1 Free particles

Consider a free spinless particle in one dimension

$$H = \frac{P^2}{2m} \tag{1}$$

- H is compatible with P $\Rightarrow$ common eigenkets of P and H

$$H|p\rangle = \frac{P^2}{2m}|p\rangle = \frac{p^2}{2m}|p\rangle \tag{2}$$

- The spectrum of H is doubly degenerate for all $E \neq 0$
- An energy eigenket is a superposition

$$|E\rangle = c_+ \, |p = \sqrt{2mE}\,\rangle \, + \, c_- \, |p = -\sqrt{2mE}\,\rangle \tag{3}$$

(i) It represents a single particle of energy E that can be caught moving either to the right or to the left with momentum $\sqrt{2mE}$.

(ii) The wave function

$$\psi_E(x) = c_+ \, \langle x|p = \sqrt{2mE}\,\rangle \, + \, c_- \, \langle x|p = -\sqrt{2mE}\,\rangle = C_+ e^{\mathrm{i}\,k\,x} + C_- e^{-\mathrm{i}\,k\,x} \tag{4}$$

$$k \equiv \frac{\sqrt{2mE}}{\hbar}\,, \quad C_\pm \equiv \frac{c_\pm}{\sqrt{2\pi\hbar}} \tag{5}$$

(iii) It is a superposition of plane waves with wavelength $\lambda = 2\pi/k = 2\pi\hbar/\sqrt{2mE}$ called the particle's de Broglie wavelength.

- The evolution operator

$$U(t) = e^{-\mathrm{i}\,\frac{P^2}{2m\hbar}\,t} \tag{6}$$

- In the Schrödinger picture the wave function evolves as

$$\psi_E(x,t) = C_+ e^{\mathrm{i}\,k\,(x - v\,t)} + C_- e^{-\mathrm{i}\,k\,(x + v\,t)}\,, \qquad v \equiv \frac{\hbar\,k}{2m} = \frac{\sqrt{2mE}}{2m} = \frac{|p|}{2m} \tag{7}$$

  (i) The plane waves move to the right and to the left with speed v.

  (ii) The speed of these waves is half the speed of a classical particle of the same mass and momenta.

  (iii) This is not a paradox because $|p\rangle$ do not represent physically realisable states.

- A normalisable state $|\psi\rangle$ at $t = 0$

$$|\psi\rangle = \int dp\,|p\rangle\psi(p)\,, \qquad \int dp\,\psi^*(p)\psi(p) = 1 \tag{8}$$

  (i) evolves as

$$|\psi(t)\rangle = \int dp\,|p\rangle e^{-\frac{\mathrm{i}}{\hbar}\frac{p^2}{2m}\,t}\psi(p) \tag{9}$$

  (ii) leads to a normalisable wave function at any t

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int dp\,e^{\frac{\mathrm{i}}{\hbar}\,(p\,x - \frac{p^2}{2m}\,t)}\,\psi(p) \tag{10}$$

  called a **wave packet**.

  (iii) In the Heisenberg picture it is obvious that

    (a) the expectation value of P and its dispersion are independent of time

    (b) $\langle X\rangle$ is linear in time and the dispersion of X increases quadratically in time.

- A wave packet of a state with small uncertainty in momentum is narrowly peaked about k
- The Gaussian wave packet

$$\psi(p) = \sqrt{\frac{\Delta}{\sqrt{\pi}\hbar}}\, e^{-\frac{\Delta^2}{2\hbar^2}(k-p)^2} \tag{11}$$

(i) If Δ is large, it is peaked at $p = k$

(ii) In the limit $\Delta \to \infty$ it becomes Dirac's delta function $\delta(p-k)$.

- Its wave function

$$\psi(x,t) = \sqrt{\frac{\Delta}{\tilde{\Delta}^2\sqrt{\pi}}}\, e^{\mathrm{i}\,\frac{k^2 t}{2m\hbar} + \frac{\mathrm{i}}{\hbar}\, k\,(x - \frac{k}{m}\,t) - \frac{1}{2\tilde{\Delta}^2}\,(x - \frac{k}{m}\,t)^2}\,, \qquad \tilde{\Delta}^2 = \Delta^2 + \frac{\mathrm{i}\,\hbar}{m}\,t \tag{12}$$

(a) The packet's velocity is p/m as expected.

(b) It is approximately true for any momentum localised wave packet.

(c) The expectation values of P and X, and their uncertainties

$$\langle P\rangle = k\,, \quad \Delta P = \sqrt{\langle P^2\rangle - \langle P\rangle^2} = \frac{\hbar}{\sqrt{2}\,\Delta} \tag{13}$$

$$\langle X\rangle = \frac{k}{m}\,t\,, \quad \Delta X = \sqrt{\langle X^2\rangle - \langle X\rangle^2} = \frac{\Delta}{\sqrt{2}}\sqrt{1 + \frac{\hbar^2}{\Delta^4\, m^2}t^2} \tag{14}$$

(d) If $\Delta \sim \sqrt{\hbar}$, both uncertainties are very small at $t = 0$.

(e) If the mass is large enough then they remain small for very long period of time, and the motion is classical with good approximation.

- Particle freely moving in three dimensions

$$H = \frac{\vec{P}^{\,2}}{2m} = \frac{P_x^2}{2m} + \frac{P_y^2}{2m} + \frac{P_z^2}{2m} \tag{15}$$

(i) All momenta are compatible with each other and H

$$|\vec{p}\rangle \equiv |p_x, p_y, p_z\rangle\,, \quad \vec{P}\,|\vec{p}\rangle = \vec{p}\,|\vec{p}\rangle \tag{16}$$

(ii) The spectrum of H is infinitely degenerate

$$H|\vec{p}\rangle = \frac{\vec{P}^{\,2}}{2m}|\vec{p}\rangle = \frac{\vec{p}^{\,2}}{2m}|\vec{p}\rangle \quad \Rightarrow \quad E = \frac{\vec{p}^{\,2}}{2m} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} \tag{17}$$

because $|\vec{p}\rangle$ and $|A\,\vec{p}\rangle$, where $A^T A = I$, have the same energy.

(a) The eigenkets with the same E are in correspondence with points of the sphere $\vec{p}^{\,2} = 2mE$

(b) An energy eigenket is a superposition

$$|E\rangle = \int d^3\vec{p}\;|\vec{p}\rangle\; c(\vec{p})\delta(\vec{p}^{\,2} - 2mE) \tag{18}$$

(c) The energy spectrum is degenerate because H commutes with $\vec{P}$, $\vec{L} = \vec{x} \times \vec{p}$ and $\mathcal{P}$.

(iii) A wave packet

$$\psi(\vec{x},t) = \left(\frac{1}{\sqrt{2\pi\hbar}}\right)^3 \int d^3\vec{p}\, e^{\frac{\mathrm{i}}{\hbar}(\vec{p}\cdot\vec{x} - \frac{\vec{p}^2}{2m}t)}\, \psi(\vec{p})\,, \quad \int d^3\vec{p}\, \psi^*(\vec{p})\psi(\vec{p}) = 1 \tag{19}$$

(a) $\psi(\vec{p}) = \psi(p_x, p_y, p_z)$ is an arbitrary normalised function.

(b) The Gaussian wave packet peaked at $\vec{p} = \vec{k}$ is a product of one-dimensional Gaussian wave packets peaked at $p_i = k_i$.

(c) One can consider wave packets localised in different momentum and coordinate directions, e.g. a packet peaked at $p_x = k_x$ and at $y = 0$, $z = 0$.

- System of N free spinless particles

$$H = \sum_{a=1}^{N} H_a\,, \quad H_a = \frac{\vec{P}_a^{\;2}}{2m_a} \tag{20}$$

(i) Mutual eigenvectors of all the momenta are also eigenvectors of H

$$\vec{P}_a\, |\vec{p}_1, \vec{p}_2, \ldots, \vec{p}_N\rangle = \vec{p}_a\, |\vec{p}_1, \vec{p}_2, \ldots, \vec{p}_N\rangle\,, \quad a = 1, 2, \ldots, N \tag{21}$$

(ii) The spectrum of H is infinitely degenerate

(iii) The eigenkets with the same energy are in one-to-one correspondence with the points of the manifold $\sum_a \vec{p}_a^{\;2}/2m_a = E$ of dimension $3N-1$.

2 Harmonic oscillator

2.1 Stationary states

The Hamiltonian of a harmonic oscillator

$$H = \frac{P^2}{2m} + \frac{m\omega^2 X^2}{2} \tag{22}$$

- Dimensionless creation and annihilation operators

$$X = \eta(a^\dagger + a)\,,\ P = \frac{\mathrm{i}\hbar}{2\eta}(a^\dagger - a)\,, \quad a = \frac{1}{2\eta}X + \mathrm{i}\,\frac{\eta}{\hbar}\,P\,,\ a^\dagger = \frac{1}{2\eta}X - \mathrm{i}\,\frac{\eta}{\hbar}\,P\,, \quad \eta = \sqrt{\frac{\hbar}{2m\omega}} \tag{23}$$

  satisfy

$$[\,a\,,\,a^\dagger\,] = 1 \tag{24}$$

- H in terms of a and $a^\dagger$

$$H = \hbar\,\omega\,(a^\dagger a + \frac{1}{2}) = \hbar\,\omega\,(N + \frac{1}{2})\,, \quad N = a^\dagger a \tag{25}$$

- The basis vectors of the Fock space

$$|n\rangle = \frac{1}{\sqrt{n!}}\,(a^\dagger)^n|0\rangle\,, \quad a|0\rangle = 0\,, \quad N\,|n\rangle = |n\rangle \tag{26}$$

- A vector $|n\rangle$ is said to be a state with n quanta.

- The creation and annihilation operators act on $|n\rangle$ as follows

$$a|n\rangle = \sqrt{n}\,|n-1\rangle\,, \quad a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{27}$$

  and they are also called **ladder** operators.

- The expectation value of $(a^\dagger)^k a^l$ in any state $|n\rangle$ does not vanish only if $k = l$.

- The spectrum of the Hamiltonian

$$H|n\rangle = E_n|n\rangle\,, \quad E_n = \hbar\,\omega\,(n + \frac{1}{2}) \tag{28}$$

  (i) The vacuum state has the lowest energy $E_0 = \hbar\omega/2$, and therefore it is the **ground state**.

  (ii) All the other states with higher energy are called **excited** states.

- H is parity invariant and $\mathcal{P} = \exp(\mathrm{i}\,\pi\,N)$ anti-commutes with a and $a^\dagger$

  (i) The eigenstates with even number of quanta are even parity and those with odd number of quanta are odd parity states.

  (ii) Since X and P anti-commute with $\mathcal{P}$ their expectation values in definite parity states vanish.

- Uncertainties of X and P in the n-th excited state

$$\begin{aligned} \langle n|X^2|n\rangle &= \eta^2\langle n|(a^\dagger+a)^2|n\rangle = \eta^2\langle n|a^\dagger a + aa^\dagger|n\rangle = \eta^2(2n+1) = \eta^2\frac{2E_n}{\hbar\omega} = \frac{E_n}{m\omega^2} \\ \langle n|P^2|n\rangle &= -\frac{\hbar^2}{4\eta^2}\langle n|(a^\dagger-a)^2|n\rangle = \frac{\hbar^2}{4\eta^2}\frac{\hbar^2}{4\eta^2}(2n+1) = \frac{\hbar^2}{4\eta^2}\frac{2E_n}{\hbar\omega} = mE_n \end{aligned} \tag{29}$$

  (i) In CM if we average x^2 and p^2 over the period of oscillations then we get the same formulae.

  (ii) The uncertainties of X and P in the ground state $|0\rangle$

$$\Delta X = \eta\,, \quad \Delta P = \frac{\hbar}{2\eta}\,, \quad \Delta X\,\Delta P = \hbar/2 \tag{30}$$

  (iii) The ground state saturates the Heisenberg uncertainty relation

- The ground state wave function is the Gaussian wave packet with $a=0$ and $p=0$

$$\psi_0(x) = \langle x|0\rangle = \frac{1}{\sqrt{\sqrt{2\pi}\eta}}\exp\Big(-\frac{x^2}{4\eta^2}\Big) \tag{31}$$

  (i) In its ground state the particle is as stationary and as close to the origin as the uncertainty principle permits

  (ii) It cannot stop moving and be at a well defined position.

  (iii) Every system that has a confining potential exhibits an analogous **zero-point motion**.

  (iv) The energy tied up in this motion is called **zero-point energy**.

  (v) Zero-point motion is an important prediction of QM

- Since $|0\rangle$ is destroyed by the annihilation operator the wave function satisfies the equation

$$a\,\psi_0(x) = (\frac{1}{2\eta}X + \mathrm{i}\,\frac{\eta}{\hbar}\,P)\,\psi_0(x) = \frac{1}{2\eta}(x + 2\eta^2\frac{d}{dx})\,\psi_0(x) = 0 \tag{32}$$

and $\psi_0(x)$ is a normalised solution of this equation.

- Compute the wave functions of excited states

$$\psi_1(x) = \langle x|1\rangle = \frac{1}{2\eta}(x - 2\eta^2\frac{d}{dx})\,\psi_0(x) = \frac{x}{\eta}\psi_0(x) \tag{33}$$

It is odd because $|1\rangle$ is an odd parity state.

- The wave function for the n-th excited state

$$\psi_n(x) = \langle x|n\rangle = \frac{1}{\sqrt{n!}}\Big(\frac{1}{2\eta}(x - 2\eta^2\frac{d}{dx})\Big)^n\,\psi_0(x) = \frac{1}{\sqrt{2^n\,n!}}H_n(\frac{x}{\sqrt{2}\eta})\,\psi_0(x) \tag{34}$$

(i) $H_n(z)$ is the n-th **Hermite polynomial**.

(ii) The **Rodrigues formula**

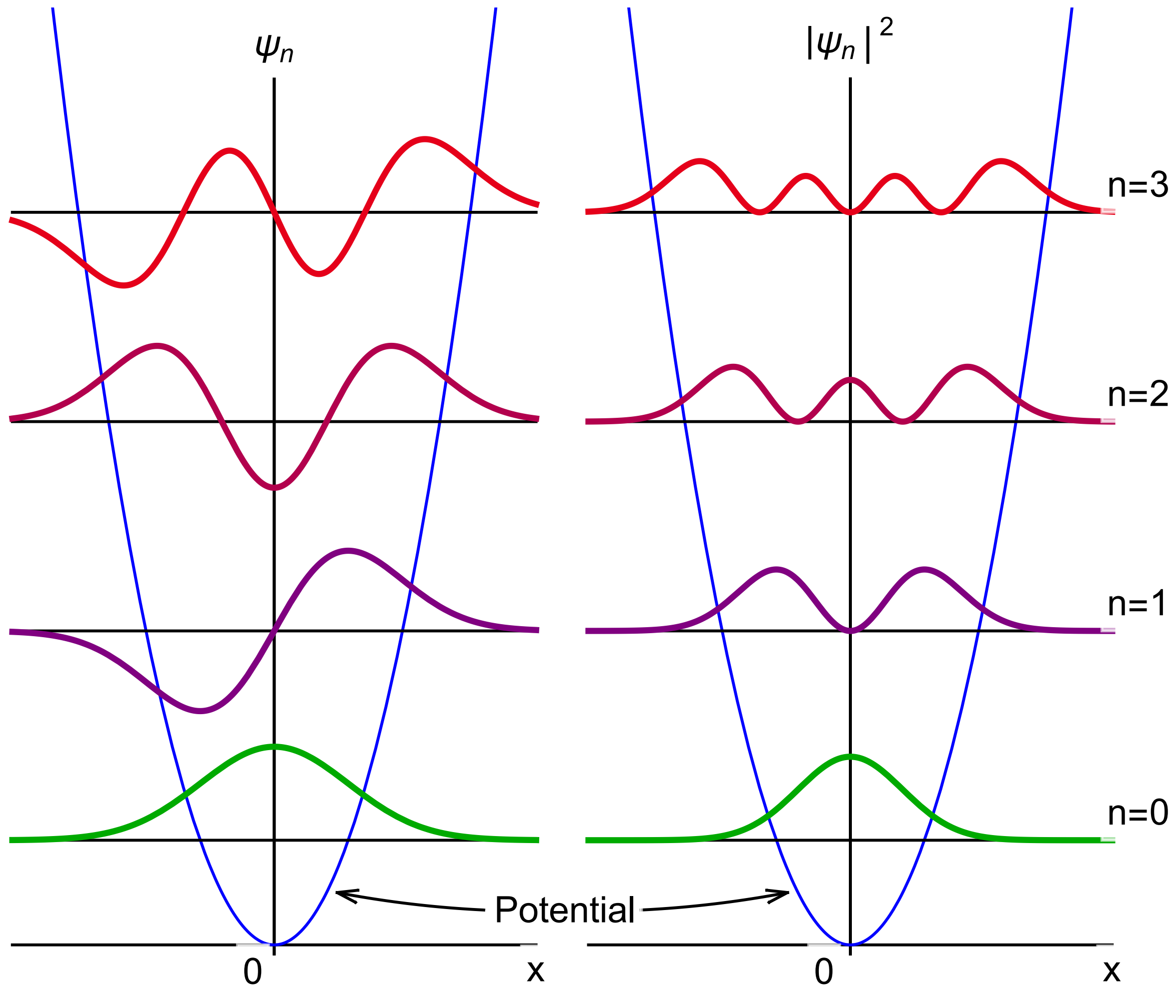
$$H_n(z) = (-1)^n e^{z^2}\left(\frac{d}{dz}\right)^n e^{-z^2} \tag{35}$$

(iii) They satisfy the recursion relation

$$H_{n+1}(z) = 2\,z\,H_n(z) - 2\,n\,H_{n-1}(z)\,, \quad H_0 = 1\,, \quad H_1 = 2z \tag{36}$$

By using the relation we get

$$H_2 = 4z^2 - 2\,, \quad H_3 = 8z^3 - 12z\,, \quad H_4 = 16z^4 - 48z^2 + 12\,, \quad \ldots \tag{37}$$



ψ_n
$|\psi_n|^2$
n=3
n=2
n=1
n=0
Potential
0
x
0
x

Let us summarise the properties of the quantum harmonic oscillator

(i) The energy is quantised. The quantum oscillator has a discrete set of levels.

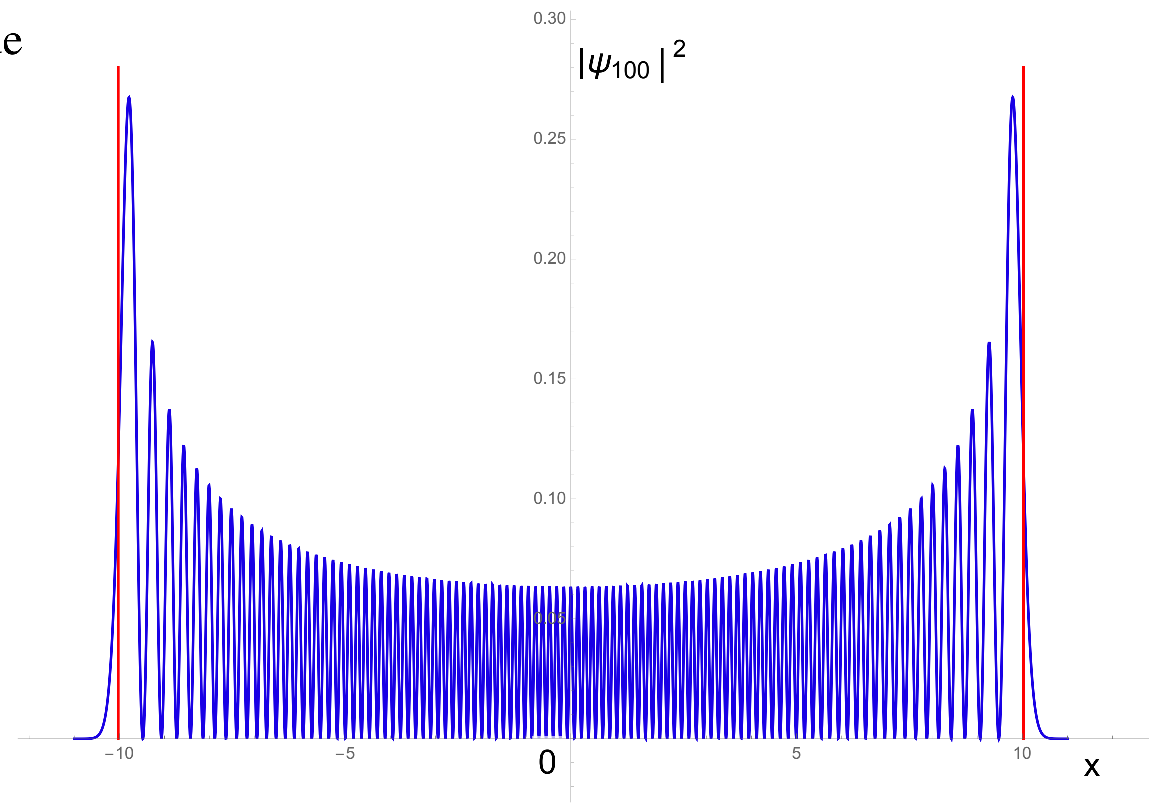
(ii) The levels are spaced uniformly.

We can think that there exist fictitious particles called quanta each endowed with energy $\hbar\omega$.

In the energy formula $E_n = \hbar\,\omega\,(n + \frac{1}{2})$ the term $\hbar\omega/2$ is the zero-point energy of the vacuum state with no quantum while $\hbar\omega\, n$ is the energy of n quanta.

(iii) The wave function does not vanish beyond the classical turning points $x_0 = \pm\eta\sqrt{4n+2}$.

The exponentially damped amplitude in the classically forbidden region is a manifestation of the tunnelling phenomena. The probability to find a particle outside the turning points is very small when n is large.



2.2 Dynamics

The Heisenberg equations

$$\frac{dX}{dt} = \frac{\mathrm{i}}{\hbar}[H, X] = \frac{P}{m}\,, \qquad \frac{dP}{dt} = \frac{\mathrm{i}}{\hbar}[H, P] = -m\omega^2 X \tag{38}$$

- The creation and annihilation operators eom

$$\frac{da}{dt} = \frac{\mathrm{i}}{\hbar}[H, a] = \frac{\mathrm{i}}{\hbar}[\hbar\omega(N + \frac{1}{2}), a] = -\mathrm{i}\,\omega\, a\,, \qquad \frac{da^\dagger}{dt} = \mathrm{i}\,\omega\, a^\dagger \tag{39}$$

are solved by

$$a(t) = a(0)\, e^{-\mathrm{i}\,\omega\, t}\,, \qquad a^\dagger(t) = a^\dagger(0)\, e^{\mathrm{i}\,\omega\, t} \tag{40}$$

- Thus,

$$X(t) = X(0)\cos\omega t + \frac{P(0)}{m\omega}\sin\omega t\,, \qquad P(t) = P(0)\cos\omega t - m\omega\, X(0)\sin\omega t \tag{41}$$

- The expectation values of $X(t)$ and $P(t)$ in any stationary state is 0

- To observe oscillations reminiscent of the classical oscillator, consider a superposition of eigenstates

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n |n\rangle \tag{42}$$

(i) The expectation value of $X(t)$ in this state

$$\langle X(t)\rangle = \eta\langle a(t) + a^\dagger(t)\rangle = \eta e^{-\mathrm{i}\,\omega\, t}\langle a\rangle + \eta e^{\mathrm{i}\,\omega\, t}\langle a^\dagger\rangle = \Re\Big(\eta e^{\mathrm{i}\,\omega\, t}\langle a^\dagger\rangle\Big) = \sum_{n=1}^{\infty} X_n \cos(\omega\, t + \phi_n) \tag{43}$$

where

$$2\eta\sqrt{n}\, c_{n+1}^* c_n = X_n e^{\mathrm{i}\,\phi_n} \tag{44}$$

and we used

$$\langle a\rangle = \sum_{m,n=0}^{\infty} c_n^* c_m \langle n|a|m\rangle = \sum_{m,n=0}^{\infty} c_n^* c_m \sqrt{m-1}\langle n|m-1\rangle = \sum_{n=0}^{\infty} c_n^* c_{n+1}\sqrt{n}\,, \quad \langle a^\dagger\rangle = \sum_{n=0}^{\infty} c_{n+1}^* c_n \sqrt{n} \tag{45}$$

(ii) Thus $\langle X(t)\rangle$ oscillates sinusoidally at the classical frequency ω for any state $|\psi\rangle$

(iii) We have recovered the classical result that the frequency at which a harmonic oscillator oscillates is independent of amplitude and equal to $\sqrt{k/m}$

- Is there a superposition of energy eigenstates that most closely imitates the classical oscillator?
- In other words we want a wave packet that bounces back and forth without spreading in shape as any free particle wave function does.
- These are **coherent states** which are eigenvectors of the annihilation operator

$$a\,|\lambda\rangle = \lambda\,|\lambda\rangle \tag{46}$$

The coherent state has many remarkable properties

(i) When expressed as a superposition of energy eigenstates

$$|\lambda\rangle = \sum_{n=0}^{\infty} f(n)\,|n\rangle \tag{47}$$

the distribution of $|f(n)|^2$ with respect to n is of the Poisson type about some mean value $\bar{n}$

$$|f(n)|^2 = \left(\frac{\bar{n}^n}{n!}\right)\exp(-\bar{n}) \tag{48}$$

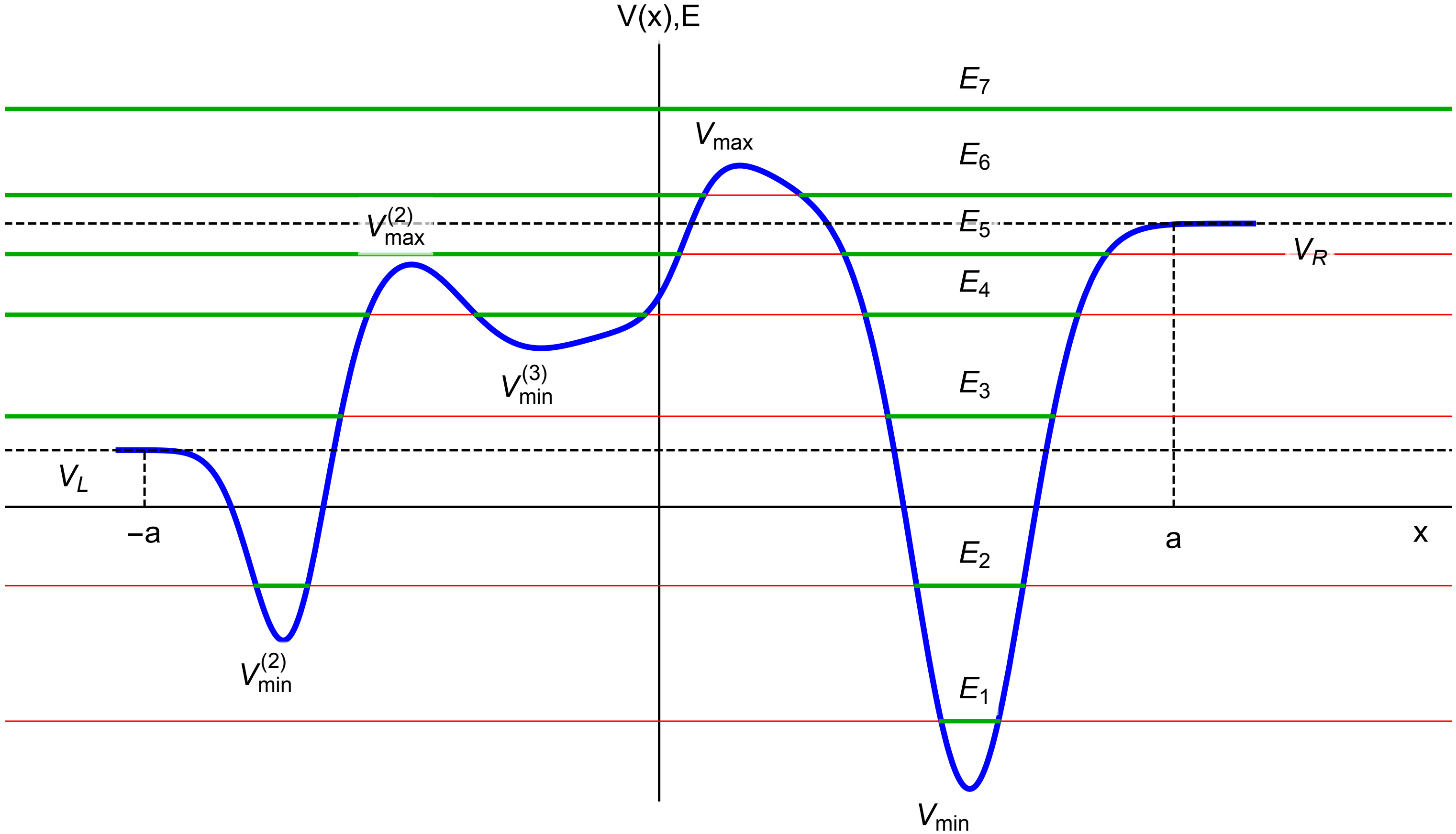
(ii) For real λ it can be obtained by translating the oscillator ground state by some finite distance

(iii) It satisfies the minimum uncertainty product relation at all times.

3 Bounded potential in one dimension

The free particle and the harmonic oscillator give us examples of systems with continuous and pure discrete spectra.

Consider the energy spectrum of a particle moving in a potential $V(x)$ which is bounded from below and above, and asymptotes to V_L for $x \to -\infty$ and to V_R for $x \to +\infty$



In CM the motion of a particle in such a potential depends on the energy and the potential shape.

- For the potential pictured there are seven clearly distinct cases.

  1. If $E > V_{\max}$ then there are no turning points and the motion is infinite – the particle moves from one infinity to another in any direction.
  2. If $V_R < E < V_{\max}$ then there are two allowed regions, and there is one turning point in each region. The motion is semi-infinite – the particle comes from $\pm$infinity, gets reflected at the turning point and goes back to $\pm$infinity.

     A particle moving in an infinite or semi-infinity region is said to be in a **scattering state**.
  3. If $V^{(2)}_{\max} < E < V_R$ then there are again two allowed regions, but there are two turning points in the right region, and the motion there is finite and periodic.

     A particle cannot escape to infinity, and is said to be in a **bound state**.
  4. If $V^{(3)}_{\min} < E < V^{(2)}_{\max}$ then there are one semi-infinite and two finite regions, and therefore, at this energy a particle can be in one scattering state and in two different bound states.
  5. If $V_L < E < V^{(3)}_{\min}$ then there are again one semi-infinite and one finite regions.
  6. If $V^{(2)}_{\min} \leq E < V_L$ then there are two finite regions.
  7. If $V_{\min} \leq E < V^{(2)}_{\min}$ then there is one finite region.

- Even if there are several allowed regions for a given energy, the particle always moves in the connected region it was at any instant of time – no jump from one allowed region to another is allowed.

In QM the energy spectrum is found by solving TISE

$$-\frac{\hbar^2}{2m}\psi'' + V(x)\psi = E\psi\,, \quad \psi'' \equiv \frac{d^2\psi}{dx^2} \tag{49}$$

- It is a second-order differential equation, and for any E it has two independent solutions.
- We are interested
  - (i) in square-integrable solutions which describe the discrete spectrum
  - (ii) in bounded solutions which are δ-function normalisable and describe continuous spectrum.
- Assume for simplicity $V(x) = V_L$ for $x < -a$ and $V(x) = V_R$ for $x > a$.
- Assume for definiteness that $V_{\min} \le V_L \le V_R$, where $V_{\min}$ is the absolute minimum of the potential.
- The expectation value of the Hamiltonian in any square-integrable state is greater than $V_{\min}$

$$\langle H\rangle = \int dx\,\Big(\frac{\hbar^2}{2m}|\psi'|^2 + V(x)|\psi|^2\Big) > \int dx\, V(x)|\psi|^2 > V_{\min} \tag{50}$$

  - (a) There is no normalisable energy eigenvector with $E \le V_{\min}$.
  - (b) If there is a **ground state**, that is a normalisable eigenvector with the lowest energy, then its energy E_0 is always greater than $V_{\min}$ which is the lowest energy allowed in CM.
  - (c) We have already seen this property in the harmonic oscillator spectrum, and discussed that it is explained by the uncertainty principle.

- Then, for $x < -a$ and for $x > a$ the Schrödinger equation (49) simplifies

$$\psi'' = \frac{2m}{\hbar^2}(V_L - E)\psi\,, \quad x < -a \tag{51}$$

$$\psi'' = \frac{2m}{\hbar^2}(V_R - E)\psi\,, \quad x > a \tag{52}$$

  (a) Contrary to CM whether a solution of TISE is square-integrable or δ-function normalisable does not depend on the precise shape of the potential.

  (b) It is only the potential's asymptotic values and the absolute minimum that matter.

- There are only three choices of energy

I. $E > V_R \geq V_L$

  (a) Solutions of (51) and (52) are superpositions of plane waves

$$\varphi_\alpha(x) = A_\alpha e^{\mathrm{i}\,k_\alpha x} + B_\alpha e^{-\mathrm{i}\,k_\alpha x}\,, \quad k_\alpha = \frac{\sqrt{2m(E - V_\alpha)}}{\hbar}\,, \quad \alpha = L, R \tag{53}$$

  (b) Both independent solutions of TISE are not square-integrable but they are bounded and δ-function normalisable.

  (c) Thus, for $E > V_R \geq V_L$ the energy spectrum is continuous and has multiplicity two.

  (d) We denote the δ-function normalised eigenkets by $|E, \pm\rangle$ where the wave functions of $|E, +\rangle$ and $|E, -\rangle$ become proportional to $e^{\mathrm{i}\,k_R x}$ for $x > a$ and $e^{-\mathrm{i}\,k_L x}$ for $x < -a$, respectively.

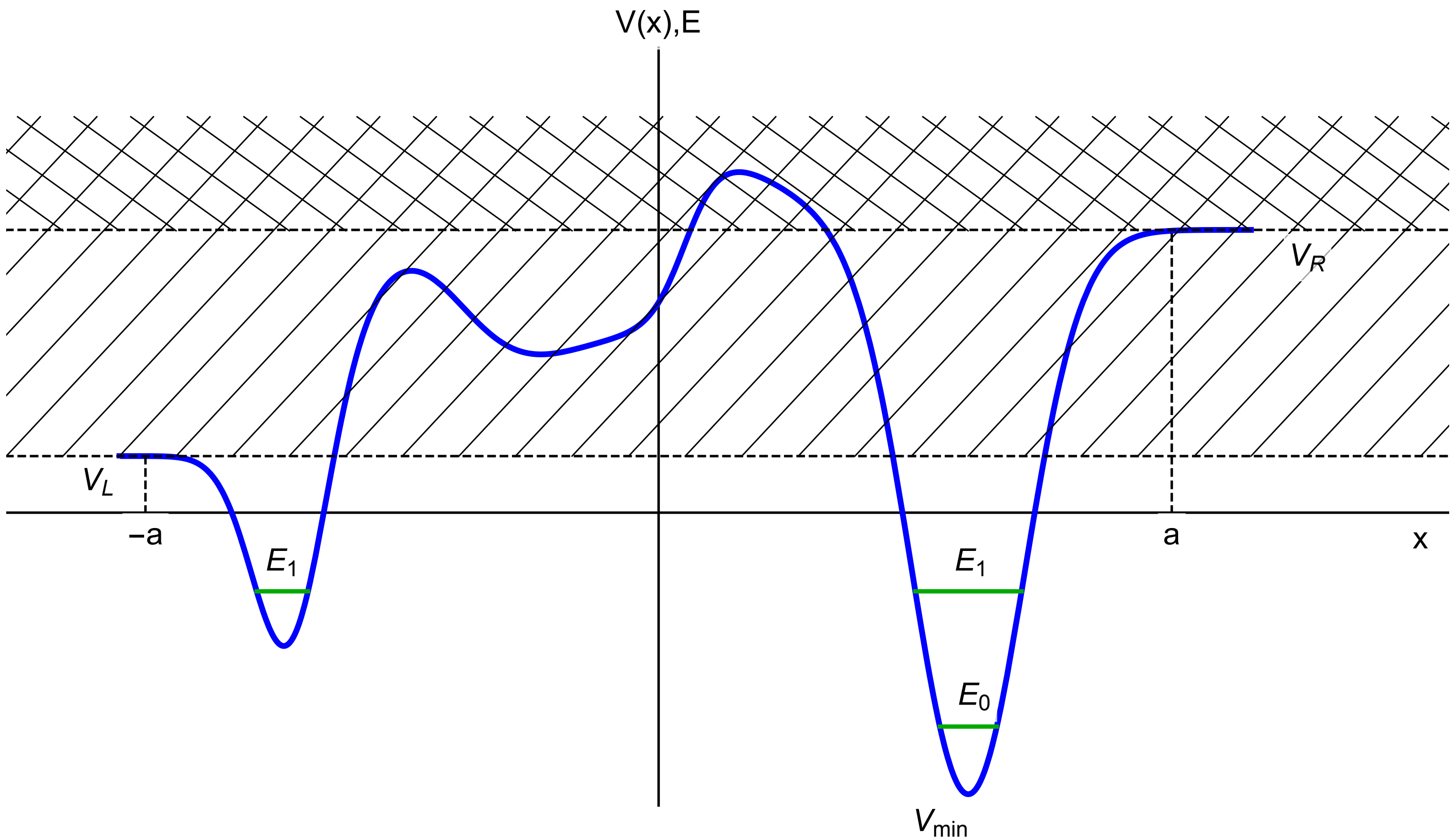


Figure. The double shading shows the region of the doubly degenerate continuous spectrum.

(e) $|E, \pm\rangle$ do not represent physically realisable states

(f) They can be used to prepare a wave packet with energies in a narrow band
$V_R < \langle E\rangle - \Delta E < E < \langle E\rangle + \Delta E$

(g) The expectation value of H and its dispersion in this wave packet are independent of time.

(h) There is no interaction at $|x| > a$ and this wave packet at large $|x|$ behaves as a free particle wave packet with momentum in a narrow band, and it is a quantum mechanical scattering state.

(i) Since the wave function does not in general vanish there is a nonzero probability to find the particle anywhere in space.

(j) This leads to the next puzzling property of quantum mechanics.

   i. The particle may be found in classically forbidden regions, and it can penetrate from one allowed region to another.

   ii. For the potential in the figure if $V_{\max} > E > V_R$

      - In CM there is a potential barrier which divides the space into two semi-infinite allowed regions.
      - In QM a particle sent from $-\infty$ to $+\infty$ has a nonvanishing probability to "leak" through the barrier and be found on its other side.

   iii. This is the phenomenon of **tunnelling** through a potential barrier.

(k) Even for $E > V_{\max}$ the behaviour of a scattering state is different from its classical counterpart.

   i. Consider a state which at $t \to -\infty$ is represented by a right-moving wave packet.
   For a generic potential this state at $t \to +\infty$ will be represented by a superposition of both left- and right-moving wave packets.

   ii. It means that a part of the wave got reflected from the potential barrier, and at large t there is a probability to find the particle moving to the left – something that is not possible in CM.

II. $V_R > E > V_L$

(a) In this case solutions of (51) are still superpositions of plane waves

$$\varphi_L(x) = A_L e^{\mathrm{i}\,k_L x} + B_L e^{-\mathrm{i}\,k_L x}\,, \quad k_L = \frac{\sqrt{2m(E - V_L)}}{\hbar} \tag{54}$$

(b) Solutions of (52) are superpositions of exponential functions

$$\varphi_R(x) = A_R e^{-\kappa_R x} + B_R e^{+\kappa_R x}\,, \quad \kappa_R = \frac{\sqrt{2m(V_R - E)}}{\hbar} > 0 \tag{55}$$

(c) Since for $x < a$, $\varphi_L(x)$ does not decrease there is no square-integrable wave function.

(d) Setting $B_R = 0$, one gets an exponentially decreasing function at large x, and, therefore, a bounded and δ-function normalisable solution of the Schrödinger equation.

(e) Since at $x \ll -a$ it is a superposition of plane waves, it is also a scattering state.

(f) In CM we could have a scattering and two different bound states for $V_{\rm min}^{(3)} < E < V_{\rm max}^{(2)}$

(g) In QM all the bound states disappear because a particle can escape to $-\infty$, and we only have a single scattering state.

(h) There is a probability to find the particle anywhere in space.

(i) A relation between A_L, B_L and A_R depends on the potential and they have to be chosen so that the wave function to be continuous everywhere.

(j) If the potential is piecewise continuous then the first derivative of ψ must be also continuous otherwise the second derivative of ψ would have δ-function singularities which contradicts the Schrödinger equation.

(k) Thus, for $V_R > E > V_L$ the energy spectrum is continuous and nondegenerate.

(l) On the figure the ordinary shading shows the region of the nondegenerate continuous spectrum.

(m) If we send V_R to infinity then κ_R diverges and the wave function vanishes for $x \geq a$.

(n) Thus, if $V_R = +\infty$ we get impenetrable barrier, in other words an ideal wall from which particles are reflected instantaneously.

(o) We denote the δ-function normalised eigenkets by $|E\rangle$.

III. $V_R \geq V_L > E \geq V_{\min}$

(a) Solutions of (51) and (52) are superpositions of exponential functions

$$\varphi_\alpha(x) = A_\alpha e^{-\kappa_\alpha x} + B_\alpha e^{+\kappa_\alpha x}, \quad \kappa_\alpha = \frac{\sqrt{2m(V_\alpha - E)}}{\hbar}, \quad \alpha = L, R \tag{56}$$

(b) We have to choose $A_L = 0$ and $B_R = 0$ to have a square-integrable solution.

- This poses a problem because just one of these conditions either $A_L = 0$ or $B_R = 0$ is sufficient to find a solution of the Schrödinger equation up to an overall factor.
- Both conditions can be satisfied only for special values of energy E, and that is the reason for the discreteness of the spectrum and energy quantisation.

(c) The quantisation condition can be found by using the following procedure.
Let ψ_1 and ψ_2 be two independent solutions of the Schrödinger equation (49).

i. The general solution can be written as

$$\psi = A\psi_1 + B\psi_2 \tag{57}$$

ii. Setting $A_L = 0$ one gets A/B as a function of energy

$$A/B = F_L(E) \tag{58}$$

iii. Setting $B_R = 0$ one gets A/B as another function of energy

$$A/B = F_R(E) \tag{59}$$

iv. $A_L = 0$ and $B_R = 0$ are satisfied for a normalisable state $\Rightarrow$ the **quantisation condition**

$$F_L(E) = F_R(E) \tag{60}$$

v. Solving this algebraic equation, one gets the discrete spectrum.

vi. This equation does not always have solutions with $V_{\min} < E < V_L$.

(d) Normalisable eigenvectors of the Hamiltonian correspond to classical finite motion and are quantum bound states.

(e) The lowest energy state is the **ground state**.

(f) The bound state with the energy E_1 on the figure occupies both classically allowed regions.

(g) Contrary to CM it is a single state, and a particle can propagate from one allowed region to another.

(h) It can also be found in classically forbidden regions but with a very small probability.

(i) If we send both V_L and V_R to infinity then we get two impenetrable walls, and the whole energy spectrum will be discrete.

(j) We denote the normalised eigenkets by $|E_n\rangle$ where $E_n < E_{n+1}$, $n = 0, 1, \ldots, N_E$ where N_E is the number of excited states.

The completeness relation

$$\hat{I} = \sum_{n=0}^{N_E} |E_n\rangle\langle E_n| + \int_{V_L}^{V_R} dE\, |E\rangle\langle E| + \int_{V_R}^{\infty} dE\, (|E,+\rangle\langle E,+| \,+\, |E,-\rangle\langle E,-|) \tag{61}$$

can be used to show that the expectation value of the Hamiltonian in any normalisable state is greater than or equal to the ground state energy

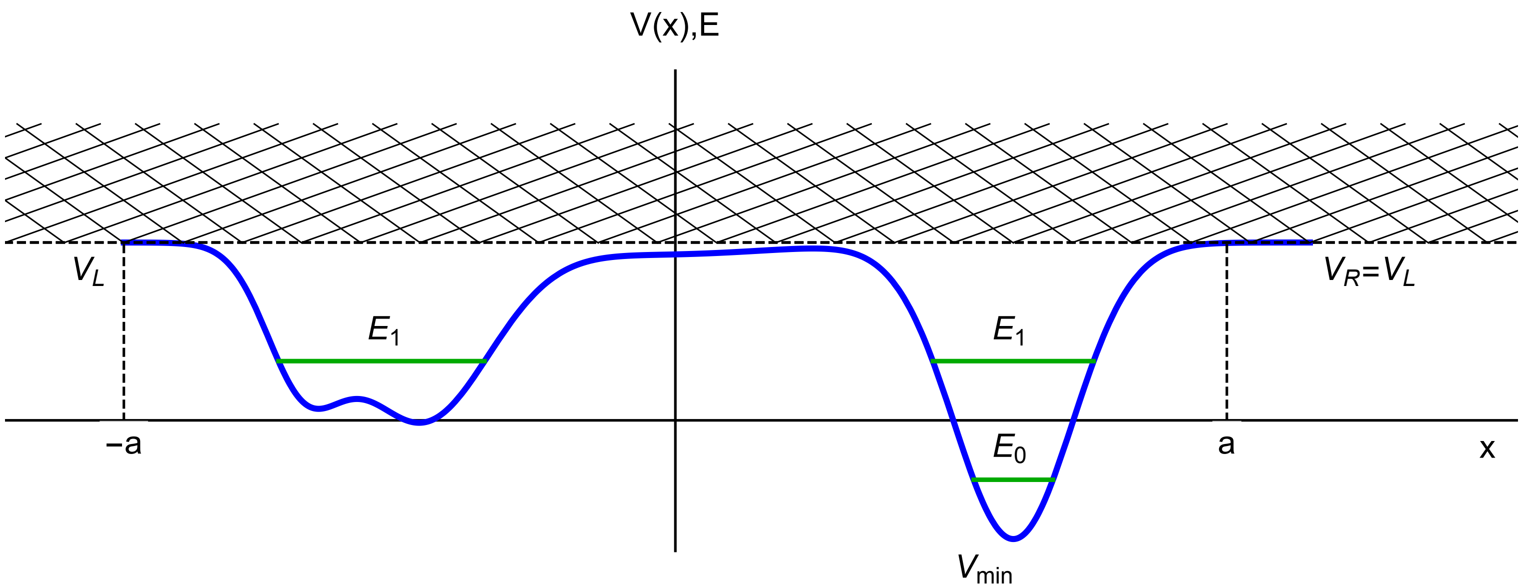
$$\langle\psi|H|\psi\rangle \geq E_0 \tag{62}$$

or to V_L if there is no ground state.

This inequality can be used to show that for any attractive potential, that is a potential with

$$V_{\rm min} < V_L = V_R \;\text{ and }\; V(x) \leq V_L \;\text{ for all }\; x \tag{63}$$

there is at least one bound state.



1. Choose the wave function ψ to be

$$\psi(x) = \sqrt{\alpha}\, e^{-\alpha\,|x|}\,, \quad \alpha > 0 \tag{64}$$

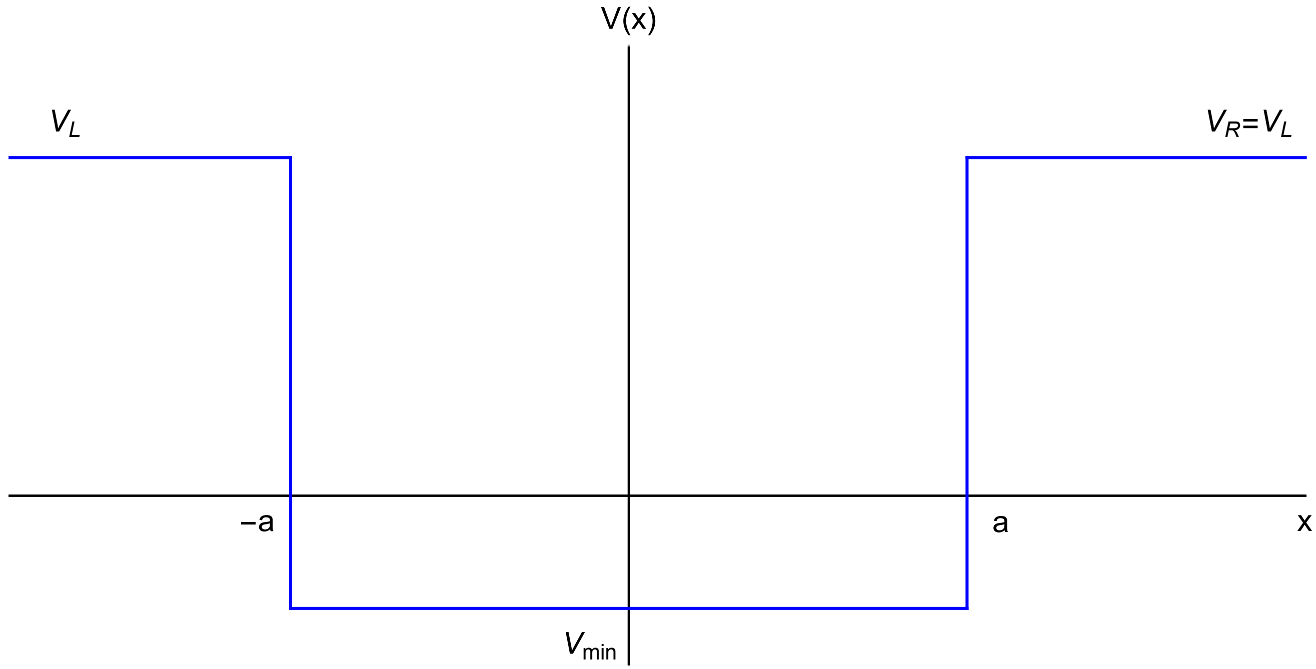
2. Get

$$\begin{aligned} E_0 \leq \langle\psi|H|\psi\rangle &= \int dx\, \Big(\frac{\hbar^2}{2m}|\psi'|^2 + V|\psi|^2\Big) = \int dx\, \Big(\frac{\hbar^2}{2m}\alpha^2 + V - V_L + V_L\Big)|\psi|^2 \\ &= \frac{\hbar^2}{2m}\alpha^2 - \alpha \int_{-a}^{a} dx\, \Big(V_L - V\Big)e^{-2\alpha\,|x|} + V_L \\ &= \Big(\frac{\hbar^2}{2m} + \int_{-a}^{a} dx\,(V_L - V)|x|\Big)\alpha^2 - \alpha \int_{-a}^{a} dx\,(V_L - V) + V_L + \mathcal{O}(\alpha^3) \end{aligned} \tag{65}$$

3. $\int_{-a}^{a} dx\,(V_L - V) > 0$, and if we choose α to be small enough the r.h.s. of the equation above becomes smaller than V_L which implies that $E_0 < V_L$, and the existence of at least a ground state.

4. If the potential well is very shallow, $V_L/V_{\min} \sim 1$, then the particle is not confined within the well; there is a non-negligible probability of finding the particle in the classically forbidden region $|x| > a$.

4 Square potential well: discrete spectrum



One of the simplest potentials of the type discussed in previous section is the potential of a rectangular well

$$V(x) = \begin{cases} V_L & \text{for } |x| > a \\ V_{\min} & \text{for } |x| < a \end{cases} \tag{66}$$

4.1 Bound states

$V_L > E > V_{\min}$, and we have to glue the following solutions of the Schrödinger equation (49)

$$\begin{aligned}&\varphi_L(x) = B_L e^{+\kappa\, x}\,,\ \ x < -a\,,\quad \varphi_R(x) = A_R e^{-\kappa\, x}\,,\ \ x > a\,,\quad \kappa = \frac{\sqrt{2m(V_L - E)}}{\hbar}\\ &\psi_M(x) = A_M e^{\mathrm{i}\, k\, x} + B_M e^{-\mathrm{i}\, k\, x}\,,\quad k = \frac{\sqrt{2m(E - V_{\min})}}{\hbar}\,,\quad |x| < a\end{aligned} \tag{67}$$

Since the potential is an even function of x, the Hamiltonian commutes with the parity operator $\mathcal{P}$, and therefore wave functions can be chosen to be either even or odd:

I. Even wave functions: $\psi_{\text{even}}(-x) = \psi_{\text{even}}(x)$

- Due to this condition

$$B_L = A_R \equiv A\,,\quad A_M = B_M \equiv \frac{B}{2}\,,\quad \varphi_R(x) = A\, e^{-\kappa\, x}\,,\quad \psi_M(x) = B\cos(k\, x) \tag{68}$$

- The continuity of the wave function and its derivative at $x = a$ gives

$$A\, e^{-\kappa\, a} = B\cos(k\, a)\,,\quad A\,\kappa\, e^{-\kappa\, a} = B\, k\sin(k\, a) \tag{69}$$

- The energy quantisation condition

$$\kappa = k\tan(k\, a)\,,\quad \kappa^2 = \frac{2m}{\hbar^2}(V_L - V_{\min}) - k^2\,,\quad E - V_{\min} = \frac{\hbar^2}{2m}k^2 \tag{70}$$

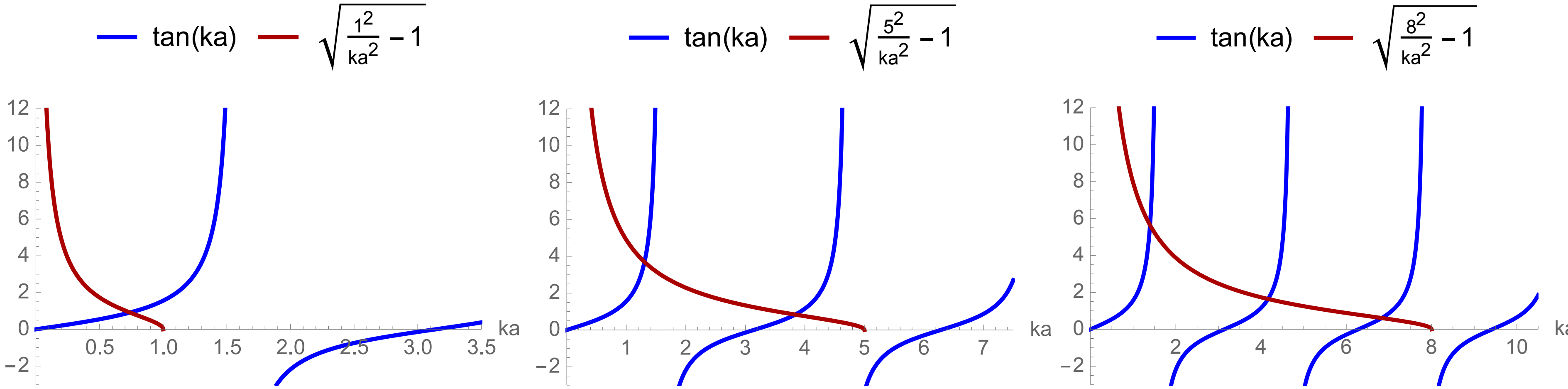


Figure 1: Plots of the left and right sides of (71) for $W = 1, 5, 8$.

- Rewrite it in terms of dimensionless quantities ka and W

$$\tan(ka) = \sqrt{\frac{W^2}{(ka)^2} - 1} \quad \text{where} \quad W^2 \equiv \frac{2m\,a^2}{\hbar^2}(V_L - V_{\min}) > 0 \tag{71}$$

(i) W controls the depth of the potential well.

(ii) Real roots of (71) exist only for $0 < ka \leq W$.

(iii) The left and right sides of eq.(71) are plotted in figure 1.

(iv) Since $\tan 0 = 0$, $\tan(\pi/2 - 0) = +\infty$ and $\tan ka$ is an increasing function of ka for $ka < \pi/2$ while $\sqrt{\frac{W^2}{(ka)^2} - 1}$ asymptotes to $+\infty$ as $ka \to 0$, and it is a decreasing function vanishing at $ka = W$, eq.(71) has at least one root no matter how small W is.

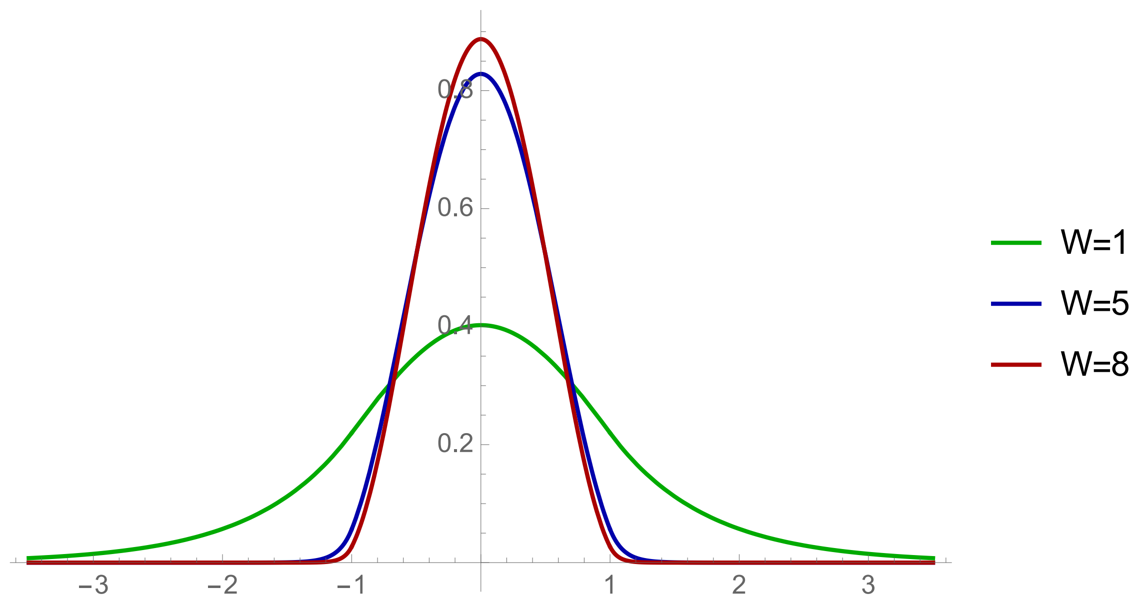
(v) Since $\tan ka$ is periodic with period π, the number of roots of eq.(71) is easy to find.

- For $0 < W < \pi$ there is only one root
- At $W = \pi$ the second root equal to π appears, and for $\pi \leq W < 2\pi$ there are two roots.
- For $(n-1)\pi \leq W < n\pi$ there are n roots.

- The constants A and B are expressed in terms of k and κ as

$$A = B\, e^{\kappa\, a} \cos(k\, a)\,, \qquad B = \frac{1}{\sqrt{\frac{\cot(ak)}{k} + a}} \tag{72}$$

- The probability densities ψ^2 of finding the particle at x for the ground state for $W = 1, 5, 8$ and $a = 1$



For $W = 1$ the particle can be easily found outside of the classically allowed region.

II. Odd wave functions: $\psi_{\rm odd}(-x) = -\psi_{\rm odd}(x)$

Imposing this condition we get

$$B_L = -A_R \equiv A\,, \quad A_M = -B_M \equiv -\frac{\mathrm{i}\,B}{2}\,, \quad \varphi_R(x) = A\,e^{-\kappa\,x}\,, \quad \psi_M(x) = B\sin(k\,x) \tag{73}$$

and the continuity of the wave function and its derivative at $x = a$ gives

$$A\,e^{-\kappa\,a} = B\sin(k\,a)\,, \quad A\,\kappa\,e^{-\kappa\,a} = -B\,k\cos(k\,a) \tag{74}$$

Taking the ratio of these equation and using the dimensionless quantities ka and W, we get the energy quantisation condition for odd parity states

$$-\cot(ka) = \sqrt{\frac{W^2}{(ka)^2} - 1} \tag{75}$$

The analysis of this equation is similar to (71). One can easily show that the first odd parity state appears at $W = \pi/2$, the second at $W = 3\pi/2$, and so on. The probability densities ψ^2 for odd parity states look similar to those of even parity states.

To summarise, the number of even and odd parity bound states for $0 < W < \pi/2$ is equal to 1, for $\pi/2 \le W < \pi$ is equal to 2, for $\pi \le W < 3\pi/2$ is equal to 3, and so on , for $(n-1)\pi/2 \le W < n\pi/2$ is equal to n.

4.2 Infinitely deep well: $V_L - V_{\min} \to \infty$, a is fixed

- The walls of the well become impenetrable, and the energy quantisation conditions give

$$
\begin{aligned}
W = \infty \quad &\Rightarrow \quad \tan ka = +\infty \quad \Rightarrow \quad ka = \frac{\pi}{2} + \pi n \quad \Rightarrow \quad E_{2n} - V_{\min} = \frac{\hbar^2}{2m}(2n+1)^2\frac{\pi^2}{4a^2} \\
W = \infty \quad &\Rightarrow \quad \cot ka = -\infty \quad \Rightarrow \quad ka = \pi n \quad \Rightarrow \quad E_{2n-1} - V_{\min} = \frac{\hbar^2}{2m}n^2\frac{\pi^2}{a^2}
\end{aligned}
\tag{76}
$$

$$
E_n - V_{\min} = \frac{\hbar^2\pi^2}{8m\,a^2}(n+1)^2\,, \qquad n = 0, 1, 2, \ldots \tag{77}
$$

- Contrary to the harmonic oscillator the distance between the energy levels is proportional to $2n+1$.

- The wave functions

$$
\begin{aligned}
\psi_{\text{even}}(x) &= \begin{cases} \frac{1}{\sqrt{a}}\cos k_{2n}x & \text{for } |x| < a \text{ where } k_{2n} \equiv (2n+1)\frac{\pi}{2a} \\ 0 & \text{for } |x| > a \end{cases} \\
\psi_{\text{odd}}(x) &= \begin{cases} \frac{1}{\sqrt{a}}\sin k_{2n-1}x & \text{for } |x| < a \text{ where } k_{2n-1} \equiv n\frac{\pi}{a} \\ 0 & \text{for } |x| > a \end{cases}
\end{aligned}
\tag{78}
$$

- As $a \to 0$ the ground state wave function becomes $\delta(x)$, and the particle is confined to $x = 0$
- If we choose $V_{\min} = -\frac{\hbar^2\pi^2}{8m\,a^2}$ then the energy of the ground state remains equal to zero for all a.
- The energy of all exited states diverges as $a \to 0$, and they completely decouple.
- Thus, we can use the Infinitely deep well potential with very small a to model quantum mechanical constrained motion.

4.3 The delta-function well: $a \to 0$, $V_{\rm min} \to -\infty$ and $aV_{\rm min}$ remains finite

We set $V_L = 0$ for definiteness.

- The square-well potential becomes

$$V(x) = -\nu\,\delta(x)\,, \quad \nu \equiv -2\,a\,V_{\rm min} \tag{79}$$

- W^2 becomes

$$W^2 = -\frac{2m\,a^2}{\hbar^2}V_{\rm min} = a\,w^2\,, \quad w^2 \equiv \frac{m\,\nu}{\hbar^2} \tag{80}$$

- This, $W^2 \to 0$, and therefore there exists only one bound state.

- The bound state is the ground state and its wave function is

$$\psi(x) = A\,e^{-\kappa\,|x|}\,, \quad \kappa^2 = -\frac{2m}{\hbar^2}V_{\rm min} - k^2 = \frac{w^2}{a} - k^2\,, \quad E = V_{\rm min} + \frac{\hbar^2}{2m}k^2 = -\frac{\hbar^2}{2m}\kappa^2 \tag{81}$$

- Since κ should have finite limit as $a \to 0$ it is convenient to rewrite (71) in terms of κ

$$\tan\left(w\,\sqrt{a}\sqrt{1 - a\frac{\kappa^2}{w^2}}\right) = \frac{\kappa}{w}\,\sqrt{a}\frac{1}{\sqrt{1 - a\frac{\kappa^2}{w^2}}} \tag{82}$$

- In the limit $a \to 0$ the equation becomes

$$w = \frac{\kappa}{w} \quad \Rightarrow \quad \kappa = w^2 = \frac{m\,\nu}{\hbar^2} \tag{83}$$

- Thus, the ground state solution to TISE with the δ-function potential

$$-\frac{\hbar^2}{2m}\psi'' - \nu\,\delta(x)\psi = E\psi \tag{84}$$

is

$$\psi(x) = \sqrt{\kappa}\,e^{-\kappa\,|x|}\,, \quad \kappa = \frac{m\,\nu}{\hbar^2}\,, \quad E = -\frac{m\,\nu^2}{2\hbar^2} \tag{85}$$

- Let us check that it is the solution.

(i) The first derivative of ψ is

$$\psi'(x) = -\kappa^{3/2)}\,\mathfrak{s}(x)\,e^{-\kappa\,|x|}\,, \quad \mathfrak{s}(x) = \begin{cases} -1 & \text{for } x < 0 \\ 1 & \text{for } x > 0 \end{cases} \tag{86}$$

(ii) The first derivative is discontinuous, and the second derivative gives

$$\psi''(x) = -2\kappa^{3/2}\,\delta(x) + \kappa^{5/2}\,e^{-\kappa\,|x|} \tag{87}$$

(iii) Substituting it into (84), we get

$$\frac{\hbar^2}{m}\kappa^{3/2}\,\delta(x) - \frac{\hbar^2\kappa^{5/2}}{2m}\,e^{-\kappa\,|x|} - \nu\sqrt{\kappa}\,\delta(x) = E\sqrt{\kappa}\,e^{-\kappa\,|x|} \tag{88}$$

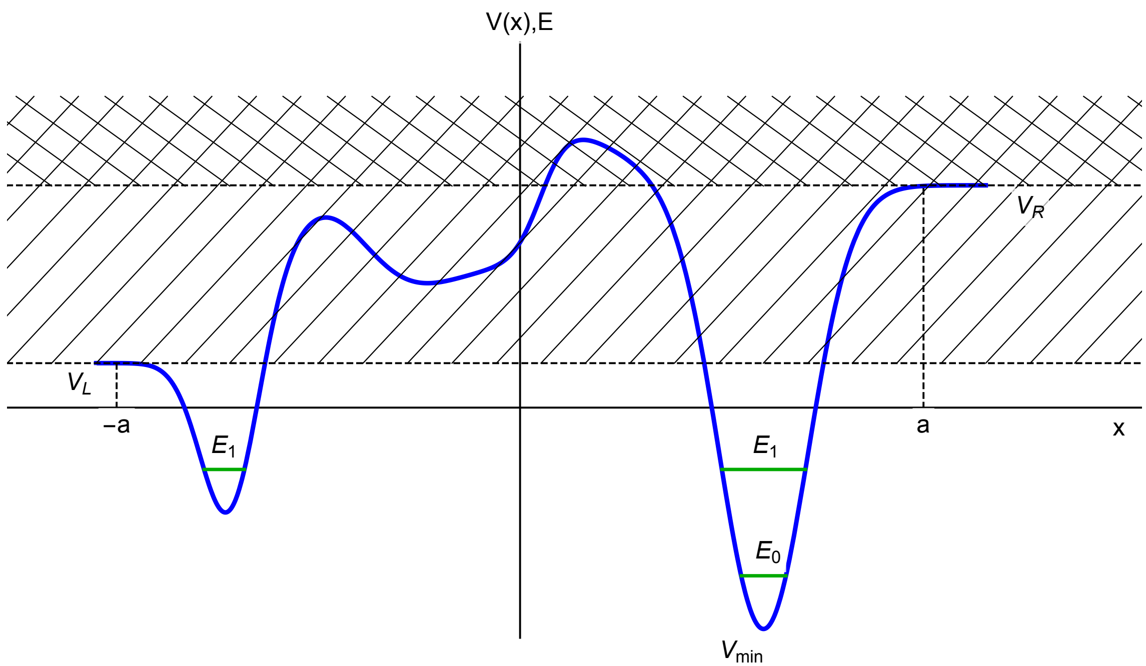
(iv) The δ-function terms give $\kappa = m\nu/\hbar^2$, and the $e^{-\kappa|x|}$ terms give the energy $E = \hbar^2\kappa^2/2m$.

(v) Thus, solutions of the Schrödinger equation with δ-function potentials are continuous functions with discontinuous first derivatives.

5 Scattering in one dimension

5.1 Scattering matrix

Consider scattering states for a particle moving in a generic bounded potential



Consider the most interesting case $E > \max(V_R\,,\,V_L)$ where the spectrum is doubly degenerate.

- Solutions of TISE for $|x| > a$ are superpositions of plane waves $\exp(\pm\mathrm{i}\,k\,x)$.
- If $V_L \neq V_R$ then the momentum is not conserved $\Rightarrow$ normalise the plane waves not with $\delta(p_1 - p_2)$ but with $\delta(E_1 - E_2)$.

- Introduce the functions

$$\varphi_\alpha^\pm(E,x) \equiv \sqrt{\frac{m}{2\pi\,\hbar^2}}\,\frac{e^{\pm \mathrm{i}\,k_\alpha\,x}}{\sqrt{k_\alpha}}\,, \quad k_\alpha \equiv \frac{\sqrt{2m(E-V_\alpha)}}{\hbar}\,, \quad \alpha = L, R \tag{89}$$

(i) solve TISE for $|x| > a$,

$$-\frac{\hbar^2}{2m}\psi'' + V(x)\psi = E\psi\,, \quad \psi'' \equiv \frac{d^2\psi}{dx^2} \tag{90}$$

(ii) are normalised as

$$\int dx\,\bar{\varphi}_L^a(E_1,x)\varphi_L^b(E_2,x) = \delta_{ab}\delta(E_1-E_2)\,, \quad a,b = +,-\,, \tag{91}$$

where $\bar{\varphi}$ denotes the complex conjugate of φ, and φ_R^a satisfy the same normalisations.

- Wave function solving TISE

$$\psi_E(x) = \begin{cases} A_L\varphi_L^+(E,x) + B_L\varphi_L^-(E,x) & \text{for } x < -a \\ A_R\varphi_R^+(E,x) + B_R\varphi_R^-(E,x) & \text{for } x > a \\ A_M\varphi_1(x) + B_M\varphi_2(x) & \text{for } |x| < a \end{cases} \tag{92}$$

where φ_1 and φ_2 are any two independent solutions of TISE in the interval $[-a,a]$.

- The continuity of $\psi_E(x)$ and $\psi'_E(x)$ at $x = \pm a$ allows one to express four of the coefficients A_α, B_α, $\alpha = L, M, R$ in terms of the other two $\Rightarrow$ the double degeneracy of the spectrum.

- Let us choose A_L and B_R as the two independent coefficients.
- Setting one of them to zero, and the other to one, one gets the following two independent solutions

$$\varphi_L(E,x) = \begin{cases} \varphi_L^+(E,x) + S_{LL}\varphi_L^-(E,x) & \text{for } x < -a \\ S_{RL}\varphi_R^+(E,x) & \text{for } x > a \\ A_{ML}\varphi_1(x) + B_{ML}\varphi_2(x) & \text{for } |x| < a \end{cases} \tag{93}$$

and

$$\varphi_R(E,x) = \begin{cases} S_{LR}\varphi_L^-(E,x) & \text{for } x < -a \\ S_{RR}\varphi_R^+(E,x) + \varphi_R^-(E,x) & \text{for } x > a \\ A_{MR}\varphi_1(x) + B_{MR}\varphi_2(x) & \text{for } |x| < a \end{cases} \tag{94}$$

(i) Multiplying the wave function (92) by $\exp(-\mathrm{i}\,E\,t/\hbar)$, one sees that $e^{\mathrm{i}\,k_\alpha\,x}$ and $e^{-\mathrm{i}\,k_\alpha\,x}$ give rise to a wave function propagating to the right and to the left, respectively

(ii) In a scattering experiment a particle can be fired only from one direction, say from the left.

(a) In that case the amplitude B_R of the left-moving wave coming from the right will be zero

$$B_R = 0 \quad \text{for scattering from the left} \tag{95}$$

(b) Then, A_L is the amplitude of the **wave incident** from the left

(c) B_L is the amplitude of the **wave reflected** to the left

(d) A_R is the amplitude of the **wave transmitted** to the right.

(e) Up to a normalisation factor φ_L is the wave function of the wave incident from the left.

(iii) Similarly, if a particle is fired from the right

(a) the amplitude A_L of the right-moving wave coming from the left will be zero, $A_L = 0$

(b) B_R is the amplitude of the **wave incident** from the right

(c) A_R is the amplitude of the **wave reflected** to the right

(d) B_L is the amplitude of the **wave transmitted** to the left

(e) Up to a normalisation factor φ_R is the wave function of the wave incident from the right.

- The general wave function (92) can be written as a superposition of φ_L and φ_R

$$\psi = A_L\varphi_L + B_R\varphi_R \tag{96}$$

- Comparing the coefficients, we get the relations

$$\begin{pmatrix} B_L \\ A_R \end{pmatrix} = \begin{pmatrix} S_{LL} & S_{LR} \\ S_{RL} & S_{RR} \end{pmatrix} \begin{pmatrix} A_L \\ B_R \end{pmatrix} \tag{97}$$

- The four coefficients $S_{\alpha\beta}$, $\alpha, \beta = L, R$ which depend on the energy and the potential are the entries of a 2×2 matrix S called the **scattering matrix** or simply the **S-matrix**.

- The S-matrix allows one to find the outgoing amplitudes B_L and A_R in terms of the incoming amplitudes A_L and B_R.

- The coefficients $S_{\alpha\beta}$ have important properties which can be derived by using the **Wronskian**

$$W(f_1, f_2) \equiv f_1 f_2' - f_1' f_2 \tag{98}$$

(i) $W(f_1, f_2)$ of any two functions satisfying TISE does not depend on x.

(ii) $W(\psi, \psi^*)$ is proportional to the probability current density, and therefore it is independent of x.

- Consider the four pairs (φ_L, φ_L^*), (φ_R, φ_R^*), (φ_L, φ_R^*) and (φ_L, φ_R), and compute their Wronskians for $x < -a$ and $x > a$.

1. $\frac{2\pi\hbar^2}{m} W(\varphi_L, \varphi_L^*)\Big|_{x<-a} = -2\mathrm{i} + 2\mathrm{i}\, S_{LL} S_{LL}^*\,, \quad \frac{2\pi\hbar^2}{m} W(\varphi_L, \varphi_L^*)\Big|_{x>a} = -2\mathrm{i}\, S_{RL} S_{RL}^*$

$$|S_{LL}|^2 + |S_{RL}|^2 = 1 \tag{99}$$

2. $\frac{2\pi\hbar^2}{m} W(\varphi_R, \varphi_R^*)\Big|_{x>a} = 2\mathrm{i} - 2\mathrm{i}\, S_{RR} S_{RR}^*\,, \quad \frac{2\pi\hbar^2}{m} W(\varphi_R, \varphi_R^*)\Big|_{x<-a} = 2\mathrm{i}\, S_{LR} S_{LR}^*$

$$|S_{RR}|^2 + |S_{LR}|^2 = 1 \tag{100}$$

3. $\frac{2\pi\hbar^2}{m} W(\varphi_L, \varphi_R^*)\Big|_{x<-a} = 2\mathrm{i}\, S_{LL} S_{LR}^*\,, \quad \frac{2\pi\hbar^2}{m} W(\varphi_L, \varphi_R^*)\Big|_{x>a} = -2\mathrm{i}\, S_{RL} S_{RR}^*$

$$S_{LL} S_{LR}^* + S_{RL} S_{RR}^* = 0 \tag{101}$$

4. $\frac{2\pi\hbar^2}{m} W(\varphi_L, \varphi_R)\Big|_{x<-a} = -2\mathrm{i}\, S_{LR}\,, \quad \frac{2\pi\hbar^2}{m} W(\varphi_L, \varphi_R)\Big|_{x>a} = -2\mathrm{i}\, S_{RL} \quad \Rightarrow \quad S_{LR} = S_{RL}$

- These conditions are equivalent to the statement that the S-matrix is unitary and symmetric

$$S S^\dagger = S^\dagger S = I\,, \quad S^t = S\,, \tag{102}$$

- These properties of the S-matrix are closely related to the time reversal symmetry
  If $\psi(x,t)$ is a solution of the Schrödinger equation with time-independent potential then $\psi^*(x,-t)$ is also its solution.
  (i) For solutions of TISE this becomes the statement that $\psi^*(x)$ is a solution.
  (ii) The unitarity of the S-matrix follows from the first three conditions which can be obtained from the x independence of the probability current density
    (a) The first two conditions are derived by using φ_L and φ_R
    (b) The third condition is derived by using $\varphi_L + \varphi_R$ and $\varphi_L + \mathrm{i}\,\varphi_R$
  (iii) The S-matrix symmetry condition is derived by using $\varphi_L + \varphi_R^*$ and $\varphi_L + \mathrm{i}\,\varphi_R^*$.
- If a potential is parity invariant, then $S_{22} = S_{11}$.
- The conditions the S-matrix elements satisfy can be used to find the normalisations of the two independent solutions $\varphi_L(E,x)$ and $\varphi_R(E,x)$

$$\int_{-\infty}^{\infty} dx\, \varphi_L^*(E_1,x)\varphi_L(E_2,x) = \delta(E_1 - E_2) \tag{103}$$

  φ_R has the same normalisation.

5.2 Reflection and transmission coefficients

Any square-integrable solution of the Schrödinger equation can be decomposed over φ_α (93) and (94).

- Consider a time-dependent wave packet constructed from $\varphi_L(E,x)$

$$\psi_L(x,t) = \int_{E_{\min}}^{\infty} dE\, C(E)\, \varphi_L(E,x)\, e^{-\mathrm{i}\, E\, t/\hbar}\,, \qquad \int_{E_{\min}}^{\infty} dE\, |C(E)|^2 = 1 \tag{104}$$

  (i) $E_{\min} = \max(V_R\,,\, V_L)$

  (ii) $\psi_L(x,t)$ has norm 1

- $\psi_L(x,t)$ can be split into incident, reflected and transmitted waves, and a collision wave in the interaction region $|x| < a$

$$\psi_L(x,t) = \begin{cases} \psi_{\mathrm{inc}}(x,t) + \psi_{\mathrm{ref}}(x,t) & \text{for } \; x < -a \\ \psi_{\mathrm{trans}}(x,t) & \text{for } \; x > a \\ \psi_{\mathrm{coll}}(x,t) & \text{for } \; |x| < a \end{cases} \tag{105}$$

$$\psi_{\mathrm{inc}}(x,t) = \int_{E_{\min}}^{\infty} dE\, C(E)\, \varphi_L^{+}(E,x)\, e^{-\mathrm{i}\, E\, t/\hbar} = \sqrt{\frac{m}{2\pi\, \hbar^2}} \int_{E_{\min}}^{\infty} dE\, \frac{C(E)}{\sqrt{k_L}}\, e^{\mathrm{i}\, k_L\, x - \mathrm{i}\, E\, t/\hbar} \tag{106}$$

$$\psi_{\mathrm{ref}}(x,t) = \int_{E_{\min}}^{\infty} dE\, C(E)\, S_{LL}(E) \varphi_L^{-}(E,x)\, e^{-\mathrm{i}\, E\, t/\hbar} = \sqrt{\frac{m}{2\pi\, \hbar^2}} \int_{E_{\min}}^{\infty} dE\, \frac{C(E)}{\sqrt{k_L}}\, S_{LL}(E)\, e^{-\mathrm{i}\, k_L\, x - \mathrm{i}\, E\, t/\hbar} \tag{107}$$

$$\psi_{\mathrm{trans}}(x,t) = \int_{E_{\min}}^{\infty} dE\, C(E)\, S_{RL}(E) \varphi_R^{+}(E,x)\, e^{-\mathrm{i}\, E\, t/\hbar} = \sqrt{\frac{m}{2\pi\, \hbar^2}} \int_{E_{\min}}^{\infty} dE\, \frac{C(E)}{\sqrt{k_R}}\, S_{RL}(E)\, e^{\mathrm{i}\, k_R\, x - \mathrm{i}\, E\, t/\hbar} \tag{108}$$

  The explicit form of the collision wave is not relevant for the subsequent discussion.

- $\psi_L(x,t)$ describes a scattering process and we are interested in its behaviour at $t \to \pm\infty$.
   (i) $\psi_{\rm coll}(x,t) \to 0$ as $t \to \pm\infty$ because of rapid oscillations of $e^{-{\rm i}\,E\,t/\hbar}$ in the integrand of (104) and the finite range of x in $\psi_{\rm coll}$.
   (ii) Similarly, if $t \to -\infty$ then $\psi_{\rm ref}(x,t) \to 0$ and $\psi_{\rm trans}(x,t) \to 0$.
   (iii) $\psi_{\rm inc}(x,t)$ survives in the limit $t \to -\infty$
      (a) It is concentrated very far to the left otherwise it would vanish as $t \to -\infty$.
      (b) The probability of observing the particle as $t \to -\infty$ to the left from the origin is 1.
   (iv) If $t \to +\infty$ then $\psi_{\rm inc}(x,t) \to 0$ but the reflected and transmitted wave functions survive and are concentrated very far to the left and to the right from the origin, respectively.
- The conditions that $\psi_{\rm ref}$ is defined only for $x < -a$, and $\psi_{\rm trans}$ is defined only for $x > a$ are satisfied automatically as $t \to +\infty$, and we can simply write

$$\psi_L(x,t) = \psi_{\rm ref}(x,t) + \psi_{\rm trans}(x,t) \quad \text{for} \quad t \to +\infty \tag{109}$$

- The probability of finding the particle to the left from the origin in the distant future, i.e. the probability of reflection is called the **reflection coefficient**

$$R = \int dx\, |\psi_{\rm ref}(x,t)|^2\,, \quad t \to +\infty \tag{110}$$

- The probability of finding the particle to the right from the origin in the distant future, i.e. the probability of transmission is called the **transmission coefficient**

$$T = \int dx\, |\psi_{\rm trans}(x,t)|^2\,, \quad t \to +\infty \tag{111}$$

- The reflection and transmission coefficients can be computed by using (107) and (108)

  (i) The reflection coefficient

$$\begin{aligned} R &= \int dx\, |\psi_{\rm ref}(x,t)|^2 \\ &= \int dx \int_{E_{\min}}^{\infty} dE dE'\, C(E)\bar{C}(E')\, S_{LL}(E)\bar{S}_{LL}(E')\varphi_L^-(E,x)\bar{\varphi}_L^-(E',x)\, e^{\mathrm{i}\,(E'-E)\,t/\hbar} \\ &= \int_{E_{\min}}^{\infty} dE dE'\, \delta(E-E')\, C(E)\bar{C}(E')\, S_{LL}(E)\bar{S}_{LL}(E')\, e^{\mathrm{i}\,(E'-E)\,t/\hbar} \end{aligned} \tag{112}$$

$$R = \int_{E_{\min}}^{\infty} dE\, |C(E)|^2\, |S_{LL}(E)|^2 \tag{113}$$

  (ii) The transmission coefficient

$$T = \int_{E_{\min}}^{\infty} dE\, |C(E)|^2\, |S_{RL}(E)|^2 \tag{114}$$

  (iii) The sum of the reflection and transmission coefficients

$$R+T = \int_{E_{\min}}^{\infty} dE\, |C(E)|^2\, (|S_{LL}(E)|^2 + |S_{RL}(E)|^2) = \int_{E_{\min}}^{\infty} dE\, |C(E)|^2 = 1 \tag{115}$$

- In general R and T depend on the detailed shape of the wave function.
- In a scattering experiment a particle has $\langle P\rangle$ equal to some $\bar{p}$, and a very small uncertainty.
- The function $C(E)$ is nonzero only in a small neighbourhood of the point $\bar{E} = \bar{p}^2/2m + V_L$.
- R and T can be approximated by

$$R = \int_{E_{\min}}^{\infty} dE\, |C(E)|^2\, |S_{LL}(E)|^2 \approx |S_{LL}(\bar{E})|^2 \int_{E_{\min}}^{\infty} dE\, |C(E)|^2 = |S_{LL}(\bar{E})|^2\,, \quad T \approx |S_{RL}(\bar{E})|^2 \tag{116}$$

  They are independent of $C(E)$: it is important only that the interval in which it is nonzero be small.

- Consider the incident wave function (106), and use the momentum representation
- We make the substitution

$$E = \frac{p^2}{2m} + V_L = \frac{\hbar^2 k^2}{2m} + V_L \tag{117}$$

and get the following representation

$$\psi_{\rm inc}(x,t) = \frac{1}{\sqrt{2\pi}} \int_{k_{\rm min}}^{\infty} dk\, A(k)\, e^{{\rm i}\, k\, x}\, e^{-{\rm i}\, E\, t/\hbar}\,, \quad \int_{k_{\rm min}}^{\infty} dk\, |A(k)|^2 = 1 \tag{118}$$

(i) $k_{\rm min} = E_{\rm min} - V_L$

(ii) $A(k)$ is related to $C(E)$ as

$$A(k) = \sqrt{\frac{\hbar^2}{m}}\, \sqrt{k}\, C(E) \tag{119}$$

- Let $A(k)$ do not vanish in a small interval $[\,\bar{k} - \Delta k\,,\ \bar{k} + \Delta k\,]$, where $\Delta k/\bar{k} \ll 1$. Then,

$$\begin{aligned} \psi_{\rm inc}(x,t) &= \frac{1}{\sqrt{2\pi}} \int_{\bar{k}-\Delta k}^{\bar{k}+\Delta k} dk\, A(k)\, e^{{\rm i}\, k\, x - {\rm i}\, E\, t/\hbar} = \frac{1}{\sqrt{2\pi}} \int_{-\Delta k}^{\Delta k} dk\, A(\bar{k}+k)\, e^{{\rm i}\,(\bar{k}+k)\, x - {\rm i}\, E(\bar{k}+k)\, t/\hbar} \\ &= \frac{e^{{\rm i}\,\bar{k}\, x - {\rm i}\,\bar{E}\, t/\hbar}}{\sqrt{2\pi}} \int_{-\Delta k}^{\Delta k} dk\, A(\bar{k}+k)\, e^{{\rm i}\, k\,(x - \frac{\hbar\,\bar{k}}{m} t) - {\rm i}\, \frac{\hbar\, k^2}{2m}\, t} \\ &\approx \frac{e^{{\rm i}\,\bar{k}\,(x-\bar{v}\, t) - {\rm i}\, \frac{\bar{E} - m\bar{v}^2}{\hbar}\, t}}{\sqrt{2\pi}} \int_{-\Delta k}^{\Delta k} dk\, A(\bar{k}+k)\, e^{{\rm i}\, k\,(x-\bar{v}\, t)} = e^{{\rm i}\, \frac{\bar{E}-m\bar{v}^2}{\hbar}\, t} \psi_{\rm inc}(x - \bar{v}\, t\,,\ 0) \end{aligned} \tag{120}$$

(i) The group speed $\bar{v} \equiv \frac{\hbar\,\bar{k}}{m} = d\bar{E}/d\bar{p}$ is equal to the classical particle speed.

(ii) Apart from the phase factor in front which does not affect the probability density the wave packet moves along at the group speed $\bar{v}$.

- The reflected and transmitted wave functions can be analysed in the same way by taking into account that the phases of S-matrix coefficients may undergo rapid changes

$$S_{LR}(E) = \sqrt{T(E)}\, e^{\mathrm{i}\,\phi(E)}\,, \quad S_{LL}(E) = \sqrt{R(E)}\, e^{\mathrm{i}\,\xi_\ell(E)}\,, \quad S_{RR}(E) = \sqrt{R(E)}\, e^{\mathrm{i}\,\xi_r(E)} \tag{121}$$

- The S-matrix is unitary $\Rightarrow\ 2\phi - \xi_\ell - \xi_r = \pm\pi$
- Repeating for the reflected wave the calculation, we get

$$\begin{aligned}\psi_{\rm ref}(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{\bar k-\Delta k}^{\bar k+\Delta k} dk\, A(k) S_{LL}(E)\, e^{-\mathrm{i}\,k\,x-\mathrm{i}\,E\,t/\hbar} \\ &\approx \frac{e^{\mathrm{i}\,\bar k\,(-x-\bar v\,(t-\hbar\xi_\ell'(\bar E))-\mathrm{i}\,\frac{\bar E-m\bar v^2}{\hbar}\,t+\mathrm{i}\,\xi_\ell(\bar E)-\mathrm{i}\,m\bar v^2\xi_\ell'(\bar E)}}{\sqrt{2\pi}}\sqrt{R(\bar E)}\int_{-\Delta k}^{\Delta k} dk\, A(\bar k+k)\, e^{\mathrm{i}\,k\,\left(-x-\bar v\,(t-\hbar\xi_\ell'(\bar E))\right)} \\ &= e^{\mathrm{i}\,\frac{\bar E-m\bar v^2}{\hbar}\,t+\mathrm{i}\,\xi_\ell(\bar E)-\mathrm{i}\,m\bar v^2\xi_\ell'(\bar E)}\sqrt{R(\bar E)}\psi_{\rm inc}(-x-\bar v\,(t-\hbar\,\xi_\ell'(\bar E))\,,\,0)\end{aligned} \tag{122}$$

where $\xi_\ell'(E) = d\xi_\ell(E)/dE$.

(i) The probability density of the reflected wave packet

$$|\psi_{\rm ref}(x,t)|^2 \approx R(\bar E)|\psi_{\rm inc}(-x-\bar v\,(t-\hbar\,\xi_\ell'(\bar E)\,,\,0)|^2 \tag{123}$$

(ii) The reflected wave packet is of the same shape but smaller as the incident one

(iii) It moves along to the left at the group speed $\bar v$

(iv) There is a **time delay** given by

$$\text{time delay of the reflected wave} \;=\; \hbar\,\xi_\ell'(\bar E) \tag{124}$$

- For the transmitted wave we get

$$\psi_{\text{trans}}(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\bar{k}_R-\Delta k}^{\bar{k}_R+\Delta k} dk_R\, \widetilde{A}(k_R) S_{LR}(E)\, e^{\mathrm{i}\, k_R\, x - \mathrm{i}\, E\, t/\hbar}$$
$$\approx \frac{e^{\mathrm{i}\,\bar{k}_R\,(x-\bar{v}_R\,(t-\hbar\xi'_\phi(\bar{E}))-\mathrm{i}\,\frac{\bar{E}-m\bar{v}_R^2}{\hbar}\,t+\mathrm{i}\,\phi(\bar{E})-\mathrm{i}\,m\bar{v}_R^2\phi'(\bar{E})}}{\sqrt{2\pi}} \sqrt{T(\bar{E})} \int_{-\Delta k}^{\Delta k} dk_R\, \widetilde{A}(\bar{k}_R+k)\, e^{\mathrm{i}\,k_R\left(x-\bar{v}_R\,(t-\hbar\phi'(\bar{E}))\right)} \tag{125}$$

where

$$\widetilde{A}(k_R) = \sqrt{\frac{\hbar^2}{m}}\,\sqrt{k_R}\, C(E) \tag{126}$$

(i) The shape of the transmitted wave is different from the incident one unless $V_L = V_R$

(ii) It moves along to the right at the group speed $\bar{v}_R$ with a time delay given by

$$\text{time delay of the transmitted wave} \;=\; \hbar\,\phi'(\bar{E}) \tag{127}$$

- The consideration generalises to a time-dependent wave packet constructed only from $\varphi_R(E,x)$.

(i) It describes a particle approaching the origin from the right.

(ii) The reflection and transmission coefficients of the wave incident from the right are

$$\begin{aligned} R_r &\approx |S_{RR}(\bar{E})|^2 = |S_{LL}(\bar{E})|^2 = R \\ T_r &\approx |S_{LR}(\bar{E})|^2 = |S_{RL}(\bar{E})|^2 = T \end{aligned} \tag{128}$$

(iii) The coefficients do not depend on where the incident wave comes from.

(iv) This is clearly related to the time reversal symmetry.

- Finally, let us comment on the case where $V_L < E < V_R$.

  (i) There is only a wave incident from the left because $\psi(x) \to 0$ exponentially for $x > a$.

  (ii) At $t \to +\infty$ there will be only the reflected wave and the reflection coefficient is equal to 1.

  (iii) Thus, $|S_{LL}| = 1$ and $S_{LL} = \exp(\mathrm{i}\,\xi(E))$.

  (iv) The incident and reflected waves only differ by a phase factor.

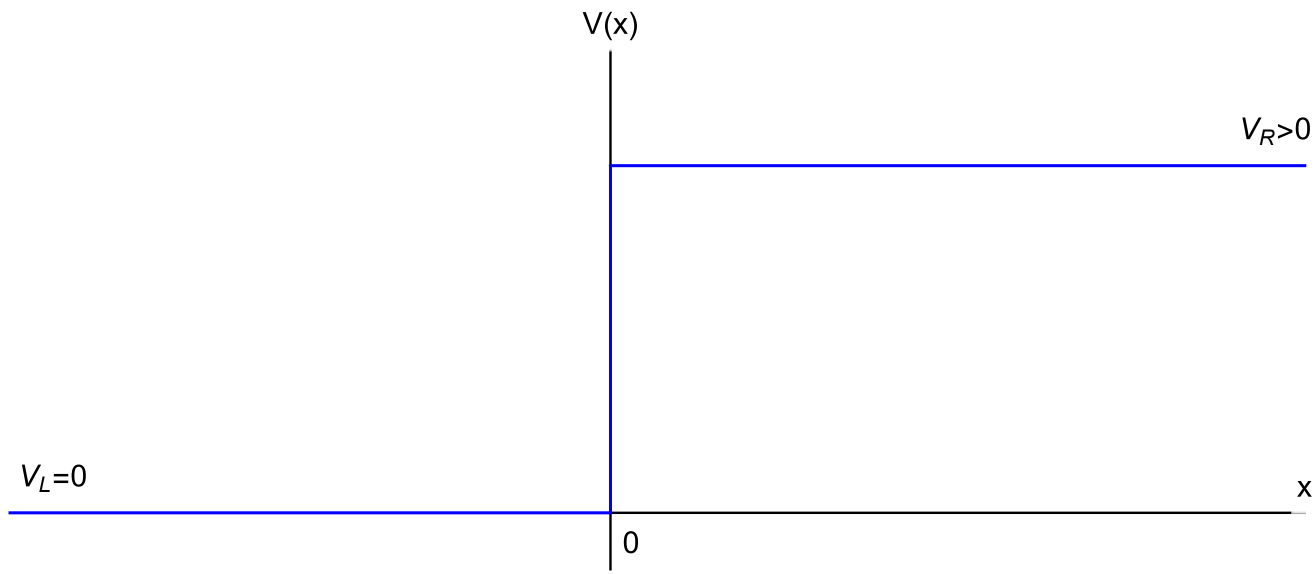
  (v) If we consider the wave packet (118), and repeat for the reflected wave the calculation done in (120), we get

$$\psi_{\mathrm{ref}}(x,t) \approx e^{\mathrm{i}\,\frac{\bar{E}-m\bar{v}^2}{\hbar}\,t+\mathrm{i}\,\xi(\bar{E})-\mathrm{i}\,m\bar{v}^2\xi'(\bar{E})}\psi_{\mathrm{inc}}(-x-\bar{v}\,(t-\hbar\xi'(\bar{E})\,,\,0) \tag{129}$$

  (vi) The probability density of the reflected wave packet

$$|\psi_{\mathrm{ref}}(x,t)|^2 \approx |\psi_{\mathrm{inc}}(-x-\bar{v}\,(t-\hbar\xi'(\bar{E})\,,\,0)|^2 \tag{130}$$

  (vii) The time delay $\hbar\,\xi'(\bar{E})$.



5.3 Step potential

Here we examine the step potential

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_R > 0 & \text{for } x > 0 \end{cases} \tag{131}$$

For this potential $a = 0$, and, therefore, we have only two regions.

I. $E > V_R$

(i) Solutions of TISE

$$\begin{aligned}
\psi_L(x) &= A_L \frac{e^{\mathrm{i}\,k_L\,x}}{\sqrt{k_L}} + B_L \frac{e^{-\mathrm{i}\,k_L\,x}}{\sqrt{k_L}}\,, \quad k_L = \frac{\sqrt{2mE}}{\hbar}\,, \quad x < 0 \\
\psi_R(x) &= A_R \frac{e^{\mathrm{i}\,k_R\,x}}{\sqrt{k_R}} + B_R \frac{e^{-\mathrm{i}\,k_R\,x}}{\sqrt{k_R}}\,, \quad k_R = \frac{\sqrt{2m(E-V_R)}}{\hbar}\,, \quad x > 0
\end{aligned} \tag{132}$$

(ii) The continuity conditions for $\psi(x)$ and $\psi'(x)$ at $x = 0$

$$\frac{A_L + B_L}{\sqrt{k_L}} = \frac{A_R + B_R}{\sqrt{k_R}}\,, \quad \sqrt{k_L}(A_L - B_L) = \sqrt{k_R}(A_R - B_R) \tag{133}$$

(iii) Solution to these equations

$$B_L = \frac{k_L - k_R}{k_L + k_R}\,A_L + \frac{2\sqrt{k_L k_R}}{k_L + k_R}\,B_R\,, \quad A_R = \frac{2\sqrt{k_L k_R}}{k_L + k_R}\,A_L - \frac{k_L - k_R}{k_L + k_R}\,B_R \tag{134}$$

(iv) The S-matrix

$$S = \begin{pmatrix} \frac{k_L - k_R}{k_L + k_R} & \frac{2\sqrt{k_L k_R}}{k_L + k_R} \\ \\ \frac{2\sqrt{k_L k_R}}{k_L + k_R} & -\frac{k_L - k_R}{k_L + k_R} \end{pmatrix} \tag{135}$$

(v) The reflection and transmission coefficients

$$R = \left(\frac{k_L - k_R}{k_L + k_R}\right)^2\,, \quad T = \frac{4 k_L k_R}{(k_L + k_R)^2} \tag{136}$$

(vi) $R + T = 1$

II. $0 < E < V_R$

(i) Solutions of TISE

$$\begin{aligned} \psi_L(x) &= A_L e^{\mathrm{i}\,k_L\,x} + B_L e^{-\mathrm{i}\,k_L\,x}\,, \quad k_L = \frac{\sqrt{2mE}}{\hbar}\,, \quad x < 0 \\ \psi_R(x) &= A_R e^{-\kappa\,x}\,, \quad \kappa = \frac{\sqrt{2m(V_R - E)}}{\hbar}\,, \quad x > 0 \end{aligned} \tag{137}$$

(ii) The continuity conditions

$$A_L + B_L = A_R\,, \quad \mathrm{i}k_L(A_L - B_L) = -\kappa A_R \tag{138}$$

(iii) Solution

$$B_L = \frac{k_L - \mathrm{i}\,\kappa}{k_L + \mathrm{i}\,\kappa}\,A_L\,, \quad A_R = \frac{2k_L}{k_L + \mathrm{i}\,\kappa}\,A_L \tag{139}$$

(iv) Thus

$$\frac{B_L}{A_L} = \frac{k_L - \mathrm{i}\,\kappa}{k_L + \mathrm{i}\,\kappa} = \frac{1 - \mathrm{i}\,\frac{\kappa}{k_L}}{1 + \mathrm{i}\,\frac{\kappa}{k_L}} = e^{\mathrm{i}\,\xi(E)}\,, \quad \xi(E) = -2\arctan\frac{\kappa}{k_L}\,, \quad \frac{\kappa}{k_L} = \sqrt{\frac{V_R}{E} - 1} \tag{140}$$

(v) The reflection coefficient is 1, and the time delay is

$$\text{time delay} \ = \ \hbar\,\xi'(\bar{E}) = \frac{\hbar}{\sqrt{E(V_R - E)}} \tag{141}$$

(vi) It has the minimum at $E = V_R/2$

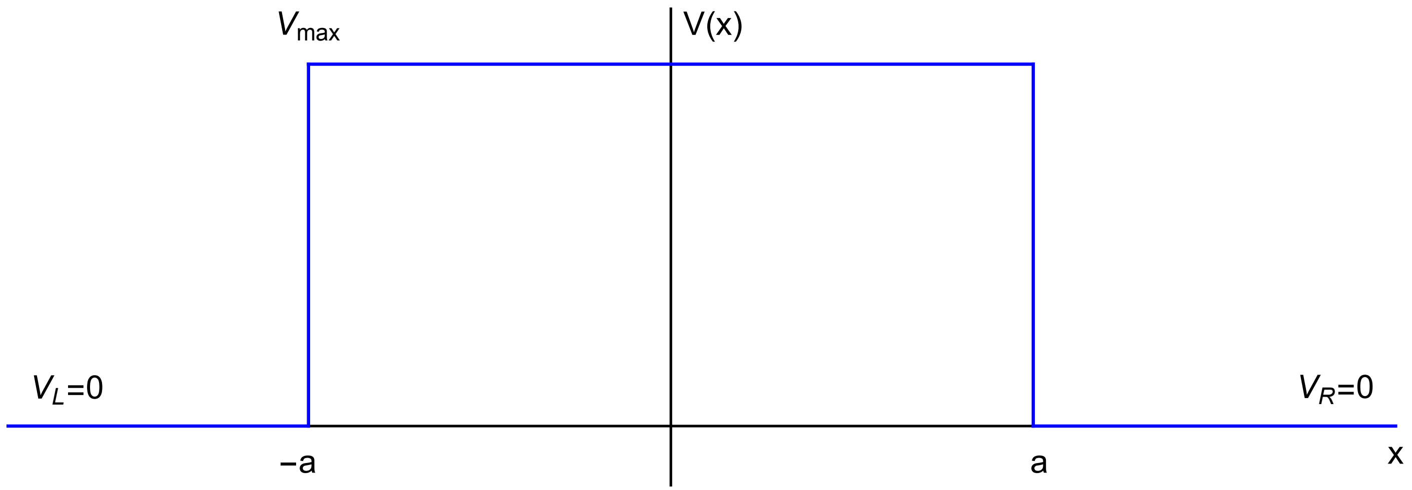


Figure 2: The square potential barrier $V(x)$.

5.4 Square potential barrier or well

Consider the scattering of a particle by a square (or rectangular) potential barrier or a well

$$V(x) = \begin{cases} 0 & \text{for } |x| > a \\ V_0 & \text{for } |x| < a \end{cases} \tag{142}$$

where $V_0 = V_{\max} > 0$ for a barrier, and $V_0 = V_{\min} < 0$ for a well.
There is no difference in the two cases.

- $V_L = V_R \;\Rightarrow\;$ use the momentum normalisation for plane waves
- Solutions of TISE

$$
\begin{aligned}
\psi_L(x) &= A_L e^{\mathrm{i}\,k\,x} + B_L e^{-\mathrm{i}\,k\,x}\,, \quad k = \frac{\sqrt{2mE}}{\hbar}\,, \quad x < -a \\
\psi_R(x) &= A_R e^{\mathrm{i}\,k\,x} + B_R e^{-\mathrm{i}\,k\,x}\,, \quad x > a \\
\psi_M(x) &= A_M e^{\mathrm{i}\,k_M\,x} + B_M e^{-\mathrm{i}\,k_M\,x}\,, \quad k_M = \frac{\sqrt{2m(E-V_0)}}{\hbar}\,, \quad |x| < a
\end{aligned}
\tag{143}
$$

- They are valid for any $E > 0$ but for $E < V_{\text{max}}$ the solution ψ_M has purely imaginary k_M.
- Continuity conditions at $x = \pm a$ allow one to express B_L, A_R, A_M, B_M in terms of A_L and B_R

$$
\begin{aligned}
B_L = S_{LL}\,A_L + S_{LR}\,B_R\,, &\quad A_R = S_{LL}\,B_R + S_{LR}\,A_L \\
A_M = K_{LL}\,A_L + K_{LR}\,B_R\,, &\quad B_M = K_{LL}\,B_R + K_{LR}\,A_L
\end{aligned}
\tag{144}
$$

(i) $S_{LL} = S_{RR},\; S_{LR} = S_{RL}$

$$
S_{LL} = \frac{e^{-2\mathrm{i}\,ak}\left(e^{4\mathrm{i}\,ak_M} - 1\right)(k^2 - k_M^2)}{e^{4\mathrm{i}\,ak_M}(k-k_M)^2 - (k+k_M)^2}\,, \quad S_{LR} = -\frac{4kk_M e^{-2\mathrm{i}\,a(k-k_M)}}{e^{4\mathrm{i}\,ak_M}(k-k_M)^2 - (k+k_M)^2}
\tag{145}
$$

(ii) K_{LL} and K_{LR}

$$
K_{LL} = \frac{(k+k_M)e^{ia(k-k_M)}}{2k_M}\,S_{LR}\,, \quad K_{LR} = \frac{(k_M-k)e^{ia(k+k_M)}}{2k_M}\,S_{LR}
\tag{146}
$$

- We do not really need K_{LL} and K_{LR}.
- The reflection and transmission coefficients

$$\begin{aligned} R = |S_{LL}|^2 &= \left(1 + \frac{4k^2k_M^2}{\left(k^2 - k_M^2\right)^2 \sin^2(2ak_M)}\right)^{-1} = \left(1 + \frac{4E(E-V_0)}{V_0^2 \sin^2(\frac{2a}{\hbar}\sqrt{2m(E-V_0)})}\right)^{-1} \\ T = |S_{LR}|^2 &= \left(1 + \frac{\left(k^2 - k_M^2\right)^2 \sin^2(2ak_M)}{4k^2k_M^2}\right)^{-1} = \left(1 + \frac{V_0^2 \sin^2(\frac{2a}{\hbar}\sqrt{2m(E-V_0)})}{4E(E-V_0)}\right)^{-1} \end{aligned} \tag{147}$$

- The transmission coefficient is equal to 1 if

$$2ak_M = \pi n \quad \Leftrightarrow \quad E_n - V_0 = \frac{\hbar^2\pi^2}{8m\,a^2}n^2\,, \quad n = n_0, n_0+1, n_0+2, \ldots \tag{148}$$

  (i) For a barrier $n_0 = 1$
  (ii) For a well n_0 is the lowest positive integer such that E_{n_0} is nonnegative.
  (iii) These values of E are precisely the energy levels of a particle in an infinitely deep well.

- The barrier or the well become transparent for these values of the energy.
- This is referred to as **resonance scattering**.
- For a potential well the transmission coefficient can be equal to 1 for $E = 0$ if there is an integer n_0 such that $|V_{\min}| = \frac{\hbar^2\pi^2}{8m\,a^2}n_0^2$.

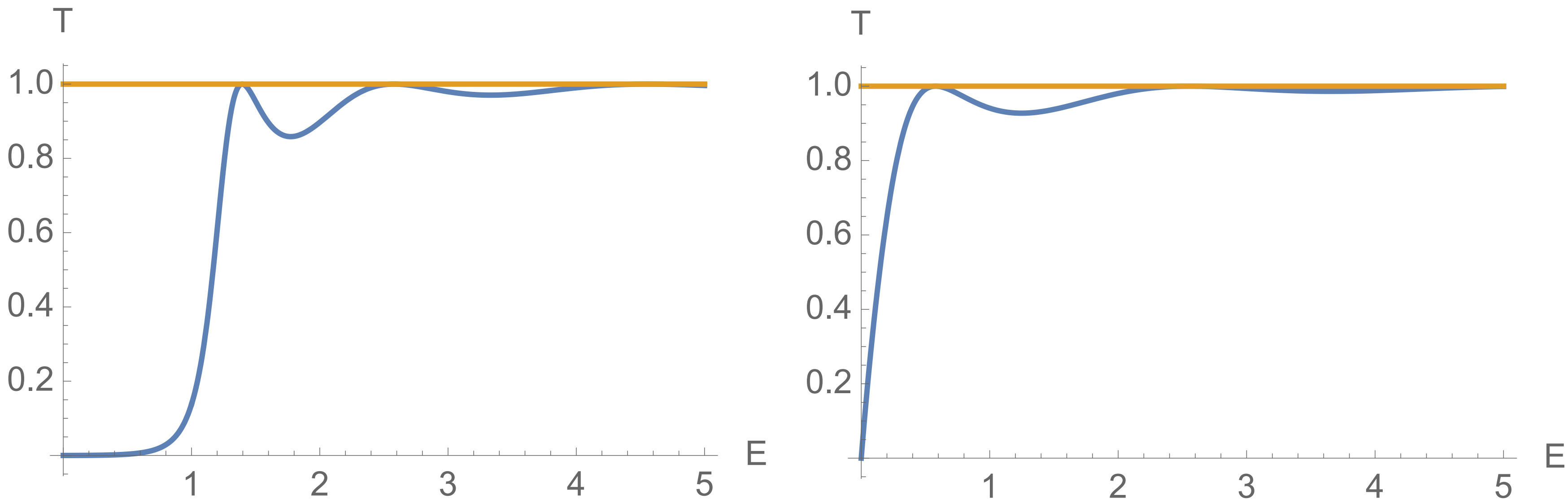


Figure 3: The transmission coefficients for a potential barrier and a well as a function of energy for $\hbar = 1$, $m = 0.5$, $a = 2.5$, $V_{\rm max} = -V_{\rm min} = 1$.

(i) For a potential barrier the transmission coefficient does not vanish if $E < V_{\rm max}$.

(ii) This is the tunnelling phenomenon.

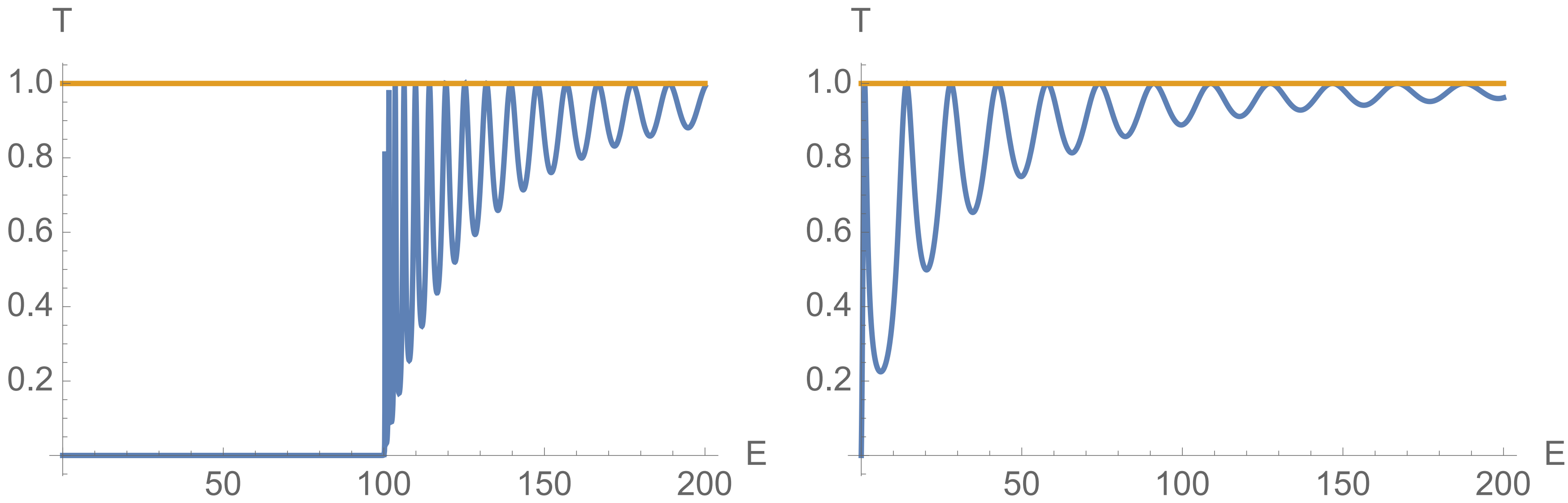


Figure 4: The transmission coefficients for a potential barrier and a well as a function of energy for $\hbar = 1$, $m = 0.5$, $a = 2.5$, $V_{\rm max} = -V_{\rm min} = 100$.

(iii) The higher the barrier is the smaller the transmission coefficient is for $E < V_{\rm max}$

(iv) For a deep well the transmission coefficient can be smaller than 1/2 for sufficiently large energy. The particle has a higher chance to be reflected by the well than to pass over it.

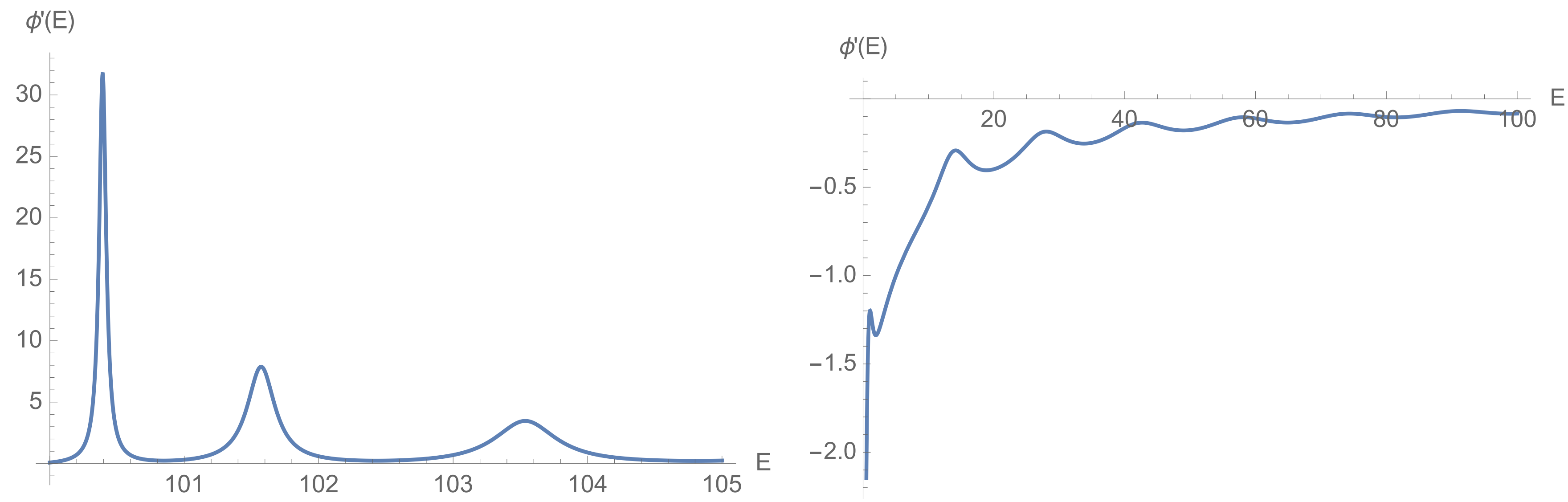


Figure 5: Time delays for a potential barrier and a well as a function of energy for $\hbar = 1$, $m = 0.5$, $a = 2.5$, $V_{\max} = -V_{\min} = 100$.

- The formula for S_{LR} allows one to find the phase shift ϕ between the incident and transmitted wave

$$\begin{aligned}\phi &= -2ak - \arctan\left(\frac{2kk_M \cot(2ak_M)}{k^2 + k_M^2}\right) \\ &= -\frac{2a}{\hbar}\sqrt{2mE} - \arctan\left(\frac{2\sqrt{E(E-V_0)}\cot(\frac{2a}{\hbar}\sqrt{2m(E-V_0)})}{2E - V_0}\right)\end{aligned} \tag{149}$$

  (i) The time delays clearly show patterns similar to the resonance patterns of figure 4.

  (ii) Since $S_{RR} = S_{LL}$ the time delays for a transmitted and reflected waves are equal.

- Another important property of the S-matrix is that for the case of a well, $V_0 < 0$, it as a function of energy has poles exactly at the bound state energies.
- Thus, poles of the S-matrix correspond to bound states.
- The formulae (147) simplify in the case of the δ-function barrier or well

  which is obtained in the limit $a \to 0,\ a\,V_{\max} = \nu = \text{const}\,,\ V(x) \to \nu\delta(x)$

$$R = \frac{1}{1 + \frac{\hbar^2}{8m\nu^2}E}\,, \quad T = \frac{1}{1 + \frac{8m\nu^2}{\hbar^2 E}} \tag{150}$$

- The coefficients depend only on ν^2, and therefore the particle is just as likely to pass through the barrier as to cross over the well.

6 Separation of variables

6.1 Particles interacting with external potentials but not with each other

The Hamiltonian of such a system of N spinless particles is given by

$$H = \sum_{a=1}^{N} H_a\,, \qquad H_a = \frac{\vec{P}_a^{\;2}}{2m_a} + V_a(\vec{X}_a) \tag{151}$$

- Since all H_a are compatible with each other and H, they can be diagonalised simultaneously.
- Denote their mutual eigenvectors by $|E_1, E_2, \ldots, E_N\rangle \equiv |E_1\rangle \otimes |E_2\rangle \otimes \ldots \otimes |E_N\rangle$

$$H_a|E_1, E_2, \ldots, E_N\rangle = E_a|E_1, E_2, \ldots, E_N\rangle\,, \quad a = 1, 2, \ldots, N \tag{152}$$

- The spectrum of H

$$H|E_1, E_2, \ldots, E_N\rangle = E|E_1, E_2, \ldots, E_N\rangle\,, \quad E = \sum_{a=1}^{N} E_a \tag{153}$$

- The variables $\vec{X}_a$ can be separated from each other
- Solve the spectrum problem for each of the N particles and find the energy spectrum of the whole system
- Dynamics is described by

$$e^{-\mathrm{i}Ht/\hbar}|E_1, E_2, \ldots, E_N\rangle = e^{-\mathrm{i}E_1/\hbar}|E_1\rangle \otimes e^{-\mathrm{i}E_2/\hbar}|E_2\rangle \otimes \ldots \otimes e^{-\mathrm{i}E_N/\hbar}|E_N\rangle \tag{154}$$

- For example, consider two particles in one dimension with the Hamiltonian

$$H = \frac{P_1^2}{2m_1} + V_1(X_1) + \frac{P_2^2}{2m_2} + V_2(X_2) = H_1 + H_2 \tag{155}$$

(i) The stationary Schrödinger equation for this system is

$$\left(-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} + V_1(X_1) - \frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_1^2} + V_2(X_2)\right)\psi_E(x_1, x_2) = E\psi_E(x_1, x_2) \tag{156}$$

(ii) The wave function can be found in the form

$$\psi_E(x_1, x_2) = \psi_{E_1}(x_1)\psi_{E_2}(x_2) \tag{157}$$

(iii) Substituting this ansatz in (156), and dividing both sides by $\psi_{E_1}(x_1)\psi_{E_2}(x_2)$, we get

$$\frac{1}{\psi_{E_1}(x_1)}\left(-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} + V_1(X_1)\right)\psi_{E_1}(x_1) + \frac{1}{\psi_{E_2}(x_2)}\left(-\frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_1^2} + V_2(X_2)\right)\psi_{E_2}(x_2) = E \tag{158}$$

(iv) The first term is a function of x_1 only, the second term is a function of x_2 only. Therefore,

$$\begin{aligned} \frac{1}{\psi_{E_1}(x_1)}\left(-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1^2} + V_1(X_1)\right)\psi_{E_1}(x_1) &= E_1 \\ \frac{1}{\psi_{E_2}(x_2)}\left(-\frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_1^2} + V_2(X_2)\right)\psi_{E_2}(x_2) &= E_2 \\ E_1 + E_2 &= E \end{aligned} \tag{159}$$

(v) ψ_{E_1} and ψ_{E_2} are eigenfunctions of the one-particle TISE with eigenvalues $E1$ and E_2.

- If V_1 and V_2 are some of the potentials we have discussed, we immediately get the spectrum of H.
- If V_1 is a harmonic oscillator potential, and V_2 is an Infinitely deep potential well

$$V_1(x_1) = \frac{m_1\omega^2 x_1^2}{2}, \quad V_2(x_2) = \begin{cases} \infty & \text{for } |x_2| > a \\ 0 & \text{for } |x_2| < a \end{cases} \tag{160}$$

(i) The spectrum is

$$E_{n_1 n_2} = \hbar\omega(n_1 + \frac{1}{2}) + \frac{\hbar^2\pi^2}{8m_2\, a^2} n_2^2 \tag{161}$$

(ii) It is in general nondegenerate.

- If both V_1 and V_2 are harmonic oscillator potentials with the same frequency ω

(i) The spectrum is

$$E_{n_1 n_2} = \hbar\omega(n_1 + n_2 + 1) \tag{162}$$

(ii) It is degenerate.

(iii) The degeneracy of a level with energy $E = \hbar\omega(n+1)$ is $n+1$.

(iv) It is explained by the rotational symmetry of H
which becomes manifest in terms of normal coordinates.

6.2 Two particles interacting with each other

Sometimes it is necessary to change coordinates to reduce a Hamiltonian to the form (151).

A system of two particles interacting with each other through translationally-invariant potential

$$H = \frac{\vec{P}_1^{\,2}}{2m_1} + \frac{\vec{P}_2^{\,2}}{2m_2} + V(\vec{X}_1 - \vec{X}_2) \tag{163}$$

- Let $m \equiv m_1 + m_2$ be the total mass, and let $\mu \equiv m_1 m_2/m$ be the reduced mass of the system.
- Introduce the centre of mass $\vec{X}_{\rm cm}$, the relative coordinate $\vec{X}$, and their conjugate momenta

$$\vec{X}_{\rm cm} = \frac{m_1}{m}\vec{X}_1 + \frac{m_2}{m}\vec{X}_2\,, \quad \vec{X} = \vec{X}_1 - \vec{X}_2\,, \quad \vec{P}_{\rm cm} = \vec{P}_1 + \vec{P}_2\,, \quad \vec{P} = \frac{m_2}{m}\vec{P}_1 - \frac{m_1}{m}\vec{P}_2 \tag{164}$$

- The new coordinates and momenta satisfy the canonical commutation relations
- The Hamiltonian takes the form

$$H = \frac{\vec{P}_{\rm cm}^{\,2}}{2m} + \frac{\vec{P}^{\,2}}{2\mu} + V(\vec{X}) \tag{165}$$

- $\vec{X}_{\rm cm}$ and $\vec{X}$ can be separated
- The eigenfunctions of H factorise

$$\psi_E(\vec{x}_{\rm cm}, \vec{x}) = \frac{e^{\mathrm{i}\,\vec{p}_{\rm cm}\cdot\vec{x}_{\rm cm}/\hbar}}{(2\pi\hbar)^{d/2}}\psi_{E_{\rm rel}}(\vec{x})\,, \quad E = \frac{\vec{p}_{\rm cm}^{\,2}}{2m} + E_{\rm rel} \tag{166}$$

  where d is the number of space dimensions.
- The total spectrum is always continuous because of the centre of mass motion.