

Numerical Solutions for Schrodinger's Equation

Integration limit: $x_{\max} := 10$ Effective mass: $\mu := 1$

Potential energy: $V_0 := 2$ atoms := 2 $V(x) := V_0 \cdot \left(\cos\left(\text{atoms} \cdot 2 \cdot \pi \cdot \frac{x}{x_{\max}} \right) + 1 \right)$

Numerical integration of Schrodinger's equation:

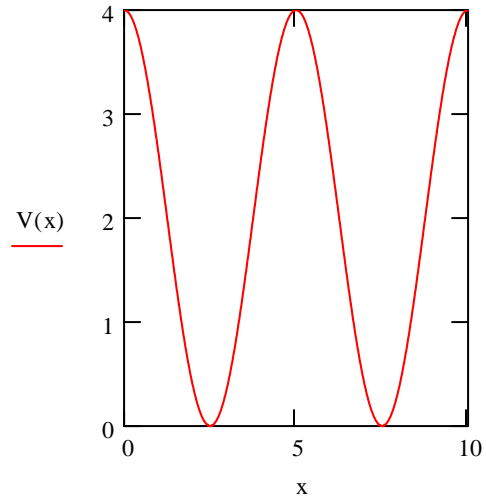
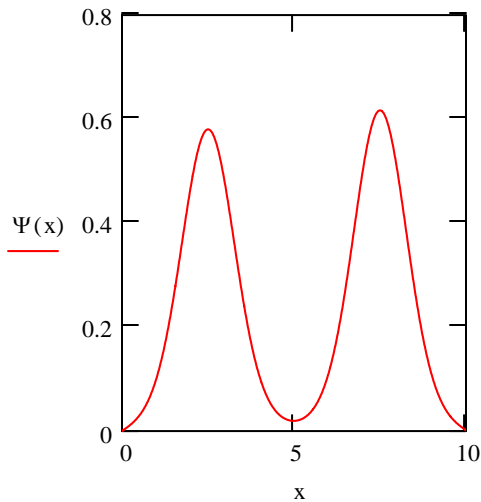
Given $\frac{-1}{2 \cdot \mu} \cdot \frac{d^2}{dx^2} \Psi(x) + V(x) \cdot \Psi(x) = E \cdot \Psi(x)$ $\Psi(0) = 0$ $\Psi'(0) = 0.1$

$\Psi := \text{Odesolve}(x, x_{\max})$

Normalize wave function:

$$\Psi(x) := \frac{\Psi(x)}{\sqrt{\int_0^{x_{\max}} \Psi(x)^2 dx}}$$

Enter energy guess: $E \equiv .83583$



Fourier transform coordinate wave function into momentum space.

$p := -10, -9.9 .. 10$ $\Phi(p) := \frac{1}{\sqrt{2 \cdot \pi}} \cdot \int_0^{x_{\max}} \exp(-i \cdot p \cdot x) \cdot \Psi(x) dx$

