Berry's Geometric Phase

Aharonov-Bohm & Related Physics

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Outline

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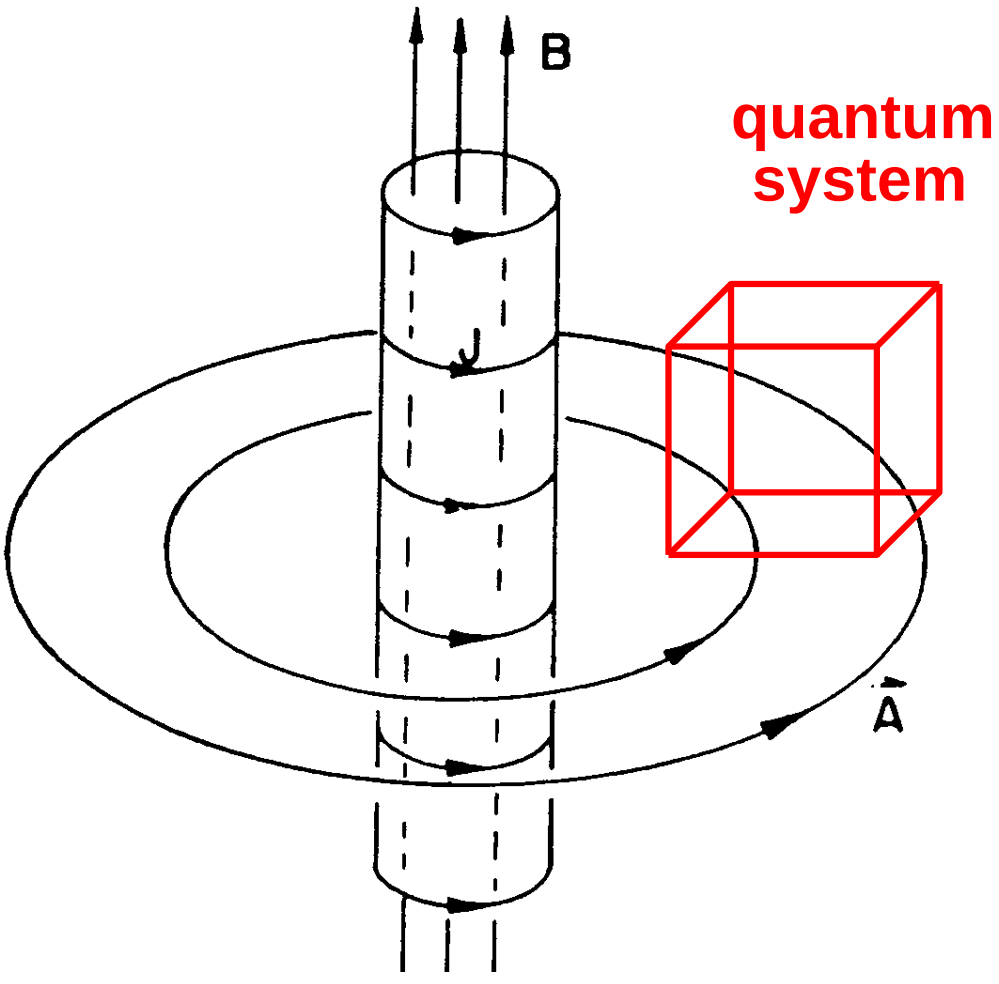
A quantum system in zero field



The parameter ξ

No magnetic field, box centered at the origin:

$$\left[\frac{1}{2}p^2 + V(\mathbf{r})\right]\chi(\mathbf{r}) = \varepsilon\chi(\mathbf{r}), \qquad \chi(\mathbf{r}) \quad \textbf{real} \text{ function}$$

Parameter $\xi \rightarrow$ the box position: $\qquad H(\mathbf{R}) = \frac{1}{2}p^2 + V(\mathbf{r}-\mathbf{R})$

$$\langle \mathbf{r}|\psi(\mathbf{R})\rangle = \chi(\mathbf{r}-\mathbf{R})$$

If there is a magnetic field (somewhere):

$$H(\mathbf{R}) = \frac{1}{2}[\,\mathbf{p} + \frac{e}{c}\mathbf{A}(\mathbf{r})\,]^2 + V(\mathbf{r}-\mathbf{R})$$

$$\langle \mathbf{r}|\psi(\mathbf{R})\rangle = \mathrm{e}^{-i\varphi(\mathbf{r})}\chi(\mathbf{r}-\mathbf{R})$$

$$\varphi(\mathbf{r}) = \frac{e}{\hbar c}\int_{\mathbf{R}}^{\mathbf{r}} \mathbf{A}(\mathbf{r}')\cdot d\mathbf{r}'$$

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Berry connection & Berry phase

Formal solution!

However: In the region where $\mathbf{B}(\mathbf{r})$ vanishes, $\varphi(\mathbf{r})$ is a single valued function of $\mathbf{r}$, and $\langle \mathbf{r}|\psi(\mathbf{R})\rangle$ is an "honest" electronic wavefunction.

What about the dependence on the "slow" parameter $\mathbf{R}$?

Berry connection:

$$i\langle\psi(\mathbf{R})|\nabla_{\mathbf{R}}\psi(\mathbf{R})\rangle = i\langle\chi(\mathbf{R})|\nabla_{\mathbf{R}}\chi(\mathbf{R})\rangle - \frac{e}{\hbar c}\mathbf{A}(\mathbf{R})$$

Berry phase:

$$\gamma = -\frac{e}{\hbar c}\oint_C \mathbf{A}(\mathbf{R})\cdot d\mathbf{R}$$

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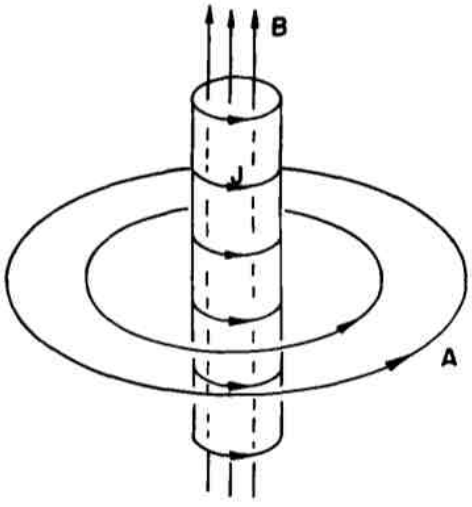

$$\gamma = -\frac{e}{\hbar c}\oint_C \mathbf{A}(\mathbf{R})\cdot d\mathbf{R} = -\frac{e}{\hbar c}\Phi$$

- In this problem (and **only** in this problem):
  The "geometric vector potential" coincides with the magnetic vector potential (times a constant)

- $\frac{e}{\hbar c}$ is the "flux quantum": $\gamma = -2\pi\frac{\Phi}{\Phi_0}$
- Only the **fractional** part of Φ/Φ_0 is relevant
- The Berry phase γ is **observable** (mod 2π)

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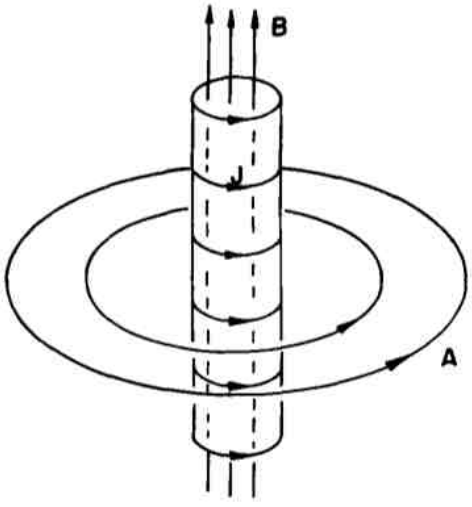

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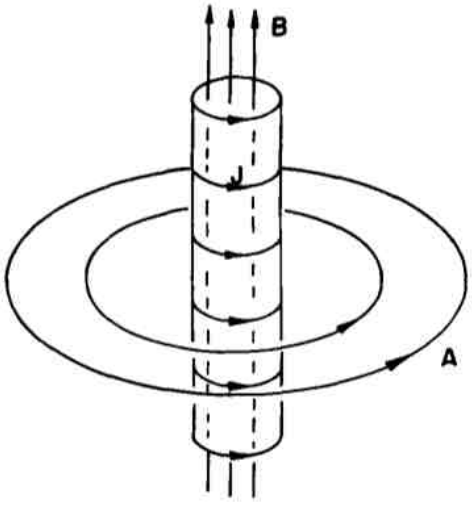

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Bottom line (no paradox!)

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Significance of Electromagnetic Potentials in the Quantum Theory

Y. AHARONOV AND D. BOHM
H. H. Wills Physics Laboratory, University of Bristol, Bristol, England
(Received May 28, 1959; revised manuscript received June 16, 1959)

In this paper, we discuss some interesting properties of the electromagnetic potentials in the quantum domain. We shall show that, contrary to the conclusions of classical mechanics, there exist effects of potentials on charged particles, even in the region where all the fields (and therefore the forces on the particles) vanish. We shall then discuss possible experiments to test these conclusions; and, finally, we shall suggest further possible developments in the interpretation of the potentials.

Outline

Reexamining the Born-Oppenheimer approximation

$$\mathcal{H}([\mathbf{R}],[\mathbf{x}]) = -\sum_j \frac{\hbar^2}{2M_j}\nabla^2_{\mathbf{R}_j} + H_{\mathrm{el}}([\mathbf{R}],[\mathbf{x}])$$

[**x**]: electronic degrees of freedom (orbital & spin)
[**R**]: nuclear coordinates $\mathbf{R}_j$
$-i\hbar\nabla_{\mathbf{R}_j}$: canonical nuclear momenta

$$\begin{aligned} H_{\mathrm{el}}([\mathbf{R}],[\mathbf{x}]) &= \text{electronic kinetic energy} \\ &+ \text{electron-electron interaction} \\ &+ \text{electron-nuclear interaction} \\ &+ \text{nuclear-nuclear interaction} \end{aligned}$$

Recipe

- Product ansatz: $\Psi([\mathbf{R}],[\mathbf{x}]) = \langle\,[\mathbf{x}]\,|\Psi_{\mathrm{el}}([\mathbf{R}])\rangle\,\Phi([\mathbf{R}])$
- Solve the electronic Schrödinger equation at **fixed** $\mathbf{R}_j$:

$$H_{\mathrm{el}}([\mathbf{R}],[\mathbf{x}])\,\langle\,[\mathbf{x}]\,|\Psi_{\mathrm{el}}([\mathbf{R}])\rangle = E_{\mathrm{el}}([\mathbf{R}])\,\langle\,[\mathbf{x}]\,|\Psi_{\mathrm{el}}([\mathbf{R}])\rangle$$

- Use $E_{\mathrm{el}}([\mathbf{R}])$ as the potential energy for nuclear motion:

$$\left(-\sum_j \frac{\hbar^2}{2M_j}\nabla^2_{\mathbf{R}_j} + E_{\mathrm{el}}([\mathbf{R}])\right)\,\Phi([\mathbf{R}]) = E\,\Phi([\mathbf{R}])$$

- **Textbook example:** Vibrational levels of a biatomic molecule.
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A closer look at the Born-Oppenheimer recipe

- Product ansatz: $\Psi([\mathbf{R}],[\mathbf{x}]) = \langle\,[\mathbf{x}]\,|\Psi_{\mathrm{el}}([\mathbf{R}])\rangle\,\Phi([\mathbf{R}])$
- The operator $\nabla_{\mathbf{R}_j}$ acting on $\Psi([\mathbf{R}],[\mathbf{x}])$:

$$\begin{aligned}\nabla_{\mathbf{R}_j}\Psi([\mathbf{R}],[\mathbf{x}]) &= \langle\,[\mathbf{x}]\,|\Psi_{\mathrm{el}}([\mathbf{R}])\rangle\nabla_{\mathbf{R}_j}\Phi([\mathbf{R}]) \\ &+ \langle\,[\mathbf{x}]\,|\nabla_{\mathbf{R}_j}\Psi_{\mathrm{el}}([\mathbf{R}])\rangle\Phi([\mathbf{R}])\end{aligned}$$

- Multiplying by $\langle\Psi_{\mathrm{el}}([\mathbf{R}])\,|\,[\mathbf{x}]\,\rangle$ and integrating in $d[\mathbf{x}]$:

$$\begin{aligned}\int d[\mathbf{x}] \quad & \langle\Psi_{\mathrm{el}}([\mathbf{R}])\,|\,[\mathbf{x}]\,\rangle\nabla_{\mathbf{R}_j}\Psi([\mathbf{R}],[\mathbf{x}]) \\ = \quad & \left(\nabla_{\mathbf{R}_j} + \langle\,\Psi_{\mathrm{el}}([\mathbf{R}])\,|\nabla_{\mathbf{R}_j}\Psi_{\mathrm{el}}([\mathbf{R}])\rangle\right)\Phi([\mathbf{R}])\end{aligned}$$

- **Nuclear kinetic energy**, after [**x**] is "integrated out":

$$\mathcal{T}_{\mathrm{N}} = \sum_j \frac{\hbar^2}{2M_j}\left(-i\hbar\nabla_{\mathbf{R}_j} - i\hbar\langle\,\Psi_{\mathrm{el}}([\mathbf{R}])\,|\nabla_{\mathbf{R}_j}\Psi_{\mathrm{el}}([\mathbf{R}])\rangle\right)^2$$

A term was missing!

- Naive Born-Oppenheimer approximation:

$$\left(\mathcal{T}_{\mathrm{N}} + E_{\mathrm{el}}([\mathbf{R}])\right) \Phi([\mathbf{R}]) = E\,\Phi([\mathbf{R}]), \qquad \mathcal{T}_{\mathrm{N}} = -\sum_j \frac{\hbar^2}{2M_j} \nabla^2_{\mathbf{R}_j}$$

- More accurate Born-Oppenheimer approximation:

$$\mathcal{T}_{\mathrm{N}} = \sum_j \frac{1}{2M_j} \left(-i\hbar\nabla_{\mathbf{R}_j} - i\hbar\langle\, \Psi_{\mathrm{el}}([\mathbf{R}])\,|\nabla_{\mathbf{R}_j}\Psi_{\mathrm{el}}([\mathbf{R}])\rangle\right)^2$$

- The electronic **Berry connection** acts as a "geometric vector potential" in the nuclear Hamiltonian

- In most cases the correction is neglected: **Why?**

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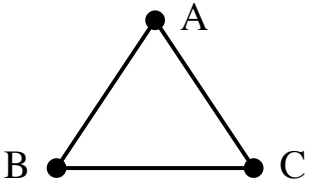
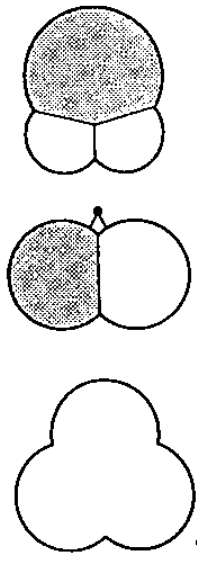
The hydrogen (or sodium) trimer, LCAO





$$|2\rangle = \frac{1}{\sqrt{6}}(\, |\mathrm{B}\rangle + |\mathrm{C}\rangle - 2 \, |\mathrm{A}\rangle \,)$$

$$|1\rangle = \frac{1}{\sqrt{2}}(\, |\mathrm{C}\rangle - |\mathrm{B}\rangle \,)$$

$$|0\rangle = \frac{1}{\sqrt{3}}(\, |\mathrm{A}\rangle + |\mathrm{B}\rangle + |\mathrm{C}\rangle \,)$$

- Equilateral geometry, 3 valence electrons: degenerate HOMO ($\varepsilon_1 = \varepsilon_2$)
- Broken-symmetry equilibrium geometry: **isosceles** Jahn-Teller splitting ($\varepsilon_1 \neq \varepsilon_2$)

$|1\rangle$ is the HOMO, $|2\rangle$ is the LUMO

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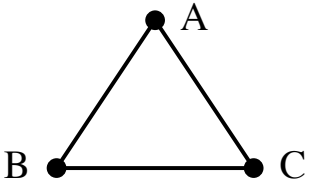

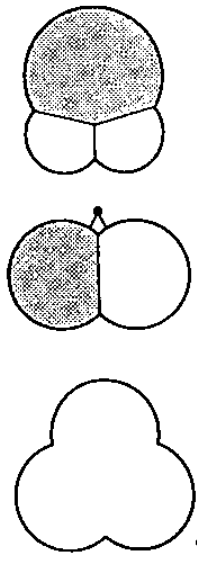

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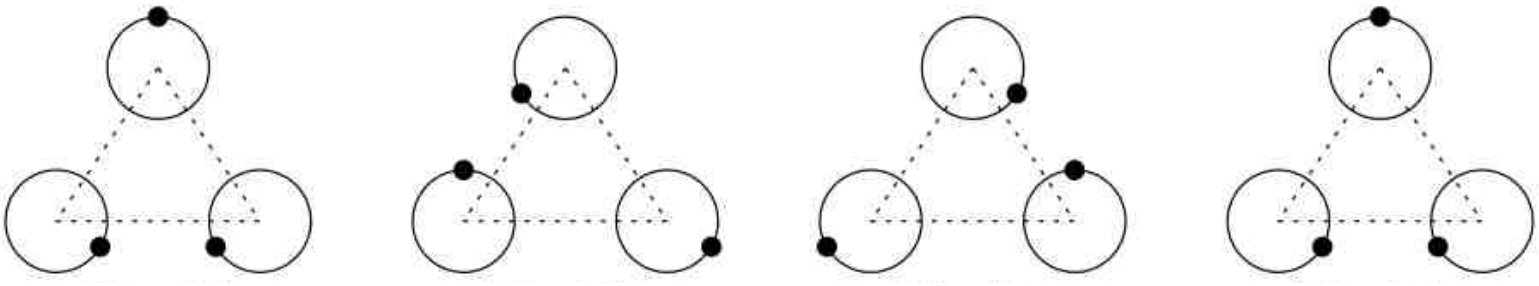
Born-Oppenheimer surfaces



pseudorotation

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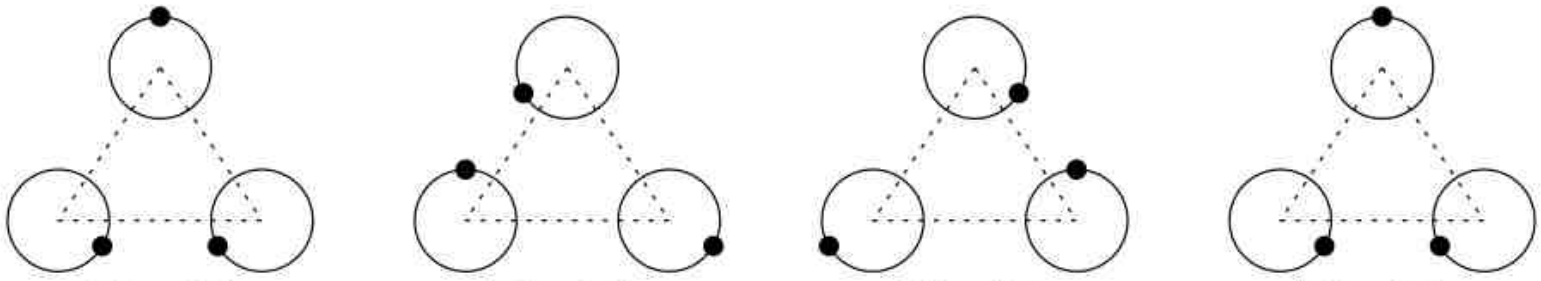

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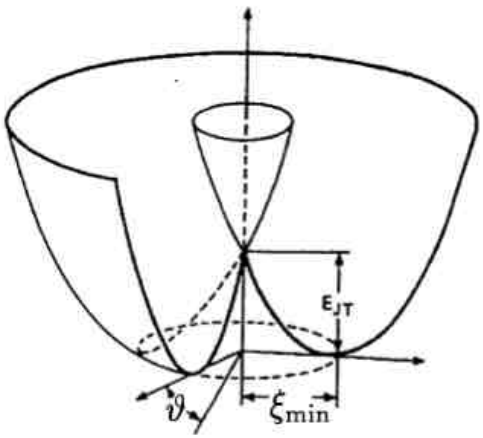
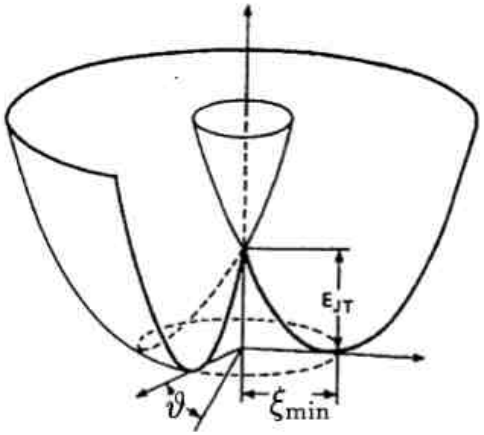


"conical intersection"

a.k.a. "diabolical point"

Nuclear dynamics



$$E_{el}(\boldsymbol{\xi}) = E_{el}(\xi) \qquad \vartheta\text{-independent}$$

$$E_{el}(\xi) = \frac{1}{2} k (\xi^2 \pm 2\,\xi_{min}\,\xi)$$

Lowest BO surface:

minimum in ξ_{min}

$$E_{el}(\xi_{min}) = -\frac{1}{2} k\,\xi_{min}^2 = -E_{JT}$$

- **Classical:** Free motion at valley's bottom, $M = 3m$ & transverse oscillations
- **Quantized pseudorotations:**

$$\Phi_{mn}(\xi, \vartheta) \propto H_n(\alpha\xi)\; \mathrm{e}^{-\frac{\omega}{2}(\xi - \xi_{min})^2}\; \mathrm{e}^{im\vartheta}$$

$m \in \mathbb{Z}, \qquad n = 0, 1, 2, \ldots$

Ground state: m=0, n=0

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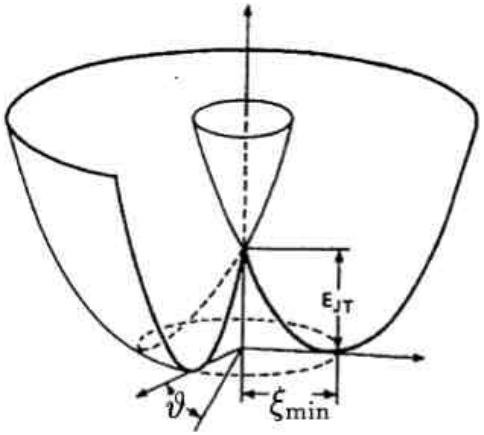

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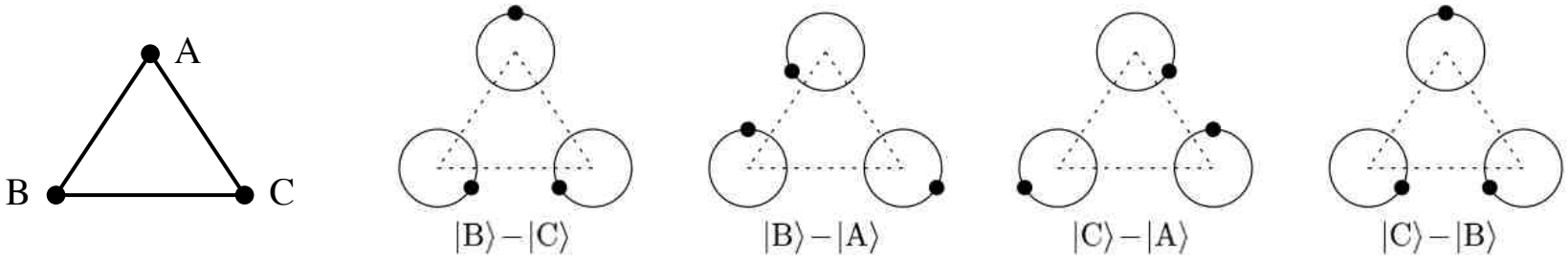

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The **total** wfn $\Psi(\boldsymbol{\xi},\mathbf{r}) = \langle \mathbf{r}|\psi_{\mathrm{el}}(\boldsymbol{\xi})\rangle\, \Phi(\boldsymbol{\xi})$ must be **single-valued**
Even the **nuclear** wfn must change sign

$\Rightarrow$ **Different quantization rules!**

$\Phi_{mn}(\xi,\vartheta) \propto H_n(\alpha\xi)\, \mathrm{e}^{-\frac{\omega}{2}(\xi-\xi_{\min})^2}\, \mathrm{e}^{im\vartheta}$
m **half-integer**, $n = 0, 1, 2, \ldots$
Ground state: $m = \frac{1}{2}, n = 0$
Observable effect in **QM**, no effect in **CM**
(the system **does not visit** the conical intersection)

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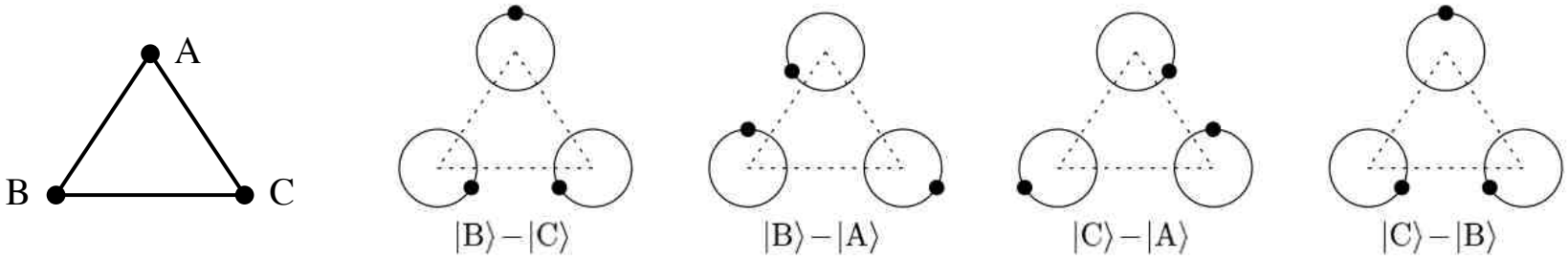

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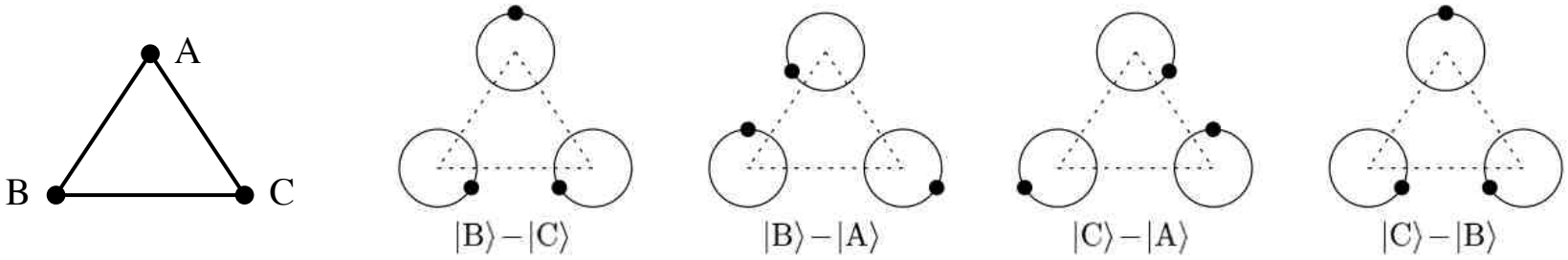

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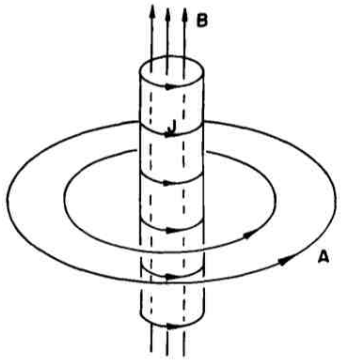
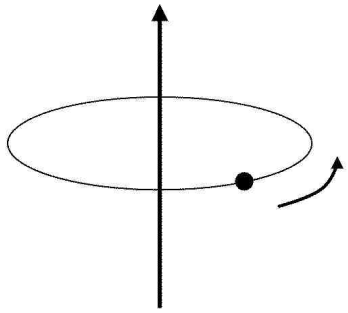
Molecular Aharonov-Bohm effect



Aharonov-Bohm effect (real **B** field):

$$\gamma = \oint_C \mathcal{A}(\xi) \cdot d\xi = -2\pi \frac{\Phi}{\Phi_0} \mod 2\pi$$



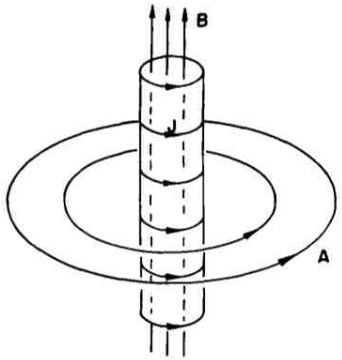
Molecular Aharonov-Bohm effect (**B** $= 0$):

$$\gamma = \oint_C \mathcal{A}(\xi) \cdot d\xi = \pi \mod 2\pi$$

Same as having a δ-like flux tube at the conical intersection

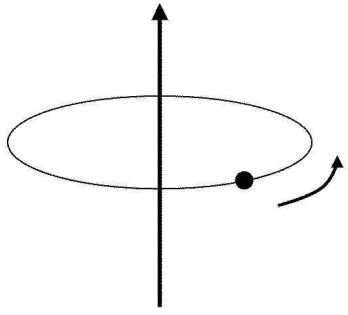
$$\Phi = \frac{\Phi_0}{2}$$ (**half-quantum**, a.k.a. "π flux")

Molecular Aharonov-Bohm effect



Aharonov-Bohm effect (real **B** field):

$$\gamma = \oint_C \mathcal{A}(\xi) \cdot d\xi = -2\pi \frac{\Phi}{\Phi_0} \mod 2\pi$$



Molecular Aharonov-Bohm effect (**B** $= 0$):

$$\gamma = \oint_C \mathcal{A}(\xi) \cdot d\xi = \pi \mod 2\pi$$

Same as having a δ-like flux tube at the conical intersection

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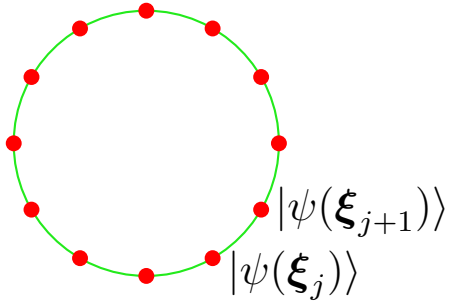
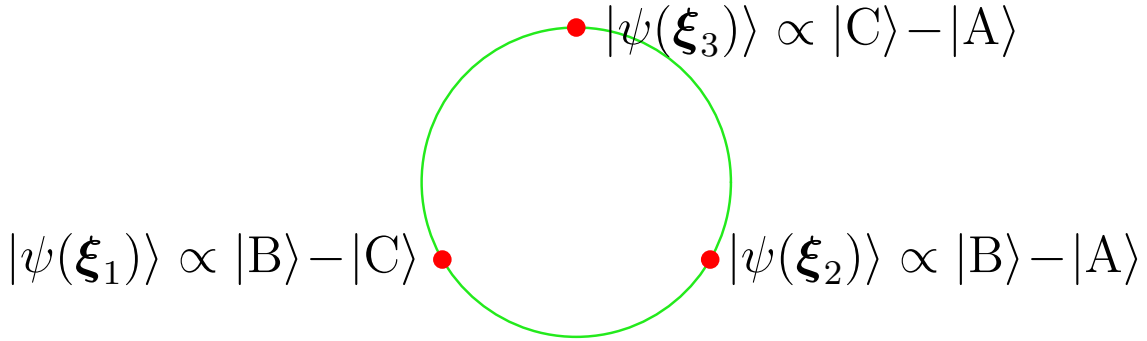
Berry phase: discrete algorithm

$$\gamma = \sum_{j=1}^{N} \Delta\varphi_{j,j+1}$$



$$= - \operatorname{Im} \log \langle\psi(\boldsymbol{\xi}_1)|\psi(\boldsymbol{\xi}_2)\rangle\langle\psi(\boldsymbol{\xi}_2)|\psi(\boldsymbol{\xi}_3)\rangle \ldots \langle\psi(\boldsymbol{\xi}_N)|\psi(\boldsymbol{\xi}_1)\rangle$$

$N = 3$



$$\langle\psi(\boldsymbol{\xi}_1)|\psi(\boldsymbol{\xi}_2)\rangle\langle\psi(\boldsymbol{\xi}_2)|\psi(\boldsymbol{\xi}_3)\rangle\langle\psi(\boldsymbol{\xi}_3)|\psi(\boldsymbol{\xi}_1)\rangle = -\frac{1}{8}$$

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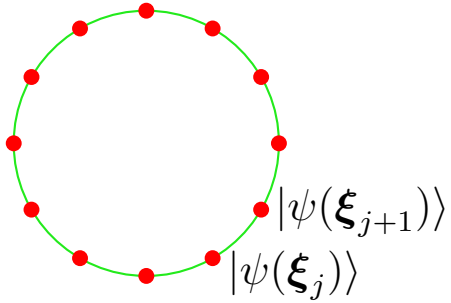

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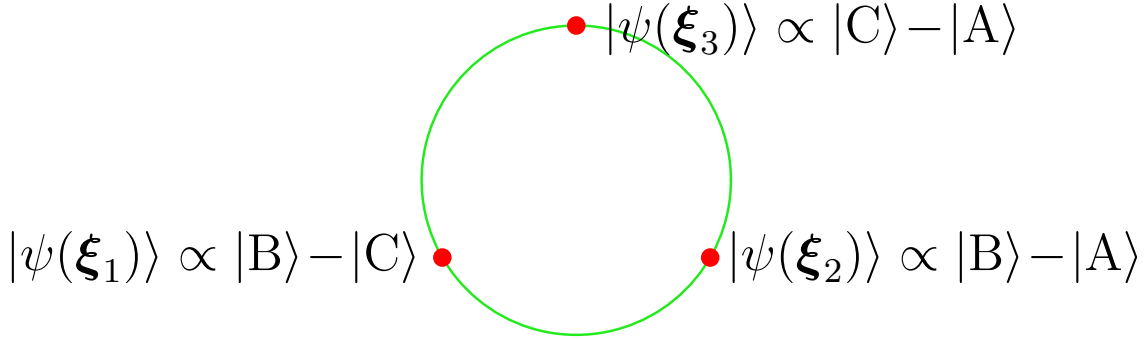

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Outline

Topology & conical intersections

Herzberg & Longuet-Higgins, 1963:

It shows that a conically self-intersecting potential surface has a different topological character from a pair of distinct surfaces which happen to meet at a point. Indeed, if an electronic wave function changes sign when we move round a closed loop in configuration space, we can conclude that somewhere inside the loop there must be a singular point at which the wave function is degenerate; in other words, there must be a genuine conical intersection, leading to an upper or lower sheet of the surface, as the case may be.

Berry phase γ

- Topologically trivial: $\gamma = 0 \bmod 2\pi = \pi \times (0 \bmod 2)$
- Topologically nontrivial: $\gamma = \pi \bmod 2\pi = \pi \times (1 \bmod 2)$
- Topological **invariant** $\in \mathbb{Z}_2$
  ($\mathbb{Z}_2$ = additive group of the integers mod 2)

Robustness of the topological invariant

Two-valued topological invariant:
The $\mathbb{Z}_2$ index is either 0 or 1 (mod 2)

- The index is robust against deformations of the path C, provided it does not cross the "obstruction"
- The index is very robust against **continuous** deformations of Hamiltonian & wave function,
  provided the HOMO-LUMO gap does not close
- We can even "continuously deformate" the wfn into the exact correlated one (if ground state non degenerate)
- Key role of **time-reversal invariance**
- In modern jargon:
  $\mathbb{Z}_2$ invariant is **"protected"** by time-reversal symmetry

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Outline

BO approx. for the H atom, $\mathbf{B} = 0$

$$\begin{aligned} \mathcal{H}(\mathbf{R},\mathbf{r}) &= -\frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}} + H_{\rm el}(\mathbf{R},\mathbf{r}) \\ H_{\rm el}(\mathbf{R},\mathbf{r}) &= -\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}} - \frac{e^2}{|\mathbf{r}-\mathbf{R}|} \end{aligned}$$

Lowest BO surface:

$$E_{\rm el}(\mathbf{R}) = \text{const} = -\frac{e^2}{2a_0}, \qquad \langle \mathbf{r}|\psi_{\rm el}(\mathbf{R})\rangle \propto \mathrm{e}^{-|\mathbf{r}-\mathbf{R}|/a_0}$$

BO Recipe: $$-\frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}}\Phi(\mathbf{R}) - \frac{e^2}{2a_0}\Phi(\mathbf{R}) = E\Phi(\mathbf{R})$$

$$E_{\rm BO}(\mathbf{k}) = \frac{\hbar^2 k^2}{2M} - \frac{e^2}{2a_0}, \qquad \Psi_{\rm BO}(\mathbf{R},\mathbf{r}) \propto \mathrm{e}^{-|\mathbf{r}-\mathbf{R}|/a_0}\ \mathrm{e}^{i\mathbf{k}\cdot\mathbf{R}}$$

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Compare exact with Born-Oppenheimer approx.

$$\mathcal{H}(\mathbf{R},\mathbf{r}) = -\frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}} - \frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}} - \frac{e^2}{|\mathbf{r}-\mathbf{R}|}$$

Separable using: $\tilde{\mathbf{R}} = \dfrac{M\,\mathbf{R} + m\,\mathbf{r}}{M+m}, \quad \tilde{\mathbf{r}} = \mathbf{r} - \mathbf{R}$

$$\begin{aligned} E(\mathbf{k}) &= \frac{\hbar^2 k^2}{2(M+m)} - \frac{\mu e^2}{2a_0}, \qquad \mu = \frac{m\,M}{m+M} \\ E_{\mathrm{BO}}(\mathbf{k}) &= \frac{\hbar^2 k^2}{2M} - \frac{e^2}{2a_0} \\ \lim_{m/M\to 0} E(\mathbf{k}) &= E_{\mathrm{BO}}(\mathbf{k}) \end{aligned}$$

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BO approx. for the H atom, $\mathbf{B} \neq 0$

(Neglecting irrelevant spin-dependent terms)

$$\mathcal{H}(\mathbf{R},\mathbf{r}) = \frac{1}{2M}\left[-i\hbar\nabla_{\mathbf{R}} - \frac{e}{c}\mathbf{A}(\mathbf{R})\right]^2 + H_{\rm el}(\mathbf{R},\mathbf{r})$$

$$H_{\rm el}(\mathbf{R},\mathbf{r}) = \frac{1}{2m}\left[-i\hbar\nabla_{\mathbf{r}} + \frac{e}{c}\mathbf{A}(\mathbf{r})\right]^2 - \frac{e^2}{|\mathbf{r}-\mathbf{R}|}$$

In a **constant** **B** field $\qquad E_{\rm el}(\mathbf{R}) = E_{\rm el} = \text{const}$

Naive recipe: $\dfrac{1}{2M}\left[-i\hbar\nabla_{\mathbf{R}} - \dfrac{e}{c}\mathbf{A}(\mathbf{R})\right]^2 \Phi(\mathbf{R}) - E_{\rm el}\,\Phi(\mathbf{R}) = E\Phi(\mathbf{R})$

- Same kinetic energy **as if** the proton were "naked"
- Classical limit: the H atom is deflected by a Lorentz force
- A neutral system is **not** deflected by a Lorentz force

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$$H_{\mathrm{el}}(\mathbf{R},\mathbf{r}) = \frac{1}{2m}\left[-i\hbar\nabla_{\mathbf{r}} + \frac{e}{c}\mathbf{A}(\mathbf{r})\right]^2 - \frac{e^2}{|\mathbf{r}-\mathbf{R}|}$$

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Solution of the paradox

"Screened" Born-Oppenheimer approximation:
Schmelcher, Cederbaum, & Meyer, 1988

Better:
Berry Connection & Berry curvature (same as for $\mathbf{B} = 0$)

$$\frac{1}{2M}\left[-i\hbar\nabla_{\mathbf{R}} - \frac{e}{c}\mathbf{A}(\mathbf{R})\right]^2 \rightarrow \frac{1}{2M}\left[-i\hbar\nabla_{\mathbf{R}} - \frac{e}{c}\mathbf{A}(\mathbf{R}) - \hbar\mathcal{A}(\mathbf{R})\right]^2$$

- $\mathbf{A}(\mathbf{R})$ genuine vector potential of magnetic origin
- $\mathcal{A}(\mathbf{R}) = i\langle\psi_{\mathrm{el}}(\mathbf{R})|\nabla_{\mathbf{R}}\psi_{\mathrm{el}}(\mathbf{R})\rangle$ Berry connection

Detailed reckoning in the central gauge

$$
\begin{aligned}
H_{\mathrm{el}}(\mathbf{R},\mathbf{r}) &= \frac{1}{2m}\left[-i\hbar\nabla_{\mathbf{r}} + \frac{e}{2c}\mathbf{B}\times\mathbf{r}\right]^2 - \frac{e^2}{|\mathbf{r}-\mathbf{R}|} \\
H_{\mathrm{el}}(0,\mathbf{r}) &= \frac{1}{2m}\left[-i\hbar\nabla_{\mathbf{r}} + \frac{e}{2c}\mathbf{B}\times\mathbf{r}\right]^2 - \frac{e^2}{r} \\
\langle\mathbf{r}|\psi_{\mathrm{el}}(0)\rangle &= \tilde{\psi}_0(\mathbf{r}) \qquad \text{complex wfn, cylindrical symmetry}
\end{aligned}
$$

$$
\langle\mathbf{r}|\psi_{\mathrm{el}}(\mathbf{R})\rangle = \mathrm{e}^{-\frac{ie}{2\hbar c}\mathbf{r}\cdot\mathbf{B}\times\mathbf{R}}\,\tilde{\psi}_0(|\mathbf{r}-\mathbf{R}|)
$$

$$
\mathcal{A}(\mathbf{R}) = i\langle\psi_{\mathrm{el}}(\mathbf{R})|\nabla_{\mathbf{R}}\psi_{\mathrm{el}}(\mathbf{R})\rangle = -\frac{e}{2\hbar c}\mathbf{B}\times\mathbf{R} = -\frac{e}{\hbar c}\mathbf{A}(\mathbf{R})
$$

$$
\mathcal{T}_{\mathrm{N}} = \frac{1}{2M}\left[-i\hbar\nabla_{\mathbf{R}} - \frac{e}{c}\mathbf{A}(\mathbf{R}) - \hbar\mathcal{A}(\mathbf{R})\right]^2 = \frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}}
$$

Detailed reckoning in the central gauge

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H_{\rm el}(\mathbf{R},\mathbf{r}) &= \frac{1}{2m}\left[-i\hbar\nabla_{\mathbf{r}}+\frac{e}{2c}\mathbf{B}\times\mathbf{r}\right]^2-\frac{e^2}{|\mathbf{r}-\mathbf{R}|}\\
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$$

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\mathcal{A}(\mathbf{R}) = i\langle\psi_{\rm el}(\mathbf{R})|\nabla_{\mathbf{R}}\psi_{\rm el}(\mathbf{R})\rangle = -\frac{e}{2\hbar c}\mathbf{B}\times\mathbf{R} = -\frac{e}{\hbar c}\mathbf{A}(\mathbf{R})
$$

$$
\mathcal{T}_{\rm N} = \frac{1}{2M}\left[-i\hbar\nabla_{\mathbf{R}}-\frac{e}{c}\mathbf{A}(\mathbf{R})-\hbar\mathcal{A}(\mathbf{R})\right]^2 = \frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}}
$$

Magnetic & geometric together

- **H atom**
  - Paradox solved (both quantum nucleus & classical nucleus)
  - In the classical limit **no Lorentz force**
  - **Hamiltonian** (quantum & classical)
    The Berry **connection** cancels the **vector potential**
  - **Newton Eq.** (gauge invariant):
    The Berry **curvature** cancels the **magnetic field**

- **Molecule** (rotations & vibrations in a **B** field)
  - The two terms **do not cancel**
  - They are of the same order of magnitude
  - The geometric term is important even for classical nuclei:
    "geometric Lorentz force" in Newton Eq.

$\mathbf{B} = 0$ vs. $\mathbf{B} \neq 0$ in Born-Oppenheimer

- $\mathbf{B} = 0$ (time-reversal symmetric)
  - Conical intersections $\Rightarrow$ nontrivial geometric effects
  - The electronic wfn **can** be chosen as **real**
  - The Berry **curvature** vanishes (or is singular)
  - Classical nuclei **not affected** by geometric effects
  - The Berry phase only shows up when quantising the nuclei

- $\mathbf{B} \neq 0$ (time-reversal symmetry absent)
  - No singularity needed in the Born-Oppenheimer surface
  - The electronic wfn must be **complex**
  - The Berry **curvature** is generally **nonzero**
  - Classical nuclei **are affected** by geometric effects
  - The Berry curvature enters the Newton Eq. for the nuclei

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