Lecture 5

Motion of a charged particle in a magnetic field
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
Lorentz force

What is effect of a static electromagnetic field on a charged particle?

- **Classically**, in electric and magnetic field, particles experience a **Lorentz force**:
  \[ F = q(E + v \times B) \]

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

- Velocity-dependent force \( qv \times B \) 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,

$$\frac{d}{dt} (\partial_{\dot{q}_i} L(q_i, \dot{q}_i)) - \partial_{q_i} L(q_i, \dot{q}_i) = 0$$

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

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- 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** $p_i = \partial q_i L$ and then set

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

- e.g. for $L(q, \dot{q}) = \frac{m\dot{q}^2}{2} - V(q)$, $p = \partial_q L = m\dot{q}$, 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.
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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}
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\( q_i \equiv x_i = (x_1, x_2, x_3) \) 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:

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no longer given by mass \( \times \) velocity – there is an extra term!
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H = \sum_i (mv_i + qA_i) v_i - \left( \frac{1}{2}mv^2 - q\varphi + qv \cdot A \right) = \frac{1}{2}mv^2 + q\varphi
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- To determine classical equations of motion, \( H \) must be expressed solely in terms of coordinates and canonical momenta, \( p = mv + qA \)

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

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m\ddot{x} = F = q (E + v \times B)
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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, \( p \to \hat{p} = -i\hbar \nabla \), \( x \to \hat{x} \) 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)
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- Gauge freedom: Note that the vector potential, \( A \), is specified only up to some gauge:

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

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

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

- In the following, we will adopt the Coulomb gauge condition,

\[
(\nabla \cdot A) = 0.
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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**),

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

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 field

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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}
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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)
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Quantum mechanics of particle in a uniform field

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Quantum mechanics of particle in a uniform field

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

- In the following, we will address two examples of electron \((q = -e)\) motion in a uniform magnetic field, \(B = B\hat{e}_z:\)
  - **Atomic hydrogen:** where electron is bound to a proton by the Coulomb potential,
    \[ V(r) = q\varphi(r) = -\frac{1}{4\pi\varepsilon_0} \frac{e^2}{r} \]
  - **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

\[ \hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \frac{eB}{2m} \hat{L}_z + \frac{e^2 B^2}{8m} (x^2 + y^2) - \frac{1}{4\pi \epsilon_0} \frac{e^2}{r} \]

- 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,

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

i.e. for bound electrons, \textit{diamagnetic term is negligible}. not so for unbound electrons or on neutron stars!

- When compared with Coulomb energy scale,

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

where \( \alpha = \frac{e^2}{4\pi \epsilon_0 \hbar c} \simeq \frac{1}{137} \) denotes fine structure constant, paramagnetic term effects only a small perturbation.
Atomic hydrogen in uniform field

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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 \( L = m_evr \),

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

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

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

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

\[
\hat{H} = \hat{H}_0 + \frac{e}{2m} B \hat{L}_z, \quad \hat{H}_0 = \frac{\hat{p}^2}{2m} - \frac{1}{4\pi\varepsilon_0} \frac{e^2}{r}
\]

- Since \([\hat{H}_0, L_z] = 0\), 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)

...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, \( A \). Since \( A \) defined only up to some gauge choice \( \Rightarrow \) wavefunction is not a gauge invariant object.
- To explore gauge freedom, consider effect of gauge transformation
  \[ A \mapsto A' = A + \nabla \Lambda, \quad \varphi \mapsto \varphi' = \varphi - \partial_t \Lambda \]
  where \( \Lambda(x, t) \) denotes arbitrary scalar function.
- Under gauge transformation: \( i\hbar \partial_t \psi = \hat{H}[A] \psi \mapsto i\hbar \partial_t \psi' = \hat{H}[A'] \psi' \)
  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.
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\[ \psi'(x, t) = \exp \left[ \frac{i q}{\hbar} \Lambda(x, t) \right] \psi(x, t) \]

**Proof:** using the identity

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

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

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

Similarly

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

Therefore, if \( i\hbar \partial_t \psi = \hat{H}[A] \psi \), we have \( i\hbar \partial_t \psi' = \hat{H}[A'] \psi' \).
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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,
  \[ \Delta \phi = \frac{q}{\hbar} \int_P A \cdot dx - \frac{q}{\hbar} \int_{P'} A \cdot dx = \frac{q}{\hbar} \oint P A \cdot dx \quad \text{Stokes} \quad \frac{q}{\hbar} \int_A B \cdot d^2x \]

  where \( \oint_A \) runs over area enclosed by loop formed from \( P \) and \( P' \).
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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

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When electrons are forced to detour around a potential barrier, conductance through the device shows Aharonov-Bohm oscillations.
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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
  \[ \varphi = -\frac{e}{\hbar} \times n \frac{h}{2e} = n\pi. \]

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

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

we derived the quantum Hamiltonian,

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

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

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

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

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

- 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**,

\[
E_{n\ell m} = -\frac{1}{n^2} R_y + \mu_B B m
\]

- However, when diamagnetic term \( O(B^2 n^3) \) competes with Coulomb energy scale \(-\frac{R_y}{n^2}\) classical dynamics becomes **irregular** and system enters “quantum chaotic regime”. 
Summary: charged particle in a field

- **Gauge invariance** of electromagnetic field \( \Rightarrow \) wavefunction not gauge invariant.

- Under gauge transformation, \( \mathbf{A} \leftrightarrow \mathbf{A}' = \mathbf{A} + \nabla \Lambda \), \( \varphi \leftrightarrow \varphi' = \varphi - \partial_t \Lambda \), wavefunction acquires additional phase,

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

- \( \leadsto \) **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.