Berry's Geometric Phase

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The landmark paper, 1983-1984

Proc. R. Soc. Lond. A **392**, 45–57 (1984)
Printed in Great Britain

Quantal phase factors accompanying adiabatic changes

By M. V. Berry, F.R.S.
H. H. Wills Physics Laboratory, University of Bristol,
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(*Received* 13 *June* 1983)

- Very simple concept, nonetheless missed by the founding fathers of QM in the 1920s and 1930s
- Nowadays in any modern elementary QM textbook

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Sakurai QM textbook, p. 464

SUPPLEMENT I

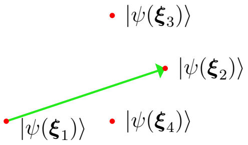
Adiabatic Change and Geometrical Phase

When the author died in 1982, this book was left in manuscript form; subsequently, there have been some new developments in quantum mechanics. The most important development is a definitive formulation of geometrical phases, introduced by M. V. Berry in 1983. The phase factors accompanying adiabatic changes are expressed in concise and elegant forms and have found universal applications in various fields of physics, thus giving a new viewpoint to quantum theory. We review here the physical consequences of these phases, which have in fact been used unconsciously in some cases already, by adding a supplement to the Japanese version of the text. (Here in the new English edition of *Modern Quantum Mechanics* we are providing a translation from Japanese of this supplement, prepared by Professor Akio Sakurai of Kyoto Sangyo University for the Japanese version of the book. The Editor deeply appreciates Professor Akio Sakurai's guidance on an initial translation provided by his student, Yasunaga Suzuki, as a term paper for the graduate quantum mechanics course here at the University of Hawaii—Manoa.)

Basics

Parametric Hamiltonian, non degenerate ground state

$$H(\xi)|\psi(\xi)\rangle = E(\xi)|\psi(\xi)\rangle \qquad \text{parameter } \xi\text{: “slow variable”}$$



$$e^{-i\Delta\varphi_{12}} = \frac{\langle\psi(\boldsymbol{\xi}_1)|\psi(\boldsymbol{\xi}_2)\rangle}{|\langle\psi(\boldsymbol{\xi}_1)|\psi(\boldsymbol{\xi}_2)\rangle|}$$

$$\Delta\varphi_{12} = -\,\mathrm{Im}\,\log\,\langle\psi(\boldsymbol{\xi}_1)|\psi(\boldsymbol{\xi}_2)\rangle$$

$$\gamma = \Delta\varphi_{12} + \Delta\varphi_{23} + \Delta\varphi_{34} + \Delta\varphi_{41}$$

$$= -\,\mathrm{Im}\,\log\,\langle\psi(\boldsymbol{\xi}_1)|\psi(\boldsymbol{\xi}_2)\rangle\langle\psi(\boldsymbol{\xi}_2)|\psi(\boldsymbol{\xi}_3)\rangle\langle\psi(\boldsymbol{\xi}_3)|\psi(\boldsymbol{\xi}_4)\rangle\langle\psi(\boldsymbol{\xi}_4)|\psi(\boldsymbol{\xi}_1)\rangle$$

Gauge-invariant!

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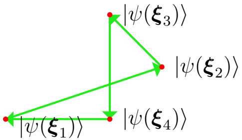

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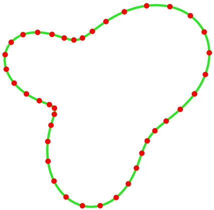
Gauge-invariant!

From discrete "geometry" to differential geometry

A smooth closed curve C in ξ space



$$\mathrm{e}^{-i\Delta\varphi} = \frac{\langle\psi(\boldsymbol{\xi})|\psi(\boldsymbol{\xi}+\Delta\boldsymbol{\xi})\rangle}{|\langle\psi(\boldsymbol{\xi})|\psi(\boldsymbol{\xi}+\Delta\boldsymbol{\xi})\rangle|}$$

If we choose a **differentiable gauge**:

$$-i\Delta\varphi \simeq \langle\psi(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}}\psi(\boldsymbol{\xi})\rangle \cdot \Delta\boldsymbol{\xi}$$

$$\gamma = \sum_{s=1}^{M} \Delta\varphi_{s,s+1} \longrightarrow \oint_C d\varphi$$

$$d\varphi = \mathcal{A}(\boldsymbol{\xi}) \cdot d\boldsymbol{\xi} = i\,\langle\psi(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}}\psi(\boldsymbol{\xi})\rangle \cdot d\boldsymbol{\xi}$$

$d\varphi$ linear differential form, $i\,\langle\psi(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}}\psi(\boldsymbol{\xi})\rangle$ vector field

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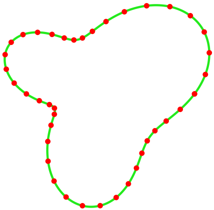

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Berry connection & Berry curvature

- Domain S: $\boldsymbol{\xi} \in S \subset \mathbb{R}^d$
- Berry **connection**
  $\boldsymbol{\mathcal{A}}(\boldsymbol{\xi}) = i \langle \psi(\boldsymbol{\xi}) | \nabla_{\boldsymbol{\xi}} \psi(\boldsymbol{\xi}) \rangle$
  - **real**, nonconservative vector field
  - gauge-dependent
  - “geometrical” vector potential
  - a.k.a. “gauge potential”
- Berry **curvature** $(\boldsymbol{\xi} \in \mathbb{R}^3)$
  $\boldsymbol{\Omega}(\boldsymbol{\xi}) = \nabla_{\boldsymbol{\xi}} \times \boldsymbol{\mathcal{A}}(\boldsymbol{\xi}) = i \langle \nabla_{\boldsymbol{\xi}} \psi(\boldsymbol{\xi}) | \times | \nabla_{\boldsymbol{\xi}} \psi(\boldsymbol{\xi}) \rangle$
  - gauge-invariant (hence observable)
  - geometric analog of a magnetic field
  - a.k.a. “gauge field”

The Berry connection is real

$$\langle\psi(\boldsymbol{\xi})|\psi(\boldsymbol{\xi})\rangle = 1 \qquad \forall\boldsymbol{\xi}$$

$$\begin{aligned}\nabla_{\boldsymbol{\xi}}\langle\psi(\boldsymbol{\xi})|\psi(\boldsymbol{\xi})\rangle &= 0\\ &= \langle\nabla_{\boldsymbol{\xi}}\psi(\boldsymbol{\xi})|\psi(\boldsymbol{\xi})\rangle + \langle\psi(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}}\psi(\boldsymbol{\xi})\rangle\\ &= 2\,\mathrm{Re}\,\langle\psi(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}}\psi(\boldsymbol{\xi})\rangle\end{aligned}$$

$\langle\psi(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}}\psi(\boldsymbol{\xi})\rangle$ purely imaginary

$$\mathcal{A}(\boldsymbol{\xi}) = i\;\langle\psi(\boldsymbol{\xi})|\nabla_{\boldsymbol{\xi}}\psi(\boldsymbol{\xi})\rangle \qquad \text{real} \qquad (1)$$

Last but not least:

What about time-reversal invariant systems?

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What about time-reversal invariant systems?

Berry connection vs. perturbation theory

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\begin{aligned}
& |\psi_0(\boldsymbol{\xi} + \Delta\boldsymbol{\xi})\rangle - |\psi_0(\boldsymbol{\xi})\rangle \\
\simeq \;\; & \sum_{n \neq 0}{}' |\psi_n(\boldsymbol{\xi})\rangle \frac{\langle \psi_n(\boldsymbol{\xi})| \, [\, H(\boldsymbol{\xi} + \Delta\boldsymbol{\xi}) - H(\boldsymbol{\xi}) \,] \, |\psi_0(\boldsymbol{\xi})\rangle}{E_0(\boldsymbol{\xi}) - E_n(\boldsymbol{\xi})}
\end{aligned}
$$

$$
|\partial_\alpha \Psi_0(\xi)\rangle = \sum_{n \neq 0}{}' |\Psi_n(\xi)\rangle \frac{\langle \Psi_n(\xi)|\partial_\alpha H(\xi)|\Psi_0(\xi)\rangle}{E_0(\xi) - E_n(\xi)}
$$

$$
\mathcal{A}_\alpha(\xi) = i\langle \psi_0(\xi)|\partial_\alpha \psi_0(\xi)\rangle = 0
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“parallel transport” gauge

Berry connection vs. perturbation theory

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“parallel transport” gauge

Parallel transport

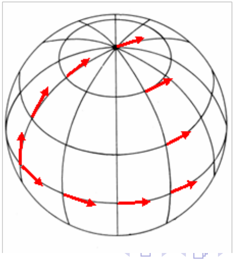
$$|\Delta\psi_0(\xi)\rangle = \sum_{n\neq 0}{}' |\psi_n(\xi)\rangle \frac{\langle\psi_n(\xi)|\,[\,H(\xi+\Delta\xi) - H(\xi)\,]\,|\psi_0(\xi)\rangle}{E_0(\xi) - E_n(\xi)}$$

$$|\psi_0(\xi+\Delta\xi)\rangle \simeq |\psi_0(\xi)\rangle + |\Delta\psi_0(\xi)\rangle$$

$|\Delta\psi_0(\xi)\rangle$ **orthogonal** to $|\psi_0(\xi)\rangle$

Differential Geometry:

Gaussian curvature of the spherical surface $\Omega = 1/R^2$



$\int_\Sigma \Omega d\sigma =$ angular mismatch

Connection?

Berry connection vs. perturbation theory, better

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|\psi_0(\xi+\Delta\xi)\rangle &\to [\,|\psi_0(\xi)\rangle + |\Delta\psi_0(\xi)\rangle\,]\,\mathrm{e}^{-i\Delta\varphi(\xi)} \\
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Berry curvature: perturbation theory is OK

The Berry curvature is **gauge invariant**

$$\begin{aligned}\boldsymbol{\Omega}(\boldsymbol{\xi}) &= \nabla_{\boldsymbol{\xi}} \times \boldsymbol{\mathcal{A}}(\boldsymbol{\xi}) \qquad (\boldsymbol{\xi} \in \mathbb{R}^3) \\ &= i{\sum_{n\neq 0}}' \frac{\langle \psi_0(\boldsymbol{\xi})|\nabla H(\boldsymbol{\xi})|\psi_n(\boldsymbol{\xi})\rangle \times \langle \psi_n(\boldsymbol{\xi})|\nabla H(\boldsymbol{\xi})|\psi_0(\boldsymbol{\xi})\rangle}{[E_0(\boldsymbol{\xi}) - E_n(\boldsymbol{\xi})]^2}\end{aligned}$$

$\Omega(\xi)$ **singular at degeneracy points**

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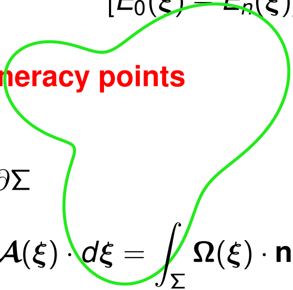

Stokes' theorem: $C = \partial\Sigma$

$$\gamma = \oint_{\partial\Sigma} \boldsymbol{\mathcal{A}}(\xi) \cdot d\xi = \int_{\Sigma} \boldsymbol{\Omega}(\xi) \cdot \mathbf{n}\, d\sigma$$

.......only if Σ is **simply connected!**

Berry phase

- Loop integral of the Berry connection on a closed path:

$$\gamma = \oint_C \boldsymbol{\mathcal{A}}(\xi) \cdot d\xi$$

- Berry phase, gauge invariant modulo 2π
- corresponds to **measurable** effects

Main message of Berry's 1984 paper:

- In quantum mechanics, **any** gauge-invariant quantity is potentially a physical observable

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Coupling to “the rest of the Universe”

- γ cannot be cast as the expectation value of **any** Hermitian operator: instead, it is a gauge-invariant **phase** of the wavefunction
- The quantum system is **not** isolated:
  the parameter ξ summarizes the effect of “the rest of the Universe”
- **Slow variables:** ξ (e.g., a nuclear coordinate).
  Fast variables: here, the electronic coordinates
- For a genuinely isolated system, no Berry phase occurs and all observable effects **are** indeed expectation values of some operators
- What about classical mechanics?

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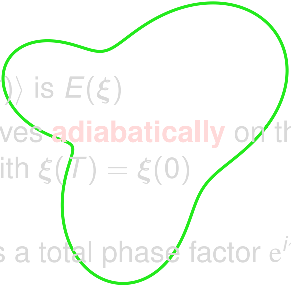
Semantics: why "Geometric"?

So far, everything **time-independent**.
Suppose instead that:

- The energy of $|\psi(\xi)\rangle$ is $E(\xi)$
- The parameter moves **adiabatically** on the closed path in time t: $\xi \to \xi(t)$, with $\xi(T) = \xi(0)$



Then the state acquires a total phase factor $e^{i\gamma} e^{i\alpha(T)}$

- The phase γ is independent of the details of motion: hence **"geometric"**
- The additional phase is the **"dynamical phase"**, and does depend on the motion: $\alpha(T) = -\frac{1}{\hbar}\int_0^T dt\, E(\xi(t))$

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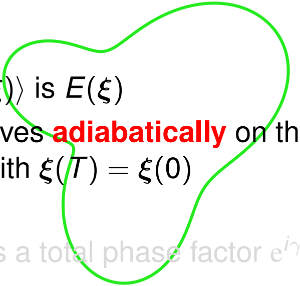

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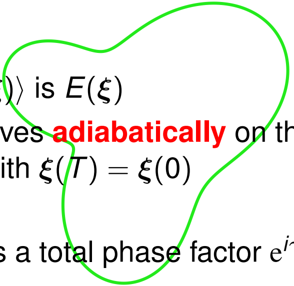

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$$\gamma = \oint_C \mathcal{A}(\xi) \cdot d\xi$$

  - Berry phase, gauge invariant **only modulo** 2π
  - corresponds to **measurable** effects

- If $C = \partial\Sigma$ is the boundary of Σ, then (Stokes th.):

$$\gamma = \oint_{\partial\Sigma} \mathcal{A}(\xi) \cdot d\xi = \int_\Sigma d\sigma \, \mathbf{\Omega}(\xi) \cdot \hat{\mathbf{n}}$$

  - requires Σ to be simply connected
  - requires $\mathcal{A}$ to be regular on Σ
  - no longer arbitrary mod 2π

- What about integrating the curvature on a **closed** surface?

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A simple example: Two level system

$$\begin{aligned} H(\boldsymbol{\xi}) &= \boldsymbol{\xi} \cdot \vec{\sigma} \qquad \text{nondegenerate for } \boldsymbol{\xi} \neq 0 \\ &= \xi \left(\sin\vartheta \cos\varphi \, \sigma_x + \sin\vartheta \sin\varphi \, \sigma_y + \cos\vartheta \, \sigma_z \right) \end{aligned}$$

lowest eigenvalue $-\xi$

lowest eigenvector $|\psi(\vartheta, \varphi)\rangle = \begin{pmatrix} \sin\frac{\vartheta}{2} e^{-i\varphi} \\ -\cos\frac{\vartheta}{2} \end{pmatrix}$

$$\begin{aligned} \mathcal{A}_\vartheta &= i\langle\psi|\partial_\vartheta\psi\rangle = 0 \\ \mathcal{A}_\varphi &= i\langle\psi|\partial_\varphi\psi\rangle = \sin^2\frac{\vartheta}{2} \\ \boldsymbol{\Omega} &= \partial_\vartheta \mathcal{A}_\varphi - \partial_\varphi \mathcal{A}_\vartheta = \frac{1}{2}\sin\vartheta \end{aligned}$$

- Ω gauge invariant
- What about $\mathcal{A}$? **Obstruction!**

A simple example: Two level system

$$\begin{aligned} H(\boldsymbol{\xi}) &= \boldsymbol{\xi}\cdot\vec{\sigma} \qquad \text{nondegenerate for } \boldsymbol{\xi}\neq 0 \\ &= \xi\left(\sin\vartheta\cos\varphi\,\sigma_x + \sin\vartheta\sin\varphi\,\sigma_y + \cos\vartheta\,\sigma_z\right) \end{aligned}$$

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lowest eigenvector $|\psi(\vartheta,\varphi)\rangle = \begin{pmatrix} \sin\frac{\vartheta}{2}e^{-i\varphi} \\ -\cos\frac{\vartheta}{2} \end{pmatrix}$

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Integrating the Berry curvature

- Gauss-Bonnet-Chern theorem (1940):

$$\frac{1}{2\pi}\int_{S^2} \mathbf{\Omega}(\xi)\cdot\mathbf{n}\, d\sigma = \text{topological integer} \in \mathbb{Z}$$

- Integrating $\Omega(\vartheta,\varphi)$ over $[0,\pi]\times[0,2\pi]$:

$$\frac{1}{2\pi}\int d\vartheta d\varphi\, \frac{1}{2}\sin\vartheta = 1 \qquad \text{Chern number } C_1$$

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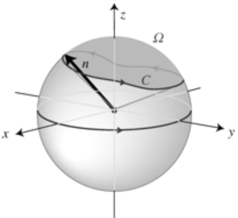

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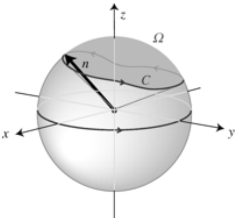

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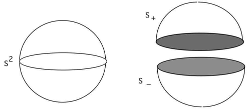
The sphere as the sum of two half spheres



$$
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2\pi C_1 &= \int_{S^2} \boldsymbol{\Omega}(\xi)\cdot\mathbf{n}\, d\sigma \\
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\end{aligned}
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Stokes: $$\int_{S_\pm} \boldsymbol{\Omega}(\xi)\cdot\mathbf{n}\, d\sigma = \pm \oint_C \boldsymbol{\mathcal{A}}_\pm(\xi)\cdot d\xi$$

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Gauge choice: $\mathcal{A}_-(\xi)$ regular in the lower hemisphere: hence it has an **obstruction** in the upper hemisphere

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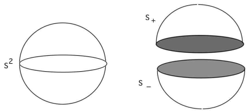

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Bloch orbitals (noninteracting electrons in this talk)

- Lattice-periodical Hamiltonian (no **macroscopic** B field); 2d, single band, spinless electrons

$$\begin{aligned} H|\psi_{\mathbf{k}}\rangle &= \varepsilon_{\mathbf{k}}|\psi_{\mathbf{k}}\rangle \\ H_{\mathbf{k}}|u_{\mathbf{k}}\rangle &= \varepsilon_{\mathbf{k}}|u_{\mathbf{k}}\rangle \qquad |u_{\mathbf{k}}\rangle = \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}|\psi_{\mathbf{k}}\rangle \quad H_{\mathbf{k}} = \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}H\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} \end{aligned}$$

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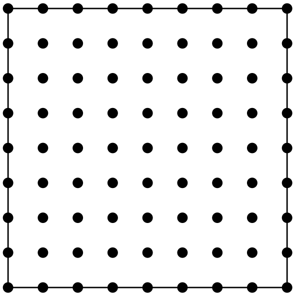
Computing the Chern number

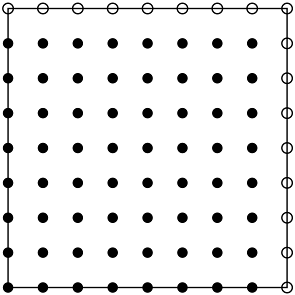
Discretized reciprocal cell



Computing the Chern number

Discretized reciprocal cell

Periodic gauge choice:
where is the obstruction?



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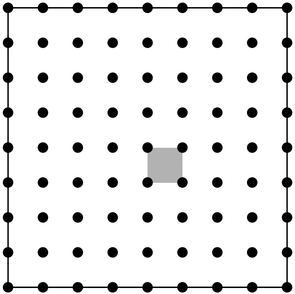

Curvature $\equiv$ Berry phase per unit (reciprocal) area
Berry phase on a small square:

$$\gamma = -\text{Im}\log \langle u_{\mathbf{k}_1}|u_{\mathbf{k}_2}\rangle\langle u_{\mathbf{k}_2}|u_{\mathbf{k}_3}\rangle\langle u_{\mathbf{k}_3}|u_{\mathbf{k}_4}\rangle\langle u_{\mathbf{k}_4}|u_{\mathbf{k}_1}\rangle$$

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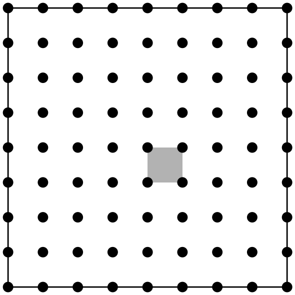

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Which branch of Im log?

Computing the Chern number

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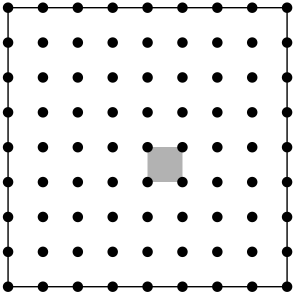

NonAbelian (many-band):

$$\gamma = -\text{Im log det } S(\mathbf{k}_1, \mathbf{k}_2) S(\mathbf{k}_2, \mathbf{k}_3) S(\mathbf{k}_3, \mathbf{k}_4) S(\mathbf{k}_4, \mathbf{k}_1)$$

$$S_{nn'}(\mathbf{k}_s, \mathbf{k}_{s'}) = \langle u_{n\mathbf{k}_s} | u_{n\mathbf{k}_{s'}} \rangle$$

Outline

The simplest geometrical property: Distance

Two state vectors $|\Psi_1\rangle$ and $|\Psi_2\rangle$ in the **same** Hilbert space

$$D_{12}^2 = -\log|\langle\Psi_1|\Psi_2\rangle|^2$$

- $D_{12}^2 = 0$ if the two quantum states coincide apart for an irrelevant phase: **gauge-invariant**
- $D_{12}^2 = \infty$ if the two states are orthogonal

A second geometrical property: Connection

$$D_{12}^2 = -\log|\langle\Psi_1|\Psi_2\rangle|^2 = -\log\langle\Psi_1|\Psi_2\rangle - \log\langle\Psi_2|\Psi_1\rangle$$

- The two terms are **not** gauge-invariant
- Each of the two terms is a complex number
- What is the meaning of $\text{Im}\log\langle\Psi_1|\Psi_2\rangle$?

$$\langle\Psi_1|\Psi_2\rangle = |\langle\Psi_1|\Psi_2\rangle| e^{i\varphi_{12}}$$

$$-\text{Im}\log\langle\Psi_1|\Psi_2\rangle = \varphi_{12}, \qquad \varphi_{21} = -\varphi_{12}$$

- The connection fixes the **phase difference**
- The connection is **arbitrary**
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Differential quantities in quantum geometry

The state vector $|\Psi_{\boldsymbol{\kappa}}\rangle$ depends on the continuous parameter $\boldsymbol{\kappa}$

- Quantum metric $g_{\alpha\beta}$:

$$d\,D^2 = D^2_{\boldsymbol{\kappa},\boldsymbol{\kappa}+d\boldsymbol{\kappa}} = g_{\alpha\beta} d\kappa_\alpha d\kappa_\beta$$

- Berry connection $\mathcal{A}_\alpha$:

$$d\,\varphi = \mathcal{A}_\alpha d\kappa_\alpha$$

- Berry curvature $\Omega_{\alpha\beta} = \partial_{\kappa_\alpha} \mathcal{A}_\beta - \partial_{\kappa_\beta} \mathcal{A}_\alpha$

$$d \times d\varphi = \Omega_{\alpha\beta}\, d\kappa_\alpha d\kappa_\beta$$

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A more general geometrical quantity

- Beside the state vectors, even the **Hamiltonian** is involved:

$$H\,|\Psi_0\rangle = E_0|\Psi_0\rangle$$

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2-form