

Tillämpningar

0.0.1 Lågpotential med oändligt stela väggar i en dimension

$$\mathcal{U}(x) = \begin{cases} \infty & x \leq 0, a \leq x \\ 0 & 0 < x < a \end{cases}$$

$$\Phi_n(x) = \begin{cases} 0 & \text{för } x \leq 0 \text{ och } a \leq x \\ \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} & \text{för } 0 < x < a \end{cases}$$

$$E_n = \frac{\pi^2 \hbar^2 n^2}{2ma^2}$$

Harmonisk oscillator 1D

$$\mathcal{U}(x) = \frac{1}{2}m\omega^2 x^2 = \frac{1}{2}kx^2$$

$$N_n = (2^n n!)^{-1/2} \left(\frac{m\omega}{\pi \hbar} \right)^{1/4}$$

Hermite's polynomial:

$$H_n(\xi) = (-1)^n \cdot e^{\xi^2} \cdot \frac{d^n e^{-\xi^2}}{d\xi^n}$$

$$\Phi_n(x) = N_n \cdot e^{-\frac{m\omega}{2\hbar}x^2} \cdot H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right)$$

$$E_n = \hbar\omega \cdot \left(n + \frac{1}{2} \right)$$

Vågfunktionerna kan alternativt skrivas:

$$u_n(x) = N \left(\frac{\partial}{\partial x} - ax \right)^n \cdot u_0(x)$$

$$u_0(x) = e^{-ax^2/2}$$

Sfärisk symmetrisk potential

$$\mathcal{U}(\mathbf{r}) = \mathcal{U}(r)$$

$$H = -\frac{\hbar}{2mr^2} \frac{\partial}{\partial r} \left[r^2 \frac{\partial}{\partial r} \right] + \frac{L^2}{2mr^2} + \mathcal{U}(r)$$

$$H\psi_{nlm}(\mathbf{r}) = E_{nlm}\psi_{nlm}(\mathbf{r})$$

$$\psi_{nlm}(\mathbf{r}) = \frac{G_{nl}(r)}{r} \Upsilon_l^m(\theta, \phi)$$

Radiella ekvationen:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} G(r) + \left[\frac{l(l+1)\hbar^2}{2mr^2} + \mathcal{U}(r) \right] G(r) = EG(r)$$

Väteliknande atom

$$\mathcal{U}(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}$$

Schrödingerekvationen blir:

$$\left[\Delta + \frac{2Z}{a_0 r} + \frac{2mE}{\hbar^2} \right] \Phi(r) = 0$$

Radiella vågfunktioner för väteliknande atomer:

n	l	$R_{nl}(r)$
1	0	$R_{10}(r) = 2 \left(\frac{Z}{a_0} \right)^{3/2} e^{-\rho/2}$
2	0	$R_{20}(r) = \frac{1}{2\sqrt{2}} \left(\frac{Z}{a_0} \right)^{3/2} (2 - \rho) e^{-\rho/2}$
2	1	$R_{21}(r) = \frac{1}{2\sqrt{6}} \left(\frac{Z}{a_0} \right)^{3/2} \rho e^{-\rho/2}$
3	0	$R_{30}(r) = \frac{1}{9\sqrt{3}} \left(\frac{Z}{a_0} \right)^{3/2} (6 - 6\rho + \rho^2) e^{-\rho/2}$
3	1	$R_{31}(r) = \frac{1}{9\sqrt{6}} \left(\frac{Z}{a_0} \right)^{3/2} \rho(4 - \rho) e^{-\rho/2}$
3	2	$R_{32}(r) = \frac{1}{9\sqrt{30}} \left(\frac{Z}{a_0} \right)^{3/2} \rho^2 e^{-\rho/2}$

$$E - n = -\frac{mZ^2 e^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} = -\frac{Z^2 \hbar^2}{2a_0^2 m n^2} = -13.6 \frac{Z^2}{n^2} \text{eV}$$

$$S(x, t) = \frac{\hbar}{2im} \left[\psi^* \cdot \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right]$$