

10.1: Trial Wavefunctions for Various Potentials

This is list of functions and the potentials for which they would be suitable trial wave functions in a variation method calculation.

$$\psi(x, \alpha) = 2 \cdot \alpha^{\frac{3}{2}} \cdot x \cdot \exp(-\alpha \cdot x)$$

$$\psi(x, \alpha) = \left(\frac{128 \cdot \alpha^3}{\pi}\right)^{\frac{1}{4}} \cdot \exp(-\alpha \cdot x^2)$$

- Particle in a gravitational field $V(z) = mgz$ ($z = 0$ to ∞)
- Particle confined by a linear potential $V(x) = ax$ ($x = 0$ to ∞)
- One-dimensional atoms and ions $V(x) = -Z/x$ ($x = 0$ to ∞)
- Particle in semi-infinite potential well $V(x) = \text{if}[x \leq a, 0, b]$ ($x = 0$ to ∞)
- Particle in semi-harmonic potential well $V(x) = kx^2$ ($x = 0$ to ∞)

$$\psi(x, \alpha) = \left(\frac{2 \cdot \alpha}{\pi}\right)^{\frac{1}{4}} \cdot \exp(-\alpha \cdot x^2)$$

- Quartic oscillator $V(x) = bx^4$ ($x = -\infty$ to ∞)
- Particle in the finite one-dimensional potential well $V(x) = \text{if}[(x \geq -1 \cdot (x \leq 1), 0, 2]$ ($x = -\infty$ to ∞)
- 1D Hydrogen atom ground state
- Harmonic oscillator ground state
- Particle in $V(x) = |x|$ potential well

$$\psi(x, \alpha) = \sqrt{\alpha} \cdot \exp(-\alpha \cdot |x|)$$

- This wavefunction is discontinuous at $x = 0$, so the following calculations must be made in momentum space
- Dirac hydrogen atom $V(x) = -\Delta(x)$
- Harmonic oscillator ground state
- Particle in $V(x) = |x|$ potential well
- Quartic oscillator $V(x) = bx^4$ ($x = -\infty$ to ∞)

$$\psi(x) = \sqrt{30} \cdot x \cdot (1 - x)$$

$$\Gamma(x) = \sqrt{105} \cdot x \cdot (1 - x)^2$$

$$\Theta(x) = \sqrt{105} \cdot x^2 \cdot (1 - x)$$

- Particle in a one-dimensional, one-bohr box
- Particle in a slanted one-dimensional box
- Particle in a semi-infinite potential well (change 1 to variational parameter)
- Particle in a gravitational field (change 1 to variational parameter)

$$\Phi(r, a) = (a - r)$$

$$\Phi(r, a) = (a - r)^2$$

$$\Phi(r, a) = \frac{1}{\sqrt{2 \cdot \pi \cdot a}} \cdot \frac{\sin \frac{\pi \cdot r}{a}}{r}$$

- Particle in a infinite spherical potential well of radius a
- Particle in a finite spherical potential well (treat a as a variational parameter)

$$\psi(r, \beta) = \left(\frac{2 \cdot \beta}{\pi}\right)^{\frac{3}{4}} \cdot \exp(-\beta \cdot r^2)$$

- Particle in a finite spherical potential well
- Hydrogen atom ground state
- Helium atom ground state

$$\psi(r, \beta) = \sqrt{\frac{3 \cdot \beta^3}{\pi^3}} \cdot \text{sech}(\beta \cdot r)$$

- Particle in a finite potential well
- Hydrogen atom ground state
- Helium atom ground state

$$\psi(x, \beta) = \sqrt{\frac{\beta}{2}} \cdot \operatorname{sech}(\beta \cdot x)$$

- Harmonic oscillator
- Quartic oscillator
- Particle in a gravitational field
- Particle in a finite potential well

$$\psi(\alpha, \beta) = \sqrt{\frac{12\alpha^3}{\pi}} \cdot x \cdot \operatorname{sech}(\alpha \cdot x)$$

- Particle in a semi-infinite potential well
- Particle in a gravitational field
- Particle in a linear potential well (same as above) $V(x) = ax$ ($x = 0$ to ∞)
- 1D hydrogen atom or one-electron ion

Some finite potential energy wells.

$$V(x) = \text{if}[(x \geq -1 \cdot (x \leq 1)), 0, V_0]$$

$$V(x) = \text{if}[(x \geq -1 \cdot (x \leq 1)), 0, |x| - 1]$$

$$V(x) = \text{if}[(x \geq -1 \cdot (x \leq 1)), 0, \sqrt{|x| - 1}]$$

Some semi-infinite potential energy well.

$$V(x) = \text{if}(x \leq a, 0, b)$$

$$V(x) = \text{if}[(x \leq 2), 0, \frac{5}{x}]$$

$$V(x) = \text{if}[(x \geq 2), 0, (x - 2)]$$

$$V(x) = \text{if}[(x \leq 2), 0, \sqrt{x - 2}]$$

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