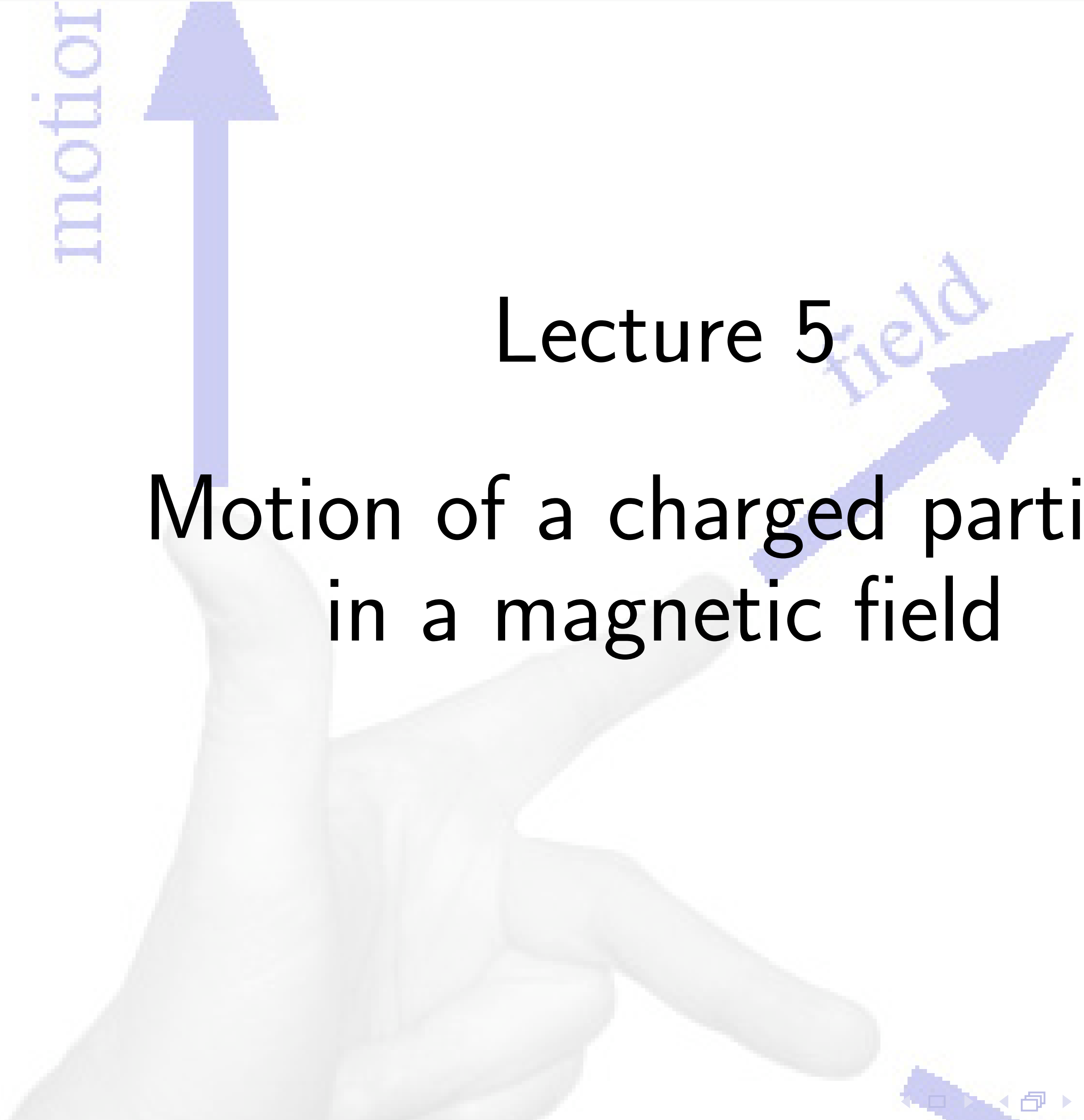
Lecture 5

Motion of a charged particle in a magnetic field



Charged particle in a magnetic field: Outline

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**:

$$\mathbf{F} = q\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right)$$

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**.

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,

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

- 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

- 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

- To determine the classical Hamiltonian H from the Lagrangian, first obtain the **canonical momentum** $\boxed{p_i = \partial_{\dot{q}_i} L}$ and then set

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

- 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:

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

- 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.

Analytical dynamics: a short primer

- 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:

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

- 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.

Analytical dynamics: a short primer

- To determine the classical Hamiltonian H from the Lagrangian, first obtain the **canonical momentum** $\boxed{p_i = \partial_{\dot{q}_i} L}$ and then set

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

- 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:

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

- 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.

Analytical dynamics: a short primer

- To determine the classical Hamiltonian H from the Lagrangian, first obtain the **canonical momentum** $\boxed{p_i = \partial_{\dot{q}_i} L}$ and then set

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

- 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:

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

- 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.

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 specifed 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:

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

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

- 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 specifed 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:

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

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

- 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 specifed 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:

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

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

- 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 × 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 specifed 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:

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

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

- 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

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

$$H = \sum_i \underbrace{(mv_i + qA_i)}_{=p_i} v_i - \underbrace{\left(\frac{1}{2}m\mathbf{v}^2 - q\varphi + q\mathbf{v}\cdot\mathbf{A}\right)}_{=L(\dot{q}_i, q_i)} = \frac{1}{2}m\mathbf{v}^2 + q\varphi$$

- To determine classical equations of motion, H must be expressed solely in terms of coordinates and canonical momenta, $\mathbf{p} = m\mathbf{v} + q\mathbf{A}$

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

- 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

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

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:

$$H = \sum_i \underbrace{(mv_i + qA_i)}_{=p_i} v_i - \underbrace{\left(\frac{1}{2}m\mathbf{v}^2 - q\varphi + q\mathbf{v}\cdot\mathbf{A}\right)}_{=L(\dot{q}_i, q_i)} = \frac{1}{2}m\mathbf{v}^2 + q\varphi$$

- To determine classical equations of motion, H must be expressed solely in terms of coordinates and canonical momenta, $\mathbf{p} = m\mathbf{v} + q\mathbf{A}$

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

- 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

$$\boxed{m\ddot{x} = \mathbf{F} = q\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right)}$$

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:

$$H = \sum_i \underbrace{(mv_i + qA_i)}_{= p_i} v_i - \underbrace{\left(\frac{1}{2}m\mathbf{v}^2 - q\varphi + q\mathbf{v}\cdot\mathbf{A}\right)}_{= L(\dot{q}_i, q_i)} = \frac{1}{2}m\mathbf{v}^2 + q\varphi$$

- To determine classical equations of motion, H must be expressed solely in terms of coordinates and canonical momenta, $\mathbf{p} = m\mathbf{v} + q\mathbf{A}$

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

- 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

$$\boxed{m\ddot{x} = \mathbf{F} = q\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right)}$$

Lessons from classical dynamics

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

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

- 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, $\mathbf{p} \to \hat{\mathbf{p}} = -i\hbar\nabla$, $\mathbf{x} \to \hat{\mathbf{x}}$ 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

$$\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} + \nabla\Lambda, \qquad \varphi \mapsto \varphi' = \varphi - \partial_t\Lambda$$

  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, $\mathbf{p} \to \hat{\mathbf{p}} = -i\hbar\nabla$, $\mathbf{x} \to \hat{\mathbf{x}}$ 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

$$\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} + \nabla\Lambda, \qquad \varphi \mapsto \varphi' = \varphi - \partial_t\Lambda$$

  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, $\mathbf{p} \to \hat{\mathbf{p}} = -i\hbar\nabla$, $\mathbf{x} \to \hat{\mathbf{x}}$ 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

$$\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} + \nabla\Lambda, \qquad \varphi \mapsto \varphi' = \varphi - \partial_t\Lambda$$

  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

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

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

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

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

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

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

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

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

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

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

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

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 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**,

$$\frac{q^2}{2m}\mathbf{A}^2 = \frac{q^2}{8m}(\mathbf{x}\times\mathbf{B})^2 = \frac{q^2}{8m}\left(\mathbf{x}^2\mathbf{B}^2 - (\mathbf{x}\cdot\mathbf{B})^2\right) = \frac{q^2B^2}{8m}(x^2+y^2)$$

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, $\mathbf{A}(\mathbf{x}) = -\frac{1}{2}\mathbf{x}\times\mathbf{B}$ (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**,

$$\frac{q^2}{2m}\mathbf{A}^2 = \frac{q^2}{8m}(\mathbf{x}\times\mathbf{B})^2 = \frac{q^2}{8m}\left(\mathbf{x}^2\mathbf{B}^2 - (\mathbf{x}\cdot\mathbf{B})^2\right) = \frac{q^2B^2}{8m}(x^2+y^2)$$

Quantum mechanics of particle in a uniform field

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

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

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

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

  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

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

- 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,

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

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

- When compared with Coulomb energy scale,

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

where $\alpha = \frac{e^2}{4\pi\epsilon_0}\frac{1}{\hbar c} \simeq \frac{1}{137}$ denotes fine structure constant, paramagnetic term effects only a small perturbation.

Atomic hydrogen in uniform field

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

- 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,

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

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

- When compared with Coulomb energy scale,

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

where $\alpha = \frac{e^2}{4\pi\epsilon_0}\frac{1}{\hbar c} \simeq \frac{1}{137}$ denotes fine structure constant, paramagnetic term effects only a small perturbation.

Atomic hydrogen in uniform field

$$\hat{H} \simeq -\frac{\hbar^2}{2m}\nabla^2 + \frac{e}{2m}\mathbf{B}\cdot\hat{\mathbf{L}} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$

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

$$\boldsymbol{\mu} = -\frac{e}{2m_e}\hat{\mathbf{L}}$$

- 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 μ set by the **Bohr magneton**,

$$\mu_{\mathrm{B}} = \frac{e\hbar}{2m_e} = 5.79\times10^{-5}\,\mathrm{eV/T}$$

Atomic hydrogen in uniform field

$$\hat{H} \simeq -\frac{\hbar^2}{2m}\nabla^2 + \frac{e}{2m}\mathbf{B}\cdot\hat{\mathbf{L}} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$

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

$$\boldsymbol{\mu} = -\frac{e}{2m_e}\hat{\mathbf{L}}$$

- 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 $\boldsymbol{\mu}$ set by the **Bohr magneton**,

$$\mu_{\rm B} = \frac{e\hbar}{2m_e} = 5.79\times 10^{-5}\,\mathrm{eV/T}$$

Atomic hydrogen in uniform field

$$\hat{H} \simeq -\frac{\hbar^2}{2m}\nabla^2 + \frac{e}{2m}\mathbf{B}\cdot\hat{\mathbf{L}} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$

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

$$\boldsymbol{\mu} = -\frac{e}{2m_e}\hat{\mathbf{L}}$$

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

- Since $\langle \hat{L}\rangle \sim \hbar$, scale of μ set by the **Bohr magneton**,

$$\mu_{\mathrm{B}} = \frac{e\hbar}{2m_e} = 5.79\times 10^{-5}\,\mathrm{eV/T}$$

Atomic hydrogen in uniform field

$$\hat{H} \simeq -\frac{\hbar^2}{2m}\nabla^2 + \frac{e}{2m}\mathbf{B}\cdot\hat{\mathbf{L}} - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$

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

$$\boldsymbol{\mu} = -\frac{e}{2m_e}\hat{\mathbf{L}}$$

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

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

$$\mu_{\rm B} = \frac{e\hbar}{2m_e} = 5.79\times 10^{-5}\,{\rm eV/T}$$

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,

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

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

$$E_{n\ell m} = -\frac{1}{n^2}\mathrm{Ry} + \hbar\omega_{\mathrm{L}} m$$

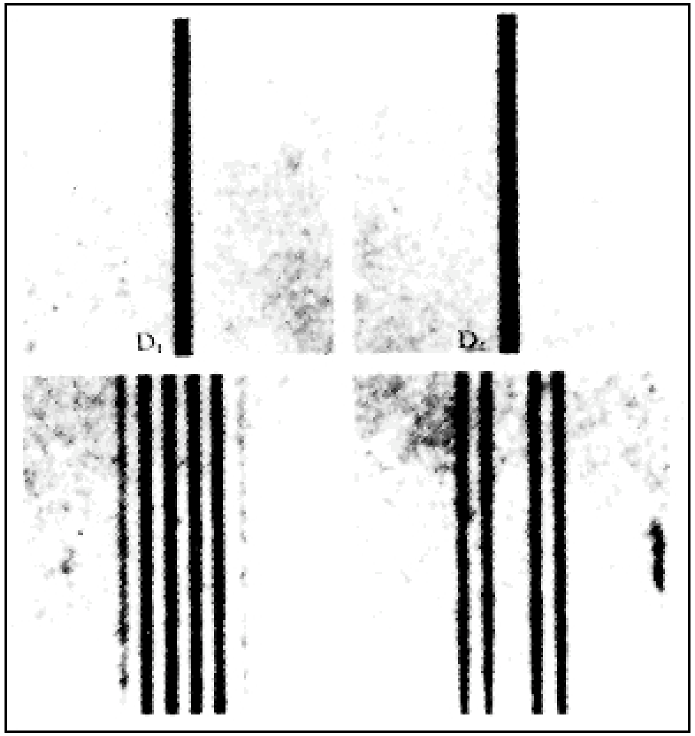
where $\omega_{\mathrm{L}} = \frac{eB}{2m}$ denotes the **Larmor frequency**.

- (Without spin contribution) uniform magnetic field $\rightsquigarrow$ splitting of $(2\ell + 1)$-fold degeneracy with multiplets separated by $\hbar\omega_{\mathrm{L}}$.

Normal Zeeman effect: experiment

- Experiment shows Zeeman splitting of spectral lines...

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



P. Zeeman, Nature **55**, 347 (1897).

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

Gauge invariance

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

- 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

$$\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} + \nabla\Lambda, \qquad \varphi \mapsto \varphi' = \varphi - \partial_t\Lambda$$

where $\Lambda(\mathbf{x}, t)$ 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,

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

but probability density, $|\psi'(\mathbf{x}, t)|^2 = |\psi(\mathbf{x}, t)|^2$ is conserved.

Gauge invariance

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

- 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

$$\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} + \nabla\Lambda, \qquad \varphi \mapsto \varphi' = \varphi - \partial_t\Lambda$$

where $\Lambda(\mathbf{x},t)$ 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,

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

but probability density, $|\psi'(\mathbf{x},t)|^2 = |\psi(\mathbf{x},t)|^2$ is conserved.

Gauge invariance

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

- **Proof:** using the identity

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

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

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

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

- **Proof:** using the identity

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

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

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

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

- **Proof:** using the identity

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

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

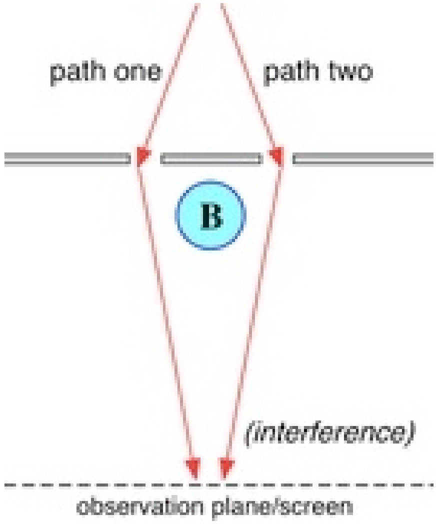
Similarly

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

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

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



- Consider particle (charge q) travelling along path, P, in which the magnetic field, $\mathbf{B} = 0$.
- However, $\mathbf{B} = 0 \not\Rightarrow \mathbf{A} = 0$:
  any $\Lambda(\mathbf{x})$ such that $\mathbf{A} = \nabla\Lambda$ leads to $\mathbf{B} = 0$.
- In traversing path, wavefunction acquires phase
  $$\phi = \frac{q}{\hbar}\int_P \mathbf{A}\cdot d\mathbf{x}.$$
- If we consider two separate paths P and P' with same initial and final points, relative phase of the wavefunction,

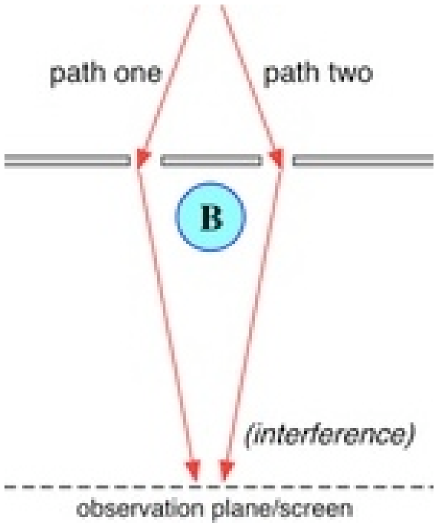
$$\Delta\phi = \frac{q}{\hbar}\int_P \mathbf{A}\cdot d\mathbf{x} - \frac{q}{\hbar}\int_{P'} \mathbf{A}\cdot d\mathbf{x} = \frac{q}{\hbar}\oint \mathbf{A}\cdot d\mathbf{x} \stackrel{\text{Stokes}}{=} \frac{q}{\hbar}\int_A \mathbf{B}\cdot d^2\mathbf{x}$$

where $\int_A$ runs over area enclosed by loop formed from P and P'

Gauge invariance: physical consequences

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

- Consider particle (charge q) travelling along path, P, in which the magnetic field, $\mathbf{B}=0$.
- However, $\mathbf{B}=0 \not\Rightarrow \mathbf{A}=0$:
  any $\Lambda(\mathbf{x})$ such that $\mathbf{A}=\nabla\Lambda$ leads to $\mathbf{B}=0$.
- In traversing path, wavefunction acquires phase
  $$\phi = \frac{q}{\hbar}\int_P \mathbf{A}\cdot d\mathbf{x}.$$



- If we consider two separate paths P and P' with same initial and final points, relative phase of the wavefunction,

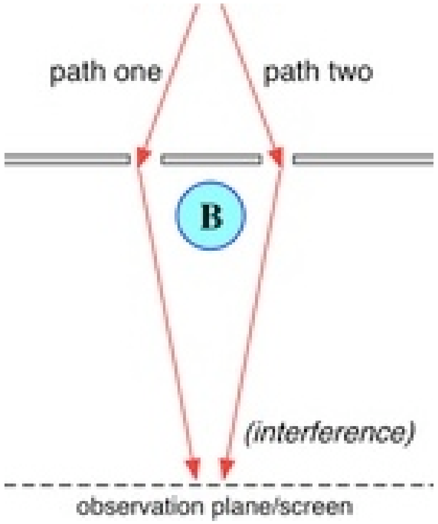
$$\Delta\phi = \frac{q}{\hbar}\int_P \mathbf{A}\cdot d\mathbf{x} - \frac{q}{\hbar}\int_{P'} \mathbf{A}\cdot d\mathbf{x} = \frac{q}{\hbar}\oint \mathbf{A}\cdot d\mathbf{x} \overset{\text{Stokes}}{=} \frac{q}{\hbar}\int_A \mathbf{B}\cdot d^2\mathbf{x}$$

where $\int_A$ 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,

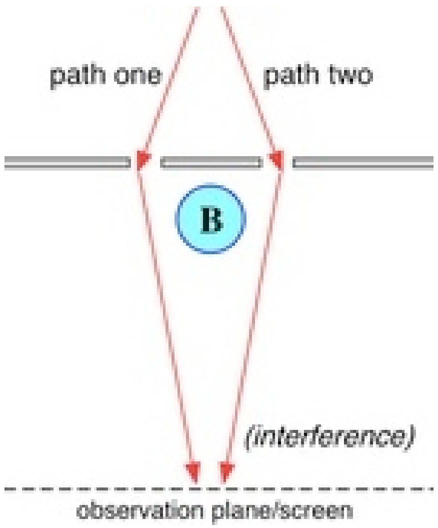


$$\Delta\phi = \frac{q}{\hbar}\times \text{magnetic flux through area}$$

- 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

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



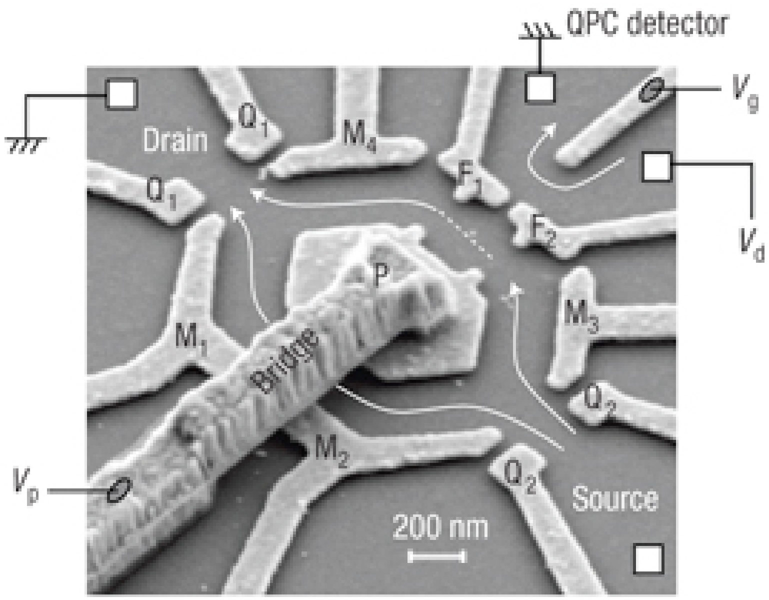
- i.e. for paths P and P', wavefunction components acquire relative phase difference,

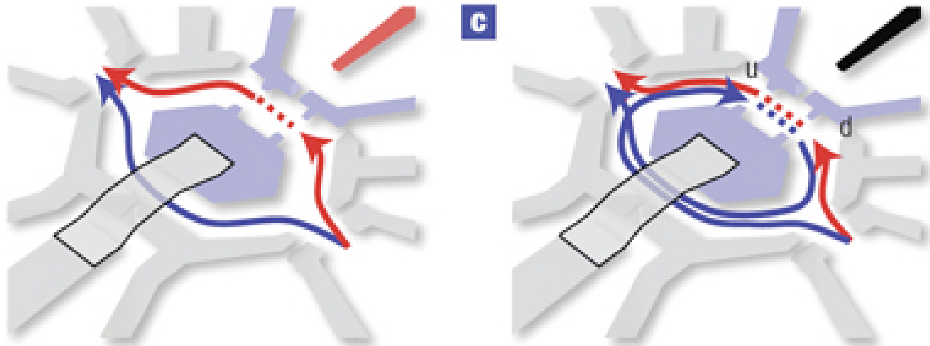
$$\Delta\phi = \frac{q}{\hbar} \times \text{magnetic flux through area}$$

- If paths enclose region of non-vanishing field, *even if* **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.

Aharanov-Bohm effect: example I

- 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.



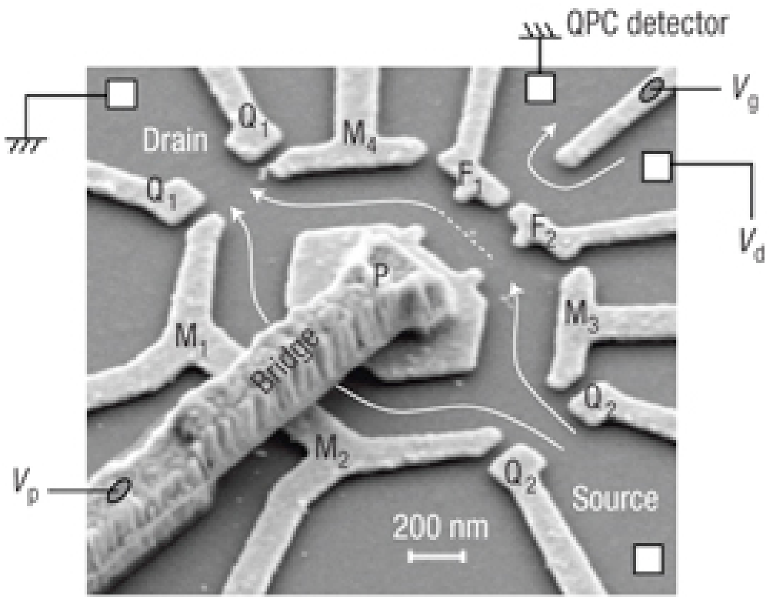


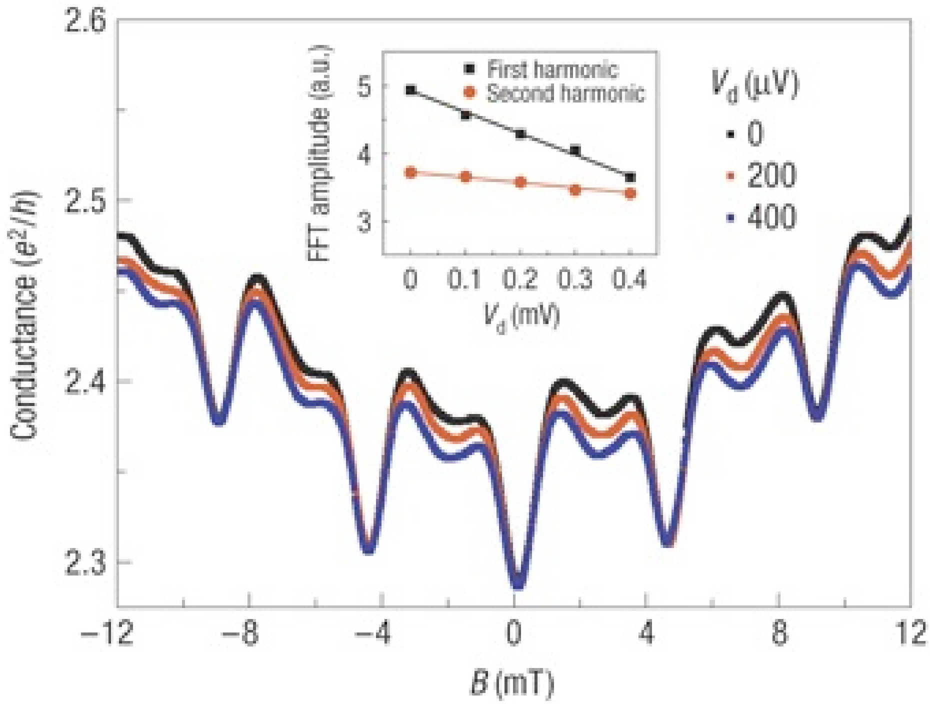
First harmonic (h/e oscillation) path information

Second harmonic ($h/2e$ oscillation) no path information

Aharanov-Bohm effect: example I

- 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.

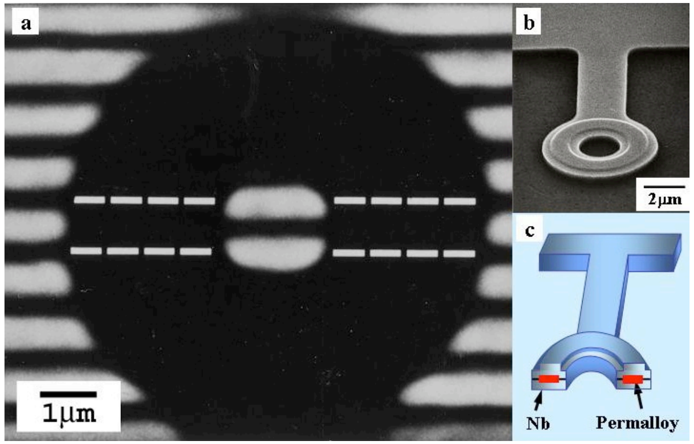




Aharanov-Bohm effect: example II

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 $h/2e$.
- 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 π.



Tonomura *et al.*, 1986

- 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 a static electromagnetic field,

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

- we derived the quantum Hamiltonian,

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

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

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

Summary: charged particle in a field

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

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

- 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**,

$$E_{n\ell m} = -\frac{1}{n^2}\mathrm{Ry} + \mu_\mathrm{B} B m$$

- However, when diamagnetic term $O(B^2 n^3)$ competes with Coulomb energy scale $-\frac{\mathrm{Ry}}{n^2}$ 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, $\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} + \nabla\Lambda$, $\varphi \mapsto \varphi' = \varphi - \partial_t\Lambda$, wavefunction acquires additional phase,

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

- $\rightsquigarrow$ **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 $\Rightarrow \frac{1}{n}\frac{h}{e}$ oscillations.