Chapter 3: Problems in One Dimension

→ Application of concept of quantum mechanics to simple systems in 1 dimension:

We consider a particle in
* an impenetrable box → only discrete energy eigenvalues exist
* a harmonic oscillator potential → zero-point energy & algebraic solution & coherent states
* a potential with steps → reflection from, transmission into a potential wall & tunneling
* δ-function potential → bound states and scattering eigenstate of the Hamilton operator

3.1. Particle in an Impenetrable Box

→ Consider particle "trapped" in a potential $V(x) = \begin{cases} 0 & ; \ 0 \le x \le L \\ \infty & ; \ x < 0 \text{ or } x > L \end{cases}$.

We need to determine all possible energy eigenvalues and the corresponding eigenfunctions from the **time-independent Schrödinger equation**:

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

→ Infinite potential region: Consider $V(x) = \Lambda$ for $\Lambda \to \infty$. The term $\frac{\partial^2}{\partial x^2}\psi$ is finite almost everywhere (i.e. everywhere except at exceptional and separated points) and we have $E < \infty$.
So $\psi(x)$ must vanish almost everywhere.
We can therefore conclude that $\psi(x) = 0$ in the region wher $V(x) = \infty$.

→ Smoothness of $\psi(x)$ at boundary points $x = 0, L$: For any finite Λ (with $\Lambda \to \infty$) $\psi(x)$ must be smooth, because if $\psi(x)$ were discontinuous (e.g. $\psi(x) \sim \Theta(x)$ for x close to zero) we had ($\frac{\partial}{\partial x}\psi(x) \sim \delta(x)$ and) $\frac{\partial^2}{\partial x^2}\psi(x) \sim \delta'(x)$, which does not appear in the time-independent Schrödinger equation. So we must have $\psi(0) = \psi(L) = 0$. $\psi(x)$ is also continuous everywhere in the region $0 \le x \le L$.

→ Zero potential region: We have to solve the following **eigenvalue problem with boundary conditions**:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) = E\,\phi(x)\ , \quad \phi(0) = \phi(L) = 0$$

$e^{ix} = \cos(x) + i\sin(x)$

↳ This is the differential equation for trigonometric functions and the general solution without yet considering the boundary conditions reads $\phi_E(x) = N\exp(\pm i(k - a))$ with $E = \frac{\hbar^2 k^2}{2m}$ and $k, a, N \in \mathbb{R}$.
The boundary conditions further restrict the possible eigenvalues and the form of the eigenfunctions.

$\phi(0) = 0$: $\phi_E(x) = N e^{ia}\sin(kx)$, $E = \frac{\hbar^2 k^2}{2m}$
$\phi(L) = 0$: $\sin(kL) = 0 \Rightarrow k_n L \overset{!}{=} n\pi$ $(n = 1, 2, \ldots)$ [$n=0$ leads to $\phi(x) = 0$]
We can further set $e^{ia} = 1$ $(a = 0)$ since an overall (constant) phase can be set to zero.

We thus obtain as the energy eigenfunctions and the associated energy eigenvalues:
$\phi_n(x) = N\sin\left(\frac{n\pi}{L}x\right)$ with $E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2\pi^2}{2mL^2}$, $n \in \mathbb{N}$

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give same results for integrals over half cycles

Normalization gives the condition: $\quad \sin^2 x + \cos^2 x = 1$

$$1 \stackrel{!}{=} N^2 \int_0^L dx \, \sin^2\left(\frac{n\pi}{L} x\right) = N^2 \frac{L}{2} \quad \longrightarrow N^2 = \frac{2}{L}$$

↳ Final result: ϕ_n: energy eigenfunctions ; E_n: energy eigenvalues

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin(k_n x) \quad , \; k_n = \frac{n\pi}{L} \quad , \; n = 1, 2, 3, \dots \quad (n \in \mathbb{N})$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} \quad , \; \text{so } E_1 = \frac{1}{2m}\left(\frac{\hbar\pi}{L}\right)^2 , \; E_2 = 4E_1 , \dots \; E_n = n^2 E_1$$

$$\langle \phi_m | \phi_n \rangle = \int_0^L dx \, \phi_m^*(x) \phi_n(x) = \delta_{nm}$$

↳ Completeness: Every continuous wave function $\psi(x)$, $x \in [0, L]$ with $\psi(0) = \psi(L) = 0$ can be expanded in the / written as a superposition of the energy eigenfunctions: (→ Fourier Analysis!)

$$\psi(x) = \sum_{n=1}^{\infty} \phi_n(x) c_n \quad , \quad c_n = \langle \phi_n | \psi \rangle = \int_0^L dx \, \phi_n^*(x) \psi(x)$$

This implies the completeness relation

$$\sum_{n=1}^{\infty} \phi_n^*(x) \phi_n(y) = \delta(x - y)$$

↳ Time evolution:

$$\psi(x,t) = e^{-i\frac{Ht}{\hbar}} \sum_{n=1}^{\infty} c_n \phi_n(x) = \sum_{n=1}^{\infty} e^{-i\frac{E_n t}{\hbar}} c_n \phi_n(x)$$

3.2. Harmonic Oscillator

→ Consider particle in the harmonic oscillator potential $V(x) = \frac{m\omega^2}{2} x^2$.

Hamilton operator : $H = \frac{P^2}{2m} + \frac{m\omega^2}{2} X^2$

→ We can easily see that the energy spectrum of H contains only real numbers $E \geq 0$, because

$$\langle \psi | H \psi \rangle = \frac{1}{2m} \langle \psi | P^2 \psi \rangle + \frac{m\omega^2}{2} \langle \psi | X^2 \psi \rangle$$

$$= \frac{1}{2m} \langle P\psi | P\psi \rangle + \frac{m\omega^2}{2} \langle X\psi | X\psi \rangle \geq 0$$

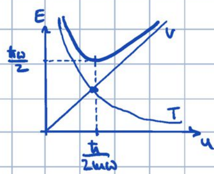
→ The ground state is the energy eigenstate with the lowest energy eigenvalue. Using Heisenberg's uncertainty principle we can show that the ground state's energy is indeed > 0.

↳ We may assume that the ground state ($|\phi_0\rangle$) has the classic property $\langle X \rangle_{\phi_0} = 0$, $\langle P \rangle_{\phi_0} = 0$ since it should be the state that simply stays at the minimum and does not move.

$\Rightarrow (\Delta X)^2_{\phi_0} = \langle X^2 \rangle_{\phi_0}$, $(\Delta P)^2_{\phi_0} = \langle P^2 \rangle_{\phi_0}$

$\Rightarrow \langle X^2 \rangle_{\phi_0} \langle P^2 \rangle_{\phi_0} \geq \left(\frac{\hbar}{2}\right)^2$ (Heisenberg's uncertainty principle)

$$\Rightarrow \langle H \rangle_{\phi_0} = \frac{1}{2m} \langle P^2 \rangle_{\phi_0} + \frac{m\omega^2}{2} \langle X^2 \rangle_{\phi_0}$$
$$\geq \frac{1}{2m} \left(\frac{\hbar}{2}\right)^2 \frac{1}{\langle X^2 \rangle_{\phi_0}} + \frac{m\omega^2}{2} \langle X^2 \rangle_{\phi_0}$$



We can now look for the minimum of the function $E(u) = \overbrace{\frac{\hbar^2}{8m} \frac{1}{u}}^{T(u)} + \overbrace{\frac{m\omega^2}{2} u}^{V(u)}$

$E'(u) = -\frac{\hbar^2}{8m} \frac{1}{u^2} + \frac{m\omega^2}{2} \overset{!}{=} 0$

↳ $u_{min} = \frac{\hbar}{2m\omega} \Rightarrow E(u_{min}) = \frac{\hbar\omega}{2}$ with $T(u_{min}) = V(u_{min})$.

So the ground state energy has the property $E_0 = \langle H \rangle_{\phi_0} \geq \frac{\hbar\omega}{2}$.

↳ It turns out that the ground state is the Gauss wave packet from Chap. 2.9. with $p_0 = 0$:

$$\boxed{\phi_0(x) = (2\pi)^{-1/4} \sigma^{-1/2} \exp\left(-\frac{x^2}{4\sigma^2}\right)}$$

$\Rightarrow \langle X \rangle_{\phi_0} = 0$, $\langle P \rangle_{\phi_0} = 0$ ✓

$\langle X^2 \rangle^{1/2}_{\phi_0} = \sigma$, $\langle P^2 \rangle^{1/2}_{\phi_0} = \frac{\hbar}{2\sigma}$ (exercises)

We check: $-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \phi_0(x) = -\frac{\hbar^2}{2m} \left(\frac{x^2}{4\sigma^4} - \frac{1}{2\sigma^2}\right) \phi_0(x)$

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \phi_0(x) + \frac{m\omega^2}{2} x^2 \phi_0(x) = x^2 \overbrace{\left[\frac{m\omega^2}{2} - \frac{\hbar^2}{8m\sigma^4}\right]}^{=0} \phi_0(x) + \frac{\hbar^2}{4m\sigma^2} \phi_0(x)$$

So we must have $\boxed{\sigma = \left(\frac{\hbar}{2m\omega}\right)^{1/2}}$ and get $\boxed{E_0 = \frac{\hbar\omega}{2}}$ as the ground state energy.

Note that $\frac{1}{2m} \langle P^2 \rangle_{\phi_0} = \frac{m\omega^2}{2} \langle X^2 \rangle_{\phi_0}$, so kinetic and potential energy average values are equal in the ground state.

↳ Note: The ground state wave function is unique (up to a global phase factor).

→ Ladder operators:

From Chp. 2.8. (→ generalized uncertainty relation) and the fact that the ground state $\phi_0(x)$ minimizes the Heisenberg's uncertainty relation it follows that

$$\underbrace{\left(\frac{X}{\Delta X} + i\frac{P}{\Delta P}\right)}_{=2a} |\phi_0\rangle = 0 \qquad \text{with } \Delta X = \left(\frac{\hbar}{2m\omega}\right)^{1/2}, \ \Delta P = \left(\frac{\hbar m\omega}{2}\right)^{1/2}$$

It turns out to be extremely useful to define the **ladder operators**

$$a := \left(\frac{m\omega}{2\hbar}\right)^{1/2} X + i\left(\frac{1}{2\hbar m\omega}\right)^{1/2} P, \quad a^+ = \left(\frac{m\omega}{2\hbar}\right)^{1/2} X - i\left(\frac{1}{2\hbar m\omega}\right)^{1/2} P$$

$$\Rightarrow X = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(a+a^+), \quad P = \left(\frac{\hbar m\omega}{2}\right)^{1/2} i(a^+-a)$$

The commutation relation of the a and a^+ reads: $\quad [X,P] = i\hbar = -[P,X], \ [a,a^+] = -\frac{i}{2\hbar}[X,P] + \frac{i}{2\hbar}[P,X]$

$$[a,a^+] = 1 \qquad \Rightarrow \qquad N = aa^+ - 1$$

We also have that the Hermitian operator $N = a^+a$, called **number operator** can be written as

$$N = \frac{m\omega}{2\hbar}X^2 + \frac{1}{2\hbar m\omega}P^2 + \frac{i}{2\hbar}[X,P] = \frac{1}{\hbar\omega}\overbrace{\left(\frac{1}{2m}P^2 + \frac{m\omega^2}{2}X^2\right)}^{=H} - \frac{1}{2} = \frac{1}{\hbar\omega}H - \frac{1}{2}$$

such that the Hamilton can be expressed as

$$H = \hbar\omega\left(a^+a + \tfrac{1}{2}\right) = \hbar\omega\left(N + \tfrac{1}{2}\right).$$

$$[AB,C] = A[B,C] + [A,C]B$$

In addition we have the following commutation relations

$$[N,a^+] = a^+, \quad [N,a] = -a$$

$$\hookrightarrow [H,a^+] = \hbar\omega a^+, \quad [H,a] = -\hbar\omega a$$

→ Algebraic construction of the energy eigenstates:

↳ We know that $a|\phi_0\rangle = 0$ with $|\phi_0\rangle$ being unique and, so we also have $N|\phi_0\rangle = 0$, i.e. $|\phi_0\rangle$ is eigenstate to N with eigenvalue 0.

$$\hookrightarrow Na^+|\phi_0\rangle = [N,a^+]|\phi_0\rangle + a^+\cancel{N|\phi_0\rangle} = a^+|\phi_0\rangle$$
$$Ha^+|\phi_0\rangle = [H,a^+]|\phi_0\rangle + a^+H|\phi_0\rangle = (E_0 + \hbar\omega)\,a^+|\phi_0\rangle$$
$$\langle a^+\phi_0|a^+\phi_0\rangle = \langle\phi_0|aa^+\phi_0\rangle = \langle\phi_0|(N+1)|\phi_0\rangle = \langle\phi_0|\phi_0\rangle = 1$$

$$[N,aa^+] = a[N,a^+] + [N,a]a^+ = aa^+ - aa^+ = 0$$

$$N\,aa^+|\phi_0\rangle = [N,aa^+]|\phi_0\rangle + aa^+\cancel{N|\phi_0\rangle} = (aa^+ - aa^+)|\phi_0\rangle = 0$$
$$\langle aa^+\phi_0|aa^+\phi_0\rangle = \langle\phi_0|a\overbrace{a^+a}^{N}a^+|\phi_0\rangle = \langle\phi_0|aa^+\phi_0\rangle = \langle\phi_0|(1+N)|\phi_0\rangle = \langle\phi_0|\phi_0\rangle = 1$$

So $|\phi_1\rangle := a^+|\phi_0\rangle$ is a normalized eigenstate of N to the eigenvalue 1 and energy eigenstate with the eigenvalue $\frac{3}{2}\hbar\omega$, and we have $a|\phi_1\rangle = |\phi_0\rangle$.

↳ $N a^+|\phi_1\rangle = [N,a^+]|\phi_1\rangle + a^+ N|\phi_1\rangle = 2\, a^+|\phi_1\rangle$
$H a^+|\phi_1\rangle = [H,a^+]|\phi_1\rangle + a^+ H|\phi_1\rangle = (E_1 + \hbar\omega)\, a^+|\phi_1\rangle$
$\langle a^+\phi_1 | a^+\phi_1\rangle = \langle \phi_1 | a a^+ \phi_1\rangle = \langle \phi_1|(N+1)|\phi_1\rangle = 2\langle\phi_1|\phi_1\rangle = 2$

$N a a^+|\phi_1\rangle = a a^+ N|\phi_1\rangle = a a^+|\phi_1\rangle = (1+N)|\phi_1\rangle = 2|\phi_1\rangle$
$\langle a a^+\phi_1 | a a^+\phi_1\rangle = \langle\phi_1| a N a^+|\phi_1\rangle = \langle\phi_1|(a a^+ + a a^+ N)\phi_1\rangle = 2\langle\phi_1|(1+N)|\phi_1\rangle = 4\langle\phi_1|\phi_1\rangle = 4$

So $|\phi_2\rangle := \frac{1}{\sqrt{2}} a^+|\phi_1\rangle = \frac{1}{\sqrt{2}}(a^+)^2|\phi_0\rangle$ is a normalized eigenstate of N to the eigenvalue 2 and energy eigenstate to the eigenvalue $\frac{5}{2}\hbar\omega$, and we have $a|\phi_2\rangle = \sqrt{2}|\phi_1\rangle$.

proof: exercises

↳ With this method we can (indeed!) construct a CONS of eigenstates of the number operator N and the Hamilton operator H:

$$a|\phi_0\rangle = 0 \quad , \quad \langle\phi_0|\phi_0\rangle = 1$$

$$|\phi_n\rangle = \frac{1}{\sqrt{n!}}(a^+)^n|\phi_0\rangle \quad ,$$

$$a^+|\phi_n\rangle = \sqrt{n+1}\,|\phi_{n+1}\rangle \quad , \quad a|\phi_n\rangle = \sqrt{n}\,|\phi_{n-1}\rangle \qquad (*)$$

$$\langle\phi_m|\phi_n\rangle = \delta_{mn} \quad , \quad \sum_{n=0}^{\infty} |\phi_n\rangle\langle\phi_n| = \mathbb{1}$$

$$N|\phi_n\rangle = n|\phi_n\rangle \qquad \leftarrow \text{"N: number operator"}$$

$$H|\phi_n\rangle = \hbar\omega(n+\tfrac{1}{2})|\phi_n\rangle \quad , \quad (n = 0,1,2,\dots)$$

Due to property (*) we call a^+ creation operator and a annihilation operator.
The state $|\phi_n\rangle$ is called the n-th excited state.

↳ We can obtain the configuration space energy eigenfunctions by applying the creation operator a^+

$$\phi_0(x) = (\sqrt{\pi}\,\tilde{x})^{-1/2} \exp\left\{-\tfrac{1}{2}\left(\tfrac{x}{\tilde{x}}\right)^2\right\} \qquad \tilde{x} \equiv \left(\frac{\hbar}{\omega m}\right)^{1/2} = \sqrt{2}\,\Delta x$$

$$\phi_n(x) = (n!\sqrt{\pi}\,\tilde{x})^{-1/2}(a^+)^n \exp\left\{-\tfrac{1}{2}\left(\tfrac{x}{\tilde{x}}\right)^2\right\}, \quad a^+ = \frac{1}{\sqrt{2}}\left(\frac{x}{\tilde{x}} - \tilde{x}\frac{d}{dx}\right), \quad a = \frac{1}{\sqrt{2}}\left(\frac{x}{\tilde{x}} + \tilde{x}\frac{d}{dx}\right)$$

$$= (2^n n!\sqrt{\pi}\,\tilde{x})^{-1/2} \exp\left\{-\tfrac{1}{2}\left(\tfrac{x}{\tilde{x}}\right)^2\right\} H_n\left(\tfrac{x}{\tilde{x}}\right)$$

"Hermite polynomials"

↳ Hermite polynomials:

$$H_n(x) = e^{x^2/2}(\sqrt{2}a^+)^n\big|_{x_0=1} e^{-x^2/2} = e^{x^2}\overbrace{e^{-x^2/2}\left(x - \frac{d}{dx}\right)^n e^{x^2/2}}^{(-1)^n \frac{d^n}{dx^n}} e^{-x^2} = (-1)^n e^{x^2}\frac{d^n}{dx^n} e^{-x^2}$$

$H_0(x) = 1$ $\qquad$ $H_3(x) = 8x^3 - 12x$

$H_1(x) = 2x$ $\qquad$ $H_4(x) = 16x^4 - 48x^2 + 12$

$H_2(x) = 4x^2 - 2$ $\qquad$ $H_5(x) = 32x^5 - 160x^3 + 120x$

Orthogonality: $\int_{-\infty}^{+\infty} dx\, e^{-x^2} H_n(x) H_m(x) = \sqrt{\pi}\, 2^n n!\, \delta_{nm}$

Generating function: $e^{-t^2+2tx} = \sum_{n=0}^{\infty} \frac{1}{n!} t^n H_n(x)$

Differential equation: $\left[\frac{d^2}{dx^2} - 2x\frac{d}{dx} + 2n\right] H_n(x) = 0$

→ **Multiparticle state interpretation:**

The energy eigenstates $|\varphi_n\rangle$ with $E_n = \hbar\omega(\frac{1}{2}+n)$ also provide the quantum mechanical description of states with n identical Bose particles each having energy $\hbar\omega$.

Example: Photons (light particles) with a fixed direction and a fixed frequency ω
↳ $|\varphi_0\rangle$: zero photon state, "vacuum" with vacuum energy $E_0 = \frac{1}{2}\hbar\omega$
$|\varphi_n\rangle$: n photon state with energy $E_n = E_0 + n\hbar\omega$
a : operator that annihilates one photon
a^+ : operator that creates one photon

→ **Coherent States:**

The energy eigenstates $|\varphi_n\rangle$ do not at all resemble at all a classical particle oscillating in the harmonic oscillator potential with $x(t) = x_0 \cos(\omega t - \delta)$ because we have at any time t $\langle\varphi_n|X|\varphi_n\rangle = 0$ and $\langle\varphi_n|P|\varphi_n\rangle = 0$ (recall: $X = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(a+a^+)$, $P = \left(\frac{\hbar m\omega}{2}\right)^{1/2} i(a^+-a)$)
We want to construct a solution of the time-dependent Schrödinger equation that describes an oscillating behavior.

↳ A solution with $\langle x\rangle = 0$ at $t=0$ may have the correct property, so we may look at a wave function that at $t=0$ satisfies the equation

$$\frac{1}{2}\left(\frac{X-x_0}{\Delta X} + i\frac{P-p_0}{\Delta P}\right)|\varphi_z\rangle = 0, \text{ where } \Delta X = \left(\frac{\hbar}{2m\omega}\right)^{1/2}, \Delta P = \left(\frac{\hbar m\omega}{2}\right)^{1/2} \text{ from the ground state } |\varphi_0\rangle$$
and $x_0, p_0 \in \mathbb{R}$ arbitrary

$$\Leftrightarrow \quad a|\varphi_z\rangle = \frac{1}{2}\left(\frac{x_0}{\Delta X} + i\frac{p_0}{\Delta P}\right)|\varphi_z\rangle = z|\varphi_z\rangle, \quad z \in \mathbb{C}$$

↳ The eigenvalue equation $a|\varphi_z\rangle = z|\varphi_z\rangle,\ z\in\mathbb{C}$, is an example of a coherent state:
* $|\varphi_z\rangle$ is obviously a superposition of states with different particle number
* destroying one photon from state $|\varphi_z\rangle$ gives $z\cdot|\varphi_z\rangle$. ⇒ $|\varphi_z\rangle$ is superposition of multiparticle states
* important for the quantum mechanical description of coherent light.

We define for convenience: $|n\rangle := |\varphi_n\rangle$, $n \in \mathbb{N}_0$ and $|z\rangle := |\varphi_z\rangle$.
We can make the ansatz $|z\rangle = f(a^+)|0\rangle$ and because of $[a, f(a^+)] = f'(a^+)$ we obtain

$$a|z\rangle = a\, f(a^+)|0\rangle = [a, f(a^+)]|0\rangle + \cancel{f(a^+)a|0\rangle} = f'(a^+)|0\rangle \overset{!}{=} z\, f(a^+)|0\rangle$$

$$\Rightarrow f'(a^+) = z f(a^+) \Rightarrow f(a^+) = c\, e^{z a^+} = c\left(1 + za^+ + \frac{1}{2}z^2(a^+)^2 + \frac{1}{3!}z^3(a^+)^3 + \dots\right), \quad c \in \mathbb{C}.$$

We see that $|z\rangle = c \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle = c \sum_{n=0}^{\infty} \frac{(z a^+)^n}{n!} |0\rangle$

Norm: $1 \stackrel{!}{=} \langle z | z \rangle = |c|^2 \sum_{n,m=0}^{\infty} \frac{(z^*)^m z^n}{\sqrt{m!}\sqrt{n!}} \overbrace{\langle m | n \rangle}^{\delta_{mn}} = |c|^2 \sum_{n=0}^{\infty} \frac{|z|^{2n}}{n!} = |c|^2 e^{|z|^2} \Rightarrow |c| = e^{-|z|^2/2}$

We set $c = |c|$.

↳ Time-dependent solution:

$$\varphi_z(x,t) = e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{(z e^{-i\omega t})^n}{\sqrt{n!}} \phi_n(x)\, e^{-i\omega t/2}$$

$$= \varphi_{z(t)}(x)\, e^{-i\omega t/2} \qquad \text{with} \quad z(t) = z e^{-i\omega t}$$

Location and momentum expectation value:

$$\langle x \rangle = \langle \varphi_{z(t)} | x\, \varphi_{z(t)} \rangle = \frac{\tilde{x}}{\sqrt{2}} \langle \varphi_{z(t)} | (a + a^+) \varphi_{z(t)} \rangle = \frac{\tilde{x}}{\sqrt{2}} (z(t) + z^*(t)), \quad \tilde{x} = \left(\frac{\hbar}{\omega m}\right)^{1/2}$$

$$= \sqrt{2}\, \tilde{x}\, |z| \cos(\omega t - \delta), \qquad z = |z| e^{i\delta}, \quad z(t) = |z| e^{-i(\omega t - \delta)} = |z| (\cos(\omega t - \delta) - i \sin(\omega t - \delta))$$

$$\langle P \rangle = \frac{-i\hbar}{\sqrt{2}\,\tilde{x}} \langle \varphi_{z(t)} | (a - a^+) \varphi_{z(t)} \rangle = \frac{-i\hbar}{\sqrt{2}\,\tilde{x}} (z(t) - z^*(t)) = \sqrt{2} \frac{\hbar}{\tilde{x}} |z| \sin(\omega t - \delta)$$

$$= \sqrt{2}\, m\, \tilde{x}\, |z|\, \omega \sin(\omega t - \delta) = m \frac{d}{dt} \langle x \rangle$$

→ Exactly corresponds to the motion of a classic particle in the harmonic oscillator potential with the amplitude $x_0 \equiv \sqrt{2}\, \tilde{x}\, |z|$.

↳ Explizit expression for wave function:

$$\varphi_z(x,t) = e^{-i\omega t/2} \sum_{n=0}^{\infty} \frac{(z(t) a^+)^n}{n!} e^{-|z|^2/2} \phi_0(x) = e^{-i\omega t/2} e^{z(t) a^+} \overbrace{e^{-|z|^2/2}}^{-\frac{1}{2}|z|^2 [a^+, -a] = -\frac{1}{2}[z(t) a^+, -z^*(t) a]} \phi_0(x)$$

gives 1 on ϕ_0

$$= e^{-i\omega t/2} e^{z(t) a^+} e^{-z^*(t) a} e^{-\frac{1}{2}[z(t) a^+, -z(t)^* a]} \phi_0(x)$$

use: $\overbrace{e^{A+B} = e^A e^B e^{-[A,B]/2}}^{\text{valid if } [[A,B],A] = [[A,B],B] = 0}$ (∗)

$$= e^{-i\omega t/2} e^{\underbrace{z(t) a^+ - z^*(t) a}} \phi_0(x)$$

$$\to -i \frac{\sqrt{2}|z| x}{\tilde{x}} \sin(\omega t - \delta) - \sqrt{2}|z| \tilde{x} \cos(\omega t - \delta) \frac{d}{dx}$$

$a^+ = \frac{1}{\sqrt{2}} \left(\frac{x}{\tilde{x}} - \tilde{x} \frac{d}{dx} \right), \quad a = \frac{1}{\sqrt{2}} \left(\frac{x}{\tilde{x}} + \tilde{x} \frac{d}{dx} \right)$

(∗) & $[x, \frac{d}{dx}] = -1$

$$= e^{-i\omega t/2} e^{-i \frac{\sqrt{2}|z| x}{\tilde{x}} \sin(\omega t - \delta)} e^{i|z|^2 \overbrace{\sin(\omega t - \delta) \cos(\omega t - \delta)}^{\frac{1}{2}\sin(2(\omega t - \delta))}} \overbrace{e^{-\sqrt{2}|z| \tilde{x} \cos(\omega t - \delta) \frac{d}{dx}}}^{T_{-\sqrt{2}|z|\tilde{x}\cos(\omega t - \delta)}} \phi_0(x)$$

$$= \frac{1}{\pi^{1/4} \tilde{x}^{1/2}} \underbrace{\exp\left\{ -i \left[\frac{\omega t}{2} - \frac{|z|^2}{2} \sin(2(\omega t - \delta)) + \frac{\sqrt{2}|z| x}{\tilde{x}} \sin(\omega t - \delta) \right] \right\}}_{\text{time-dependent pure phase}} \exp\left\{ -\frac{1}{2\tilde{x}^2} (x - x_0 \cos(\omega t - \delta))^2 \right\}$$

$$\Rightarrow |\varphi_z(x,t)|^2 = \frac{1}{\pi^{1/2} \tilde{x}} \exp\left\{ -\frac{1}{\tilde{x}^2} (x - x_0 \cos(\omega t - \delta))^2 \right\}, \quad x_0 = \sqrt{2}\, \tilde{x}\, |z|, \quad \tilde{x} = \left(\frac{\hbar}{\omega m}\right)^{1/2}$$

This is exactly a Gaussian wave packet oscillating with frequency ω, that does not broaden with time.

This does completely agree with our classic notion of a coherent light beam!

↳ Energy expectation value:

$$\langle H \rangle = \hbar\omega \langle a^+a + \tfrac{1}{2} \rangle = \frac{\hbar\omega}{2} + \hbar\omega \langle \varphi_{z(t)} | a^+a\, \varphi_{z(t)} \rangle = \frac{\hbar\omega}{2} + \hbar\omega \langle a\, \varphi_{z(t)} | a\, \varphi_{z(t)} \rangle$$

$$= \frac{\hbar\omega}{2} + \hbar\omega\, |z(t)|^2 = \hbar\omega \left(|z|^2 + \tfrac{1}{2} \right) = \hbar\omega \left(\frac{x_0^2}{2\tilde{x}^2} + \frac{1}{2} \right)$$

$$= \frac{m\omega^2}{2} x_0^2 + \frac{\hbar\omega}{2} \qquad x_0 : \text{"classic" amplitude}$$

We see that the classic limit is obtained for $|z| \gg 1$.

This is consistent with the following observation:

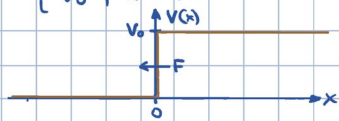
We have $\langle \varphi_z | \varphi_z \rangle = e^{-|z|^2} \sum_{n=0}^{\infty} \frac{|z|^{2n}}{n!} \underbrace{\langle \phi_n | \phi_n \rangle}^{=1}$.

The function $f_z(n) = \frac{|z|^{2n}}{n!}$ has its maximum at $n \approx |z|$, so the states $|\phi_n\rangle$ with $n \approx |z|$ dominate the coherent state for $|z| \gg 1$.

3.3. Potential With a Step

→ Consider a particle that experiences a very **localized force** at $x=0$ of the form $F(x) = -V_0\,\delta(x)$.

So the particle moves in a potential of the form $V(x) = V_0\,\theta(x) = \begin{cases} 0 & , x \le 0 \\ V_0 & , x > 0 \end{cases}$
and the force acts to the left.



Hamilton operator : $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\,\theta(x)$

We have to find all solutions of the eigenvalue problem $H\phi(x) = E\phi(x)$.
We have $\langle H \rangle \ge 0$ for any state, so $E \ge 0$ as well.

→ <u>Region $x<0$:</u> We have to solve the free particle Schrödinger equation $-\frac{\hbar^2}{2m}\phi''(x) = E\,\phi(x)$

The solution has the form : $Ae^{ikx} + Be^{-ikx}$, $p = \hbar k$, $E = \frac{\hbar^2 k^2}{2m} \ge 0$, $k \in \mathbb{R}$

Note that $Pe^{\pm ikx} = \pm p\,e^{\pm ikx}$, so $e^{\pm ikx}$ describe a right/left moving particle.

<u>Region $x>0$:</u> We solve the eigenvalue equation $-\frac{\hbar^2}{2m}\phi''(x) = (E-V_0)\,\phi(x)$

$(E-V_0)$ can be positive or negative, so we must consider 2 cases.

<u>Case $0 \le E \le V_0$:</u> Solution has the form : $Ce^{-\kappa x}$, $\kappa > 0$

with $\frac{\hbar^2\kappa^2}{2m} = \underbrace{V_0 - E}_{\ge 0} = V_0 - \frac{\hbar^2 k^2}{2m} \Rightarrow \kappa = \sqrt{\frac{2mV_0}{\hbar^2} - k^2}$, $k \le \frac{\sqrt{2mV_0}}{\hbar}$

Note that the solution $e^{+\kappa x}$ is not allowed since it diverges for large x.

<u>Case $E > V_0$:</u> Solution has the form: $Ce^{ik'x} + De^{-ik'x}$

with $\frac{\hbar^2 k'^2}{2m} = \underbrace{E - V_0}_{>0} = \frac{\hbar^2k^2}{2m} - V_0 \Rightarrow k' = \sqrt{k^2 - \frac{2mV_0}{\hbar^2}}$, $|k| \ge \frac{\sqrt{2mV_0}}{\hbar}$

<u>Continuity at $x=0$:</u> $\phi(x)$ and $\phi'(x)$ must be continuous at $x=0$, because otherwise $\phi''(x)$ would contain terms $\sim \delta(x)$ or $\sim \delta'(x)$, which however do not appear in the Schrödinger equation.

→ <u>Construction of a complete set of energy eigenfunctions</u>

We want to identify the eigenfunctions $\phi_k(x)$ with : $H\phi_k(x) = \overbrace{\frac{\hbar^2k^2}{2m}}^{E(k)}\phi_k(x)$

<u>(1) Right-moving incoming particle with $E(k) < V_0$:</u>

$$\phi_k(x) = \begin{cases} e^{ikx} + Re^{-ikx} & , x \le 0 \\ Ce^{-\kappa x} & , x > 0 \end{cases} \qquad \text{with } 0 < k < \frac{\sqrt{2mV_0}}{\hbar}, \quad \kappa = \sqrt{\frac{2mV_0}{\hbar^2} - k^2} > 0$$

Continuity of $\phi_k(x)$ at $x=0$: $1+R=C$

Continuity of $\phi_k'(x) = \begin{cases} ik\left(e^{ikx} - Re^{-ikx}\right), & x\le 0 \\ -\kappa C e^{-\kappa x}, & x>0\end{cases}$ at $x=0$ gives $ik(1-R) = -\kappa C$

$\Rightarrow C = \frac{2k}{k+i\kappa}$ $\quad R = \frac{k-i\kappa}{k+i\kappa}$ $\quad$ with $|C| = \frac{2k}{\sqrt{k^2+\kappa^2}}$ $\quad |R| = 1$

↳ $C = \frac{2k}{\sqrt{k^2+\kappa^2}}\, e^{i\delta_C} = \sqrt{\frac{2}{mV_0}}\,\hbar k\, e^{i\delta_C}$, $\delta_C = -\arctan\left(\frac{\kappa}{k}\right)$ $\quad \left(-\frac{\pi}{2} \le \delta_C \le 0\right)$

$R = e^{i\delta_R}$, $\delta_R = -2\arctan\left(\frac{\kappa}{k}\right)$ $\quad (-\pi \le \delta_R \le 0)$

↳ **Physical interpretation:** $\qquad \overleftrightarrow{\partial}_x = \overrightarrow{\partial}_x - \overleftarrow{\partial}_x$

with sharp momentum $p=\hbar k$

* $e^{ikx}\,\theta(-x)$: incoming wave coming from left with probability current $j_{in} = \frac{\hbar}{2im} e^{-ikx}\overleftrightarrow{\partial}_x e^{ikx} = \frac{\hbar k}{m}$
* $Re^{-ikx}\,\theta(x)$: **totally reflected wave** going left with probability current $j_{refl} = \frac{\hbar |R|^2}{2im} e^{ikx}\overleftrightarrow{\partial}_x e^{-ikx} = -\frac{\hbar k}{m}|R|^2$
* $Ce^{-\kappa x}\,\theta(x)$: wave function **penetrating** into the classically forbidden zone $x>0$ with probability current $j_{pene} = \frac{\hbar |C|^2}{2im} e^{-\kappa x}\overleftrightarrow{\partial}_x e^{-\kappa x} = 0$

Quantum effect! Does not exist classically.

Note: The reflected wave (as well as the penetrating wave) obtains an additional **phase shift** $e^{i\delta_R}$ ($e^{i\delta_C}$) which can be physically observed by a time delay of the reflected particle.

Important: This physical interpretation is further supported by the fact that the interference between incoming and reflected waves vanishes:

$$j_{x<0} = \frac{\hbar}{2im}\left[\left(e^{-ikx} + R^* e^{ikx}\right)(ik)\left(e^{ikx} - Re^{-ikx}\right) - \left(e^{-ikx} - R^* e^{ikx}\right)(-ik)\left(e^{ikx} + Re^{-ikx}\right)\right]$$

$$= \frac{\hbar}{2im}\left[ik\left(1 - |R|^2 - \cancel{Re^{-2ikx}} + \cancel{R^* e^{2ikx}}\right) + ik\left(1 - |R|^2 - \cancel{R^* e^{2ikx}} + \cancel{Re^{-2ikx}}\right)\right]$$

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

← The net current $j_{x<0} = 0$, due to $|R| = 1$.

↳ **Limit of infinitely high potential wall** $(V_0 \to \infty)$: $\kappa \to \infty$, $C \to 0$, $R \to -1 = e^{-i\pi}$

phase shift of reflected wave! (also for $V_0 < \infty$)

(2) Right-moving incoming particle with $E(k) > V_0$:

$\phi_k(x) = \begin{cases} e^{ikx} + Re^{-ikx}, & x \le 0 \\ Te^{ik'x}, & x > 0\end{cases}$ $\quad$ with $k > \frac{\sqrt{2mV_0}}{\hbar}$

$k' = \sqrt{k^2 - \frac{2mV_0}{\hbar^2}} < k$

Continuity of $\phi_k(x)$ and $\phi_k'(x)$ at $x=0$ gives: $1+R = T$ and $ik(1-R) = ik'T$

$\Rightarrow T = \frac{2k}{k+k'}$, $R = \frac{k-k'}{k+k'}$ $\quad$ with $\underset{k\to\infty}{1} < T < \underset{k\to\frac{2mV_0}{\hbar^2}}{2}$ and $\underset{k\to\infty}{0} < R < \underset{k\to\frac{2mV_0}{\hbar^2}}{1}$

Physical interpretation:

with sharp momentum $p = \hbar k$

* $e^{ikx}\theta(-x)$: **incoming wave** coming from left as in (1) with $j_{in} = \frac{\hbar k}{m}$
* $Re^{-ikx}\theta(-x)$: **partially reflected wave** going left with $j_{refl} = -|R|^2 \frac{\hbar k}{2m}$ ← Quantum effect! Does not exist classically.
* $Te^{ik'x}\theta(x)$: **transmitted wave** going right with $j_{trans} = |T|^2 \frac{\hbar k'}{2m}$

with sharp momentum $p' = \hbar k'$

↳ Probability that incoming particle is reflected: $\left|\frac{j_{refl}}{j_{in}}\right| = |R|^2$
Probability that incoming particle is transmitted: $\left|\frac{j_{trans}}{j_{in}}\right| = |T|^2 \frac{k'}{k}$

We indeed have $|R|^2 + |T|^2 \frac{k'}{k} = 1$:
PROBABILITY CONSERVATION
PARTICLE NUMBER CONSERVATION

↳ **Limit of infinite energy ($E \gg V_0$): $k' \to k$, $R \to 0$, $T \to 1$**

<u>(3) Left-moving incoming particle with $E(k) > V_0$:</u> → only $k > \frac{\sqrt{2mV_0}}{\hbar}$ is possible

$$\phi_k(x) = \begin{cases} T' e^{-ikx} & , x \le 0 \\ e^{-ik'x} + R' e^{ik'x} & , x > 0 \end{cases} \quad \text{with } k > \frac{\sqrt{2mV_0}}{\hbar}, \quad k' = \sqrt{k^2 - \frac{2mV_0}{\hbar^2}} < k$$

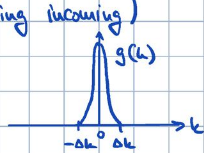
Continuity of $\phi_k(x)$ and $\phi_k'(x)$ at $x = 0$ gives: $1 + R' = T'$ and $ik'(-1+R') = -ikT$

$$\Rightarrow T' = \frac{2k}{k+k'}, \quad R' = \frac{k-k'}{k+k'}$$

Exactly the same result for the reflected and the transmitted wave amplitudes as for case (2)!

→ **Construction of scattered wave packets:**
* starts a $x = x_0$ at $t = 0$
* has group velocity $v_0 = \frac{p_0}{m}$ (right-moving incoming)

↳ We take a superposition of ϕ_k states with a strongly peaked wave number function real-valued $g(k)$ shifted to $k_0 = p_0/\hbar = mv_0/\hbar$ and an additional phase such that the wave packet is located at x_0 at $t = 0$ ($x_0 < 0$).



$$\psi(x,t) = \int_{-\infty}^{+\infty} dk\, g(k-k_0)\, e^{-ikx_0}\, e^{-i\omega(k)t}\, \phi_k(x), \quad \omega(k) = \frac{E(k)}{\hbar} = \frac{\hbar k^2}{2m}$$

phase shifting packet at x_0 at $t=0$

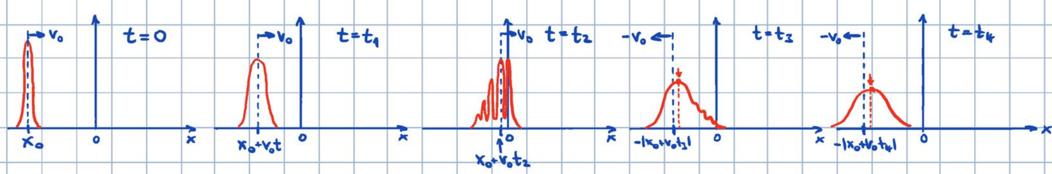
<u>Case $E(k) < V_0$:</u> We have to take $\phi_k(x)$ from case (1)

$$\phi_k(x) = \begin{cases} e^{ikx} + Re^{-ikx} & , x \le 0 \\ Ce^{-\kappa x} & , x > 0 \end{cases} \quad \text{with } 0 < k < \frac{\sqrt{2mV_0}}{\hbar}, \quad \kappa = \sqrt{\frac{2mV_0}{\hbar^2} - k^2} > 0$$

velocity
↓
$v_0 = \frac{p_0}{m} = \frac{\hbar k_0}{m}$

$$C = \frac{2k}{\sqrt{k^2+\kappa^2}} e^{i\delta_c}, \quad \delta_c = -\arctan\left(\frac{\kappa}{k}\right) \qquad \left(-\frac{\pi}{2} \le \delta_c \le 0\right)$$

$$R = e^{i\delta_R}, \quad \delta_R = -2\arctan\left(\frac{\kappa}{k}\right) \qquad (-\pi \le \delta_R \le 0)$$



$t=0$: Wave packet located at x_0, moves right with $v_0 = \frac{p_0}{m}$

$t=t_1$: Wave packet broadens, located at $x_0+v_0t_1$

$t=t_2$: Packet hits potential barrier, penetration into zone $x>0$, continued broadening. Packet pauses a bit at barrier due to k-dependence of complex phases δ_R and δ_c.

$t=t_3$: Reflected wave moves left with $v_0 = \frac{p_0}{m}$, further broadening. Wave is a bit behind the classic reflected particle due to k-dependence of complex phase δ_R. → "phase shift"

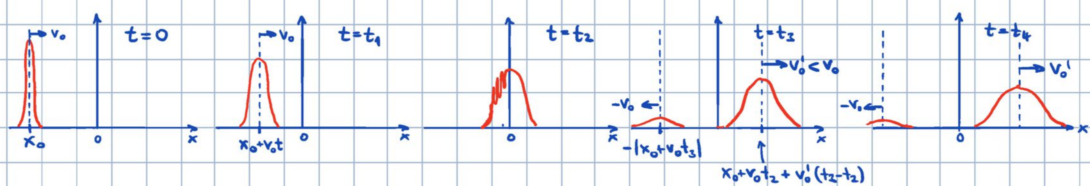
$t=t_4$: Further broadening, phase shift remains constant

<u>Case $E(k) > V_0$</u> : We have to take $\phi_k(x)$ from case (2)

$$\phi_k(x) = \begin{cases} e^{ikx} + R\,e^{-ikx} & , \; x \le 0 \\ T e^{ik'x} & , \; x > 0 \end{cases} \qquad \text{with } k > \frac{\sqrt{2mV_0}}{\hbar}, \quad v_0 = \frac{p_0}{m} = \frac{\hbar k_0}{m}, \quad v_0' = \frac{\hbar k_0'}{m} < v_0$$

$$k' = \sqrt{k^2 - \frac{2mV_0}{\hbar^2}} < k$$

$$T = \frac{2k}{k+k'}, \quad R = \frac{k-k'}{k+k'} \qquad \text{with } 1 < T < 2 \text{ and } 0 < R < 1, \quad T, R \in \mathbb{R}!$$



$t=0$: Wave packet located at x_0, moves right with $v_0 = \frac{p_0}{m}$

$t=t_1$: Wave packet broadens, located at $x_0+v_0t_1$

$t=t_2$: Packet hits potential barrier, continued broadening, transmitted and reflected wave packets separate.

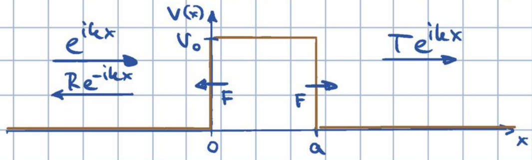
$t=t_3$: Reflected wave moves left with $-v_0 = \frac{-p_0}{m}$, further broadening. ← bounced back without delay
Transmitted wave moves right with $v_0' = \frac{\hbar k_0'}{m} < v_0$, further broadening ← follows classic motion

$t=t_4$: Further broadening.

3.4. Potential Wall

→ Consider a particle experiencing a force related to a **potential wall** of the form

$$V(x) = V_0\,\Theta(x)\,\Theta(a-x) = \begin{cases} 0, & x<0 \text{ or } x>a \\ V_0, & 0\le x\le a \end{cases}, \quad V_0>0$$



From our considerations for the potential step we expect that an incoming particle with $E<V_0$ (coming from the left) can penetrate into the classically forbidden zone $0\le x\le a$ and with some finite probability emerge for $x>a$.

→ We only consider energy eigenfunctions representing incoming particles from the left

(1) <u>Right-moving incoming particle with $E(k)<V_0$:</u>

$$\phi_k(x) = \begin{cases} e^{ikx} + R e^{-ikx}, & x\le 0 \\ A e^{\kappa x} + B e^{-\kappa x}, & 0\le x\le a \\ T e^{ikx}, & x>a \end{cases} \quad \text{with} \quad 0<k<\frac{\sqrt{2mV_0}}{\hbar}, \quad \kappa = \sqrt{\frac{2mV_0}{\hbar^2}-k^2} > 0$$

We have:
* partial reflection towards $x<0$, phase shift
* penetration into classically forbidden zone $0\le x\le a$
* classically forbidden transmission into $x>a$

} 'tunnel effect' → quantum effect that does not exist classically

(2) <u>Right-moving incoming particle with $E(k)>V_0$:</u>

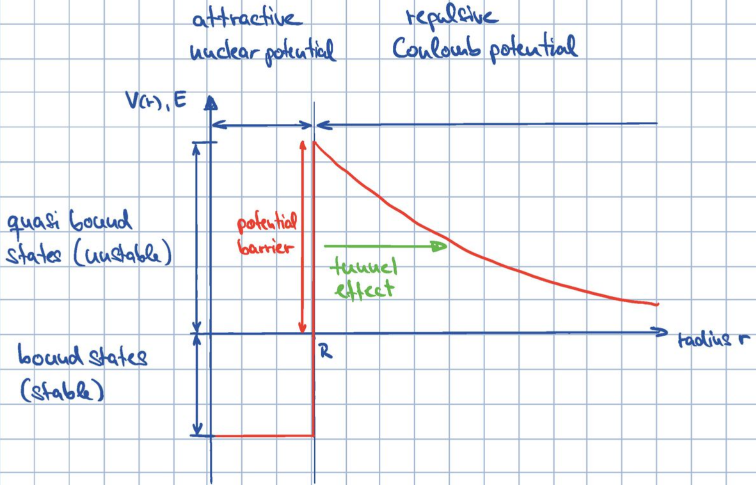
$$\phi_k(x) = \begin{cases} e^{ikx} + R e^{-ikx}, & x\le 0 \\ A e^{ik'x} + B e^{-ik'x}, & 0\le x\le a \\ T e^{ikx}, & x>a \end{cases} \quad \text{with} \quad k>\frac{\sqrt{2mV_0}}{\hbar}, \quad k' = \sqrt{k^2-\frac{2mV_0}{\hbar^2}} < k$$

We have:
* partial reflection towards $x<0$ ← quantum effect
* transmission into $x>0$, like classic particle

→ Nature's application of the tunnel effect: **α-Decay** → α-particle = ^{4}He nucleus = 

↳ Heavy nuclei are unstable and can decay by the emission of α-particles

Mechanism: Inside the nucleus ($R\le 10^{-15}\text{m}\,A^{1/3}$) the nuclear force provides an attractive potential for the α-particle generated by the other protons and neutrons.
Outside the nucleus $r>R$ the nuclear force is screened and the Coulomb-force provides a repulsive potential $V(r)\sim\frac{2(Z-2)e^2}{r}$ for the α-particle.



$^{238}_{92}U \longrightarrow {}^{234}_{90}Th + \alpha$, $E_\alpha^{inside} \simeq 4.2$ MeV , $E^{barrier} \simeq 28$ MeV , $\tau_{1/2} \simeq 4.5 \cdot 10^9$ a

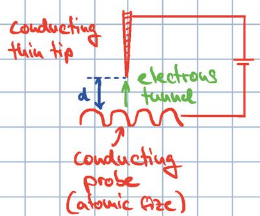
$^{232}_{90}Th$ (Thorium) $E_\alpha \simeq 4.0$ MeV $\tau_{1/2} \simeq 1.4 \cdot 10^{10}$ a

$^{226}_{88}Ra$ (Radium) $E_\alpha = 4.8$ MeV $\tau_{1/2} \simeq 1600$ a

$^{212}_{84}Po$ (Polonium) $E_\alpha \simeq 8.8$ MeV $\tau_{1/2} \simeq 3 \cdot 10^{-7}$ s

→ Physical application of the tunnel effect: Scanning Tunneling Microscopy ("Rastertunnelmikroskopie")

↳ Nobel prize 1986 for Gerd Binnig and Heinrich Rohrer



Tunnel current depends exponentially on distance d. One can picture the form of the conducting surface by scanning the surface (by moving the tip).