Schrodinger 1D Formulas

Convenience Variables for Wave Solutions: $k = \frac{2\pi}{\lambda}, \omega = 2\pi f = \frac{2\pi}{T}$

Complex Wave: $\psi(x,t) = A\exp\left(i\left[kx - \omega t\right]\right) = A\exp\left(2\pi i\left[\frac{x}{\lambda} - \frac{t}{T}\right]\right)$

Fourier Transform (physics convention) :

$$\psi(x) = \int dk\, a(k)\exp(ikx) \leftrightarrow a(k) = \frac{1}{2\pi}\int dx\, \psi(x)\exp(-ikx)$$

Fourier Transform of Gaussian:

$$\psi(x) = \frac{1}{\sqrt{2\pi}\,\sigma_x}\exp\left(\frac{-x^2}{2\sigma_x^2}\right) \leftrightarrow a(k) = \frac{1}{\sqrt{2\pi}\,\sigma_k}\exp\left(\frac{-k^2}{2\sigma_k^2}\right) \quad \sigma_x \cdot \sigma_k = 1$$

Classical Kinetic Energy: $E_{\text{kinetic}} = \frac{1}{2}mv^2 = \frac{p^2}{2m} \to p = \sqrt{2mE_{\text{kinetic}}}$

Planck-Einstein Relation: $E = hf = \frac{hc}{\lambda} = \hbar\omega$ with $\hbar = \frac{h}{2\pi}$, $\hbar c = 197.4$ eV-nm

de Broglie Relation: $\lambda = \frac{h}{p} \to p = \frac{h}{\lambda} = \frac{h}{2\pi/k} = \hbar k$

1D Time-Dependent Schrodinger: $i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\cdot\psi \to \psi(x,t)$

Free Particle $(V = 0)$ Solution: $\psi_{\text{free}}(x,t) = A\exp\left(i\left[kx - \omega t\right]\right)$ with $k = \frac{\pm\sqrt{2mE}}{\hbar}$ and $\omega = \frac{E}{\hbar}$

Probability Density (un-normalized: $\rho(x) = \psi^*\psi$, real and positive

Normalization: $\psi \to \psi\Big/\sqrt{\int dx\, \psi^*\psi}$

Momentum Operator: $p_{op}\psi = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi \;\to\; -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{\hbar^2}{2m}p_{op}^2\psi$

Probability Current Density: $\frac{\hbar}{2im}\left[\psi^*\cdot\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\cdot\psi\right] = \text{Re}\left[\psi^*\cdot\frac{p_{op}}{m}\psi\right]$

Probability Conservation: $\frac{\partial}{\partial t}\left[\psi^*\psi\right] + \frac{\partial}{\partial x}\frac{\hbar}{2im}\left[\psi^*\cdot\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\cdot\psi\right] = 0$

1D Time-Independent Schrodinger: $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x)\cdot\psi=E\psi\rightarrow\psi(x)$

$E>$ flat V solution: $\psi(x)=A\exp(ikx)$ with $k=\frac{\sqrt{2m\cdot(E-V)}}{\hbar}$

$E<$ flat V solution: $\psi(x)=A\exp(ik'x)$ with $k'=\frac{\sqrt{2m\cdot(E-V)}}{\hbar}=i\frac{\sqrt{2m\cdot|E-V|}}{\hbar}$

Boundary conditions at sharp step: $\psi_{\text{inc}}+\psi_{\text{refl}}=\psi_{\text{trans}}$ $\quad\frac{\partial}{\partial x}(\psi_{\text{inc}}+\psi_{\text{refl}})=\frac{\partial}{\partial x}\psi_{\text{trans}}$

$\rightarrow 1+R=T\quad k-kR=k'T\quad\rightarrow\quad R=\frac{k-k'}{k+k'}\quad T=\frac{2k}{k+k'}$ note that $\frac{\sqrt{2m}}{\hbar}$ cancels

Probability densities: R^*R and T^*T

For flux, multiply by $v=\frac{p}{m}=\frac{\hbar k}{m}$ or $v'=\frac{\hbar k'}{m}$

Tunnelling through $V>E$ Barrier: $\text{Probability}=G\cdot\exp\left(-2\frac{\sqrt{2m}}{\hbar}\int_{x1}^{x2}dx\sqrt{V(x)-E}\right)$

For sharp steps at x_1 and x_2: $G=16\frac{E}{V}\cdot\left(1-\frac{E}{V}\right)$

For flat top and length $=L$: $P=G\cdot\exp(-2\kappa L)$ with $\kappa=\frac{\sqrt{2m\cdot(V-E)}}{\hbar}=\frac{5.123}{\sqrt{\text{eV}}\text{-nm}}\sqrt{V-E}$ for electron

For sharp step to $V=\infty$: $\psi=0$ at step

Infinite Square Well: $V=0$ for $0<x<w$ but $V=\infty$ elsewhere

Solutions: $\psi_n(x)=A\sin\left(n\frac{\pi x}{w}\right)$ with $n=1,2,3,\ldots$ and $A=\sqrt{\frac{2}{w}}$ for normalization

Energies: $E_n=n^2\cdot\frac{1}{2m}\cdot\left(\frac{\hbar\pi}{w}\right)^2=n^2\cdot\frac{0.3763\text{ eV-nm}^2}{w^2}$ for electron

Harmonic Oscillator with spring constant k: $V(x)=\frac{1}{2}kx^2\quad\omega=\sqrt{\frac{k}{m}}$

Solutions: $\psi_n=\exp\left(-\frac{y^2}{2}\right)\cdot H_n(y)$ with $y=\frac{x}{b}$, $n=0,1,2,\ldots$

with $b^2=\frac{\hbar}{\sqrt{km}}=\frac{0.2761\sqrt{\text{eV}}\text{-nm}}{\sqrt{k}}$ for electron

Hermite Polynomials: $H_0(y)=1\quad H_1(y)=y\quad H_2(y)=y^2-\frac{1}{2}$

Energies: $E_n=\left(n+\frac{1}{2}\right)\hbar\omega=\left(n+\frac{1}{2}\right)\hbar\sqrt{\frac{k}{m}}=\left(n+\frac{1}{2}\right)\cdot\left(0.2761\sqrt{\text{eV}}\text{-nm}\right)\cdot\sqrt{k}$ for electron