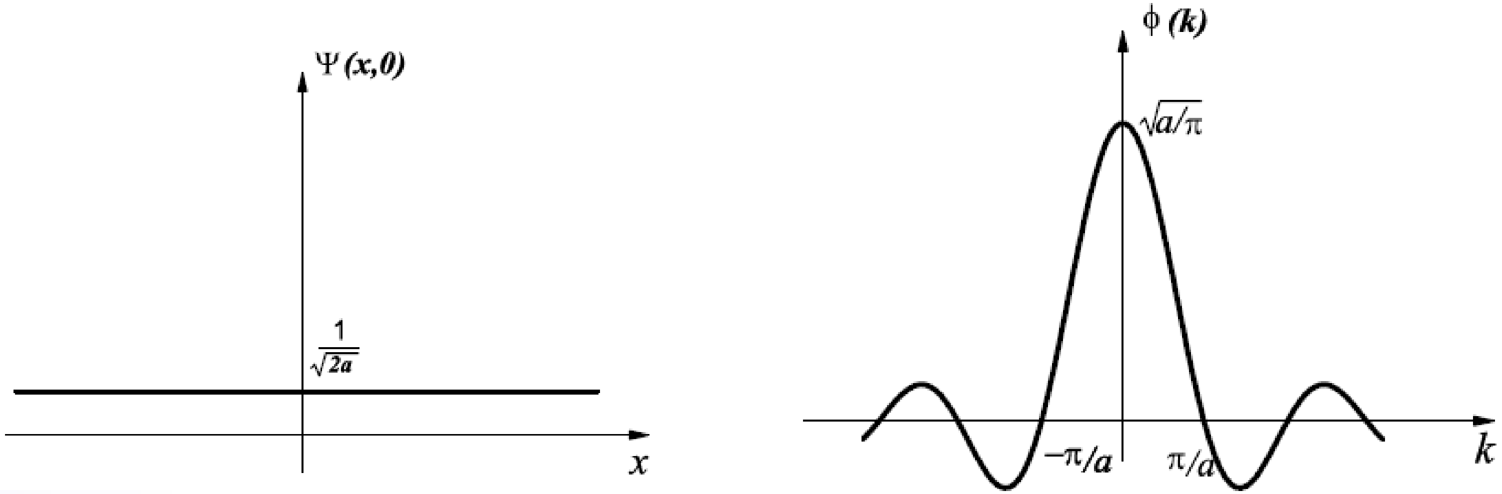
At the other extreme $a \to 1$; the spread in position is broad

$$\varphi(k) = \sqrt{\frac{a}{\pi}} \frac{\sin(ka)}{ka}$$

it is a sharp spike about $k = 0$.



For small a, graphs of $\Psi(x,0)$ and $\phi(k)$.



For large a, graphs of $\Psi(x,0)$ and $\phi(k)$.

The velocity paradox

From SE, Evidently the "stationary states" of the free particle are propagating waves; their wavelength is $\lambda = 2\pi/|k|$, and, according to the de Broglie formula, they carry momentum $\vec{p} = \hbar\vec{k}$.

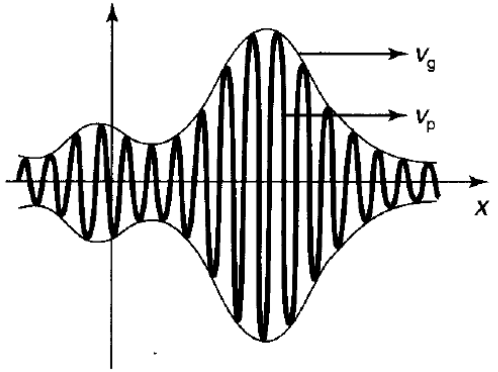
Since $k \equiv \pm\frac{\sqrt{2mE}}{\hbar}$, The speed of these waves (the coefficient of t over the coefficient of x) is

$$v_{quantum} = \frac{\hbar|k|}{2m} = \sqrt{\frac{E}{2m}}$$

On the other hand, the *classical* speed of a free particle with energy E is given by

$$v_{classical} = \sqrt{\frac{2E}{m}} = 2v_{quantum}$$

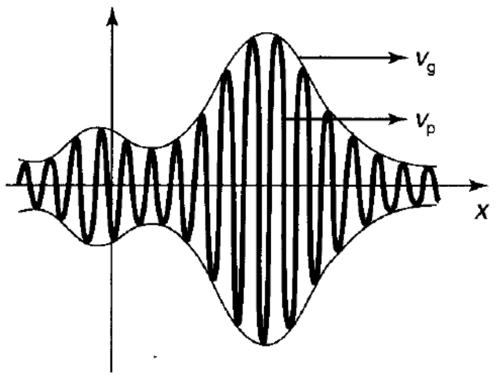
- The fact is that the separable solution $\Psi_k(x; t)$ travels at the "wrong" speed for the particle it ostensibly(表面上） represents.



- The essential idea : A wave packet is a sinusoidal function whose amplitude is modulated; it consists of "ripples" contained within an "envelope".

- What corresponds to the particle velocity is not the speed of the individual ripples (the so-called phase velocity v_p), but rather the speed of the envelope (the group velocity v_g)-- which, depending on the nature of the waves, can be greater than, less than, or equal to the velocity of the ripples that go to make it up.

- What need to show is that for the wave function of a free particle in quantum mechanics the group velocity is twice the phase velocity--just right to represent the classical particle speed.



First, we consider two combining waves

$$y_1 = A\sin(kx - \omega t)$$

$$y_2 = A\sin[(k + \Delta k)x - (\omega + \Delta\omega)t]$$

The individual phase velocities are given by $v_{ph1} = \frac{\omega}{k}$, $v_{ph2} = \frac{\omega+\Delta\omega}{k+\Delta k}$.

The combined disturbance can then be written

$$y = y_1 + y_2 = 2A\sin[(k + \frac{1}{2}\Delta k)x - (\omega + \frac{1}{2}\Delta\omega)t]\cos\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)$$

The last factor, $\cos\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)$, describes the modulation of amplitude of the resultant waveform. The velocity with which this modulation envelope moves is the group velocity v_g. This velocity is given, as for any progressive wave, by the coefficient of t divided by the coefficient of x. Thus we have

$$v_g = \frac{\Delta\omega}{\Delta k}$$

In the limit of infinitesimally small differences in frequency and wave number between the combining waves, we thus have

$$\text{(Phase velocity) } v_{ph} = \frac{\omega}{k}$$

$$\text{(Group velocity) } v_g = \frac{d\omega}{dk}$$

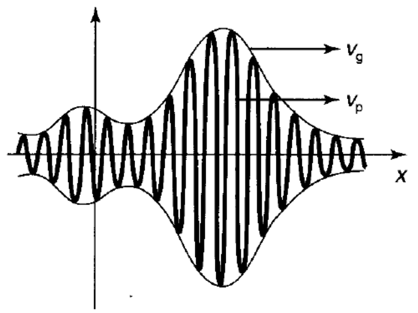
The velocity of the traveling plane wave , that is, the phase velocity is different from the classical velocity v of the particle.

The "group velocity" of the wave, however, defined in the usual classical way as the velocity of the center of a "wave packet" made of waves with wavevectors centered around k, is

$$v_g \equiv \frac{d\omega}{dk} = \frac{d\hbar\omega}{d\hbar k} = \frac{dE}{dp} = \frac{p}{m}$$

It is obviously equal to *v---the velocity of classical particle.*

Now, determine the group velocity of a wave packet with the



$$\Psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{i(kx-\omega t)}dk$$

The center of the wave packet is determined by taking the extreme value of the phase angle $\varphi = kx-\omega t$, $\frac{\partial\varphi}{\partial k}=0$, then $x-\left(\frac{d\omega}{dk}\right)t=0$. So the center of the wave packet is at

$$x=x_c=\left(\frac{d\omega}{dk}\right)t$$

its velocity is called the group velocity

$$v_g=\frac{dx}{dt}=\frac{d\omega}{dk}$$

For a free particle $$\omega = \frac{\hbar k^2}{2m}$$

$$v_g = \frac{\hbar k}{m}$$

$$v_p = \frac{\hbar k}{2m}$$

$$v_g = 2v_p$$

This confirms that it is the group velocity of the wave packet, not the phase velocity of the stationary states, that matches the classical particle velocity

Problem 2.21 ,

- 2.1 Stationary States
- 2.2 The Infinite Square Well
- 2.3 The Harmonic Oscillator
- 2.4 The Free Particle
- **2.5 The Delta-Function Potential**
- 2.6 The Finite Square Well

2.5 The Delta-Function Potential

- Two very different kinds of solutions to the TISE:

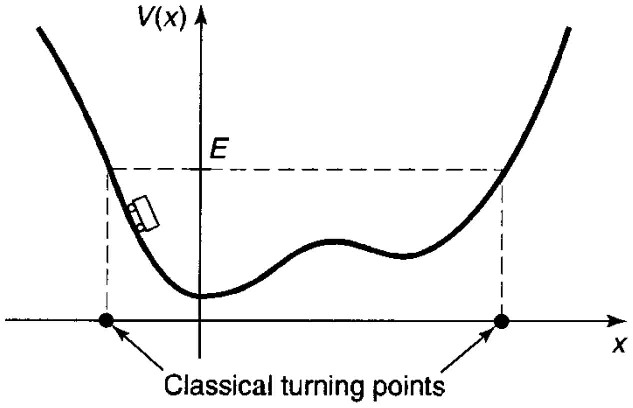
1. For the infinite square well and the harmonic oscillator they are normalizable, and labeled by a discrete index n;
2. For the free particle they are non-normalizable, and labeled by a continuous variable k.

-

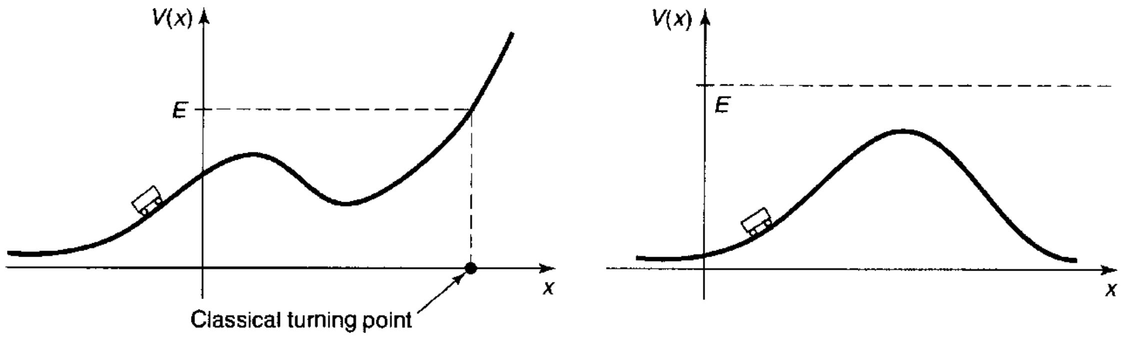
- In both cases the general solution to the TDSE is a **linear combination of stationary states**

first type takes the form of a sum (over n), whereas for the second it is an integral (over k).

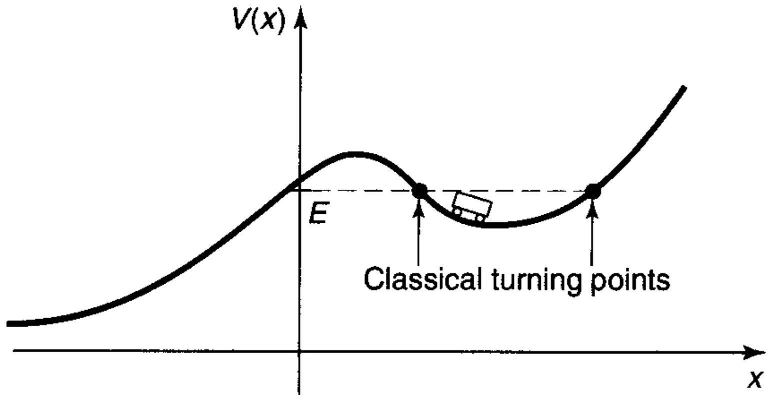
What is the physical significance of this distinction?



(a) A bound state.



(b) Scattering states.



(c)

A classical bound state, but a quantum scattering state

- Classical physics, a particle with energy $E < V_0$ could not penetrate - the region inside the barrier is classically forbidden.
- The wave function is continuous at the barrier and exponential decays inside the barrier.
- The wave function must also be continuous on the far side of the barrier, so there is a finite probability that the particle will **tunnel** through the barrier.
- The two kinds of solutions to the Schrodinger equation correspond precisely **to bound and scattering states.**

- The distinction is even cleaner in the quantum domain, because the phenomenon of **tunneling allows the particle to "leak" through any finite potential barrier**

$$\begin{cases} E < V(-\infty) \text{ and } V(+\infty) \Rightarrow \quad \text{bound state} \\ E > V(-\infty) \text{ or } V(+\infty) \Rightarrow \text{scattering state} \end{cases}$$

In "real life" **most potentials go to zero at infinity**, in which case the criterion simplifies even further:

$$\begin{cases} E < 0 \Rightarrow \quad \text{bound state} \\ E > 0 \Rightarrow \text{scattering state} \end{cases}$$

- Because the infinite square well and harmonic oscillator **potentials go to infinity** as $x \to \pm\infty$, they **admit bound states only**;
- The **free particle** potential is zero everywhere, it only **allows scattering states**.

We shall explore potentials that give rise to both kinds of states.

Let's consider a potential of the form

$$V(x) = -\alpha\delta(x),$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi.$$

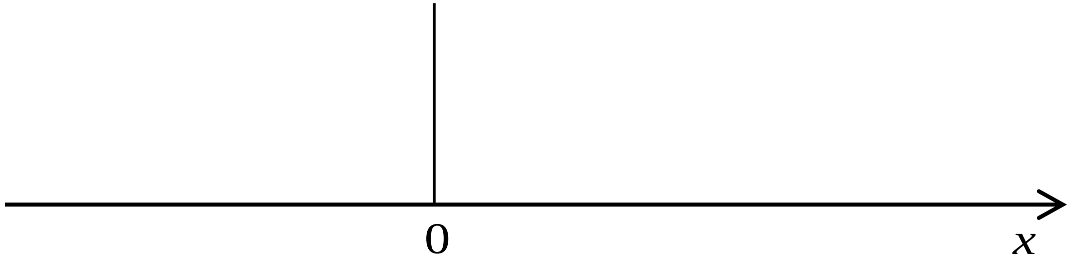
This potential yields **both bound states (E < 0)** and **scattering states (E > 0)**

The Dirac delta function, δ(x), is defined informally as follows:

$$f(x)\delta(x-a) = f(a)\delta(x-a),$$

$$\int_{-\infty}^{+\infty} f(x)\delta(x-a)\,dx = f(a)\int_{-\infty}^{+\infty}\delta(x-a)\,dx = f(a).$$

$$\delta(x) = \begin{cases} 0, & \text{if } x \neq 0 \\ \infty, & \text{if } x = 0 \end{cases}, \quad \text{with} \int_{-\infty}^{+\infty}\delta(x)\,dx = 1.$$



$$\int \delta(ax)\,dx = \frac{1}{a}\int \delta(ax)\,d(ax)$$

$$\delta(ax) = \frac{1}{a}\delta(x) \text{ (Note the dimension is correct)}$$

$$\int_{-\infty}^{x} g(x)\,dx \to \int_{-\infty}^{x}\delta(x)\,dx = \vartheta(x) = \begin{cases} 0, \text{ if } (x<0) \\ 1/2, \text{ if } (x=0) \\ 1, \text{ if } (x>0) \end{cases}$$

$$\delta(x) = \frac{d}{dx}\vartheta(x)$$

$$\frac{d}{dx}\delta(x) = \begin{cases} 0, & \text{if } (x \neq 0) \\ \pm\infty, & \text{if } (x=0) \end{cases}$$

1. The dimension of d-function is $(1/x)$
2. Always meant to appear in an integral
3. A notation of a limiting process

$$\delta(x) = \lim_{a\to 0}\frac{1}{\sqrt{2\pi a}}\exp\left(-\frac{x^2}{2a}\right)$$

$$\delta^n(\mathbf{r}) = \begin{cases} 0, & \text{if } (\mathbf{r} \neq 0) \\ \infty, & \text{if } (\mathbf{r}=0) \end{cases} \text{ and } \begin{cases} \iint \delta^2(\mathbf{r})\,dxdy = 1 \\ \iiint \delta^3(\mathbf{r})\,dxdydz = 1 \end{cases}$$

$$\delta^2(\mathbf{r}) = \delta(x)\delta(y) \text{ and } \delta^3(\mathbf{r}) = \delta(x)\delta(y)\delta(z)$$

we'll look first at the bound states. In the region $x < 0$, V(x) = 0, so

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = \kappa^2\psi, \qquad \kappa \equiv \frac{\sqrt{-2mE}}{\hbar}.$$

(E is negative, by assumption, so k is real and positive.) The general solution is

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x},$$

but the first term blows up as $x \to -\infty$, so we must choose A = 0:

$$\psi(x) = Be^{\kappa x}, \qquad (x < 0).$$

In the region $\boldsymbol{x > 0}$, V(x) is again zero, and the general solution is of the form Fexp(-kx) + Gexp(kx); this time it's the second term that blows up (as $x \to -\infty$), so

$$\psi(x) = Fe^{-\kappa x}, \quad (x > 0).$$

It remains only to stitch these two functions together, using the appropriate boundary conditions at $x = 0$.

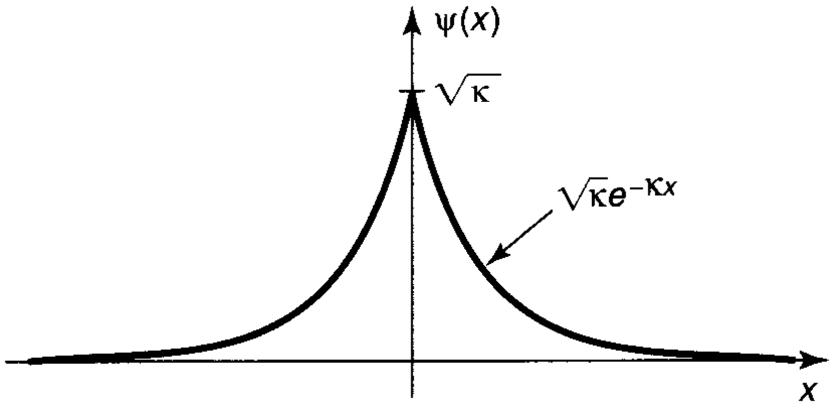
$$\begin{cases} 1.\ \psi \text{ is always continuous, and} \\ 2.\ d\psi/dx \text{ is continuous except at points} \\ \quad \text{where the potential is infinite.} \end{cases}$$

In this case the first boundary condition tells us that $F = B$, so

$$\psi(x) = \begin{cases} Be^{\kappa x}, & (x \le 0), \\ Be^{-\kappa x}, & (x \ge 0). \end{cases}$$

The second boundary condition tells us nothing; this is (like the infinite square well) the exceptional case where V is infinite at the join, and it's clear from the graph that this function has a kink at $x = 0$.

5 The Delta-function potential



- Moreover, up to this point the delta function has not come into the story at all.
- Evidently the delta function must determine the discontinuity in the derivative of ψ, at $x = 0$.
- I'll show you now how this works, and as a byproduct we'll see why $d\psi/dx$ is ordinarily continuous.

5 The Delta-function potential

- The idea is to **integrate the Schrodinger equation, from -ε to + ε,** and then take the limit as ε → 0 :

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{+\epsilon}\frac{d^2\psi}{dx^2}\,dx+\int_{-\epsilon}^{+\epsilon}V(x)\psi(x)\,dx=E\int_{-\epsilon}^{+\epsilon}\psi(x)\,dx.$$

The first integral is nothing but $d\psi/dx$.

$$\Delta\left(\frac{d\psi}{dx}\right)=\frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{-\epsilon}^{+\epsilon}V(x)\psi(x)\,dx.$$

$$\Delta\left(\frac{d\psi}{dx}\right)=-\frac{2m\alpha}{\hbar^2}\psi(0).$$

5 The Delta-function potential

$$\begin{cases} d\psi/dx = -B\kappa e^{-\kappa x}, \text{ for } (x>0), & \text{so } d\psi/dx\big|_+ = -B\kappa, \\ d\psi/dx = +B\kappa e^{+\kappa x}, \text{ for } (x<0), & \text{so } d\psi/dx\big|_- = +B\kappa, \end{cases}$$

and hence $\Delta(d\psi/dx) = -2B\kappa$. And $\psi(0) = B$. So

$$\kappa = \frac{m\alpha}{\hbar^2}, \longrightarrow E = -\frac{\hbar^2\kappa^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}.$$

Finally, we normalize ψ:

$$\int_{-\infty}^{+\infty} |\psi(x)|^2\,dx = 2|B|^2 \int_0^{\infty} e^{-2\kappa x}\,dx = \frac{|B|^2}{\kappa} = 1,$$

5 The Delta-function potential

$$\longrightarrow B = \sqrt{\kappa} = \frac{\sqrt{m\alpha}}{\hbar}.$$

Evidently the delta-function well, regardless of its "strength" α, has exactly one bound state:

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2}; \qquad E = -\frac{m\alpha^2}{2\hbar^2}.$$

What about **scattering states**, with $E > 0$? For $x < 0$ the TISE reads

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi, \qquad k \equiv \frac{\sqrt{2mE}}{\hbar}$$

5 The Delta-function potential

The general solution is

$$\psi(x) = Ae^{ikx} + Be^{-ikx},$$

Similarly, for $x > 0$,

$$\psi(x) = Fe^{ikx} + Ge^{-ikx}.$$

The continuity of $\psi(x)$ at $x = 0$ requires that

$$F + G = A + B.$$

5 The Delta-function potential

The derivatives are

$$\begin{cases} d\psi/dx = ik\left(Fe^{ikx} - Ge^{-ikx}\right), \text{ for } (x > 0), & \text{so } d\psi/dx\big|_+ = ik(F - G), \\ d\psi/dx = ik\left(Ae^{ikx} - Be^{-ikx}\right), \text{ for } (x < 0), & \text{so } d\psi/dx\big|_- = ik(A - B), \end{cases}$$

and hence $\Delta(d\psi/dx) = ik(F - G - A + B)$. Meanwhile, $\psi(0) = (A + B)$, so the second boundary condition says

$$ik(F - G - A + B) = -\frac{2m\alpha}{\hbar^2}(A + B),$$

or, more compactly,

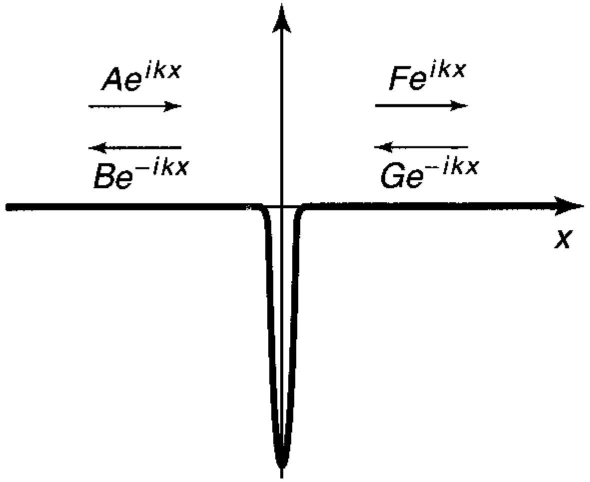
$$F - G = A(1 + 2i\beta) - B(1 - 2i\beta), \quad \text{where } \beta \equiv \frac{m\alpha}{\hbar^2 k}.$$

5 The Delta-function potential

- Having imposed the boundary conditions, we are left with two equations in four unknowns (A, B, F, and G)--five, if you count k. Normalization won't helps, this isn't a normalizable state.
- Recall that exp(ikx) gives rise [when coupled with the time-dependent factor exp($-iEt/h$)] to a wave function propagating to the right, and exp($-ikx$) leads to a wave propagating to the left.
- It follows that A is the amplitude of a wave coming in from the left, B is the amplitude of a wave returning to the left, F is the amplitude of a wave traveling off to the right, and G is the amplitude of a wave coming in from the right.

5 The Delta-function potential

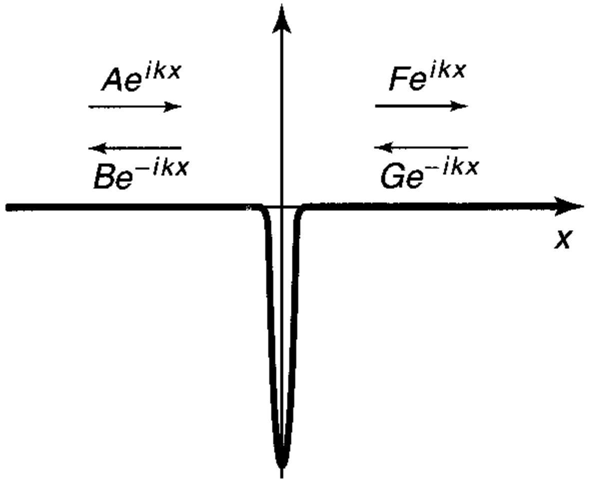
- In a typical scattering experiment particles are fired in from one direction--let's say, from the left. In that case the amplitude of the wave coming in from the right will be zero: G = 0 (for scattering from the left).



***A* is then the amplitude of the incident wave, *B* is the amplitude of the reflected wave, and *F* is the amplitude of the transmitted wave**. Then

$$B = \frac{i\beta}{1 - i\beta}A, \qquad F = \frac{1}{1 - i\beta}A.$$

5 The Delta-function potential



reflection coefficient.

$$R \equiv \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta^2}.$$

transmission coefficient

$$T \equiv \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2}.$$

$$R + T = 1.$$

$$R = \frac{1}{1 + (2\hbar^2 E/m\alpha^2)}, \quad T = \frac{1}{1 + (m\alpha^2/2\hbar^2 E)}.$$

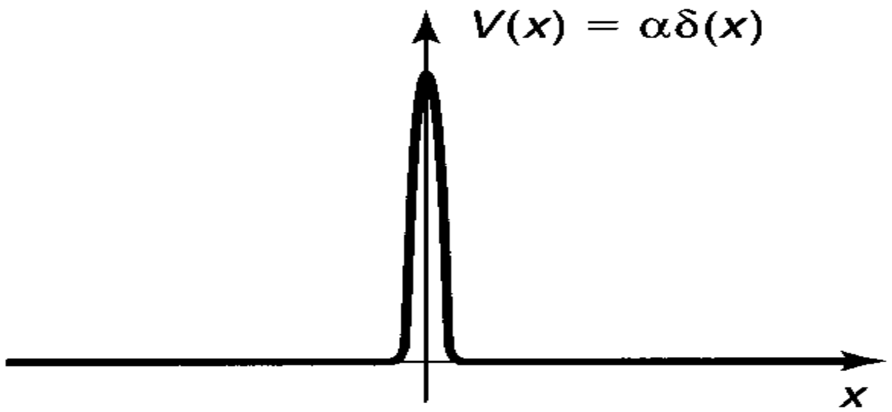
Remarks:

- These scattering wave functions are not normalizable, so they don't actually represent possible particle states.

- But we know what the resolution to this problem is: We must form normalizable linear **combinations of the stationary states,**

just as we did for the free particle--**true physical particles** are represented by the resulting **wave packets**.

- Meanwhile, since it is impossible to create a normalizable free particle wave function without **involving a range of energies**, R and T should be interpreted as the approximate reflection and transmission probabilities for particles in a narrow energy range.



- Look briefly at the case of a delta-function barrier. Formally, all we have to do is change the sign of α. ***This kills the bound state***, of course.

- But, the reflection and transmission coefficients, which depend only on α^2, are unchanged. **the particle is just as likely to pass through the barrier as to cross over the well**!

- Classically, the particle could not make it over an infinitely high barrier, regardless of its energy. In fact, the classical scattering problem is pretty dull:

If $E > V_{max}$, then T = 1 and R = 0---the particle certainly makes it over; conversely,

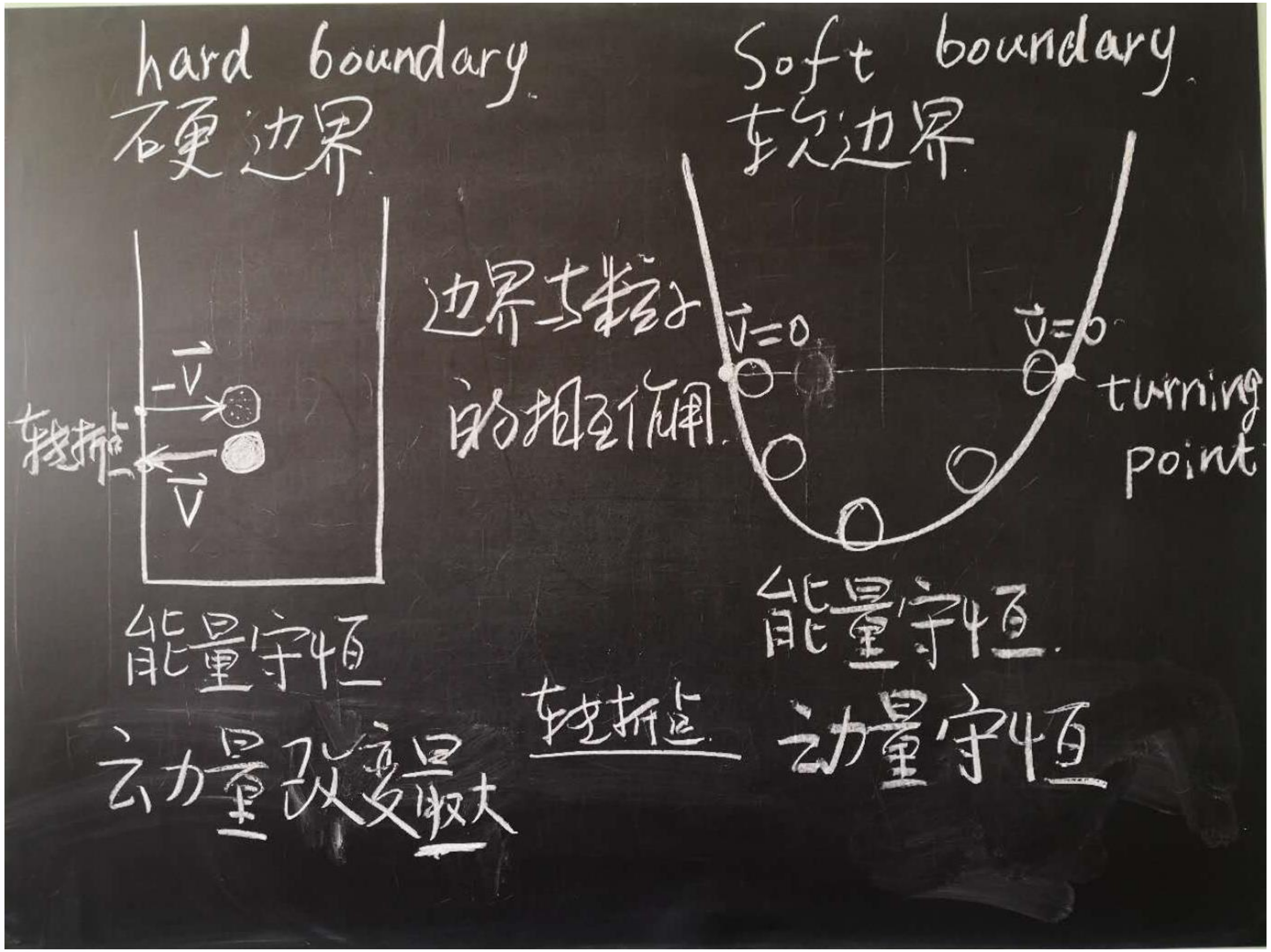
if $E < V_{max}$, then T = 0 and R = 1---it rides "up the hill" until it runs out of energy, and then returns the same way it came.

- The quantum scattering problem is much richer; the particle has some nonzero probability of passing through the potential even if $E < V_{max}$. We call this phenomenon tunneling; it is the mechanism that makes possible much of modem electronics--not to mention spectacular recent advances in microscopy. Conversely, even if $E > V_{max}$, there is a possibility that the particle will bounce back though.

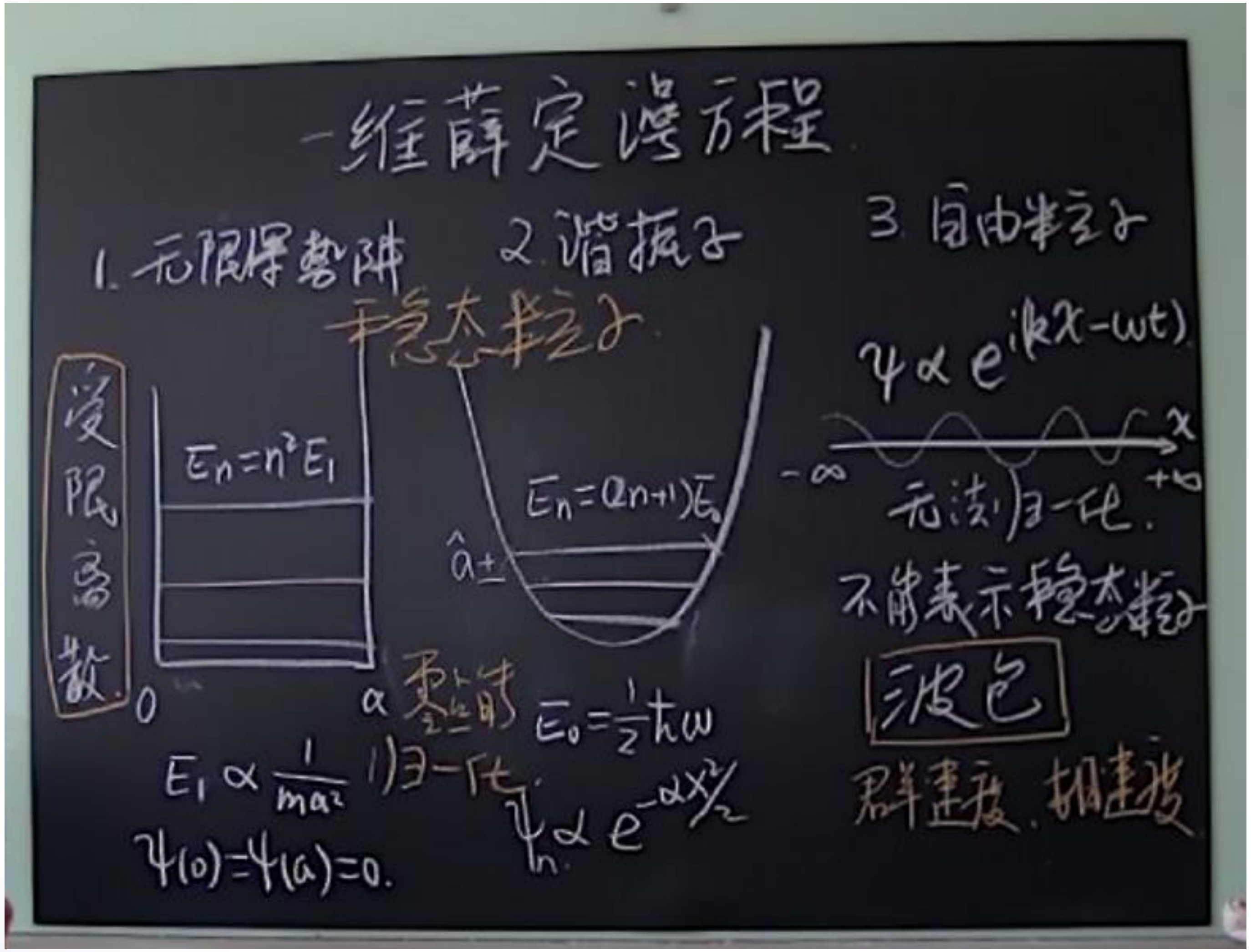
Problem: 2.24, 2.50, 2.52

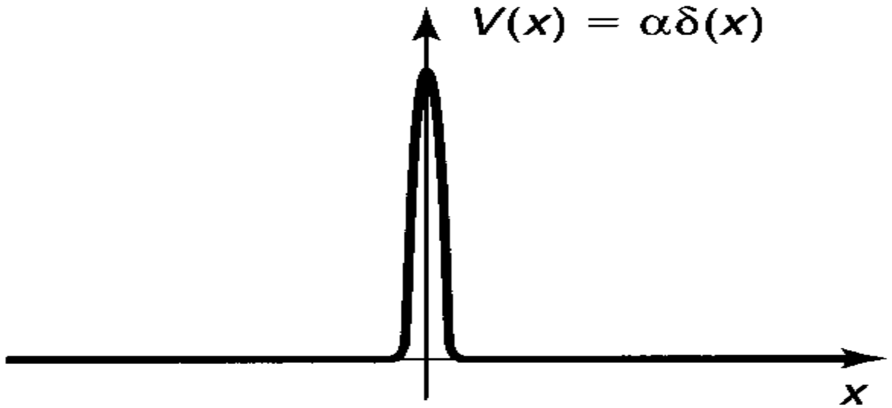
- 2.1 Stationary States
- 2.2 The Infinite Square Well
- 2.3 The Harmonic Oscillator
- 2.4 The Free Particle
- 2.5 The Delta-Function Potential
- **2.6 The Finite Square Well**

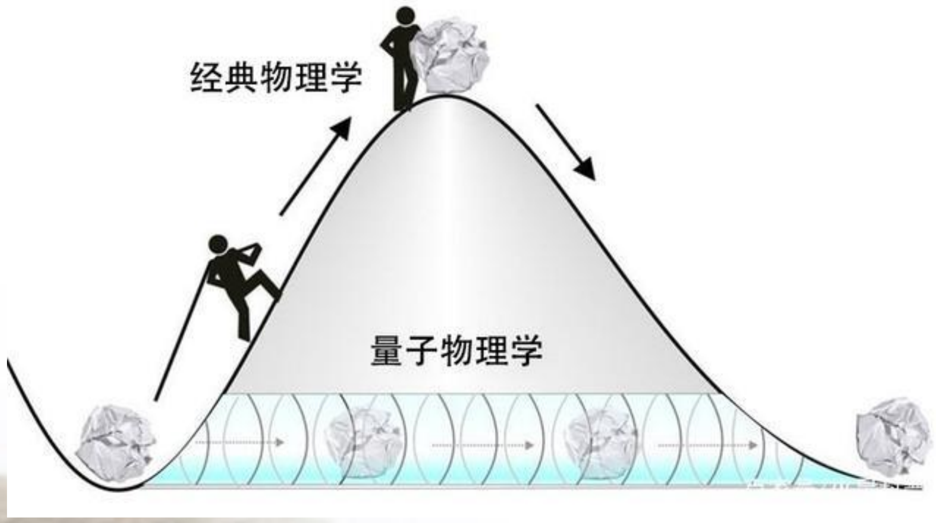
Review

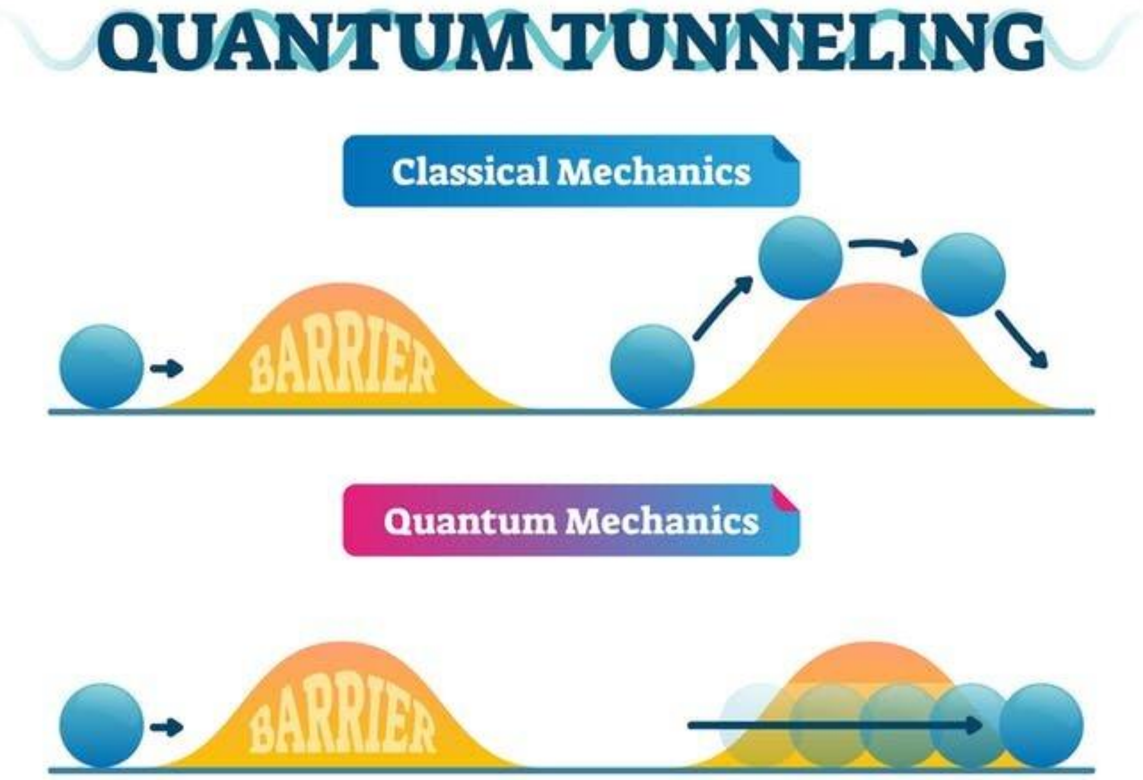

hard boundary
硬边界
Soft boundary
软边界
边界与粒子的相互作用
转折点
$-\vec{v}$
$\vec{v}$
$v=0$
$v=0$
turning point
能量守恒
动量改变最大
转折点
能量守恒
动量守恒

Review

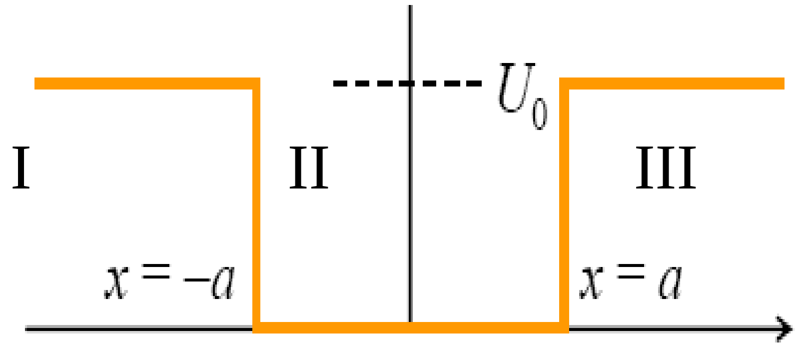

一维薛定谔方程
1. 无限深势阱
2. 谐振子
3. 自由粒子
$E_n=n^2E_1$
$E_1 \propto \frac{1}{ma^2}$
$\psi(0)=\psi(a)=0.$
$E_n=(2n+1)E_0$
$\hat{a}_\pm$
零点能
$E_0=\frac{1}{2}\hbar\omega$
归一化
$\psi_n \propto e^{-\alpha x^2/2}$
$\psi \propto e^{i(kx-\omega t)}$
无法归一化.
不能表示稳态粒子
波包
群速度. 相速度


$V(x) = \alpha\delta(x)$
x


经典物理学
量子物理学


QUANTUM TUNNELING
Classical Mechanics
BARRIER
Quantum Mechanics
BARRIER

2.6 The Finite Square Well



$$
U(x)=\begin{cases} U_0 & x<-a & \text{Region I} \\ 0 & -a\le x\le a & \text{Region II} \\ U_0 & x>a & \text{Region III} \end{cases}
$$

- We are interested only in the states whose energies are positive and smaller than U_0 ($0 < E < U_0$). These states are ***bound states***. (For $E > U_0$, the wave functions are quite similar to those of a free particle and the energies are not quantized.)

- A *classical particle* with energy $E < U_0$ is permanently bound to the region $-a \le x \le a$. Quantum mechanics, however, tells us that there is some non-vanishing probability that the particle can be found *outside* the region!

- As before, we solve the TISE.
- For region II ($-a \le x \le a$): $U(x) = 0$

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} &= E\psi, \\ \Rightarrow \frac{\partial^2\psi}{\partial x^2} &= -k^2\psi, \\ \text{where } k^2 &= \frac{2mE}{\hbar^2}. \end{aligned}$$

- Thus we get

$$\psi(x) = A \sin kx + B \cos kx$$

for some constants A and B.

- For regions I ($x < -a$) and III ($x > a$): $U(x) = U_0 > E > 0$

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+U_0\psi &= E\psi, \\
\Rightarrow \frac{\partial^2\psi}{\partial x^2} &= \frac{2m}{\hbar^2}\left(U_0-E\right)\psi \equiv \alpha^2\psi, \\
\therefore \psi(x) &= Ce^{\alpha x}+De^{-\alpha x}.
\end{aligned}
$$

- For region I, $\psi(x)$ has to remain *finite*, in particular when $x \to -\infty$, therefore $D = 0$.
- Similarly, for region III, $\psi(x)$ has to remain finite, in particular when $x \to +\infty$, $\therefore$ $C = 0$.

$$\psi(x) = \begin{cases} Ce^{\alpha x} & x < -a \\ A\sin kx + B\cos kx \quad \text{for} & -a \le x \le a\,. \\ De^{-\alpha x} & x > a \end{cases}$$

- To proceed, we use the continuity conditions of ψ and $d\psi/dx$ at $x = \pm a$.

Why?

Continuity of ψ at $x = -a$:

$$-A \sin ka + B \cos ka = Ce^{-\alpha a} \qquad (1)$$

Continuity of $d\psi/dx$ at $x = -a$:

$$kA \cos ka + kB \sin ka = \alpha Ce^{-\alpha a} \qquad (2)$$

Continuity of ψ at $x = +a$:

$$A \sin ka + B \cos ka = De^{-\alpha a} \qquad (3)$$

Continuity of $d\psi/dx$ at $x = +a$:

$$kA \cos ka - kB \sin ka = \alpha De^{-\alpha a} \qquad (4)$$

$$(1) + (3) \Rightarrow 2B \cos ka = (C + D)e^{-\alpha a} \qquad (5)$$

$$(2) - (4) \Rightarrow 2kB \sin ka = \alpha(C + D)e^{-\alpha a} \qquad (6)$$

$$(3) - (1) \Rightarrow 2A \sin ka = -(C - D)e^{-\alpha a} \qquad (7)$$

$$(2) + (4) \Rightarrow 2kA \cos ka = \alpha(C - D)e^{-\alpha a} \qquad (8)$$

From (5): If $(C + D) \neq 0$, then $B \neq 0$

$$(6)/(5) \Rightarrow k \tan ka = \alpha \qquad (9)$$

– Substitute (9) into (8):

$$2kA \cos ka = k \tan ka(C - D)e^{-\alpha a}$$

$$\Rightarrow 2A \cos^2 ka = \sin ka(C - D)e^{-\alpha a}$$

$$\Rightarrow 2A \sin ka \cos^2 ka = \sin^2 ka(C - D)e^{-\alpha a}$$

$(7) \Rightarrow$

$$-\cos^2 ka(C - D)e^{-\alpha a} = \sin^2 ka(C - D)e^{-\alpha a}$$

$$\Rightarrow (C - D)e^{-\alpha a} = 0$$

$$\Rightarrow C = D$$

– Substitute (10) into (8) gives

$$A = 0 \qquad (11)$$

– Substitute (10) into (5) gives

$$C = D = B \cos ka\, e^{\alpha a} \qquad (12)$$

– Hence (9), (11) and (12) give one type of solutions.

Another type of solutions exists for $(C-D)\neq 0$ and $A\neq 0$:

$$(8)/(7) \quad \Rightarrow \quad k\cot ka = -\alpha \qquad (13)$$

– Substitute (13) into (6):

$$2kB\sin ka = -(C+D)k\cot(ka)e^{-\alpha a}$$

$$\Rightarrow \quad 2B\cos ka \sin 2ka = -(C+D)\cos^2(ka)e^{-\alpha a}$$

$$(5)\Rightarrow$$

$$(C+D)\sin^2 ka e^{-\alpha a} = -(C+D)\cos^2 ka e^{-\alpha a}$$

$$\Rightarrow \quad (C+D)e^{-\alpha a} = 0$$

$$\Rightarrow \quad C = -D \qquad (14)$$

– Substitute (14) into (5)

$$\Rightarrow \quad B = 0 \qquad (15)$$

– Substitute (14) into (7)

$$\Rightarrow \quad -D = C$$

$$= -A\sin ka\, e^{\alpha a} \qquad (16)$$

–Hence (13), (15) and (16) give the other type of solutions.

- For the first type of solutions, the wavefunctions are:

$$\psi(x) = \begin{cases} B\cos ka e^{\alpha(a+x)} & x<-a \\ B\cos kx \quad \text{for} & -a\le x\le a \\ B\cos ka e^{\alpha(a-x)} & x>a \end{cases} \qquad (17)$$

- We see that

$$\boxed{\psi(x) = \psi(-x);}$$

$\psi(x)$ are said to have *even parity*.

- For the second type of solutions, the wavefunctions are:

$$\psi(x) = \begin{cases} -A\sin ka e^{\alpha(a+x)} & x<-a \\ A\sin kx \quad \text{for} & -a\le x\le a \\ A\sin ka e^{\alpha(a-x)} & x>a \end{cases} \qquad (18)$$

- We see that

$$\boxed{\psi(x) = -\psi(-x);}$$

$\psi(x)$ are said to have *odd parity*.

- The fact that the wavefunctions have a definite *parity* (even or odd) is a *consequence of the symmetry* of the potential: $V(x) = V(-x)$. With this symmetry, if $\psi(x)$ is a solution, then $\psi(-x)$ is also a solution of the Schrödinger equation.
- Optional:
- Mathematical speaking: when the Hamiltonian is *invariant* under certain kinds of *transformation*, its eigenfunctions can be classified into different kinds of *modes*.

Recall $k = \frac{\sqrt{2mE}}{\hbar} \quad \alpha = \frac{\sqrt{2m(U_0 - E)}}{\hbar},$

$$\therefore \left(k^2 + \alpha^2\right)a^2 = \frac{2mU_0 a^2}{\hbar^2} = \frac{U_0}{\Delta}, \qquad (19)$$

where $\Delta \equiv \frac{\hbar^2}{2ma^2}.$

Thus, the first type of solutions, which correspond to the *even* wavefunctions, satisfy (9) and (19):

$$\boxed{\begin{aligned} \alpha &= k \tan ka, && (9) \\ \left(k^2 + \alpha^2\right)a^2 &= \frac{U_0}{\Delta}. && (19) \end{aligned}}$$

Similarly, the second type of solutions, which correspond to the *odd* wavefunctions, satisfy (13) and (19):

$$\boxed{\begin{aligned} \alpha &= -k \cot ka, && (13) \\ \left(k^2 + \alpha^2\right)a^2 &= \frac{U_0}{\Delta}. && (19) \end{aligned}}$$

- Thus the energy eigenvalues E of the even and odd wavefunctions are found by solving the two corresponding sets of equations.
- These equations cannot be solved exactly. We shall solve for E graphically.
- Let us look at the case of the even wavefunctions first.
- – Since α and k are positive, $\tan ka$ has to be positive; hence only values of ka lying in the intervals

$$2n\frac{\pi}{2} \le ka \le (2n+1)\frac{\pi}{2}, \qquad (20)$$

for $n = 0, 1, 2, \ldots$ are allowed.

– Substitute (9) into (19) gives:

$$\Delta \equiv \frac{\hbar^2}{2ma^2}.$$

$$\boxed{k^2a^2\sec^2(ka) = \frac{U_0}{\Delta} \Rightarrow |\cos ka| = \sqrt{\frac{\Delta}{U_0}}ka.} \quad (21)$$

We take the absolute sign for cos *ka* because the right hand side of the equation is known to be positive.

– Thus for the even wavefunctions, the allowed values of *ka* are given by certain specific discrete values satisfying both (20) and (21).

– These special values are determined by the intersection of the straight line $(\Delta/U_0)^{1/2}ka$ with the curves for $|\cos ka|$ in the regions specified by (20).

We repeat a similar procedure for the case of the odd wavefunctions.

– First, cot *ka* has to be negative, so we have

$$\boxed{(2n-1)\frac{\pi}{2} \le ka \le 2n\frac{\pi}{2}, \qquad (22)}$$

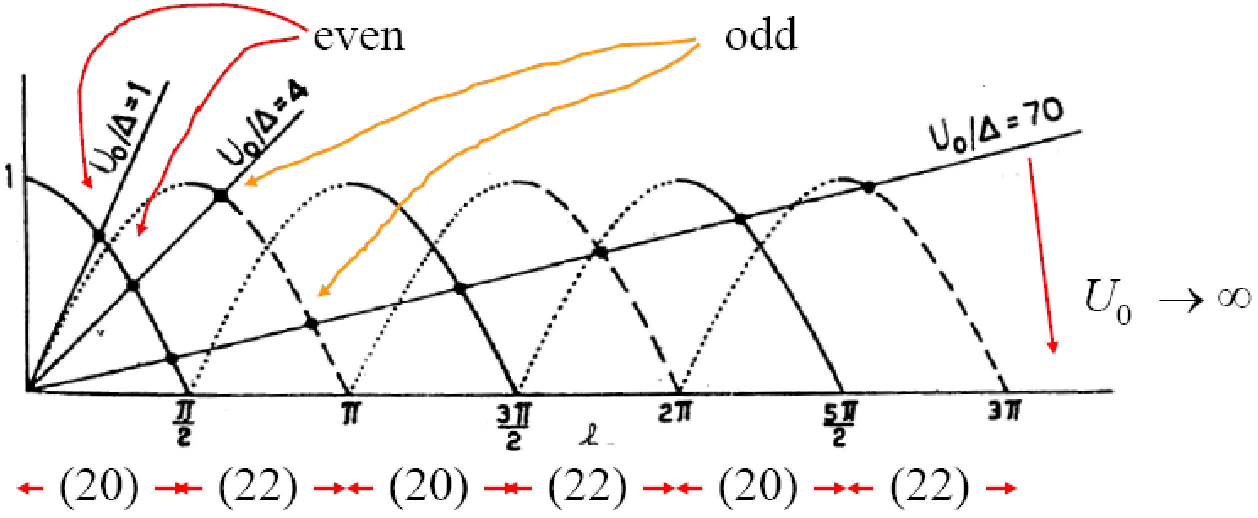
for n = 1, 2, 3 . . . are allowed.

Second,

$$\boxed{|\sin ka| = \sqrt{\frac{\Delta}{U_0}}ka. \qquad (23)}$$

Thus for the odd wavefunctions, the allowed values of *ka* are determined by the intersection of the straight line $(\Delta/U_0)^{1/2}ka$ with the curves for $|\sin ka|$ in the regions specified by (22).

The graphical solutions for the two cases are



– The parts of |cos *ka*| and |sin *ka*| which lie within the respective allowed regions are shown as solid lines and dashed lines. The not allowed parts are indicated by dotted lines.

– From the figure, we can see that only certain specific discrete values of *k* are allowed,

∴ *E* are quantized.

- Remarks:

1. There is always at least *one* solution of even wavefunction.

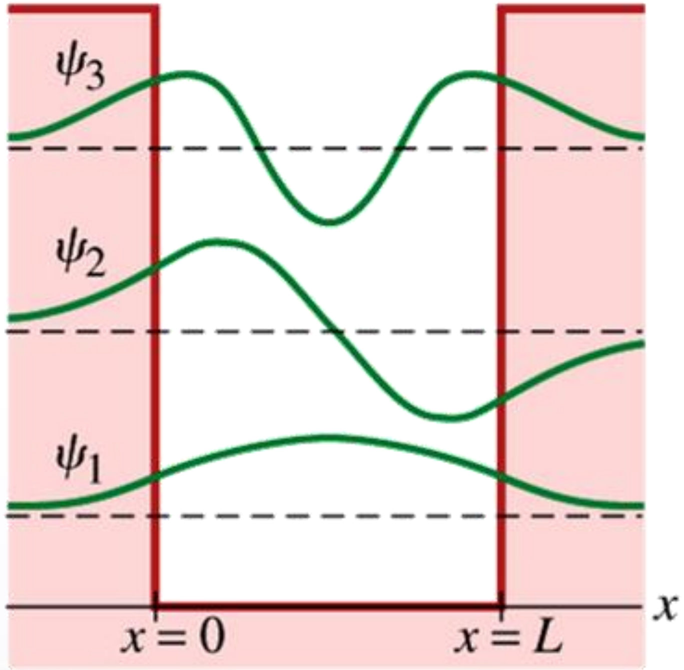
2. For larger U_0/Δ , there can be more than one solutions with even parity.

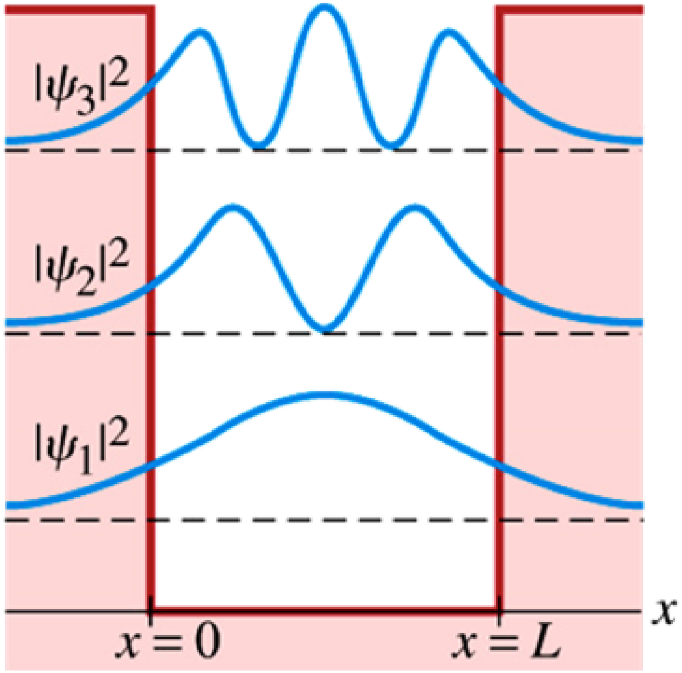
3. Only for *large enough* U_0/Δ will there be solution of odd parity. (Then, what is the minimum U_0?)

4. The number of bound states depends on U_0 and a but is always finite for a given U_0/Δ.

The constants A and B in (17) and (18) are determined by the normalization condition.

- The wave functions and probability densities penetrate the walls with an exponential decay





- Note the following features:
- – Alternate parity of the wavefunctions.
- – Number of nodes increases for states with higher energies

– $\psi(x) \neq 0$ outside the well. This is a *quantum effect*. This leads to the possibility of *quantum tunneling* (penetration) through a finite-width barrier.

Final comment:

– Even for a problem as simple as an 1D finite square well, there is no exact analytical solutions for the energy eigenvalues --- they have to be found numerically or graphically. There are not many exactly soluble QM problems.

- Classically, for any combination of a and U_0, one can always have a particle with *any* value of E (= K.E. + P.E.). Then if $0 < E < U_0$, the particle always stays inside the well, and the probability of finding the particle inside the well (region II) at any position (x) should be equal.

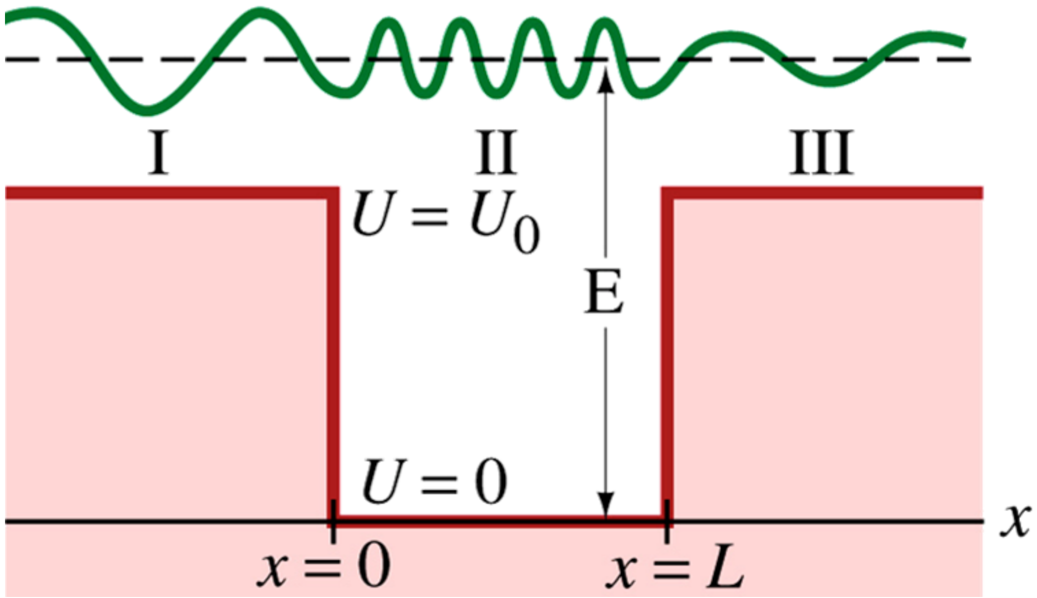
- However, by solving the Schrödinger Equation, there is a *minimum allowed E* for any value of U_0. In addition, when U_0 is large enough, then for certain position(s) in region II, the probability of finding the particle will be *zero*. One may also find the particle in regions I and III.

- Case where E>U_0
- In all regions the wave function has the form of a sinusoid.
- The potential in region II is different from I and II.
- The boundary conditions allow the wavefunction to be determined in each region, though the system has a continuum in energy.
- Regions I and III have

$$KE = E - U_0 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

$$\lambda_{\mathrm{I,III}} = \frac{h}{p} = \frac{h}{\sqrt{2m(E-U_0)}}$$

$$\lambda_{\mathrm{II}} = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$$



- Region II has U_0=0

势垒贯穿及扩展

一维势垒问题扩展

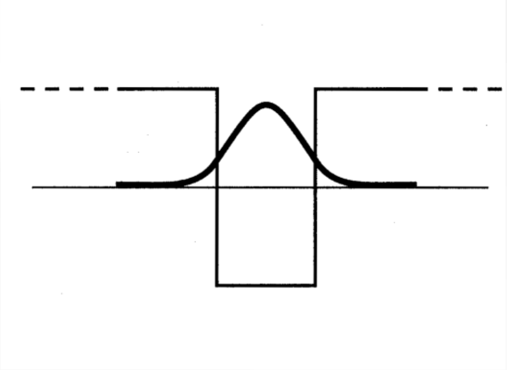
一维量子力学问题

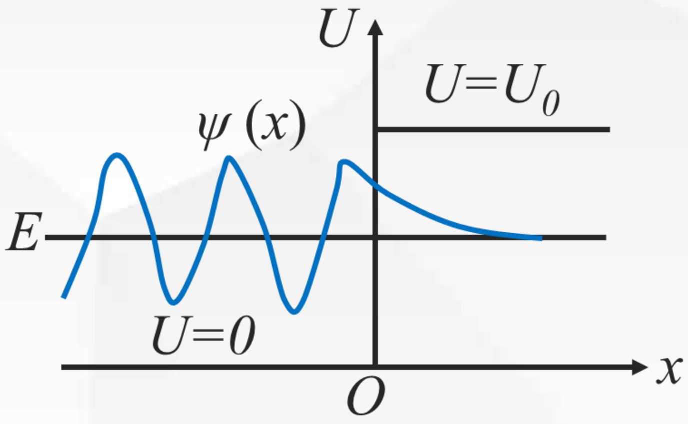
- 自由粒子波函数对应于平面波，能谱是连续的。
- 无限深势阱，波函数对应驻波，能谱离散，束缚态，基态零点能。
- 半自由空间和半空间的有限高势垒（真空和导体的电子输运问题）的散射和渗漏，能谱是连续谱。

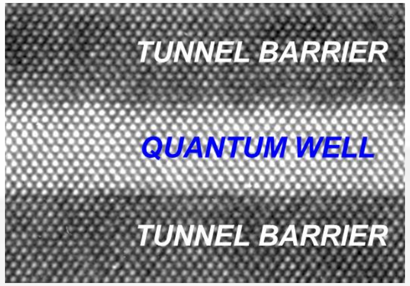
一维势垒问题扩展

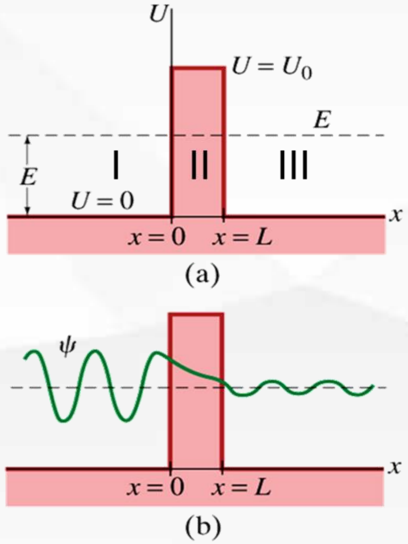
- 有限宽度、有限高势垒（半导体结、金属岛）的电子透射及全透射（隧穿效应）
- 一边半无线空间高势垒和一边半无限空间的低势垒中间存在有限深（高）势垒的电子透射和隧穿效应，束缚态和散射态共存的情况
- Delta函数势的透射
- 周期性势垒带来的能带结构

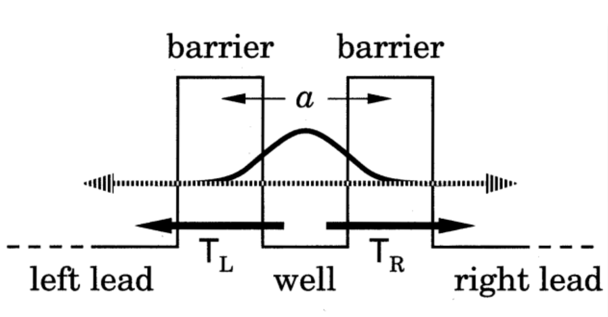
The Square Barrier

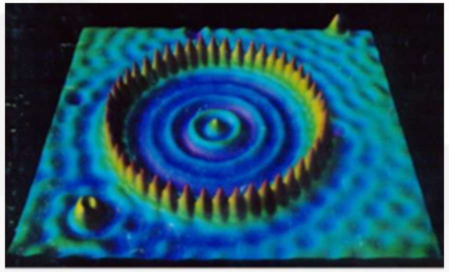








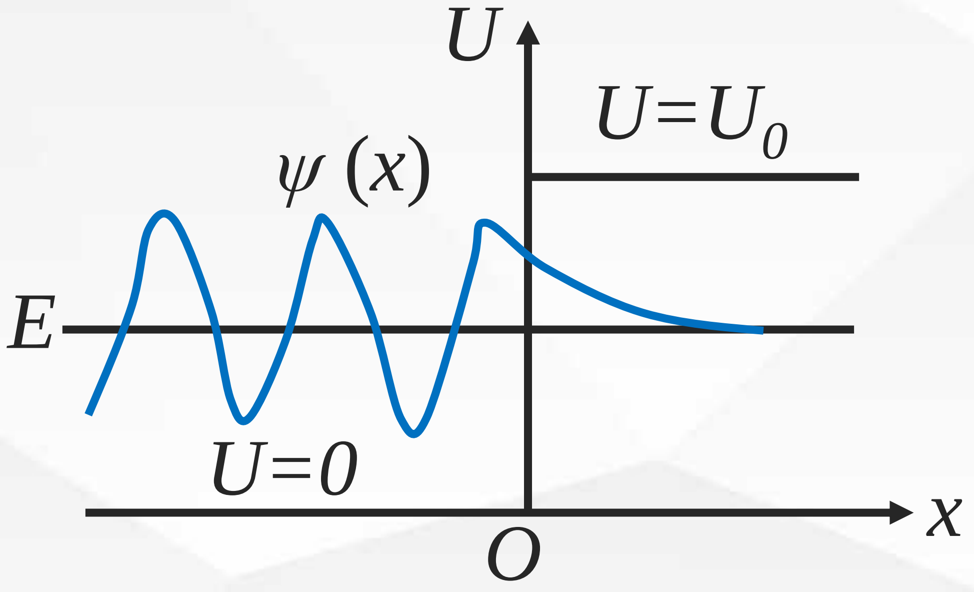




一维常势问题拓展

电子逸出金属表面的模型

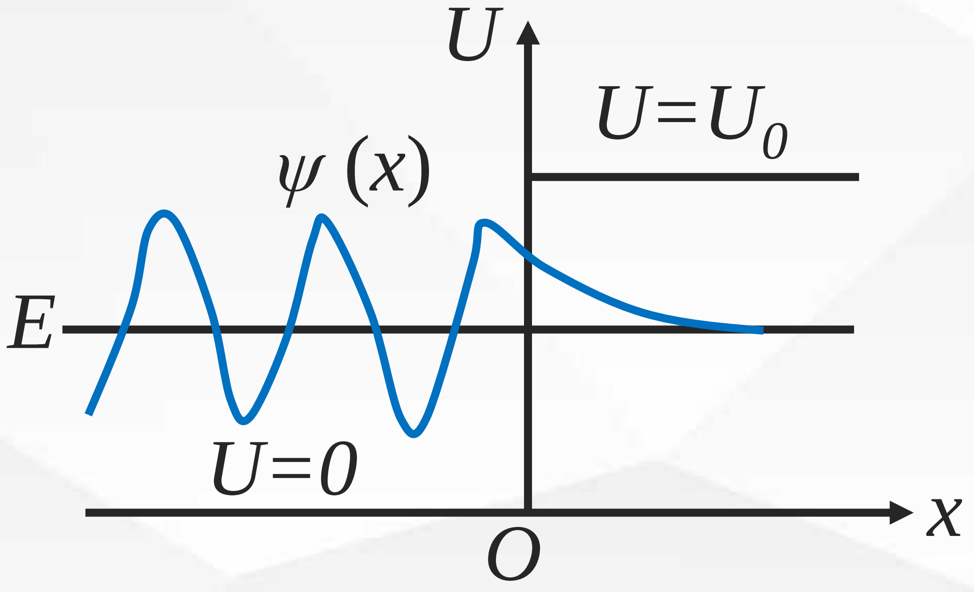
如果粒子能量小于势能U_0，在经典力学中显然不可能进入$x>0$的区域。只有当粒子能量大于势能U_0，粒子才能进入。但是在量子力学中，即使能量很小，也允许部分粒子有在$x>0$区域出现。



一维常势问题拓展

$$V(x)=\begin{cases}0, & x<0\\ \mathrm{U}_0, & x\geq 0\end{cases}$$

$$\frac{d^2\psi(x)}{dx^2}+\frac{2m(E-V)}{\hbar^2}\psi(x)，\quad \frac{2m(E-V)}{\hbar^2}=k^2,$$



通解

$$\psi(x)=Ae^{ikx}+Be^{-ikx}$$

一维常势问题拓展

$x < 0, V = 0$		$x \geq 0, V = U_0$	
$\sqrt{2mE}/\hbar = k$		$\lambda = \sqrt{2m(V-E)}/\hbar$	
$\psi(x) = Ae^{ikx}$ 入射波	$+ \quad Be^{-ikx}$ 反射波	$\psi(x) = Ce^{\lambda x}$ 指数增大	$+ \quad De^{-\lambda x}$ 指数衰减
边界条件：$\psi(\infty) = 0$ ： $C = 0$, $\psi_-(0) = \psi_+(0)$: $D = A + B$, $\psi'_-(0) = \psi'_+(0)$: $ikA - ikB = -\lambda D$			
$B = -\dfrac{\lambda + ik}{\lambda - ik}A, \quad D = \dfrac{2ik}{\lambda - ik}A$			

一维常势问题拓展

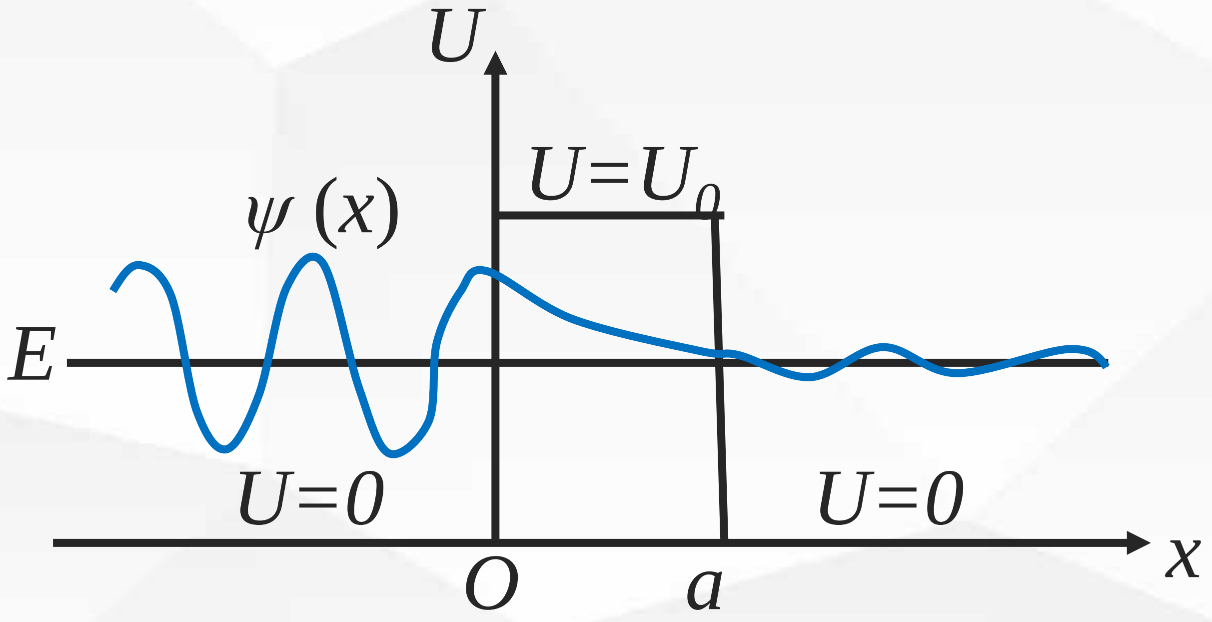
	$x < 0, V = 0$	$x \geq 0, V = U_0$
$\Psi(x,t) = \psi(x)e^{-\frac{i}{\hbar}Et}$	$\psi(x) = A\left(e^{ikx} - \frac{\lambda + ik}{\lambda - ik}e^{-ikx}\right)$	$\psi(x) = \frac{2ik}{\lambda - ik}Ae^{-\lambda x}$
$\rho(x,t) = \Psi^*(x,t)\Psi(x,t)$	$\rho = 2\|A\|^2\left[1 - \frac{\lambda^2 - k^2}{\lambda^2 + k^2}\cos(2kx) - \frac{2\lambda k}{\lambda^2 + k^2}\sin(2kx)\right]$ 驻波	$\rho = \|A\|^2\frac{4k^2}{\lambda^2 + k^2}e^{-2\lambda x}$ 渗透
$\boldsymbol{J} = \frac{i\hbar}{2m}(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi)$	入射流：$\frac{\hbar k}{m}\|A\|^2$,反射流：$-\frac{\hbar k}{m}\|B\|^2$	0

一维常势问题拓展

势垒隧穿

$$V(x)=\begin{cases}0, & x<0\\ U_0, a>x\geq 0\\ 0, & x>a\end{cases}$$

$$\frac{d^2\psi(x)}{dx^2}+k^2\psi(x)=0$$



一维常势问题拓展

<table>
<tr><th colspan="2">$x < 0, V = 0$</th><th colspan="2">$a > x \geq 0, V = U_0$</th><th colspan="2">$x > a, V = 0$</th></tr>
<tr><td colspan="2">$\sqrt{2mE}/\hbar = k_1$</td><td colspan="2">$k_2 = \sqrt{2m(E-V)}/\hbar$</td><td colspan="2">$\sqrt{2mE}/\hbar = k_1$</td></tr>
<tr><td colspan="2">$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x}$</td><td colspan="2">$\psi(x) = Ce^{\lambda x} + De^{-\lambda x}$</td><td colspan="2">$\psi(x) = Fe^{ik_1x} + Ge^{-ik_1x}$</td></tr>
<tr><td colspan="3">$\psi_-(0) = \psi_+(0): C + D = A$
$\psi'_-(0) = \psi'_+(0): k_1(A-B) = k_2(C-D)$</td><td colspan="3">$\psi_-(a) = \psi_+(a):\ Ce^{ik_2a} + De^{-ik_2a} = Fe^{ik_1a}$
$\psi'_-(a) = \psi'_+(a): k_2(Ce^{ik_2a} - De^{-ik_2a}) = k_1Fe^{ik_1a}$</td></tr>
<tr><td colspan="6">$B = -\dfrac{2i(k_1^2 - k_2^2)\sin k_2a}{(k_1+k_2)^2e^{-ik_2a} - (k_1-k_2)^2e^{ik_2a}}A,\quad F = \dfrac{4k_1k_2e^{-ik_1a}}{(k_1+k_2)^2e^{-ik_2a} - (k_1-k_2)^2e^{ik_2a}}A$</td></tr>
</table>

一维常势问题拓展

	$x < 0, V = 0$	$a > x \geq 0$	$x > a, V = 0$
$\Psi(x,t)$	$A\left(e^{ik_1x} - \frac{2i(k_1^2 - k_2^2)\sin k_2a}{(k_1+k_2)^2e^{-ik_2a} - (k_1-k_2)^2e^{ik_2a}}e^{-ik_1x}\right)$	?	$\frac{4k_1k_2Ae^{ik_1(x-a)}}{(k_1+k_2)^2e^{-ik_2a} - (k_1-k_2)^2e^{ik_2a}}$
$\rho(x,t)$	?	?	?
J	入射流：$\frac{\hbar k}{m}\lvert A\rvert^2$,反射流：$-\frac{\hbar k}{m}\lvert B\rvert^2$	?	出射流：$\frac{\hbar k}{m}\lvert F\rvert^2$

$$E < V, \frac{\sqrt{2mE}}{\hbar} = k_1 = k, k_2 = \frac{\sqrt{2m(E-V)}}{\hbar} = -i\lambda,\ F = \frac{2i\lambda k e^{-ik_1a}}{(k^2-\lambda^2)\sinh ka + 2i\lambda k\cosh ka}A$$

一维常势问题拓展

透射系数 $T=\frac{J_D}{J}=\frac{|C|^2}{|A|^2}=\frac{4k_1^2k_2^2}{(k_1^2-k_2^2)^2\sin^2 ak_2+4k_1^2k_2^2}$

$ik_3=k_2$ $T=\frac{4k_1^2k_2^2}{(k_1^2+k_3^2)^2 sh^2k_3a+4k_1^2k_3^2}$

反射系数 $R=\frac{J_R}{J}=\frac{|A'|^2}{|A|^2}=\frac{(k_1^2-k_2^2)^2\sin^2 k_2a}{(k_1^2-k_2^2)^2\sin^2 ak_2+4k_1^2k_2^2}=1-D$

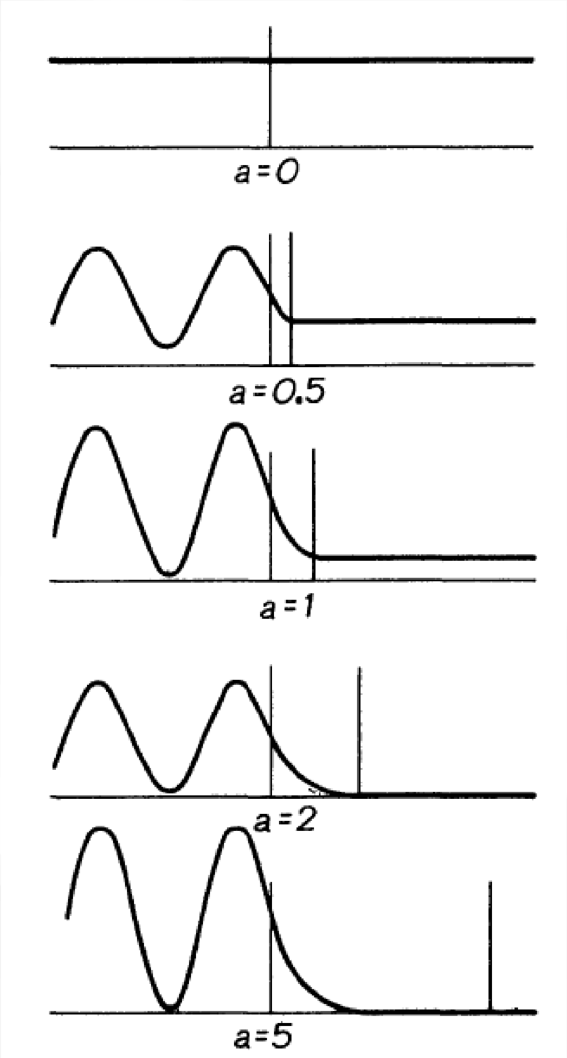
$$T = \left\{1 + \frac{1}{4}\frac{V_0^2}{E(V_0 - E)}\sinh^2 \alpha L\right\}^{-1}$$

For high and wide barriers such that $\alpha L >> 1$,

$$\sinh \alpha L = \frac{e^{\alpha L} - e^{-\alpha L}}{2} \approx \frac{e^{\alpha L}}{2} \gg 1$$

$$T \approx 16\frac{E(V_0 - E)}{V_0^2} e^{-2\alpha L}$$

the tunneling probability *falls off exponentially* and depends sensitively on E, V_0 and L.



Question: A 50 eV electron approaches a square barrier potential 70 eV high and (a) 1.0 nm thick (b) 0.10 nm thick. What is the probability that the electron will tunnel through?

Answer:

(a) First convert to SI units

$$V_0 - E = (70eV - 50eV) \times 1.6 \times 10^{-19}\,\frac{\mathrm{J}}{\mathrm{eV}} = 3.2 \times 10^{-18}\,\frac{\mathrm{J}}{\mathrm{eV}}$$

$$2\alpha L = 2\sqrt{\frac{2(9.11 \times 10^{-31}\mathrm{kg}) \times 3.2 \times 10^{-18}\,\frac{\mathrm{J}}{\mathrm{eV}}}{1.06 \times 10^{-34}\mathrm{J \cdot s}}} \times 1.0 \times 10^{-9}\mathrm{m} = 46$$

$$T \approx 16\frac{E(V_0 - E)}{V_0^2}e^{-2\alpha L} \approx 3.3 \times 10^{-20}$$

which is extremely small!

(b) for L=0.1nm, $2\alpha L = 4.6$, $T \approx 3.3 \times 10^{-2}$, so by decreasing the barrier width by a factor of 10, the probability of tunnelling has increased by 18 orders of magnitude.

Example : A rectangular potential barrier has a width L=0.15nm. Find the barrier height V_0 and the electron energy E for which the electron's total probability of transmission through the barrier is equal to T=0.4 and 16 $\frac{E(V_0-E)}{V_0^2}$=1.

Solution: form 16 $\frac{E(V_0-E)}{V_0^2}$=1, wen can find the ratio $\gamma = E/V_0$,$\gamma = \frac{1}{2} \pm \frac{\sqrt{3}}{4}$.

since now, $T \approx e^{-\frac{2L\sqrt{2m(V_0-E)}}{\hbar}} = e^{-\frac{2L\sqrt{2mV_0(1-\gamma)}}{\hbar}}$, so $\ln T = -\frac{2L\sqrt{2mV_0(1-\gamma)}}{\hbar}$,

$$V_0 = \frac{\hbar^2}{1-\gamma}\frac{(\ln T)^2}{8mL^2}$$

After the substitution of the given parameters we obtain two values of V_0

$$V_{01} = 8.51 \times 10^{-19}\mathrm{J} = 5.31\mathrm{eV}$$
$$V_{02} = 0.61 \times 10^{-19}\mathrm{J} = 0.38\mathrm{eV}$$

The corresponding values of the electron's energy are

$$E_1 = 7.94 \times 10^{-19}\mathrm{J} = 4.95\mathrm{eV}$$
$$E_2 = 0.4 \times 10^{-19}\mathrm{J} = 0.25\mathrm{eV}$$

一维常势问题拓展

隧道效应

粒子在能量E小于势垒高度时仍能贯穿势垒的现象

经典力学中，动能为负是无意义的。但在微观世界，由于粒子的波粒二象性，动能和势能是无法同时确定的，上述等式是不成立的。因此可以可出，隧道效应是微观粒子所特有的量子效应。

- Problem 2.30, 2.32, 2.47, 2.48, 2.52

Problem 3.4. An electron is in a one-dimensional rectangular potential well with barriers of infinite height. The width of the well is equal to $L = 5$ nm. Find the wavelengths of photons emitted during electronic transitions from the excited states with quantum numbers $n = 2$, λ_{21}, and $n = 3$, λ_{31}, to the ground state with $n = 1$. (Answer: $\lambda_{21} \approx 1.15$ μm and $\lambda_{31} \approx 0.43$ μm.)

Problem 3.8. An electron is in a symmetric rectangular potential well with width $L = 10$ nm and with barriers of finite height: $U_0 = 10$ eV. The electron wavefunction is symmetric with respect to the coordinate origin placed at the center of the well (see Fig. 3.15), in contrast to the case shown in Fig. 3.5. For which values of quantum numbers, n, can we apply the approximation of barriers with infinite height? (Answer: $n \ll 52$.)

Problem 3.9. An electron with energy $E = 32$ eV, which is moving in the positive direction along the x-direction, encounters an obstacle – an infinitely long rectangular potential step. Find the reflection, R, and transmission, D, coefficients of the electron de Broglie waves for a given potential step in two cases: (a) the height of the potential step is lower than the electron energy ($U_1 = 30$ eV) and (b) the height of the potential step is higher than the electron energy ($U_2 = 34$ eV). (Answer: (a) $R \approx 0.36$ and $D \approx 0.64$; (b) $R \approx 1.0$ and $D \approx 0$.)

Problem 3.10. Estimate the transmission coefficient, D, of an electron with energy $E = 18$ eV for passage through a potential barrier with the following dependence of potential energy on coordinate:

$$U(x) = U_0 \left(1 - \frac{x^2}{L^2}\right) \tag{3.196}$$

in the region $|x| \leq L$ and

$$U(x) = 0 \tag{3.197}$$

in the region $|x| > L$. Here, $U_0 = 20$ eV and $L = 2$ nm. (Answer: $D \approx 0.24$.)

The Dirac delta function, δ(x), is defined informally as follows:

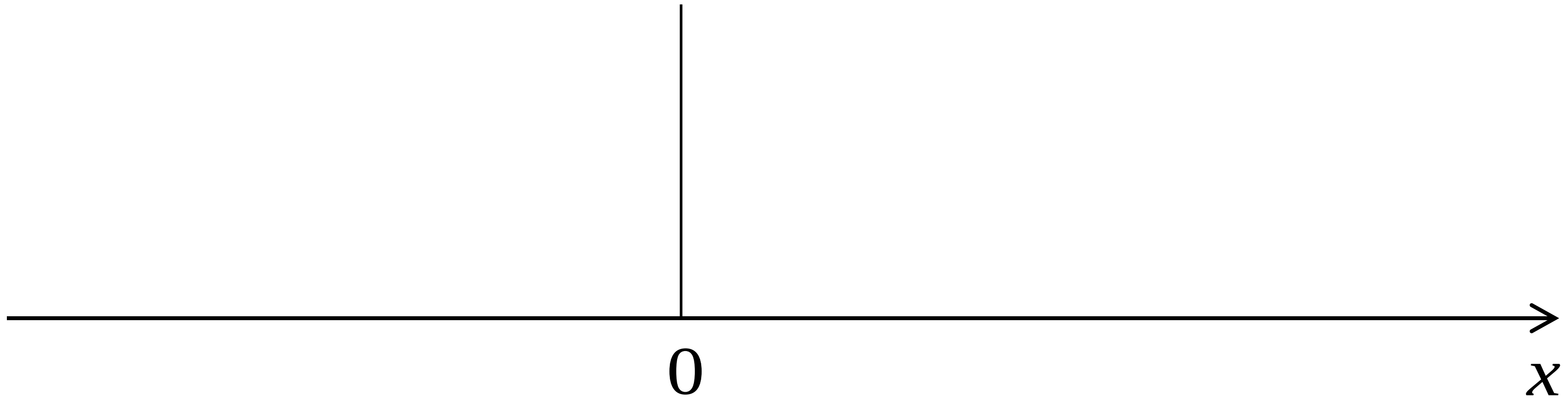
$$\delta(x) = \begin{Bmatrix} 0, & \text{if } x \neq 0 \\ \infty, & \text{if } x = 0 \end{Bmatrix}, \text{ with } \int_{-\infty}^{+\infty} \delta(x)\, dx = 1.$$

Supplement Dirac δ-function

- Definition
- Calculus
- 2D and 3D
- In curvilinear coordinates

Definition of δ-function

$$\delta(x)=\begin{cases}0, & \text{if } (x\neq 0)\\ \infty, & \text{if } (x=0)\end{cases} \quad \text{and} \quad \int \delta(x)\,dx=1$$

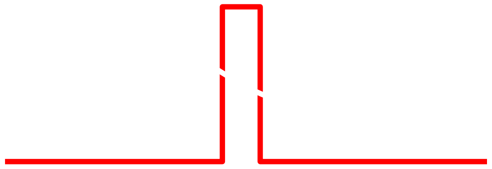


1. The dimension of d-function is $(1/x)$
2. Always meant to appear in an integral
3. A notation of a limiting process

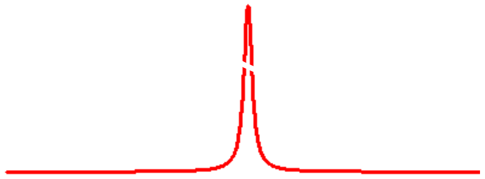
Definition of δ-function

If $f(x)$ is smooth and $g(x)$ is a sharp peak at $x=0$

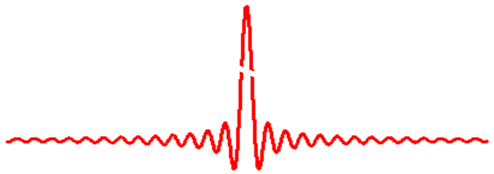
and $\int g(x)dx = 1$, then $\int f(x)g(x)dx \approx f(0)$



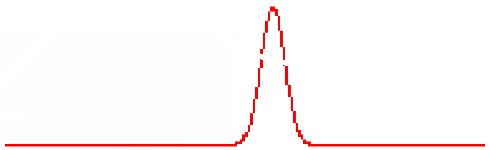
$$g(x)=\begin{cases} 0, & (|x|>\gamma/2) \\ \gamma^{-1}, & (|x|<\gamma/2) \end{cases}$$



$$g(x)=\frac{\gamma/\pi}{x^2+\gamma^2}$$



$$g(x)=\frac{\sin(x/\gamma)}{x}$$



$$g(x)=\frac{1}{\gamma\sqrt{\pi}}\exp\left(-\frac{x^2}{\gamma^2}\right)$$

$$\gamma \to 0$$

$$g(x)\to\delta(x)$$

$$f(x)g(x)\to f(0)\delta(x)$$

$$\int f(x)g(x)dx \to f(0)\int\delta(x)dx = f(0)$$

Definition of δ-function

Even function

$$g(x)=\frac{g(x)+g(-x)}{2}+\frac{g(x)-g(-x)}{2}=g^{+}(x)+g^{-}(x)$$

$$g^{+}(x)\to\delta(x)$$

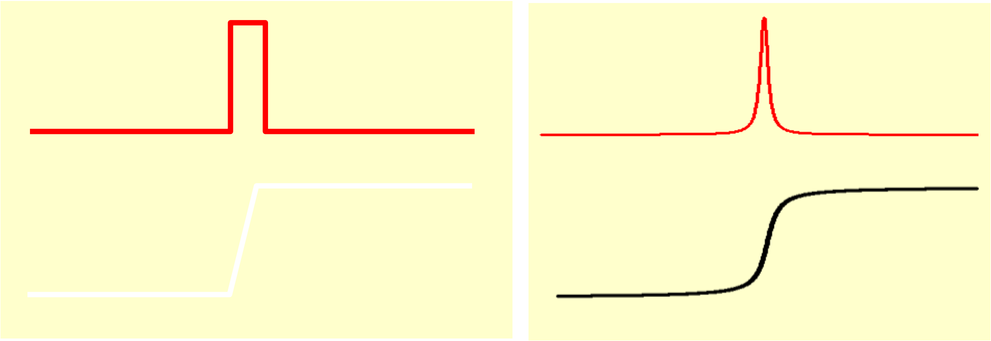
$$\delta(x)=\delta(-x)$$ since the integral of the odd part vanishes

Scaling property

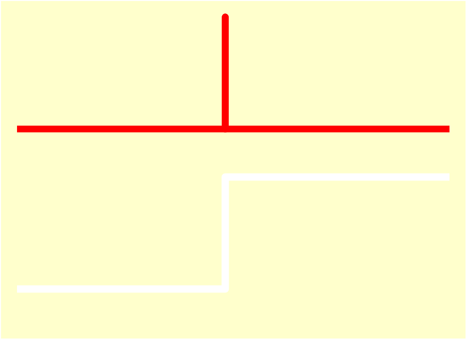
$$\int\delta(ax)\,dx=\frac{1}{a}\int\delta(ax)\,d(ax)$$

$$\delta(ax)=\frac{1}{a}\delta(x)$$ (Note the dimension is correct)

Integral of δ-function



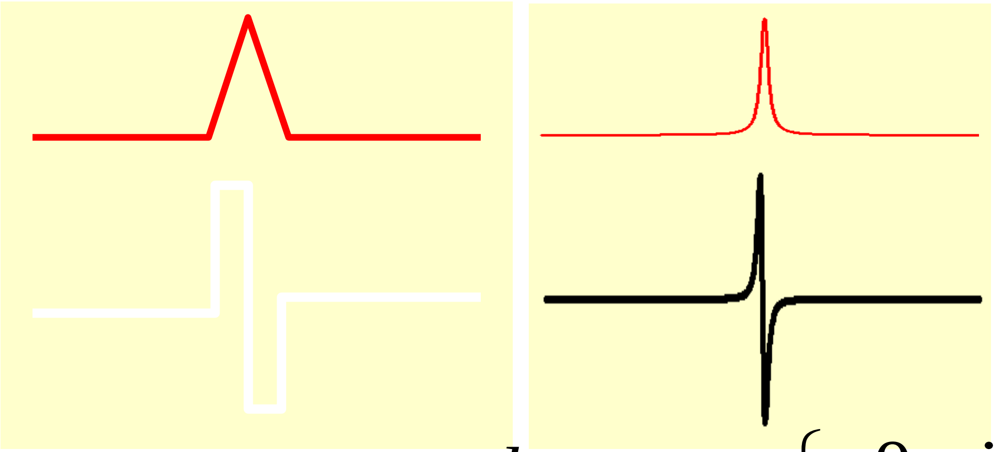
$\gamma \to 0$



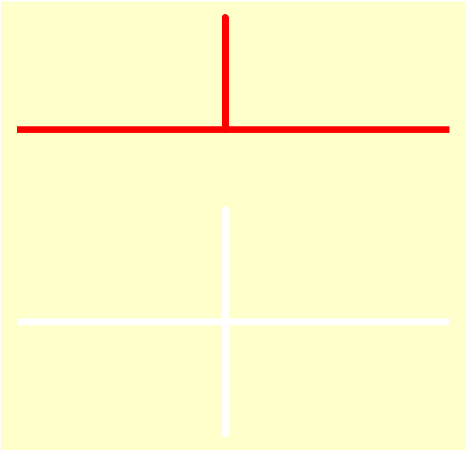
$$\int_{-\infty}^{x} g(x)\,dx \to \int_{-\infty}^{x} \delta(x)\,dx = \vartheta(x) = \begin{cases} 0, \text{ if } (x<0) \\ 1/2, \text{ if } (x=0) \\ 1, \text{ if } (x>0) \end{cases}$$

$$\delta(x) = \frac{d}{dx}\vartheta(x)$$

Derivative of δ-function



$\gamma \to 0$



$$\frac{d}{dx}\delta(x) = \begin{cases} 0, & \text{if } (x \neq 0) \\ \pm\infty, & \text{if } (x = 0) \end{cases}$$

It is not even a single-value function, but it is useful for partial integration

$$\int_{-\infty}^{+\infty} f(x)\frac{d}{dx}\delta(x)\,dx = f(x)\delta(x)\Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \delta(x)\frac{d}{dx}f(x)dx = -\frac{d}{dx}f(x)\Big|_{x=0}$$

Watch out: $\int_{-\infty}^{+\infty} f(x)\frac{d}{dx}\delta(x)\,dx \neq \int_{-\infty}^{+\infty} f(0)\frac{d}{dx}\delta(x)\,dx$

δ-function in 2D & 3D

$$\delta^n(\mathbf{r}) = \begin{cases} 0, & \text{if } (\mathbf{r} \neq 0) \\ \infty, & \text{if } (\mathbf{r} = 0) \end{cases} \quad \text{and} \quad \begin{cases} \iint \delta^2(\mathbf{r})\, dxdy = 1 \\ \iiint \delta^3(\mathbf{r})\, dxdydz = 1 \end{cases}$$

$$\delta^2(\mathbf{r}) = \delta(x)\delta(y) \quad \text{and} \quad \delta^3(\mathbf{r}) = \delta(x)\delta(y)\delta(z)$$

δ-function in curvilinear coordinates

$$\iiint \delta^3(\mathbf{r})\,d\tau = 1$$

Spherical coordinates

$$d\tau = r^2 \sin\theta\, dr\, d\theta\, d\varphi$$

$$\delta^3(\mathbf{r}) = g(r)\delta(r)$$

$$\iiint g(r)\delta(r) r^2 \sin\theta\, dr\, d\theta\, d\varphi$$

$$= 4\pi \int g(r)\delta(r) r^2 dr = 1$$

$$\delta^3(\mathbf{r}) = \frac{1}{4\pi r^2}\delta(r)$$

Cylindrical coordinates

$$d\tau = s\,dz\,ds\,d\theta$$

$$\delta^3(\mathbf{r}) = g(s)\delta(s)\delta(z)$$

$$\iiint g(s)\delta(s)\delta(z)\, s\,dz\,ds\,d\theta$$

$$= 2\pi \int g(s)\delta(s)\, s\,ds = 1$$

$$\delta^3(\mathbf{r}) = \frac{1}{2\pi s}\delta(s)\delta(z)$$

Example: Fourier transformation

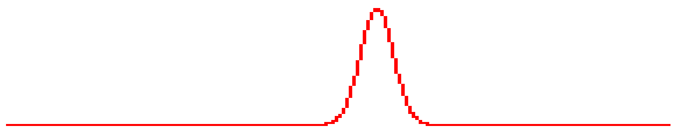
$$\int e^{ikx}dx = \lim_{\gamma\to 0}\left(\int e^{ikx-\gamma|x|}dx\right) = \lim_{\gamma\to 0}\left(\frac{2\gamma}{k^2+\gamma^2}\right) = 2\pi\delta(k)$$

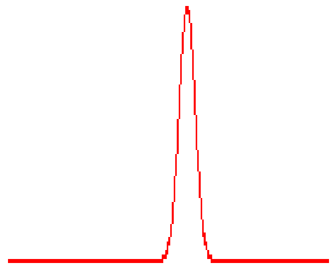
$$f(x) \equiv \int \tilde{f}(k)e^{ikx}\frac{dk}{2\pi}$$

$$\begin{aligned}\int f(x)e^{-ikx}dx &= \int dx\int \tilde{f}(k')e^{ik'x}e^{-ikx}\frac{dk'}{2\pi} \\ &= \int \frac{dk'}{2\pi}\int \tilde{f}(k')e^{i(k'-k)x}dx \\ &= \int \tilde{f}(k')\delta(k'-k)dk' \\ &= \tilde{f}(k)\end{aligned}$$

Example: Gaussian integral

$$\delta(x) = \lim_{a\to 0} \frac{1}{\sqrt{2\pi a}} \exp\left(-\frac{x^2}{2a}\right)$$





$$\lim_{a\to 0} \frac{1}{\sqrt{2\pi a}} \exp\left(-\frac{x^2}{2a}\right) = \begin{cases} \infty & x = 0 \\ 0 & x \neq 0 \end{cases}$$

and $\int \frac{1}{\sqrt{2\pi a}} \exp\left(-\frac{x^2}{2a^2}\right) dx = 1$

$\lim_{a\to 0} \frac{1}{\sqrt{2\pi a}} \exp\left(-\frac{x^2}{2a}\right)$ has the same modulus (∞) if a is pure imaginary.

Is the definition still okay?

Example: Gaussian integral

Yes. since $\int f(x)\lim_{a\to 0}\frac{1}{\sqrt{2\pi a}}\exp\left(-\frac{x^2}{2a}\right)dx = f(0)$ still hold.

$$\lim_{a\to 0}\frac{1}{\sqrt{2\pi a}}\exp\left(i\frac{x^2}{2|a|}\right)$$ has fast-varying phase for $x \neq 0$

$$\int f(x)\lim_{a\to 0}\frac{1}{\sqrt{2\pi a}}\exp\left(-\frac{x^2}{2a}\right)dx = f(0)\int \lim_{a\to 0}\frac{1}{\sqrt{2\pi a}}\exp\left(-\frac{x^2}{2a}\right)dx.$$

$$\int \frac{1}{\sqrt{2\pi a}}\exp\left(-\frac{x^2}{2a^2}\right)dx = 1$$

Consider the contour integral to calculate the Gaussian integral with imaginary a.

If you multiply $\delta(x - a)$ by an ordinary function $f(x)$, it's the same as multiplying by $f(a)$:

$$f(x)\delta(x-a) = f(a)\delta(x-a),$$

because the product is zero anyway except at the point *a*. In particular,

$$\int_{-\infty}^{+\infty} f(x)\delta(x-a)\,dx = f(a)\int_{-\infty}^{+\infty}\delta(x-a)\,dx = f(a).$$