Foundations of Physics 3A

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Part I

Quantum Mechanics

Lecture 1

1. Hilbert spaces 2. von Neumanns axioms 3. Hermitian ops 4. T.D. Schrodinger Eq -> T.I. Schrodinger Eq 5. 1 particle in 3D 6. Ang momentum ops, commutators, spin angular momentumo

1.1 von Neumanns axioms

1. In QM, every observable is represented by a Hermitian operator. 2. The state of the system is represented by a wavefunction. - Scalar multiple of the wavefunction still represents system, convenient to choose to be normalised though. 3. Usual bra-ket stuff

$$\langle\psi|Q\psi\rangle = \int dx \psi^*(x)(Q\psi(x)) \tag{1.1}$$

$$\langle\psi|Q\psi\rangle^* = \langle Q\psi|\psi\rangle = \int dx (Q\psi(x))^* \psi(x) \tag{1.2}$$

$$\langle Q\rangle = \langle\psi|Q\psi\rangle = \langle Q\psi|\psi\rangle = \langle\psi|Q|\psi\rangle \tag{1.3}$$

4. Usual orthonormal eigen stuff

1.1.1 Example

See Pauli spin operators and stuff Find result of $\omega = \gamma B$, the angular momentum around a magnetic field

Lecture 2

nothing

Lecture 3

1. Study motion of charged particle in magnetic fields 2. Study means to solve S.E. - we need H for B, E, $H = \frac{1}{2m}(-i\hbar\nabla - qA)^2 + q\phi$ 3. It turns out H contains ϕ, A, not E, B, $E = -\nabla\phi$, $B = \nabla \times A$ 4. But different As may gave same B 5. Solve examples 1. 2D motion of q in uniform mag field (cyclotron freq) 2. Explore A vs B - 1D example where $B = 0, A \neq 0$

3.1 Guage freedom

$$\vec{A} = \frac{B}{2}(-y\hat{x} + x\hat{y} \implies \vec{\nabla} \times \vec{A} = B\hat{z} \tag{3.1}$$

$$\vec{A}' = -By\hat{x} \implies \vec{\nabla} \times \vec{A}' = B\hat{z} \tag{3.2}$$

$$\vec{A} - \vec{A}' = \frac{By}{2}\hat{x} + \frac{Bx}{2}\hat{y} = \vec{\nabla}\left(-\frac{Bxy}{2}\right) \implies \vec{A} = \vec{A}' + \vec{\nabla} \times (x, y, z) \tag{3.3}$$

$$\vec{\nabla} \times \vec{A} = \vec{\nabla} \times \vec{A} + \cancel{\vec{\nabla}} \times \vec{\nabla} \times (\vec{r}) \tag{3.4}$$

3.1.1 Time deriv of fn

$$\phi' = \phi + \frac{\partial}{\partial t} \times (r, t) \tag{3.5}$$

$$\vec{A}' = \vec{A} + \vec{\nabla} \times (r, t) \tag{3.6}$$

$$(\phi', \vec{A}'), (\phi, \vec{A}) \rightarrow \vec{E}, \vec{B} \tag{3.7}$$

Convenient to choose $\vec{A}$ s.t. $\vec{\nabla} \cdot \vec{A} = 0$.

3.2 2D motion (x,y) of q in mag field, B along z

$$H = \frac{1}{2m}\left(-i\hbar\vec{\nabla} - q\vec{A}\right)^2 \tag{3.8}$$

$$= \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\hat{x} - i\hbar\frac{\partial}{\partial y}\hat{y} + qBy\hat{x}\right)^2 \tag{3.9}$$

$$= \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial y}\hat{y} + \left(-i\hbar\frac{\partial}{\partial x} + qBy\right)\hat{x}\right)^2 \tag{3.10}$$

$$E\psi(x, y) = \frac{1}{2m}\left(-\hbar^2\frac{\partial}{\partial x^2} - 2i\hbar qBy\frac{\partial}{\partial x} + q^2B^2y^2 - \hbar^2\frac{\partial^2}{\partial y^2}\right)\psi(x, y) \tag{3.11}$$

$$\psi(x, y) = e^{-ikx}\phi(y) \tag{3.12}$$

$$\implies \frac{1}{2m}\left(\hbar^2k^2 - 2\hbar kqBy + q^2B^2y^2 - \hbar^2\frac{\partial^2}{\partial y^2}\right)\cancel{e^{-ikx}}\phi(y) = E\cancel{e^{-ikx}}\phi(y) \tag{3.13}$$

$$\implies \frac{1}{2m}(qBy - \hbar k)^2\phi(y) = E\phi(y), y_0 = \frac{\hbar k}{qB} \tag{3.14}$$

$$\implies \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{m}{2}\frac{q^2B^2}{m^2}(y - y_0)^2\right]\psi(y) = E\psi(y) \tag{3.15}$$

This is Simple harmonic motion with $\frac{qB}{m} = \omega$, and energy $E = \left(n + \frac{1}{2}\right)\hbar\omega$. These are the Landau levels.

3.2.1 Periodic boundary conditions

$$e^{-ik(x+L)} = e^{-ikx} \tag{3.16}$$
$$e^{-ikL} = 1 \tag{3.17}$$
$$kL = 2\pi j \tag{3.18}$$
$$k_j = \frac{2\pi}{L} j, j \in Z \tag{3.19}$$
$$0 < y_0 < L \tag{3.20}$$
$$0 < \frac{\hbar k_j}{qB} < L \tag{3.21}$$
$$0 < \frac{\hbar 2\pi j}{qBL} < L \tag{3.22}$$
$$0 < j < \frac{qBL^2}{h} \tag{3.23}$$
$$0 < j < \frac{\Phi}{h/q} \tag{3.24}$$
$$j_{max} = \frac{\Phi}{h/q} \tag{3.25}$$

3.3 A vs B, Aharanov-Bohm

$$H = \frac{L_z^2}{2I} = -\frac{\hbar^2}{2mb^2}\frac{\partial^2}{\partial\phi^2} \tag{3.26}$$
$$-frac\hbar^2 2mb^2 \frac{\partial^2}{\partial\phi^2}\psi(\phi) = E\psi(\phi) \tag{3.27}$$
$$E = \frac{\hbar^2 k^2}{2mb^2} \tag{3.28}$$

Single valued: $e^{ik\phi}$ soln, $e^{ik(\phi+2\pi)} = e^{ik\phi}$. k is integer.

Lecture 4

4.1 Particle moving on ring, radius b in xy plane

Without magnetic field:

$$H = -\frac{\hbar^2}{2mb^2}\frac{\partial^2}{\partial\phi^2} \tag{4.1}$$

$$\implies E\Psi(\phi) = -\frac{\hbar^2}{2mb^2}\frac{\partial^2}{\partial\phi^2}\Psi(\phi) \tag{4.2}$$

$$\frac{L_z^2}{2I}, \Psi(\phi) = \frac{e^{2n\phi}}{\sqrt{2\pi}}, 0 \le \phi \le 2\pi \tag{4.3}$$

$$e^{in(\phi+2\pi)} = e^{in\phi} \tag{4.4}$$

$$\implies e^{in2\pi} = 1 \implies n \in \mathbb{Z} \tag{4.5}$$

$$\Psi_n(\phi) = \frac{e^{in\phi}}{\sqrt{2\pi}} \tag{4.6}$$

$$E_n = \frac{\hbar^2 n^2}{2mb^2} \tag{4.7}$$

With magnetic field:

$$\vec{A} = \begin{cases} \frac{\Phi\dot{\rho}}{2\pi a^2}\hat{\phi} & \rho < a \\ \frac{\Phi}{2\pi a}\hat{\phi} & \rho > a \end{cases} \tag{4.8}$$

$$\rho < a, \vec{\nabla}\times\vec{A} = \frac{\hat{z}}{\rho}\frac{\partial}{\partial\rho}(\rho A_\phi) \tag{4.9}$$

$$= \hat{z}\frac{\Phi}{\pi a^2} = \hat{z}B\rho > a, \vec{\nabla}\times\vec{A} \qquad = 0 \implies B = 0 \tag{4.10}$$

$$H = \frac{1}{2m}\left[\left(-i\hbar\frac{1}{\rho}\frac{\partial}{\partial\phi} - q\frac{\Phi}{2\pi a^2}\right)\hat{\phi}\right]^2 \tag{4.11}$$

$$= \frac{\hbar^2}{2mb^2}\left[-\frac{\partial^2}{\partial\phi^2} + 2i\frac{q\Phi}{h}\frac{\partial}{\partial\phi} + \left(\frac{q\Phi}{h}\right)^2\right] \tag{4.12}$$

$$H\Psi(\phi) = E\Psi(\phi) \tag{4.13}$$

$$E_n = \frac{\hbar^2}{2mb^2}\left[n^2 - 2\frac{q\Phi n}{h} + \left(\frac{q\Phi}{h}\right)^2\right] \tag{4.14}$$

$$= \frac{\hbar^2}{2mb^2}\left(n - \frac{q\Phi}{h}\right)^2 \tag{4.15}$$

Energy will be parabolas with minimum of zero on a plot of flux and energy. Increasing n will shift the centre of parabola along axis.

4.2 Guage Invariance

1. The same $\vec{E}, \vec{B}$ can be given from different $\phi, \vec{A}$

$$\vec{E} = -\vec{\nabla} - \frac{\partial}{\partial t}\vec{A} \tag{4.16}$$

$$\vec{B} = \vec{\nabla} \times \vec{A} \tag{4.17}$$

$$\phi' = \phi - \frac{\partial A}{\partial t} \tag{4.18}$$

$$\vec{A}' = \vec{A} + \vec{\nabla} A \tag{4.19}$$

2. Same $\vec{E}, \vec{B}$ have different H, so different wavefns

3. Do measurable quantities depend on choice of guage?

$$\rho(r,t) = |\Psi(r,t)|^2 \tag{4.20}$$

$$j(r,t) = \text{ probability current density} \tag{4.21}$$

$$\frac{\partial \rho(r,t)}{\partial t} + \vec{\nabla} \vec{j}(r,t) = 0 \tag{4.22}$$

$$\int dx \left[\frac{\partial \rho}{\partial t} + \frac{d}{dx} j(x) \right] = \frac{\partial}{\partial t} \int_A^B \rho(x)\, dx + \int_A^B \frac{d}{dx} j\, dx = 0 \tag{4.23}$$

$$\frac{\partial}{\partial t} N_{AB} = j(A) - j(B) \tag{4.24}$$

Lecture 5

5.1 Equation for conservation of probability

$$\Psi^*(\vec{r})i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = \Psi^*(\vec{r})\left(\frac{-\hbar^2}{2m}\right)\left(\nabla^2\Psi(\vec{r},t)\right) + \Psi^*(\vec{r})V(r)\Psi(\vec{r},t) \tag{5.1}$$

$$i\hbar\left[\Psi^*\frac{\partial\Psi}{\partial t} + \Psi\frac{\partial\Psi^*}{\partial t}\right] = -\frac{\hbar^2}{2m}\left[\Psi^*\left(\nabla^2\Psi\right) - \Psi\left(\nabla^2\Psi^*\right)\right] \tag{5.2}$$

$$= \frac{i\hbar i\hbar}{2m}\nabla\cdot\left[\Psi^*\left(\nabla\Psi\right) - \Psi\left(\nabla\Psi^*\right)\right] \tag{5.3}$$

$$\frac{\partial}{\partial t}\rho(\vec{r},t) + \nabla\left(\frac{-i\hbar}{2m}\right)\left[\Psi\left(\nabla\Psi\right) - \Psi\left(\nabla\Psi^*\right)\right] = 0 \tag{5.4}$$

5.2 Rayleigh-Ritz variational principle

1. Approximation method (useful and powerful). Find approx. for solution of S.E.
2. Powerful theoretical tool/concept. Equivalent to S.E.

For one particle,

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r) \tag{5.5}$$

$$H\Psi_n(\vec{r}) = E_n\Psi_n(\vec{r}) \tag{5.6}$$

$$\Psi(\vec{r}) = \sum_n c_n\Psi_n(\vec{r}) \tag{5.7}$$

$$\Psi^*(\vec{r}) = \sum_m c_m^*\Psi_m^*(\vec{r}) \tag{5.8}$$

$$\langle\Psi|H|\Psi\rangle \geq E_0 \tag{5.9}$$

$$= \int d^3r\Psi^*(r)H\Psi(r) = \int d^3r\sum_m c_m^*\Psi^*(r)H\sum_n c_n\Psi_n(r) \tag{5.10}$$

$$= \sum_{m,n} c_m^*c_n\int d^3r\Psi_m^*(r)\left(H\Psi_n(r)\right) = \sum_{m,n} c_m^*c_nE_n\int d^3r\Psi_m^*(r)\Psi_n(r) \tag{5.11}$$

$$\langle\Psi|H|\Psi\rangle = \sum_n |c_n|^2E_n\delta_{nm} = |c_0|^2E_0 + |c_1|^2E_1 + \cdots \geq E_0\sum_n |c_n|^2 \tag{5.12}$$

$$\implies \langle\Psi|H|\Psi\rangle \geq E_0\sum_n |c_n|^2 \tag{5.13}$$

$$\geq E_0 \ \forall\ \Psi \tag{5.14}$$

For Lagrange multipliers, see notes on DUO.

Lecture 6

Find the minimum of

$$G[\phi] = [\langle\phi|H|\phi\rangle - \lambda\langle\phi|\phi\rangle] \tag{6.1}$$

$$\lim_{\epsilon\to 0}\frac{G[\phi+\epsilon u]-G[\phi]}{\epsilon} = 0,\ \forall\ u(\vec{r}) \tag{6.2}$$

$$G[\phi+\epsilon u] = \langle\phi+\epsilon u|H|\phi+\epsilon u\rangle - \lambda\langle\phi+\epsilon u|\phi+\epsilon u\rangle \tag{6.3}$$

$$= \int dr(\phi^*(\vec{r})+\epsilon u^*(\vec{r}))H(\phi(\vec{r})+\epsilon u(\vec{r})) - \lambda\int dr|\phi(\vec{r})+\epsilon u(\vec{r})|^2 \tag{6.4}$$

$$\begin{aligned} &= \left[\int d^3r\phi^*(\vec{r})H\phi(\vec{r}) - \lambda\int dr|\phi(r)|^2\right] + \epsilon\left[\int dr\ u^*(\vec{r})H\phi(\vec{r}) - \lambda\int dr\ u^*(\vec{r})\phi(\vec{r})\right] \\ &+ \epsilon\left[\int dr\phi^*(\vec{r})Hu(\vec{r}) - \lambda\int dr\ \phi^*(\vec{r})u(\vec{r})\right] \end{aligned} \tag{6.5}$$

$$= G[\phi] + \epsilon(\langle u|H\phi\rangle - \lambda\langle u|\phi\rangle) + \epsilon(\langle\phi|H|u\rangle - \lambda\langle\phi|u\rangle) + O(\epsilon^2) \tag{6.6}$$

$$\frac{G[\phi+\epsilon u]-G[\phi]}{\epsilon} = \lim_{\epsilon\to 0}\frac{\epsilon(\langle u|H|\phi\rangle - \lambda\langle u|\phi\rangle) + \epsilon(\langle\phi|H|u\rangle - \lambda\langle\phi|u\rangle)}{\epsilon} \tag{6.7}$$

$$\implies \int dr\ u^*(\vec{r})[H\phi(\vec{r}) - \lambda\phi(\vec{r})] = 0 \tag{6.8}$$

$$\implies H\phi(\vec{r}) - \lambda\phi(\vec{r}) = 0 \tag{6.9}$$

Lecture 7

there may be one or two missing lectures here

1. Example - 2 electrons without repulsion, ground and first excited states
2. Switch on electron interaction
3. N electrons, no interaction - Slater determinants
4. Introduce interaction, electron strucutre theory, many body
5. mean field, Hartree-Fock