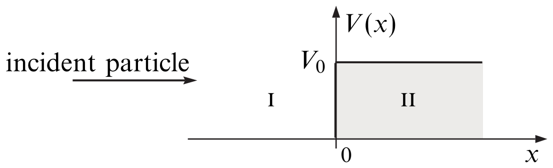
4.3 Wave mechanics

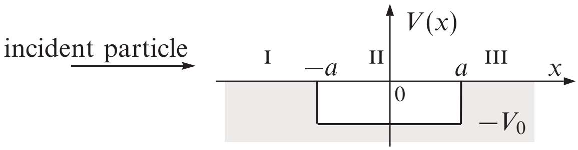
Potential step[a]



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

[a]One-dimensional interaction with an incident particle of total energy $E=\text{KE}+V$. If $E<V_0$ then q is imaginary and $|r|^2=1$. $1/|q|$ is then a measure of the tunnelling depth.
[b]Particle flux with the sign of increasing x.

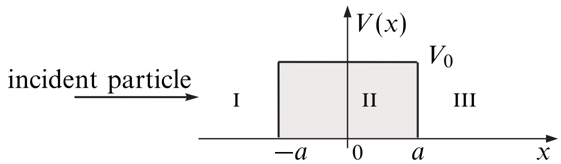
Potential well[a]



Potential function	$$V(x)=\begin{cases}0 & (\lvert x\rvert>a)\\ -V_0 & (\lvert x\rvert\le a)\end{cases} \quad (4.45)$$	V particle potential energy V_0 well depth $\hbar$ (Planck constant)/(2π) $2a$ well width
Wavenumbers	$$\hbar^2k^2=2mE \quad (\lvert x\rvert>a) \quad (4.46)$$ $$\hbar^2q^2=2m(E+V_0) \quad (\lvert x\rvert<a) \quad (4.47)$$	k,q particle wavenumbers m particle mass E total particle energy
Amplitude reflection coefficient	$$r=\frac{\mathrm{i}e^{-2\mathrm{i}ka}(q^2-k^2)\sin 2qa}{2kq\cos 2qa-\mathrm{i}(q^2+k^2)\sin 2qa} \quad (4.48)$$	r amplitude reflection coefficient
Amplitude transmission coefficient	$$t=\frac{2kqe^{-2\mathrm{i}ka}}{2kq\cos 2qa-\mathrm{i}(q^2+k^2)\sin 2qa} \quad (4.49)$$	t amplitude transmission coefficient
Probability currents[b]	$$j_{\mathrm{I}}=\frac{\hbar k}{m}(1-\lvert r\rvert^2) \quad (4.50)$$ $$j_{\mathrm{III}}=\frac{\hbar k}{m}\lvert t\rvert^2 \quad (4.51)$$	j_{I} particle flux in zone I 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]	$$\tan qa=\begin{cases}\lvert k\rvert/q & \text{even parity}\\ -q/\lvert k\rvert & \text{odd parity}\end{cases} \quad (4.53)$$ $$q^2-\lvert k\rvert^2=2mV_0/\hbar^2 \quad (4.54)$$	

[a] One-dimensional interaction with an incident particle of total energy $E=\mathrm{KE}+V>0$.
[b] Particle flux in the sense of increasing x.
[c] Incident energy for which $2qa=n\pi$, $\lvert r\rvert=0$, and $\lvert t\rvert=1$.
[d] When $E<0$, k is purely imaginary. $\lvert k\rvert$ and q are obtained by solving these implicit equations.

Barrier tunnelling[a]

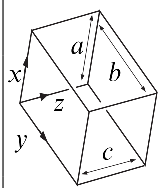


Potential function	$V(x)=\begin{cases}0 & (\lvert x\rvert>a)\\ V_0 & (\lvert x\rvert\le a)\end{cases}$ (4.55)	V V_0 $\hbar$ $2a$	particle potential energy well depth (Planck constant)/(2π) barrier width
Wavenumber and tunnelling constant	$\hbar^2k^2=2mE \quad (\lvert x\rvert>a)$ (4.56) $\hbar^2\kappa^2=2m(V_0-E)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

[a] By a particle of total energy $E=\mathrm{KE}+V$, through a one-dimensional rectangular potential barrier height $V_0>E$.
[b] Particle flux in the sense of increasing x.

Particle in a rectangular box[a]

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



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

[a] E_0 is the zero-point energy of the oscillator.