Physics 492 M Gold

<u>Lecture 1</u>

This semester is mostly <u>atomic physics</u>

(1) $V(r) = -\frac{\alpha \hbar c}{r}$ central potential
no spin

$\alpha \hbar c = \left(\frac{1}{137.036}\right) 197 \text{ eV}\cdot\text{nm} = e^2 = \frac{e'^2}{4\pi\epsilon_0}$

(2) relativistic corrections
perturbation theory

(3) External $\vec{E}, \vec{B}$ fields

(4) Multi electron atoms

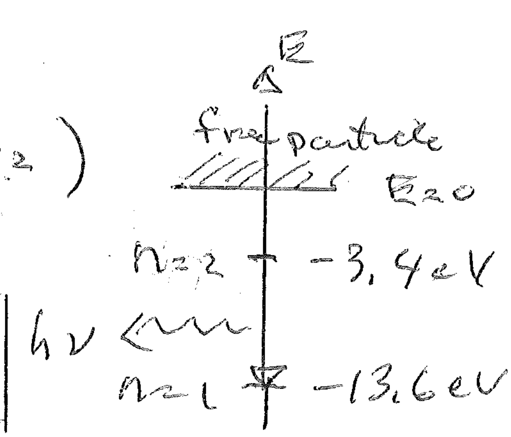
(5) atomic bonding

(6) scattering theory

(7) spontaneous emission

$$\nu = \frac{\Delta E}{\hbar} = R_\infty \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

$$\boxed{2\pi\hbar c R_\infty = 13.6 \text{ eV} = \frac{1}{2} m_e c^2 \alpha^2}$$



$$V(r) = -\frac{\alpha\hbar c}{r}$$

In hydrogen C.m. frame with $\Delta p \Delta r \sim \hbar$
minimize $E(r)$ for ground state.

gives exact Q.M. answer

$$\Delta p = \sqrt{\langle p^2 \rangle} \sim \frac{\hbar}{r}$$

$$E(r) = \frac{\hbar^2}{r^2}\frac{1}{2m} - \frac{\alpha\hbar c}{r}$$

$$\left.\frac{dE}{dr}\right|_{r=r_0} = 0 = \frac{\hbar^2}{2m}\left(\frac{-2}{r^3}\right) + \frac{\alpha\hbar c}{r^2}$$

$$r_0 = \frac{\hbar}{\alpha m c}$$ Bohr radius

$$E(r_0) = \frac{\hbar^2}{2m}\left(\frac{\alpha m c}{\hbar}\right)^2 - \alpha\hbar c\left(\frac{\alpha m c}{\hbar}\right)$$

$$E_0 = -\frac{1}{2}\alpha^2 \underbrace{mc^2}$$

energy

coupling squared

$$V(r) = k\frac{q_1 q_2}{r}$$ $k = \frac{1}{4\pi\varepsilon_0}$ SI

$e_{SI} = 1.60\times10^{-19}\,C$

$ke^2 = \alpha\hbar c$

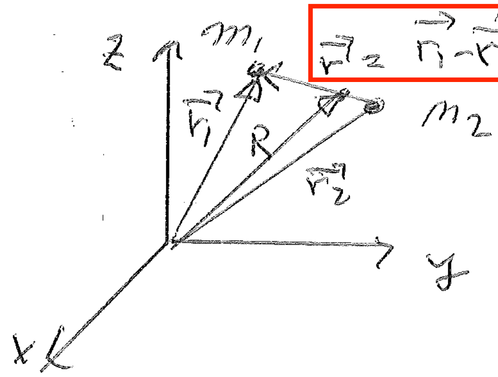
$\alpha \cong 1/137.0$

$k = 1$ Gaussian

$e_G = 4.80\times10^{-10}$ esu

$\hbar c = 197$ eV.nm = MeV.fm

Two Body Central Force



$$\boxed{\vec{r} = \vec{r}_1 - \vec{r}_2}$$

in absence of external forces, total momentum is conserved.

$$\vec{P}_{cm} = \vec{P}_1 + \vec{P}_2 = \text{constant}$$

$$\vec{P}_{cm} \quad (m_1+m_2)\dot{\vec{R}}_{cm} = m_1\dot{\vec{r}}_1 + m_2\dot{\vec{r}}_2$$

$$\boxed{\vec{R}_{cm} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1+m_2}}$$

$V(\vec{r})$ for central potential. We will always have a spherically symmetric potential,

$$V(\vec{r}) = V(|\vec{r}|) = V(r)$$

Rewrite kinetic energy,

$$\frac{1}{2}m_1|\dot{\vec{r}}_1|^2 + \frac{1}{2}m_2|\dot{\vec{r}}_2|^2 = \frac{1}{2}M_T|\dot{\vec{R}}_{cm}|^2 + \frac{1}{2}\mu|\dot{\vec{r}}|^2$$

where $M_T = m_1+m_2$, $\mu = \frac{m_1 m_2}{m_1+m_2}$

μ is reduced mass

The Hamiltonian needed for Q.M. is given in terms of momenta,

$$\vec{p} \equiv \mu \dot{\vec{r}} = \frac{m_2 \vec{p}_1 - m_1 \vec{p}_2}{m_1 + m_2}$$

$$\vec{P}_{cm} = m_T \dot{\vec{R}}_{cm}$$

$$\hat{H} = \frac{\hat{P}_{cm}^2}{2 m_T} + \frac{\hat{p}^2}{2\mu} + V(r) = \hat{H}_{cm} + \hat{H}_{rel}$$

In homework show:

$$[\hat{x}_i, \hat{p}_j] = i\hbar \delta_{ij}$$

$$[\hat{X}_i, \hat{P}_{cm_j}] = i\hbar \delta_{ij}$$

$$[\hat{X}_i, \hat{P}_{cm_j}] = 0$$

$$[\hat{x}_i, \hat{P}_j] = 0$$

notation from text

$$\vec{r} = \sum_i x_i \hat{e}_i$$

$$\vec{R}_{cm} = \sum_i X_i \hat{e}_i$$

$\hat{e}_i$ an Euclidean orthogonal unit vector

so that $[\hat{H}_{cm}, \hat{H}_{rel}] = 0$

$$\Psi(\vec{r}, \vec{R}) = \psi_{cm}(\vec{R}) \psi_{rel}(\vec{r})$$

$$E = E_{cm} + E_{rel}$$

Total system is a free particle, so wave function is plane wave:

$$\psi_{cm}(\vec{R}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{R}\cdot\vec{P}_{cm}/\hbar}$$

We will therefore deal exclusively with the relative wave function and drop the subscript "rel".

Generalizing from 1D to 3D,

$$\hat{T}(\vec{a})\,|\vec{r}\rangle \equiv |\vec{r}+\vec{a}\rangle$$

$$\left[\hat{T}(a_x\hat{x}),\hat{T}(a_y\hat{y})\right] = 0 \quad \text{from } [\hat{P}_x,\hat{P}_y]=0$$

thus, $\hat{T}(\vec{a}) = \exp(-i\,\vec{a}\cdot\hat{\vec{P}}/\hbar)$

$$\langle\vec{r}|\,\hat{T}(\vec{\varepsilon})\,|\psi\rangle = \langle\vec{r}-\vec{\varepsilon}\,|\psi\rangle$$

expand to first order in $\vec{\varepsilon}$.

$$\langle\vec{r}|\left(1-\frac{i}{\hbar}\vec{\varepsilon}\cdot\hat{\vec{P}}\right)|\psi\rangle = \psi(\vec{r}) - \vec{\varepsilon}\cdot\vec{\nabla}\psi(\vec{r})$$

$$\langle\vec{r}|\hat{\vec{P}}|\psi\rangle = \frac{\hbar}{i}\vec{\nabla}\psi(r)$$

$$\hat{\vec{p}} \xrightarrow[\vec{r}\text{ basis}]{} \frac{\hbar}{i}\vec{\nabla}$$

Orbital angular momentum

You show that $\hat{L}_i = \sum_{jk} \varepsilon_{ijk} \hat{X}_j \hat{P}_k$

satisfy $[L_i, L_j] = i\hbar \sum_k \varepsilon_{ijk} \hat{L}_k$

So are generators of rotations in Hilbert space. Eigenvalues of $\hat{L}_i$ are components of a Euclidean vector. A general vector operator $\hat{\vec{V}}$ transforms under a rotation as

$$\langle \vec{r} \,|\, \hat{V}_i \,|\, \vec{r} \rangle = \langle \vec{r} \,|\, \hat{R} \hat{R}^{+} \hat{V}_i \hat{R} \hat{R}^{+} \,|\, \vec{r} \rangle$$

$$= \langle \vec{r}\,' \,|\, \hat{V}_i' \,|\, \vec{r}_i\,' \rangle$$

with $$\hat{V}_i' = \hat{R}^{+} \hat{V}_i \hat{R} = \sum_j [\hat{R}]_{ij} \hat{V}_j$$

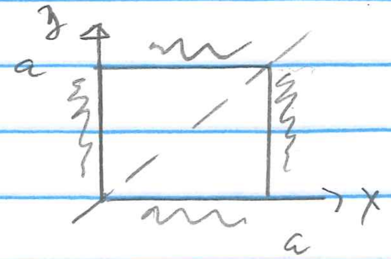
You can use the infinitessimal form of the rotation operator about $\hat{z}$,

$$\hat{R}_z = 1 - i\theta \frac{\hat{L}_z}{\hbar} \quad \text{to}$$

prove

$$[\hat{L}_z, \hat{V}_x] = i\hbar \hat{V}_y \qquad \text{(HW 9.6)}$$

Example: particle in 2D box



$$\hat{H} = \frac{1}{2m}\hat{P}_x^2 + \frac{1}{2m}\hat{P}_y^2 \quad \text{since } [\hat{P}_x, \hat{P}_y] = 0$$

$$|E\rangle = |n_1\rangle_x |n_2\rangle_y \equiv |n_1 n_2\rangle$$

$$\psi_{n_1 n_2}(x,y) = \langle x,y|n_1 n_2\rangle = \left(\sqrt{\frac{2}{a}}\right)^2 \sin\frac{n_1\pi x}{a}\sin\frac{n_2\pi y}{a}$$

$|n_1 n_2\rangle$ & $|n_2 n_1\rangle$ are degenerate

$$E = \frac{\hbar^2}{2m}\left(\frac{n_1\pi}{a}\right)^2 + \frac{\hbar^2}{2m}\left(\frac{n_2\pi}{a}\right)^2$$

This degeneracy is due to reflection symmetry.

Even and odd eigenstates under symmetry

$$\psi_\pm(x,y) \equiv \psi_{n_1 n_2}(x,y) \pm \psi_{n_2 n_1}(x,y)$$

Reflection operator $\hat{R}$ takes $x \leftrightarrow y$; $\psi_{n_2 n_1}(x,y) = \psi_{n_1 n_2}(y,x)$

So $\psi_\pm(x,y) = \psi_{n_1 n_2}(x,y) \pm \psi_{n_1 n_2}(y,x)$

$$\hat{R}\psi_\pm(x,y) = \pm\psi_\pm(x,y)$$

probability $|\psi_\pm|^2$ unchanged under reflection

Example: 2 particles in 1D box

$$\hat{H} = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} + V(x_1) + V(x_2) = \hat{H}_1 + \hat{H}_2$$

1, 2 label particles. Since $[\hat{H}_1, \hat{H}_2] = 0$

Energy is $E = E_1 + E_2$

$$\psi_{n_1, n_2}(x_1, x_2) = \phi_{n_1}(x_1)\, \phi_{n_2}(x_2)$$

$$\phi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

$$E = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 \left(n_1^2 + n_2^2\right)$$

again we find degeneracies. Here they are due to the particle exchange operator.

$$\hat{\mathcal{E}}_{12} \psi(x_1, x_2) = \psi(x_2, x_1)$$

$$[\hat{H}, \hat{\mathcal{E}}_{12}] = 0$$

We can define symmetric, antisymmetric states

$$\psi_{S,A} = \frac{1}{\sqrt{2}}\left(\psi_{n_1}(x_1)\psi_{n_2}(x_2) \pm \psi_{n_1}(x_2)\psi_{n_2}(x_1)\right)$$

When particles are identical we must require <u>fermions</u> to be antisymmetric and <u>bosons</u> to be symmetric

For particles with spin, the total wave function |space>|spin> must be symmetrized/antisymmetrized according to Bose/Fermi statistics.