

4.3 Wave mechanics

Potential step^a

Potential function	$V(x) = \begin{cases} 0 & (x < 0) \\ V_0 & (x \geq 0) \end{cases} \quad (4.38)$	V particle potential energy V_0 step height $\hbar$ (Planck constant)/(2 π)
Wavenumbers	$\hbar^2 k^2 = 2mE \quad (x < 0) \quad (4.39)$	k, q particle wavenumbers
	$\hbar^2 q^2 = 2m(E - V_0) \quad (x > 0) \quad (4.40)$	m particle mass E total particle energy
Amplitude reflection coefficient	$r = \frac{k - q}{k + q} \quad (4.41)$	r amplitude reflection coefficient
Amplitude transmission coefficient	$t = \frac{2k}{k + q} \quad (4.42)$	t amplitude transmission coefficient
Probability currents ^b	$j_I = \frac{\hbar k}{m} (1 - r ^2) \quad (4.43)$	j_I particle flux in zone I
	$j_{II} = \frac{\hbar q}{m} t ^2 \quad (4.44)$	j_{II} particle flux in zone II

^aOne-dimensional interaction with an incident particle of total energy $E = KE + V$. If $E < V_0$ then q is imaginary and $|r|^2 = 1$. $1/|q|$ is then a measure of the tunnelling depth.

^bParticle flux with the sign of increasing x .

Potential well^a

Potential function	$V(x) = \begin{cases} 0 & (x > a) \\ -V_0 & (x \leq a) \end{cases} \quad (4.45)$	V particle potential energy V_0 well depth $\hbar$ (Planck constant)/(2π) $2a$ well width
Wavenumbers	$\hbar^2 k^2 = 2mE \quad (x > a) \quad (4.46)$ $\hbar^2 q^2 = 2m(E + V_0) \quad (x < a) \quad (4.47)$	k, q particle wavenumbers m particle mass E total particle energy
Amplitude reflection coefficient	$r = \frac{\mathbf{i}e^{-2ika}(q^2 - k^2)\sin 2qa}{2kq \cos 2qa - \mathbf{i}(q^2 + k^2)\sin 2qa} \quad (4.48)$	r amplitude reflection coefficient
Amplitude transmission coefficient	$t = \frac{2kqe^{-2ika}}{2kq \cos 2qa - \mathbf{i}(q^2 + k^2)\sin 2qa} \quad (4.49)$	t amplitude transmission coefficient
Probability currents ^b	$j_{\text{I}} = \frac{\hbar k}{m}(1 - r ^2) \quad (4.50)$	j_{I} particle flux in zone I
	$j_{\text{III}} = \frac{\hbar k}{m} t ^2 \quad (4.51)$	j_{III} particle flux in zone III
Ramsauer effect ^c	$E_n = -V_0 + \frac{n^2 \hbar^2 \pi^2}{8ma^2} \quad (4.52)$	n integer > 0 E_n Ramsauer energy
Bound states ($V_0 < E < 0$) ^d	$\tan qa = \begin{cases} k /q & \text{even parity} \\ -q/ k & \text{odd parity} \end{cases} \quad (4.53)$	
	$q^2 - k ^2 = 2mV_0/\hbar^2 \quad (4.54)$	

^aOne-dimensional interaction with an incident particle of total energy $E = KE + V > 0$.

^bParticle flux in the sense of increasing x .

^cIncident energy for which $2qa = n\pi$, $|r| = 0$, and $|t| = 1$.

^dWhen $E < 0$, k is purely imaginary. $|k|$ and q are obtained by solving these implicit equations.

Barrier tunnelling^a

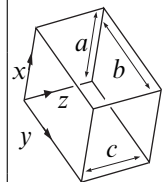
Potential function	$V(x) = \begin{cases} 0 & (x > a) \\ V_0 & (x \leq a) \end{cases} \quad (4.55)$	V particle potential energy V_0 well depth $\hbar$ (Planck constant)/(2π) $2a$ barrier width
Wavenumber and tunnelling constant	$\hbar^2 k^2 = 2mE \quad (x > a) \quad (4.56)$	k incident wavenumber
	$\hbar^2 \kappa^2 = 2m(V_0 - E) \quad (x < a) \quad (4.57)$	κ tunnelling constant
		m particle mass
		E total energy ($< V_0$)
Amplitude reflection coefficient	$r = \frac{-i e^{-2ika} (k^2 + \kappa^2) \sinh 2\kappa a}{2k\kappa \cosh 2\kappa a - i(k^2 - \kappa^2) \sinh 2\kappa a} \quad (4.58)$	r amplitude reflection coefficient
Amplitude transmission coefficient	$t = \frac{2k\kappa e^{-2ika}}{2k\kappa \cosh 2\kappa a - i(k^2 - \kappa^2) \sinh 2\kappa a} \quad (4.59)$	t amplitude transmission coefficient
Tunnelling probability	$ t ^2 = \frac{4k^2 \kappa^2}{(k^2 + \kappa^2)^2 \sinh^2 2\kappa a + 4k^2 \kappa^2} \quad (4.60)$ $\simeq \frac{16k^2 \kappa^2}{(k^2 + \kappa^2)^2} \exp(-4\kappa a) \quad (t ^2 \ll 1) \quad (4.61)$	$ t ^2$ tunnelling probability
Probability currents ^b	$j_I = \frac{\hbar k}{m} (1 - r ^2) \quad (4.62)$	j_I particle flux in zone I
	$j_{III} = \frac{\hbar k}{m} t ^2 \quad (4.63)$	j_{III} particle flux in zone III

^aBy a particle of total energy $E = KE + V$, through a one-dimensional rectangular potential barrier height $V_0 > E$.

^bParticle flux in the sense of increasing x .

Particle in a rectangular box^a

Eigenfunctions	$\Psi_{lmn} = \left(\frac{8}{abc} \right)^{1/2} \sin \frac{l\pi x}{a} \sin \frac{m\pi y}{b} \sin \frac{n\pi z}{c} \quad (4.64)$	Ψ_{lmn} eigenfunctions a, b, c box dimensions l, m, n integers ≥ 1
Energy levels	$E_{lmn} = \frac{h^2}{8M} \left(\frac{l^2}{a^2} + \frac{m^2}{b^2} + \frac{n^2}{c^2} \right) \quad (4.65)$	E_{lmn} energy h Planck constant M particle mass
Density of states	$\rho(E) dE = \frac{4\pi}{h^3} (2M^3 E)^{1/2} dE \quad (4.66)$	$\rho(E)$ density of states (per unit volume)



^aSpinless particle in a rectangular box bounded by the planes $x=0$, $y=0$, $z=0$, $x=a$, $y=b$, and $z=c$. The potential is zero inside and infinite outside the box.

Harmonic oscillator

Schrödinger equation	$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \psi_n = E_n \psi_n \quad (4.67)$	$\hbar$ (Planck constant)/(2 π) m mass ψ_n n th eigenfunction x displacement
Energy levels ^a	$E_n = \left(n + \frac{1}{2}\right) \hbar \omega \quad (4.68)$	n integer ≥ 0 ω angular frequency E_n total energy in n th state
Eigen-functions	$\psi_n = \frac{H_n(x/a) \exp[-x^2/(2a^2)]}{(n! 2^n a \pi^{1/2})^{1/2}} \quad (4.69)$ where $a = \left(\frac{\hbar}{m\omega}\right)^{1/2}$	H_n Hermite polynomials
Hermite polynomials	$\begin{aligned} H_0(y) &= 1, & H_1(y) &= 2y, & H_2(y) &= 4y^2 - 2 \\ H_{n+1}(y) &= 2yH_n(y) - 2nH_{n-1}(y) \end{aligned} \quad (4.70)$	y dummy variable

^a E_0 is the zero-point energy of the oscillator.