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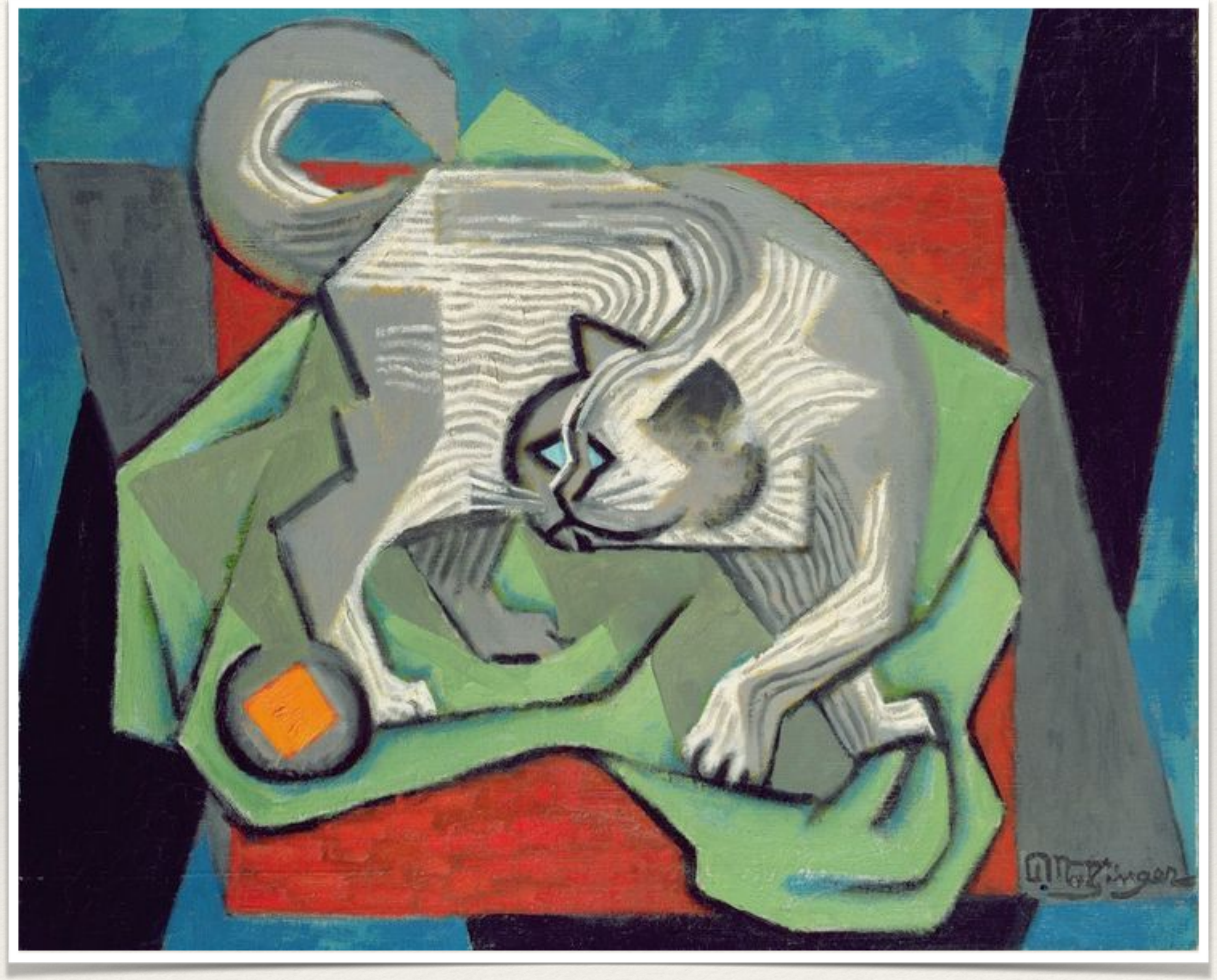
Quantum Mechanics

Lecture 14

Quiz 3;
Quantum Hamiltonian for the EM field;
Zeeman splitting;
Aharonov-Bohm effect.



Classical electrodynamics

The classical Lorentz force law is a velocity-dependent force

$$\mathbf{F} = q\left(\mathbf{E} + \frac{\mathbf{v} \times \mathbf{B}}{c}\right) \qquad \text{(classical Lorentz force)}$$

This is **not a conservative force**, i.e. it cannot be derived from a potential. Deriving the quantum Hamiltonian for the EM field is therefore delicate.

Recall that the **B** and **E** fields can be expressed in terms of a scalar and vector potential, ϕ and **A**:

$$\mathbf{B} = \nabla \times \mathbf{A} \qquad \mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}$$

The Lagrangian, from which we derive equations of motion, is given by:

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

Classical equations of motion

The classical equations of motion are given by the Euler-Lagrange equations. The Hamiltonian formulation, with $\dot{x}_i = v_i$, has canonical momentum:

$$p_i = \frac{\partial L}{\partial \dot{x}_i} = mv_i + \frac{q}{c}A_i$$

Thus, **canonical momentum is not just *mv***! The classical Hamiltonian is

$$\begin{aligned} H(x_i, p_i) = \sum_i p_i \dot{x}_i - L(x_i, \dot{x}_i) &= \sum_i \left(mv_i + \frac{q}{c}A_i \right) v_i - \frac{1}{2}mv^2 + q\phi - \frac{q}{c}\mathbf{v} \cdot \mathbf{A} \\ &= \frac{1}{2}mv^2 + q\phi \\ &= \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A} \right)^2 + q\phi \end{aligned}$$

Quantum Hamiltonian

Thus we expect that the correct quantum Hamiltonian is obtained by:

$$H = \frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A}(\hat{\mathbf{r}}, t)\right)^2 + q\phi(\hat{\mathbf{r}}, t)\,, \qquad \hat{\mathbf{p}} = -i\hbar\nabla\,, \qquad [\hat{x}_j, \hat{p}_k] = i\hbar\delta_{jk}$$

However, in the presence of the **B** field, **velocities don't commute**:

$$m^2[v_j, v_k] = [mv_j, mv_k] = \left[-i\hbar\frac{\partial}{\partial x_j} - \frac{q}{c}A_j, -i\hbar\frac{\partial}{\partial x_k} - \frac{q}{c}A_k\right] = \frac{i\hbar q}{c}\sum_i \epsilon_{ijk}B_i$$

Let's expand the square:

$$H = \frac{-\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{2mc}\big(\mathbf{A}\cdot\nabla + \nabla\cdot\mathbf{A}\big) + \frac{q^2}{2mc^2}\mathbf{A}^2 + q\phi$$

Gauge transformations

We can simplify this Hamiltonian be a careful choice of gauge.

$$H = \frac{-\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{2mc}\left(\mathbf{A}\cdot\nabla + \nabla\cdot\mathbf{A}\right) + \frac{q^2}{2mc^2}\mathbf{A}^2 + q\phi$$

Any transformation on the gauge fields of the following form leaves **B**, **E** alone:

Gauge transformation $$A \to A + \nabla\Lambda \qquad \phi \to \phi - \frac{1}{c}\frac{\partial\Lambda}{\partial t}$$

$$B = \nabla \times A \qquad E = -\nabla\phi - \frac{1}{c}\frac{\partial A}{\partial t}$$ **Gauge invariant**

The **Coulomb gauge** is a choice that sets: $\nabla\cdot\mathbf{A} = 0 \;\Rightarrow (\nabla\cdot\mathbf{A})f + A\cdot\nabla f = A\cdot\nabla f$

In the Coulomb gauge the Hamiltonian becomes:

$$H = \frac{-\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{mc}\mathbf{A}\cdot\nabla + \frac{q^2}{2mc^2}\mathbf{A}^2 + q\phi$$

Constant B-field (Coulomb gauge)

The result is:

$$H = \frac{-\hbar^2}{2m}\nabla^2 + \underset{\uparrow}{\frac{i\hbar q}{mc}\mathbf{A}\cdot\nabla} + \underset{\nwarrow}{\frac{q^2}{2mc^2}\mathbf{A}^2} + q\phi$$

"paramagnetic term" "diamagnetic term"

Let's consider an example with constant **B**-field.

The vector potential can be expressed as: $\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}$ (check: $\nabla\times\mathbf{A} = \mathbf{B}$)

Paramagnetic term:

$$\frac{i\hbar q}{mc}\mathbf{A}\cdot\nabla = \frac{i\hbar q}{2mc}(\mathbf{B}\times\mathbf{r})\cdot\nabla$$

$$= \frac{i\hbar q}{2mc}(\mathbf{r}\times\nabla)\cdot\mathbf{B}$$

$$= \frac{-q}{2mc}\mathbf{L}\cdot\mathbf{B}$$

AM coupled to B field

Diamagnetic term:

$$\frac{q^2}{2mc^2}\mathbf{A}^2 = \frac{q^2}{8mc^2}\left(r^2B^2 - (\mathbf{r}\cdot\mathbf{B})^2\right)$$

$$\rightarrow \frac{q^2B^2}{8mc^2}\left(x^2+y^2\right)$$

If B field is along z-axis.

Zeeman splitting

The ratio of the dia- and paramagnetic terms is tiny in any case where an electron is bound to an atom and when B is less than a few Tesla.

$$\langle x^2+y^2\rangle \sim a_0^2\,, \quad \langle L_z\rangle \sim \hbar \qquad\qquad \frac{\frac{q^2B^2}{8mc^2}\langle x^2+y^2\rangle}{\frac{q}{2mc}B\langle L_z\rangle} = \frac{ea_0^2B^2}{4c\hbar B} = 10^{-6}B/T$$

The paramagnetic term is small compared to the Coulomb energy scale:

$$V \sim \frac{e^2}{\langle r\rangle}\,, \quad \langle r\rangle \sim a_0 \qquad\qquad \frac{e\hbar B/2mc}{e^2/a_0} = 10^{-5}B/T$$

We therefore want to solve:

$$H = H_0 + H_1\,, \qquad H_0 = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{e^2}{|\hat{\mathbf{r}}|}\,, \qquad H_1 = \frac{eB}{2mc}L_z$$

Zeeman splitting

Notice that L_z still commutes with H, so m_l is still a good quantum number:

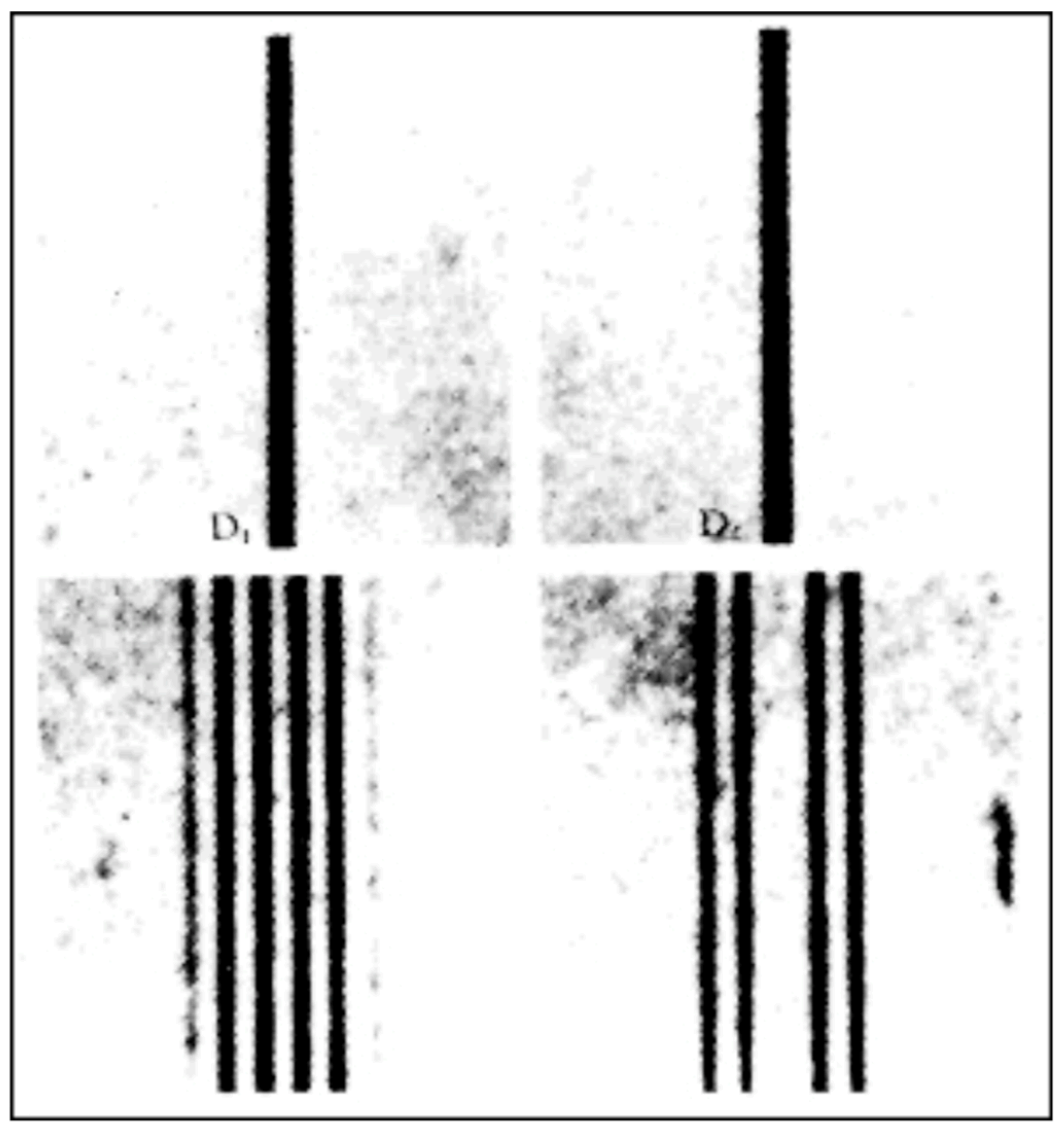
$$H = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{e^2}{|\hat{\mathbf{r}}|} + \frac{eB}{2mc}L_z$$

The new eigenstates are unchanged.

$$\langle n, l, m_l | \frac{eB}{2mc} L_z | n, l, m_l \rangle = \frac{eBm_l\hbar}{2mc} = \hbar\omega_L m_l$$

$$\omega_L = \frac{eB}{2mc}$$ Larmor frequency

Magnetic field leads to splitting of degeneracy of the (2*l*+1) states in the *l* subspace.



Splitting of Sodium D lines, from Zeeman's original paper (1897)

Consequences of gauge invariance

Gauge transformations change the wavefunction, but not in an observable way:

$$A' = A + \nabla \Lambda$$
$$\phi' = \phi - \frac{1}{c}\frac{\partial \Lambda}{\partial t}$$

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

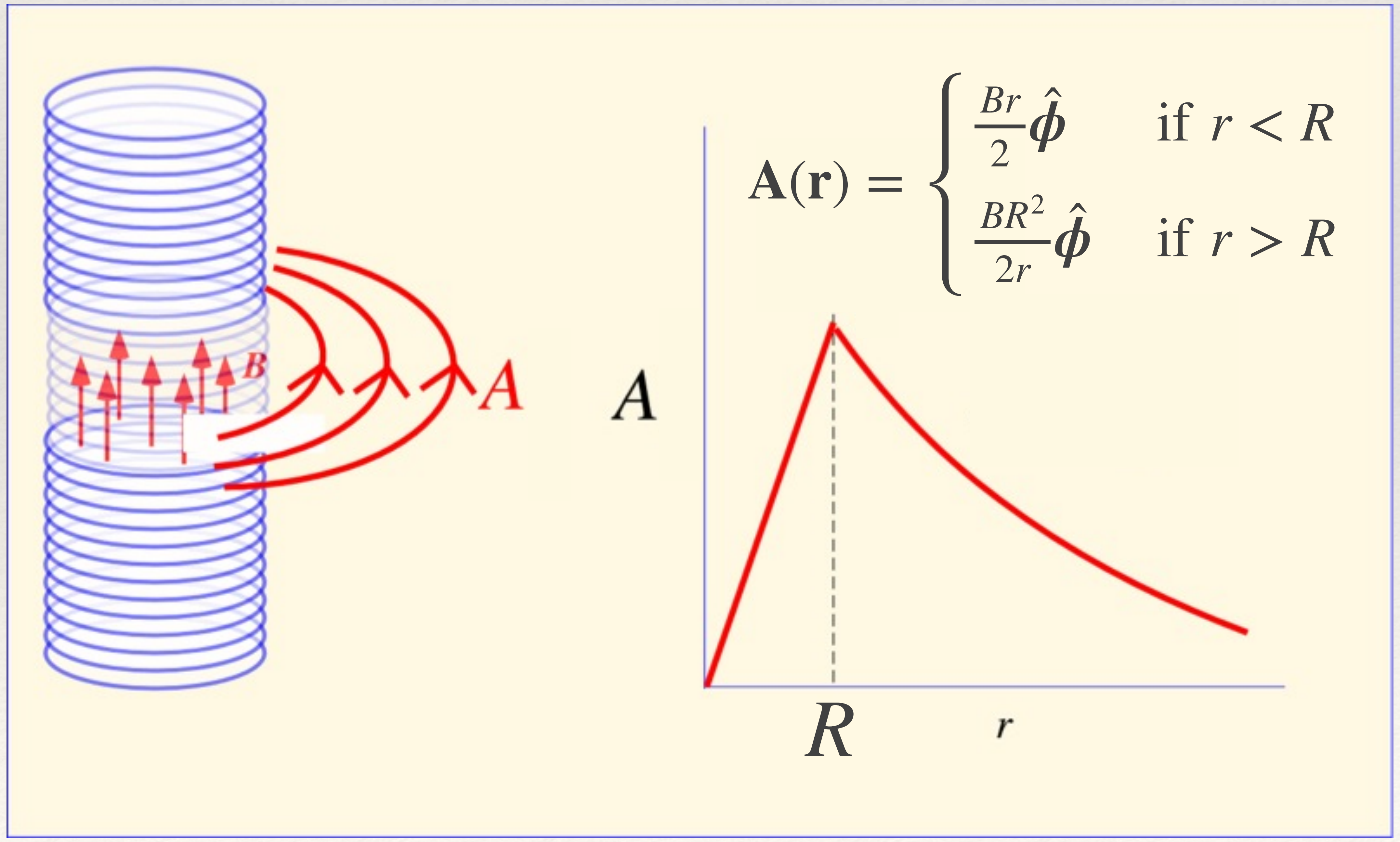
Overall phase

All probabilities are invariant:

$$|\psi'(\mathbf{r}, t)|^2 = |\psi(\mathbf{r}, t)|^2$$

Of course, we can have non-zero **A** even if the magnetic field **B** is zero. Consider a solenoid:

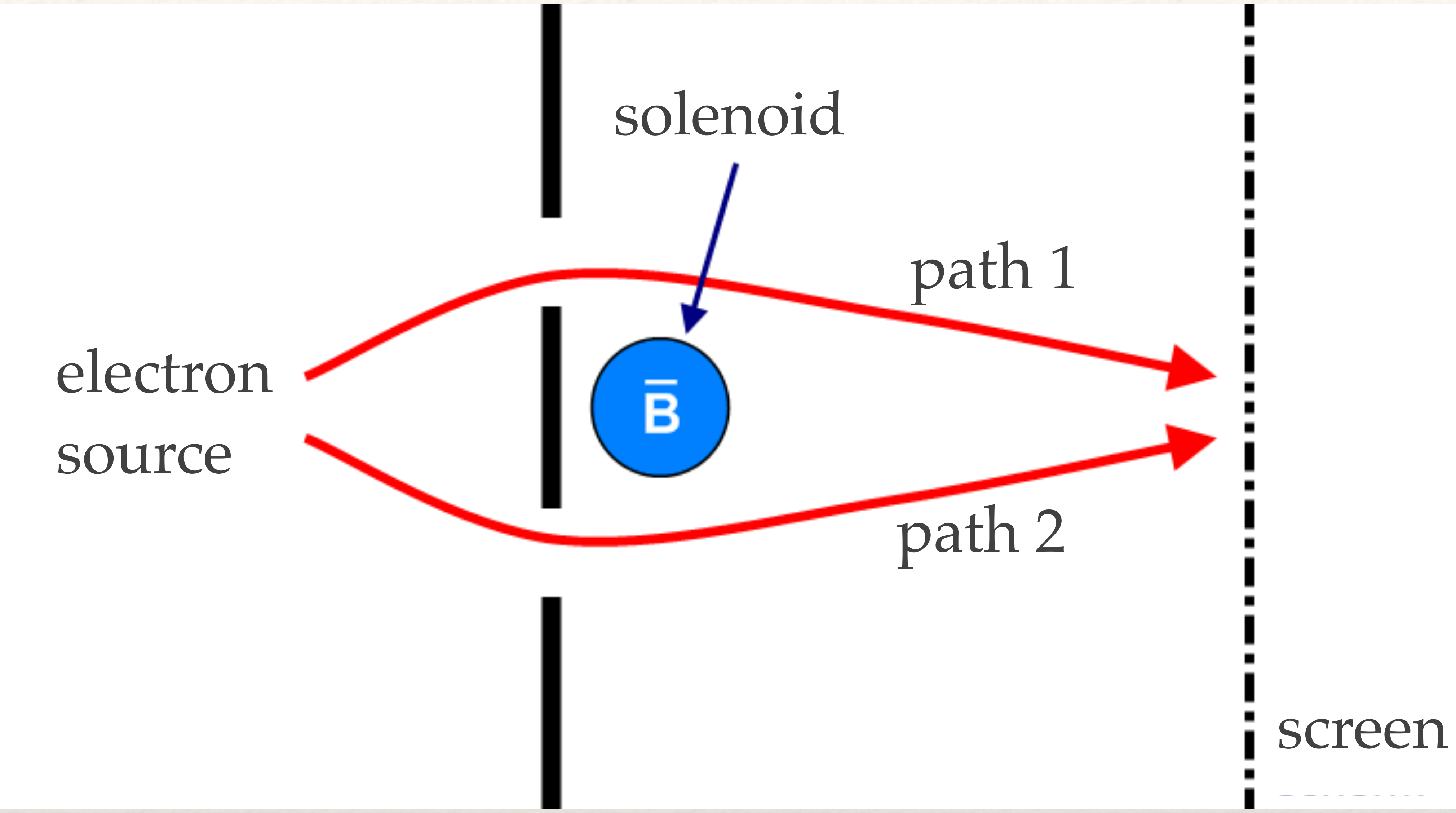
$$\mathbf{B}(\mathbf{r}) = \begin{cases} B\hat{\mathbf{z}} & \text{if } r < R \\ 0 & \text{if } r > R \end{cases}$$



$$\mathbf{A}(\mathbf{r}) = \begin{cases} \frac{Br}{2}\hat{\boldsymbol{\phi}} & \text{if } r < R \\ \frac{BR^2}{2r}\hat{\boldsymbol{\phi}} & \text{if } r > R \end{cases}$$

Aharonov-Bohm effect

Consider the following double slit experiment:



With each path P, an electron will pick up a different phase factor that depends on the vector potential:

$$\gamma_P = \frac{e}{\hbar c}\int_P \mathbf{A}\cdot\mathrm{d}\mathbf{r} \qquad \psi \to \exp(i\gamma_P)\psi$$

(note: this is a real number.)

The **phase difference** is observable as interference fringes on the screen!

$$\Delta\gamma = \frac{e}{\hbar c}\int_{P_1}\mathbf{A}\cdot\mathrm{d}\mathbf{r} - \frac{e}{\hbar c}\int_{P_2}\mathbf{A}\cdot\mathrm{d}\mathbf{r} = \frac{e}{\hbar c}\oint_{P_1-P_2}\mathbf{A}\cdot\mathrm{d}\mathbf{r} = \frac{e}{\hbar c}\int_{\mathrm{A}(P)}\mathbf{B}\cdot\mathrm{d}^2\mathbf{r}$$

$$\Rightarrow \quad \Delta\gamma = \frac{e}{\hbar c}\Phi$$

Phase shift depends on the flux Φ through the area enclosed by the paths.