Quantum Mechanics (KEMS401)

Lecture 2

Free particle wave functions

momentum operator in 1 D

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

wave function

$$\psi_p(x) = |p\rangle = \frac{1}{\sqrt{2\pi}}\exp[i\frac{p}{\hbar}x] = \frac{1}{\sqrt{2\pi}}\exp[ikx] = |k\rangle$$ **note:** $$\langle k| = \frac{1}{\sqrt{2\pi}}\exp[-ikx]$$

superposition principle: wave packet

$$\psi(x) = |x\rangle = \int_{-\infty}^{\infty} f(k)|k\rangle dk = \int_{-\infty}^{\infty} f(k)\exp[ikx]dk$$

time dependent wave packet (in lecture 4)

$$\psi_k(x,t) = |x,t\rangle = \int_{-\infty}^{\infty} f(k)|k\rangle\exp\left[-i\frac{E_k}{\hbar}t\right]dk = \int_{-\infty}^{\infty} f(k)\exp[ikx - i\omega(k)t]dk$$

Quantum Mechanics (KEMS401)

lectures 5 & 6:

Harmonic oscillator in Schrödinger representation

$$F(x) = -kx \qquad V(x) = \frac{1}{2}kx^2 \qquad \omega = \sqrt{\frac{k}{m}}$$

important model in chemistry

- Infra-red spectroscopy
- thermodynamics & kinetics

boundary conditions

- wave function needs to be zero at infinity

two step solution strategy

- find solution for $x \to \infty$
- multiply by a polynomial
- use boundary conditions to set limits on the polynomial

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

photochemistry

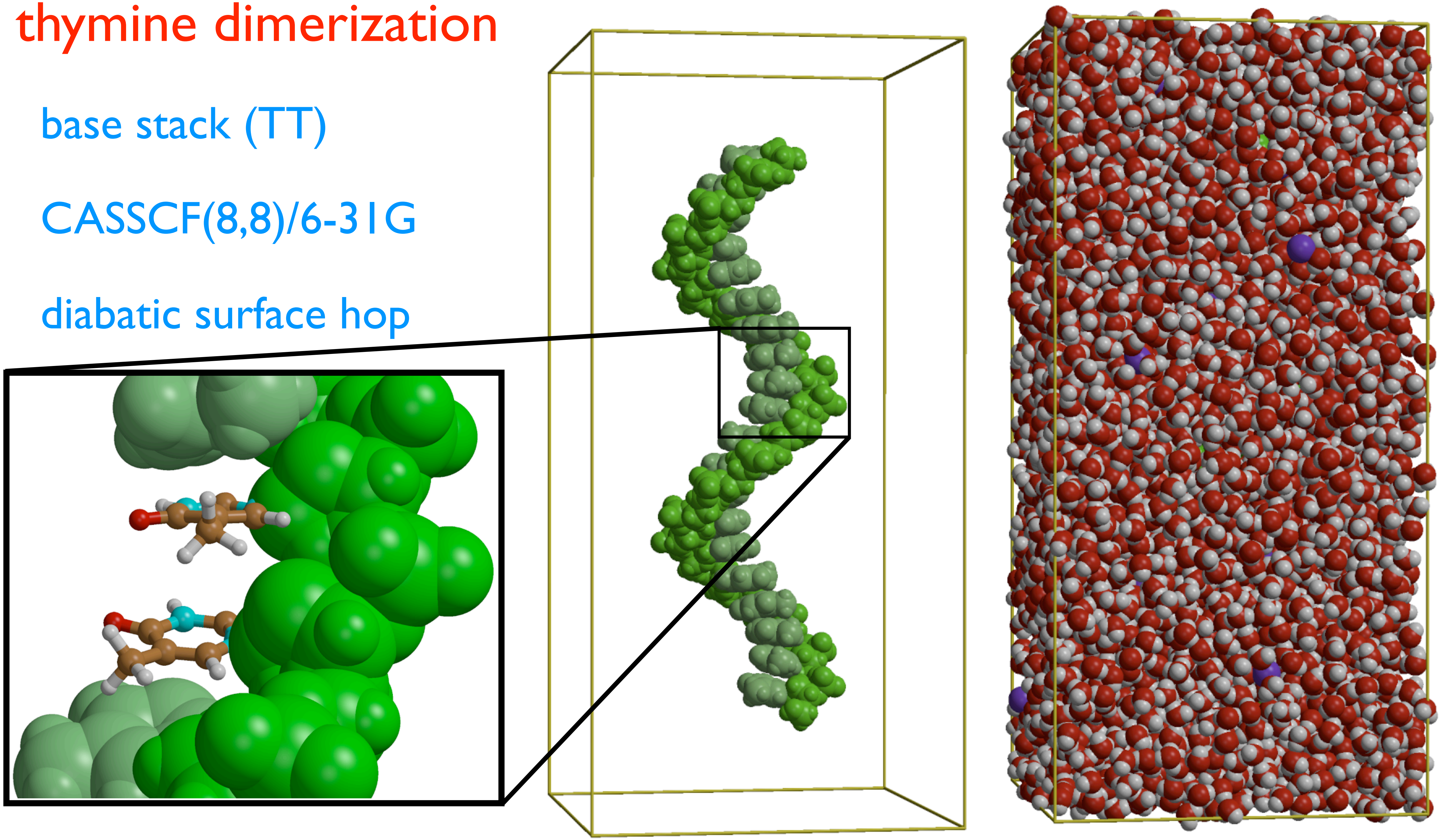
example: radiation damage in DNA

thymine dimerization

base stack (TT)

CASSCF(8,8)/6-31G

diabatic surface hop

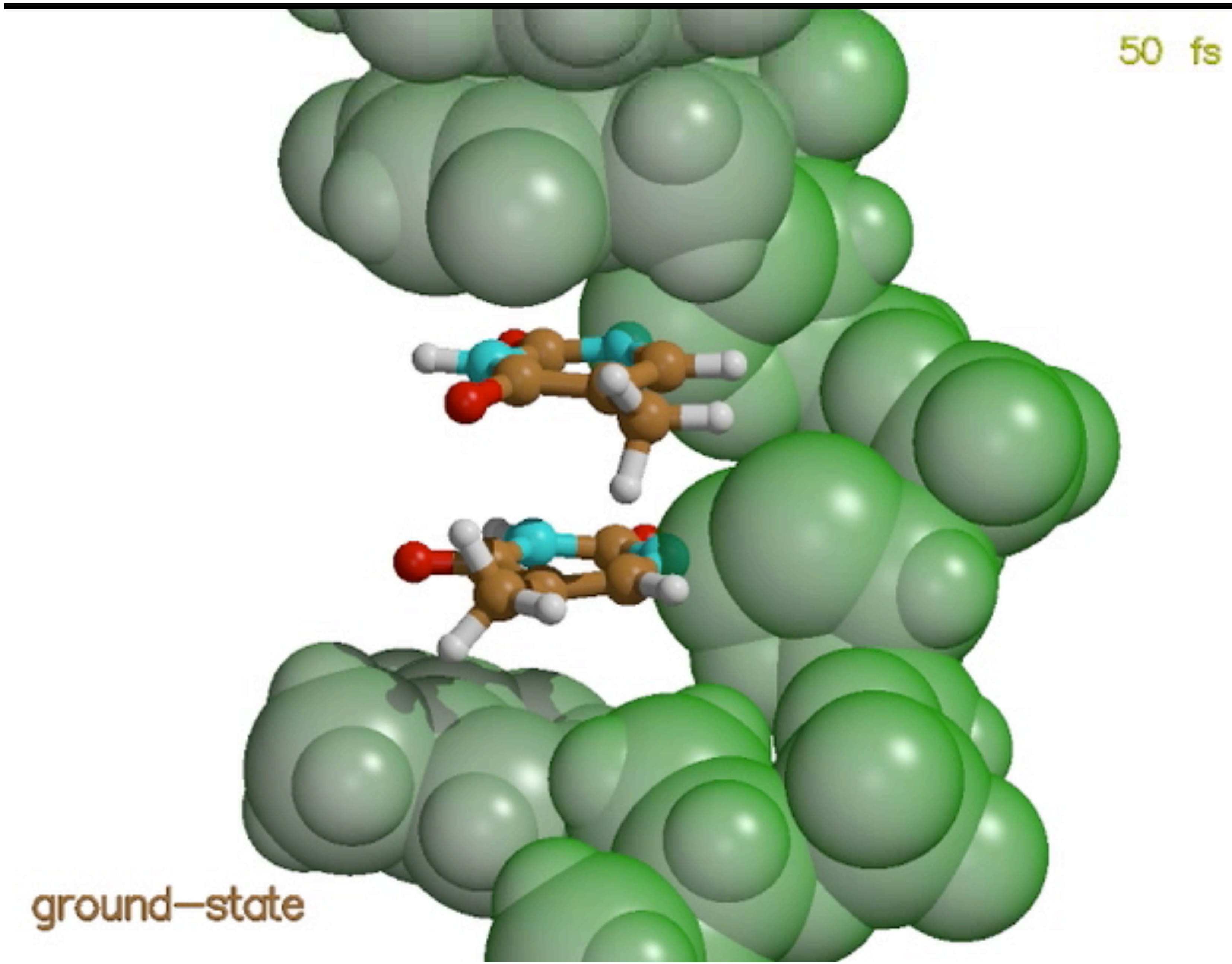


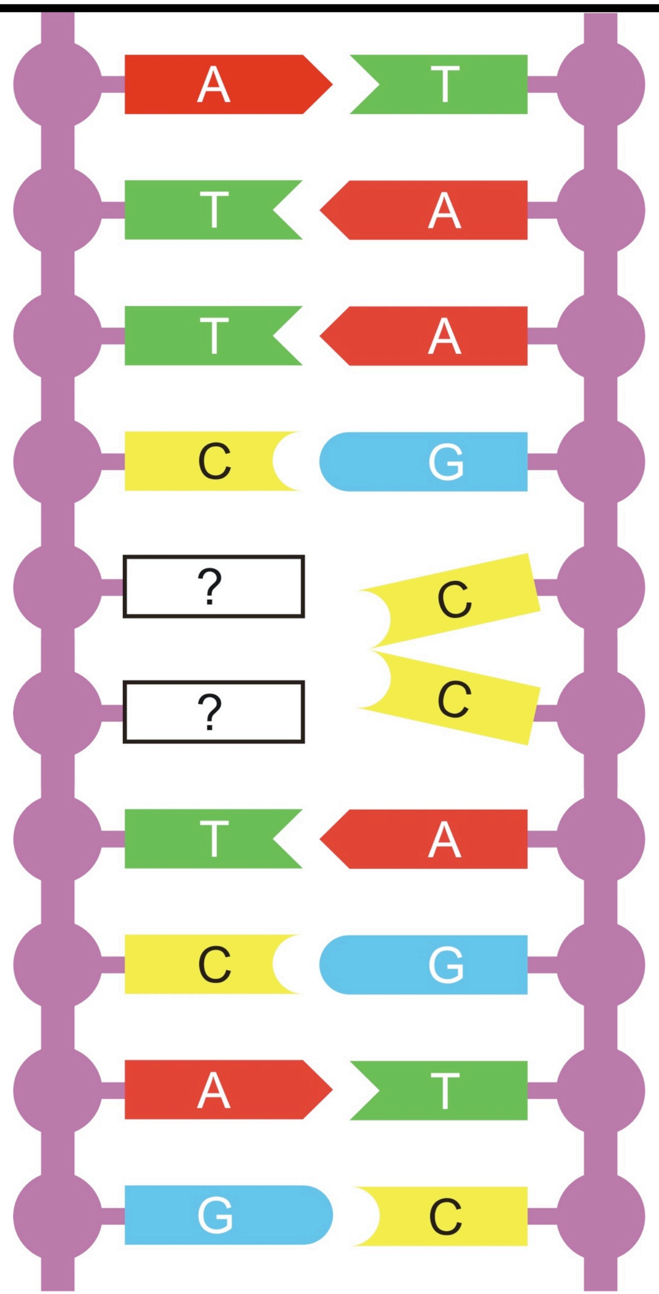
Radiation damage: UV absorption in DNA

thymine dimerization

cell dead?

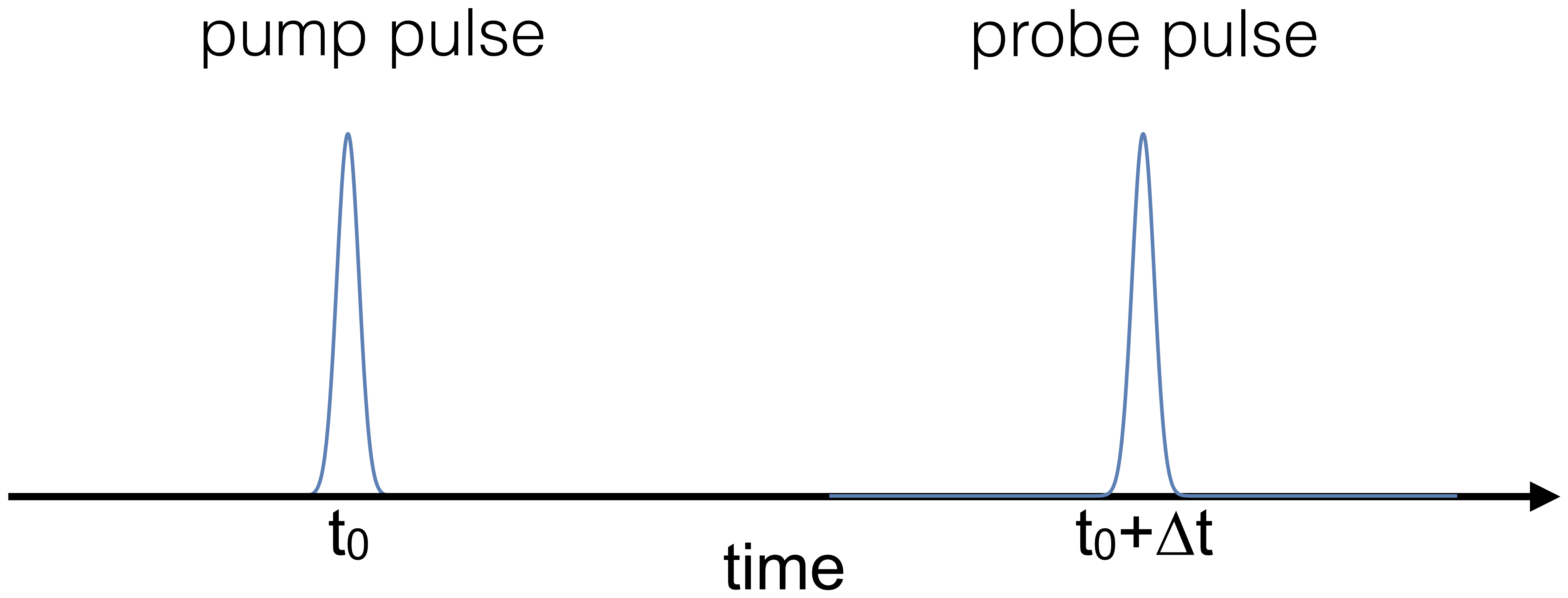
mutation?





Time-resolved spectroscopy

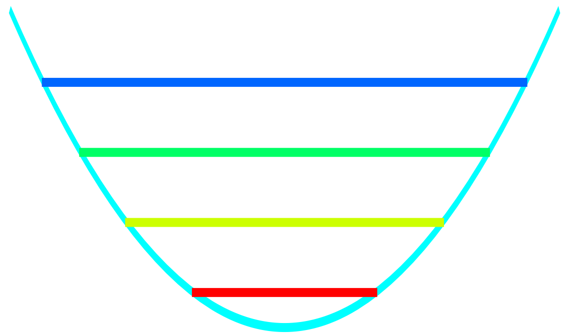
linear pump-probe spectroscopy

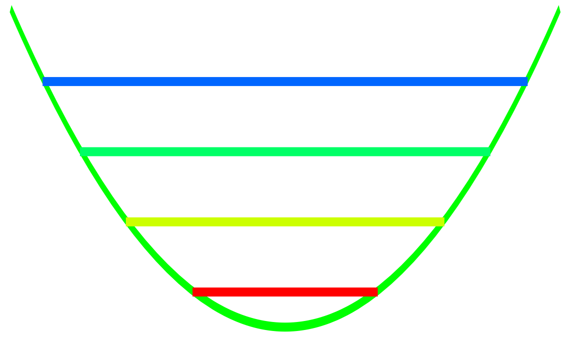


Time-resolved spectroscopy

some issues (out of many)

fs pump pulses have large bandwidth





Time-resolved spectroscopy

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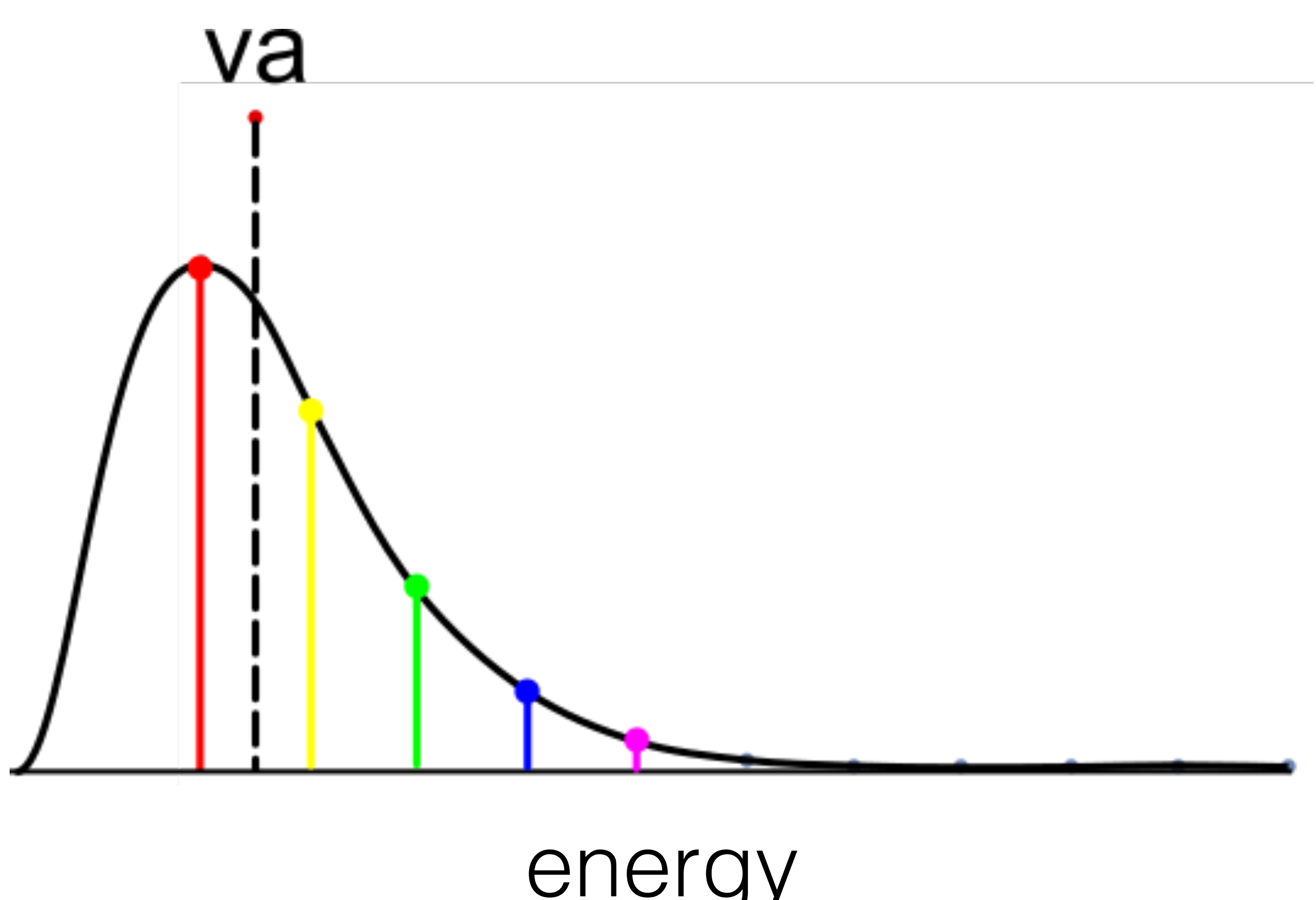

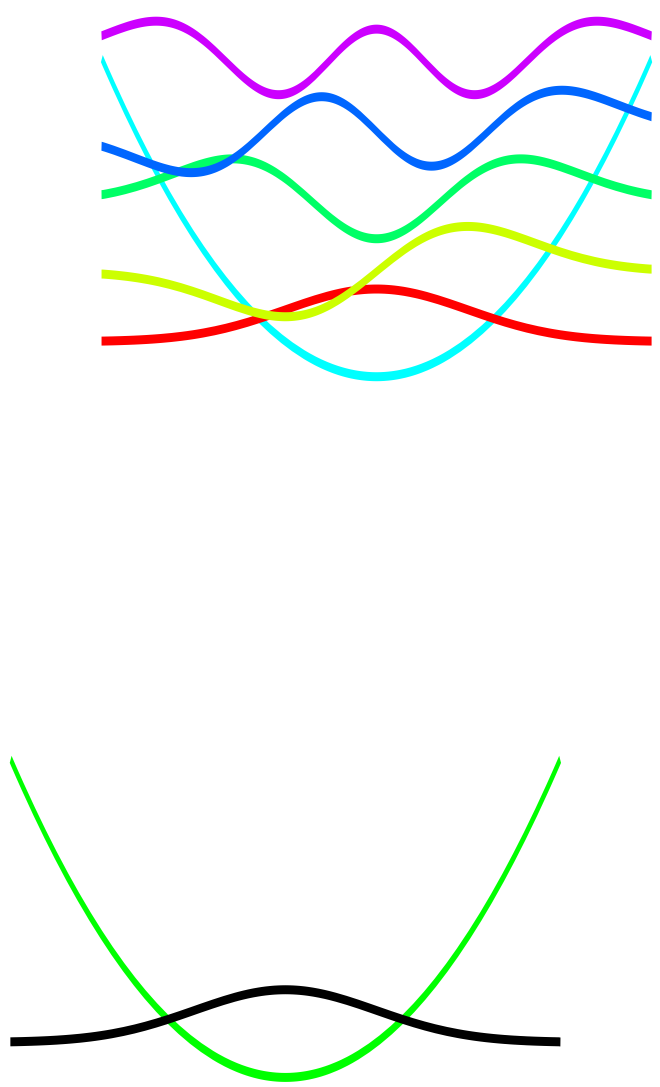

Time-resolved spectroscopy

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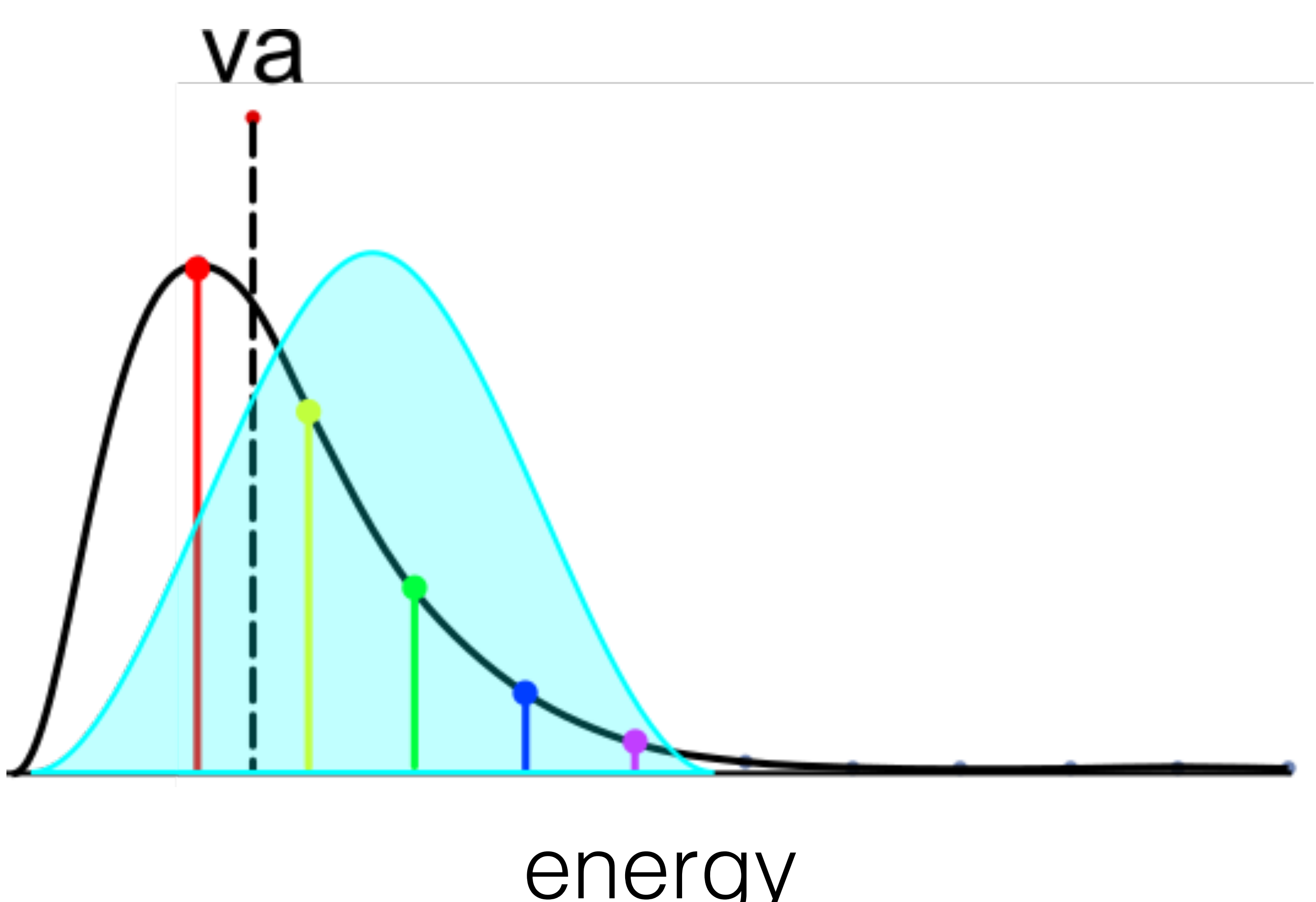
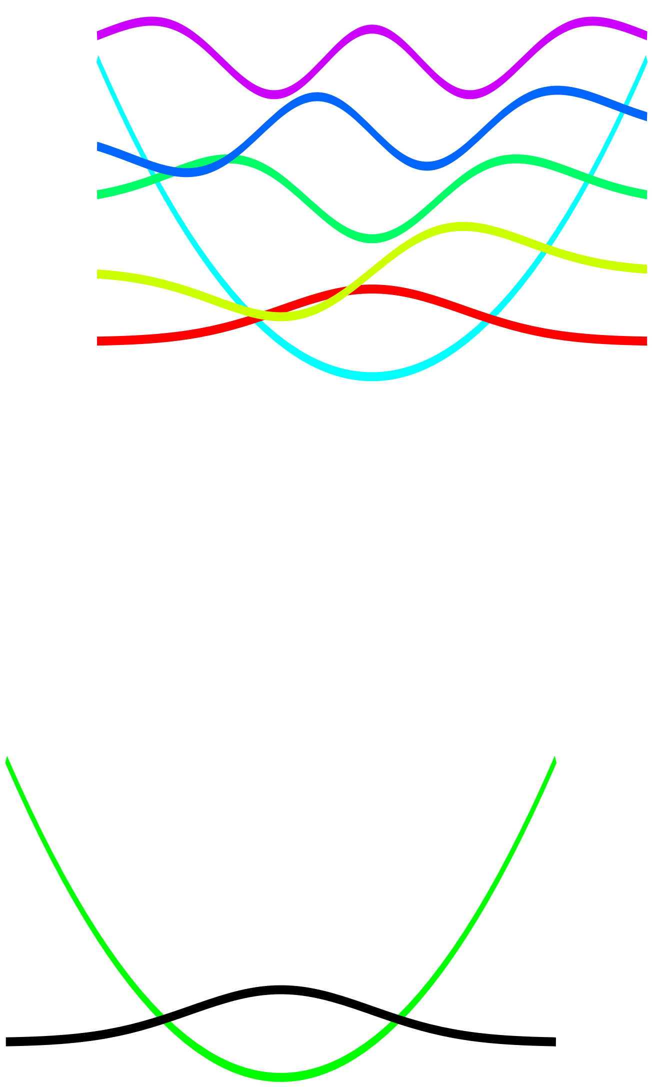


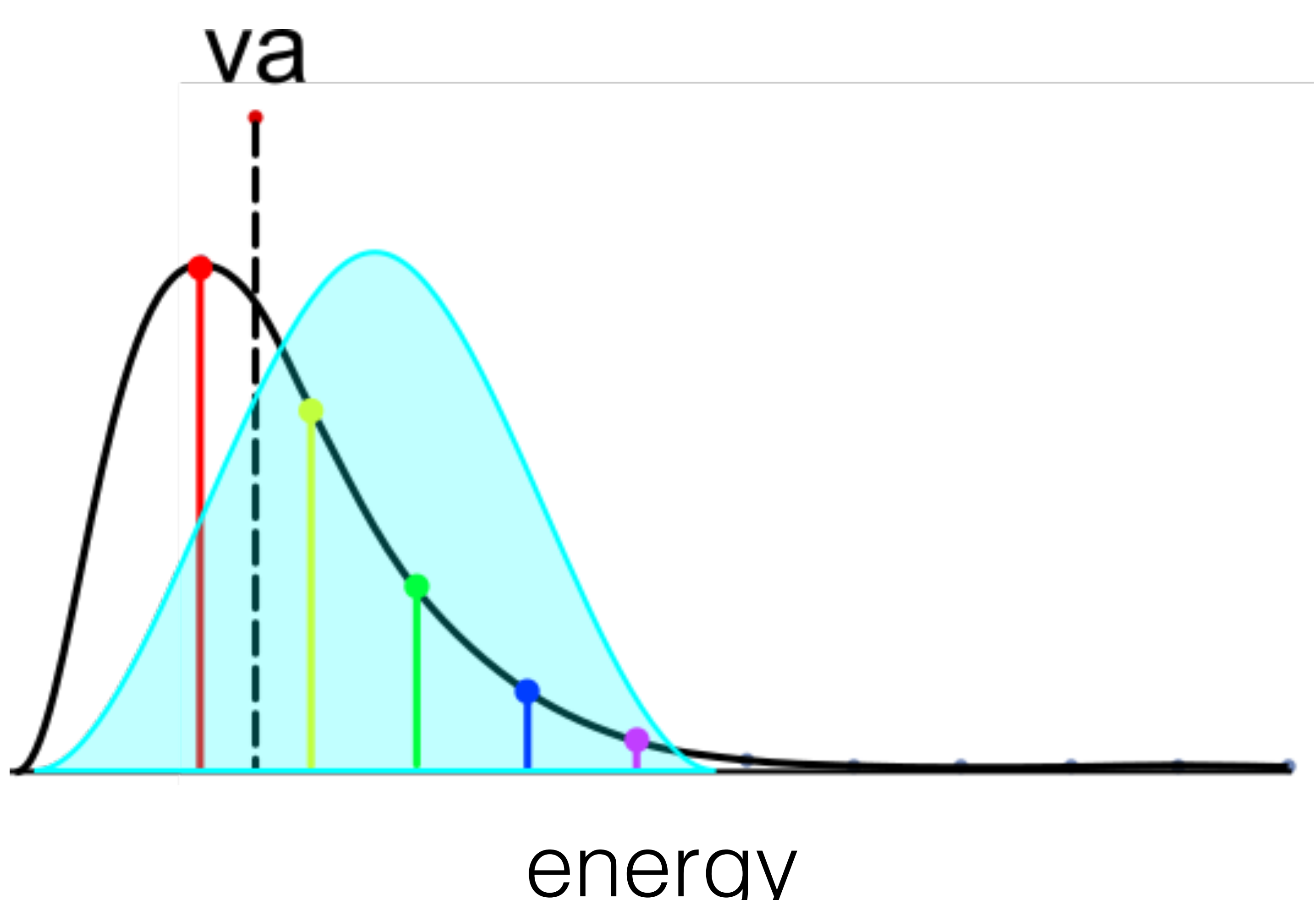


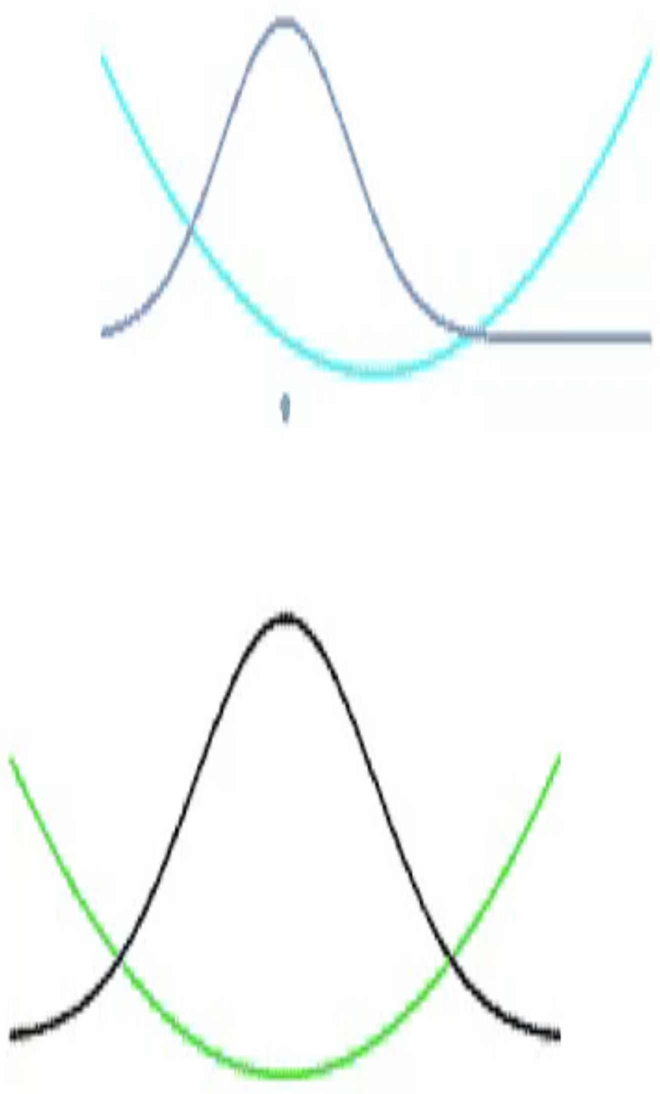
Time-resolved spectroscopy

some issues (out of many)

fs pump pulses have large bandwidth

coherent vibrations in ground and excited state





Time-resolved spectroscopy

some issues (out of many)

fs pump pulses have large bandwidth

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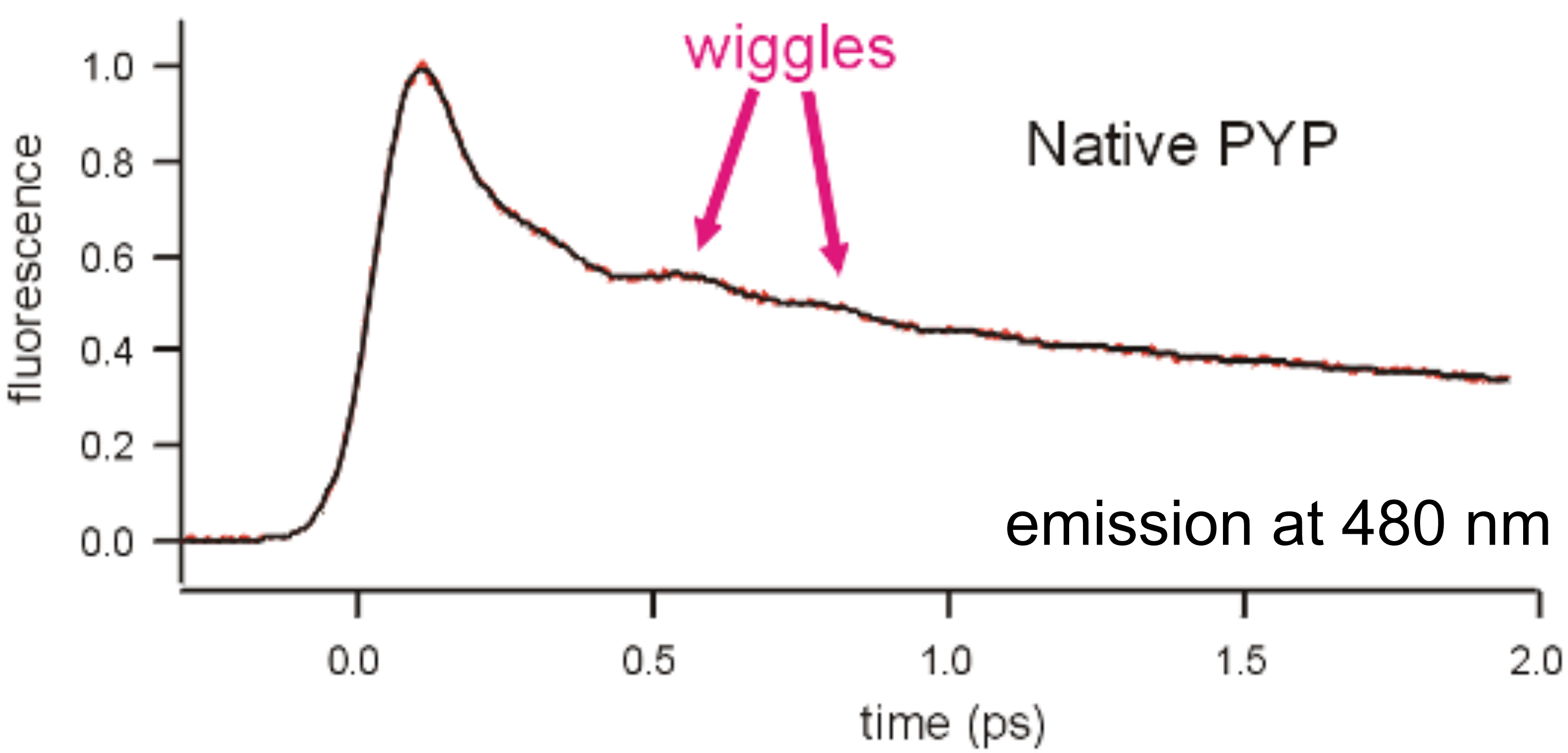

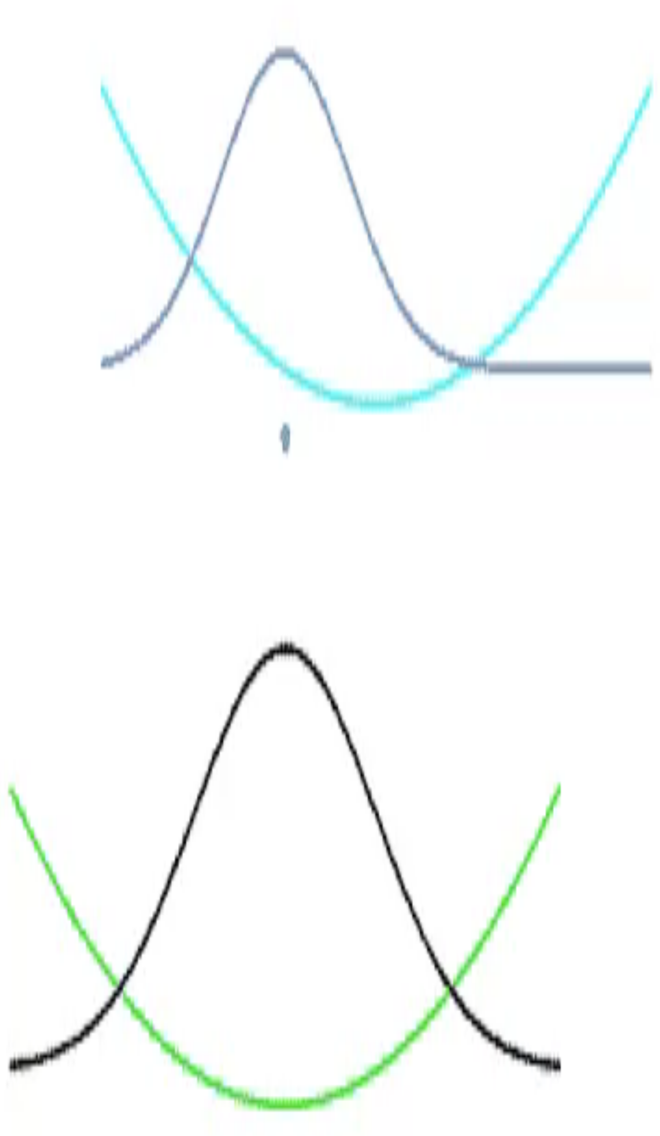

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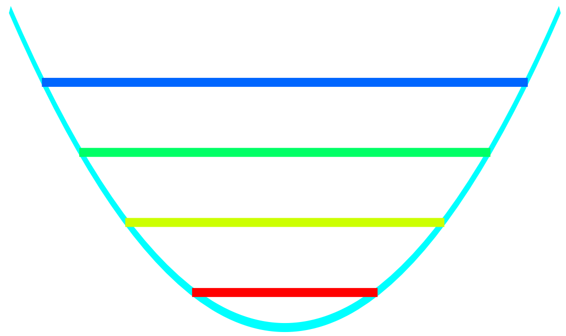
Time-resolved spectroscopy

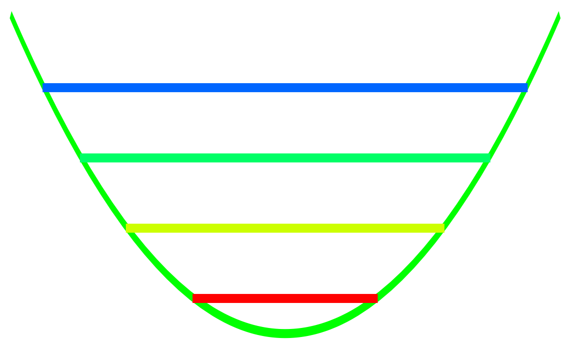
some issues (out of many)

fs pump pulses have large bandwidth

coherent vibrations in ground and excited state

stimulated emission limits population transfer





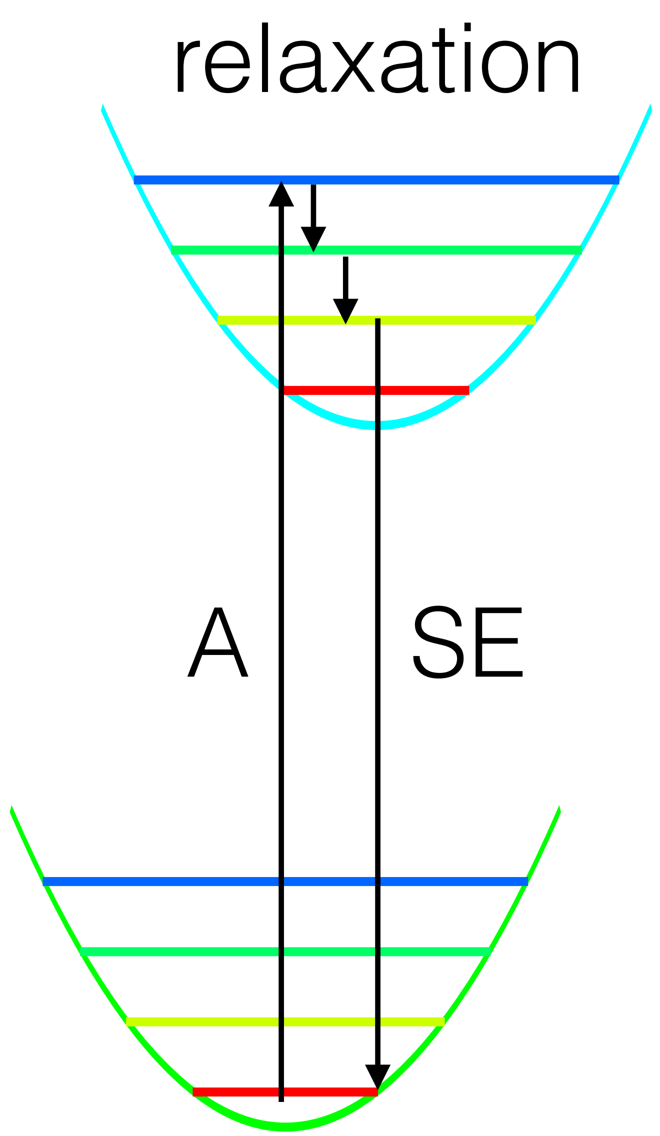
Time-resolved spectroscopy

some issues (out of many)

fs pump pulses have large bandwidth

coherent vibrations in ground and excited state

stimulated emission limits population transfer



Time-resolved spectroscopy

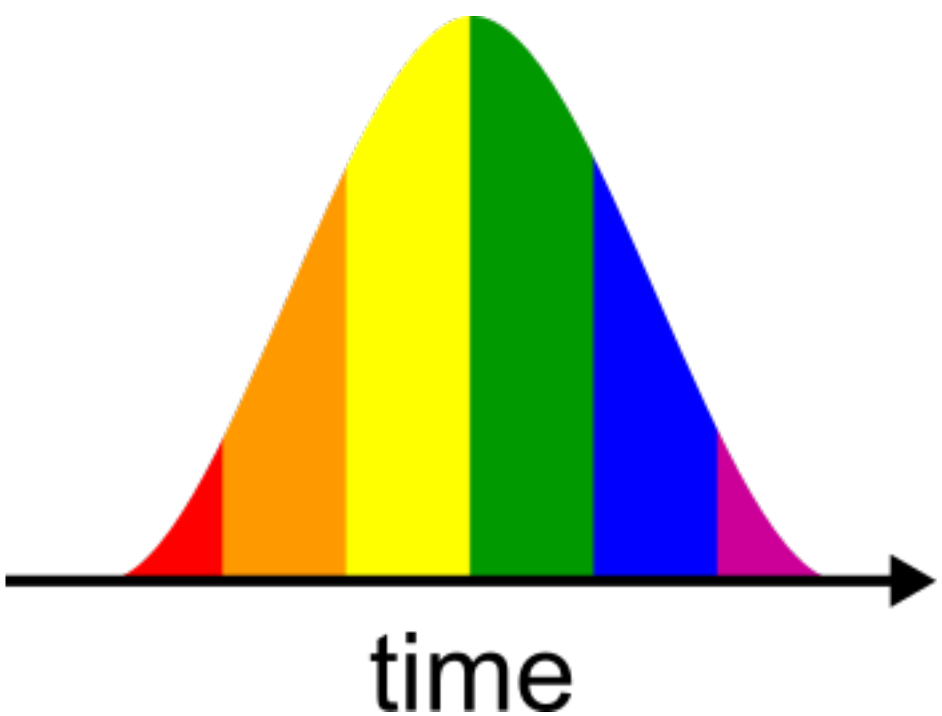
some issues (out of many)

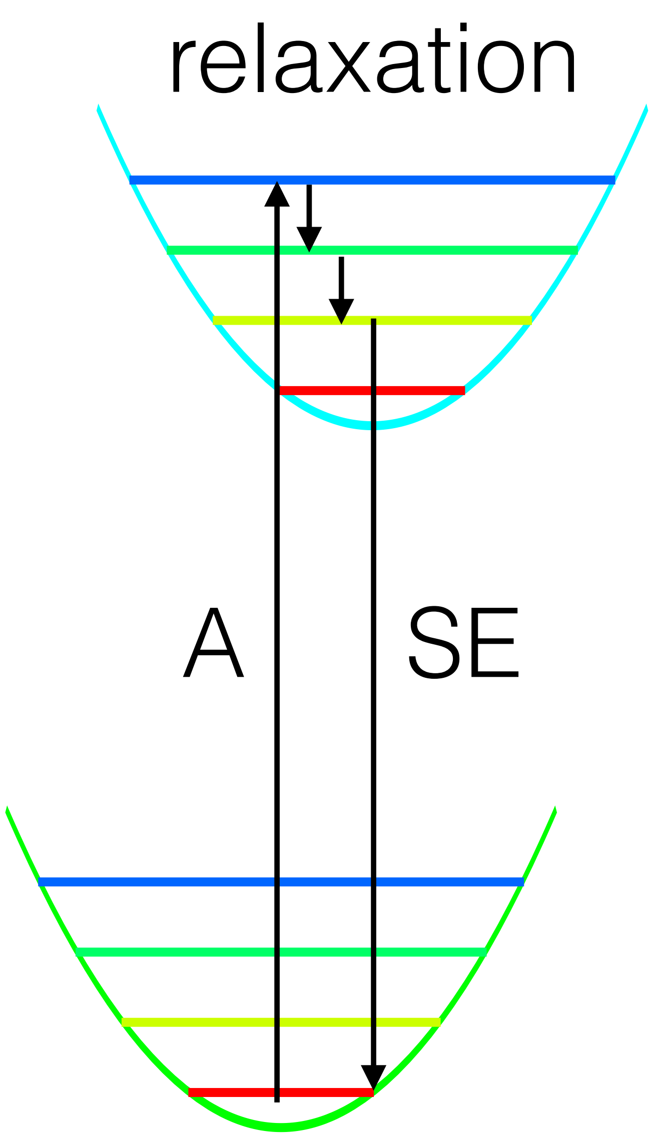
fs pump pulses have large bandwidth

coherent vibrations in ground and excited state

stimulated emission limits population transfer

chirped pulses





Quantum Mechanics (KEMS401)

lecture 6:

Harmonic oscillator in Dirac Representation

ladder operators

atomic units: $\hbar = m = k = 1$

$$\hat{a} = \frac{i}{\sqrt{2}}\left(\hat{p} - i\hat{x}\right) \qquad \hat{a}^{+} = \frac{1}{i\sqrt{2}}\left(\hat{p} + i\hat{x}\right) \qquad \hat{a}\hat{a}^{+} = \hat{H} + \frac{1}{2} \qquad \hat{a}^{+}\hat{a} = \hat{H} - \frac{1}{2}$$

$$\hat{H} = \frac{1}{2}\left(\hat{a}\hat{a}^{+} + \hat{a}^{+}\hat{a}\right)$$

commutation relations

$$[\hat{a}, \hat{a}^{+}] = 1$$

$$[\hat{a}, \hat{H}] = \hat{a}$$

$$[\hat{a}^{+}, \hat{H}] = \hat{a}^{+}$$

raising and lowering operator

$$\hat{a}^{+}\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad \hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle$$

Quantum Mechanics (KEMS401)

lecture 6:

Harmonic oscillator in Dirac Representation

ladder operators

$$\hat{a}^{+}|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad \hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$$

number operator

$$\hat{a}^{+}\hat{a}|n\rangle = n|n\rangle$$

real units

$$\hat{H} = \frac{1}{2}\hbar\omega(\hat{a}\hat{a}^{+} + \hat{a}^{+}\hat{a})$$

$$\hat{a} = \frac{i}{\sqrt{2\hbar\omega}}\left(\frac{1}{\sqrt{m}}\hat{p} - i\sqrt{k}\hat{x}\right) \qquad \hat{a}^{+} = \frac{1}{i\sqrt{2\hbar\omega}}\left(\frac{1}{\sqrt{m}}\hat{p} + i\sqrt{k}\hat{x}\right)$$

$$\hat{x} = \sqrt{\frac{\hbar\omega}{2k}}\left(\hat{a} + \hat{a}^{+}\right) \qquad \hat{p} = -i\sqrt{\frac{\hbar\omega m}{2}}\left(\hat{a} - \hat{a}^{+}\right)$$

Quantum Mechanics (KEMS401)

lecture 7:

Particle on ring

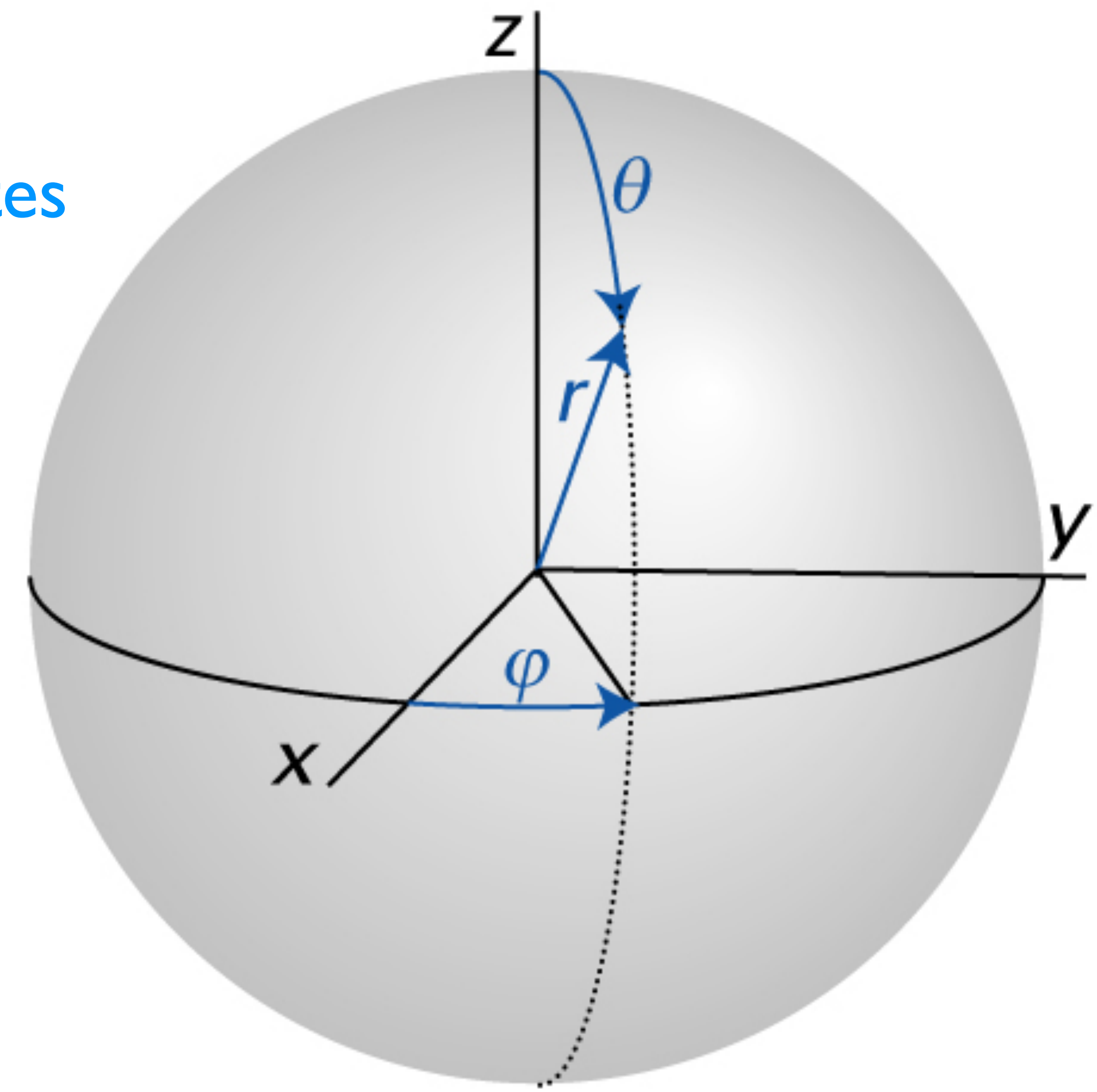
Hamiltonian in Cartesian coordinates

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)$$

polar coordinates (2D)

$$x = r\cos\varphi$$

$$y = r\sin\varphi$$



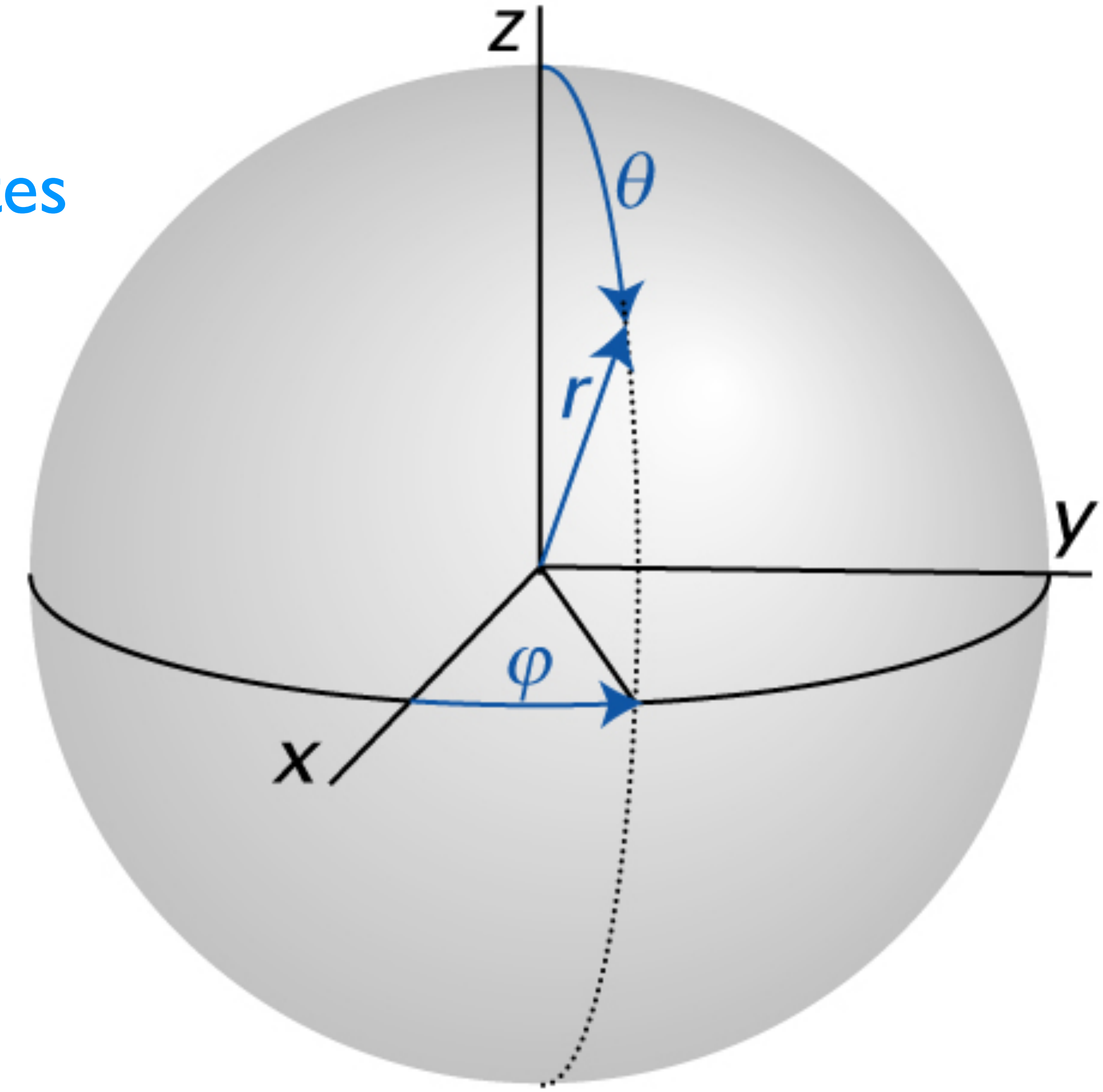
Hamiltonian in polar coordinates

$$\hat{H} = -\frac{\hbar^2}{2m}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right\}$$

Quantum Mechanics (KEMS401)

lecture 7/8:

Particle on sphere



Hamiltonian in Cartesian coordinates

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

spherical coordinates (3D)

$$x = r\sin\theta\cos\varphi$$

$$y = r\sin\theta\sin\varphi$$

$$z = r\cos\theta$$

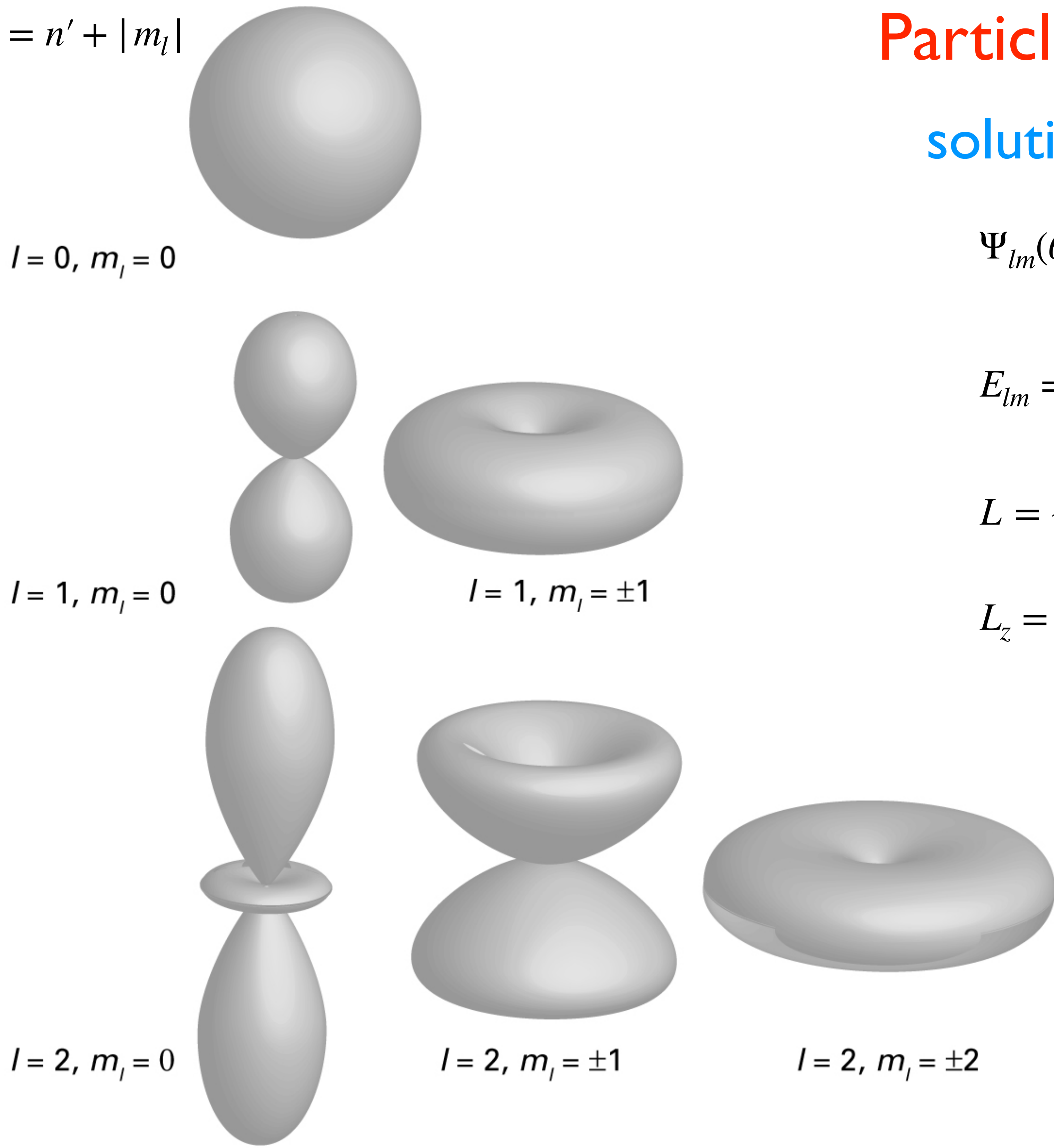
Hamiltonian in spherical coordinates

$$\hat{H} = -\frac{\hbar^2}{2m}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right\}$$

Quantum Mechanics (KEMS401)

lecture 8:

$l = n' + |m_l|$



Particle on sphere

solutions: spherical harmonics

$$\Psi_{lm}(\theta, \varphi) = \Theta_{lm}(\theta)\Phi_m(\varphi)$$

$$E_{lm} = l(l+1)\frac{\hbar}{2I}$$ 2l+1 degeneracies

$$L = \sqrt{l(l+1)}\hbar$$

$$L_z = m_l \hbar \qquad m_l \in [-l, l]$$

Quantum Mechanics (KEMS401)

lecture 8/9:

Hydrogen atom

Hamiltonian of electron and proton (6D)

$$\hat{H} = -\frac{\hbar^2}{2m_p}\left(\frac{\partial^2}{\partial x_p^2} + \frac{\partial^2}{\partial y_p^2} + \frac{\partial^2}{\partial z_p^2}\right) - \frac{\hbar^2}{2m_e}\left(\frac{\partial^2}{\partial x_e^2} + \frac{\partial^2}{\partial y_e^2} + \frac{\partial^2}{\partial z_e^2}\right) - \frac{Ze^2}{4\pi\epsilon_0\sqrt{(x_e - x_p)^2 + (y_e - y_p)^2 + (z_e - z_p)^2}}$$

center of mass coordinates (3D)

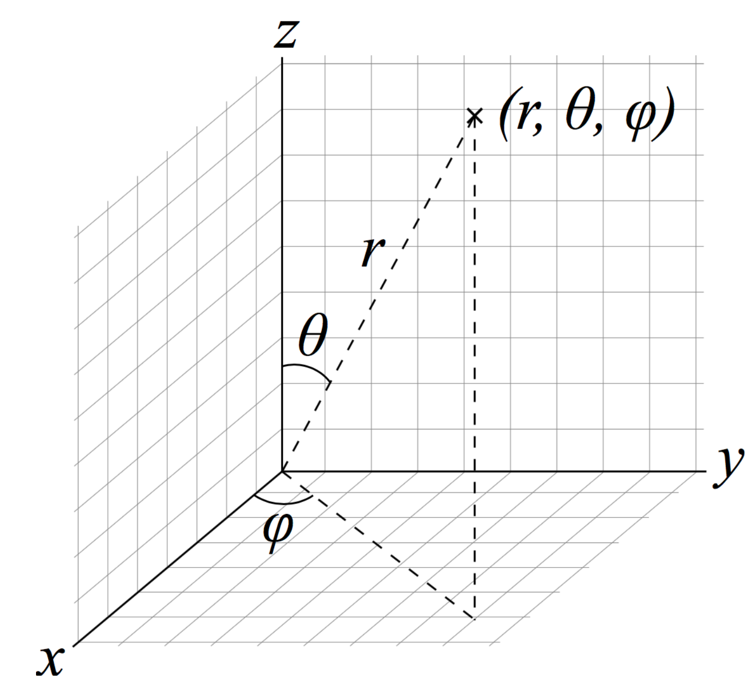
$$X = \frac{m_p x_p + m_e x_e}{m_p + m_e} \qquad Y = \frac{m_p y_p + m_e y_e}{m_p + m_e} \qquad Z = \frac{m_p z_p + m_e z_e}{m_p + m_e}$$

spherical coordinates (3D)

$$x = x_e - x_p = r \sin\theta \cos\phi$$

$$y = y_e - y_p = r \sin\theta \sin\phi$$

$$z = z_e - z_p = r \cos\theta$$



Quantum Mechanics (KEMS401)

lecture 8/9:

Hydrogen atom

Hamiltonian of electron and proton (6D)

$$\hat{H} = \hat{H}_{\mathrm{COM}}(X, Y, Z) + \hat{H}_{\mathrm{int}}(x, y, z)$$

free particle: COM

$$\hat{H}_{\mathrm{COM}} = -\frac{\hbar^2}{2(m_p + m_2)}\left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2}\right)$$

internal

$$\hat{H}_{\mathrm{int}} = -\frac{\hbar^2}{2\mu}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right\} + V(r)$$

reduced mass

$$\mu = \frac{m_p m_e}{m_p + m_e}$$

Quantum Mechanics (KEMS401)

lecture 8/9:

Hydrogen atom

free particle: COM

$$\hat{H}_{\text{COM}} = -\frac{\hbar^2}{2(m_p + m_2)}\left(\frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2}\right)$$

$$\hat{H}_{\text{COM}}\Psi_{\text{COM}}(X, Y, Z) = E_{\text{COM}}\Psi_{\text{COM}}(X, Y, Z)$$

internal

$$\hat{H}_{\text{int}} = -\frac{\hbar^2}{2\mu}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right\} + V(r)$$

$$\hat{H}_{\text{int}}\Psi_{\text{int}}(r, \theta, \phi) = E_{\text{int}}\Psi_{\text{int}}(r, \theta, \phi)$$

total wave function

$$\Psi(x, y, z, r, \theta, \phi) = \Psi_{\text{COM}} \cdot \Psi_{\text{int}}$$

Quantum Mechanics (KEMS401)

lecture 8/9:

Hydrogen atom

internal

$$\hat{H}_{\text{int}} = -\frac{\hbar^2}{2\mu}\left\{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial}{\partial\phi^2} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right\} - \frac{Ze^2}{4\pi\epsilon_0 r}$$

$$\hat{H}_{\text{int}}\Psi_{\text{int}}(r,\theta,\phi) = E_{\text{int}}\Psi_{\text{int}}(r,\theta,\phi)$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi_{\text{int}}}{\partial r}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Psi_{\text{int}}}{\partial\phi^2} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi_{\text{int}}}{\partial\theta}\right) + \frac{2\mu}{\hbar^2}\left(E_{\text{int}} + \frac{Ze^2}{4\pi\epsilon_0 r}\right)\Psi_{\text{int}} = 0$$

product of 1D functions:

$$\Psi_{\text{int}}(r,\theta,\phi) = \Phi(\phi)\Theta(\theta)R(r)$$

Quantum Mechanics (KEMS401)

lecture 8/9:

Hydrogen atom

product of 1D functions:

$$\Psi_{\text{int}}(r, \theta, \phi) = \Phi(\phi)\Theta(\theta)R(r)$$

divide:

$$\frac{1}{\Psi_{\text{int}}}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \Psi_{\text{int}}}{\partial r}\right) + \frac{1}{\Psi_{\text{int}}}\frac{1}{r^2 \sin^2\theta}\frac{\partial^2 \Psi_{\text{int}}}{\partial \phi^2} + \frac{1}{\Psi_{\text{int}}}\frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial \Psi_{\text{int}}}{\partial \theta}\right) + \frac{2\mu}{\hbar^2}\left(E_{\text{int}} + \frac{Ze^2}{4\pi\epsilon_0 r}\right) = 0$$

$$\frac{1}{R(r)}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right) + \frac{1}{\Phi(\phi)}\frac{1}{r^2 \sin^2\theta}\frac{\partial^2 \Phi(\phi)}{\partial \phi^2} + \frac{1}{\Theta(\theta)}\frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial \Theta(\theta)}{\partial \theta}\right) + \frac{2\mu}{\hbar^2}\left(E_{\text{int}} + \frac{Ze^2}{4\pi\epsilon_0 r}\right) = 0$$

Quantum Mechanics (KEMS401)

lecture 8/9:

Hydrogen atom

product of 1D functions:

$$\Psi_{\text{int}}(r, \theta, \phi) = \Phi(\phi)\Theta(\theta)R(r)$$

$$\frac{1}{R(r)}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right) + \frac{1}{\Phi(\phi)}\frac{1}{r^2\sin^2\theta}\frac{\partial^2\Phi(\phi)}{\partial\phi^2} + \frac{1}{\Theta(\theta)}\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta}\right) + \frac{2\mu}{\hbar^2}\left(E_{\text{int}} + \frac{Ze^2}{4\pi\epsilon_0 r}\right) = 0$$

divide, multiply, re-arrange etc.

$$\sin^2\theta\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right) + \frac{1}{\Phi(\phi)}\frac{\partial^2\Phi(\phi)}{\partial\phi^2} + \frac{1}{\Theta(\theta)}\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta}\right) + \frac{2\mu}{\hbar^2}r^2\sin^2\theta\left(E_{\text{int}} + \frac{Ze^2}{4\pi\epsilon_0 r}\right) = 0$$

equation for $\Phi(\phi)$

$$\frac{1}{\Phi(\phi)}\frac{\partial^2\Phi(\phi)}{\partial\phi^2} = -m^2$$

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi} \qquad m = 0, \pm 1, \pm 2, \pm 3,..$$

Quantum Mechanics (KEMS401)

lecture 8/9:

Hydrogen atom

$$\sin^2\theta \frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right) - m^2 + \frac{1}{\Theta(\theta)}\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta}\right) + \frac{2\mu}{\hbar^2}r^2\sin^2\theta\left(E_{\text{int}} + \frac{Ze^2}{4\pi\epsilon_0 r}\right) = 0$$

divide, multiply, re-arrange etc. once more

$$\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right) - \frac{m^2}{\sin^2\theta} + \frac{1}{\Theta(\theta)}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta}\right) + \frac{2\mu}{\hbar^2}r^2\left(E_{\text{int}} + \frac{Ze^2}{4\pi\epsilon_0 r}\right) = 0$$

equation for $\Theta(\theta)$

$$\frac{1}{\Theta(\theta)}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{m^2}{\sin^2\theta} = -\beta$$

$$\Theta_{lm}(\theta) = (1-z^2)^{\frac{|m|}{2}}G(z) \qquad z = \cos\theta$$

$$\beta = l(l+1) \qquad l = \nu + |m| \qquad \nu = 0,1,2,3,4,..$$

Quantum Mechanics (KEMS401)

lecture 9:

Hydrogen atom

$$\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right) - l(l+1) + \frac{2\mu}{\hbar^2}r^2\left(E_{\text{int}} + \frac{Ze^2}{4\pi\epsilon_0 r}\right) = 0$$

divide, multiply, re-arrange etc. for the last time

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R(r)}{\partial r}\right) + \left[-\frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2}\left(E_{\text{int}} + \frac{Ze^2}{4\pi\epsilon_0 r}\right)\right] = 0$$

equation for $R(r)$

$$R_{nl}(r) = e^{-\frac{1}{2}\rho}\rho^l L(\rho) \quad \rho = 2\alpha r \qquad \alpha^2 = -\frac{2\mu E}{\hbar^2} \qquad E_n = -\frac{\mu Z^2 e^4}{8\epsilon_0^2 h^2 n^2}$$

energies

$$E_n = -\frac{\mu Z^2 e^4}{8\epsilon_0^2 h^2 n^2} \qquad n = 1,2,3,... \quad l = 0,1,..,n-2,n-1 \quad m = -l, -(l-1),...,0,..(l-1), l$$

$$n = s, p, d, \ldots$$

Quantum Mechanics (KEMS401)

lecture 9:

Hydrogen atom

$$\Phi_m(\phi) = \frac{1}{2\pi} e^{im\phi}$$

$$\Theta_{lm}(\theta) = \sqrt{\frac{(2l+1)}{2}\frac{(l-|m|)!}{(l+|m|)!}} P_l^{|m|}(\cos\theta)$$

$$R_{nl}(r) = -\sqrt{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}} e^{-\rho/2}\rho^l L_{n+l}^{2l+1}(\rho) \qquad \rho = 2\alpha r \qquad \alpha^2 = -\frac{2\mu E}{\hbar^2}$$

$$E_n = -\frac{\mu Z^2 e^4}{8\epsilon_0^2 h^2 n^2}$$

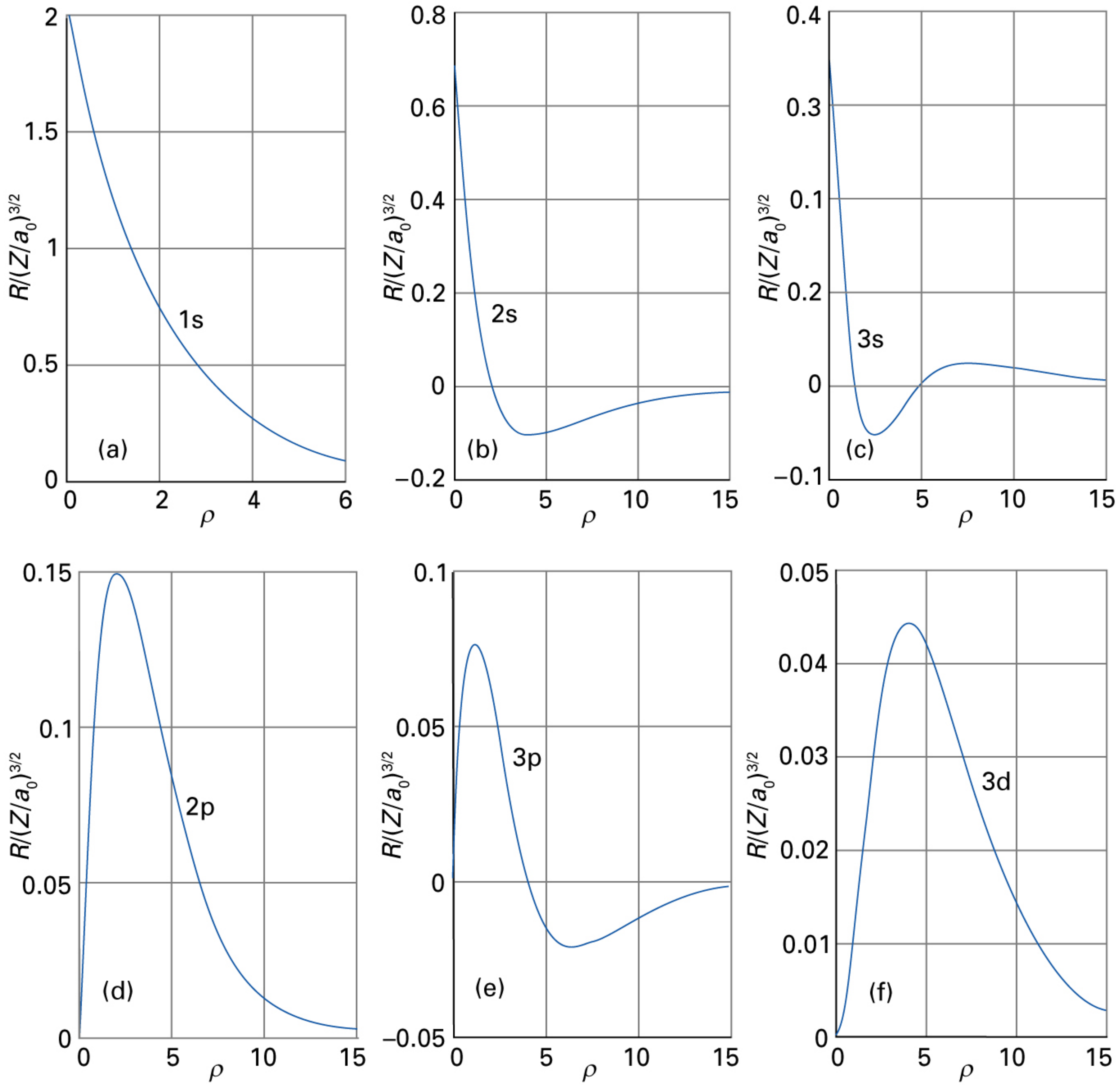
1S orbital

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

Quantum Mechanics (KEMS401)

lecture 9:

Hydrogen atom



$$\rho = 2\alpha r$$

$$\alpha^2 = -\frac{2\mu E}{\hbar^2}$$

$$E_n = -\frac{\mu Z^2 e^4}{8\epsilon_0^2 h^2 n^2}$$

$$a_0 = \frac{\epsilon_0 h^2}{\pi \mu e^2}$$

Quantum Mechanics (KEMS401)

lecture 9:

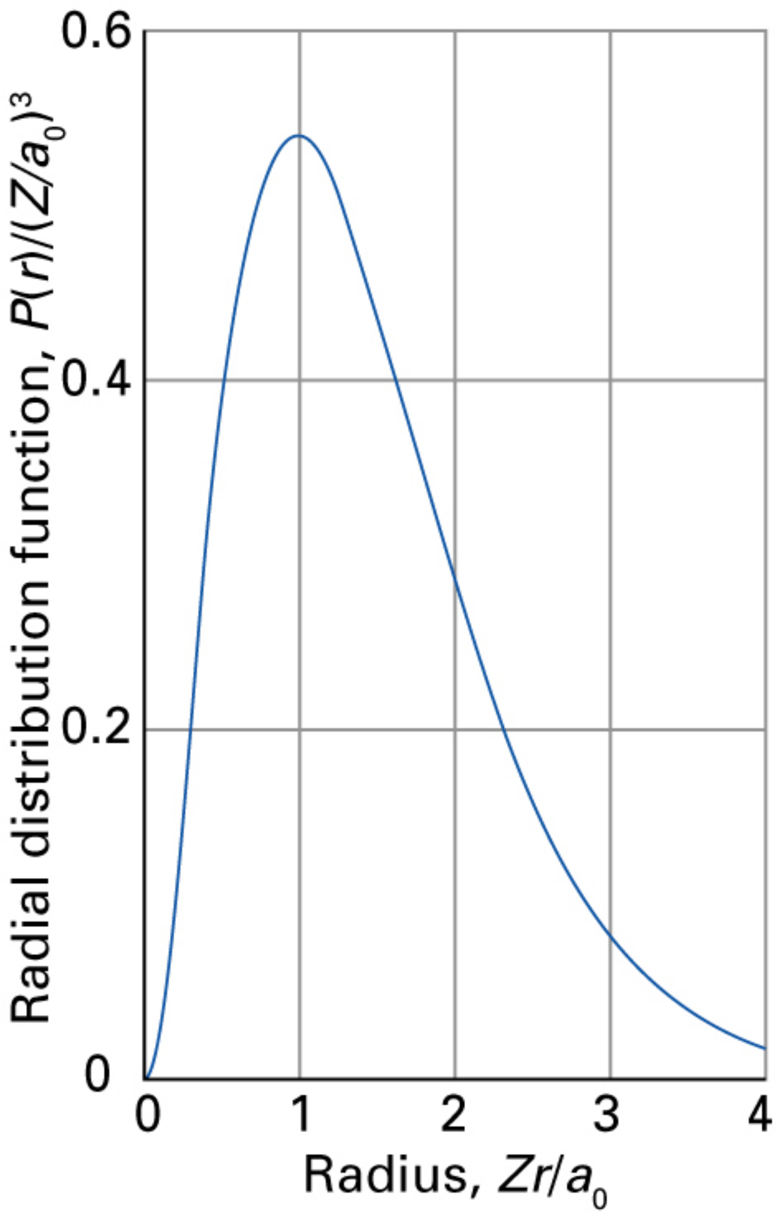
Hydrogen atom

1s radial distribution function

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

$$P(r)dr = 4\pi r^2 \psi^*_{100}(r)\psi_{100}(r)$$

$$P(r) = \frac{4r^2}{a_0^3} e^{-2r/a_0}$$



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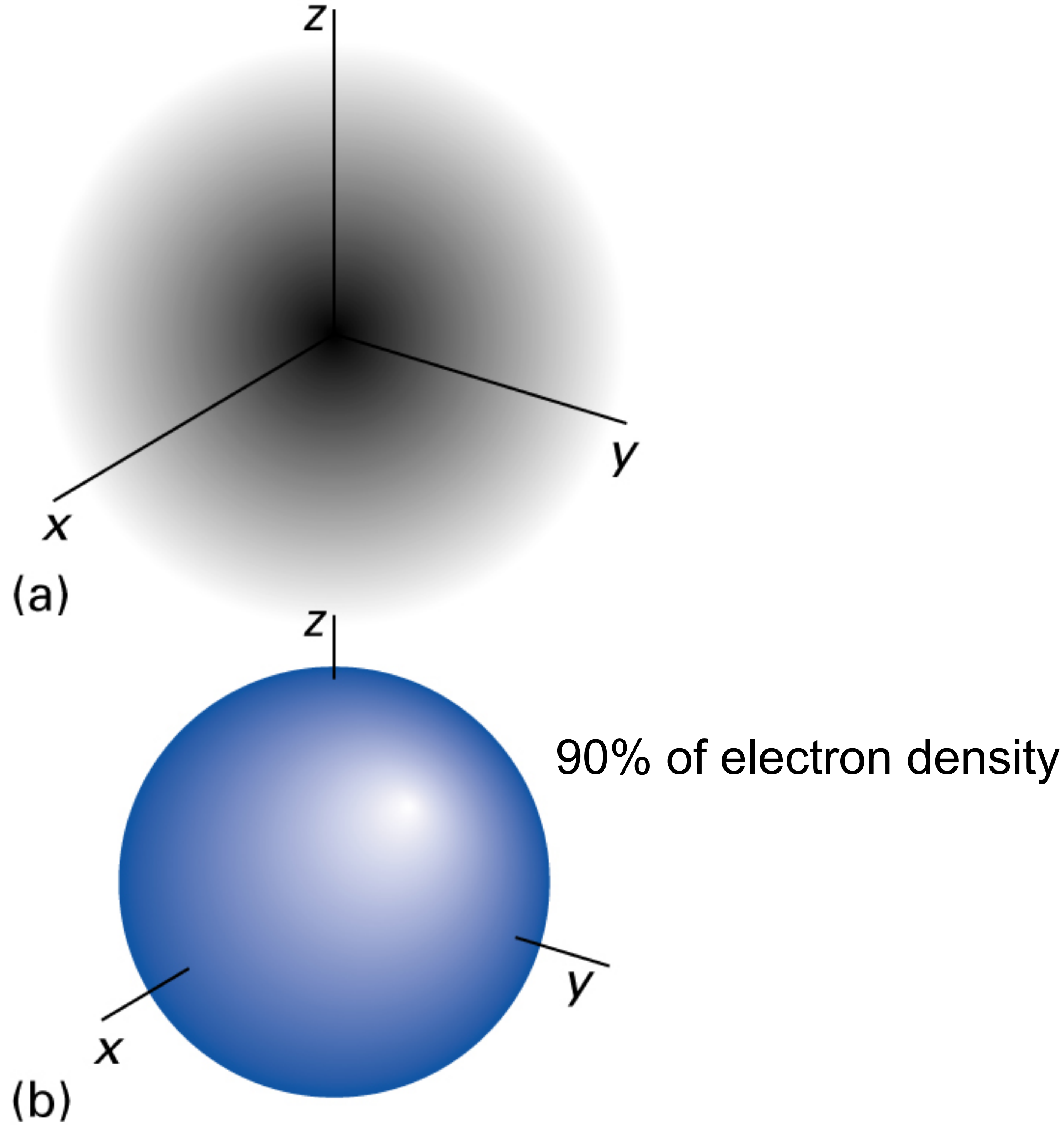
Quantum Mechanics (KEMS401)

lecture 9:

Hydrogen atom

1s orbital

$$\psi_{100}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$



Quantum Mechanics (KEMS401)

lecture 9:

Hydrogen atom

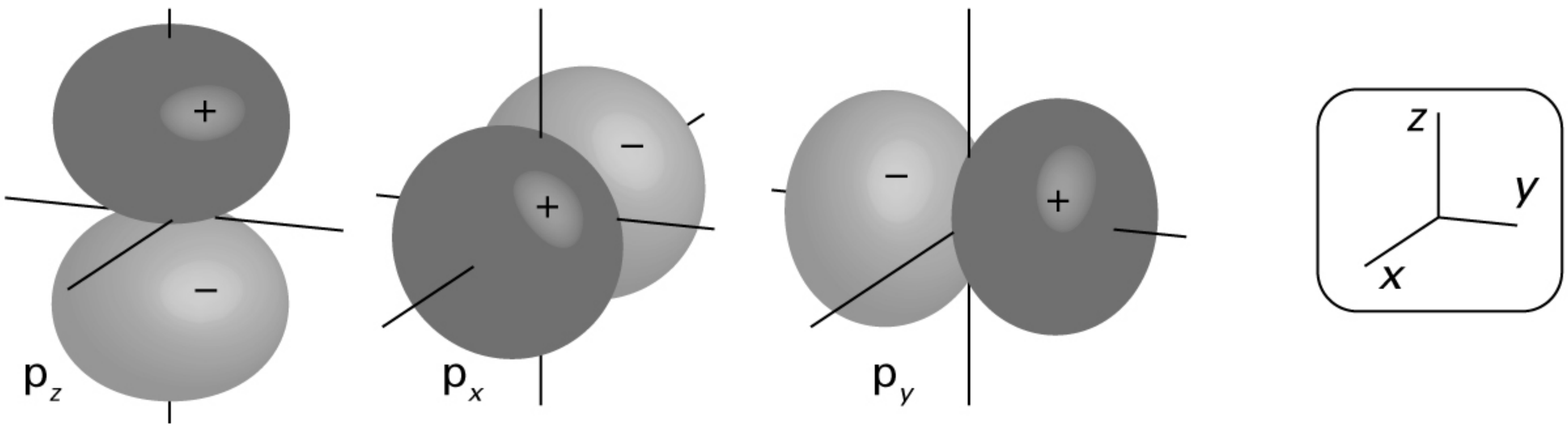
$$x = x_e - x_p = r\sin\theta\cos\phi$$

$$y = y_e - y_p = r\sin\theta\sin\phi$$

$$z = z_e - z_p = r\cos\theta$$

p orbitals (3) $\quad n > 1$

90% of electron density



$Y_{l=1,m=0}(\theta,\varphi)$ $\qquad p_0 = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} R_{n1}(r)\cos\theta$ $\qquad p_z = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} R_{n1}(r)\cos\theta$

$Y_{l=1,m=1}(\theta,\varphi)$ $\qquad p_{+1} = -\left(\frac{3}{8\pi}\right)^{\frac{1}{2}} R_{n1}(r)\sin\theta e^{i\varphi}$ $\qquad p_x = \frac{1}{\sqrt{2}}(p_{-1} - p_{+1}) = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} R_{n1}(r)\sin\theta\cos\varphi$

$Y_{l=-1,m=-1}(\theta,\varphi)$ $\qquad p_{-1} = \left(\frac{3}{8\pi}\right)^{\frac{1}{2}} R_{n1}(r)\sin\theta e^{-i\varphi}$ $\qquad p_y = \frac{i}{\sqrt{2}}(p_{-1} + p_{+1}) = \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} R_{n1}(r)\sin\theta\sin\varphi$

Quantum Mechanics (KEMS401)

lecture 9:

$$x = x_e - x_p = r\sin\theta\cos\phi$$

$$y = y_e - y_p = r\sin\theta\sin\phi$$

$$z = z_e - z_p = r\cos\theta$$

Hydrogen atom

d orbitals (5)

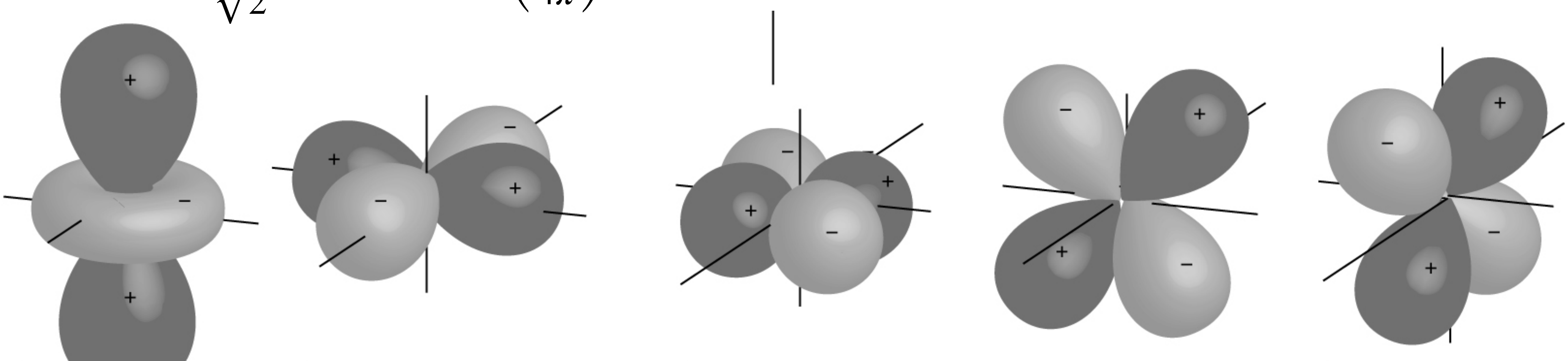
$n > 2 \qquad Y_{l=2,m=-2}(\theta,\varphi)\ldots Y_{l=2,m=2}(\theta,\varphi)$

$$d_{z^2} = \left(\frac{5}{16\pi}\right)^{\frac{1}{2}} R_{n2}(r)(3\cos^2\theta - 1) = \left(\frac{5}{16\pi}\right)^{\frac{1}{2}} R_{n2}(r)(3z^2 - r^2)/r^2$$

$$d_{x^2-y^2} = \frac{1}{\sqrt{2}}(d_{+2} + d_{-2}) = \left(\frac{15}{16\pi}\right)^{\frac{1}{2}} R_{n2}(r)(x^2 - y^2)/r^2$$

$$d_{xy} = \frac{1}{i\sqrt{2}}(d_{+2} - d_{-2}) = \left(\frac{15}{4\pi}\right)^{\frac{1}{2}} R_{n2}(r)xy/r^2 \qquad d_{yz} = \frac{1}{i\sqrt{2}}(d_{+} + d_{-1}) = -\left(\frac{15}{4\pi}\right)^{\frac{1}{2}} R_{n2}(r)yz/r^2$$

$$d_{zx} = \frac{1}{\sqrt{2}}(d_{+} - d_{-1}) = -\left(\frac{15}{4\pi}\right)^{\frac{1}{2}} R_{n2}(r)zx/r^2$$



d_{z^2} $\qquad$ $d_{x^2-y^2}$ $\qquad$ d_{xy} $\qquad$ d_{yz} $\qquad$ d_{zx}