XXVII. Solution of Schrödinger Wave Equation for Propagation of an Electron

Given an electron of mass, m_e, velocity, v_e, kinetic energy of 1 eV

By Quantum Mechanics. it has an associated de Broglie wavelength, λ_e, and wavenumber k_0

Planck's Constant: $h := 6.626 \cdot 10^{-34} J \cdot s$

Given: $m_e := 9.10938 \cdot 10^{-31} kg$ $\quad v := 1 \cdot 10^3 \frac{m}{s}$ $\quad T := 1 eV$ $\quad \lambda_e := \frac{h}{\sqrt{2 \cdot m_e \cdot T}} = 12.265 \cdot A$

Consider a monochromatic E Field plane wave associated with an electron which propagates in an isotropic and homogeneous medium: $E(r,t) = E_0 \cdot e^{[i \cdot (k \cdot r - \omega \cdot t)]}$

Associated with this electron is a wavenumber, k_e, amplitude, A

$k_e := 8.637 \cdot 10^6 \cdot \frac{1}{m}$ $\quad A := \frac{1}{\sqrt{a \cdot \sqrt{\pi}}}$ $\quad h_{bar} := \frac{h}{2 \cdot \pi}$ $\quad A_m := A \cdot \sqrt{m}$

$eV := 1.602 \cdot 10^{-19} J$

The electron has Kinetic Energy: $E := \frac{h_{bar}{}^2 \cdot k_e{}^2}{2.m_e}$ $\quad E = 4.554 \times 10^{-25} J$ $\quad$ **Electron Frequency:** $\omega = 2\pi \cdot f$

Equation of Traveling Wave: $\psi(x) = A \cdot e^{i \cdot (k \cdot x - \omega \cdot t)} + B \cdot e^{-i \cdot (k \cdot x + \omega \cdot t)}$

To solve the one-dimensional Schrödinger equation for a free particle of mass m moving with velocity v, we can proceed a follows:

Solve Schrödinger's Wave Equation for the Quantum Wavefunction, Ψ(x, t)

$$\frac{-\hbar^2}{2 \cdot m_e} \cdot \frac{\partial^2}{\partial x^2} \Psi = i \cdot \hbar \cdot \frac{\partial}{\partial t} \Psi$$

$$\Psi(x,t) = \int_{-\infty}^{\infty} \psi(k,x,t)\, dk$$

$$\Psi(x,t) = \frac{A \cdot a}{\sqrt{2\pi}} \cdot \int_{-\infty}^{\infty} exp\left[\frac{-1}{2} a^2 \cdot (k - k_0)^2 + i \cdot k \cdot x - \frac{i \cdot h_{bar} \cdot t}{2 \cdot m_e} \cdot k^2\right] dk$$

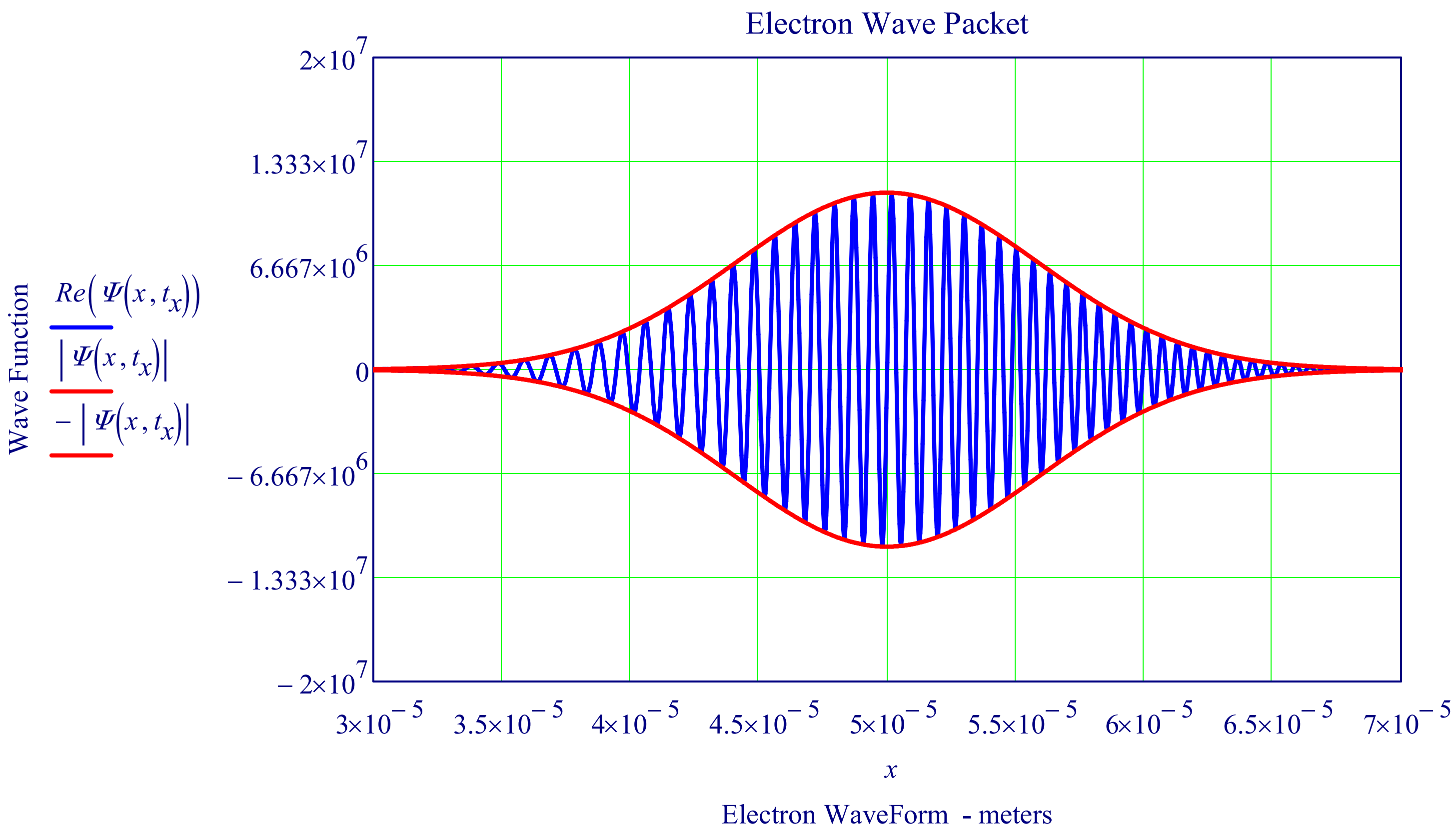
Evaluate the Wavefunction over the Space and Time Region: $\quad a := 1 \cdot \mu m \quad t_x := 50ns$

Solution for Ψ(x,t):

$$\Psi(x,t) := \frac{A_m}{\sqrt{1 + \frac{i \cdot h_{bar} \cdot t}{m_e \cdot a^2}}} \cdot exp\left[\frac{-\left(x^2 - 2 \cdot i \cdot a^2 \cdot k_e \cdot x + \frac{i \cdot h_{bar} \cdot t}{2.m_e} \cdot k_e{}^2 \cdot a^2\right)}{2 \cdot a^2 \cdot \left(1 + \frac{i \cdot h_{bar} \cdot t}{m_e \cdot a^2}\right)}\right]$$

Plot Wavefunction Ψ(x,t) over Distance Range, x

Distance Range: $x := 10^{-5} \cdot 2m, 10^{-5} \cdot 2m + \left(\frac{10^{-5} \cdot 8 \cdot m - 10^{-5} \cdot 2m}{2000} \right) .. 10^{-5} \cdot 8m$



Numerical Schrödinger Equation Solutions for 3-D Harmonic Oscillator

Parameters:

$E := 7.5$ $L := 0$

Reduced mass: $\mu := 1$ Angular momentum: $L := 0$ Integration limit: $r_{max} := 6$ $r := 0, 0.01 .. r_{max}$

Force constant: $k := 1$

Solve Schrödinger's equation numerically. Use Mathcad's ODE solve block:

Given

$$\frac{-1}{2\cdot\mu}\cdot\frac{d^2}{dr^2}\Psi(r) - \frac{1}{r\cdot\mu}\cdot\frac{d}{dr}\Psi(r) + \left[\frac{L\cdot(L+1)}{2\cdot\mu\cdot r^2} + \frac{1}{2}\cdot k\cdot r^2\right]\cdot\Psi(r) = E\cdot\Psi(r)$$

$$\Psi(.001) = .1 \qquad \Psi'(.001) = .1$$

$$\Psi := Odesolve\left(r, r_{max}\right)$$

Energy guess: $E \equiv 7.5$

Normalize the wavefunction: $\Psi(r) := \left(\int_0^{r_{max}} \Psi(r)^2\cdot 4\cdot\pi\cdot r^2\, dr\right)^{\frac{-1}{2}}\cdot\Psi(r)$