Lecture 27 – Schrödinger's Equation in Electromagnetic Fields

1. Schrödinger's equation in EM fields
2. Current | Conservation

1. Schrödinger's Equation in EM fields

$\Pi = p - \frac{eA}{c}$, the kinematic momentum

$$\mathcal{H} = \frac{\Pi^2}{2m} + e\varphi(x,t)$$

Writing the Hamiltonian this way allows us to recover the Lorentz force law

$$m\frac{d^2x}{dt^2} = \frac{m\,d\Pi}{dt} = e\left[\vec{E} + \frac{1}{2c}\left(\overbrace{\frac{d\vec{x}}{dt}}^{\vec{v}} \times \vec{B} - \vec{B}\times\frac{d\vec{x}}{dt}\right)\right]$$

Classically, $\vec{B}$ & $\vec{v}$ commute (and this would cancel), but Quantum Mechanically, if $\vec{B}$ is dependent on direction | position, you get this expression

Wave equation:
(prime implies not the operator)

$$\langle x'|\hat{H}|\psi\rangle = i\hbar\underbrace{\langle x'|\partial_t|\psi\rangle}_{\partial_t\psi(x',t)}$$

$$e\underbrace{\langle x'|\varphi(x')|\psi\rangle}_{\varphi(x')\psi(x')} + \frac{1}{2m}\langle x'|\Pi^2|\psi\rangle = i\hbar\partial_t\psi(x',t)$$

* A and φ are classical fields – ψ is the only thing that is quantum mechanical

$$\langle x'|\Pi^2|\psi\rangle = \langle x'|\left[\hat{p} - \frac{e}{c}\hat{A}(\hat{x})\right]\underbrace{\left[\hat{p} - \frac{e}{c}\hat{A}(\hat{x})\right]|\psi\rangle}_{|\psi_1\rangle}$$

$$= \langle x'|\hat{p} - \frac{e}{c}\hat{A}(\hat{x})|\psi_1\rangle$$

$$= \underbrace{\langle x'|\hat{p}|\psi_1\rangle}_{\text{normal momentum operator}} - \frac{e}{c}A(x')\langle x'|\psi_1\rangle$$

$$= -i\hbar\partial_{x'}\langle x'|\psi_1\rangle - \frac{e}{c}A(x')\langle x'|\psi_1\rangle$$

$$= \underbrace{\left[-i\hbar\partial_{x'} - \frac{e}{c}A(x')\right]}_{\text{"covariant derivative"}}\underbrace{\langle x'|\psi_1\rangle}_{\langle x'|\hat{p} - \frac{e}{c}\hat{A}(\hat{x})|\psi\rangle}$$

$$= \left[-\hbar i\partial_{x'} - \frac{e}{c}A(x')\right]\left[-i\hbar\partial_{x'} - \frac{e}{c}A(x')\right]\underbrace{\psi(x')}_{\langle x'|\psi\rangle}$$

$(\partial_{x'}A)(\psi(x'))$ don't forget this term!

We can now write the wave equation:

$$\left\{\frac{1}{2m}\left[-i\hbar\partial_{x'} - \frac{e}{c}A(x';t)\right]^2 + e\varphi(x';t)\right\}\Psi(x';t) = i\hbar\partial_t\Psi(x';t)$$

potentials may be static or time-dependent

2. Current/conservation

Recall:

$\rho(x,t) = |\Psi(x,t)|^2$ — probability density

$\vec{j}(x';t) \sim \hbar/m \, \mathrm{Im}\{\Psi^* \vec{\nabla}\Psi\} \sim (j_{ch}/e)$ — charged current density

$\vec{j}$: current density

$\vec{\nabla}$: need to replace this somehow with $(p - \frac{e}{c}A)$

From the wave equation above, we can obtain the continuity equation

$$\partial_t\rho + \vec{\nabla}\cdot\vec{j} = 0$$

- Derivation of a new current density -

We expect j to be related to what would be a "velocity" operator

$$j(x';t) \simeq \underbrace{\hat{v}(x';t)}_{\sim\langle\Psi|\hat{v}|\Psi\rangle}\rho(x';t)$$

need to replace this with quantum density, $\delta(\hat{x}-x')$

$$= \frac{1}{m}\langle\Psi|\underbrace{\frac{d\hat{x}}{dt}}_{\hat{p}-\frac{e}{c}A(\hat{x})}|\Psi\rangle$$

real

$$= \frac{1}{m}\langle\Psi|\hat{p}|\Psi\rangle - \frac{e}{c}\langle\Psi|A(\hat{x})|\Psi\rangle$$

$$= \underbrace{\frac{-i\hbar}{m}\Psi^*\vec{\nabla}\Psi}_{\text{but this isn't real!}} - \frac{e}{c}A(x')|\Psi|^2$$

but this isn't real! $(i\Psi^*\vec{\nabla}\Psi)^* = -i\Psi\vec{\nabla}\Psi^* \neq (i\Psi^*\vec{\nabla}\Psi)$

but $\int(i\Psi^*\vec{\nabla}\Psi)dx' = \int(i\Psi^*\vec{\nabla}\Psi)^*dx'$

due to integration by parts

General prescription:

$$\underbrace{j(x';t)}_{\text{current density at a specific point } x'} = \frac{1}{2m}\left\{\frac{d\hat{x}}{dt}, \delta(\hat{x}-x')\right\}$$

anti-commutator (AB+BA)

current density at a specific point x'

$$j(x',t) = \frac{1}{2m}\{\Pi, \delta(\hat{x}-x')\}$$

This delta-function solves the problem of the expectation value of $\hat{p}$ over all space yielding a non-real answer by demanding a specific location, x'

$$\frac{1}{2m}\langle\psi|\left\{\hat{p}-\frac{e}{c}\hat{A}(\hat{x}),\ \delta(\hat{x}-x')\right\}|\psi\rangle$$

$$= \frac{1}{2m}\langle\psi|\left(\hat{p}-\frac{e}{c}\hat{A}(\hat{x})\right)\delta(\hat{x}-x')|\psi\rangle + \frac{1}{2m}\langle\psi|\delta(\hat{x}-x')\left(\hat{p}-\frac{e}{c}\hat{A}(\hat{x})\right)|\psi\rangle$$

$$j(x',t) = \frac{-eA(x')}{c}|\psi|^2 + \frac{1}{2m}\left\{\langle\psi|\hat{p}\,\delta(\hat{x}-x')|\psi\rangle + \langle\psi|\delta(\hat{x}-x')\,\hat{p}|\psi\rangle\right\}$$

$$\int dx''\,\psi^*(x'')\,(-i\hbar\partial_{x''})\left(\delta(x''-x')\psi(x')\right)$$

integration by parts

$$\rightarrow +i\hbar(\partial_{x'}\psi^*)\psi(x')$$

$$\int dx''\,\psi^*(x'')\,\delta(x''-x')\left(-i\hbar\partial_{x''}\psi(x'')\right)$$

delta function in the integral kills the integral

$$\rightarrow -i\hbar\psi^*\vec{\nabla}\psi$$

$$\Rightarrow\ j(x',t) = \frac{\hbar}{m}\,\mathrm{Im}\left\{\psi^*\vec{\nabla}\psi\right\} - \frac{eA}{mc}|\psi|^2$$

By deriving this from a classical standpoint, you've removed ambiguity of relating the field to the curl of A by creating a form that represents the physical current so that you might understand the electromagnetic response of a quantum material

Next: Check that this is actually gauge invariance

Gauge redundancy – multiple A's and φ's