Lecture 14

Solutions of Schrodinger's equation in d>1

Announcements:

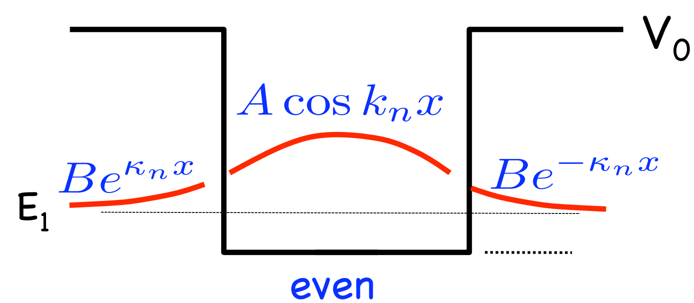
- lecture 13 is posted
- http://tinyurl.com/2170SP10POSTSTURVEY
- homework 9 solutions are posted
- homework 10 is due April 12
- reading for this week is:
  - Ch 8 in TZD

recall lecture 13:

Last Time

Simple Schrödinger's equation problems in 1d

- mathematical generalities:
  - *exponential (oscillating and decaying) solutions*
  - *continuity of ψ and ψ'*
- free particle: $\psi_E(x) = Ae^{ikx} + Be^{-ikx}$
- particle in an infinite square-well
  - $\psi_k(x) = \sqrt{\frac{2}{L}} \sin k_n x, \quad \text{for } 0 < x < L$ $\qquad E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2$
- particle in a finite square-well:



- harmonic oscillator:

  $E_n = \hbar\omega_0(n + 1/2), \quad n = 0, 1, 2, \ldots$

  $\psi_n(x) = H_n(x/\ell) e^{-x^2/2\ell^2}, \;\; \ell = \sqrt{\frac{\hbar}{m\omega_0}}$
- potential barrier, tunneling: $t \approx A_R/A_L \approx e^{-\kappa x_2}/e^{-\kappa x_1} \approx e^{-\kappa d}$

  $\kappa d = d\sqrt{2m(V_0 - E)/\hbar^2}$

Today

Simple Schrödinger's equation problems in 2d, 3d

- separation of variables
- free particle
- particle in an infinite square-well
- harmonic oscillator
- Hydrogen atom

Mathematical background

- separation of variables, possible when:

$$V(x,y,z) = v_1(x) + v_2(y) + v_3(z)$$

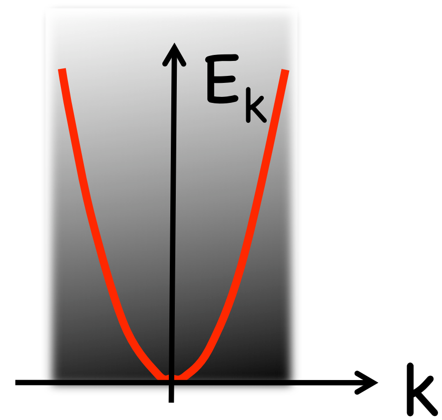
or

$$V(x,y,z) = v_1(r) + v_2(\theta) + v_3(\varphi)$$

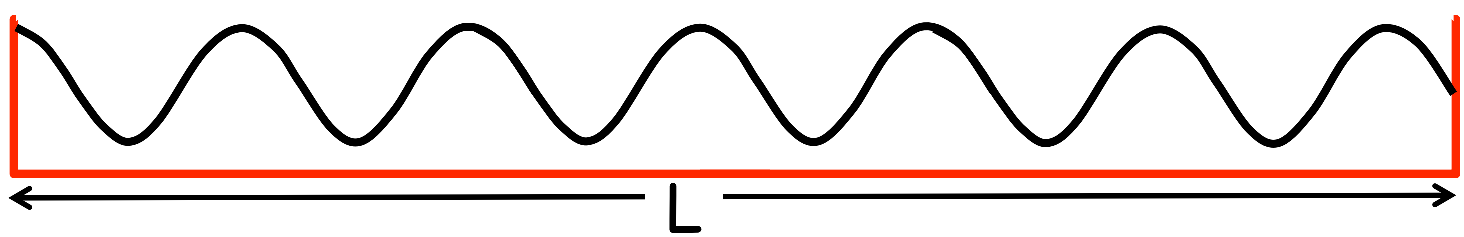
or...

Free particle in d-dimensions: V = 0

- $-\frac{\hbar^2}{2m}\frac{\partial^2\psi_E}{\partial x^2} + V(x)\psi_E = E\psi_E \Longrightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\psi_E}{\partial x^2} = E\psi_E$
- plane-wave: $\psi_k(x) = A\, e^{ikx}$, with $E_k = \frac{\hbar^2 k^2}{2m}$
- continuum spectrum: E = $p^2/2m$



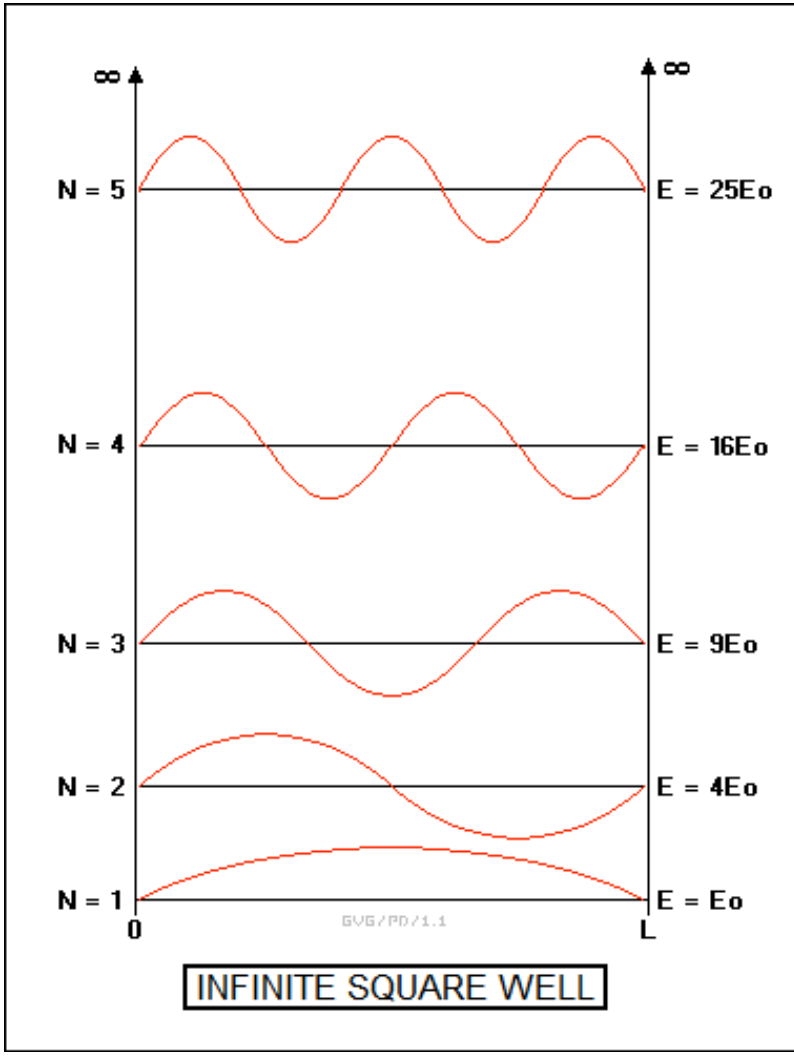
- normalization in a box: *A* = ? *only determined up to a phase* $e^{i\varphi}$



$$1 = \int_{-\infty}^{+\infty} |\psi|^2 = \int_{-L/2}^{+L/2} |A|^2 \Longrightarrow A = 1/\sqrt{L}$$

Particle in an infinite square-well in d-dimensions

- V = 0 , for 0 < x < L, and ∞ outside the well
- $$\psi_k(x) = \sqrt{\frac{2}{L}} \sin k_n x, \quad \text{for } 0 < x < L$$
  $$= 0, \quad \text{otherwise}$$
- with $k_n = n\pi/L$, *n = 1, 2, 3,... (number nodes)*
- discrete spectrum: $$E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2$$
- degeneracy in 3d: $n_x^2 + n_y^2 + n_z^2$ = const
- $$P_n(x) = |\psi_n(x)|^2, = \frac{2}{L}\sin^2\frac{\pi n x}{L}, \quad \text{for } 0 < x < L$$
- "crude" path to solution: p ≈ n h/L and minimize E(x) over x



Lecture 15 **Solutions in polar and spherical coordinates**

Announcements:

- lecture 13 is posted
- http://tinyurl.com/2170SP10POSTSTURVEY
- homework 11 is due April 23
- please begin reviewing for the final
- reading for this week is:
  - Ch 8 in TZD

Today

Harmonic oscillator and hydrogen atom

- separation of variables in polar coordinates
- harmonic oscillator in polar coordinates
- separation of variables in spherical coordinates
- Hydrogen atom

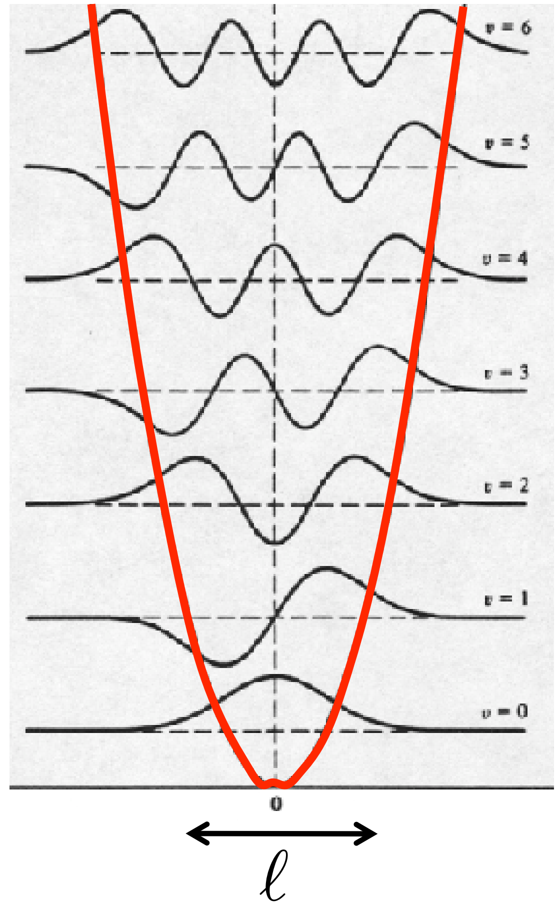
Harmonic oscillator in d-dimensions

- S.Eqn: $$-\frac{\hbar^2}{2m}\nabla^2\psi_E + \frac{1}{2}m\omega_0^2 r^2\psi_E = E\psi_E$$
- spectrum: $$E_{n_1,n_2,\ldots} = \hbar\omega_0(n_1+n_2+\ldots)$$
- eigenstates: $$\psi_n(x) = H_n(x/\ell)e^{-x^2/2\ell^2}, \; \ell = \sqrt{\frac{\hbar}{m\omega_0}}$$

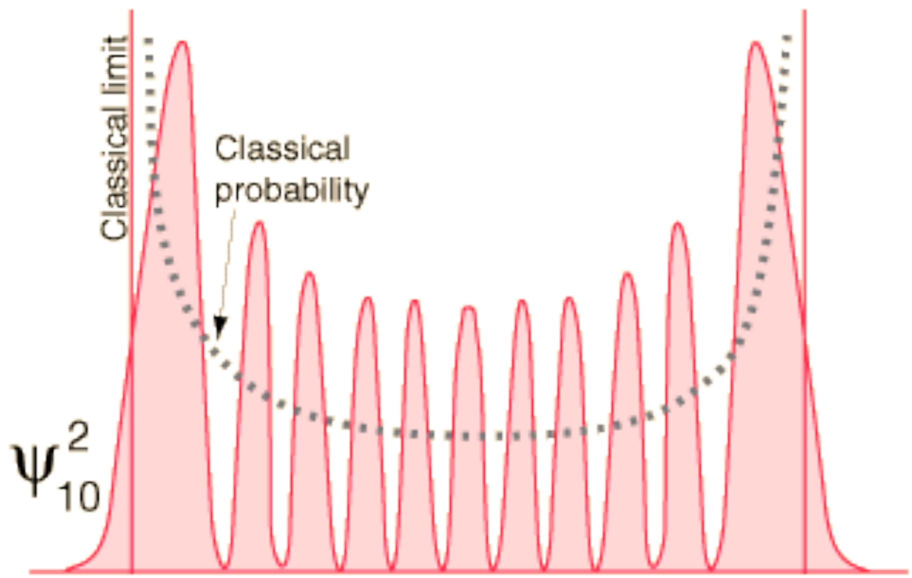
$$\psi_0(x) = e^{-\hat{x}^2/2}, \quad E_0 = \frac{1}{2}\hbar\omega_0,$$

$$\psi_1(x) = \hat{x}e^{-\hat{x}^2/2}, \quad E_1 = \frac{3}{2}\hbar\omega_0,$$

$$\psi_2(x) = (1-2\hat{x}^2)e^{-\hat{x}^2/2}, \quad E_2 = \frac{5}{2}\hbar\omega_0$$

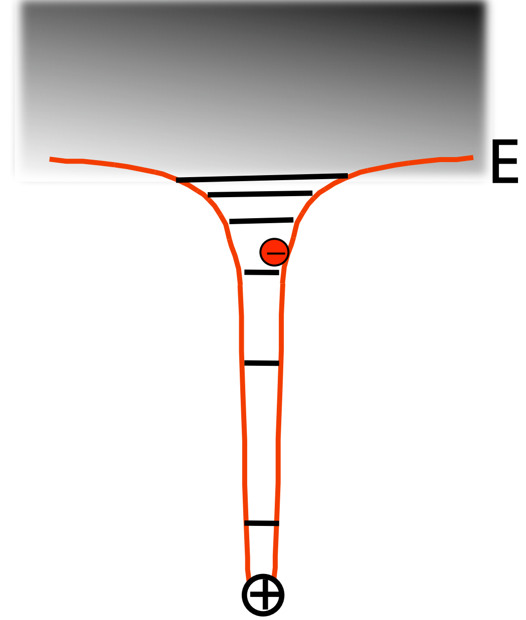


- degeneracy for states $n_x\, n_y\, n_z$:
  - $D_{2d} = n+1$, $D_{3d} = (n+1)(n+2)/2$

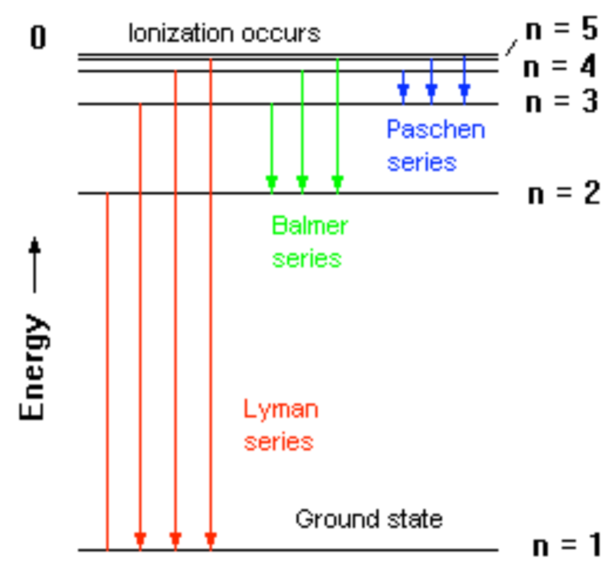


- "crude" path to solution: $p \approx n\, h/x$ and minimize $E(x)$ over x

Hydrogen atom: V= -1/r



- S.Eqn: $$-\frac{\hbar^2}{2m}\nabla^2\psi_E - \frac{e^2}{r}\psi_E = E\psi_E$$
- spectrum: $$E_n = -\frac{e^4 m}{2\hbar^2}\frac{1}{n^2} = -\frac{13.6eV}{n^2}, \quad n = 1, 2, 3, \ldots$$
  $$\ell = 0, 1, 2, \ldots, n-1, \quad -\ell \le m \le \ell$$
- eigenstates: $$\psi_{n\ell m}(r,\theta,\phi) = Y_\ell^m(\theta,\phi)\hat{r}^\ell e^{-\hat{r}/2} L_{n-\ell-1}^{2\ell+1}(\hat{r})$$ $$\hat{r} = \frac{2r}{na_0}$$
  - $Y_l^m(\theta,\phi)$ – *spherical harmonics*
  - $L_a^b(r)$ – *generalized Laguerre polynomials*

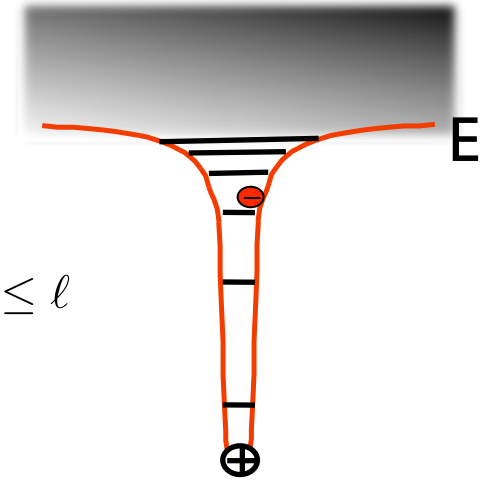


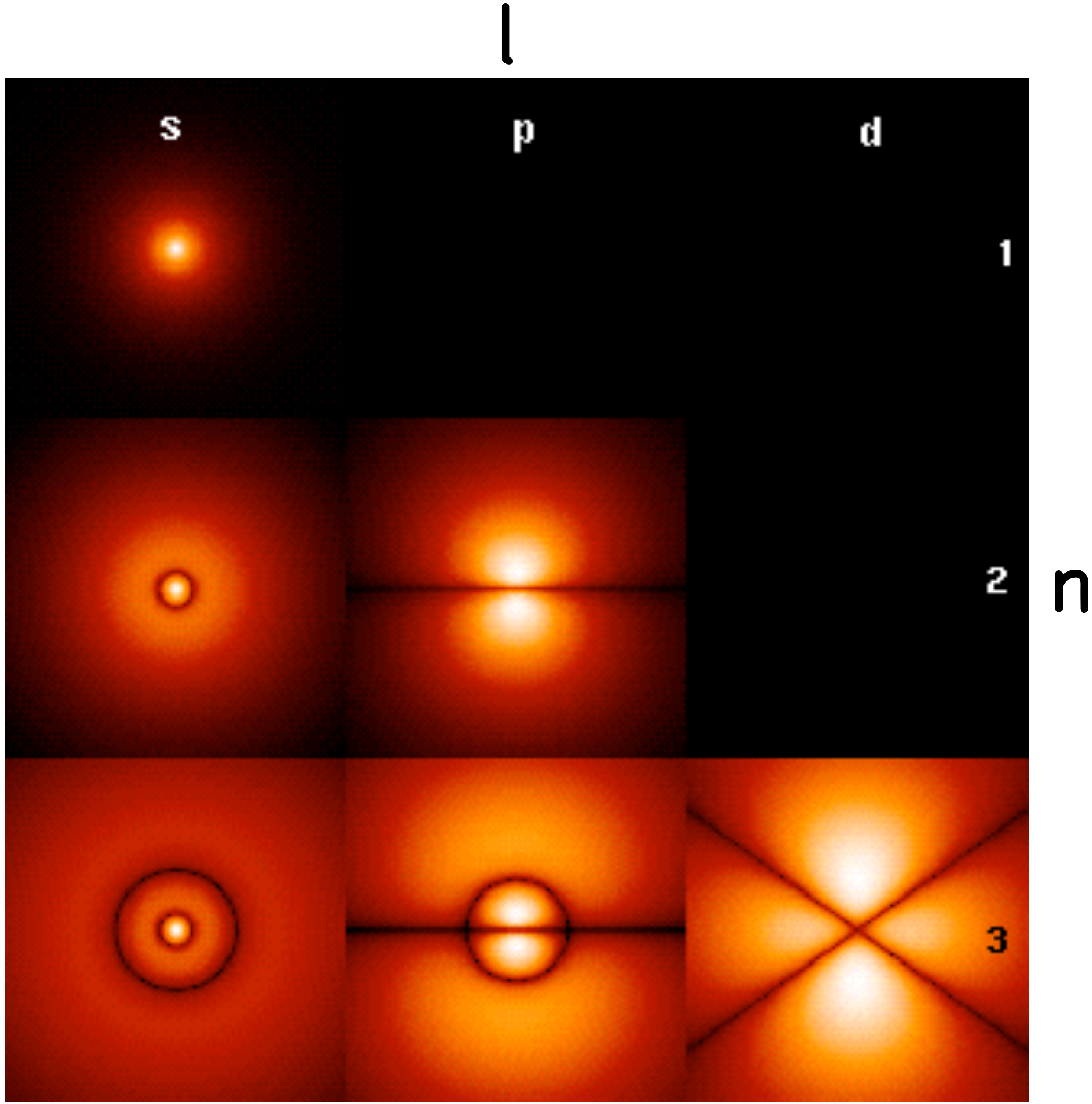
- degeneracy for state n, l, m:
  - *m degeneracy: 2l+1*
  - *total degeneracy: n^2 ($2n^2$, with spin)*
- "crude" path to solution: p ≈ n h/r and minimize E(r) over r

Hydrogen atom wavefunctions

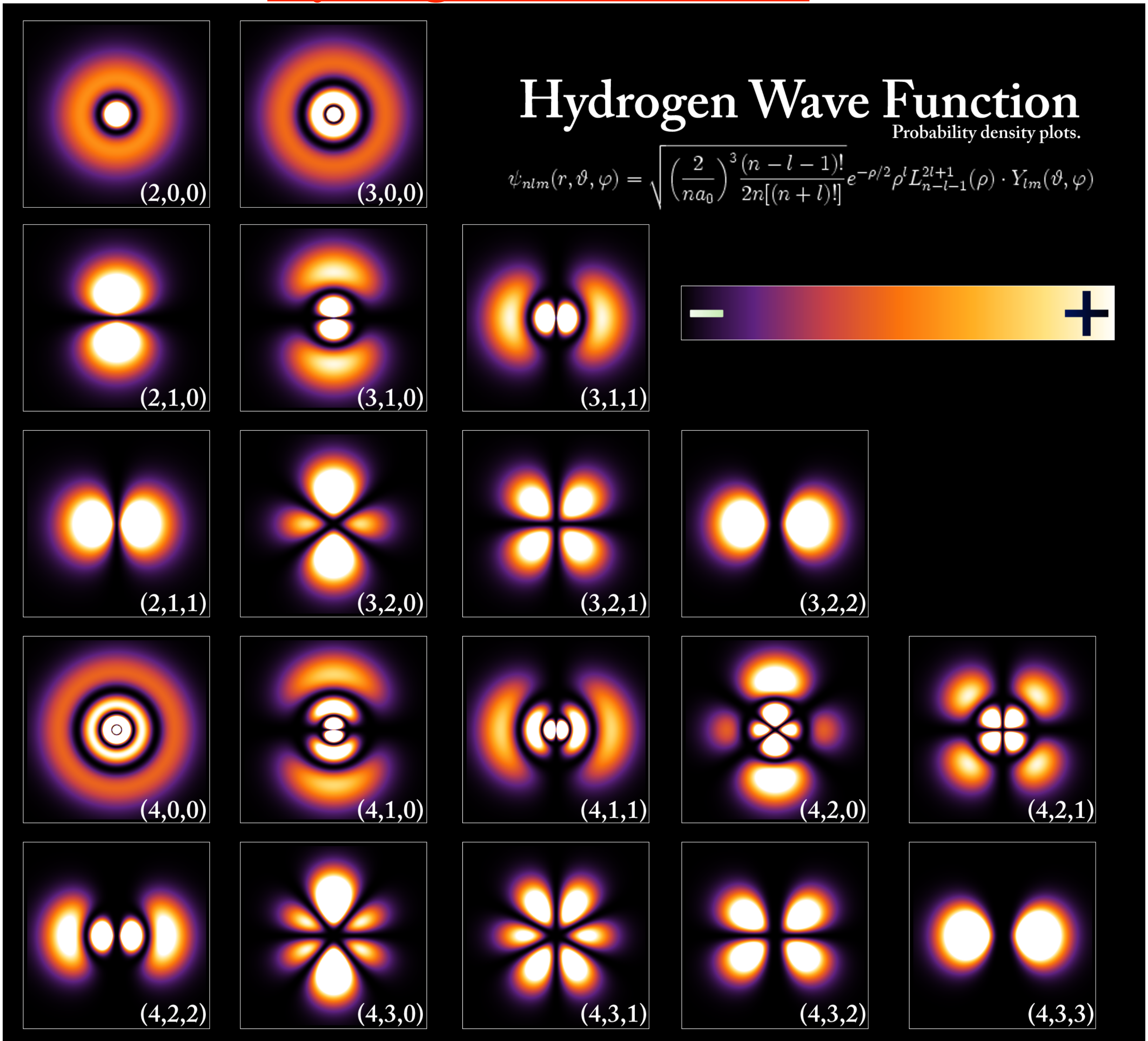
- eigenstates labeled by n, l, m quantum numbers

$$E_n = -\frac{e^4 m}{2\hbar^2}\frac{1}{n^2} = -\frac{13.6eV}{n^2}, \quad n = 1, 2, 3, \ldots \quad \ell = 0, 1, 2, \ldots, n-1, \quad -\ell \le m \le \ell$$



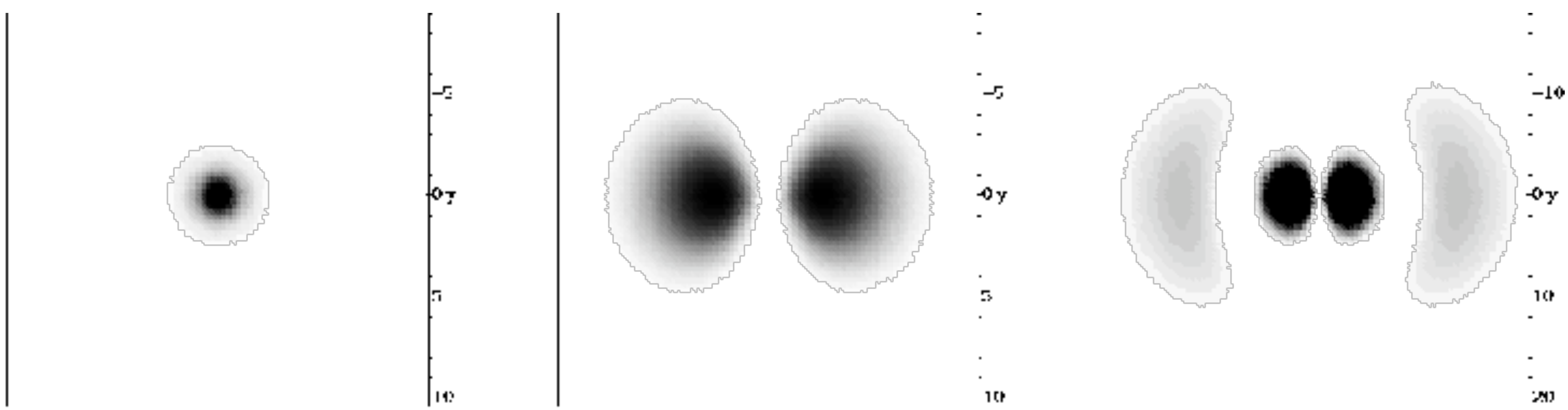


Hydrogen atom details



Hydrogen atom details

n	ℓ	m	$R_{n\ell}$	$Y_{\ell m}$	$\psi_{n\ell m} = R_{n\ell} Y_{\ell m}$
1	0	0	$2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$	$\frac{1}{2\sqrt{\pi}}$	$\frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$
2	0	0	$\left(\frac{1}{2a_0}\right)^{3/2}\left(2-\frac{r}{a_0}\right) e^{-r/2a_0}$	$\frac{1}{2\sqrt{\pi}}$	$\frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(2-\frac{r}{a_0}\right) e^{-r/2a_0}$
2	1	0	$\left(\frac{1}{2a_0}\right)^{3/2} \frac{1}{\sqrt{3}}\frac{r}{a_0} e^{-r/2a_0}$	$\frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$	$\frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0} e^{-r/2a_0}\cos\theta$
2	1	±1	$\left(\frac{1}{2a_0}\right)^{3/2} \frac{1}{\sqrt{3}}\frac{r}{a_0} e^{-r/2a_0}$	$\pm\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{\pm i\phi}$	$\frac{1}{8}\sqrt{\frac{1}{\pi}}\left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0} e^{-r/2a_0}\sin\theta e^{\pm i\phi}$



Hydrogen atom details