

# La fase de Berry

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# Fase de Berry

$$H(x; \xi)\Psi(x; \xi) = E(\xi)\Psi(x; \xi) \quad \xi \longrightarrow \text{paràmetres}$$

$$\Psi(x; \xi) \equiv \Psi(\xi) \quad \text{No degenerat } \forall \xi$$

$$\Psi(\xi) \quad \text{determinat excepte una fase } e^{-i\varphi} \text{ (gauge)}$$

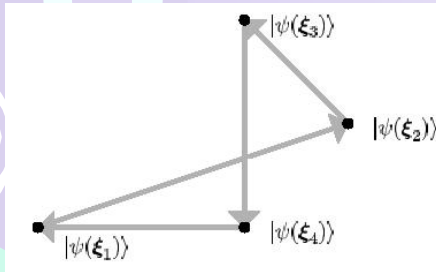
Definició: Diferència de fase entre  $|\Psi(\xi_1)\rangle$  i  $|\Psi(\xi_2)\rangle$

$$e^{-i\Delta\varphi_{12}} = \frac{\langle \Psi(\xi_1) | \Psi(\xi_2) \rangle}{|\langle \Psi(\xi_1) | \Psi(\xi_2) \rangle|}$$

$$\Delta\varphi_{12} = -\text{Im} \text{Log} \langle \Psi(\xi_1) | \Psi(\xi_2) \rangle \in \mathfrak{R}$$

$\Delta\varphi_{12}$  no té sentit físic (és funció del gauge)

# Fase de Berry



Definició: fase total  $\gamma$

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

$$\gamma = -\text{Im} \text{Log} \langle \Psi(\xi_1) | \Psi(\xi_2) \rangle \langle \Psi(\xi_2) | \Psi(\xi_3) \rangle \langle \Psi(\xi_3) | \Psi(\xi_4) \rangle \langle \Psi(\xi_4) | \Psi(\xi_1) \rangle$$

$\gamma$  és funció del camí triat ... Però independent de gauge (INVARIANT) ... ¿observable?

# Fase de Berry

Diferencia de fase entre punts infinitament pròxims:  $e^{-id\varphi} = \frac{\langle \Psi(\xi) | \Psi(\xi + d\xi) \rangle}{|\langle \Psi(\xi) | \Psi(\xi + d\xi) \rangle|}$

$$-i d\varphi \approx \text{Log}\left(1 + \langle \Psi(\xi) | \nabla_{\xi} \Psi(\xi) \rangle d\xi\right)$$

$$d\varphi \approx i \langle \Psi(\xi) | \nabla_{\xi} \Psi(\xi) \rangle d\xi = X(\xi) d\xi$$

$$X(\xi) \in \mathfrak{R} \quad \text{Connexió de Berry}$$

Definició: Fase  $\gamma$  de Berry

$$\gamma = \oint d\varphi = \oint X(\xi) d\xi \in \mathfrak{R}$$

Gauge independent

# Analogia magnètica

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$$\left. \begin{array}{l} \vec{\xi} \in D \subset \mathbb{R}^3 \\ D \text{ connex} \end{array} \right\}$$

Teorema de Stokes:  $\gamma = \oint X(\xi) d\xi = \iint Y(\xi) dS$

$$Y(\xi) = \nabla_{\xi} \wedge X(\xi)$$

$X(\xi) \Rightarrow$  potencial vector  $A$

$Y(\xi) \Rightarrow$  camp magnètic  $B$

$\gamma \Rightarrow$  flux magnètic  $\Phi$

## Cas general

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$$\gamma = \oint X(\xi) d\xi = \int_{\sigma} Y(\xi) d\sigma$$

connexió de Berry  $\Rightarrow X(\xi) = i \langle \Psi(\xi) | \nabla_{\xi} \Psi(\xi) \rangle \in \mathfrak{R}^N$

curvatura  $\Rightarrow Y_{\alpha\beta}(\xi) = \frac{\partial}{\partial \xi_{\alpha}} X_{\beta}(\xi) - \frac{\partial}{\partial \xi_{\beta}} X_{\alpha}(\xi)$

$$Y_{\alpha\beta}(\xi) = i \left[ \left\langle \frac{\partial \psi}{\partial \xi_{\alpha}} \middle| \frac{\partial \psi}{\partial \xi_{\beta}} \right\rangle + \left\langle \frac{\partial \psi}{\partial \xi_{\beta}} \middle| \frac{\partial \psi}{\partial \xi_{\alpha}} \right\rangle \right] = 2 \operatorname{Im} \left\langle \frac{\partial \psi}{\partial \xi_{\alpha}} \middle| \frac{\partial \psi}{\partial \xi_{\beta}} \right\rangle$$

La curvatura Y és gauge independent (similar a B) .... ¿Observable?

## Cas general (cont.)

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Si és possible triar  $\psi \in \mathfrak{R} \longrightarrow Y_{\alpha\beta}(\xi) = 0$



En dominis connexos

$$\gamma = 0$$



$\gamma$  no trivial (e.g.  $\gamma = \pi$ ) únicament en dominis múltiplement connexos.

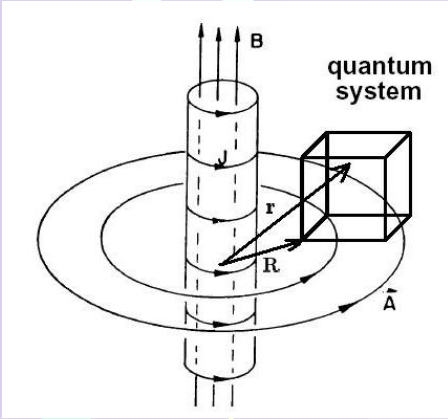


Si  $\Psi$  inevitablement complexa  $\longrightarrow Y_{\alpha\beta}(\xi) \neq 0$  (en general)



Podem trobar  $\gamma \neq 0$  fins i tot en dominis simplement connexos

# Efecte Aharonov Bohm



$$H(R) = \frac{p^2}{2m} + V(r - R)$$

$$\Psi(r - R) \in \mathfrak{R} \quad (\text{gauge possible})$$

➡ En presència de camp B:  $p \rightarrow p - eA$

$$\tilde{H}(R) = \frac{1}{2m} [p - eA]^2 + V(r - R)$$

$$\tilde{\psi}(r - R) = \exp \left[ \frac{ie}{\hbar} \int_R^r A(r') dr' \right] \psi(r - R)$$

{ Si  $B \neq 0$  en el solenoide (fora del sistema)  
 Si  $B = 0$  en la resta de l'espai

➡ Domini R doblement connex

$\gamma$  no trivial





## Efecte Aharonov-Bohm (cont.)

$$X(R) = i \langle \tilde{\Psi}(r-R) | \nabla_R \tilde{\Psi}(r-R) \rangle = \dots = i \int \Psi(r-R) \nabla_R \Psi(r-R) dr + \frac{eA(R)}{\hbar}$$

però  $\int \Psi(r-R) \nabla_R \Psi(r-R) dr = \frac{1}{2} \nabla_R \int \Psi(r-R)^2 dr = \frac{1}{2} \nabla_R (1) = 0$

$$\gamma = \oint X(R) dR = \frac{e}{\hbar} \oint A(R) dR = \frac{e}{\hbar} \Phi = \frac{\Phi}{\Phi_0}$$

$$e^{im\theta} \Rightarrow e^{i(m\theta + \frac{\Phi}{\Phi_0})}$$

# Born-Oppenheimer. Interseccions còniques

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$$H(x; \xi) = T_N(\xi) + H_e(x; \xi)$$

$$\Psi_{B.O.} = \Psi_e(x; \xi) R(\xi)$$

on:  $H_e(x; \xi) \Psi_e(x; \xi) = E_e(\xi) \Psi_e(x; \xi)$

i  $R(\xi)$  és solució d'un Hamiltonià efectiu per al moviment nuclear

$$H_{eff}(\xi) R(\xi) = E R(\xi)$$

$$H_{eff}(\xi) = \frac{1}{2} \pi^2 + V(\xi) \quad ?$$

## Born-Oppenheimer (cont.)

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Si escrivim:  $H(x; \xi) \Psi_{B.O.} = T_N(\xi) \Psi_e(x; \xi) R(\xi) + E_e(\xi) \Psi_e(x; \xi) R(\xi)$

multipliquem per  $\Psi_e(x; \xi)^*$  i integrem les coordenades electròniques:

$$\begin{aligned} \langle \Psi_e(x; \xi) | H(x; \xi) | \Psi_e(x; \xi) \rangle_x R(\xi) &\equiv H_{eff}(\xi) R(\xi) = \\ &= \langle \Psi_e(x; \xi) | T_N(\xi) | \Psi_e(x; \xi) \rangle_x R(\xi) + E_e(\xi) R(\xi) = E R(\xi) \end{aligned}$$

De seguida identifiquem:  $V(\xi) = E_e(\xi)$

En una aproximació d'ordre zero:  $\nabla_\xi [\Psi_e(x; \xi) R(\xi)] \approx \Psi_e(x; \xi) \nabla_\xi R(\xi)$

  $\pi = p = -i \nabla_\xi$

## Born-Oppenheimer (cont.)

En una aproximació de primer ordre, atès que:

$$\langle \Psi_e(x; \xi) | \hat{p} \Psi_e(x; \xi) R(\xi) \rangle_x = -i \left( \nabla_\xi + \langle \Psi_e(x; \xi) | \nabla_\xi \Psi_e(x; \xi) \rangle_x \right) R(\xi)$$

definim:  $\pi = -i \left( \nabla_\xi + \langle \Psi_e(x; \xi) | \nabla_\xi \Psi_e(x; \xi) \rangle_x \right)$


i de seguida identifiquem, en comparar amb efecte AB, la connexió:

$$X(\xi) = i \langle \Psi_e(x; \xi) | \nabla_\xi \Psi_e(x; \xi) \rangle_x$$

## Born-Oppenheimer (cont.)

➡ En absència de camps i termes LS, les funcions  $\Psi_e(x; \xi)$  poden ser reals

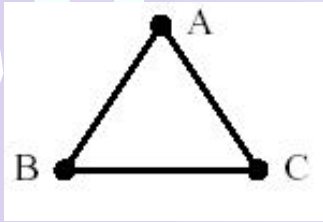
➡ 
$$X(\xi) = i \int dx \Psi_e(x; \xi) \nabla_\xi \Psi_e(x; \xi) = \frac{i}{2} \nabla_\xi \int dx \Psi_e(x; \xi)^2 = \frac{i}{2} \nabla_\xi (1) = 0$$


$$\pi = p = -i \nabla_\xi$$

➡ Pot ocórrer però que en efectuar un cicle adiabàtic la funció electrònica canvie de signe (i.e.  $\gamma = \pi$ )

➡ S'ha encerclat una singularitat, i.e., un punt o regió on  $X(\xi)$  no està definida (intersecció cònica)

# Un exemple: Jahn-Teller $E \otimes \varepsilon$



$\left\{ \begin{array}{l} \text{Tres nuclis idèntics (D}_{3h}\text{)} \\ \text{Tres electrons: Aproximem } \Psi_e(x; \xi) \text{ per una funció PI} \end{array} \right.$

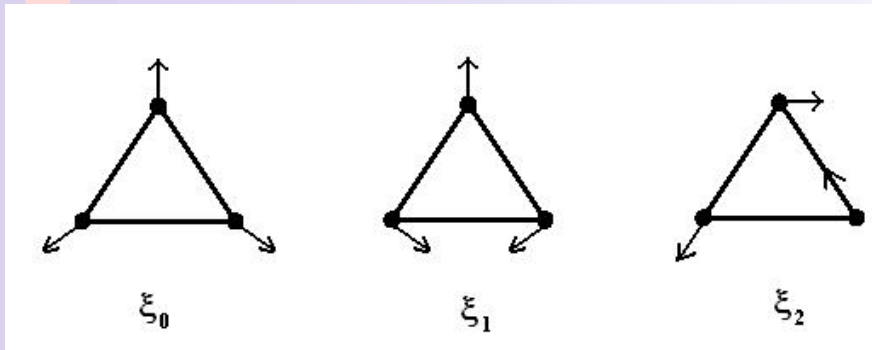
Els MOs:

$$\begin{aligned}
 |0\rangle &= \frac{1}{\sqrt{3}}(A + B + C) \\
 |1\rangle &= \frac{1}{\sqrt{2}}(B - C) \\
 |2\rangle &= \frac{1}{\sqrt{6}}(2A - B - C)
 \end{aligned}$$

L'estat fonamental:  $|0^2 e\rangle \rightarrow \boxed{2E}$

$$|e\rangle = \cos \alpha |1\rangle + \sin \alpha |2\rangle \quad \forall \alpha$$

Els modes normals:



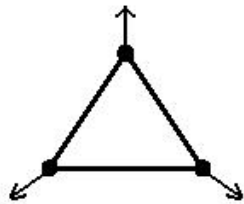
$\left\{ \begin{array}{l} \xi_0 \text{ totalment simètric} \\ (\xi_1, \xi_2) \text{ simetria } \varepsilon \end{array} \right.$

## Jahn-Teller $E \otimes \varepsilon$ (cont.)

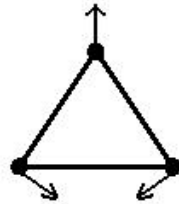
Els modes normals en coordenades:

$$\xi_1 = \begin{cases} x_A = 0 & y_A = 1 \\ x_B = \frac{\sqrt{3}}{2} & y_B = -\frac{1}{2} \\ x_C = -\frac{\sqrt{3}}{2} & y_C = -\frac{1}{2} \end{cases}$$

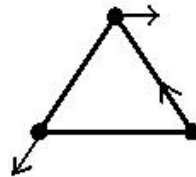
$$\xi_2 = \begin{cases} x_A = 1 & y_A = 1 \\ x_B = -\frac{1}{2} & y_B = -\frac{\sqrt{3}}{2} \\ x_C = -\frac{1}{2} & y_C = \frac{\sqrt{3}}{2} \end{cases}$$



$\xi_0$



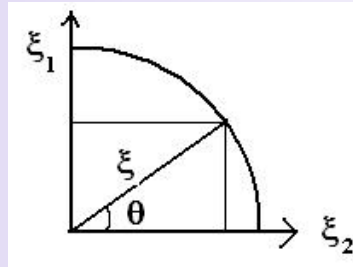
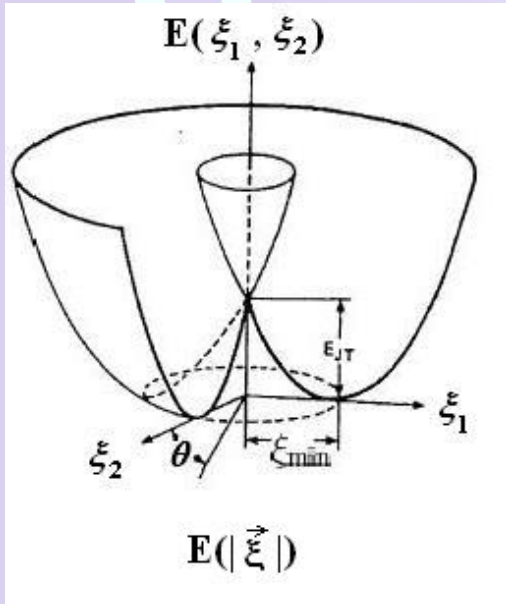
$\xi_1$



$\xi_2$

Únicament  $\vec{\xi} = a\xi_1 + b\xi_2$  disminueix la simetria i trenca la degeneració

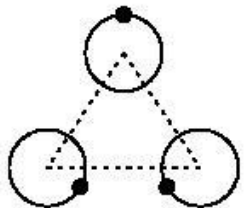
# Jahn-Teller $E \otimes \varepsilon$ (cont.)



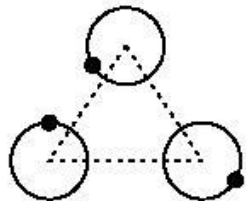
Triem  $|\vec{\xi}| = 1$

$$\vec{\xi} = \sin \theta \vec{\xi}_1 + \cos \theta \vec{\xi}_2$$

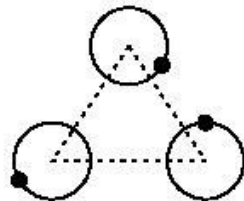
$$\vec{\xi} = \begin{cases} x_A = \sin \theta & y_A = \cos \theta \\ x_B = -\frac{1}{2} \sin \theta + \frac{\sqrt{3}}{2} \cos \theta & y_B = -\frac{\sqrt{3}}{2} \sin \theta - \frac{1}{2} \cos \theta \\ x_C = -\frac{1}{2} \sin \theta - \frac{\sqrt{3}}{2} \cos \theta & y_C = \frac{\sqrt{3}}{2} \sin \theta - \frac{1}{2} \cos \theta \end{cases}$$



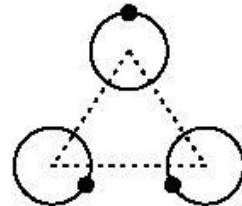
$\theta = 0^\circ$



$\theta = 120^\circ$



$\theta = 240^\circ$

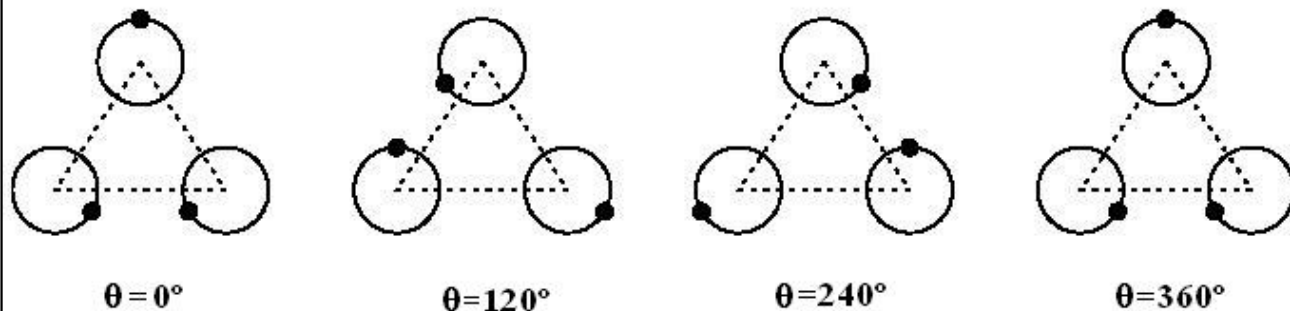


$\theta = 360^\circ$

ISOENERGÈTICS



# Jahn-Teller $E \otimes \varepsilon$ (cont.)



**Triem** en  $\theta = 0$

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

Cal esperar que:  $|e\rangle = \pm \frac{1}{\sqrt{2}}(A - B)$      $|e\rangle = \pm \frac{1}{\sqrt{2}}(A - C)$      $|e\rangle = \pm \frac{1}{\sqrt{2}}(B - C)$

Triem el gauge diferenciable:  $\alpha = \theta/2$      $\longrightarrow$      $|e\rangle = \cos \frac{\theta}{2} |1\rangle + \sin \frac{\theta}{2} |2\rangle$

$$\left. \begin{array}{l} \theta = 0 \rightarrow |e\rangle = |1\rangle \\ \theta = 360 \rightarrow |e\rangle = -|1\rangle \end{array} \right\}$$

$$\longrightarrow \gamma = \pi$$

Canvi de fase  
que envolta la  
**SINGULARITAT**  
(intersecció cònica)

Versió naïve del teorema de Longuet-Higgins  
(Proc. R. Soc. London A 344 (1975) 147-156)