T.O.C.: The Math

T.O.C.: Physical Systems

Section 1

The Irrelevant Phase

The Irrelevant Phase

1. All quantum mechanical observables correspond to Hermitian operators $(\hat{O})$.
2. All Hermitian operators have a spectral decomposition $(\hat{O} = \sum_n a_n |\Psi_n\rangle \langle\Psi_n|)$.
3. The projector components $(|\Psi_n\rangle \langle\Psi_n|)$ of the spectrally decomposed operator $\hat{O}$ are all invariant under the gauge transformation $|\Psi_n\rangle \rightarrow \exp(i\alpha_n) |\Psi_n\rangle$.

$\Rightarrow$ Phase is not physical!

$$\Psi = \Psi \cdot exp(i\phi) \qquad\qquad \phi \in \{0, 2\pi\}$$

Section 2

The Berry Phase

The Relative Phase

- The relative phase between two states can be uniquely defined for a given gauge.
- The relative phase is not invariant under local gauge transformations (i.e. multiplication of the state by a phase factor).

Relative Phase:

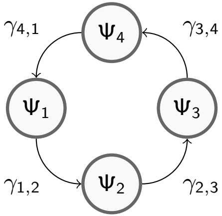
$$\gamma_{1,2} = -arg \langle \Psi_1 | \Psi_2 \rangle \qquad \gamma_{1,2} \in (-\pi, \pi]$$

Gauge Transformation:

$$|\Psi_j\rangle \to \exp(i\alpha_j) |\Psi_j\rangle$$
$$\exp(-i\gamma_{1,2}) \to \exp(-i\gamma_{1,2} + i(\alpha_2 - \alpha_1))$$

The Berry Phase

- Summation of a non-gauge invariant quantity ($\gamma_{i,j}$) along closed loops results in a gauge-invariant result!
- The Berry Phase can be expressed in terms of gauge-invariant operators.



The Berry Phase:

$$\gamma_L = \sum_{i=0}^{N-1} \gamma_{i \bmod N, i+1 \bmod N}$$

Invariance:

$$\gamma_L = \mathrm{Tr}\left(\prod_{i=0}^{N-1} |\Psi_i\rangle \langle \Psi_i| \right)$$

By Analogy

Discrete:

- Parameter Space: $\mathbb{P} = \mathbb{N}_0$

Continuous:

- Parameter Space: $\mathbb{P} = \mathcal{M}$

By Analogy

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- Parameter Space: $\mathbb{P} = \mathbb{N}_0$
- Wave Function
  $\Psi : \mathbb{P} \to \mathcal{H}, \quad n \mapsto |\Psi_n\rangle$

Continuous:

- Parameter Space: $\mathbb{P} = \mathcal{M}$
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  $\Psi : \mathbb{P} \to \mathcal{H}, \quad \boldsymbol{R} \mapsto |\Psi(\boldsymbol{R})\rangle$

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  $\Psi : \mathbb{P} \to \mathcal{H}, \quad \boldsymbol{R} \mapsto |\Psi(\boldsymbol{R})\rangle$
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- Berry Phase:
  $\gamma(\mathcal{C}) = \sum_{i=0}^{N} \gamma_{n_i \bmod N, n_{i+1} \bmod N}$

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  $\gamma(\mathcal{C}) = \sum_{i=0}^{N} \gamma_{n_i \bmod N, n_{i+1} \bmod N}$

The sum of the relative phases of each wave function connected by the path $\mathcal{C}$.

Continuous:

- Parameter Space: $\mathbb{P} = \mathcal{M}$
- Wave Function
  $\Psi : \mathbb{P} \to \mathcal{H}, \quad \boldsymbol{R} \mapsto |\Psi(\boldsymbol{R})\rangle$
- Path: $\mathcal{C} : [0,1) \to \mathcal{M}, \quad t \mapsto \boldsymbol{R}(t)$
- Berry Phase:
  $\gamma(\mathcal{C}) = \lim_{dt \to 0} \oint \gamma_{\mathcal{C}(t), \mathcal{C}(t+dt)} d\boldsymbol{R}$

The integrated relative phase of all the wave functions connected by the path $\mathcal{C}$.

The Berry Connection

Relative Phase: $\lim_{\boldsymbol{r}\to 0}\gamma_{\boldsymbol{R},\boldsymbol{R}+\boldsymbol{r}} = \lim_{\boldsymbol{r}\to 0} -arg\,\langle\Psi(\boldsymbol{R}|\Psi(\boldsymbol{R}+\boldsymbol{r})\rangle$

$$\lim_{\boldsymbol{r}\to 0}\exp(-i\gamma_{\boldsymbol{R},\boldsymbol{R}+\boldsymbol{r}}) = \lim_{\boldsymbol{r}\to 0}\frac{\langle\Psi(\boldsymbol{R})|\Psi(\boldsymbol{R}+\boldsymbol{r})\rangle}{|\langle\Psi(\boldsymbol{R})|\Psi(\boldsymbol{R}+\boldsymbol{r})\rangle|}$$

$$1 - i\gamma_{\boldsymbol{R},\boldsymbol{R}+\boldsymbol{r}} = \langle\Psi(\boldsymbol{R})|\left(|\Psi(\boldsymbol{R})\rangle + \nabla_{\boldsymbol{R}}|\Psi(\boldsymbol{R})\rangle\right)$$

$$\Rightarrow \gamma_{\boldsymbol{R},\boldsymbol{R}+\boldsymbol{dr}} = i\,\langle\Psi(\boldsymbol{R})|\nabla_{\boldsymbol{R}}|\Psi(\boldsymbol{R})\rangle$$

$$\gamma(\mathcal{C}) = \oint i\,\langle\Psi(\boldsymbol{R})|\nabla_{\boldsymbol{R}}|\Psi(\boldsymbol{R})\rangle\, d\boldsymbol{R}$$

The Berry Connection and Curvature

- Discrete relative phase quantities in the discrete case are replaced by the Berry Connection in the continuous case.
- The Berry Connection is non-gauge invariant under gauge transformations.

Berry Connection:

$\mathcal{A} := i \langle \Psi(\boldsymbol{R}) | \nabla | \Psi(\boldsymbol{R}) \rangle$

Gauge Transformation:

$|\Psi(\boldsymbol{R})\rangle \rightarrow \exp(i\alpha(\boldsymbol{R})) |\Psi(\boldsymbol{R})\rangle$

$\mathcal{A} \rightarrow \mathcal{A} - \nabla\alpha(\boldsymbol{R})$

The Berry Connnection and Curvature

- Stokes' theorem can be utilized to reformulate the path integral to a surface integral.

Stokes' Theorem:

$$\gamma(\mathcal{C}) = \sum_{\mu,\nu} \int_{\mathcal{S}(\mathcal{C})} \frac{1}{2} \partial_\mu \mathcal{A}_\nu - \partial_\nu \mathcal{A}_\mu dR^\mu \wedge dR^\nu$$

The Berry Connection and Curvature

- The resulting integrand defines what is known as the Berry Curvature.
- The Berry Curvature is gauge-invariant under gauge transformations.

Berry Curvature:

$$\Omega_{\mu,\nu}(\boldsymbol{R}) := \partial_\mu \mathcal{A}_\nu - \partial_\nu \mathcal{A}_\mu$$

Gauge Transformation:

$$|\Psi(\boldsymbol{R})\rangle \to \exp(i\alpha(\boldsymbol{R}))\,|\Psi(\boldsymbol{R})\rangle$$

$$\Omega_{\mu,\nu}(\boldsymbol{R}) \to \partial_\mu(\mathcal{A}_\nu - \partial_\nu \alpha(\boldsymbol{R})) - \partial_\nu(\mathcal{A}_\mu - \partial_\mu \alpha(\boldsymbol{R}))$$

Magnetic Analogies

- The relationship between the Berry Phase (γ), Berry Connection ($\boldsymbol{\mathcal{A}}$) and Berry Curvature ($\boldsymbol{\Omega}$) is analogous to the relationship between the magnetic flux (Φ), magnetic vector potential ($\boldsymbol{A}$) and magnetic flux density ($\boldsymbol{B}$).

Phase:

$$\begin{aligned}\gamma(C) &= \oint \boldsymbol{\mathcal{A}} \cdot d\boldsymbol{R} \\ &= \int_{\mathcal{S}(\mathcal{C})} \nabla \times \boldsymbol{\mathcal{A}} \cdot d\boldsymbol{s} \\ &= \int_{\mathcal{S}(\mathcal{C})} \boldsymbol{\Omega} \cdot d\boldsymbol{s}\end{aligned}$$

Flux:

$$\begin{aligned}\Phi(C) &= \oint \boldsymbol{A} \cdot d\boldsymbol{R} \\ &= \int_{\mathcal{S}(\mathcal{C})} \nabla \times \boldsymbol{A} \cdot d\boldsymbol{s} \\ &= \int_{\mathcal{S}(\mathcal{C})} \boldsymbol{B} \cdot d\boldsymbol{s}\end{aligned}$$

Section 3

The Adiabatic Theorem

Statement

Theorem

Under a slowly changing Hamiltonian with instantaneous eigenstates $|n(t)\rangle$ and energies $E_n(t)$, the state of a quantum system evolves ($\Psi(t) = \sum_n c_n(t) |n(t)\rangle$) such that the amplitudes of the instantaneous eigenstates composing the wave function are given by:

$$c_n(t) = c_n(0) e^{i\theta_n(t)} e^{i\gamma_n(t)}$$

$$\theta_n(t) = -\hbar^{-1} \int_0^t E_n(t')dt'$$

$$\gamma_n(t) = i \int_0^t \langle m(t')|\dot{m}(t')\rangle \, dt'$$

Assumptions

1. $i\hbar |\dot{\Psi}(t)\rangle = \boldsymbol{H} |\Psi(t)\rangle$
2. $\dfrac{\langle m(t)|\dot{\boldsymbol{H}}(t)|n(t)\rangle}{E_m(t) - E_n(t)} = 0$

Proof: Part I

1. Begin with the time-dependent Schrödinger equation.
2. Expand $|\Psi(t)\rangle$ and apply the Hamiltonian $\boldsymbol{H}$ to the eigenstates $|n(t)\rangle$.
3. Take the inner product of both sides of the equation with $|m(t)\rangle$.

$$i\hbar\,|\dot{\Psi}(t)\rangle = \boldsymbol{H}(t)\,|\Psi(t)\rangle$$

$$\boldsymbol{L.H.S} = \sum_n c_n(t)E_n(t)\,|n(t)\rangle$$

$$i\hbar\sum_n \left[\dot{c}_n(t)\,|n(t)\rangle + c_n(t)\,|\dot{n}(t)\rangle\right] = \boldsymbol{R.H.S}$$

$$i\hbar\dot{c}_m(t) + i\hbar\sum_n \langle m(t)|\dot{n}(t)\rangle = c_m(t)E_m(t)$$

Proof: Part II

4. Differentiate the time-independent Schrödinger equation with respect to time.
5. Take the inner product of both sides of the equation with $|m(t)\rangle$.
6. Rearrange in terms of the inner product $\langle m(t)|\dot{n}(t)\rangle$.

$$\boldsymbol{L.H.S} = \dot{E}_n(t)\,|n(t)\rangle + E_n(t)\,|\dot{n}(t)\rangle$$

$$\dot{\boldsymbol{H}}(t)\,|n(t)\rangle + \boldsymbol{H}(t)\,|\dot{n}(t)\rangle = \boldsymbol{R.H.S}$$

$$\boldsymbol{L.H.S} = E_n(t)\,\langle m(t)|\dot{n}(t)\rangle$$

$$\langle m(t)|\dot{\boldsymbol{H}}(t)|n(t)\rangle + E_m\,\langle m(t)|\dot{n}(t)\rangle = \boldsymbol{R.H.S}$$

$$\langle m(t)|\dot{n}(t)\rangle = \frac{\langle m(t)|\dot{\boldsymbol{H}}(t)|n(t)\rangle}{E_n(t) - E_m(t)} \quad (m \neq n)$$

Proof: Conclusion

7. Insert the result from Part II into the result from Part I.
8. For $\langle m(t)|\dot{\boldsymbol{H}}(t)|n(t)\rangle \ll E_m(t) - E_n(t)$ and $\forall n \quad \forall t : E_m(t) - E_n(t) \neq 0$.
9. Solving the resulting differential equation for $c_m(t)$.

$$\boldsymbol{L.H.S} = \sum_{\substack{n \\ n\neq m}} \frac{\langle m(t)|\dot{\boldsymbol{H}}(t)|n(t)\rangle}{E_m(t) - E_n(t)}$$

$$\dot{c}_m(t) + \left(\frac{i}{\hbar}E_m(t) + \langle m(t)|\dot{m}(t)\rangle\right) c_m(t) = \boldsymbol{R.H.S}$$

$$\dot{c}_m(t) = i\left(-\frac{1}{\hbar}E_m(t) + i\,\langle m(t)|\dot{m}(t)\rangle\right) c_m(t)$$

$$c_m(t) = c_m(0)e^{-i\frac{1}{\hbar}\int_0^t E_m(t')dt'}\, e^{i\int_0^t i\langle m(t')|\dot{m}(t')\rangle dt'}$$

Proof: The Berry Phase

Time evolution given by the variation of parameters $\boldsymbol{R} \in \mathbb{P}$:

$$\boldsymbol{H}(t) = \boldsymbol{H}(\boldsymbol{R}(t)) \quad \Psi(t) = \Psi(\boldsymbol{R}(t))$$

Therefore:

$$\begin{aligned}\gamma &= \int_0^t i \langle m(\boldsymbol{R}(t)) | \dot{m}(\boldsymbol{R}(t)) \rangle \, dt \\ &= \int_0^t i \langle m(\boldsymbol{R}(t)) | \nabla_{\boldsymbol{R}} | m(\boldsymbol{R}(t)) \rangle \, \dot{\boldsymbol{R}}(t) dt \\ &= \oint i \langle m(\boldsymbol{R}) | \nabla_{\boldsymbol{R}} | m(\boldsymbol{R}) \rangle \, d\boldsymbol{R}\end{aligned}$$

Section 4

Magnetic Moment in a Precessing Field

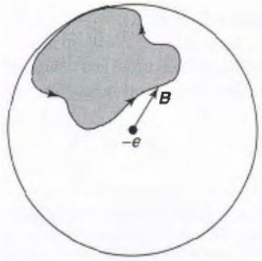
Defining the System

System:
Magnetic moment at the origin in the presence of a magnetic field B of fixed magnitude, moving along some closed path $\mathcal{C}$.

$$\boldsymbol{B}(t) = B_0 \begin{pmatrix} \sin\theta(t)\cos\phi(t) \\ \sin\theta(t)\sin\phi(t) \\ \cos\theta(t) \end{pmatrix} \qquad \boldsymbol{H}(t) = \frac{\hbar e}{2m}\boldsymbol{B}\cdot\boldsymbol{\sigma}$$

$$\chi_+(t) = \begin{pmatrix} \cos\frac{\theta(t)}{2} \\ e^{i\phi(t)}\sin\frac{\theta(t)}{2} \end{pmatrix} \qquad E_+ = \frac{\hbar\omega_1}{2}$$

$$\chi_-(t) = \begin{pmatrix} e^{-i\phi(t)}\sin\frac{\theta(t)}{2} \\ -\cos\frac{\theta(t)}{2} \end{pmatrix} \qquad E_- = -\frac{\hbar\omega_1}{2}$$



Calculating the Berry Phase

The adiabatic approximation applies:

$$\gamma = \int_{\mathcal{C}} i \langle \chi_+ | \nabla_{r,\theta,\phi} | \chi_+ \rangle \cdot d\boldsymbol{B}$$

$$\langle \chi_+ | \nabla_{r,\theta,\phi} | \chi_+ \rangle = i \frac{\sin^2(\theta/2)}{r \sin(\theta)} \hat{\phi}$$

Applying Stokes' theorem:

$$\gamma = \int_{\mathcal{S}(\mathcal{C})} i \nabla_{r,\theta,\phi} \times \langle \chi_+ | \nabla_{r,\theta,\phi} | \chi_+ \rangle \cdot d\boldsymbol{s}$$

$$\nabla_{r,\theta,\phi} \times \langle \chi_+ | \nabla_{r,\theta,\phi} | \chi_+ \rangle = \frac{i}{2r^2} \hat{r}$$

$$\gamma = -\frac{\Omega}{2}$$

Section 5

The Aharonov-Bohm Effect

The Electric Effect

1. Electron beam is split at point A.
2. Dual beams pass through *Faraday Cages* to which a voltage is applied.
3. Electron beams are recombined at point F.

$$\boldsymbol{H}(\boldsymbol{t}) = \boldsymbol{H}_0 + V(t)$$
$$\Psi(t) = \Psi_0 \exp(-i\mathcal{S})$$
$$\mathcal{S} = \int V(t)dt$$

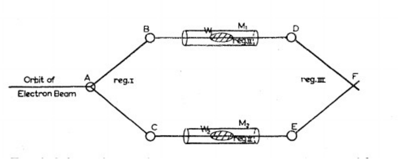


Figure: Electric effect schematic.

The Magnetic Effect

1. Electron beam is split at point A.
2. Dual beams pass over and under a solenoid coil producing a constant magnetic field in a infinitesimally small region at the origin.
3. Electron beams are recombined at point F.

$$\boldsymbol{H} = \frac{\left[\boldsymbol{P} - \frac{e}{c}\boldsymbol{A}\right]^2}{2m}$$

$$\Psi(t) = \Psi_0 \exp(-i\mathcal{S})$$

$$\mathcal{S} = \int \boldsymbol{A} \cdot d\boldsymbol{x}$$

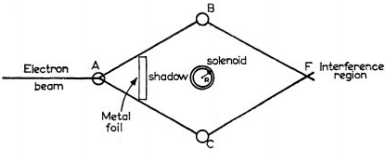


Figure: Magnetic effect schematic.

The Berry Phase

The General Case:

$$\boldsymbol{H} = \frac{\left[\boldsymbol{P} - \frac{e}{c}\boldsymbol{A}\right]^2}{2m} + V(t)$$

$$\Psi(t) = \Psi_0 \exp(-i\mathcal{S})$$

$$\triangle\mathcal{S} = \oint V(t)dt + \boldsymbol{A}\cdot d\boldsymbol{x}$$

The Berry Phase:

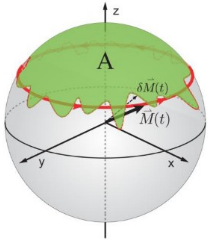
$$\gamma = \oint i \langle \Psi(t) | \nabla_{\boldsymbol{r}} | \Psi(t) \rangle \, d\boldsymbol{r} = \mathcal{S}$$

Section 6

Outlook

Quantum Information

- Use of the geometric phase in a universal set of quantum gates
- Fault tolerance because of geometric nature

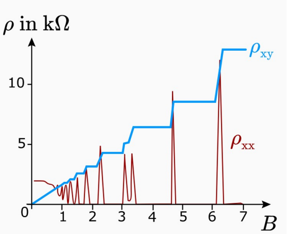


$$\hat{H} = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \qquad \hat{\phi} = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix} \qquad \hat{U}_{cphase} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{bmatrix}$$

Quantum Hall Effect

- Quantized conductivity closely related to the Berry curvature (Ω_n) in the Thoules, Kohomoto, Nightingale and den Nijs (TKNN) formalism.

$$\sigma_{xy} = \frac{e^2}{\hbar} \sum_n \int \frac{dk}{2\pi} \Omega_z^n$$



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- The Berry Phase arises naturally in the adiabatic theorem describing the quantum evolution of a state in a system undergoing infinitesimally small changes to its parameters.
- The Berry Phase is just one example of the much wider phenomena of holonomy.