Physics 115B at UCLA ◇ Formula Sheet (1 of 2)

Three Dimensional QM

The TISE still holds as $H\psi = E\psi$, and the extension from 1D to 3D follows:

$$x \implies x, y, z \iff r, \theta, \varphi$$
$$\psi(x) \implies \psi(x,y,z) \iff \psi(r,\theta,\varphi)$$
$$V(x) \implies V(x,y,z) \iff V(r,\theta,\varphi)$$
$$p = -i\hbar\frac{\partial}{\partial x}|\psi\rangle\,\hat{\boldsymbol{x}} \implies p = -i\hbar\nabla|\psi\rangle$$
$$\Psi_n(x,t) \implies \Psi_n(\boldsymbol{r},t) = \psi_n(\boldsymbol{r})e^{-iE_nt/\hbar}$$

Particle in a Box

Assume separable $\psi = X(x)\,Y(y)\,Z(z)$, which for a free particle becomes:

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2} = -\frac{2mE}{\hbar^2}$$

The solutions are sines and cosines of wavenumber k_i, where the energy is:

$$E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$$

Box of size a^3 at the origin removes cos terms, so wave function for $A_i = \sqrt{2/a}$:

$$\psi(x,y,z) = \prod_{i=1}^{3} A_i \sin\left(\frac{n_i\pi}{a}x_i\right)$$

Spherical Schrödinger Eq

Hamiltonian is chosen as $H = p^2/2m + V$. The Laplacian in spherical coordinates:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\varphi^2}\right)$$

With potential $V(r)$, the Schrödinger equation is then solved by separation of variables and power series expansion:

- Separate $\psi(r,\theta,\varphi) = R(r)Y(\theta,\varphi)$
- Substitute, divide, and cancel
- Separate variables (equate to 0)
  - Set equal to $\pm\ell(\ell+1)$
- Separate $Y(\theta,\varphi) = \Theta(\theta)\Phi(\varphi)$
- Substitute, divide, and cancel
- Separate variables (equate to 0)
  - Set equal to $\pm m^2$
- Solve for Φ with sep. of variables
- Solve for Θ with power series
- Solve for R with power series for a specific potential energy $V(r)$
- Multiply $\psi = R(r)\,\Theta(\theta)\,\Phi(\varphi)$

The solutions $Y(\theta,\varphi) = \Theta(\theta)\,\Phi(\varphi)$ are spherical harmonics for integers $|m| \le l$:

$$Y_l^m = \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}\,e^{im\varphi}P_l^m(\cos\theta)$$

P_l^m is the associated Legendre function for $\epsilon = -1^m$ for $0 < m$ and 1 otherwise:

$$P_l^m = \epsilon\frac{(1-x^2)^{|m|/2}}{2^l l!}\left(\frac{d}{dx}\right)^{l+|m|}(x^2-1)^l$$

Infinite Spherical Well

Radial equation for $R(r)$, with $u = rR(r)$:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left(V + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right)u = Eu$$

For the spherical well, the potential is:

$$V(r) = \begin{cases} 0 & r \le a \\ \infty & a < r \end{cases}$$

For $\ell = 0$ the solution is simple:

$$\frac{d^2u}{dr^2} = -k^2u \implies u(r) = A\sin(kr)$$
$$\psi_{n,0,0} = \frac{\sin(n\pi r/a)}{\sqrt{2\pi a}\,r};\; E_{n,0} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

R, with spherical Bessel functions j_ℓ:

$$R(r) = A\,j_\ell(kr)$$

The spherical Bessel functions are:

$$j_\ell(x) = (-x)^\ell\left(\frac{1}{x}\frac{d}{dx}\right)^\ell\frac{\sin(x)}{x}$$

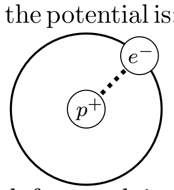
The Bessel functions have multiple (∞) zeros, $\beta_{n\ell}$, where $k = \beta_{n\ell}/a$, and so:

$$\psi_{n,\ell,m} = A_{n\ell}\,j_\ell(\beta_{n\ell}r/a)\,Y_\ell^m;\; E_{n,\ell} = \frac{\hbar^2\beta_{n\ell}^2}{2ma^2}$$

The Hydrogen Atom

For the Hydrogen atom, the potential is:

$$V(r) = -\frac{1}{4\pi\epsilon_0}\cdot\frac{e^2}{r} = -\frac{e^2}{r}\ \text{(CGS)}$$



Bound states are found from solving the radial equation for $u = rR$ with $\kappa = \sqrt{-2mE/\hbar^2}$, $\rho = \kappa r$, $\rho_0 = 2me^2/\hbar^2\kappa$:

$$\frac{d^2u}{d\rho^2} = \left(1 - \frac{\rho_0}{\rho} + \frac{\ell(\ell+1)}{\rho^2}\right)u$$

Using limits of ρ large and small, guess:

$$u(\rho) = \rho^{\ell+1}e^{-\rho}v(\rho) \text{ for some } v(\rho)$$

Guess the power series ansatz:

$$v(\rho) = \sum_{j=0}^{\infty} a_j\rho^j$$

Plugging into the ODE and solving, the solutions blow up unless series ends at n:

$$a_{j+1} = \frac{2(j+\ell+1-n)}{(j+1)(j+2\ell+2)}a_j$$

End is from $\rho_0 = 2n$, which sets E as:

$$E_n = -\frac{1}{n^2}\left(\frac{me^4}{2\hbar^2}\right) = \frac{E_1}{n^2} = -\frac{13.61}{n^2}\text{ eV}$$

The ground state energy is not at $-\infty$ because of the uncertainty principle.

The Bohr Radius, of state E_1 is:

$$a = \frac{\hbar^2}{me^2} = 0.529\text{ Å}$$

Quantum numbers $|m| \le l \le n-1$.

Angular Momentum

Radial momentum is, from $\boldsymbol{L} = \boldsymbol{r}\times\boldsymbol{p}$:

$$p_r = \frac{1}{2}\left(\frac{1}{r}r\cdot p + p\cdot r\frac{1}{r}\right) = \frac{\hbar}{i}\frac{1}{r}\frac{\partial}{\partial r}r$$

Some angular momentum operators:

$$L_z = xp_y - yp_z$$
$$L_\pm = L_x \pm iL_y$$
$$L^2 = L_x^2 + L_y^2 + L_z^2$$
$$= L_\pm L_\mp + L_z^2 \mp \hbar L_z$$

Their representations as operators:

$$L_z = \frac{\hbar}{i}\frac{\partial}{\partial\varphi}$$
$$L_\pm = \pm\hbar e^{\pm i\varphi}\left(\frac{\partial}{\partial\theta} \pm i\cot(\theta)\frac{\partial}{\partial\varphi}\right)$$
$$L^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)$$

Commutator identities:

$$[A,B] \equiv AB - BA$$
$$[A,B] = -[B,A]$$
$$[A,B-C] = [A,B] - [A,C]$$
$$[A,BC] = [A,B]C + B[A,C]$$

These commutation relations hold:

$$[L_i, L_j] = \varepsilon_{ijk}i\hbar L_k$$
$$[L_z, L_\pm] = \pm\hbar L_\pm$$
$$[L_i, L^2] = 0$$
$$[L_\pm, L_\mp] = \pm 2\hbar L_z$$
$$[L_\pm, L^2] = 0$$

Hamiltonian for a central potential:

$$H = \frac{p_r^2}{2m} + \frac{L^2}{2mr^2} + V(r)$$

Simultaneous observables of $Y_\ell^m = |\ell, m\rangle$:

$$L^2|\ell,m\rangle = \hbar^2\ell(\ell+1)|\ell,m\rangle$$
$$L_z|\ell,m\rangle = \hbar m|\ell,m\rangle$$
$$H|\ell,m\rangle = E|\ell,m\rangle$$

Raising/lowering operators act on m:

$$L_z(L_\pm|\ell,m\rangle) = \hbar(m\pm1)(L_\pm|\ell,m\rangle)$$
$$L^2(L_\pm|\ell,m\rangle) = \hbar^2\ell(\ell+1)(L_\pm|\ell,m\rangle)$$

For $\ell = n/2$, $m = \{-\ell, -\ell+1, \ldots, \ell-1, \ell\}$

Matrix elements are found as:

$$\langle\ell,m'|L_+|\ell,m\rangle = \hbar\sqrt{\ell(\ell+1)-m(m+1)}\,\delta_{m',m+1}$$
$$\langle\ell,m'|L_-|\ell,m\rangle = \hbar\sqrt{\ell(\ell+1)-m(m-1)}\,\delta_{m',m-1}$$
$$\langle\ell,m'|L_z|\ell,m\rangle = \hbar m\delta_{m',m}$$

Ex. m_1 and m_2, separated by r_0, and $\mu = m_1m_2/(m_1+m_2)$, thence $I = \mu r_0^2$:

$$H = \frac{L^2}{2I} \Rightarrow E_{n,\ell} = (n+1/2)\hbar\omega + \frac{\ell(\ell+1)}{2I}\hbar^2$$

Expectation values, and time evolution may be calculated for a given state.

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Spin

Spin is an additional degree of freedom. For two states, it may be expressed as:

$$|\uparrow\rangle = |\tfrac{1}{2}, \tfrac{1}{2}\rangle \text{ and } |\downarrow\rangle = |\tfrac{1}{2}, -\tfrac{1}{2}\rangle$$

$$\text{(or)} \qquad \chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+^z + b\chi_-^z$$

Spin operators commute as:

$$[S_i, S_j] = i\hbar S_k \epsilon_{ijk}$$

Eigenvalue relations are just like for L.

The spin measurement operators, or the Pauli Matrices are with $\hbar/2 = 1$:

$$S_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, S_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, S_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Expectation values may be found with:

$$\langle S_i \rangle = \chi^\dagger S_i \chi$$

S_i matrices are unitary, so $\langle S_i^2 \rangle = \hbar^2/4$. The eigenvectors may be set as a basis of eigenvectors of S_i, and the probabilities of measurement thence calculated:

$$\chi_+^y = \begin{pmatrix} 1 \\ -i \end{pmatrix}, \chi_-^y = \begin{pmatrix} 1 \\ i \end{pmatrix}, \chi_+^x = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \chi_-^x = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Spins in a Magnetic Field

With magnetic field in $\hat{\boldsymbol{z}}$, spins rotate:

$$H = -\gamma \boldsymbol{B} \cdot S_z$$

Spinor states have an energy splitting, and so are time dependent, and rotates at angle α, with frequency $\omega = \gamma \|\boldsymbol{B}\|$:

$$\chi(t) = \begin{pmatrix} \cos(\alpha/2)\exp(i\gamma B_0 t/2) \\ \sin(\alpha/2)\exp(-i\gamma B_0 t/2) \end{pmatrix}$$

Even an infinitesimal field may flip S:

$$\left\{ \begin{array}{l} \langle S_x \rangle = \frac{\hbar}{2}\sin(\alpha)\cos(\omega t) \\ \langle S_y \rangle = -\frac{\hbar}{2}\sin(\alpha)\sin(\omega t) \\ \langle S_z \rangle = \frac{\hbar}{2}\cos(\alpha) \end{array} \right\}$$

Force arises in an inhomogeneous field and leads to the Stern-Gerlach result.

Adding Angular Momenta

Multiple particles: spin operators act on each particle to yield the usual eigenvalue relations, and $m = m_1 + m_2$.

Two particles: $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, so, considering the lowering operator S_-, one arrives at "triplets" and "singlets":

$$\left\{ \begin{array}{ll} |1,1\rangle & = |\uparrow\uparrow\rangle \\ |1,0\rangle & = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |1,-1\rangle & = |\downarrow\downarrow\rangle \end{array} \right\} s = 1$$

$$\left\{ |0,0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \right\} s = 0$$

Operators may act on these to yield eigenvalue relations, and determine s.

Electromagnetic Effects

With both electric scalar potential ϕ, and magnetic vector potential $\boldsymbol{A}$, find:

$$H = \frac{(\boldsymbol{p} - e\boldsymbol{A})^2}{2m} + q\phi + V(x)$$

With $\phi = 0$, and $\boldsymbol{A} = B/2 \cdot (-y\hat{\boldsymbol{x}} + x\hat{\boldsymbol{y}})$, the Landau Level quantization arises:

$$H = \frac{p^2}{2m} + \frac{m\omega_0^2 Q^2}{2}; \; E = (n + \tfrac{1}{2})\hbar\omega_0$$

Gauge transformation $\boldsymbol{A} \to \boldsymbol{A} + \nabla\Lambda$, as in AB Effect where a beam is split:

$$\Psi \to \Psi e^{iq\Lambda/\hbar} \xrightarrow{\text{Aharonov-Bohm}} \Lambda = \Phi$$

Identical Particles

For multiple particles, H generalizes:

$$H = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 + V(r_1, r_2)$$

Particles are identical in QM, so they cannot be labeled, so two possibilities. Particles with integer spin are bosons, and particles with half-integer spin are fermions. Wave functions follow from a Slater Determinant and Permanent:

$$\Psi_F = A \det\begin{vmatrix} \psi_1(r_1) & \psi_2(r_1) \\ \psi_1(r_2) & \psi_2(r_2) \end{vmatrix} = A(\psi_1(r_1)\psi_2(r_2) - \psi_1(r_2)\psi_2(r_1))$$

$$\Psi_B = A \operatorname{perm}\begin{vmatrix} \psi_1(r_1) & \psi_2(r_1) \\ \psi_1(r_2) & \psi_2(r_2) \end{vmatrix} = A(\psi_1(r_1)\psi_2(r_2) + \psi_1(r_2)\psi_2(r_1))$$

Noting that if $\psi_1 = \psi_2$, then $\Psi = 0$, which is the Pauli exclusion principle. Exchange relations then become clear:

$$\Psi_F(r_1, r_2) = -\Psi_F(r_2, r_1)$$

$$\Psi_B(r_1, r_2) = +\Psi_B(r_2, r_1)$$

Exchange forces can be calculated, viz, bosons cluster and fermions don't:

$$\langle (x_1 - x_2)^2 \rangle_F^B = \langle x^2 \rangle_1 + \langle x^2 \rangle_2 - 2\langle x \rangle_1 \langle x \rangle_2 \mp \text{exch}$$

$$\text{exch} = 2\left| \int_{x_1} \psi_2^*(x_1) x_1 \psi_1(x_1) \int_{x_2} \psi_1^*(x_2) x_2 \psi_2(x_2) \right|^2$$

Non-Interacting Particles

For non-interacting particles, one may pretend that they are separate, so that $V(r_1, r_2) = V(r_1) + V(r_2)$, so ψ_1 and ψ_2 each, fulfill the one-particle S. Eqn, and have total energy of $E = E_1 + E_2$.

Total wave functions are products of the single wave functions. Linearity of $\Psi = \psi_1\psi_2$, implies entanglement, where a particle's state and another can be linked: measure one get one free!

Free Electron Gas

Begin by assuming that electrons are non-interacting, and that they reside in a periodic solid modeled by an $L \times L \times L$ box with periodic boundaries. If this is the case, then for a single particle solved for by separation of variables, normalized by $A = \sqrt{8/L^3}$, and with wave vectors $k_i = n_i\pi/L$, for $n_i \in \mathbb{N}$:

$$\psi_{k_x k_y k_z} = A\sin(k_x x)\sin(k_y y)\sin(k_z z)$$

Whose energy eigenvalue is evidently:

$$E_{k_x k_y k_z} = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) = \frac{\hbar^2 \boldsymbol{k} \cdot \boldsymbol{k}}{2m}$$

The highest occupied energy relates to a wave vector k_F known as the Fermi radius, which is for N electrons in real volume V, accounting for the 2 spins:

$$2 \cdot \frac{4\pi}{3} k_F^3 = N\left(\frac{2\pi}{L}\right)^3 \Longrightarrow k_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3}$$

Related Fermi quantities are defined:

$p_F = \hbar k_F$	
$v_F = p_F/m = \hbar k_F/m$	$\sim 10^6$ m/s
$\epsilon_F = p_F^2/2m = \hbar^2 k_F^2/2m$	$1 - 10$ eV
$T_F = \epsilon_F/k_B = \hbar^2 k_F^2/2mk_B$	$\sim 10^5$ K

The degeneracy pressure is outwards:

$$P = -\frac{\partial E_{\text{tot}}}{\partial V} = \frac{2}{3}\frac{E_{\text{tot}}}{V} = \frac{2}{3}\frac{\hbar^2 k_F^5}{10\pi^2 m}$$

Kronig-Penney Model

Bloch's Theorem reduces periodic potential problems to solving withing one unit cell. For an a-periodic potential:

$$\psi(x+a)e^{iKa} = \psi(x), \text{ ring: } \psi(x)e^{iNKa} = \psi(x)$$

The KP Model assumes a potential:

$$V(x) = \alpha \sum_{j=0}^{N-1} \delta(x - ja)$$

The general solution in the free region:

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

With Bloch's Theorem and boundaries:

$$\cos(qa) = \cos(ka) + \frac{m\alpha}{\hbar^2 k}\sin(ka)$$

Non-dimensional consistency relation:

$$f(z) \equiv \cos(z) + \beta\,\text{sinc}(z)$$

For negative energies and z, one finds:

$$f(z) \equiv \cosh(z) + \beta\,\text{sinhc}(z)$$

This is a quantitative description of bands and gaps in an energy spectrum. There are N states between $z = \pm 1$, which effectively form a continuum.