Charged Particles in Electromagnetic Fields

Quantum Mechanics II

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- Starting from the Maxwell equation: $\nabla \cdot \mathbf{B} = 0$, we deduce that $\mathbf{B}$ can locally be expressed as the curl of a vector potential $\mathbf{A}$:

$$\mathbf{B} = \nabla \times \mathbf{A}.$$

- The second source-free Maxwell equation is:

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

- Substituting $\mathbf{B} = \nabla \times \mathbf{A}$ and rearranging, we get:

$$\nabla \times \left(\mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} \right) = 0.$$

- Since the curl of a field vanishes, the field can be expressed as the gradient of a scalar:

$$\mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} = -\nabla \Phi,$$

  where Φ is the scalar potential. The electric field $\mathbf{E}$ can be expressed:

$$\mathbf{E} = -\nabla \Phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}.$$

Gauge Transformations and Electromagnetic Potentials

- Potentials are not uniquely defined. They can be transformed without altering the resulting fields **E** and **B**. For a scalar function $\Lambda(\mathbf{x}, t)$, the transformations are:

$$\mathbf{A}' = \mathbf{A} + \nabla\Lambda, \quad \Phi' = \Phi - \frac{1}{c}\frac{\partial\Lambda}{\partial t}.$$

- The primed potentials yield the same electric and magnetic fields:

$$\mathbf{E}(\mathbf{A}', \Phi') = \mathbf{E}(\mathbf{A}, \Phi), \quad \mathbf{B}(\mathbf{A}', \Phi') = \mathbf{B}(\mathbf{A}, \Phi).$$

- An electromagnetic field configuration can be imagined as an **equivalence class** of potentials, all of which differ from each other by gauge transformations and with any element of the class a valid representative.
- Implications of this equivalence:
  - Different sets of potentials $(\mathbf{A}, \Phi)$ and $(\mathbf{A}', \Phi')$ can produce identical fields $(\mathbf{E}, \mathbf{B})$, but may not be gauge-equivalent. The Aharonov-Bohm effect demonstrates how potentials can have physical significance, even when fields are identical.
  - Consider the fields $(\mathbf{E}, \mathbf{B})$ that satisfy Maxwell's equations. Suppose, however, that there are no potentials $(\mathbf{A}, \Phi)$ from which $(\mathbf{E}, \mathbf{B})$ arise as usual. We must then conclude that $(\mathbf{E}, \mathbf{B})$, despite satisfying Maxwell's equations, are not valid fields.

Schrödinger Equation with Electromagnetic Potentials

Schrödinger Equation with Electromagnetic Potentials

To incorporate electromagnetic fields in the Schrödinger equation for a particle with charge q:

- Adding to the Hamiltonian a term $q\Phi(\hat{\mathbf{x}}, t)$
- The canonical momentum operator $\hat{\mathbf{p}}$ is replaced as (**minimal coupling**):

$$\hat{\mathbf{p}} \to \hat{\mathbf{p}} - \frac{q}{c}\mathbf{A}(\hat{\mathbf{x}}, t).$$

- Here, $\mathbf{A}(\hat{\mathbf{x}}, t)$ is the vector potential, and $\Phi(\hat{\mathbf{x}}, t)$ is the scalar potential.
- The basic commutation relations are not be changed:

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}, \quad \hat{\mathbf{p}} = -i\hbar\nabla \text{ (in coordinate space)}.$$

Schrödinger Equation with Electromagnetic Potentials (cont.)

The Hamiltonian for minimal coupling becomes:

$$\hat{H} = \frac{1}{2m}\left(\hat{\mathbf{p}} - \frac{q}{c}\mathbf{A}(\hat{\mathbf{x}}, t)\right)^2 + q\Phi(\hat{\mathbf{x}}, t).$$

In coordinate space, this is expressed as:

$$\hat{H} = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{q}{c}\mathbf{A}(\mathbf{x}, t)\right)^2 + q\Phi(\mathbf{x}, t).$$

The corresponding Schrödinger equation for the wave function $\Psi(\mathbf{x}, t)$ is:

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{q}{c}\mathbf{A}(\mathbf{x}, t)\right)^2 + q\Phi(\mathbf{x}, t)\right]\Psi.$$

Gauge Invariance in the Schrödinger Equation

Here is the way we state the gauge invariance. For gauge-transformed potentials:

$$\mathbf{A}' = \mathbf{A} + \nabla\Lambda, \quad \Phi' = \Phi - \frac{1}{c}\frac{\partial\Lambda}{\partial t},$$

the wave function transforms as:

$$\Psi' = \exp\left(\frac{iq\Lambda}{\hbar c}\right)\Psi.$$

Substituting these transformations, the Schrödinger equation remains unchanged:

$$i\hbar\frac{\partial\Psi'}{\partial t} = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{q}{c}\mathbf{A}'\right)^2 + q\Phi'\right]\Psi'.$$

The transformation of the wave function can be expressed as:

$$U(\Lambda) = \exp\left(\frac{iq\Lambda}{\hbar c}\right), \quad \Psi' = U(\Lambda)\Psi.$$

This ensures that the probability density $\rho(\mathbf{x}, t) = \Psi^*(\mathbf{x}, t)\Psi(\mathbf{x}, t)$ is invariant under gauge transformations.

Gauge-Covariant Operators

In this theory, we aim to ensure that the result of measurements does not depend on the choice of gauge. Not all Hermitian operators achieve this, so we consider a class of operators called **gauge-covariant operators**, which yield gauge-invariant measurements.
Under a gauge transformation with parameter $\Lambda(x, t)$, an operator $\mathcal{O}[\Phi, \mathbf{A}]$, written as $\mathcal{O}$ for brevity, transforms into a new operator $\mathcal{O}'$ given by:

$$\text{Gauge transformation:} \quad \mathcal{O}[\Phi, \mathbf{A}] \to \mathcal{O}'[\Phi', \mathbf{A}'].$$

Definition of Gauge-Covariant Operators: Physical observables are Hermitian operators $\mathcal{O}$ that are **gauge covariant**—namely, they satisfy the condition:

$$\mathcal{O}' = U(\Lambda)\mathcal{O}U^{-1}(\Lambda).$$

Or more explicitly:

$$\mathcal{O}'[\Phi', \mathbf{A}'] = U(\Lambda)\mathcal{O}[\Phi, \mathbf{A}]U^{-1}(\Lambda).$$

Gauge-Invariant Measurements

We now demonstrate that **gauge-covariant observables** yield **gauge-invariant measurements**.
Suppose $|\Psi\rangle$ is an eigenstate of a gauge-covariant operator $\mathcal{O}$ with eigenvalue $\lambda_{\mathcal{O}}$:

$$\mathcal{O}|\Psi\rangle = \lambda_{\mathcal{O}}|\Psi\rangle.$$

Under a gauge transformation, we find that:

$$\mathcal{O}'|\Psi'\rangle = U\mathcal{O}U^{-1}U|\Psi\rangle = U\mathcal{O}|\Psi\rangle = U\lambda_{\mathcal{O}}|\Psi\rangle = \lambda_{\mathcal{O}}|\Psi'\rangle,$$

showing that a measurement with the gauge-transformed operator $\mathcal{O}'$ on the gauge-transformed state $|\Psi'\rangle$ gives the same result.
Similarly, we verify that the expectation value of a gauge-covariant observable $\mathcal{O}$ is gauge-invariant:

$$\langle\Psi'|\mathcal{O}'|\Psi'\rangle = \langle\Psi|U^{-1}(U\mathcal{O}U^{-1})U|\Psi\rangle = \langle\Psi|\mathcal{O}|\Psi\rangle.$$

This establishes that both eigenvalues and expectation values of gauge-covariant observables remain unchanged under a gauge transformation, ensuring gauge invariance of physical measurements.

Heisenberg Picture

This picture incorporates the time dependence of states into the operators.

- Given a Schrödinger operator $\hat{A}_S$, the corresponding Heisenberg operator $\hat{A}_H(t)$ is defined as:

$$\hat{A}_H(t) = U^\dagger(t)\hat{A}_S U(t),$$

  where $U(t)$ is the unitary time evolution operator, evolving states as $|\Psi(t)\rangle = U(t)|\Psi(0)\rangle$.
- Heisenberg operators satisfy the equations of motion:

$$\frac{d\hat{A}_H(t)}{dt} = \frac{i}{\hbar}[\hat{H}_H(t), \hat{A}_H(t)] + \frac{\partial \hat{A}_H(t)}{\partial t}.$$

- This equation is analogous to classical equations of motion. The additional term arises when $\hat{A}_S$ has explicit time dependence.
- If the Schrödinger Hamiltonian is:

$$\hat{H}_S = H(\hat{\mathbf{x}}, \hat{\mathbf{p}}, A(\hat{\mathbf{x}}, t), \Phi(\hat{\mathbf{x}}, t)),$$

  the Heisenberg Hamiltonian takes the form:

$$\hat{H}_H = H(\hat{\mathbf{x}}_H(t), \hat{\mathbf{p}}_H(t), A(\hat{\mathbf{x}}_H(t), t), \Phi(\hat{\mathbf{x}}_H(t), t)).$$

Heisenberg Velocity Operator and Lorentz Force Law

- The Heisenberg equation of motion for $\hat{\mathbf{x}}_H$ is given by:

$$\frac{d\hat{\mathbf{x}}_{H,i}}{dt} = \frac{i}{\hbar}\left[\hat{H}_H, \hat{\mathbf{x}}_{H,i}\right].$$

- Using the definition $\mathbf{A}_H = \mathbf{A}(\hat{\mathbf{x}}_H, t)$, the commutator is computed as $([AA, B] = A[A, B] + [A, B]A)$:

$$\frac{d\hat{\mathbf{x}}_{H,i}}{dt} = \frac{i}{\hbar}\sum_j \left(\hat{\mathbf{p}}_H - \frac{q}{c}\mathbf{A}_H\right)_j \left[\left(\hat{\mathbf{p}}_H - \frac{q}{c}\mathbf{A}_H\right)_j, \hat{\mathbf{x}}_{H,i}\right].$$

- Simplifying with $[\hat{\mathbf{p}}_{H,j}, \hat{\mathbf{x}}_{H,i}] = -i\hbar\delta_{ij}$, we find:

$$\frac{d\hat{\mathbf{x}}_{H,i}}{dt} = \frac{1}{m}\left(\hat{\mathbf{p}}_H - \frac{q}{c}\mathbf{A}_H\right)_i.$$

- Combining with the previous result, we have the relation:

$$m\hat{\mathbf{v}}_H = \hat{\mathbf{p}}_H - \frac{q}{c}\mathbf{A}_H.$$

- Quantum version of the Lorentz force law

$$m\frac{d\hat{\mathbf{v}}_H}{dt} = q\mathbf{E}_H + \frac{q}{c}\frac{1}{2}\left(\hat{\mathbf{v}}_H \times \mathbf{B}_H - \mathbf{B}_H \times \hat{\mathbf{v}}_H\right)$$

Magnetic Fields on a Torus

Magnetic Fields on a Torus

- A two-dimensional torus T^2 is defined by the space (x, y) with the identifications:

$$(x, y) \sim (x + L_x, y), \quad (x, y) \sim (x, y + L_y).$$

- The torus can be visualized as a rectangular region $0 \leq x \leq L_x$ and $0 \leq y \leq L_y$, with periodic boundary conditions.

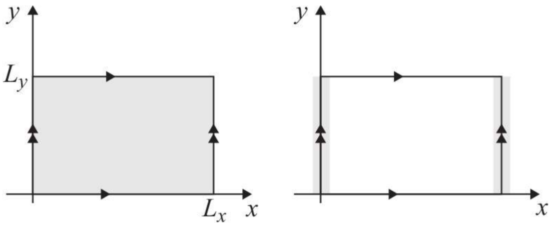

Figure: Left: A two-dimensional torus as a rectangular region with boundaries identified. Right: The candidate gauge potential $A_y(x, y) = B_0 x$ takes different values on the left and right vertical boundaries.

Constant Magnetic Field on a Torus

- Consider a constant magnetic field B_0 along the z-direction on the torus.
- Maxwell's equations for B_0:

$$\nabla \cdot \mathbf{B} = 0, \quad \nabla \times \mathbf{B} = 0.$$

  For point charges with charge q, the magnetic flux $B_0 L_x L_y$ must be quantized in multiples of a flux quantum $\Phi_0 \propto \hbar c/q$.
- With B_0 in the z-direction, we have:

$$B_0 = \partial_x A_y - \partial_y A_x.$$

- A simple solution for the vector potential:

$$A_x(x,y) = 0, \quad A_y(x,y) = B_0 x.$$

- Periodicity conditions for A_y:

$$A_y(x,y) = A_y(x+L_x,y), \quad A_y(x,y) = A_y(x,y+L_y).$$

- The second condition is satisfied, but the first is not.

Periodic Gauge Transformation

- Periodicity is not strictly necessary; gauge transformations allow A_y on the left ($x = 0$) and right ($x = L_x$) vertical boundary lines to differ by a gauge transformation.
- Define $A_y^R(y)$ as A_y on the right boundary $x = L_x$:

$$A_y^R(y) = A_y(x = L_x, y) = B_0 L_x.$$

  Define $A_y^L(y)$ as A_y deduced from $x = 0$:

$$A_y^L(y) = A_y(x = 0, y) = 0.$$

- Gauge transformation ensures:

$$A_y^R(y) = A_y^L(y) + \partial_y \Lambda(x, y).$$

- Solving for $\Lambda(x, y)$:

$$\Lambda(x, y) = B_0 L_x y + f(x),$$

- To maintain periodicity for A_x, set $f(x) = 0$, giving:

$$\Lambda(x, y) = B_0 L_x y.$$

- This gauge parameter is not periodic in this circle.

Periodic Gauge Transformation and Quantization

- The gauge transformations for the potentials and the wave function are written in terms of the phase factor $U(x, y)$:

$$U(x, y) = \exp\left(i\frac{q\Lambda}{\hbar c}\right).$$

- For the wave function, this is manifest as $\Psi' = U\Psi$. For the potentials:

$$\mathbf{A}' = \mathbf{A} + \nabla\Lambda = \mathbf{A} - \frac{i\hbar c}{q}U^{-1}\nabla U,$$

$$\Phi' = \Phi - \frac{1}{c}\frac{\partial\Lambda}{\partial t} = \Phi + \frac{i\hbar}{q}U^{-1}\frac{\partial U}{\partial t}.$$

- The gauge parameter Λ does not need to be periodic; instead, $U(x, y)$ must satisfy periodicity conditions. Using the previously determined $\Lambda(x, y)$:

$$U(x, y) = \exp\left(i\frac{q}{\hbar c}B_0 L_x y\right),$$

- The periodicity in y requires:

$$U(x, y) = U(x, y + L_y) \implies \frac{q}{\hbar c}B_0 L_x L_y = 2\pi n, \quad n \in \mathbb{Z}.$$

- This is the quantization condition: $B_0 L_x L_y = \frac{2\pi\hbar c}{q}n$.

Flux Quantization

- Define the flux of B_0 through the torus as $\Phi_B \equiv B_0 L_x L_y$. The quantization condition can be expressed as:
$$\Phi_B = \frac{2\pi\hbar c}{q} n = \hat{\Phi}_0 n,$$
where we introduced the **flux quantum** $\hat{\Phi}_0$:
$$\hat{\Phi}_0 \equiv \frac{2\pi\hbar c}{q}.$$
- This is the smallest nonzero flux allowed. The magnetic field on the torus must have a flux that is an integer multiple of $\hat{\Phi}_0$, which depends on the charge q of the particle.
- In superconductivity, Cooper pairs of electrons ($q = 2e$) define the magnetic flux quantum Φ_0 (without a hat):
$$\Phi_0 \equiv \frac{2\pi\hbar c}{2e} = \frac{hc}{2e} \approx 2.067 \times 10^{-7}\,\text{gauss} \cdot \text{cm}^2.$$
- The well-known value of Φ_0 allows computation of $\hat{\Phi}_0$ for arbitrary charges q:
$$\hat{\Phi}_0 = \left(\frac{2e}{q}\right) \Phi_0.$$

Landau Levels

Particles in Uniform Magnetic Field: classical results

- Consider a particle of mass m and charge q moving in a constant uniform magnetic field in the z-direction.
- The charged particle undergoes circular motion in the (x, y)-plane with a constant angular velocity, called the **cyclotron frequency**, ω_c.
- Using the Lorentz force and centripetal acceleration, the relation is:

$$q\frac{v}{c}B = m\frac{v^2}{r} \quad \rightarrow \quad \frac{v}{r} = \frac{qB}{mc} = \omega_c.$$

- Larger orbits correspond to higher velocity and greater kinetic energy for the particle.

Particles in Uniform Magnetic Field: Quantum results

- Consider the motion of a particle of mass m and charge q in a constant magnetic field B along the z-direction.
- The **Landau gauge** is given by:

$$\mathbf{A} = (-By, 0, 0), \quad \Phi = 0.$$

- The Hamiltonian becomes:

$$\hat{H} = \frac{1}{2m}\left(\hat{p}_x + q\frac{B}{c}y\right)^2 + \frac{1}{2m}\hat{p}_y^2.$$

- Motion is assumed in the (x, y)-plane, ignoring $\hat{p}_z$.
- Energy eigenstates can be assumed to be $\hat{p}_x$ eigenstates. The wavefunction takes the form:

$$\psi(x, y) = \psi(y)e^{ik_x x}, \quad p_x = \hbar k_x.$$

- The Hamiltonian reduces to:

$$\hat{H}_{k_x} = \frac{1}{2m}\left[\hat{p}_y^2 + \left(\frac{qB}{c}y + \hbar k_x\right)^2\right].$$

Landau Levels (cont.)

- The reduced Hamiltonian is identified as that of a harmonic oscillator in the y-direction:

$$\hat{H}_{k_x} = \frac{1}{2m}\hat{p}_y^2 + \frac{1}{2}m\left(\frac{qB}{mc}\right)^2\left(y - \frac{-\hbar k_x c}{qB}\right)^2.$$

- The frequency of the harmonic oscillator is the cyclotron frequency $\omega_c = \frac{qB}{mc}$, and the equilibrium position is shifted to:

$$y_0 = -\frac{\hbar k_x c}{qB}.$$

- The square of the length scale for a harmonic oscillator is given by:

$$\ell_B^2 = \frac{\hbar}{m\omega_c} = \frac{\hbar c}{qB}.$$

- In terms of the magnetic length ℓ_B, the equilibrium position can be rewritten as:

$$y_0 = -k_x \ell_B^2.$$

- For a harmonic oscillator wavefunction $\psi(y)$ centered at $y_0 > 0$ with $k_x < 0$, the energy eigenstate $\psi(x, y)$ is delocalized in the x-direction, with a width approximately ℓ_B.

Landau Levels (cont.)

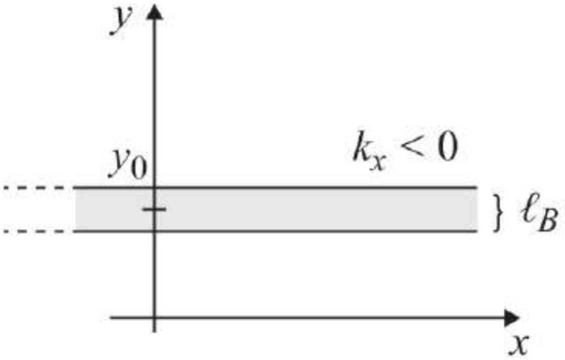

Figure: The wave function $\psi(x, y)$ is supported in a band of width ℓ_B centered at $y_0 > 0$ if $k_x < 0$.

Landau Levels (cont.)

- Using the n-th state ϕ_n of the harmonic oscillator for $\psi(y)$, the wavefunction becomes:

$$\psi(x, y) = \phi_n(y - y_0)e^{ik_x x},$$

  or in ket notation:

$$|\psi\rangle = e^{ik_x x}|n\rangle_y.$$

- The energy E_{n,k_x} of these states is:

$$E_{n,k_x} = \hbar\omega_c \left(\frac{1}{2} + n\right).$$

Comments:

1. Remarkably, the energy does not depend on k_x. Instead, k_x determines the value of y_0. For a fixed n, there is an infinite degeneracy corresponding to the continuum of k_x values. These energy levels are known as **Landau levels**. For $n = 0$, this is the first Landau level; for $n = 1$, the second, and so on.
2. Our Landau-gauge solution can be thought of as the coherent superposition of infinitely many circular orbits centered on the $y = y_0$ line, at all possible values of x.

Landau Levels in a Finite Sample

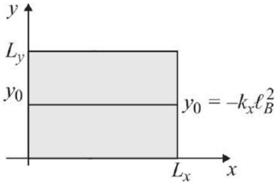

Figure: A finite rectangular sample. The minimum of the harmonic oscillator is shifted by an amount proportional to k_x. With k_x quantized, the degeneracy of the Landau levels is finite.

- For a finite rectangular sample with sides L_x and L_y, the quantization of k_x arises from the periodicity condition:

$$k_x L_x = 2\pi n_x, \quad n_x \in \mathbb{Z}.$$

- To ensure that the states are confined within $0 \leq y_0 \leq L_y$, with $y_0 = -k_x\ell_B^2$, the quantization gives the lowest value of n_x as $-D$, where D is a positive integer.
- Using the condition $y_0 = L_y$, we find:

$$L_y = -k_x\ell_B^2 = \frac{2\pi(-D)}{L_x}\ell_B^2, \quad D = \frac{L_x L_y}{2\pi\ell_B^2}.$$

Degeneracy of Landau Levels

- The degeneracy D corresponds to the number of allowed n_x values, which equals the number of degenerate energy eigenstates in each Landau level.
- Using the relation for $\ell_B^2 = \frac{\hbar c}{qB}$, and with the area $A = L_x L_y$, we can write:

$$D = \frac{AB}{\Phi_0},$$

  where $\Phi_0 = \frac{2\pi\hbar c}{q}$ is the flux quantum.
- This implies:

$$D = \frac{\Phi_B}{\Phi_0},$$

  where $\Phi_B = BA$ is the magnetic flux through the sample.

Example: For a sample area of $1\,\mathrm{cm}^2$ under a 1 gauss magnetic field, the degeneracy is approximately 2.4 million.

The Pauli Equation

Pauli Equation

- The Schrödinger equation for a free particle is:

$$i\hbar\frac{\partial\Psi}{\partial t} = \frac{\hat{\mathbf{p}}^2}{2m}\Psi.$$

- For a spin one-half particle has two degrees of freedom, we expect the following equation:

$$i\hbar\frac{\partial\chi}{\partial t} = \frac{\hat{\mathbf{p}}^2}{2m}\chi, \quad \text{with} \quad \chi = \begin{pmatrix}\chi_1\\ \chi_2\end{pmatrix}.$$

- Here, χ is the Pauli spinor. The Hamiltonian takes the form:

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m}\mathbf{1}_{2\times 2} = \begin{pmatrix}\frac{\hat{\mathbf{p}}^2}{2m} & 0\\ 0 & \frac{\hat{\mathbf{p}}^2}{2m}\end{pmatrix}.$$

- Using minimal coupling $\hat{\mathbf{p}} \to \hat{\mathbf{p}} - \frac{q}{c}\mathbf{A}$, the correct Hamiltonian for a particle with spin coupled to electromagnetic fields is required.
- Rewriting the Hamiltonian using Pauli matrices, recall the identity:

$$(\boldsymbol{\sigma} \cdot \mathbf{a})(\boldsymbol{\sigma} \cdot \mathbf{b}) = \mathbf{a} \cdot \mathbf{b}\, \mathbf{1}_{2\times 2} + i\boldsymbol{\sigma} \cdot (\mathbf{a} \times \mathbf{b}),$$

  valid for arbitrary vector operators $\mathbf{a}$ and $\mathbf{b}$.
- For $\mathbf{a} = \mathbf{b} = \hat{\mathbf{p}}$, and recognizing $\hat{\mathbf{p}} \times \hat{\mathbf{p}} = 0$, we have:

$$(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}})(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}) = \hat{\mathbf{p}}^2 \mathbf{1}_{2\times 2}.$$

- The Hamiltonian can now be written as:

$$\hat{H} = \frac{1}{2m}(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}})(\boldsymbol{\sigma} \cdot \hat{\mathbf{p}}).$$

Pauli Hamiltonian

- With the replacement $\hat{\mathbf{p}} \to \hat{\boldsymbol{\pi}} \equiv \hat{\mathbf{p}} - \frac{q}{c}\mathbf{A}(\hat{\mathbf{x}}, t)$, and including the scalar potential, we define the Pauli Hamiltonian:

$$\hat{H}_{\text{Pauli}} = \frac{1}{2m}(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{\pi}})(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{\pi}}) + q\Phi(\hat{\mathbf{x}}, t).$$

- Expanding the first term, the Hamiltonian becomes:

$$\hat{H}_{\text{Pauli}} = \frac{1}{2m}\hat{\boldsymbol{\pi}} \cdot \hat{\boldsymbol{\pi}}\mathbb{I} + \frac{i}{2m}\boldsymbol{\sigma} \cdot (\hat{\boldsymbol{\pi}} \times \hat{\boldsymbol{\pi}}) + q\Phi(\hat{\mathbf{x}}, t).$$

- The commutator $(\hat{\boldsymbol{\pi}} \times \hat{\boldsymbol{\pi}})$ is nonzero:

$$[\hat{\pi}_i, \hat{\pi}_j] = \left[\hat{p}_i - \frac{q}{c}A_i, \hat{p}_j - \frac{q}{c}A_j\right] = -i\hbar\frac{q}{c}\epsilon_{ijk}B_k.$$

- Thus, in vector notation:

$$(\hat{\pi} \times \hat{\pi})_k = \epsilon_{ijk}\hat{\pi}_i\hat{\pi}_j = \frac{1}{2}\epsilon_{ijk}\left[\hat{\pi}_i, \hat{\pi}_j\right] = -i\hbar\frac{q}{c}B_k.$$

- Substituting back into $\hat{H}_{\text{Pauli}}$, with $q = -e$ and $m = m_e$, we have:

$$\hat{H}_{\text{Pauli}} = \frac{1}{2m_e}\left(\hat{\mathbf{p}} + \frac{e}{c}\mathbf{A}\right)^2 + \frac{e\hbar}{2m_e c}\boldsymbol{\sigma} \cdot \mathbf{B} - e\Phi(\hat{\mathbf{x}}, t),$$

The second term gives the coupling of the electron spin to the magnetic field.

The Dirac Equation

The Dirac Equation

- As discovered by Dirac, a relativistic description of the electron requires the use of matrices and upgrading the Pauli spinor to a four-component spinor.
- The analysis begins with the relationship between relativistic energy and momentum:

$$E^2 - c^2 p^2 = m^2 c^4 \quad \Rightarrow \quad E = \sqrt{c^2 p^2 + m^2 c^4}.$$

- This suggests a relativistic Hamiltonian $\hat{H}$ for a free particle could be written as:

$$\hat{H} = \sqrt{c^2 \hat{\mathbf{p}}^2 + m^2 c^4}.$$

- The associated Schrödinger equation would then be:

$$i\hbar \frac{\partial \Psi}{\partial t} = \sqrt{c^2 \hat{\mathbf{p}}^2 + m^2 c^4}\, \Psi.$$

Dirac Hamiltonian

- Dirac sought to avoid square roots in the Hamiltonian by rewriting the relativistic energy as the square of a linear function of momentum:

$$c^2\hat{\mathbf{p}}^2 + m^2c^4 = (c\alpha_1\hat{p}_1 + c\alpha_2\hat{p}_2 + c\alpha_3\hat{p}_3 + \beta mc^2)^2.$$

- Here, $\alpha_1, \alpha_2, \alpha_3, \beta$ are to be determined. The expression inside the parentheses is the candidate for the energy operator:

$$\hat{H}_{\text{Dirac}} = \sum_i \alpha_i \hat{p}_i + \beta mc^2.$$

- Expanding the square and equating coefficients yields the following conditions:

$$\alpha_1^2 = \alpha_2^2 = \alpha_3^2 = \beta^2 = 1,$$

$$\alpha_i\alpha_j + \alpha_j\alpha_i = \{\alpha_i, \alpha_j\} = 0, \quad i \neq j,$$

$$\alpha_i\beta + \beta\alpha_i = \{\alpha_i, \beta\} = 0.$$

- These anticommutator relations imply that α_i and β cannot be numbers. They must instead be matrices.

Dirac Equation

- A solution for α_i and β is achieved using 4×4 Hermitian matrices:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbb{I}_{2\times 2} & 0 \\ 0 & -\mathbb{I}_{2\times 2} \end{pmatrix}.$$

- The Dirac equation becomes:

$$i\hbar \frac{\partial}{\partial t}\Psi = \left(\sum_i \alpha_i \cdot \hat{p}_i + \beta mc^2 \right) \Psi,$$

where Ψ is a Dirac spinor, a four-component column vector composed of two two-component vectors:

$$\Psi = \begin{pmatrix} \chi \\ \eta \end{pmatrix}, \quad \chi = \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix}, \quad \eta = \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}.$$

Dirac Equation

- The spinors χ and η correspond to the top and bottom components of the Dirac spinor. At low energies, η is negligible, and the evolution of χ follows the Pauli Hamiltonian.
- Coupling the Dirac equation to electromagnetic fields, with $\hat{\mathbf{p}} \to \hat{\mathbf{p}} + \frac{e}{c}\mathbf{A}$, the equation becomes:

$$i\hbar\frac{\partial}{\partial t}\Psi = \left[c\boldsymbol{\alpha}\cdot\left(\hat{\mathbf{p}} + \frac{e}{c}\mathbf{A}\right) + \beta mc^2 + V(r)\right]\Psi,$$

  where $V(r) = -e\Phi(r)$.
- The great advantage of the Dirac equation is that the relativistic corrections to the hydrogen Bohr Hamiltonian can be derived systematically.