Off-diagonal geometric phases

Nicola Manini - Università degli Studi di Milano, Italy

Fabio Pistolesi - CNRS, Grenoble, France

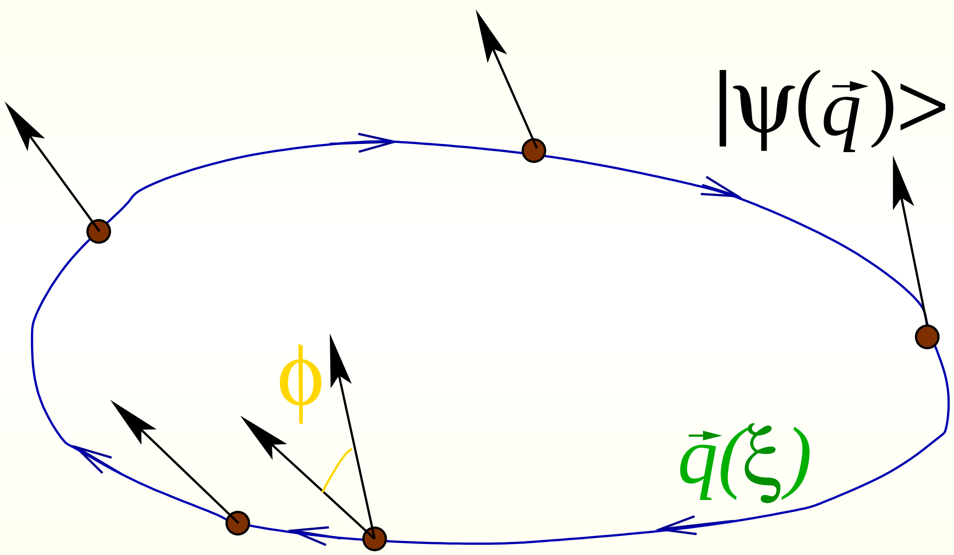
Phys. Rev. Lett. **85**, 1585 (2000)
$\longrightarrow$ Phys. Rev. Lett. **85**, 3067 (2000) $\longleftarrow$
Phys. Rev. A **65**, 052111 (2002)

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 $\vec{q}$



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 $\langle\psi(\vec{q}_{\text{in}})|\,\psi(\vec{q}_{\text{fin}})\rangle \,/\, |\langle\psi(\vec{q}_{\text{in}})|\,\psi(\vec{q}_{\text{fin}})\rangle|$

Original formulation [Berry 1984]

The path $\vec{q} = \vec{q}(s)$ is time-parameterized and closes to an adiabatic loop.

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

The Berry phase associated to the loop is

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

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 $\phi_j = \mathrm{Im}\log\langle\psi(\vec{q}_{\rm in})|\psi(\vec{q}_{\rm fin})\rangle$

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

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

Formulation in terms of Bargmann invariants

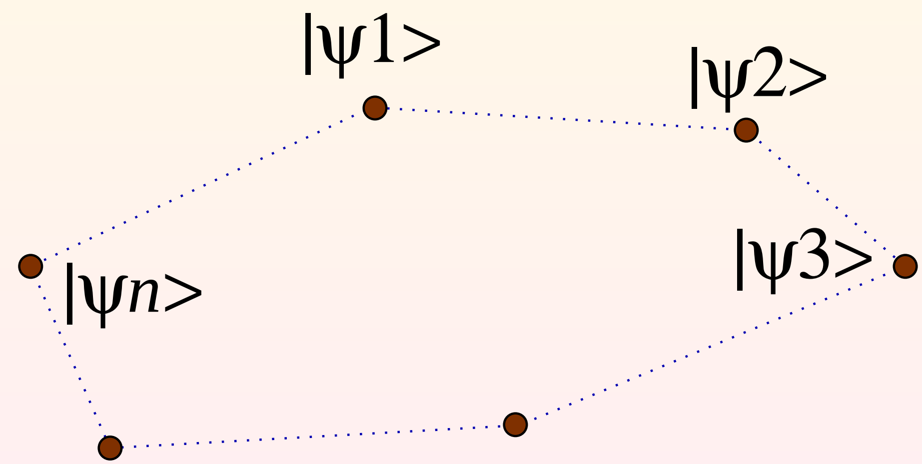
[Simon Mukunda 1993]

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:

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

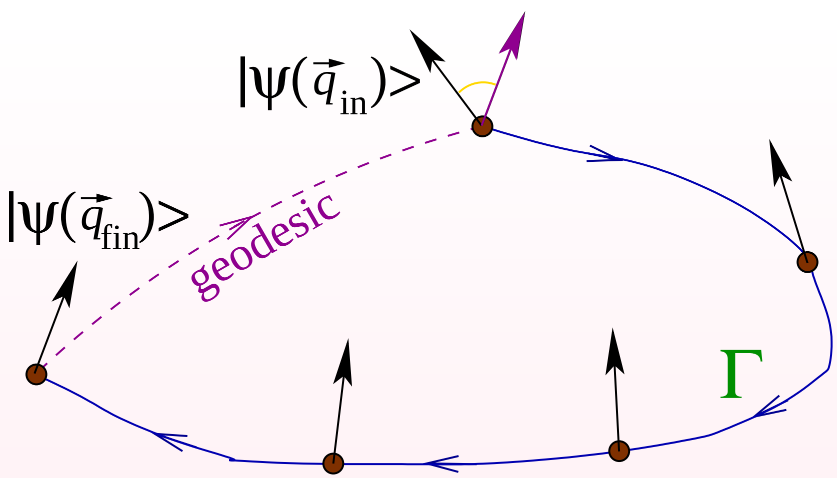
with $\Phi(z) = z/|z|$
for complex $z \neq 0$.



Phase tracking algorithms

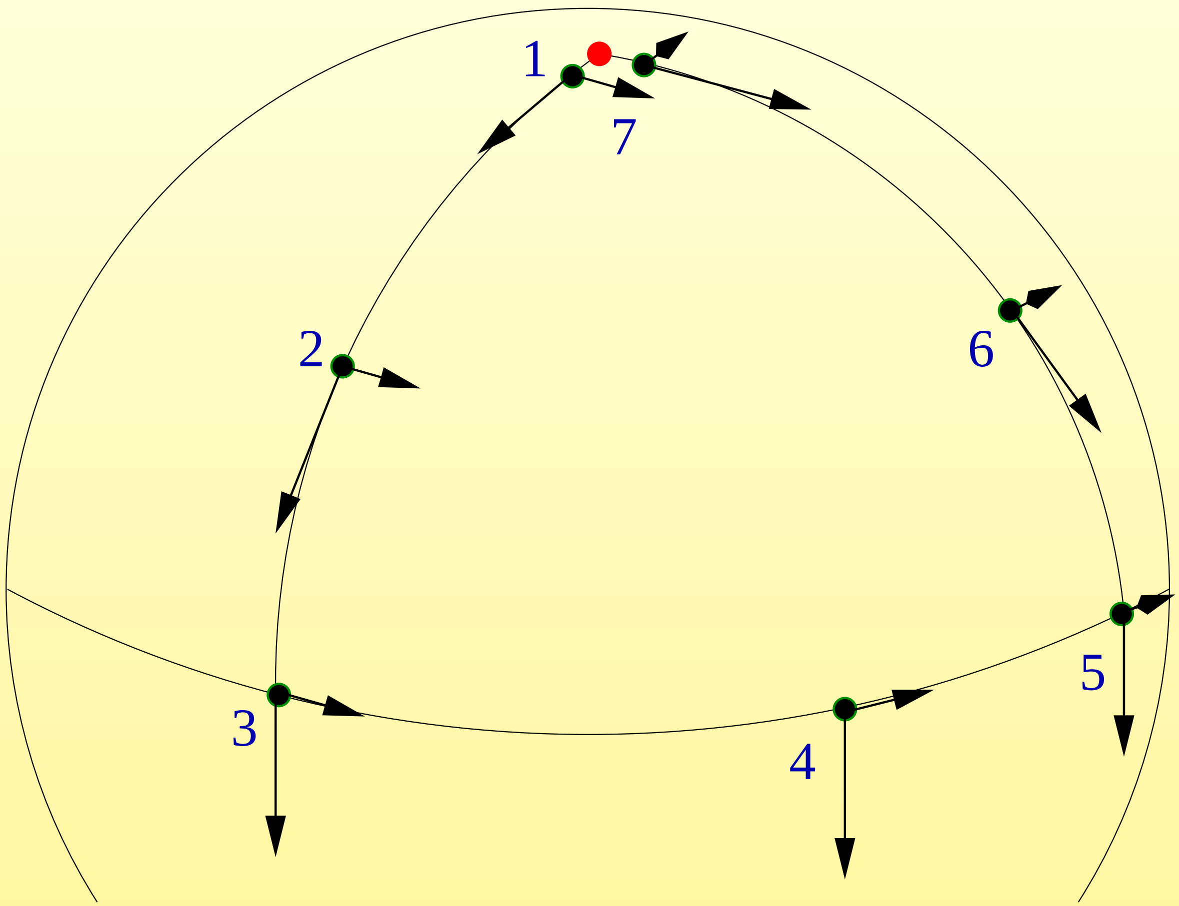
Extensions

- 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 Γ 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 $\langle\psi(\vec{q}_{\text{in}})|\psi(\vec{q}_{\text{fin}})\rangle \neq 0$

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 $\vec{q}_{\rm in}$ to $\vec{q}_{\rm fin}$ along path Γ: their Berry-Pancharatnam phase factor are

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

For n states, consider the parallel-evolution matrix

$$U_{jk}^\Gamma = \langle\psi_j^{\parallel}(\vec{q}_{\rm in})|\psi_k^{\parallel}(\vec{q}_{\rm fin})\rangle, \qquad \begin{pmatrix} U_{11}^\Gamma & U_{12}^\Gamma & \cdots \\ U_{21}^\Gamma & U_{22}^\Gamma & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

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

This is all is there for cyclic evolutions (matrix U^Γ is diagonal).

What about the information contents of the off-diagonal elements U_{jk}^Γ?

Is the phase factor $\sigma^{\Gamma}_{jk} \equiv \Phi\Big(U^{\Gamma}_{jk}\Big) = \Phi\Big(\langle\psi^{\parallel}_{j}(\vec{q}_{\rm in})|\psi^{\parallel}_{k}(\vec{q}_{\rm fin})\rangle\Big)$ measurable?

NO!

It depends on arbitrary choices of the initial phases of two different eigenstates $|\psi^{\parallel}_{j}(\vec{q}_{\rm in})\rangle$ and $|\psi^{\parallel}_{k}(\vec{q}_{\rm in})\rangle$.

σ^{Γ}_{jk} is not gauge-invariant $\longrightarrow$ it is arbitrary, thus non-measurable.

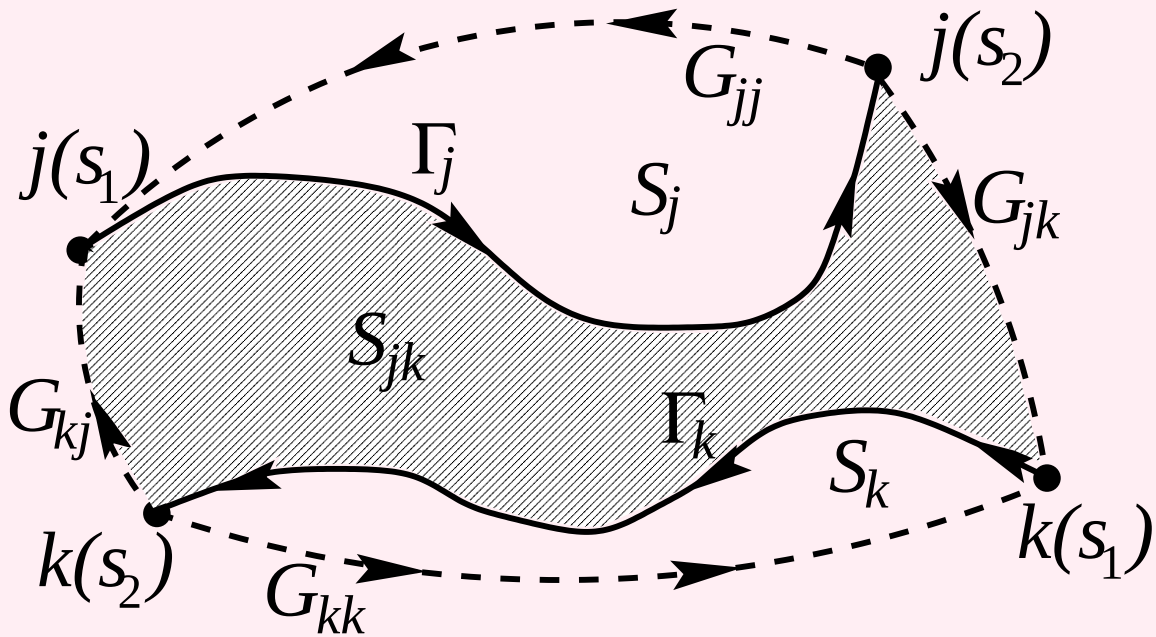
Idea: combine two σ's in the product:

$$\gamma^{\Gamma}_{jk} = \sigma^{\Gamma}_{jk}\,\sigma^{\Gamma}_{kj} = \Phi\Big(\langle\psi^{\parallel}_{j}(\vec{q}_{\rm in})|\psi^{\parallel}_{k}(\vec{q}_{\rm fin})\rangle\langle\psi^{\parallel}_{k}(\vec{q}_{\rm in})|\psi^{\parallel}_{j}(\vec{q}_{\rm fin})\rangle\Big)$$

γ^{Γ}_{jk} is clearly gauge invariant.

MAIN FINDING: γ^{Γ}_{jk} is a measurable geometric quantity!

Geometric interpretation [in projective Hilbert space]



dashed curves
G = geodesics

$$\gamma_j = \exp\left(-i\ \mathrm{Im} \iint_{S_j} dS \, \langle \nabla_1 \psi_j | \times | \nabla_2 \psi_j \rangle \right) \quad \text{(diagonal)}$$

$$\gamma_{jk} = \exp\left(-i\ \mathrm{Im} \iint_{S_{jk}} dS \, \langle \nabla_1 \psi_j | \times | \nabla_2 \psi_j \rangle \right) \quad \text{(off-diagonal)}$$

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

More measurable phases, general expression

$$\gamma^{(l)\,\Gamma}_{j_1 j_2 j_3 \ldots j_l} = \sigma^{\Gamma}_{j_1 j_2}\, \sigma^{\Gamma}_{j_2 j_3}\, \cdots\, \sigma^{\Gamma}_{j_{l-1} j_l}\, \sigma^{\Gamma}_{j_l j_1}$$

$l = 1$: 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 $\gamma^{(l')}\,\gamma^{(l-l')} \quad \longrightarrow \quad l \leq n$
- n^2 real numbers fix the unitary matrix U^{Γ}: only a finite number of $\gamma^{(l)}$'s are algebraically independent

Crucial example: Permutational case

$$\begin{cases} H(\vec{q}_1^{\,P}) & = & \sum_j E_j |\psi_j\rangle\langle\psi_j| \\ H(\vec{q}_2^{\,P}) & = & \sum_j E'_j |\psi_{P_j}\rangle\langle\psi_{P_j}| \end{cases}$$

$P =$ permutation of the n eigenstates

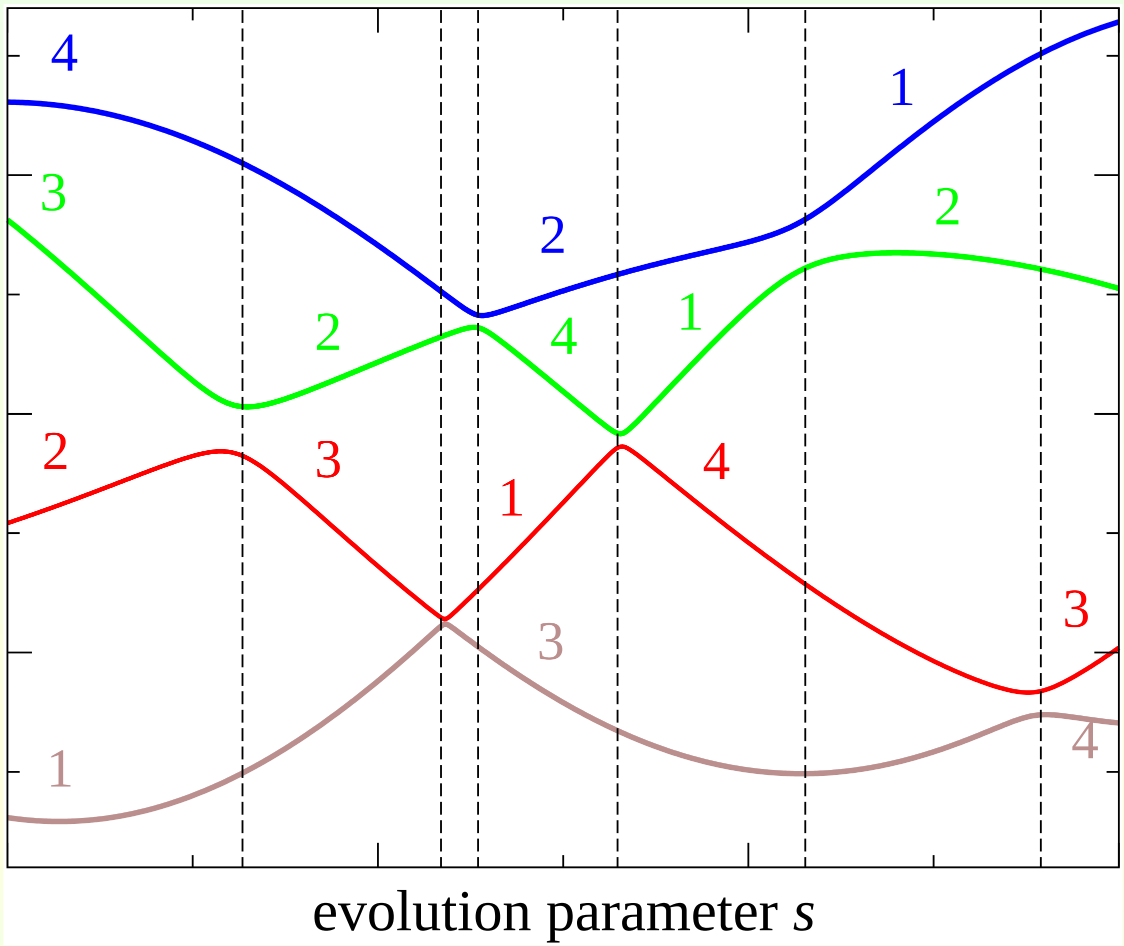
The only meaningful σ^{Γ}_{jk}'s are the n phase factors $\sigma^{\Gamma}_{j\,P_j}$.
For example:

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

Only well-defined $\gamma^{(l)}$: $\gamma^{(3)}_{123} = \sigma_{12}\sigma_{23}\sigma_{31} = e^{i(\alpha_1+\alpha_2+\alpha_3)}$

n	P	geometric phase factors	condition $\det U^{\Gamma} = 1$	# of Re cases
1	1	γ_1	$\gamma_1 = 1$	1
2	1 2	$\gamma_1 \ \gamma_2$	$\gamma_1 \gamma_2 = 1$	2
	2 1	γ_{12}	$\gamma_{12} = -1$	1
3	1 2 3	$\gamma_1 \ \gamma_2 \ \gamma_3$	$\gamma_1 \gamma_2 \gamma_3 = 1$	4
	2 1 3	$\gamma_{12} \ \gamma_3$	$\gamma_{12} \gamma_3 = -1$	2
	3 2 1	$\gamma_{13} \ \gamma_2$	$\gamma_{13} \gamma_2 = -1$	2
	1 3 2	$\gamma_{23} \ \gamma_1$	$\gamma_{23} \gamma_1 = -1$	2
	2 3 1	γ_{123}	$\gamma_{123} = 1$	1
	3 1 2	γ_{132}	$\gamma_{132} = 1$	1
4	1 2 3 4	$\gamma_1 \ \gamma_2 \ \gamma_3 \ \gamma_4$	$\gamma_1 \gamma_2 \gamma_3 \gamma_4 = 1$	8
	2 1 3 4	$\gamma_{12} \ \gamma_3 \ \gamma_4$	$\gamma_{12} \gamma_3 \gamma_4 = -1$	4
		....		
	2 3 4 1	γ_{1234}	$\gamma_{1234} = -1$	1
		....		

Application 1: Approximate permutational case



$$U^{\Gamma} \simeq \begin{pmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} & e^{i\alpha_1} \\ \epsilon_{21} & \epsilon_{22} & e^{i\alpha_2} & \epsilon_{24} \\ \epsilon_{31} & e^{i\alpha_3} & \epsilon_{32} & \epsilon_{34} \\ e^{i\alpha_4} & \epsilon_{41} & \epsilon_{42} & \epsilon_{44} \end{pmatrix}$$

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:

$$\gamma_1 = \Phi(U_{11}) = \mathrm{sgn}(\cos\alpha)\, e^{i\beta} \qquad \gamma_2 = \Phi(U_{22}) = \mathrm{sgn}(\cos\alpha)\, e^{-i\beta}$$

$$\gamma_{12} = \Phi(U_{12}U_{21}) = -\mathrm{sgn}\big(\sin^2\alpha\big)\, e^{i\chi}e^{-i\chi} = -1$$

"trivial" case, like diagonal phase of single state

Application 3: $H(\vec{q}_2) \longrightarrow -H(\vec{q}_1)$

A special permutational case:

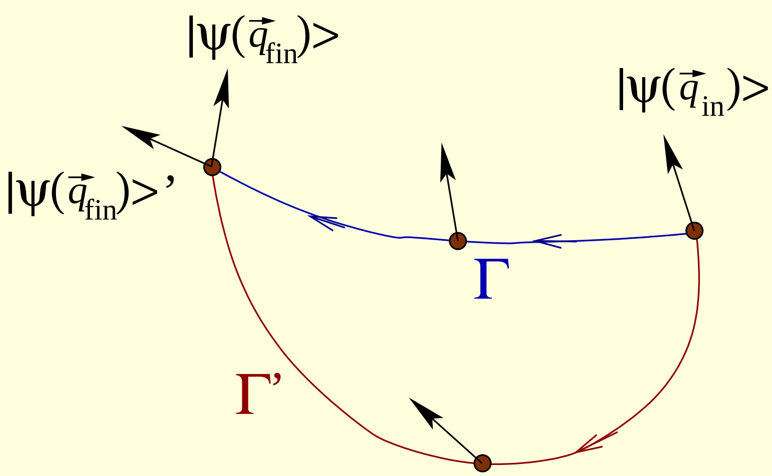
$$U = \begin{pmatrix} 0 & 0 & 0 & 0 & e^{i\alpha_1} \\ 0 & 0 & 0 & e^{i\alpha_2} & 0 \\ 0 & 0 & e^{i\alpha_3} & 0 & 0 \\ 0 & e^{i\alpha_4} & 0 & 0 & 0 \\ e^{i\alpha_5} & 0 & 0 & 0 & 0 \end{pmatrix}$$

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...)

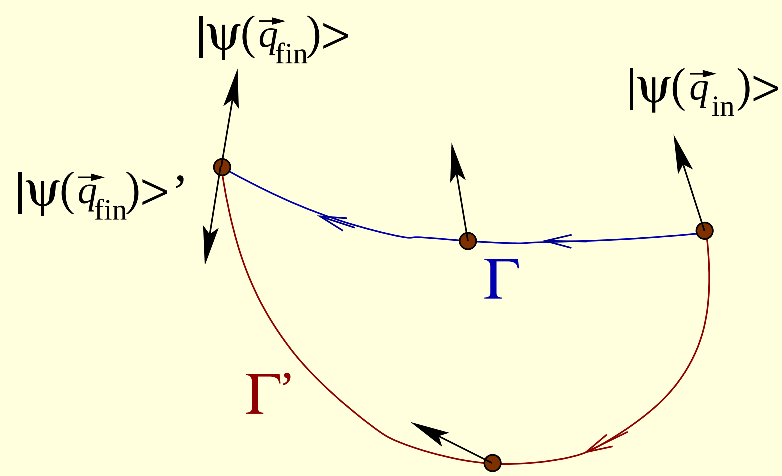
Comparison with nonabelian phases

Nonabelian



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

Abelian



nondegenerate evolution. The final states $|\psi^{\parallel}_k(\vec{q}_{\rm fin})\rangle$ are fixed up to a phase for any path leading to $\vec{q}_{\rm fin} \longrightarrow U^{\Gamma}$ is essentially fixed, except for some phase information captured by the diagonal and off-diagonal phases $\gamma^{(l)\,\Gamma}_{j_1 j_2 j_3 \ldots j_l}$. Invariance group: $\mathrm{U}(1)\times\mathrm{U}(1)\times\mathrm{U}(1)\times\mathrm{U}(1)\times\ldots$.

Further theoretical work

- Relation with Bargmann invariants [Mukunda *et al.*, PRA 2001]:
  The structure of $\gamma^{(l)\,\Gamma}_{j_1 j_2 j_3 \ldots j_l} = \Phi\big(\langle\psi^{\rm in}_{j_1}|\psi^{\rm fin}_{j_2}\rangle\langle\psi^{\rm in}_{j_2}|\psi^{\rm fin}_{j_3}\rangle \ldots \langle\psi^{\rm in}_{j_l}|\psi^{\rm fin}_{j_1}\rangle\big)$ is that of a Bargmann invariant!
  All off-diag phases can be expressed in terms of the 4-vertex invariants $\Delta_{jk} = \langle\psi^{\rm in}_j|\psi^{\rm fin}_k\rangle\langle\psi^{\rm in}_k|\psi^{\rm fin}_k\rangle\langle\psi^{\rm in}_k|\psi^{\rm fin}_j\rangle\langle\psi^{\rm in}_j|\psi^{\rm fin}_j\rangle$ + 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 ρ. The corresponding off-diagonal phase factor is $\gamma_{\rho\rho^{\perp}} = \Phi\Big[\mathrm{Tr}(U^{\parallel}\sqrt{\rho}\, U^{\parallel}\sqrt{\rho^{\perp}})\Big]$
  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 χ, 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 ϕ in $e^{i\phi} = \Phi(\langle\psi_I||\psi_{II}\rangle)$

Start with a pure spinor state

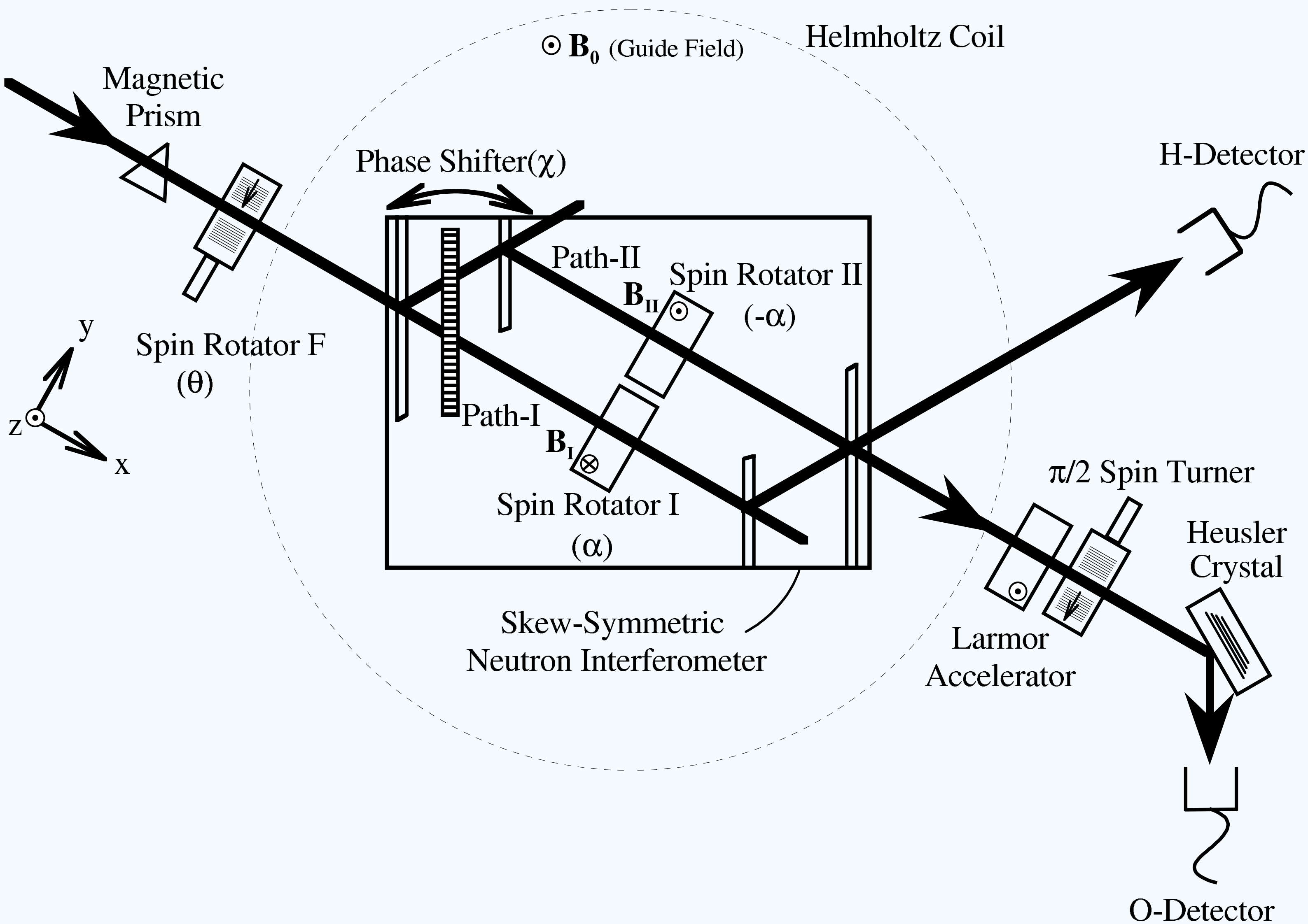
$|\psi^+\rangle = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix} \to U$-evolve $\to$ compare with $|\psi^-\rangle = \begin{pmatrix} -\sin(\theta/2) \\ \cos(\theta/2) \end{pmatrix}$

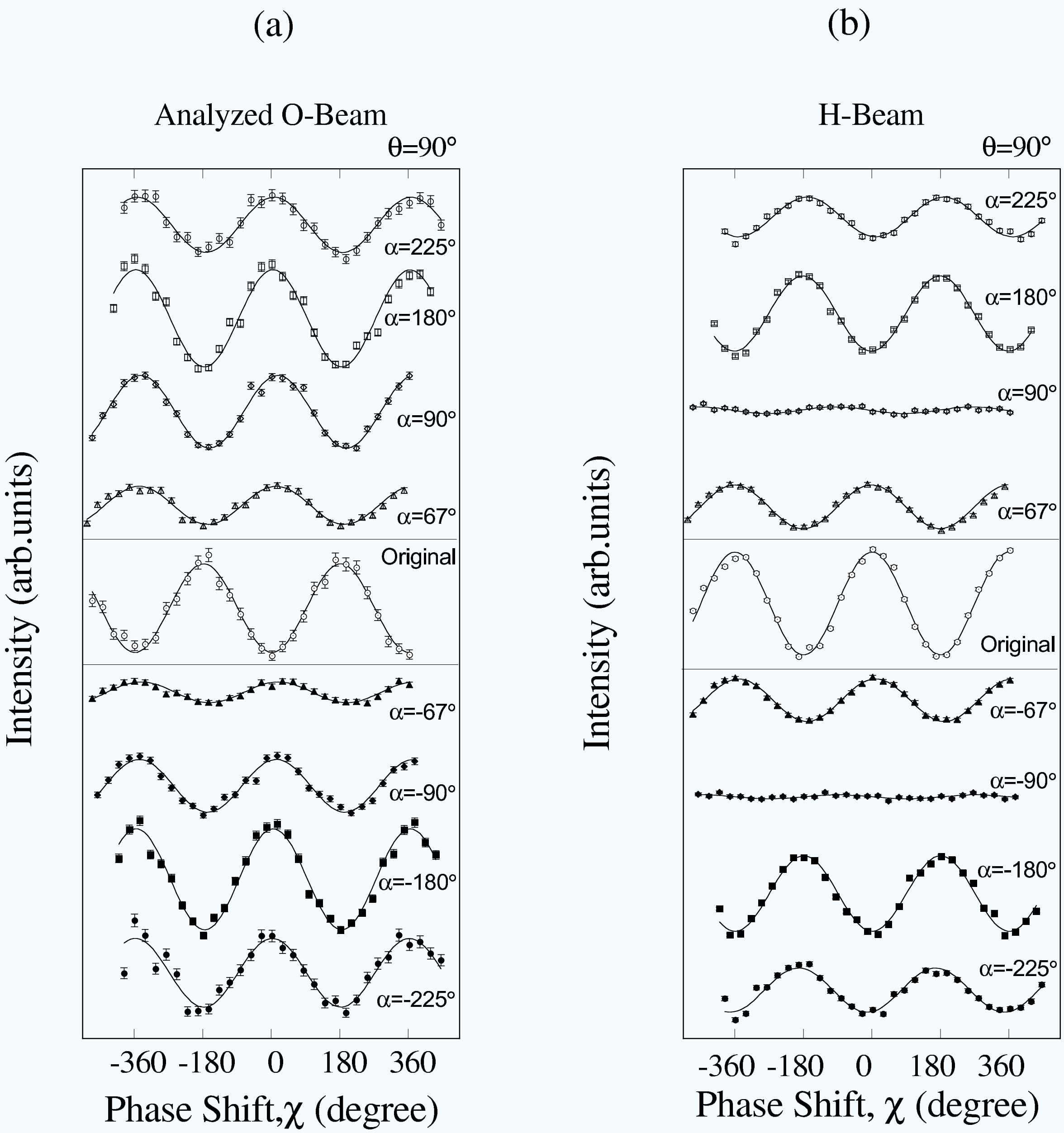
Trick: take $|\psi_I\rangle = |\psi^-\rangle\langle\psi^-|\,U^{-1}|\psi^+\rangle$ and $|\psi_{II}\rangle = |\psi^-\rangle\langle\psi^-|\,U\,|\psi^+\rangle$, with U=α-rotation along $\hat{z}$.

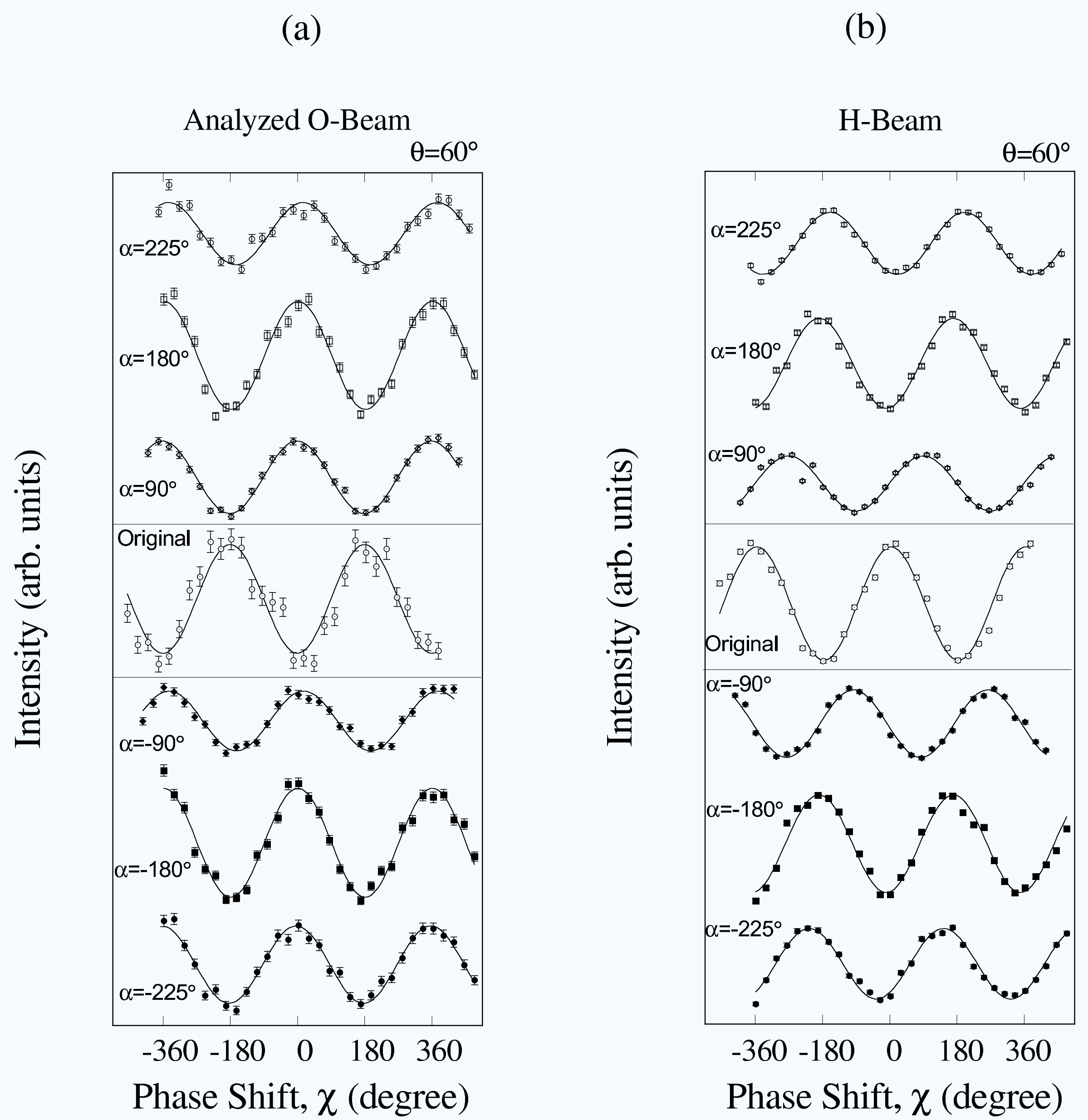
Result: $I = 2\sin^2(\theta)\sin^2(\alpha/2)[1 + \cos(\chi - \pi)]$

The off-diagonal phase of $\gamma_{12} = \pi$ should appear as complete anti-phase of the recombined intensity I, independent of α-rotation.

The setup for neutron interferometry

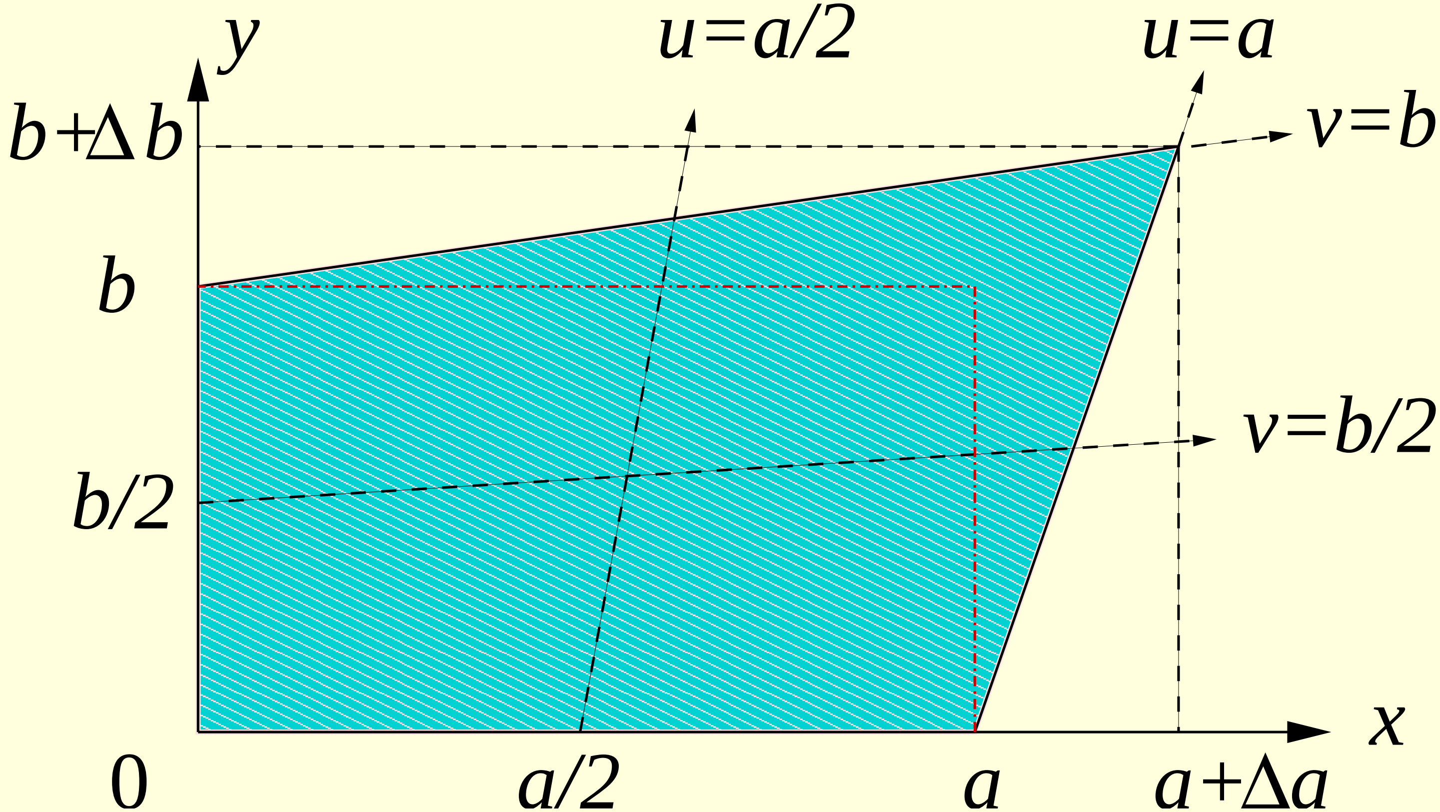



(a)
Analyzed O-Beam
θ=90°
α=225°
α=180°
α=90°
α=67°
Original
α=-67°
α=-90°
α=-180°
α=-225°
Intensity (arb.units)
-360 -180 0 180 360
Phase Shift,χ (degree)
(b)
H-Beam
θ=90°
α=225°
α=180°
α=90°
α=67°
Original
α=-67°
α=-90°
α=-180°
α=-225°
Intensity (arb.units)
-360 -180 0 180 360
Phase Shift, χ (degree)


(a)
(b)
Analyzed O-Beam
H-Beam
θ=60°
θ=60°
α=225°
α=180°
α=90°
Original
α=-90°
α=-180°
α=-225°
Intensity (arb. units)
-360 -180 0 180 360
Phase Shift, χ (degree)

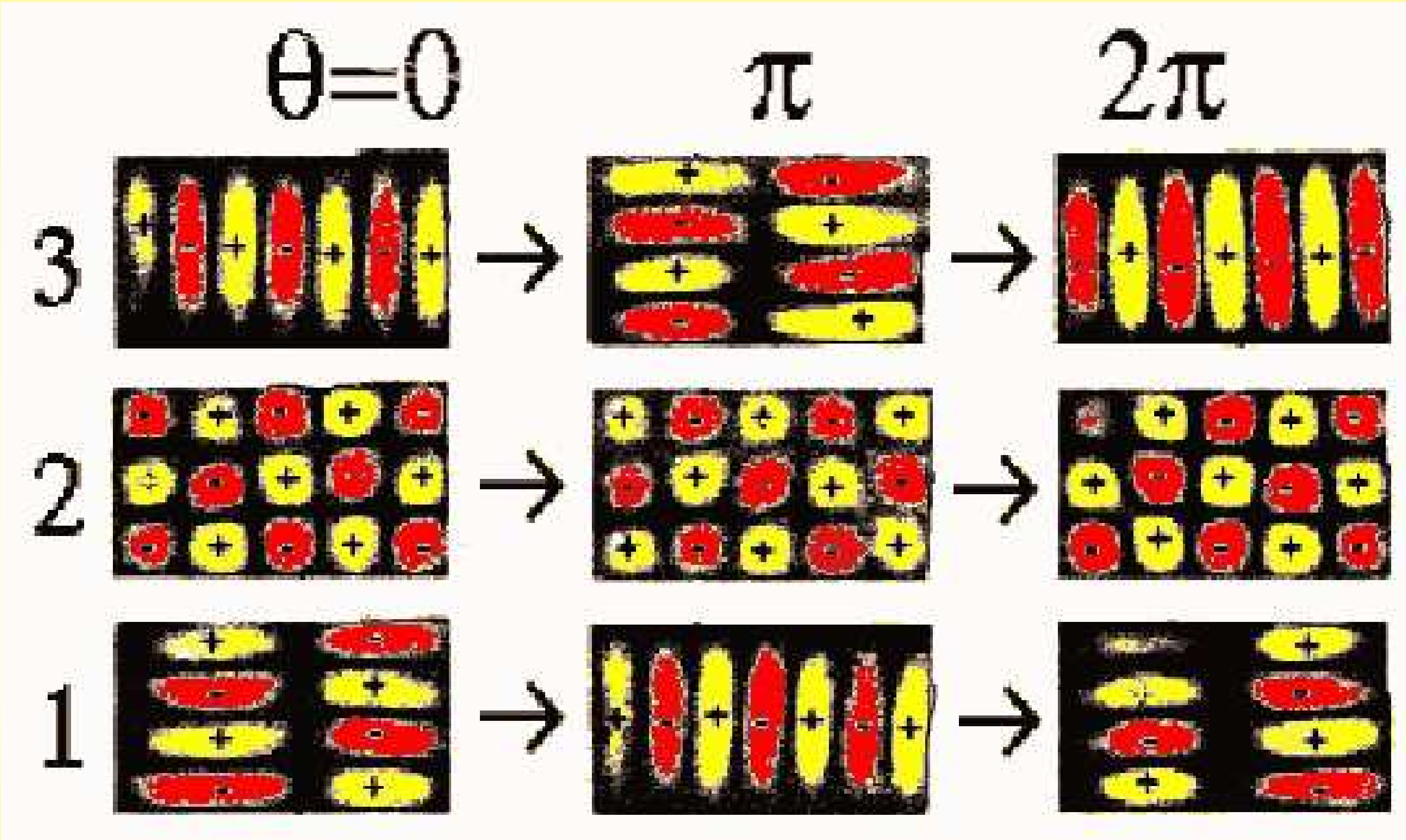
EXPERIMENTAL EVIDENCE 2 – quantum billiard

2D deformable rectangular microwave cavity

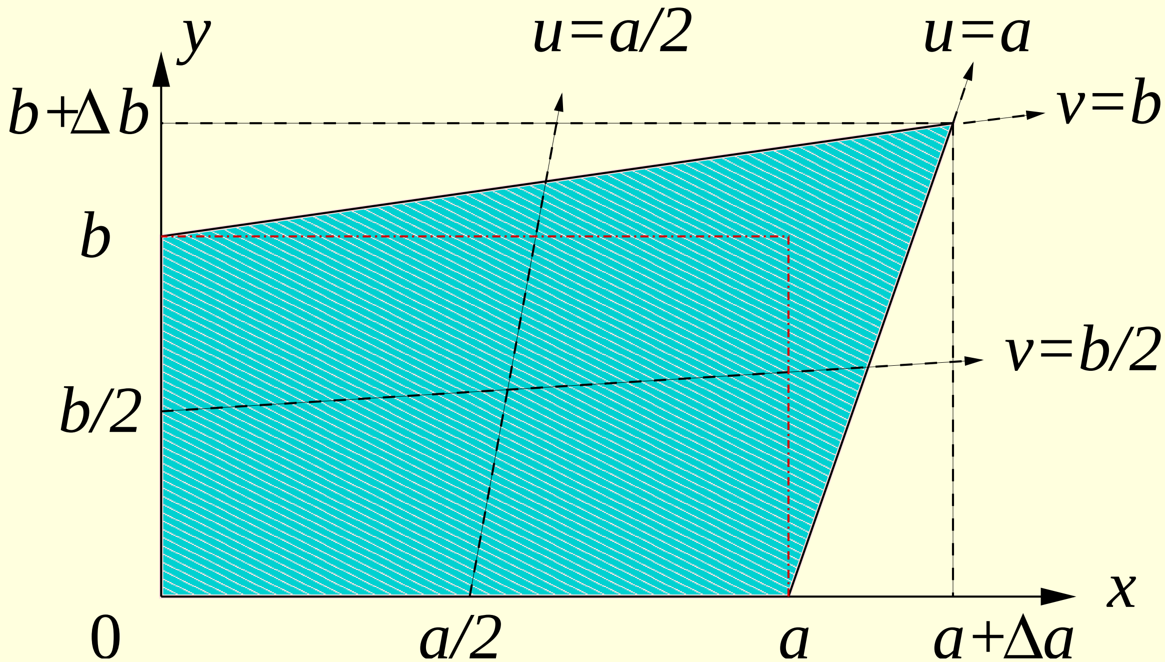


[Lauber Wiedenhammer Dubbers PRL 1990]

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



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

rectangular domain for u and v $\quad 0 \leq u \leq a \quad 0 \leq v <\leq b$

Laplace operator in (u, v) coordinates

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

where A, B, C, D are complicate functions of u, v, a, b, Δa, Δb

[see D.E. Manolopoulos and M.S. Child, Phys. Rev. Lett. **82**, 2223 (1999)]

Approximate treatment:

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

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

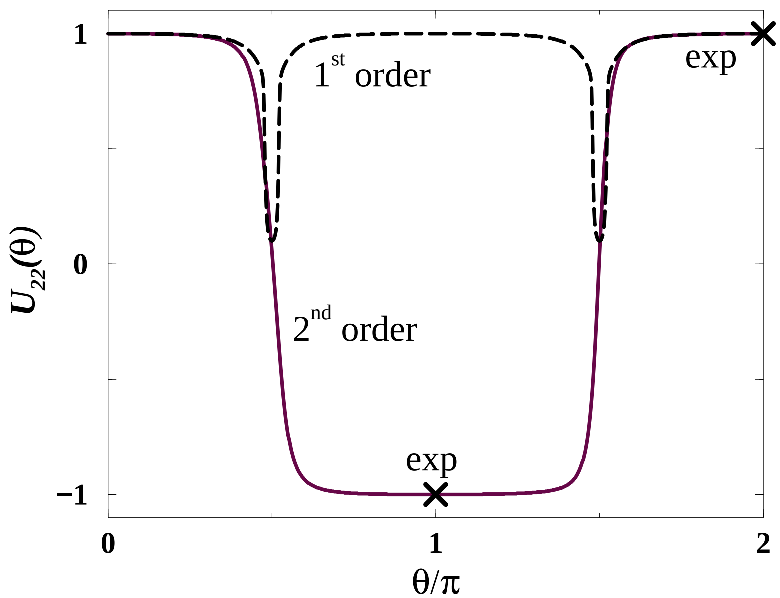
unperturbed basis: $\psi_{(n_x,n_y)}(u,v) = \frac{2}{\sqrt{ab}} \sin(\frac{n_x u}{a}) \sin(\frac{n_y v}{b})$

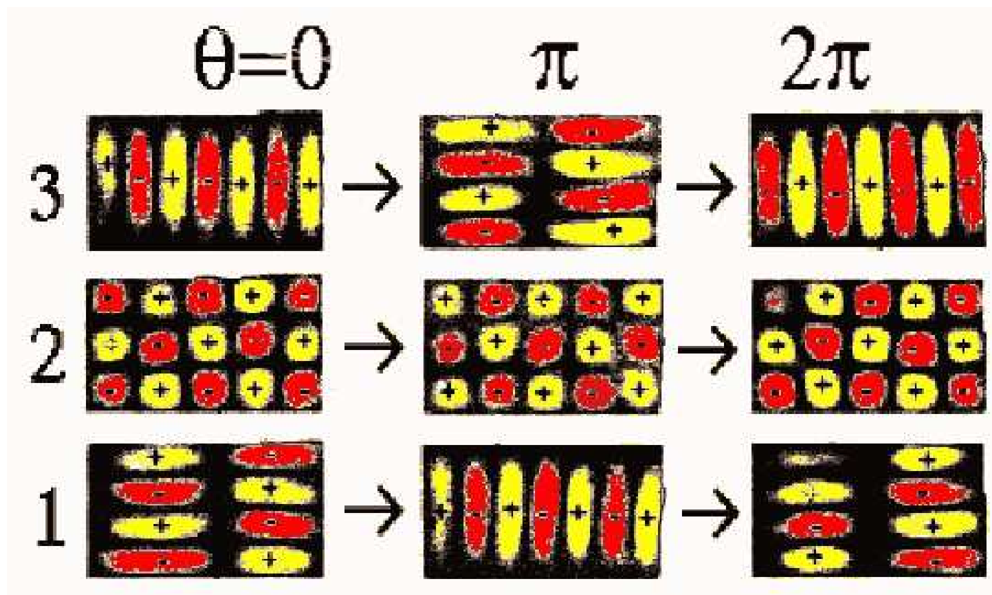
Interesting case: degenerate multiplets

example: if $a/b = \sqrt{3}$ "geometrical degeneracies" appear, for $(n_x, n_y) = (2,4)$, $(5,3)$, and $(7,1)$:

$$\begin{aligned}
H^{(0)} \quad &\rightarrow \quad \text{const} = 52\pi^2/3 \\
H^{(1)} \quad &\rightarrow \quad \text{a } 3\times 3 \text{ matrix} = \cos\theta\ F + \sin\theta\ F' \\
H^{(2)} \quad &\rightarrow \quad \langle\psi_i|H^{(2)}|\psi_j\rangle + \sum_{k\neq 1,2,3} \frac{\langle\psi_i|H^{(1)}|\psi_k\rangle\langle\psi_k|H^{(1)}|\psi_j\rangle}{E_i - E_k} \\
\vdots \quad & \qquad \vdots
\end{aligned}$$

Perturbation theory vs. Observed



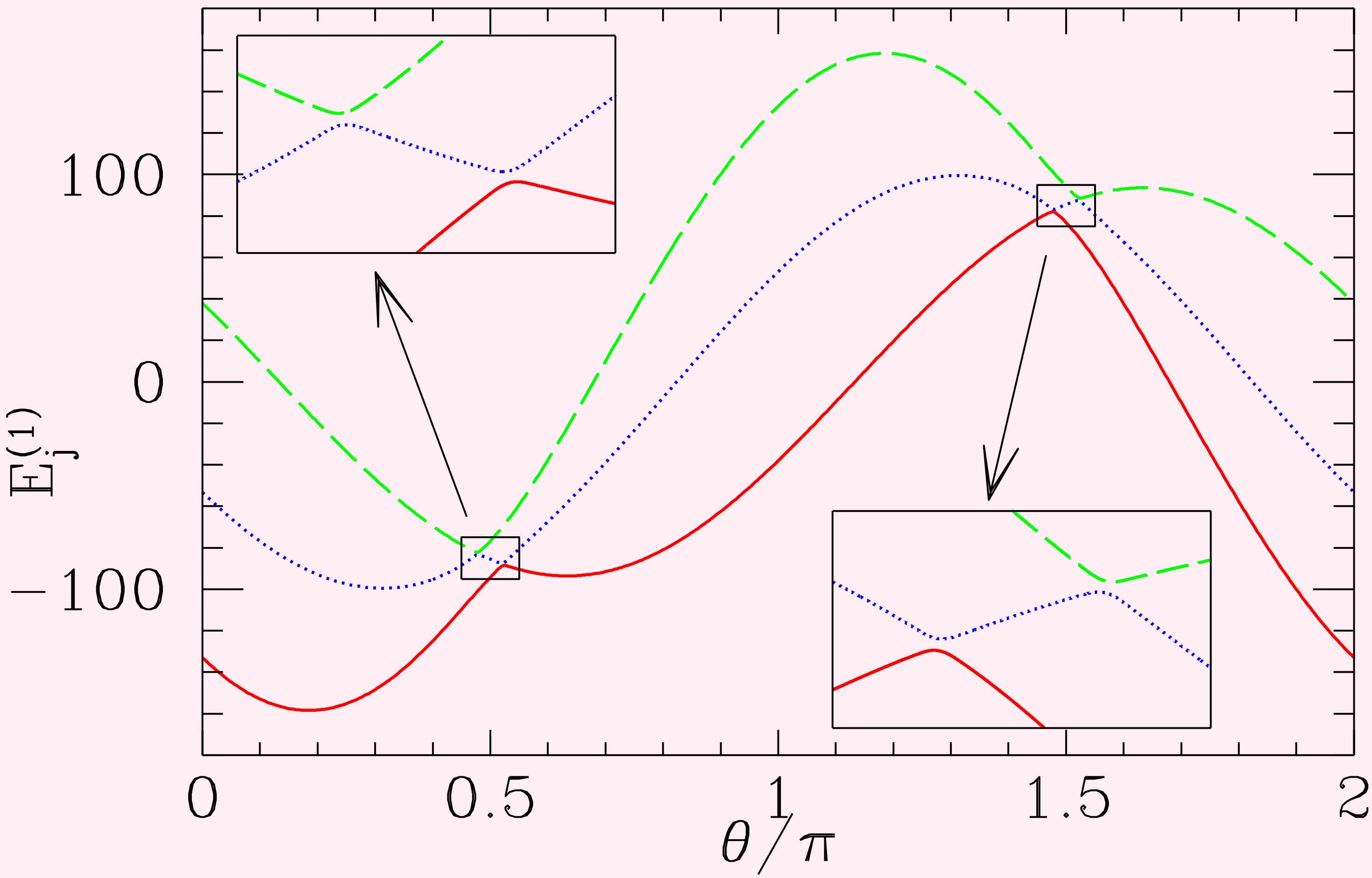


for the path $\theta = 0 \longrightarrow \pi$

observed $\gamma_2 = -1$, while 1^{st} order gives $\gamma_2 = 1$

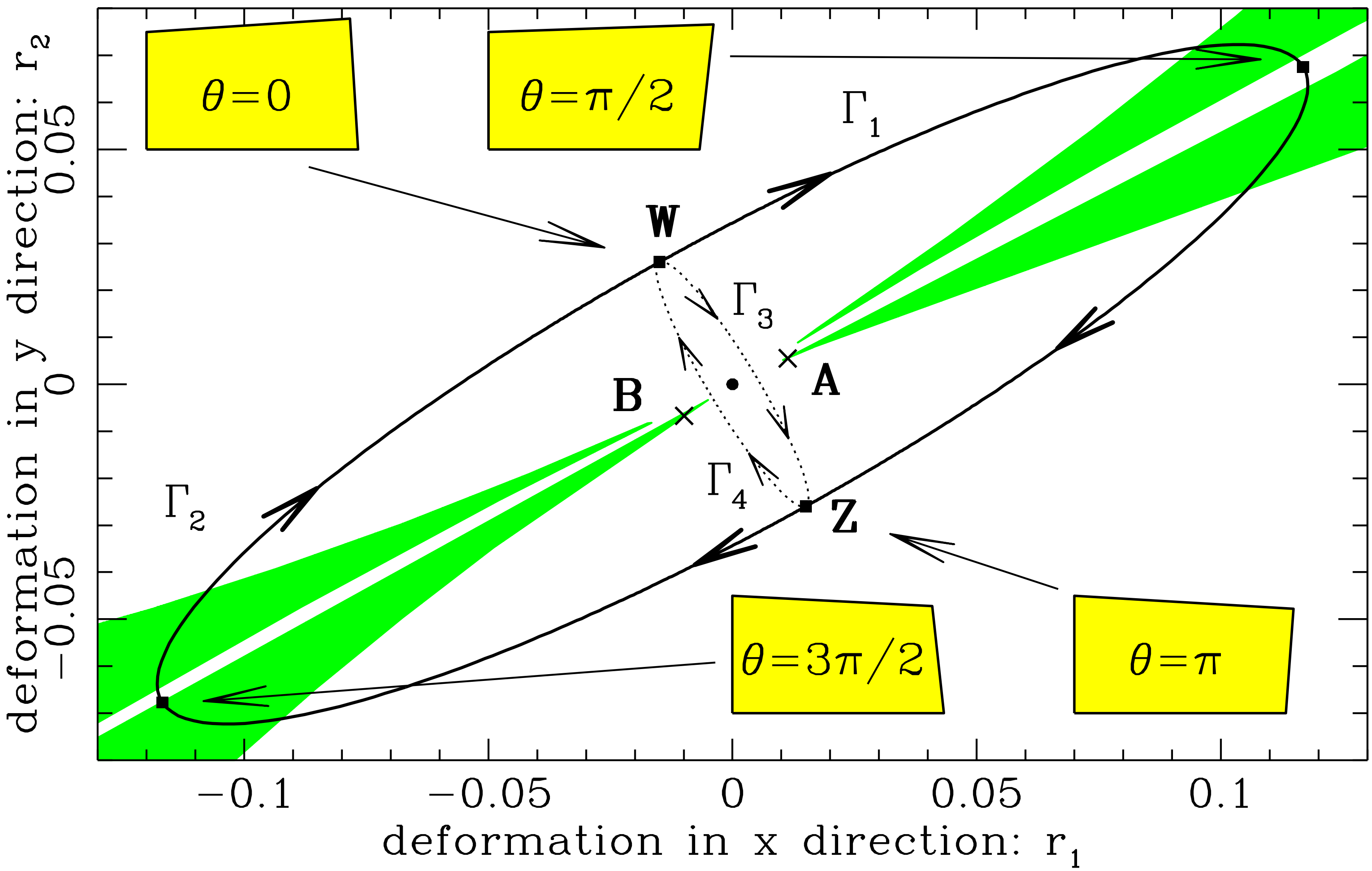
observed $\gamma_{13} = 1$, while 1^{st} order gives $\gamma_{13} = -1$

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