

Condensed Matter Physics IV

Chapter 2

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Recap: Topology in Quantum Mechanics, Aharonov-Bohm, Dirac monopole

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We continue the discussion of Dirac's magnetic monopole.

Our motivation is:

1. Application of gauge transformation to a physical problem
2. Quantization of a physical quantity, here the electric charge of an electron or the magnetic monopole charge of a magnetic monopole, due to single-valued nature of the wavefunction
3. Example of a topological charge without introducing the emergent magnetic field / Berry phase formalism; here we can use entirely the (well-known) electromagnetic fields.

Recap from the previous lecture:

Consider the enhanced symmetry that would be introduced to Maxwell's classical electrodynamics by the presence of a new elementary particle, the magnetic monopole or magnetic charge density ρ_m in vacuum

$$\begin{aligned}\nabla \cdot \mathbf{B} &= \rho_m & \nabla \cdot \mathbf{E} &= \rho_e/\varepsilon_0 \\ \nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} - \mathbf{j}_m & \nabla \times \mathbf{B} &= \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{j}_e\end{aligned}\tag{1}$$

where $c = 1/\sqrt{\mu_0\varepsilon_0}$, μ_0 , and ε_0 are the speed of light, the magnetic permeability of vacuum, and the electric permittivity of vacuum, respectively. We also have the continuity equations for the charges, $\partial\rho_e/\partial t + \nabla \cdot \mathbf{j}_e = 0$ and $\partial\rho_m/\partial t + \nabla \cdot \mathbf{j}_m = 0$.

The modified Lorentz force:

The currents $\mathbf{j}_e$ and $\mathbf{j}_m$ are the electric and magnetic current densities. A modified Lorentz force can be derived as

$$\mathbf{F} = q_e (\mathbf{E} + \mathbf{v} \times \mathbf{B}) + \frac{q_m}{\mu_0} \left(\mathbf{B} - \frac{1}{c^2} \mathbf{v} \times \mathbf{E} \right),\tag{2}$$

where the symmetry of the dependence on $q = q_e$ and q_m is quite apparent. The magnetic charge is measured in Webers, $[\text{Wb}] = \text{kg m}^2/\text{A s}^2$.

2.4.1 Vector potential for motion in field of magnetic monopole

Contrary to the familiar case of classical electrodynamics, $\nabla \cdot \mathbf{B} = 0$ is now violated due to the presence of magnetic monopoles. While the electromagnetic vector potential $\mathbf{A}$ is still related to the observable magnetic field as $\mathbf{B} = \nabla \times \mathbf{A}$, the mathematical identity $\nabla \cdot (\nabla \times \mathbf{A}) = 0$ breaks down at singular locations $\mathbf{x}_i$, i.e. at the locations of the monopoles.

Purpose / summary: We are interested in the stationary behavior of a QM particle on the two-dimensional surface of a sphere of radius R around a magnetic monopole. We show that the point-like singularity of $\mathbf{B}$ at the center of the sphere requires that no unique function $\mathbf{A}(\mathbf{x})$ can be defined on the entire spherical surface; instead, we must define $\mathbf{A}$ in at least two separate, but overlapping patches. Drawing an analogy to the previous section: even if the QM particle does not have any probability density at the location of the monopole, its quantum-phase properties are affected by the monopole through geometrical constraints on the vector potential $\mathbf{A}$.

First, we choose an ansatz for the magnetic field of a monopole in analogy to the electric field of a point charge,

$$\mathbf{B} = \frac{q_m}{4\pi r^2} \frac{\mathbf{r}}{r} \quad (3)$$

where $\mathbf{r}/r = \hat{e}_r$ in spherical coordinates. This gives, according to Gauss' theorem with a spherical surface $\mathcal{S}$ of radius R surrounding the point charge,

$$\int_{\mathcal{S}} dr^2 \mathbf{B} \cdot \hat{n} = q_m \quad (4)$$

A possible ansatz for the vector potential is

$$\mathbf{A}^N(\mathbf{x}) = \frac{q_m}{4\pi} \frac{1 - \cos \theta}{r \sin \theta} \hat{e}_\varphi \quad (5)$$

which is tangential to the spherical surface and diverges at $\theta = \pi$. In spherical coordinates (r, θ, φ) , the curl operation is

$$\nabla \times \mathbf{A} = \frac{1}{r \sin \theta} \left(\frac{\partial}{\partial \theta} (A_\varphi \sin \theta) - \frac{\partial A_\theta}{\partial \varphi} \right) \hat{e}_r + \frac{1}{r} \left(\frac{1}{\sin \theta} \frac{\partial A_r}{\partial \varphi} - \frac{\partial}{\partial r} (r A_\varphi) \right) \hat{e}_\theta + \frac{1}{r} \left(\frac{\partial}{\partial r} (r A_\theta) - \frac{\partial A_r}{\partial \theta} \right) \hat{e}_\varphi \quad (6)$$

But our expression only includes A_φ and rA_φ is independent of r , so that

$$\frac{4\pi}{q_m} \nabla \times \mathbf{A}^N = \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} \left(\frac{1 - \cos \theta}{r} \right) \hat{e}_r = \frac{1}{r^2} \hat{e}_r \quad (7)$$

as expected for the monopole field. At the south pole $\theta = \pi$ however, the vector potential breaks down and the magnetic field cannot be well defined from $\mathbf{A}^N$ (although $\mathbf{B}$ does not diverge on the spherical surface at radius R). Likewise, it is possible to define a south-pole potential

$$\mathbf{A}^S(\mathbf{x}) = \frac{q_m}{4\pi} \left(\frac{-1 - \cos \theta}{r \sin \theta} \right) \hat{e}_\varphi \quad (8)$$

which diverges at the north pole, i.e., at $\theta = 0$.

These two vector potentials result in the same magnetic field $\mathbf{B}$, so they must be connected by a gauge transformation

$$\mathbf{A}^N - \mathbf{A}^S = \frac{q_m}{2\pi} \frac{1}{r \sin \theta} \hat{e}_\varphi \stackrel{!}{=} \nabla \Lambda(\mathbf{x}) \quad (9)$$

with $\Lambda = (q_m/2\pi)\varphi$ and φ is the scalar spherical coordinate related to $\hat{e}_\varphi$. It can be confirmed that

$$\nabla \Lambda(\mathbf{x}) = \hat{e}_r \frac{\partial \Lambda}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial \Lambda}{\partial \theta} + \hat{e}_\varphi \frac{1}{r \sin \theta} \frac{\partial \Lambda}{\partial \varphi} = \frac{q_m}{2\pi} \cdot \frac{1}{r \sin \theta} \quad (10)$$

There is thus no single vector potential that is non-divergent everywhere on the sphere around the monopole. However, we can 'cover the sphere in patches'.

The situation is quite different from an electric monopole, which has a well-defined scalar potential A_0 , despite the apparent 'symmetry' of the modified Maxwell equations.

2.4.2 Quantization of electric and magnetic charges

Say that ψ corresponds to a solution of the static Schroedinger equation for a particle with electric charge q under the influence of the magnetic monopole of charge q_m :

$$\mathcal{H}\psi = E\psi \quad \rightarrow \quad \frac{1}{2m} (-i\hbar \nabla - q\mathbf{A})^2 \psi = E\psi \quad (11)$$

We use $\mathbf{A}^N$ at $0 \leq \theta \leq \pi - \varepsilon$ and $\mathbf{A}^S$ for $\varepsilon \leq \theta \leq \pi$ with a finite $\varepsilon > 0$. In the overlap region, either one of them is suitable. According to the gauge transformation between the vector potentials, discussed above, the

wavefunctions transform as

$$\psi \rightarrow \exp [iq\Lambda(\mathbf{x})/\hbar] \psi \quad (12)$$

so that the wavefunctions in the two patches are related by

$$\psi^N = \exp \left[+\frac{iq}{\hbar} \left(\frac{q_m}{2\pi} \right) \phi \right] \psi^S \quad (13)$$

Considering a loop around the equator, we demand that the wavefunction must return onto itself at $\Delta\varphi = 2\pi N_0$, where $N_0 \in \mathbb{Z}$ (in a later section we derive the same result for bosonic wavefunctions without making this assumption). Hence,

$$\frac{q}{\hbar} \frac{q_m}{2\pi} \stackrel{!}{=} N_0 \quad \rightarrow \quad q_m q = h N_0 \quad (14)$$

and the product of the two charges is quantized. We note that, for the product to be quantized, neither $q = q_e$ nor q_m can take on continuous values.

Comment 1: The quantization of the electric and magnetic charges also implies the quantization of magnetic flux. The total magnetic flux through the surface of our sphere (radius R) is

$$\int d^2r \mathbf{B} \cdot \hat{n} = \int d^3\mathbf{r} \nabla \cdot \mathbf{B} = q_m = \frac{h N_0}{q} = \frac{h}{q} N_0 = \phi_0 N_0 \quad (15)$$

where ϕ_0 is the flux quantum for a single particle (not superconducting flux quantum). The first equality arises from the divergence theorem, and the second equality to the modified Maxwell equations.

Comment 2: If there is no magnetic monopole charge, $q_m = 0$, then $A^S = A^N$ and the argument breaks down. We need the monopole at the center to use the argument about the gauge transformation.

3 Berry phase and Berry curvature (nondegenerate case)

3.1 Definition of the Berry curvature

We consider a parameter space $\mathbf{R}(t)$, where t is an intrinsic parameter which allows us to traverse a path in the parameter space. For the purpose of the present discussion, $\mathbf{R}$ is a position in a three-dimensional

vector space. For parameter-dependent Hamiltonian $\hat{\mathcal{H}}(\mathbf{R}(t))$, eigenstates $|n(\mathbf{R}(t))\rangle$, and energy spectrum $E_n(\mathbf{R}(t))$, we search solutions to the time-dependent S.-Eq.,

$$i\hbar\partial_t |\psi_n[\mathbf{R}(t)]\rangle = \hat{\mathcal{H}}[\mathbf{R}(t)] |\psi_n[\mathbf{R}(t)]\rangle, \quad (16)$$

while traversing a path in $\mathbf{R}$ space 'sufficiently slow' so as to ensure that a system which starts in an eigenstate $|n\rangle$ at time $t = 0$ remains in the corresponding eigenstate at $t > 0$. According to the adiabatic theorem, there is a threshold speed for traversing any parameter path, below which this condition is met.

The full expression for the wavefunction is

$$|\psi(\mathbf{R})\rangle = \exp(i\gamma_n(t)) \exp\left(-\frac{i}{\hbar} \int_0^t dt' E_n[\mathbf{R}(t')]\right) |n[\mathbf{R}(t)]\rangle \quad (17)$$

where $|n[\mathbf{R}(t)]\rangle$ satisfies the time-independent Schroedinger equation,

$$\hat{\mathcal{H}}[\mathbf{R}(t)] |n[\mathbf{R}(t)]\rangle = E_n |n[\mathbf{R}(t)]\rangle \quad (18)$$

Besides the dynamical phase factor, an additional phase term γ_n is necessary to fulfill the S.-Eq. as we will show in the following. This phase is called geometrical phase or Berry phase.

From here, we abbreviate $\mathbf{R}(t) \equiv \mathbf{R}$ and have

$$\begin{aligned} i\hbar\partial_t |\psi(\mathbf{R})\rangle &= e^{i\gamma_n(t)} e^{-\frac{i}{\hbar} \int_0^t dt' E_n[\mathbf{R}(t')]} i\hbar \left[i \frac{\partial \gamma_n}{\partial t} - \frac{i}{\hbar} E_n[\mathbf{R}] + \frac{\partial}{\partial t} \right] |n(\mathbf{R})\rangle \\ &= e^{i\gamma_n(t)} e^{-\frac{i}{\hbar} \int_0^t dt' E_n[\mathbf{R}(t')]} \hat{\mathcal{H}}(\mathbf{R}) |n(\mathbf{R})\rangle \end{aligned} \quad (19)$$

Now to simplify, we remove the dynamical phase factor and multiply this equation by $\langle n(\mathbf{R})|$ from the left-hand side, yielding

$$\frac{\partial \gamma_n}{\partial t} = i \langle n(\mathbf{R})| \frac{\partial}{\partial t} |n(\mathbf{R})\rangle = i \langle n(\mathbf{R})| \frac{\partial}{\partial \mathbf{R}} |n(\mathbf{R})\rangle \cdot \frac{\partial \mathbf{R}}{\partial t} \quad (20)$$

and we can define the shorthand for the parameter-space velocity $\dot{\mathbf{R}} = \partial \mathbf{R} / \partial t$ (sufficiently slow to satisfy the adiabatic condition). Note that the bra/ket expression is a contraction of wavefunctions in Hilbert space, but also a 3-vector in the parameter space of $\mathbf{R}$.

As will be shown below, the expression for γ_n is not gauge-invariant in the general case; however, when considering a closed loop $\mathcal{C}$ in $\mathbf{R}$ -space, a physically meaningful quantity is obtained:

$$\begin{aligned}\gamma_n[\mathcal{C}] &= \int_0^T \frac{\partial \gamma_n}{\partial t} dt = i \int_0^T dt \langle n(\mathbf{R}) | \frac{\partial}{\partial \mathbf{R}} | n(\mathbf{R}) \rangle \cdot \dot{\mathbf{R}} = i \oint_{\mathcal{C}} d\mathbf{l}_{\mathbf{R}} \cdot \langle n(\mathbf{R}) | \frac{\partial}{\partial \mathbf{R}} | n(\mathbf{R}) \rangle \\ &\equiv - \oint_{\mathcal{C}} d\mathbf{l}_{\mathbf{R}} \cdot \mathbf{A}_n(\mathbf{R})\end{aligned}\quad (21)$$

where the Berry vector potential, Berry connection, or emergent vector potential was introduced:

$$\mathbf{A}_n = -i \langle n(\mathbf{R}) | \frac{\partial}{\partial \mathbf{R}} | n(\mathbf{R}) \rangle \quad (22)$$

This is a vector in the $\mathbf{R}$ -space. Further in the 3D case, the Berry curvature or emergent magnetic field is defined as $\boldsymbol{\Omega}_n(\mathbf{R}) = \nabla_{\mathbf{R}} \times \mathbf{A}_n$ so that

$$\gamma_n = - \int d^2\mathbf{R} \boldsymbol{\Omega}_n(\mathbf{R}) \cdot \hat{n}_{\mathbf{R}} \quad (23)$$

where $\hat{n}_{\mathbf{R}}$ is a normal vector on the surface of integration in $\mathbf{R}$ space.

3.2 Berry curvature (not Berry phase) is gauge invariant

Consider a gauge transformation of the eigenstates

$$|n(\mathbf{R})\rangle \rightarrow \exp(i\Lambda(\mathbf{R})) |n(\mathbf{R})\rangle \quad (24)$$

The associated change of the Berry connection is

$$\begin{aligned}\mathbf{A}'_n &= -i \langle n(\mathbf{R}) | e^{-i\Lambda} \frac{\partial}{\partial \mathbf{R}} e^{i\Lambda} | n(\mathbf{R}) \rangle \\ &= -i \langle n | \frac{\partial}{\partial \mathbf{R}} | n \rangle - i \langle n | i \frac{\partial \Lambda}{\partial \mathbf{R}} | n \rangle = \mathbf{A}_n + \frac{\partial \Lambda}{\partial \mathbf{R}}\end{aligned}\quad (25)$$

i.e. mathematically equivalent to a gauge transformation of the electromagnetic field with a spatially dependent scalar function $\Lambda(\mathbf{x})$. The Berry curvature $\boldsymbol{\Omega}_n$ remains gauge invariant.

Gauge transformation and Berry phase:

We further illustrate how the Berry *phase* is gauge invariant only modulo 2π (in contrast to $\boldsymbol{\Omega}_n$, a locally gauge invariant object). As deduced above, we have $\gamma_n = - \oint_{\mathcal{C}} d\mathbf{l}_{\mathbf{R}} \cdot \mathbf{A}_n(\mathbf{R})$. Under gauge transformation,

$\gamma'_n = \gamma_n - \oint_{\mathcal{C}} d\mathbf{l}_{\mathbf{R}} \cdot (\nabla_{\mathbf{R}} \Lambda)$ and $\Lambda(t=T) - \Lambda(t=0) = 2\pi N$ where $N \in \mathbb{Z}$ is required to ensure that the wave function is single-valued at a fixed point in $\mathbf{R}$ -space.

3.3 Gauge transformation and singularities in parameter space

Unlike the case of a 'real' magnetic field, there can be sinks and sources (monopoles) of $\boldsymbol{\Omega}_n(\mathbf{r})$:

$$\nabla_{\mathbf{R}} \cdot \boldsymbol{\Omega}_n(\mathbf{R}) \neq 0 \quad (26)$$

due to emergent monopoles in parameters space. In this case, no single vector potential $\mathbf{A}_n(\mathbf{R})$ exists which could satisfy $\nabla_{\mathbf{R}} \times \mathbf{A}_n(\mathbf{R}) = \boldsymbol{\Omega}_n(\mathbf{R})$ everywhere in parameter space, without becoming singular at some points.

Comment 1: Stokes' theorem for $\mathbf{A}_n(\mathbf{R})$,

$$\oint_{\mathcal{C}} d\mathbf{l}_{\mathbf{R}} \cdot \mathbf{A}_n(\mathbf{R}) = \int_{\mathcal{S}(\mathcal{C})} d^2\mathbf{R} (\nabla_{\mathbf{R}} \times \mathbf{A}_n(\mathbf{R})) \cdot \hat{n}_{\mathbf{R}} \quad (27)$$

is only valid if the loop and surface are in a region of $\mathbf{R}$ -space where $\boldsymbol{\Omega}_n(\mathbf{R}) = \nabla_{\mathbf{R}} \times \mathbf{A}_n(\mathbf{R})$ has no singularities.

Comment 2: "Moving $\mathcal{S}(\mathcal{C})$ across a monopole"; we start with a loop $\mathcal{C}$ and the narrow surface (neck) $\mathcal{S}_1(\mathcal{C})$ that is the tightest surface surrounded by the loop. Let a monopole be situated above this surface. We let the surface expand upwards; then we let the surface "catch" the monopole and finally envelop the monopole.

Recall the previous problem of an electron in the environment of a magnetic monopole, with two vector potentials $\mathbf{A}^S$ and $\mathbf{A}^N$. In this language, we can use $\mathbf{A}^S$ for $\mathcal{S}_1(\mathcal{C})$, but should use $\mathbf{A}^N$ for $\mathcal{S}_2(\mathcal{C})$; this is because the former surface is located entirely below the monopole, and the latter surface does not include the south pole.

In summary: When calculating the Berry phase, the correct gauge for the vector potential depends on the surface of integration. What is more, the gauge transformation for going from $\mathbf{A}^S$ to $\mathbf{A}^N$ changes $\gamma_n(\mathcal{C})$

by $2\pi N$, with $N \in \mathbb{Z}$. The gauge degree of freedom corresponds to a choice of surface of integration in the Berry phase formula.

Comment:

1. The emergent magnetic field $\mathbf{\Omega}_n(\mathbf{R})$ is a *local* quantity, whereas γ_n is only properly defined on a loop.
2. $\mathbf{\Omega}_n(\mathbf{R})$ is gauge invariant and physically observable, whereas γ_n is affected by a gauge transformation and not directly observable (only modulo 2π).