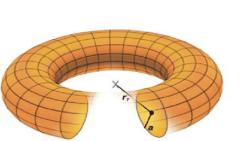
The Berry Phase Jacob MacWilliams

Universität Konstanz



 $S_r = 4\pi^2 r_r a$

 $V_T = 2\pi^2 r_T a^2$

 $V_s = 4/3\pi r_s^3$ $S_s = 4\pi r^2$

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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 $|\Psi_n\rangle \to \exp(i\alpha_n) |\Psi_n\rangle$.
- ⇒ Phase is not physical!

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

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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:

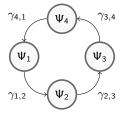
$$\gamma_{1,2} = -\text{arg} \langle \Psi_1 | \Psi_2 \rangle$$
 $\gamma_{1,2} \in (-\pi, \pi]$

Gauge Transformation:

$$|\Psi_{j}\rangle
ightarrow \exp(i\alpha_{j}) |\Psi_{j}\rangle \ \exp(-i\gamma_{1,2})
ightarrow \exp(-i\gamma_{1,2} + i(\alpha_{2} - \alpha_{1}))$$

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:

$$\gamma_L = \operatorname{Tr}\left(\prod_{i=0}^{N-1} \ket{\Psi_i}ra{\Psi_i}\right)$$

Discrete:

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

Continuous:

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

Discrete:

- ▶ Parameter Space: $\mathbb{P} = \mathbb{N}_0$
- ► Wave Function

$$\Psi: \mathbb{P} \to \mathcal{H}, \quad n \mapsto |\Psi_n\rangle$$

Continuous:

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

$$\Psi: \mathbb{P} \to \mathcal{H}, \quad \mathbf{R} \mapsto |\Psi(\mathbf{R})\rangle$$

Discrete:

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

$$\Psi: \mathbb{P} \to \mathcal{H}, \quad n \mapsto |\Psi_n\rangle$$

▶ Path: $C = [n_0, n_1, ..., n_{N-1}]$

Continuous:

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

$$\Psi: \mathbb{P} \to \mathcal{H}, \quad \mathbf{R} \mapsto |\Psi(\mathbf{R})\rangle$$

▶ Path: $C: [0,1) \rightarrow \mathcal{M}, \quad t \mapsto R(t)$

Discrete:

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

$$\Psi: \mathbb{P} \to \mathcal{H}, \quad n \mapsto |\Psi_n\rangle$$

- ▶ Path: $C = [n_0, n_1, ..., n_{N-1}]$
- ► Berry Phase: $\gamma(\mathcal{C}) = \sum_{i=0}^{N} \gamma_{n_{i \bmod N}, n_{i+1 \bmod N}}$

Continuous:

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

$$\Psi: \mathbb{P} o \mathcal{H}, \quad \textit{\textbf{R}} \mapsto |\Psi(\textit{\textbf{R}})
angle$$

- ▶ Path: $C: [0,1) \to \mathcal{M}, \quad t \mapsto R(t)$
- Berry Phase:

$$\gamma(\mathcal{C}) = \lim_{dt \to 0} \oint \gamma_{\mathcal{C}(t), \mathcal{C}(t+dt)} d\mathbf{R}$$

Discrete:

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

$$\Psi: \mathbb{P} \to \mathcal{H}, \quad n \mapsto |\Psi_n\rangle$$

- ▶ Path: $C = [n_0, n_1, ..., n_{N-1}]$
- ► Berry Phase:

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

The sum of the relative phases of each wave function connected by the path C.

Continuous:

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

$$\Psi: \mathbb{P} \to \mathcal{H}, \quad \textit{\textbf{R}} \mapsto |\Psi(\textit{\textbf{R}})\rangle$$

- ▶ Path: $C: [0,1) \to \mathcal{M}, \quad t \mapsto R(t)$
- ▶ Berry Phase:

$$\gamma(\mathcal{C}) = \lim_{dt \to 0} \oint \gamma_{\mathcal{C}(t), \mathcal{C}(t+dt)} d\mathbf{R}$$

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

The Berry Connection

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

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

$$1 - i\gamma_{R,R+r} = \langle \Psi(R) | (|\Psi(R) \rangle + \nabla_R |\Psi(R) \rangle)$$

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

$$\gamma(\mathcal{C}) = \oint i \langle \Psi(R) | \nabla_R | \Psi(R) \rangle dR$$

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:

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

Gauge Transformation:

$$|\Psi(\emph{\textbf{R}})
angle
ightarrow \exp(ilpha(\emph{\textbf{R}}))\,|\Psi(\emph{\textbf{R}})
angle \ \mathcal{A}
ightarrow \mathcal{A}-
ablalpha(\emph{\textbf{R}})$$

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:

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

Gauge Transformation:

$$egin{aligned} |\Psi(\pmb{R})
angle &
ightarrow \exp(ilpha(\pmb{R}))\,|\Psi(\pmb{R})
angle \ \Omega_{\mu,
u}(\pmb{R}) &
ightarrow \partial_{\mu}(\mathcal{A}_{
u}-\partial_{
u}lpha(\pmb{R})) - \partial_{
u}(\mathcal{A}_{\mu}-\partial_{\mu}lpha(\pmb{R})) \end{aligned}$$

Magnetic Analogies

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

Phase:

$$\gamma(C) = \oint \mathbf{A} \cdot d\mathbf{R}$$
$$= \int_{\mathcal{S}(C)} \nabla \times \mathbf{A} \cdot d\mathbf{s}$$
$$= \int_{\mathcal{S}(C)} \mathbf{\Omega} \cdot d\mathbf{s}$$

Flux:

$$\Phi(C) = \oint \mathbf{A} \cdot d\mathbf{R}$$
$$= \int_{S(C)} \nabla \times \mathbf{A} \cdot d\mathbf{s}$$
$$= \int_{S(C)} \mathbf{B} \cdot d\mathbf{s}$$

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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.
$$\frac{\langle m(t)|\dot{H}(t)|n(t)\rangle}{E_m(t)-E_n(t)}=0$$

Proof: Part I

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

$$i\hbar \ket{\dot{\Psi}(t)} = \boldsymbol{H}(t)\ket{\Psi(t)}$$

$$L.H.S = \sum_{n} c_n(t) E_n(t) |n(t)|$$

$$egin{aligned} extbf{\textit{L.H.S}} &= \sum_n c_n(t) E_n(t) \ket{n(t)} \ i\hbar \sum_n \left[\dot{c}_n(t) \ket{n(t)} + c_n(t) \ket{\dot{n}(t)}
ight] = extbf{\textit{R.H.S}} \end{aligned}$$

$$i\hbar\dot{c}_{m}(t)+i\hbar\sum_{n}\langle m(t)|\dot{n}(t)\rangle=c_{m}(t)E_{m}(t)$$

Proof: Part II

- 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 $\langle m(t)|\dot{n}(t)\rangle$.

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

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

$$\begin{split} \textbf{\textit{L.H.S}} &= \textit{E}_{\textit{n}}(t) \left\langle \textit{m}(t) | \dot{\textit{n}}(t) \right\rangle \\ \left\langle \textit{m}(t) | \dot{\textit{H}}(t) | \textit{n}(t) \right\rangle + \textit{E}_{\textit{m}} \left\langle \textit{m}(t) | \dot{\textit{n}}(t) \right\rangle = \textit{R.H.S} \end{split}$$

$$\langle m(t)|\dot{n}(t)\rangle = rac{\langle m(t)|\dot{H}(t)|n(t)
angle}{E_n(t)-E_m(t)} \quad (m
eq n)$$

Proof: Conclusion

8. For
$$\langle m(t)|\dot{H}(t)|n(t)\rangle \ll E_m(t) - E_n(t)$$
 and $\forall n \quad \forall t : E_m(t) - E_n(t) \neq 0$.

9. Solving the resulting differential equation for $c_m(t)$.

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

$$\dot{c}_m(t) + \left(rac{i}{\hbar} \mathcal{E}_m(t) + \langle m(t) | \dot{m}(t)
angle
ight) c_m(t) = extbf{\textit{R.H.S}}$$

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

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

Proof: The Berry Phase

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

$$H(t) = H(R(t)) \quad \Psi(t) = \Psi(R(t))$$

Therefore:

$$\gamma = \int_0^t i \langle m(R(t)) | \dot{m}(R(t)) \rangle dt$$

$$= \int_0^t i \langle m(R(t)) | \nabla_R | m(R(t)) \rangle \dot{R}(t) dt$$

$$= \oint i \langle m(R) | \nabla_R | m(R) \rangle dR$$

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Defining the System

System:

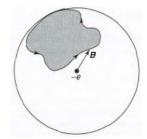
Magnetic moment at the origin in the presence of a magnetic field B of fixed magnitude, moving along some closed path \mathcal{C} .

$$m{B}(t) = B_0 egin{pmatrix} \sin heta(t) \cos \phi(t) \ \sin heta(t) \sin \phi(t) \ \cos heta(t) \end{pmatrix}$$

$$\boldsymbol{H}(t) = \frac{\hbar e}{2m} \boldsymbol{B} \cdot \boldsymbol{\sigma}$$

$$\chi_{+}(t) = \begin{pmatrix} \cos \frac{\theta(t)}{2} \\ e^{i\phi(t)} \sin \frac{\theta(t)}{2} \end{pmatrix} \qquad E_{+} = \frac{\hbar\omega_{1}}{2}$$

$$\chi_{-}(t) = \begin{pmatrix} e^{-i\phi(t)} \sin \frac{\theta(t)}{2} \\ -\cos \frac{\theta(t)}{2} \end{pmatrix} \qquad E_{-} = -\frac{\hbar\omega_{1}}{2}$$



Calculating the Berry Phase

The adiabatic approximation applies:

$$\gamma = \int_{\mathcal{C}} i \langle \chi_{+} | \nabla_{r,\theta,\phi} | \chi_{+} \rangle \cdot d\mathbf{B}$$
$$\langle \chi_{+} | \nabla_{r,\theta,\phi} | \chi_{+} \rangle = i \frac{\sin^{2}(\theta/2)}{r \sin(\theta)} \hat{\phi}$$

Applying Stokes' theorem:

$$\begin{split} \gamma &= \int_{\mathcal{S}(\mathcal{C})} i \nabla_{r,\theta,\phi} \times \langle \chi_+ | \nabla_{r,\theta,\phi} | \chi_+ \rangle \cdot d\mathbf{s} \\ \nabla_{r,\theta,\phi} \times \langle \chi_+ | \nabla_{r,\theta,\phi} | \chi_+ \rangle &= \frac{i}{2r^2} \hat{r} \\ \gamma &= -\frac{\Omega}{2} \end{split}$$

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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.

$$egin{aligned} m{H}(t) &= m{H}_0 + V(t) \ m{\Psi}(t) &= m{\Psi}_0 \exp(-i\mathcal{S}) \ m{\mathcal{S}} &= \int V(t) dt \end{aligned}$$

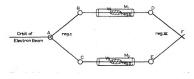


Figure: Electric effect schematic.

The Magnetic Effect

- 1. Electron beam is split at point A.
- 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.

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

$$\Psi(t) = \Psi_{0} \exp(-iS)$$

$$S = \int A \cdot dx$$

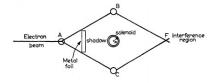


Figure: Magnetic effect schematic.

The Berry Phase

The General Case:

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

$$\Psi(t) = \Psi_{0} \exp(-iS)$$

$$\triangle S = \oint V(t)dt + A \cdot dx$$

The Berry Phase:

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

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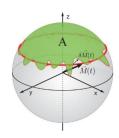
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Quantum Information

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

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

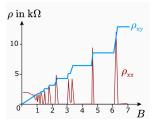


$$\hat{U}_{cphase} = egin{bmatrix} 1 & 0 & 0 & 0 \ 0 & 1 & 0 & 0 \ 0 & 0 & 1 & 0 \ 0 & 0 & 0 & e^{i\phi} \end{bmatrix}$$

Quantum Hall Effect

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

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



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- The Berry Phase is a gauge-invariant property of the manifold describing the parameter space of the system.
- It is given as the integral of the berry connection over the parametrized path $(\oint i \langle \Psi(\mathbf{R})|\nabla|\Psi(\mathbf{R})\rangle)$ which can be considered as the relative phase of two infinitesimally close states.

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- It is given as the integral of the berry connection over the parametrized path $(\oint i \langle \Psi(\mathbf{R})|\nabla|\Psi(\mathbf{R})\rangle)$ which can be considered as the relative phase of two infinitesimally close states.
- ▶ 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.

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Conclusion

- The Berry Phase is a gauge-invariant property of the manifold describing the parameter space of the system.
- It is given as the integral of the berry connection over the parametrized path $(\oint i \langle \Psi(\mathbf{R}) | \nabla | \Psi(\mathbf{R}) \rangle)$ which can be considered as the relative phase of two infinitesimally close states.
- 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.