

Wohl Ch. 3: Simple Approximations

1. Dimensions & Scaling

2. Fitting Wavelengths in a Well: WKB

3. Guessing the Ground State: Variational Method

Dimensions & Scaling

$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$ All 3 terms have to have same dimensions

Energies of hydrogen atom ($E_n = -\frac{1}{n^2} \frac{\hbar^2}{2ma_0^2}$) & infinite square well ($E_n = n^2 \pi^2 \frac{\hbar^2}{2mL^2}$)

$a_0 = \frac{\hbar^2}{mke^2}$ is the Bohr radius & L is the width of the square well.

Schrödinger for harmonic oscillator: $-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi$

Let M, L, T represent the fundamental physical dimensions of mass, length, time.

$$\dim(E) = ML^2T^{-2} \quad \dim(m) = M \quad \dim(\omega) = T^{-1} \quad \dim(\hbar) = ML^2T^{-1}$$

$$\dim(k) = MT^{-2}$$

$$\text{Ex: } \dim(E) = [\dim(\hbar)]^a [\dim(m)]^b [\dim(k)]^c$$

$$\Rightarrow ML^2T^{-2} = (ML^2T^{-1})^a M^b (MT^{-2})^c$$

$$1 = a + b + c \quad 2 = 2a + 3c \quad -2 = -a - 2c \quad \text{solve. } E \propto \text{result}$$

Fitting Wavelengths in a Well: The WKB Method

- For many potential wells of interest, no solutions to the Schrödinger eqns. can be solved in closed form
WKB method:

1) Calculate # of de Broglie Wavelengths between turning points of a well as a function of an arbitrary value of the energy.

2) How many wavelengths correspond to the quantized energy levels of the infinite square well & the oscillator, where we already know the answers?

Ex: infinite square well

$$\lambda = \frac{h}{p} = \frac{2\pi\hbar}{\sqrt{2mE}} \quad (E = \frac{p^2}{2m})$$

$$\# \text{ wavelengths between } 0 \text{ \& } L = \int_0^L \frac{dx}{\lambda} = \frac{L}{\lambda} = \frac{\sqrt{2mE}}{2\pi\hbar} L$$

quantized energy levels: # wavelengths = $\frac{n}{2}$

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

Ex: A bouncing ball: $V(z) = \begin{cases} mgz & z \geq 0 \\ \infty & z < 0 \end{cases}$ $\lambda(z) = \frac{h}{p(z)} = \frac{2\pi\hbar}{\sqrt{2m(E-V(z))}}$ ($\frac{p}{2m} = E - V(z)$)

\Rightarrow turning points at $z=0, z = \frac{E}{mg} \equiv z_0$

$$\int_0^{z_0} \frac{dz}{\lambda(z)} = \frac{1}{2\pi\hbar} \int_0^{z_0} \sqrt{2m(E-mgz)} dz$$

$$y \equiv z/z_0$$

$$\Rightarrow \frac{\sqrt{2mE}}{2\pi\hbar} \frac{E}{mg} \int_0^1 \sqrt{1-y} dy = \frac{1}{2\pi\hbar} \sqrt{\frac{2E^3}{m}} \left(-\frac{2}{3}\right) (1-y)^{3/2} \Big|_0^1 = \frac{1}{3\pi\hbar} \sqrt{\frac{2E^3}{m}}$$

want $(n/2 - 1/8)$ wavelengths $\Rightarrow \frac{1}{3\pi\hbar} \sqrt{\frac{2E_n^3}{m}} \approx \frac{1}{2} (n - \frac{1}{4})$

offset chosen by: $\begin{cases} 2 \text{ hard turning points: } n=0, 1, 2; \frac{1}{4}, \frac{3}{4}, \frac{5}{4} \\ 1 \text{ soft, 1 hard: } n=1, 2, 3; \frac{3}{8}, \frac{7}{8}, \frac{11}{8} \\ 2 \text{ soft: } n=0, 1, 2, \dots; \frac{1}{4}, \frac{3}{4}, \frac{5}{4} \end{cases}$

Guessing the Ground State: The Variational Method

- Used mainly to get a good approximation for the ground-state energy of a system.
- If ψ_1 is the true ground state ~~wavefunction~~ wavefunction & \hat{H} is the Hamiltonian, then $\hat{H}\psi_1 = E_1\psi_1$

$$\int_{-\infty}^{\infty} \psi_1^* (\hat{H}\psi_1) dx = E_1 \int_{-\infty}^{\infty} \psi_1^* \psi_1 dx = E_1$$

- We don't know ψ_1 , so we guess a trial wavefunction ψ_T .

$$E_T = \int_{-\infty}^{\infty} \psi_T^* (\hat{H}\psi_T) dx$$

$$\psi_T = \sum_{n=1}^{\infty} c_n \psi_n \quad \text{where } \sum |c_n|^2 = 1 \quad E_T = \sum_{n=1}^{\infty} E_n |c_n|^2 \geq \sum_{n=1}^{\infty} E_1 |c_n|^2 = E_1 \rightarrow E_T \geq E_1$$

Ex: hydrogen: $\psi_T(r) = c e^{-br}$ (true ground state wavefunction has $b = 1/a_0$)

$$\int_0^{\infty} r^n e^{-ar} dr = \frac{n!}{a^{n+1}}, \quad \int_{\text{space}} |\psi_T(r)|^2 r^2 \sin\theta dr d\theta d\phi = 4\pi |c|^2 \int_0^{\infty} e^{-2br} r^2 dr = 4\pi |c|^2 \frac{2}{(2b)^3} = \frac{\pi |c|^2}{b^3} = 1$$

$V(r) = -ke^2/r \rightarrow$ potential energy part of integral of $\psi_T(\hat{H}\psi_T) = -4\pi ke^2 |c|^2 \int_0^{\infty} e^{-2br} r dr = -ke^2 b$

Kinetic energy integral: $\nabla\psi_T = c \frac{d(e^{-br})}{dr} \hat{r} = -b\psi_T \hat{r}$

$$-\frac{\hbar^2}{2m} \int_{\text{space}} \psi_T^* \nabla^2 \psi_T d^3r = +\frac{\hbar^2}{2m} b^2 \int_{\text{space}} |\psi_T|^2 d^3r = \frac{\hbar^2 b^2}{2m}$$

$$E_T(b) = \frac{\hbar^2 b^2}{2m} - ke^2 b$$

$$\frac{dE_T}{db} = \frac{\hbar^2 b}{m} - ke^2 = 0$$

$$\Rightarrow b = \frac{mke^2}{\hbar^2} = \frac{1}{a_0}$$

Wohl Ch. 10: Spin-1/2 Particles

1. Spinors, Eigenvals & Eigenstates
2. Polarization Vector
3. Magnetic Moments & Magnetic Fields
4. Time Dependence: Precessing the Polarization
5. Time Dependence: Flipping the Polarization
6. Stern-Gerlach Experiments

- In a magnetic field, the spin-up & down states w.r.t. the field direction have different energies (Zeeman Effect)
- In a static magnetic field, the spin precesses about the field direction (Larmor precession)
- In a properly arranged time-dependent field, the spin will spiral back & forth between spin-up & down states (magnetic resonance)
- In an inhomogeneous field, the spin-up & down states can be separated into two beams (Stern-Gerlach)

Spinors

The only simultaneous eigenstates of the angular momentum operators \hat{S}^2 & \hat{S}_z are:

$$|s, m\rangle = |1/2, \pm 1/2\rangle$$

shorthand: $|+\rangle = |1/2, 1/2\rangle = |\uparrow\rangle$

$|-\rangle = |1/2, -1/2\rangle = |\downarrow\rangle$

* In spin up, $|+\rangle$, \hat{S} is 55° w.r.t. $+z$

Two component vectors (spinors): $|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $|-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $|+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ $|-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$
 $|X\rangle = c_+ |+\rangle + c_- |-\rangle$ $|+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ $|-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

$$\hat{S}_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \hat{S}_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \hat{S}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad [\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z$$

General Eigenstates

$a\hat{I} + b\hat{\sigma}$ eigenstates belonging to eigenvals $a \pm b$ are associated w/ $\hat{b} = b\hat{n}$

$$(b_x, b_y, b_z) = (b \sin\theta \cos\phi, b \sin\theta \sin\phi, b \cos\theta)$$

$$a\hat{I} + b\hat{\sigma} = \begin{pmatrix} a + b \cos\theta & b e^{-i\phi} \sin\theta \\ b e^{i\phi} \sin\theta & a - b \cos\theta \end{pmatrix}$$

eigenvals $\lambda_{\pm} = a \pm b \rightarrow$ eigenstates $|+\rangle = \begin{pmatrix} \cos \frac{\theta}{2} \\ e^{i\phi} \sin \frac{\theta}{2} \end{pmatrix}, |-\rangle = \begin{pmatrix} \sin \frac{\theta}{2} \\ -e^{i\phi} \cos \frac{\theta}{2} \end{pmatrix}$

Polarization Vector

\underline{P} points along direction which, were a measurement made of the component of \underline{S} , the result would be $\pm\hbar/2$ w/ certainty. \underline{P} points in direction along which spin is up.

$$(P_x, P_y, P_z) = (\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta), \quad P_x^2 + P_y^2 + P_z^2 = 1$$

$$\underline{P} = \begin{pmatrix} \cos \frac{\theta}{2} \\ e^{i\phi} \sin \frac{\theta}{2} \end{pmatrix} \quad \text{(spin up/down amplitudes)}$$

or write in x, y, z / r, θ , ϕ

$$c_+ = \langle +z | X \rangle \quad c_- = \langle -z | X \rangle$$

$$P_x = 2\text{Re}(c_+^* c_-) \quad P_y = 2\text{Im}(c_+^* c_-) \quad P_z = |c_+|^2 - |c_-|^2$$

$$\underline{P} = \begin{pmatrix} \sin\theta \cos\phi \\ \sin\theta \sin\phi \\ \cos\theta \end{pmatrix} = \begin{pmatrix} 2\text{Re}(c_+^* c_-) \\ 2\text{Im}(c_+^* c_-) \\ |c_+|^2 - |c_-|^2 \end{pmatrix}$$

- Suppose, knowing an initial \underline{P} , want the probability of getting $\pm\hbar/2$ on measuring along the direction of arbitrary \underline{d} .

$$P(\text{spin up along } \underline{d}) = \frac{1 + \cos\beta}{2} = \cos^2\left(\frac{\beta}{2}\right) \quad \text{where } \beta \text{ is angle between } \underline{P} \text{ \& } \underline{d}.$$

Wohl Ch. 11: Two Angular Momenta

1. Hyperfine Structure of the Hydrogen Ground State
2. The 21-cm Line & Astronomy
3. Total Spin of Two Spin-1/2 Particles
4. Coupling Any Two Angular Momenta
5. Clebsch-Gordan Coefficients
6. Particle Multiplets & Isospin

Hyperfine

Two spin-1/2 particles

basis states: $|++\rangle, |+-\rangle, |-+\rangle, |--\rangle$

Ex) $|+-\rangle \rightarrow |s_e, s_p; m_e, m_p\rangle = |1/2, 1/2; +1/2, -1/2\rangle$

$$|++\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad |+-\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad |-+\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad |--\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Grnd st. of Hydrogen

$$\Rightarrow \Psi_{100}(r)|\chi\rangle = \frac{1}{\sqrt{\pi} a_0^3} e^{-r/a_0} \begin{pmatrix} c_{++} \\ c_{+-} \\ c_{-+} \\ c_{--} \end{pmatrix}$$

Two magnetic moments associated w/ the spins of electron & proton

$$\hat{\mu}_e = -\mu_B \hat{S}_e \quad \hat{\mu}_p = \mu_p \hat{S}_p \quad E_{\text{hydrogen}} = \frac{-13.6 \text{ eV}}{n^2}$$

$$\hat{H}_{\text{hf}} = A \hat{S}_e \cdot \hat{S}_p = A (\hat{S}_x^e \hat{S}_x^p + \hat{S}_y^e \hat{S}_y^p + \hat{S}_z^e \hat{S}_z^p)$$

$$\hat{S}_x |+\rangle = +|-\rangle \quad \hat{S}_y |+\rangle = i|-\rangle \quad \hat{S}_z |+\rangle = +|+\rangle$$

$$\hat{S}_x |-\rangle = -|+\rangle \quad \hat{S}_y |-\rangle = -i|+\rangle \quad \hat{S}_z |-\rangle = -|-\rangle$$

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} \otimes \begin{pmatrix} a_2 \\ b_2 \end{pmatrix} = \begin{pmatrix} a_1 b_1 \\ a_1 b_2 \\ b_1 a_2 \\ b_1 b_2 \end{pmatrix}$$

$$\begin{pmatrix} a_1 & c_1 \\ b_1 & d_1 \end{pmatrix} \otimes \begin{pmatrix} a_2 & c_2 \\ b_2 & d_2 \end{pmatrix} = \begin{pmatrix} a_1 a_2 & a_1 c_2 & c_1 a_2 & c_1 c_2 \\ a_1 b_2 & a_1 d_2 & c_1 b_2 & c_1 d_2 \\ b_1 a_2 & b_1 c_2 & d_1 a_2 & d_1 c_2 \\ b_1 b_2 & b_1 d_2 & d_1 b_2 & d_1 d_2 \end{pmatrix}$$

21-cm line

splits to $+A$ and $-3A$

$$\nu = 4A/h, \quad \lambda = c/\nu \approx 21.1 \text{ cm}$$

Total Spin of Two Spin-1/2 Particles

$$\hat{S}_x = \hat{S}_x^e + \hat{S}_x^p \quad \hat{S}_y = \hat{S}_y^e + \hat{S}_y^p, \quad \hat{S}^2 = (\hat{S}^e + \hat{S}^p)^2 = (\hat{S}^e)^2 + (\hat{S}^p)^2 + 2\hat{S}^e \cdot \hat{S}^p \quad [\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z$$

$$\hat{J}^2 |j, m\rangle = j(j+1)\hbar^2 |j, m\rangle$$

$$\hat{J}_1 \cdot \hat{J}_2 = \frac{1}{2} (\hat{J}^2 - \hat{J}_1^2 - \hat{J}_2^2)$$

$$\hat{J}_z |j, m\rangle = m\hbar |j, m\rangle$$

$$\hat{J}_+ |j, m\rangle = \sqrt{(j-m)(j+m+1)} \hbar |j, m+1\rangle$$

$$\hat{J}_- |j, m\rangle = \sqrt{(j+m)(j-m+1)} \hbar |j, m-1\rangle$$

Coupling any Two Angular Momenta

Ex) Spin=1 & Spin=1/2

$$|m_1, m_2\rangle = |+1, +1/2\rangle$$

$$|+1, -1/2\rangle, |0, +1/2\rangle$$

$$|0, -1/2\rangle, |-1, +1/2\rangle$$

$$|-1, -1/2\rangle$$

$$m_1 + m_2 = M = +3/2$$

$$+1/2$$

$$-1/2$$

$$-3/2$$

$$|J, m\rangle = |3/2, +3/2\rangle$$

⋮
⋮
⋮
⋮

$$\hat{J}_- |j, m\rangle = \sqrt{(j+m)(j-m+1)} \hbar |j, m-1\rangle$$

$$\hat{J}_- |3/2, +3/2\rangle = (\hat{j}_{1-} + \hat{j}_{2-}) |1, +1/2\rangle$$