Off-diagonal geometric phases

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OUTLINE

- Parallel transport & geometric phases

- **Off-diagonal phases**
  - Definition
  - Generalizations
  - Applications
  - Further work
  - Examples

- Experimental evidence
  - Neutron spin interferometry
  - Conical intersections in “quantum billiards”

- Conclusions
Parallel transport and geometric phase

A vector field $|\psi\rangle$ depending on a multidimensional parameter $\vec{q}$

$$|\psi(\vec{q})\rangle$$

ex.: $H_{\vec{q}}|\psi^j(\vec{q})\rangle = E^j(\vec{q})|\psi^j(\vec{q})\rangle$

$|\psi(\vec{q})\rangle$ is parallel-transported along a path $\vec{q}(\xi)$ if $\langle\psi(\vec{q}(\xi))| \frac{d}{d\xi} |\psi(\vec{q}(\xi))\rangle = 0$

$|\psi(\vec{q})\rangle$ acquires a geometric phase factor $\langle\psi(\vec{q}_{\text{fin}})|\psi(\vec{q}_{\text{fin}})\rangle / |\langle\psi(\vec{q}_{\text{in}})|\psi(\vec{q}_{\text{fin}})\rangle|$
The path $\vec{q} = \vec{q}(s)$ is time-parameterized and closes to an adiabatic loop.

The vectors involved are single-valued eigenstates of $H_{\vec{q}}|\psi^j_{\vec{q}}\rangle = E^j(q)|\psi^j_{\vec{q}}\rangle$.

The Berry phase associated to the loop is

$$\phi_j = \int_{s_{\text{in}}}^{s_{\text{fin}}} i \langle \psi^j(\vec{q}) | \nabla_{\vec{q}} \psi^j(\vec{q}) \rangle \cdot \dot{\vec{q}} \, ds = \int_\Gamma i \langle \psi^j(\vec{q}) | \nabla_{\vec{q}} \psi^j(\vec{q}) \rangle \cdot d\vec{q}$$

If $|\psi^j_{\vec{q}}\rangle$ is parallel transported then $\phi_j = 0$, but then generally $|\psi^j_{\vec{q}}\rangle$ is not single valued, and the BP is precisely $\phi_j = \text{Im} \log \langle \psi(\vec{q}_{\text{in}}) | \psi(\vec{q}_{\text{fin}}) \rangle$

The circuit integral of the 1-form (connection) can be recast into a surface integral of the 2-form (curvature) [Simon 1983]:

$$\phi_j = -\text{Im} \int_{S(\Gamma)} \langle \nabla_{\vec{q}} \psi^j(\vec{q}) \rangle \wedge | \nabla_{\vec{q}} \psi^j(\vec{q}) \rangle \cdot dS = \int_{S(\Gamma)} -\text{Im} \sum_{a < b} \langle \partial_{q_a} \psi^j | \partial_{q_b} \psi^j \rangle dq_a \wedge dq_b$$
Formulation in terms of Bargmann invariants

[Simon Mukunda 1993]

The continuous adiabatic evolution could be replaced by a discrete sequence of nonorthogonal states.
The evolution \( |\psi_k\rangle \longrightarrow |\psi_{k+1}\rangle \) need not even be unitary.
The geometric phase factor associated to this sequence of \( n \) states is:

\[
e^{i\phi} = \gamma = \Phi(\langle \psi_1 | \psi_2 \rangle \langle \psi_2 | \psi_3 \rangle \ldots \langle \psi_{n-1} | \psi_n \rangle \langle \psi_n | \psi_1 \rangle)
\]

with \( \Phi(z) = z/|z| \)
for complex \( z \neq 0 \).

Phase tracking algorithms
Extensions

- The single-state $|\psi^j\rangle$ may be replaced by a degenerate $n$-dimensional space: the “phase” relation becomes a whole unitary matrix in $SU(n)$, an element of a non abelian group [Wilczek Zee 1984].

- The path $\Gamma$ need not be closed (Pancharathnam 1956).

the open-path phase can be reduced to a closed-path phase by closing it with a geodesic [Samuel Bhandari 1988] provided that $\langle \psi(q_{\text{in}})|\psi(q_{\text{fin}}) \rangle \neq 0$
What about the relative phases of several vectors $|\psi_1(\vec{q})\rangle$, $|\psi_2(\vec{q})\rangle$, ... in a nondegenerate context? Anything measurable there?
Another generalization!?! 

Take states $|\psi_j^\parallel(\vec{q})\rangle$ parallel-transported from $\vec{q}_{\text{in}}$ to $\vec{q}_{\text{fin}}$ along path $\Gamma$: their Berry-Pancharatnam phase factor are

$$e^{i\phi_j^\Gamma} = \gamma_j^\Gamma \equiv \Phi\left(\langle \psi_j^\parallel(\vec{q}_{\text{in}})|\psi_j^\parallel(\vec{q}_{\text{fin}})\rangle\right) \quad \text{with } \Phi(z) = z/|z|$$

For $n$ states, consider the parallel-evolution matrix

$$U_{jk}^\Gamma = \langle \psi_j^\parallel(\vec{q}_{\text{in}})|\psi_k^\parallel(\vec{q}_{\text{fin}})\rangle,$$

the traditional Berry phase factor is just the diagonal element $\gamma_j^\Gamma \equiv \Phi(U_{jj}^\Gamma)$.

This is all is there for cyclic evolutions (matrix $U^\Gamma$ is diagonal). What about the information contents of the off-diagonal elements $U_{jk}^\Gamma$?
Is the phase factor $\sigma_{jk}^\Gamma \equiv \Phi\left(U_{jk}^\Gamma\right) = \Phi\left(\langle \psi_j^\parallel (q_{\text{in}}) | \psi_k^\parallel (q_{\text{fin}}) \rangle \right)$ measurable?

**NO!**

It depends on arbitrary choices of the initial phases of two different eigenstates $|\psi_j^\parallel (q_{\text{in}})\rangle$ and $|\psi_k^\parallel (q_{\text{in}})\rangle$.

$\sigma_{jk}^\Gamma$ is not gauge-invariant $\longrightarrow$ it is arbitrary, thus non-measurable.

Idea: combine two $\sigma$'s in the product:

$$\gamma_{jk}^\Gamma = \sigma_{jk}^\Gamma \sigma_{kj}^\Gamma = \Phi\left(\langle \psi_j^\parallel (q_{\text{in}}) | \psi_k^\parallel (q_{\text{fin}}) \rangle \langle \psi_k^\parallel (q_{\text{in}}) | \psi_j^\parallel (q_{\text{fin}}) \rangle \right)$$

$\gamma_{jk}^\Gamma$ is clearly gauge invariant.

MAIN FINDING: $\gamma_{jk}^\Gamma$ is a measurable geometric quantity!
Geometric interpretation [in projective Hilbert space]

\[ \gamma_j = \exp \left( -i \ \text{Im} \int_{S_j} dS \langle \nabla_1 \psi_j | \times | \nabla_2 \psi_j \rangle \right) \quad \text{(diagonal)} \]

\[ \gamma_{jk} = \exp \left( -i \ \text{Im} \int_{S_{jk}} dS \langle \nabla_1 \psi_j | \times | \nabla_2 \psi_j \rangle \right) \quad \text{(off-diagonal)} \]

Like standard single-state open-path geometric phase is reduced to a loop with the help of geodesics

\[ G = \text{geodesics} \]

\[ G_{jj}, G_{jk}, G_{kk} \]

\[ j(s_1), j(s_2), k(s_1), k(s_2) \]

\[ S_j, S_k, S_{jk}, \Gamma_j, \Gamma_k \]

\[ \text{dashed curves} \]
More measurable phases, general expression

\[ \gamma_{j_1 j_2 j_3 \ldots j_l}^{(l)} \Gamma = \sigma_{j_1 j_2}^{\Gamma} \sigma_{j_2 j_3}^{\Gamma} \cdots \sigma_{j_{l-1} j_l}^{\Gamma} \sigma_{j_l j_1}^{\Gamma} \]

\( l = 1 \): one-state “diagonal” phase

\( l = 2 \): two-states off-diagonal as above \( \sigma_{j_1 j_2} \sigma_{j_2 j_1} \)

\( l > 2 \): more intricate phase relations among off-diagonal components

Notes:

- any cyclic permutation of the indexes \( j_1 j_2 j_3 \ldots j_l \) is immaterial
- if one index is repeated, the associated \( \gamma^{(l)} \) can be decomposed into a product \( \gamma^{(l')} \gamma^{(l-l')} \) \( \rightarrow \) \( l \leq n \)
- \( n^2 \) real numbers fix the unitary matrix \( U^\Gamma \): only a finite number of \( \gamma^{(l)} \)'s are algebraically independent
Crucial example: Permutational case

\[
\begin{align*}
H(\vec{q}_1^P) &= \sum_j E_j |\psi_j\rangle \langle \psi_j| \\
H(\vec{q}_2^P) &= \sum_j E'_j |\psi_{P_j}\rangle \langle \psi_{P_j}|
\end{align*}
\]

\[P = \text{permutation of the } n \text{ eigenstates}\]

The only meaningful \(\sigma_{jk}^\Gamma\)'s are the \(n\) phase factors \(\sigma_{jP_j}^\Gamma\).
For example:

\[P_1 = 2; \ P_2 = 3; \ P_3 = 1 \quad \longrightarrow \quad U^\Gamma = \begin{pmatrix}
0 & e^{i\alpha_1} & 0 \\
0 & 0 & e^{i\alpha_2} \\
e^{i\alpha_3} & 0 & 0
\end{pmatrix}\]

Only well-defined \(\gamma^{(l)}\):

\[\gamma^{(3)}_{123} = \sigma_{12} \sigma_{23} \sigma_{31} = e^{i(\alpha_1 + \alpha_2 + \alpha_3)}\]
<table>
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<th>condition det $U^\Gamma = 1$</th>
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Application 1: Approximate permutational case

\[ U^\Gamma \approx \begin{pmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} & e^{i\alpha_1} \\ \epsilon_{21} & \epsilon_{22} & e^{i\alpha_2} & \epsilon_{24} \\ \epsilon_{31} & e^{i\alpha_3} & \epsilon_{32} & \epsilon_{34} \\ e^{i\alpha_4} & \epsilon_{41} & \epsilon_{42} & \epsilon_{44} \end{pmatrix} \]
Application 2: two-state system (qubit)

\[
U = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} = \begin{pmatrix} e^{i\beta} \cos \alpha & e^{i\chi} \sin \alpha \\ -e^{-i\chi} \sin \alpha & e^{-i\beta} \cos \alpha \end{pmatrix}
\]

Thus:

\[
\gamma_1 = \Phi(U_{11}) = \text{sgn}(\cos \alpha) e^{i\beta} \quad \gamma_2 = \Phi(U_{22}) = \text{sgn}(\cos \alpha) e^{-i\beta}
\]

\[
\gamma_{12} = \Phi(U_{12}U_{21}) = -\text{sgn}(\sin^2 \alpha) e^{i\chi} e^{-i\chi} = -1
\]

“trivial” case, like diagonal phase of single state
Application 3: \( H(\vec{q}_2) \longrightarrow -H(\vec{q}_1) \)

A special permutational case:

\[
U = \begin{pmatrix}
0 & 0 & 0 & 0 & e^{i\alpha_1} \\
0 & 0 & 0 & e^{i\alpha_2} & 0 \\
0 & 0 & e^{i\alpha_3} & 0 & 0 \\
0 & e^{i\alpha_4} & 0 & 0 & 0 \\
e^{i\alpha_5} & 0 & 0 & 0 & 0
\end{pmatrix}
\]

**Exact** because of symmetry (ex. spin systems, \( \vec{q} = \vec{B} \))

**Approximate** in perturbative expansion \( H(\vec{q}) = \vec{q} \cdot H^{(1)} + \ldots \) when for \( \vec{q} = 0 \) \( n \) states are degenerate (ex. quantum billiards...)
Comparison with nonabelian phases

Nonabelian

\[ |\psi(\vec{q}_{\text{fin}})\rangle \]

\[ |\psi(\vec{q}_{\text{in}})\rangle \]

\[ |\psi(\vec{q}_{\text{fin}})\rangle^\prime \]

\[ \Gamma \]

\[ \Gamma' \]

Abelian

\[ |\psi(\vec{q}_{\text{fin}})\rangle \]

\[ |\psi(\vec{q}_{\text{in}})\rangle \]

\[ |\psi(\vec{q}_{\text{fin}})\rangle^\prime \]

\[ \Gamma \]

\[ \Gamma' \]

\( n \) vectors remain *degenerate* along the evolution. The states can recombine within the \( n \)-dimensional subspace. Following a different path \( \Gamma' \) from \( \vec{q}_{\text{in}} \) to \( \vec{q}_{\text{fin}} \) one obtains a different mix of the final states \( \vec{q}_{\text{fin}} \): a completely different \( U_{jk}^{\Gamma} = \langle \psi_j^\parallel(\vec{q}_{\text{in}}) | \psi_k^\parallel(\vec{q}_{\text{fin}}) \rangle \) could be realized (invariance group \( SU(n) \)).

*nondegenerate* evolution. The final states \( |\psi_k^\parallel(\vec{q}_{\text{fin}})\rangle \) are fixed up to a phase for any path leading to \( \vec{q}_{\text{fin}} \rightarrow U^\Gamma \) is essentially fixed, except for some phase information captured by the diagonal and off-diagonal phases \( \gamma_{j_1j_2j_3...j_l}^{(1)} \). Invariance group: \( U(1) \times U(1) \times U(1) \times U(1) \times ... \).
Further theoretical work

- Relation with Bargmann invariants [Mukunda et al., PRA 2001]:
  The structure of $\gamma^{(l)}_{j_1 j_2 j_3 \ldots j_l} = \Phi \left( \langle \psi^{\text{in}}_{j_1} | \psi^{\text{fin}}_{j_2} \rangle \langle \psi^{\text{in}}_{j_2} | \psi^{\text{fin}}_{j_3} \rangle \ldots \langle \psi^{\text{in}}_{j_l} | \psi^{\text{fin}}_{j_1} \rangle \right)$ is that of a Bargmann invariant!

  All off-diag phases can be expressed in terms of the 4-vertex invariants
  $\Delta_{jk} = \langle \psi^{\text{in}}_{j} | \psi^{\text{fin}}_{k} \rangle \langle \psi^{\text{in}}_{k} | \psi^{\text{fin}}_{k} \rangle \langle \psi^{\text{in}}_{k} | \psi^{\text{fin}}_{j} \rangle \langle \psi^{\text{in}}_{j} | \psi^{\text{fin}}_{j} \rangle + \text{the diagonal phases.}$

  Only $j < k < n$ needed $\longrightarrow \frac{1}{2} (n - 1)(n - 2)$ independent off-diag phases.

- Generalization to mixed states [Filipp Siöqvist PRL 2003] Define an density matrix $\rho^\perp$ as orthogonal as possible to $\rho$. The corresponding off-diagonal phase factor is $\gamma_{\rho \rho^\perp} = \Phi \left[ \text{Tr} \left( U^\| \sqrt{\rho} \ U^\| \sqrt{\rho^\perp} \right) \right]$

  and similar definition for $\gamma^{(l)}$
EXPERIMENTAL EVIDENCE 1 – neutron spin

2-state system: the off-diagonal phase factor $\gamma_{12} \equiv e^{i\pi} = -1$ is trivial.

Interferometry: split a beam and insert a controlled phase $\chi$, recombine the beam $|\psi\rangle = e^{i\chi} |\psi_I\rangle + |\psi_{II}\rangle$, producing an intensity:

$$I = \langle \psi | \psi \rangle = \langle \psi_I | \psi_I \rangle + \langle \psi_{II} | \psi_{II} \rangle + 2|\langle \psi_I | \psi_{II} \rangle| \cos(\chi - \phi)$$

The offset of the oscillation measures the phase $\phi$ in $e^{i\phi} = \Phi(\langle \psi_I | \psi_{II} \rangle)$

Start with a pure spinor state

$|\psi^+\rangle = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix} \rightarrow U$-evolve $\rightarrow$ compare with $|\psi^-\rangle = \begin{pmatrix} -\sin(\theta/2) \\ \cos(\theta/2) \end{pmatrix}$

Trick: take $|\psi_I\rangle = |\psi^-\rangle\langle \psi^- | U^{-1} |\psi^+\rangle$ and $|\psi_{II}\rangle = |\psi^-\rangle\langle \psi^- | U |\psi^+\rangle$, with $U=\alpha$-rotation along $\hat{z}$.

Result: $I = 2 \sin^2(\theta) \sin^2(\alpha/2)[1 + \cos(\chi - \pi)]$

The off-diagonal phase of $\gamma_{12} = \pi$ should appear as complete anti-phase of the recombined intensity $I$, independent of $\alpha$-rotation.
The setup for neutron interferometry
(a) Analyzed O-Beam

(b) H-Beam

Intensity (arb. units)

Phase Shift, $\chi$ (degree)

Intensity (arb. units)

Phase Shift, $\chi$ (degree)
EXPERIMENTAL EVIDENCE 2 – quantum billiard

2D deformable rectangular microwave cavity

[Lauber Wiedenhammer Dubbers PRL 1990]
Parallel transport in quantum billard: follow nodal structure adiabatically along the distortion path, and keep phase real. Open-path result: at $\theta = \pi$, $\psi_1 \longleftrightarrow \psi_3$, state 2 changes sign.
Coordinate transformation for the deformed domain

\[ x = u \left( 1 + v \frac{\Delta a}{ab} \right) \]
\[ y = v \left( 1 + u \frac{\Delta b}{ab} \right) \]

rectangular domain for \( u \) and \( v \)
\[ 0 \leq u \leq a \quad 0 \leq v \ll b \]
Laplace operator in \((u, v)\) coordinates

\[
\nabla^2 = \partial_x^2 + \partial_y^2 \quad \longrightarrow \quad \nabla^2 = \underbrace{(\partial_u, \partial_v)}_{A\ B} \begin{pmatrix} A & B \\ B & C \end{pmatrix} \begin{pmatrix} \partial_u \\ \partial_v \end{pmatrix} + D
\]

where \(A, B, C, D\) are complicate functions of \(u, v, a, b, \Delta a, \Delta b\)

Approximate treatment:

degenerate perturbation theory in $\vec{q} = (\Delta a, \Delta b) = q(\cos \theta, \sin \theta)$:

$$H(\vec{q}) = -\text{Laplacian} = H^{(0)} + q H^{(1)}(\theta) + q^2 H^{(2)}(\theta) + \ldots$$

unperturbed basis: $\psi_{(n_x,n_y)}(u,v) = \frac{2}{\sqrt{ab}} \sin\left(\frac{n_x u}{a}\right) \sin\left(\frac{n_y v}{b}\right)$

Interesting case: degenerate multiplets

example: if $a/b = \sqrt{3}$ “geometrical degeneracies” appear, for

$(n_x, n_y) = (2, 4), (5, 3), \text{ and } (7, 1)$:

$$H^{(0)} \rightarrow \text{const} = \frac{52\pi^2}{3}$$

$$H^{(1)} \rightarrow \text{a } 3 \times 3 \text{ matrix } = \cos \theta \ F + \sin \theta \ F'$$

$$H^{(2)} \rightarrow \langle \psi_i | H^{(2)} | \psi_j \rangle + \sum_{k \neq 1, 2, 3} \frac{\langle \psi_i | H^{(1)} | \psi_k \rangle \langle \psi_k | H^{(1)} | \psi_j \rangle}{E_i - E_k}$$

$$\vdots \qquad \vdots$$
Perturbation theory vs. Observed

observed $\gamma_2 = -1$,
observed $\gamma_{13} = 1$,

for the path $\theta = 0 \longrightarrow \pi$

while 1st order gives $\gamma_2 = 1$
while 1st order gives $\gamma_{13} = -1$
Why?

eigenvalues of first-order term $H^{(1)}(\theta)$: almost degeneracies in 4 directions
First order fails completely in green region in figure.
General observations on quantum billard experiments

- Satellite degeneracies (degeneracies within the range of validity of perturbation theory, involving minor components on states outside the multiplet) do often appear.

- Whenever in a degenerate multiplet one state is near some states [so that second-order coupling is large] for which selection rule 
  \((-1)^{n_x+n'_x} = (-1)^{n_y+n'_y} = 1\) makes first-order coupling vanish, and at the same time it is far from all remaining states [so that \(\Delta E^{(1)}\) is small], one is likely to find satellite degeneracies.

- Wide scope: Laplacian
SUMMARY

Off-diagonal geometric phases:  [PRL 85, 3067 (2000)]

- only appear in open-path evolution
- complete the set of phase infos of diagonal phases
- in the case of permutations are the only available info

- seen in  neutron-spin interferometry  [PRA 65, 052111 (2002)]
  - trick of forward-backward evolution
  - trivial case: $\gamma_{12} \equiv -1$

- seen in “quantum billiards”  [PRL 85, 1585 (2000)]
  - discovered previously overlooked satellite degeneracies
  - through higher-order expansion + exact numerical solution

- to be seen & used in  quantum computers  [???, ???, ????? (?????)]

http://www.mi.infm.it/manini