Lecture 9: Macroscopic Quantum Model

Outline

1. Development of Quantum Mechanics
2. Schrödinger's Equation
   - Free particle
   - With forces
   - With Electromagnetic force
3. Physical meaning of Wavefunction
   - Probability density and Probability Current density
4. Macroscopic Quantum Model

October 6, 2005

Macroscopic Quantum Model

Superconductivity is a Quantum Phenomenon on a macroscopic length scale.

Development of Quantum Mechanics

Free Particle (no forces or potentials)

Wave-like properties | *Particle-like properties*

$$\mathcal{E} = \hbar\omega \qquad \mathbf{p} = \hbar\mathbf{k}$$

frequency, wavenumber

$$\mathcal{E} = \frac{1}{2}m\,(\mathbf{v}\cdot\mathbf{v}) = \frac{\mathbf{p}\cdot\mathbf{p}}{2m}$$

energy

momentum $\rightarrow \mathbf{p} = m\mathbf{v}$

Planck's constatnt $\hbar \equiv \frac{h}{2\pi} = 1.0546 \times 10^{-34}\ \text{J} - \text{sec}$

Combine wave and particle properties, to find the dispersion relation:

$$\hbar\omega = \frac{\hbar^2}{2m}\,(\mathbf{k}\cdot\mathbf{k})$$

Schrödinger's Equation (free particle)

$$\hbar\omega = \frac{\hbar^2}{2m}\,(\mathbf{k}\cdot\mathbf{k})$$

Assume that this results from a uniform plane wave solution

$$\psi = \widehat{\psi}\,e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$$

Then a good guess of the differential equation that gives the dispersion relation is

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi$$

This guess is justified by experimental confirmation; this is *not* a derivation.

Schrödinger's Equation (with forces)

We present a plausibility argument, not a derivation, relating the classical formulation to the quantum formulation.

The energy for a particle in a force is, classically,

$$\mathcal{E} = \frac{1}{2} m \; (\mathbf{v} \cdot \mathbf{v}) \; + \; V(\mathbf{r})$$

Energy is conserved since the potential is independent of time.

$$0 = \frac{d\mathcal{E}}{dt} = m\mathbf{v} \cdot \frac{d\mathbf{v}}{dt} \; + \; \frac{d}{dt} V(\mathbf{r})$$

$$= m\mathbf{v} \cdot \frac{d\mathbf{v}}{dt} + \frac{\partial}{\partial t} V(\mathbf{r}) + (\mathbf{v} \cdot \nabla) \, V(\mathbf{r}) \quad \left(\frac{\partial}{\partial t} V(\mathbf{r}) \rightarrow 0\right)$$

$$= \mathbf{v} \cdot \left(m \frac{d\mathbf{v}}{dt} + \nabla V \right) \;\Rightarrow\; m \frac{d\mathbf{v}}{dt} = -\nabla V$$

Canonical Momentum & Schrödinger's Equation

$$\frac{d\mathbf{p}}{dt} = -\nabla V$$

$$\frac{d}{dt} (\text{canonical momentum}) = -\nabla (\text{generalized potential})$$

$$\mathbf{p} = m\mathbf{v} \qquad\qquad \text{V}$$

Here, the canonical momentum equals the kinematic momentum; and the generalized potential, the scalar potential.

$$\mathcal{E} = \frac{1}{2m} \; (\mathbf{p} \cdot \mathbf{p}) \; + \; V(\mathbf{r})$$

$$\hbar\omega = \frac{\hbar^2}{2m} \; (\mathbf{k} \cdot \mathbf{k}) \; + \; V(\mathbf{r}) \;\Rightarrow\; \underbrace{i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi \; + \; V(\mathbf{r})\psi}_{\text{Schrödinger's Equation}}$$

Rules for Classical to Quantum

1. Write the classical equation of motion in terms of the canonical momentum, $\mathbf{p}$, and generalized potential, V:
$$\frac{d\mathbf{p}}{dt} = -\nabla V\,.$$
Indeed, this form identifies the precise expressions for $\mathbf{p}$ and V.

2. Use these quantities to write the energy of the system:
$$\mathcal{E} = \frac{\mathbf{p}\cdot\mathbf{p}}{2m} + V\,.$$

3. Transform the classical expression into a quantum mechanical one by appealing to the Einstein-de Broglie relations. Since Schrödinger's equation is linear, these transformations are
$$\mathcal{E} = \hbar\omega \Longrightarrow i\hbar\frac{\partial}{\partial t}$$
and
$$\mathbf{p} = \hbar\mathbf{k} \Longrightarrow -i\hbar\nabla\,.$$

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{r})\psi$$

The wave function Ψ : Real or Complex?

Compare the plane wave solutions for QM and E&M

$$\psi = \hat{\psi}\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \qquad \mathbf{H} = \mathrm{Re}\left\{\hat{\mathbf{H}}\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\right\}$$

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{r})\psi \qquad \nabla^2\mathbf{H} - \frac{1}{c^2}\frac{\partial}{\partial t}\mathbf{H} = 0$$

Ψ must be a complex function; it is not a mathematical convenience.

What does it mean to have a complex wave function?

H is a real function; it is only a mathematical convenience to consider it a complex function. The real part must be taken.

The physical meaning of the wave function Ψ

The absolute phase of a plane wave should *not* influence the overall physics of a system.
So Max Born hypothesized in ~1927 that the square of the magnitude of the wave function Ψ was equal to the *probability* of a quantum mechanical particle to be at the location **r** at time t.

$$\wp(\mathbf{r},t) \equiv |\psi(\mathbf{r},t)|^2 = \psi^*(\mathbf{r},t)\psi(\mathbf{r},t)$$

With the normalization condition (particle must be somewhere)

$$\int d\mathbf{r}\, \psi^*(\mathbf{r},t)\psi(\mathbf{r},t) = 1$$

Evolution of Probability

Multiply the S-Eqn by Ψ* and (S-Eqn)* by Ψ

$$i\hbar\psi^* \frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\psi^*\nabla^2\psi + V\psi^*\psi$$

$$- \quad -i\hbar\psi \frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\psi\nabla^2\psi^* + V\psi\psi^*$$

$$i\hbar \frac{\partial}{\partial t}(\psi\psi^*) = -\frac{\hbar^2}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right)$$

$$i\hbar \underbrace{\frac{\partial}{\partial t}(\psi\psi^*)}_{\mathcal{P}} = -\frac{\hbar^2}{2m}\underbrace{\left(\nabla\cdot(\psi^*\nabla\psi - \psi\nabla\psi^*)\right)}_{\nabla\cdot\mathbf{J}_{\mathcal{P}}}$$

Probability Current

Therefore we find that the probability

$$\wp(\mathbf{r},t) \equiv |\psi(\mathbf{r},t)|^2 = \psi^*(\mathbf{r},t)\psi(\mathbf{r},t)$$

and the probability current

$$\mathbf{J}_\wp \equiv \frac{\hbar}{2im}(\psi^*\nabla\psi - \psi\nabla\psi^*) = \mathrm{Re}\left\{\psi^*\frac{\hbar}{im}\nabla\psi\right\}$$

satisfy a continuity relation

$$\frac{\partial\wp}{\partial t} = -\nabla\cdot\mathbf{J}_\wp$$

Schrödinger's Equation with E&M Fields

For a charged particle, we want the classical equations such that

$$\frac{d}{dt}(\text{canonical momentum}) = -\nabla(\text{generalized potential})$$

Start with the Lorentz Force Law

$$m\frac{d\mathbf{v}}{dt} = q\left(\mathbf{E} + (\mathbf{v}\times\mathbf{B})\right)$$

and use the vector and scalar potentials

$$\mathbf{B} = \nabla\times\mathbf{A} \quad \text{and} \quad \mathbf{E} = -\frac{\partial\mathbf{A}}{\partial t} - \nabla\phi \quad \text{to find}$$

Canonical Momentum and Energy

$$\frac{d\mathbf{p}}{dt} = -\nabla \underbrace{\left(q\phi - \frac{q}{m}\mathbf{p}\cdot\mathbf{A} + \frac{q^2}{2m}\mathbf{A}\cdot\mathbf{A} \right)}_{V}$$

where the canonical momentum is

$$\mathbf{p} = m\mathbf{v} + q\mathbf{A}$$

Kinematic momentum ($m\mathbf{v}$) Field momentum ($q\mathbf{A}$)

The energy follows from the above to be

$$\mathcal{E} = \frac{\mathbf{p}\cdot\mathbf{p}}{2m} + \left(q\phi - \frac{q}{m}\mathbf{p}\cdot\mathbf{A} + \frac{q^2}{2m}\mathbf{A}\cdot\mathbf{A} \right)$$

Classical to Quantum

The energy can be written as

$$\mathcal{E} = \frac{1}{2m}(\mathbf{p} - q\mathbf{A})\cdot(\mathbf{p} - q\mathbf{A}) + q\phi$$

The transition to quantum mechanics is done as before

$$\mathcal{E} \Longrightarrow i\hbar\frac{\partial}{\partial t} \quad \text{and} \quad \mathbf{p} \Longrightarrow -i\hbar\nabla$$

The S-Eqn becomes

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - q\mathbf{A}\right)^2\psi + q\phi\,\psi$$

With probability current

$$\mathbf{J}_{\wp} = \mathrm{Re}\left\{\psi^*\left(\frac{\hbar}{im}\nabla - \frac{q}{m}\mathbf{A}\right)\psi\right\}$$

Macroscopic Quantum Model

1. The wave function describes the whole ensemble of superelectrons such that

$$\Psi^*(\mathbf{r},t)\Psi(\mathbf{r},t) = n^\star(\mathbf{r},t) \longrightarrow \text{density}$$

and

$$\int d\mathbf{r}\, \Psi^*(\mathbf{r},t)\Psi(\mathbf{r},t) = \mathsf{N}^\star \longrightarrow \text{Total number}$$

2. The flow of probability becomes the flow of particles, with the physical current density given by

$$\mathbf{J}_\mathsf{S} = q^\star\, \mathsf{Re}\left\{\Psi^*\left(\frac{\hbar}{im^\star}\nabla - \frac{q^\star}{m^\star}\mathbf{A}\right)\Psi\right\}$$

MQM cont.

3. This macroscopic quantum wavefunction follows

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \frac{1}{2m^\star}\left(\frac{\hbar}{i}\nabla - q^\star\mathbf{A}(\mathbf{r},t)\right)^2\Psi(\mathbf{r},t) + q^\star\phi(\mathbf{r},t)\,\Psi(\mathbf{r},t)$$

Writing $\Psi(\mathbf{r},t) = \sqrt{n^\star(\mathbf{r},t)}\, e^{i\theta(\mathbf{r},t)}$, we find

$$\mathbf{J}_\mathsf{S} = q^\star n^\star(\mathbf{r},t)\left(\frac{\hbar}{m^\star}\nabla\theta(\mathbf{r},t) - \frac{q^\star}{m^\star}\mathbf{A}(\mathbf{r},t)\right)$$

The Supercurrent Equation

The Supercurrent Equation

$$\mathbf{J}_{\mathrm{S}} = q^\star n^\star(\mathbf{r},t)\left(\frac{\hbar}{m^\star}\nabla\theta(\mathbf{r},t) - \frac{q^\star}{m^\star}\mathbf{A}(\mathbf{r},t)\right)$$

$\mathbf{J}_s$ is a unique physical quantity, but **A** and θ are not.

If a new vector and scalar potential are found in another gauge such that

$$\mathbf{A}' \equiv \mathbf{A} + \nabla\chi \qquad \phi' \equiv \phi - \frac{\partial\chi}{\partial t}$$

Then $\mathbf{B} = \nabla \times \mathbf{A}'$ $\qquad \mathbf{E} = -\frac{\partial \mathbf{A}'}{\partial t} - \nabla\phi'$

and $\theta' = \theta + \frac{q^\star}{\hbar}\chi$ $\qquad \mathbf{J}_{\mathrm{S}} = q^\star n^\star(\mathbf{r},t)\left(\frac{\hbar}{m^\star}\nabla\theta'(\mathbf{r},t) - \frac{q^\star}{m^\star}\mathbf{A}'(\mathbf{r},t)\right)$

B, **E**, and **J** are *gauge invariant*, **A**, ϕ, and θ are not.