Lecture 5

Motion of a charged particle in a magnetic field
Charged particle in a magnetic field: Outline

1. Canonical quantization: lessons from classical dynamics
2. Quantum mechanics of a particle in a field
3. Atomic hydrogen in a uniform field: Normal Zeeman effect
4. Gauge invariance and the Aharonov-Bohm effect
5. Free electrons in a magnetic field: Landau levels
6. Integer Quantum Hall effect
What is effect of a static electromagnetic field on a charged particle?

- **Classically**, in electric and magnetic field, particles experience a **Lorentz force**:

  \[ F = q(E + \mathbf{v} \times \mathbf{B}) \]

  \( q \) denotes charge (notation: \( q = -e \) for electron).

- Velocity-dependent force \( q\mathbf{v} \times \mathbf{B} \) very different from that derived from scalar potential, and programme for transferring from classical to quantum mechanics has to be carried out with more care.

- As preparation, helpful to revise(?) how the Lorentz force law arises classically from **Lagrangian formulation**.
For a system with $m$ degrees of freedom specified by coordinates $q_1, \cdots q_m$, **classical action** determined from Lagrangian $L(q_i, \dot{q}_i)$ by

\[
S[q_i] = \int dt \ L(q_i, \dot{q}_i)
\]

For conservative forces (those which conserve mechanical energy), $L = T - V$, with $T$ the kinetic and $V$ the potential energy.

**Hamilton’s extremal principle:** trajectories $q_i(t)$ that minimize action specify classical (Euler-Lagrange) equations of motion,

\[
\frac{d}{dt} \left( \partial_{q_i} L(q_i, \dot{q}_i) \right) - \partial_{q_i} L(q_i, \dot{q}_i) = 0
\]

e.g. for a particle in a potential $V(q)$, $L(q, \dot{q}) = \frac{m\dot{q}^2}{2} - V(q)$ and from Euler-Lagrange equations, $m\ddot{q} = -\partial_q V(q)$
Analytical dynamics: a short primer

- For a system with \( m \) degrees of freedom specified by coordinates \( q_1, \cdots, q_m \), **classical action** determined from Lagrangian \( L(q_i, \dot{q}_i) \) by

\[
S[q_i] = \int dt \, L(q_i, \dot{q}_i)
\]

- For conservative forces (those which conserve mechanical energy), \( L = T - V \), with \( T \) the kinetic and \( V \) the potential energy.

- **Hamilton’s extremal principle**: trajectories \( q_i(t) \) that minimize action specify classical (Euler-Lagrange) equations of motion,

\[
\frac{d}{dt} \left( \partial_{\dot{q}_i} L(q_i, \dot{q}_i) \right) - \partial_{q_i} L(q_i, \dot{q}_i) = 0
\]

- e.g., for a particle in a potential \( V(q) \), \( L(q, \dot{q}) = \frac{m\dot{q}^2}{2} - V(q) \) and from Euler-Lagrange equations, \( m\ddot{q} = -\partial_q V(q) \)
To determine the classical Hamiltonian $H$ from the Lagrangian, first obtain the **canonical momentum** $p_i = \partial_{\dot{q}_i} L$ and then set

$$H(q_i, p_i) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i)$$

- e.g. for $L(q, \dot{q}) = \frac{m\dot{q}^2}{2} - V(q)$, $p = \partial_{\dot{q}} L = m\dot{q}$, and
  $$H = p\dot{q} - L = p\frac{p}{m} - (\frac{p^2}{2m} - V(q)) = \frac{p^2}{2m} + V(q).$$

- In Hamiltonian formulation, minimization of classical action
  $$S = \int dt \left( \sum_i p_i \dot{q}_i - H(q_i, p_i) \right),$$
  leads to Hamilton’s equations:

  $$\dot{q}_i = \partial_{p_i} H, \quad \dot{p}_i = -\partial_{q_i} H$$

- i.e. if Hamiltonian is independent of $q_i$, corresponding momentum $p_i$ is conserved, i.e. $p_i$ is a constant of the motion.
To determine the classical Hamiltonian $H$ from the Lagrangian, first obtain the **canonical momentum** $p_i = \partial_{\dot{q}_i} L$ and then set

$$H(q_i, p_i) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i)$$

e.g. for $L(q, \dot{q}) = \frac{m\dot{q}^2}{2} - V(q)$, $p = \partial_{\dot{q}} L = m\dot{q}$, and

$$H = p\dot{q} - L = p\frac{p}{m} - \left(\frac{p^2}{2m} - V(q)\right) = \frac{p^2}{2m} + V(q).$$

In Hamiltonian formulation, minimization of classical action

$$S = \int dt \left( \sum_i p_i \dot{q}_i - H(q_i, p_i) \right),$$

leads to Hamilton’s equations:

$$\dot{q}_i = \partial_{p_i} H, \quad \dot{p}_i = -\partial_{q_i} H$$

i.e. if Hamiltonian is independent of $q_i$, corresponding momentum $p_i$ is conserved, i.e. $p_i$ is a constant of the motion.
To determine the classical Hamiltonian $H$ from the Lagrangian, first obtain the **canonical momentum** $p_i = \partial_{\dot{q}_i} L$ and then set

$$H(q_i, p_i) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i)$$

E.g. for $L(q, \dot{q}) = \frac{m\dot{q}^2}{2} - V(q)$, $p = \partial_{\dot{q}} L = m\dot{q}$, and

$$H = p\dot{q} - L = p \frac{p}{m} - (\frac{p^2}{2m} - V(q)) = \frac{p^2}{2m} + V(q).$$

In Hamiltonian formulation, minimization of classical action

$$S = \int dt \left( \sum_i p_i \dot{q}_i - H(q_i, p_i) \right),$$

leads to Hamilton’s equations:

$$\dot{q}_i = \partial_{p_i} H, \quad \dot{p}_i = -\partial_{q_i} H$$

I.e. if Hamiltonian is independent of $q_i$, corresponding momentum $p_i$ is conserved, i.e. $p_i$ is a constant of the motion.
To determine the classical Hamiltonian $H$ from the Lagrangian, first obtain the **canonical momentum** $p_i = \partial_{\dot{q}_i} L$ and then set

$$H(q_i, p_i) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i)$$

- E.g. for $L(q, \dot{q}) = \frac{m \dot{q}^2}{2} - V(q)$, $p = \partial_{\dot{q}} L = m \dot{q}$, and
  $$H = p \dot{q} - L = p \frac{\dot{q}}{m} - (\frac{\dot{q}^2}{2m} - V(q)) = \frac{p^2}{2m} + V(q).$$

- In Hamiltonian formulation, minimization of classical action
  $$S = \int dt \left( \sum_i p_i \dot{q}_i - H(q_i, p_i) \right),$$
  leads to Hamilton’s equations:
  $$\dot{q}_i = \partial_{p_i} H, \quad \dot{p}_i = -\partial_{q_i} H$$

- I.e. if Hamiltonian is independent of $q_i$, corresponding momentum $p_i$ is conserved, i.e. $p_i$ is a constant of the motion.
As Lorentz force $\mathbf{F} = q\mathbf{v} \times \mathbf{B}$ is velocity dependent, it can not be expressed as gradient of some potential – nevertheless, classical equations of motion still specified by principle of least action.

With electric and magnetic fields written in terms of scalar and vector potential, $\mathbf{B} = \nabla \times \mathbf{A}$, $\mathbf{E} = -\nabla \varphi - \partial_t \mathbf{A}$, Lagrangian:

$$L = \frac{1}{2}mv^2 - q\varphi + q\mathbf{v} \cdot \mathbf{A}$$

$q_i \equiv x_i = (x_1, x_2, x_3)$ and $\dot{q}_i \equiv v_i = (\dot{x}_1, \dot{x}_2, \dot{x}_3)$

N.B. form of Lagrangian more natural in relativistic formulation: $-qv^\mu A_\mu = -q\varphi + q\mathbf{v} \cdot \mathbf{A}$ where $v^\mu = (c, \mathbf{v})$ and $A^\mu = (\varphi/c, \mathbf{A})$

Canonical momentum: $p_i = \partial_{\dot{x}_i} L = mv_i + qA_i$

no longer given by mass $\times$ velocity – there is an extra term!
Analytical dynamics: Lorentz force

- As Lorentz force $\mathbf{F} = q\mathbf{v} \times \mathbf{B}$ is velocity dependent, it can not be expressed as gradient of some potential – nevertheless, classical equations of motion still specified by principle of least action.

- With electric and magnetic fields written in terms of scalar and vector potential, $\mathbf{B} = \nabla \times \mathbf{A}$, $\mathbf{E} = -\nabla \varphi - \partial_t \mathbf{A}$, Lagrangian:

$$L = \frac{1}{2}mv^2 - q\varphi + q\mathbf{v} \cdot \mathbf{A}$$

$q_i \equiv x_i = (x_1, x_2, x_3)$ and $\dot{q}_i \equiv v_i = (\dot{x}_1, \dot{x}_2, \dot{x}_3)$

- N.B. form of Lagrangian more natural in relativistic formulation: 

  $$-qv^\mu A_\mu = -q\varphi + q\mathbf{v} \cdot \mathbf{A}$$

  where $v^\mu = (c, \mathbf{v})$ and $A^\mu = (\varphi/c, \mathbf{A})$

- Canonical momentum: 

  $$p_i = \partial_{\dot{x}_i} L = mv_i + qA_i$$

  no longer given by mass $\times$ velocity – there is an extra term!
Analytical dynamics: Lorentz force

- As Lorentz force \( F = qv \times B \) is velocity dependent, it can not be expressed as gradient of some potential – nevertheless, classical equations of motion still specified by principle of least action.

- With electric and magnetic fields written in terms of scalar and vector potential, \( B = \nabla \times A, E = -\nabla \varphi - \partial_t A \), Lagrangian:

\[
L = \frac{1}{2}mv^2 - q\varphi + v \cdot A
\]

- N.B. form of Lagrangian more natural in relativistic formulation:

\[-qv^{\mu} A_{\mu} = -q\varphi + v \cdot A\] where \( v^{\mu} = (c, v) \) and \( A^{\mu} = (\varphi/c, A) \)

- Canonical momentum:

\[
p_i = \partial_{\dot{x}_i} L = mv_i + qA_i
\]

no longer given by mass \( \times \) velocity – there is an extra term!
Analytical dynamics: Lorentz force

- As Lorentz force $\mathbf{F} = q\mathbf{v} \times \mathbf{B}$ is velocity dependent, it can not be expressed as gradient of some potential – nevertheless, classical equations of motion still specified by principle of least action.

- With electric and magnetic fields written in terms of scalar and vector potential, $\mathbf{B} = \nabla \times \mathbf{A}$, $\mathbf{E} = -\nabla \varphi - \partial_t \mathbf{A}$, Lagrangian:

$$L = \frac{1}{2} m \mathbf{v}^2 - q \varphi + q \mathbf{v} \cdot \mathbf{A}$$

$$q_i \equiv x_i = (x_1, x_2, x_3) \text{ and } q_i \equiv v_i = (\dot{x}_1, \dot{x}_2, \dot{x}_3)$$

- N.B. form of Lagrangian more natural in relativistic formulation:

$$-qv^\mu A_\mu = -q \varphi + q \mathbf{v} \cdot \mathbf{A} \text{ where } v^\mu = (c, \mathbf{v}) \text{ and } A^\mu = (\varphi/c, \mathbf{A})$$

- Canonical momentum: $p_i = \partial x_i L = m v_i + q A_i$

  no longer given by mass $\times$ velocity – there is an extra term!
Analytical dynamics: Lorentz force

From $H(q_i, p_i) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i)$, Hamiltonian given by:

$$H = \sum_i \left( mv_i + qA_i \right) v_i - \left( \frac{1}{2} m v^2 - q \varphi + q \mathbf{v} \cdot \mathbf{A} \right) = \frac{1}{2} m v^2 + q \varphi$$

To determine classical equations of motion, $H$ must be expressed solely in terms of coordinates and canonical momenta, $p = mv + qA$

$$H = \frac{1}{2m} (p - qA(x, t))^2 + q \varphi(x, t)$$

Then, from classical equations of motion $\dot{x}_i = \partial_{p_i} H$ and $\dot{p}_i = -\partial_{x_i} H$, and a little algebra, we recover Lorentz force law

$$m \ddot{x} = F = q \left( E + \mathbf{v} \times \mathbf{B} \right)$$
Analytical dynamics: Lorentz force

- From $H(q_i, p_i) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i)$, Hamiltonian given by:

  $$H = \sum_i \left( mv_i + q A_i \right) v_i - \left( \frac{1}{2} mv^2 - q \varphi + q v \cdot A \right) = \frac{1}{2} mv^2 + q \varphi$$

  $$= L(\dot{q}_i, q_i)$$

- To determine classical equations of motion, $H$ must be expressed solely in terms of coordinates and canonical momenta, $p = mv + qA$

  $$H = \frac{1}{2m} \left( p - q A(x, t) \right)^2 + q \varphi(x, t)$$

- Then, from classical equations of motion $\dot{x}_i = \partial_{p_i} H$ and $\dot{p}_i = -\partial_{x_i} H$, and a little algebra, we recover Lorentz force law

  $$m\ddot{x} = F = q \left( E + v \times B \right)$$
Analytical dynamics: Lorentz force

- From $H(q_i, p_i) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i)$, Hamiltonian given by:

\[
H = \sum_i \left( mv_i + qA_i \right) v_i - \left( \frac{1}{2} mv^2 - q\varphi + qv \cdot A \right) = \frac{1}{2} mv^2 + q\varphi
\]

- To determine classical equations of motion, $H$ must be expressed solely in terms of coordinates and canonical momenta, $p = mv + qA$

\[
H = \frac{1}{2m} (p - qA(x, t))^2 + q\varphi(x, t)
\]

- Then, from classical equations of motion $\dot{x}_i = \partial_{p_i} H$ and $\dot{p}_i = -\partial_{x_i} H$, and a little algebra, we recover Lorentz force law

\[
m\ddot{x} = F = q (E + v \times B)
\]
Lessons from classical dynamics

So, in summary, the classical Hamiltonian for a charged particle in an electromagnetic field is given by

\[ H = \frac{1}{2m} (p - qA(x, t))^2 + q\varphi(x, t) \]

This is all that you need to recall – its first principles derivation from the Lagrangian formulation is not formally examinable!

Using this result as a platform, we can now turn to the quantum mechanical formulation.
Quantum mechanics of particle in a field

- Canonical quantization: promote conjugate variables to operators, 
  \( \mathbf{p} \rightarrow \hat{\mathbf{p}} = -i\hbar \nabla, \quad \mathbf{x} \rightarrow \hat{\mathbf{x}} \) with commutation relations 
  \( [\hat{p}_i, \hat{x}_j] = -i\hbar \delta_{ij} \)

\[
\hat{H} = \frac{1}{2m} (\hat{p} - qA(x, t))^2 + q\varphi(x, t)
\]

- Gauge freedom: Note that the vector potential, \( \mathbf{A} \), is specified only up to some gauge:

For a given vector potential \( \mathbf{A}(x, t) \), the gauge transformation

\[
\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} + \nabla \Lambda, \quad \varphi \mapsto \varphi' = \varphi - \partial_t \Lambda
\]

with \( \Lambda(x, t) \) an arbitrary (scalar) function, leads to the same physical magnetic and electric field, \( \mathbf{B} = \nabla \times \mathbf{A} \), and \( \mathbf{E} = -\nabla \varphi - \partial_t \mathbf{A} \).

- In the following, we will adopt the Coulomb gauge condition,
  \( (\nabla \cdot \mathbf{A}) = 0 \).
Quantum mechanics of particle in a field

- Canonical quantization: promote conjugate variables to operators, \( \mathbf{p} \rightarrow \hat{\mathbf{p}} = -i\hbar \nabla \), \( \mathbf{x} \rightarrow \hat{\mathbf{x}} \) with commutation relations \([\hat{p}_i, \hat{x}_j] = -i\hbar \delta_{ij}\)

\[
\hat{H} = \frac{1}{2m}(\hat{\mathbf{p}} - q\mathbf{A}(\mathbf{x}, t))^2 + q\varphi(\mathbf{x}, t)
\]

- **Gauge freedom**: Note that the vector potential, \( \mathbf{A} \), is specified only up to some gauge:
  
  For a given vector potential \( \mathbf{A}(\mathbf{x}, t) \), the gauge transformation
  
  \[
  \mathbf{A} \leftrightarrow \mathbf{A}' = \mathbf{A} + \nabla \Lambda , \quad \varphi \leftrightarrow \varphi' = \varphi - \partial_t \Lambda
  \]

  with \( \Lambda(\mathbf{x}, t) \) an arbitrary (scalar) function, leads to the same physical magnetic and electric field, \( \mathbf{B} = \nabla \times \mathbf{A} \), and \( \mathbf{E} = -\nabla \varphi - \partial_t \mathbf{A} \).

- In the following, we will adopt the **Coulomb gauge condition**, \( (\nabla \cdot \mathbf{A}) = 0 \).
Quantum mechanics of particle in a field

- Canonical quantization: promote conjugate variables to operators, $\mathbf{p} \rightarrow \hat{\mathbf{p}} = -i\hbar \nabla$, $\mathbf{x} \rightarrow \hat{\mathbf{x}}$ with commutation relations $[\hat{p}_i, \hat{x}_j] = -i\hbar \delta_{ij}$

$$\hat{H} = \frac{1}{2m}(\hat{\mathbf{p}} - q\mathbf{A}(\mathbf{x}, t))^2 + q\varphi(\mathbf{x}, t)$$

- **Gauge freedom**: Note that the vector potential, $\mathbf{A}$, is specified only up to some gauge:

For a given vector potential $\mathbf{A}(\mathbf{x}, t)$, the gauge transformation

$$\mathbf{A} \leftrightarrow \mathbf{A}' = \mathbf{A} + \nabla \Lambda, \quad \varphi \leftrightarrow \varphi' = \varphi - \partial_t \Lambda$$

with $\Lambda(\mathbf{x}, t)$ an arbitrary (scalar) function, leads to the same physical magnetic and electric field, $\mathbf{B} = \nabla \times \mathbf{A}$, and $\mathbf{E} = -\nabla \varphi - \partial_t \mathbf{A}$.

- In the following, we will adopt the **Coulomb gauge condition**, $(\nabla \cdot \mathbf{A}) = 0$. 
Quantum mechanics of particle in a field

\[ \hat{H} = \frac{1}{2m} (\hat{p} - qA(x, t))^2 + q\varphi(x, t) \]

- Expanding the Hamiltonian in \( A \), we can identify two types of contribution: the cross-term (known as the **paramagnetic term**),

\[ -\frac{q}{2m} (\hat{p} \cdot A + A \cdot \hat{p}) = \frac{iq\hbar}{2m} (\nabla \cdot A + A \cdot \nabla) = \frac{iq\hbar}{m} A \cdot \nabla \]

where equality follows from Coulomb gauge condition, \((\nabla \cdot A) = 0\).

- And the diagonal term (known as the **diamagnetic term**) \( \frac{q^2}{2m} A^2 \).

- Together, they lead to the expansion

\[ \hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \frac{iq\hbar}{m} A \cdot \nabla + \frac{q^2}{2m} A^2 + q\varphi \]
Expanding the Hamiltonian in $\mathbf{A}$, we can identify two types of contribution: the cross-term (known as the \textbf{paramagnetic term}),

$$-rac{q}{2m} (\hat{\mathbf{p}} \cdot \mathbf{A} + \mathbf{A} \cdot \hat{\mathbf{p}}) = \frac{i q \hbar}{2m} (\nabla \cdot \mathbf{A} + \mathbf{A} \cdot \nabla) = \frac{i q \hbar}{m} \mathbf{A} \cdot \nabla$$

where equality follows from Coulomb gauge condition, $(\nabla \cdot \mathbf{A}) = 0$.

And the diagonal term (known as the \textbf{diamagnetic term}) $\frac{q^2}{2m} \mathbf{A}^2$.

Together, they lead to the expansion

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \frac{i q \hbar}{m} \mathbf{A} \cdot \nabla + \frac{q^2}{2m} \mathbf{A}^2 + q \varphi$$
Quantum mechanics of particle in a field

\[ \hat{H} = \frac{1}{2m}(\hat{p} - q\mathbf{A}(x, t))^2 + q\varphi(x, t) \]

- Expanding the Hamiltonian in \( \mathbf{A} \), we can identify two types of contribution: the cross-term (known as the **paramagnetic term**),

  \[-\frac{q}{2m}(\hat{p} \cdot \mathbf{A} + \mathbf{A} \cdot \hat{p}) = \frac{iq}{2m} (\nabla \cdot \mathbf{A} + \mathbf{A} \cdot \nabla) = \frac{iq\hbar}{m} \mathbf{A} \cdot \nabla \]

  where equality follows from Coulomb gauge condition, \((\nabla \cdot \mathbf{A}) = 0\).

- And the diagonal term (known as the **diamagnetic term**) \( \frac{q^2}{2m} \mathbf{A}^2 \).

- Together, they lead to the expansion

\[ \hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \frac{iq\hbar}{m} \mathbf{A} \cdot \nabla + \frac{q^2}{2m} \mathbf{A}^2 + q\varphi \]
Quantum mechanics of particle in a uniform field

\[
\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \frac{iq\hbar}{m} \mathbf{A} \cdot \nabla + \frac{q^2}{2m} \mathbf{A}^2 + q\varphi
\]

- For a stationary uniform magnetic field, \( \mathbf{A}(\mathbf{x}) = -\frac{1}{2} \mathbf{x} \times \mathbf{B} \) (known as the symmetric gauge), the **paramagnetic** component of \( \hat{H} \) given by,

\[
\frac{iq\hbar}{m} \mathbf{A} \cdot \nabla = -\frac{iq\hbar}{2m} (\mathbf{x} \times \mathbf{B}) \cdot \nabla = \frac{iq\hbar}{2m} (\mathbf{x} \times \nabla) \cdot \mathbf{B} = -\frac{q}{2m} \hat{\mathbf{L}} \cdot \mathbf{B}
\]

where \( \hat{\mathbf{L}} = \mathbf{x} \times (-i\hbar \nabla) \) denotes the angular momentum operator.

- For field, \( \mathbf{B} = B\hat{\mathbf{e}}_z \) oriented along \( z \), **diamagnetic term**, 

\[
\frac{q^2}{2m} \mathbf{A}^2 = \frac{q^2}{8m} (\mathbf{x} \times \mathbf{B})^2 = \frac{q^2}{8m} (\mathbf{x}^2 \mathbf{B}^2 - (\mathbf{x} \cdot \mathbf{B})^2) = \frac{q^2 B^2}{8m} (x^2 + y^2)
\]
Quantum mechanics of particle in a uniform field

\[ \hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \frac{iq\hbar}{m} \mathbf{A} \cdot \nabla + \frac{q^2}{2m} \mathbf{A}^2 + q\varphi \]

- For a stationary uniform magnetic field, \( \mathbf{A}(x) = -\frac{1}{2} x \times \mathbf{B} \) (known as the symmetric gauge), the **paramagnetic** component of \( \hat{H} \) given by,

\[ \frac{iq\hbar}{m} \mathbf{A} \cdot \nabla = -\frac{iq\hbar}{2m} (x \times \mathbf{B}) \cdot \nabla = \frac{iq\hbar}{2m} (x \times \nabla) \cdot \mathbf{B} = -\frac{q}{2m} \hat{\mathbf{L}} \cdot \mathbf{B} \]

where \( \hat{\mathbf{L}} = x \times (-i\hbar\nabla) \) denotes the angular momentum operator.

- For field, \( \mathbf{B} = B\hat{\mathbf{e}}_z \) oriented along \( z \), **diamagnetic term**,

\[ \frac{q^2}{2m} \mathbf{A}^2 = \frac{q^2}{8m} (x \times \mathbf{B})^2 = \frac{q^2}{8m} \left( x^2 B^2 - (x \cdot \mathbf{B})^2 \right) = \frac{q^2 B^2}{8m} (x^2 + y^2) \]
Quantum mechanics of particle in a uniform field

\[ \hat{H} = -\frac{\hbar^2}{2m} \nabla^2 - \frac{qB}{2m} \hat{L}_z + \frac{q^2 B^2}{8m} (x^2 + y^2) + q\varphi \]

- In the following, we will address two examples of electron \((q = -e)\) motion in a uniform magnetic field, \(\mathbf{B} = B\mathbf{\hat{z}}:\)

1. **Atomic hydrogen:** where electron is bound to a proton by the Coulomb potential,

   \[ V(r) = q\varphi(r) = -\frac{1}{4\pi\epsilon_0} \frac{e^2}{r} \]

2. **Free electrons:** where the electron is unbound, \(\varphi = 0.\)

- In the first case, we will see that the diamagnetic term has a negligible role whereas, in the second, both terms contribute significantly to the dynamics.
Atomic hydrogen in uniform field

\[
\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \frac{eB}{2m} \hat{L}_z + \frac{e^2B^2}{8m}(x^2 + y^2) - \frac{1}{4\pi\varepsilon_0} \frac{e^2}{r}
\]

With \(\langle x^2 + y^2 \rangle \simeq a_0^2\), where \(a_0\) is Bohr radius, and \(\langle L_z \rangle \simeq \hbar\), ratio of paramagnetic and diamagnetic terms,

\[
\frac{(e^2/8m_e)\langle x^2 + y^2 \rangle B^2}{(e/2m_e)\langle L_z \rangle B} = \frac{e}{4\hbar} a_0^2 B \simeq 10^{-6} \text{ B/T}
\]

i.e. for bound electrons, diamagnetic term is negligible.

not so for unbound electrons or on neutron stars!

When compared with Coulomb energy scale,

\[
\frac{(e/2m)\hbar B}{m_e c^2 \alpha^2 / 2} = \frac{e\hbar}{(m_e c \alpha)^2} B \simeq 10^{-5} \text{ B/T}
\]

where \(\alpha = \frac{e^2}{4\pi\varepsilon_0} \frac{1}{\hbar c} \simeq \frac{1}{137}\) denotes fine structure constant,

paramagnetic term effects only a small perturbation.
Atomic hydrogen in uniform field

\[
\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \frac{eB}{2m} \hat{L}_z + \frac{e^2 B^2}{8m} (x^2 + y^2) - \frac{1}{4\pi\varepsilon_0} \frac{e^2}{r}
\]

- With \(\langle x^2 + y^2 \rangle \simeq a_0^2\), where \(a_0\) is Bohr radius, and \(\langle L_z \rangle \simeq \hbar\),
  ratio of paramagnetic and diamagnetic terms,

\[
\frac{(e^2/8m_e)\langle x^2 + y^2 \rangle B^2}{(e/2m_e)\langle L_z \rangle B} = \frac{e}{4\hbar} a_0^2 B \simeq 10^{-6} \frac{B}{T}
\]

i.e. for **bound** electrons, **diamagnetic term is negligible**.
not so for unbound electrons or on neutron stars!

- When compared with Coulomb energy scale,

\[
\frac{(e/2m)\hbar B}{m_e c^2 \alpha^2 / 2} = \frac{e\hbar}{(m_e c \alpha)^2} B \simeq 10^{-5} \frac{B}{T}
\]

where \(\alpha = \frac{e^2}{4\pi\varepsilon_0} \frac{1}{\hbar c} \simeq \frac{1}{137}\) denotes fine structure constant,
paramagnetic term effects only a small perturbation.
Atomic hydrogen in uniform field

\[ \hat{H} \simeq -\frac{\hbar^2}{2m} \nabla^2 + \frac{e}{2m} \mathbf{B} \cdot \hat{\mathbf{L}} - \frac{1}{4\pi \varepsilon_0} \frac{e^2}{r} \]

- In general, term linear in \( \mathbf{B} \) defines magnetic dipole moment \( \mu \):
  \( \hat{H}_M = -\mu \cdot \mathbf{B} \). Result above shows that orbital degrees of freedom of the electron lead to a magnetic moment,

  \[ \mu = -\frac{e}{2m_e} \hat{\mathbf{L}} \]

- cf. classical result: for an electron in a circular orbit around a proton, \( I = -e/\tau = -ev/2\pi r \). With angular momentum \( L = m_e vr \),

  \[ \mu = IA = -\frac{ev}{2\pi r} \pi r^2 = -\frac{e}{2m_e} m_e vr = -\frac{e}{2m_e} L \]

- Since \( \langle \hat{L} \rangle \sim \hbar \), scale of \( \mu \) set by the Bohr magneton,

  \[ \mu_B = \frac{e\hbar}{2m_e} = 5.79 \times 10^{-5} \text{ eV/T} \]
Atomic hydrogen in uniform field

\[
\hat{H} \simeq -\frac{\hbar^2}{2m} \nabla^2 + \frac{e}{2m} \mathbf{B} \cdot \hat{\mathbf{L}} - \frac{1}{4\pi \varepsilon_0} \frac{e^2}{r}
\]

- In general, term linear in \( \mathbf{B} \) defines magnetic dipole moment \( \mu \):
  \( \hat{H}_M = -\mu \cdot \mathbf{B} \). Result above shows that orbital degrees of freedom of the electron lead to a magnetic moment,

  \[
  \mu = -\frac{e}{2m_e} \hat{\mathbf{L}}
  \]

- cf. classical result: for an electron in a circular orbit around a proton, \( I = -e/\tau = -ev/2\pi r \). With angular momentum \( L = m_e vr \),

  \[
  \mu = IA = -\frac{ev}{2\pi r} \pi r^2 = -\frac{e}{2m_e} m_e vr = -\frac{e}{2m_e} L
  \]

- Since \( \langle \hat{L} \rangle \sim \hbar \), scale of \( \mu \) set by the Bohr magneton,

  \[
  \mu_B = \frac{e\hbar}{2m_e} = 5.79 \times 10^{-5} \text{ eV/T}
  \]
\[
\hat{H} \simeq -\frac{\hbar^2}{2m} \nabla^2 + \frac{e}{2m} \mathbf{B} \cdot \hat{\mathbf{L}} - \frac{1}{4\pi\epsilon_0} \frac{e^2}{r}
\]

- In general, term linear in \( \mathbf{B} \) defines magnetic dipole moment \( \mu \): \( \hat{H}_M = -\mu \cdot \mathbf{B} \). Result above shows that orbital degrees of freedom of the electron lead to a magnetic moment,

\[
\mu = -\frac{e}{2m_e} \hat{\mathbf{L}}
\]

- In the next lecture, we will see that there is an additional intrinsic contribution to the magnetic moment of the electron which derives from quantum mechanical spin.

- Since \( \langle \hat{\mathbf{L}} \rangle \sim \hbar \), scale of \( \mu \) set by the Bohr magneton,

\[
\mu_B = \frac{e\hbar}{2m_e} = 5.79 \times 10^{-5} \text{ eV/T}
\]
Atomic hydrogen in uniform field

\[
\hat{H} \simeq -\frac{\hbar^2}{2m} \nabla^2 + \frac{e}{2m} \mathbf{B} \cdot \hat{\mathbf{L}} - \frac{1}{4\pi\varepsilon_0} \frac{e^2}{r}
\]

- In general, term linear in \( \mathbf{B} \) defines magnetic dipole moment \( \mu \): 
  \( \hat{H}_M = -\mu \cdot \mathbf{B} \). Result above shows that orbital degrees of freedom of the electron lead to a magnetic moment,

\[
\mu = -\frac{e}{2m_e} \hat{\mathbf{L}}
\]

- In the next lecture, we will see that there is an additional intrinsic contribution to the magnetic moment of the electron which derives from quantum mechanical spin.

- Since \( \langle \hat{L} \rangle \sim \hbar \), scale of \( \mu \) set by the Bohr magneton,

\[
\mu_B = \frac{e\hbar}{2m_e} = 5.79 \times 10^{-5} \text{ eV/T}
\]
Atomic hydrogen: Normal Zeeman effect

- So, in a uniform magnetic field, \( \mathbf{B} = B\hat{\mathbf{e}}_z \), the electron Hamiltonian for atomic hydrogen is given by,

\[
\hat{H} = \hat{H}_0 + \frac{e}{2m} B \hat{L}_z, \quad \hat{H}_0 = \frac{\hat{p}^2}{2m} - \frac{1}{4\pi\epsilon_0} \frac{e^2}{r}
\]

- Since \([\hat{H}_0, \hat{L}_z] = 0\), eigenstates of unperturbed Hamiltonian, \( \hat{H}_0 \), defined by \( \psi_{n\ell m}(x) \), remain eigenstates of \( \hat{H} \), with eigenvalues,

\[
E_{n\ell m} = -\frac{1}{n^2} \text{Ry} + \hbar \omega_L m
\]

where \( \omega_L = \frac{eB}{2m} \) denotes the Larmor frequency.

- (Without spin contribution) uniform magnetic field \( \sim \) splitting of \( (2\ell + 1)\)-fold degeneracy with multiplets separated by \( \hbar \omega_L \).
Normal Zeeman effect: experiment

- Experiment shows Zeeman splitting of spectral lines...

  e.g. Splitting of Sodium D lines (involving $3p$ to $3s$ transitions)

  ![Image showing Zeeman splitting of spectral lines]


- ...but the reality is made more complicated by the existence of spin and relativistic corrections – see later in the course.
Gauge invariance

\[ \hat{H} = \frac{1}{2m} (\hat{p} - qA(x, t))^2 + q\varphi(x, t) \]

- Hamiltonian of charged particle depends on vector potential, \( \mathbf{A} \). Since \( \mathbf{A} \) defined only up to some gauge choice \( \Rightarrow \) \textbf{wavefunction is not a gauge invariant object.}

- To explore gauge freedom, consider effect of gauge transformation
  \[ \mathbf{A} \rightarrow \mathbf{A}' = \mathbf{A} + \nabla \Lambda, \quad \varphi \rightarrow \varphi' = \varphi - \partial_t \Lambda \]
  
  where \( \Lambda(x, t) \) denotes arbitrary scalar function.

- Under gauge transformation: \( i\hbar \partial_t \psi = \hat{H}[A] \psi \rightarrow i\hbar \partial_t \psi' = \hat{H}[A'] \psi' \)
  
  where wavefunction acquires additional phase,
  \[ \psi'(x, t) = \exp \left[ i \frac{q}{\hbar} \Lambda(x, t) \right] \psi(x, t) \]

  but probability density, \( |\psi'(x, t)|^2 = |\psi(x, t)|^2 \) is conserved.
Gauge invariance

\[ \hat{H} = \frac{1}{2m}(\hat{p} - q\mathbf{A}(x, t))^2 + q\varphi(x, t) \]

- Hamiltonian of charged particle depends on vector potential, \( \mathbf{A} \). Since \( \mathbf{A} \) defined only up to some gauge choice \( \Rightarrow \) wavefunction is not a gauge invariant object.

- To explore gauge freedom, consider effect of gauge transformation

\[
\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} + \nabla \Lambda, \quad \varphi \mapsto \varphi' = \varphi - \partial_t \Lambda
\]

where \( \Lambda(x, t) \) denotes arbitrary scalar function.

- Under gauge transformation: \( i\hbar \partial_t \psi = \hat{H}[\mathbf{A}]\psi \mapsto i\hbar \partial_t \psi' = \hat{H}[\mathbf{A}']\psi' \)

where wavefunction acquires additional phase,

\[
\psi'(x, t) = \exp \left[ i \frac{q}{\hbar} \Lambda(x, t) \right] \psi(x, t)
\]

but probability density, \( |\psi'(x, t)|^2 = |\psi(x, t)|^2 \) is conserved.
Gauge invariance

\[ 
\psi'(x, t) = \exp \left[ i \frac{q}{\hbar} \Lambda(x, t) \right] \psi(x, t) 
\]

**Proof:** using the identity

\[ 
(\hat{p} - qA - q\nabla \Lambda) \exp \left[ i \frac{q}{\hbar} \Lambda \right] = \exp \left[ i \frac{q}{\hbar} \Lambda \right] (\hat{p} - qA) 
\]

\[ 
\hat{H}[A']\psi' = \left[ \frac{1}{2m} (\hat{p} - qA - q\nabla \Lambda)^2 + q\varphi - q\partial_t \Lambda \right] \exp \left[ i \frac{q}{\hbar} \Lambda \right] \psi 
\]

\[ 
= \exp \left[ i \frac{q}{\hbar} \Lambda \right] \left[ \frac{1}{2m} (\hat{p} - qA)^2 + q\varphi - q\partial_t \Lambda \right] \psi 
\]

\[ 
= \exp \left[ i \frac{q}{\hbar} \Lambda \right] \left[ \hat{H}[A] - q\partial_t \Lambda \right] \psi 
\]

Similarly

\[ 
\ i\hbar \partial_t \psi' = \exp \left[ i \frac{q}{\hbar} \Lambda \right] (i\hbar \partial_t - q\partial_t \Lambda) \psi 
\]

Therefore, if \( i\hbar \partial_t \psi = \hat{H}[A] \psi \), we have \( i\hbar \partial_t \psi' = \hat{H}[A'] \psi' \).
Gauge invariance

\[ \psi'(x, t) = \exp \left[ i \frac{q}{\hbar} \Lambda(x, t) \right] \psi(x, t) \]

**Proof:** using the identity

\[ (\hat{p} - qA - q\nabla \Lambda) \exp \left[ i \frac{q}{\hbar} \right] = \exp \left[ i \frac{q}{\hbar} \right] (\hat{p} - qA) \]

\[ \hat{H}[A'] \psi' = \left[ \frac{1}{2m} (\hat{p} - qA - q\nabla \Lambda)^2 + q\varphi - q\partial_t \Lambda \right] \exp \left[ i \frac{q}{\hbar} \right] \psi \]

\[ = \exp \left[ i \frac{q}{\hbar} \right] \left[ \frac{1}{2m} (\hat{p} - qA)^2 + q\varphi - q\partial_t \Lambda \right] \psi \]

\[ = \exp \left[ i \frac{q}{\hbar} \right] \left[ \hat{H}[A] - q\partial_t \Lambda \right] \psi \]

Similarly

\[ i\hbar \partial_t \psi' = \exp \left[ i \frac{q}{\hbar} \right] (i\hbar \partial_t - q\partial_t \Lambda) \psi \]

Therefore, if \( i\hbar \partial_t \psi = \hat{H}[A] \psi \), we have \( i\hbar \partial_t \psi' = \hat{H}[A'] \psi' \).
Gauge invariance

\[ \psi'(x, t) = \exp \left[ i \frac{q}{\hbar} \Lambda(x, t) \right] \psi(x, t) \]

**Proof:** using the identity

\[(\hat{p} - qA - q\nabla \Lambda) \exp \left[ i \frac{q}{\hbar} \Lambda \right] = \exp \left[ i \frac{q}{\hbar} \Lambda \right] (\hat{p} - qA)\]

\[\hat{H}[A'] \psi' = \left[ \frac{1}{2m} (\hat{p} - qA - q\nabla \Lambda)^2 + q\varphi - q\partial_t \Lambda \right] \exp \left[ i \frac{q}{\hbar} \Lambda \right] \psi\]

\[= \exp \left[ i \frac{q}{\hbar} \Lambda \right] \left[ \frac{1}{2m} (\hat{p} - qA)^2 + q\varphi - q\partial_t \Lambda \right] \psi\]

\[= \exp \left[ i \frac{q}{\hbar} \Lambda \right] \left[ \hat{H}[A] - q\partial_t \Lambda \right] \psi\]

Similarly

\[i\hbar \partial_t \psi' = \exp \left[ i \frac{q}{\hbar} \Lambda \right] (i\hbar \partial_t - q\partial_t \Lambda) \psi\]

Therefore, if \(i\hbar \partial_t \psi = \hat{H}[A] \psi\), we have \(i\hbar \partial_t \psi' = \hat{H}[A'] \psi'\).
Gauge invariance: physical consequences

\[ \psi'(x, t) = \exp \left[ i \frac{q}{\hbar} \Lambda(x, t) \right] \psi(x, t) \]

- Consider particle (charge \( q \)) travelling along path, \( P \), in which the magnetic field, \( B = 0 \).

- However, \( B = 0 \nRightarrow A = 0 \):
  any \( \Lambda(x) \) such that \( A = \nabla \Lambda \) leads to \( B = 0 \).

- In traversing path, wavefunction acquires phase
  \[ \phi = \frac{q}{\hbar} \int_P A \cdot dx. \]

- If we consider two separate paths \( P \) and \( P' \) with same initial and final points, relative phase of the wavefunction,
  \[ \Delta \phi = \frac{q}{\hbar} \int_P A \cdot dx - \frac{q}{\hbar} \int_{P'} A \cdot dx = \frac{q}{\hbar} \oint A \cdot dx \quad \text{Stokes} \quad \frac{q}{\hbar} \int_A B \cdot d^2x \]
  where \( \int_A \) runs over area enclosed by loop formed from \( P \) and \( P' \).
Gauge invariance: physical consequences

\[ \psi'(x, t) = \exp \left[ i \frac{q}{\hbar} \Lambda(x, t) \right] \psi(x, t) \]

- Consider particle (charge \( q \)) travelling along path, \( P \), in which the magnetic field, \( B = 0 \).

- However, \( B = 0 \not\Rightarrow A = 0 \): any \( \Lambda(x) \) such that \( A = \nabla\Lambda \) leads to \( B = 0 \).

- In traversing path, wavefunction acquires phase
  \[ \phi = \frac{q}{\hbar} \int_P A \cdot dx. \]

- If we consider two separate paths \( P \) and \( P' \) with same initial and final points, relative phase of the wavefunction,
  \[ \Delta\phi = \frac{q}{\hbar} \int_P A \cdot dx - \frac{q}{\hbar} \int_{P'} A \cdot dx = \frac{q}{\hbar} \oint_A A \cdot d\mathbf{x} \overset{\text{Stokes}}{=} \frac{q}{\hbar} \int_A B \cdot d^2x \]
  where \( \oint_A \) runs over area enclosed by loop formed from \( P \) and \( P' \).
Gauge invariance: physical consequences

\[ \Delta \phi = \frac{q}{\hbar} \int_A \mathbf{B} \cdot d^2 \mathbf{x} \]

- i.e. for paths $P$ and $P'$, wavefunction components acquire relative phase difference,

\[ \Delta \phi = \frac{q}{\hbar} \times \text{magnetic flux through area} \]

- If paths enclose region of non-vanishing field, even if $\mathbf{B}$ identically zero on paths $P$ and $P'$, $\psi(\mathbf{x})$ acquires non-vanishing relative phase.

- This phenomenon, known as the **Aharonov-Bohm effect**, leads to quantum interference which can influence observable properties.
Gauge invariance: physical consequences

\[ \Delta \phi = \frac{q}{\hbar} \int_A B \cdot d^2x \]

- i.e. for paths \( P \) and \( P' \), wavefunction components acquire relative phase difference,

\[ \Delta \phi = \frac{q}{\hbar} \times \text{magnetic flux through area} \]

- If paths enclose region of non-vanishing field, even if \( B \) identically zero on paths \( P \) and \( P' \), \( \psi(x) \) acquires non-vanishing relative phase.

- This phenomenon, known as the **Aharonov-Bohm effect**, leads to quantum interference which can influence observable properties.
Influence of quantum interference effects is visible in transport properties of low-dimensional semiconductor devices.

When electrons are forced to detour around a potential barrier, conductance through the device shows Aharonov-Bohm oscillations.
Influence of quantum interference effects is visible in transport properties of low-dimensional semiconductor devices.

When electrons are forced to detour around a potential barrier, conductance through the device shows Aharonov-Bohm oscillations.
Aharanov-Bohm effect: example II

But can we demonstrate interference effects when electrons transverse region where $B$ is truly zero? Definitive experimental proof provided in 1986 by Tonomura:

- If a superconductor completely encloses a toroidal magnet, flux through superconducting loop quantized in units of $\hbar/2e$.

- Electrons which pass inside or outside the loop therefore acquire a relative phase difference of $\varphi = -\frac{e}{\hbar} \times \frac{\hbar}{2e} = n\pi$.

- If $n$ is even, there is no phase shift, while if $n$ is odd, there is a phase shift of $\pi$.

- Experiment confirms both Aharonov-Bohm effect and the phenomenon of flux quantization in a superconductor!
Summary: charged particle in a field

- Starting from the classical Lagrangian for a particle moving in a static electromagnetic field,

\[ L = \frac{1}{2} m v^2 - q \varphi + q v \cdot A \]

- we derived the quantum Hamiltonian,

\[ H = \frac{1}{2m} (p - qA(x, t))^2 + q\varphi(x, t) \]

- An expansion in \( A \) leads to a paramagnetic and diamagnetic contribution which, in the Coulomb gauge (\( \nabla \cdot A = 0 \)), is given by

\[ \hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \frac{iq\hbar}{m} A \cdot \nabla + \frac{q^2}{2m} A^2 + q\varphi \]
Summary: charged particle in a field

- Applied to atomic hydrogen, a uniform magnetic field, $\mathbf{B} = B\hat{z}$
  leads to the Hamiltonian

$$\hat{H} = \frac{1}{2m} \left[ \hat{p}_r^2 + \frac{\hat{L}^2}{r^2} + eB\hat{L}_z + \frac{1}{4}e^2B^2(x^2 + y^2) \right] - \frac{1}{4\pi\epsilon_0} \frac{e^2}{r}$$

- For weak fields, diamagnetic contribution is negligible in comparison with paramagnetic and can be dropped.

Therefore, (continuing to ignore electron spin), magnetic field splits orbital degeneracy leading to normal Zeeman effect,

$$E_{n\ell m} = -\frac{1}{n^2}\text{Ry} + \mu_B Bm$$

However, when diamagnetic term $O(B^2 n^3)$ competes with Coulomb energy scale $-\frac{\text{Ry}}{n^2}$ classical dynamics becomes irregular and system enters “quantum chaotic regime”.

Gauge invariance of electromagnetic field $\Rightarrow$ wavefunction not gauge invariant.

Under gauge transformation, $A \mapsto A' = A + \nabla \Lambda$, $\varphi \mapsto \varphi' = \varphi - \partial_t \Lambda$, wavefunction acquires additional phase,

$$\psi'(x, t) = \exp \left[ i \frac{q}{\hbar} \Lambda(x, t) \right] \psi(x, t)$$

$\rightsquigarrow$ Aharanov-Bohm effect: (even if no orbital effect) particles encircling magnetic flux acquire relative phase, $\Delta \phi = \frac{q}{\hbar} \int_A \mathbf{B} \cdot d^2 \mathbf{x}$.

i.e. for $\Delta \phi = 2\pi n$ expect constructive interference $\Rightarrow \frac{1}{n} \frac{\hbar}{e}$ oscillations.