Texture-induced spin-orbit coupling and skyrmion-electron bound states in a Néel antiferromagnet

with Naïmo Davier (PhD 2023, LPT Toulouse)

Phys. Rev. B **107**, 014406 (2023) and **109**, 224425 (2024)

Revaz Ramazashvili (LPT Toulouse)

IMPACT, Cargèse, August 29, 2024

Motivation :

Motivation :

– Much interest in antiferromagnets

Motivation :

– Much interest in antiferromagnets

– Much interest in topological textures

Motivation :

– Much interest in antiferromagnets

– Much interest in topological textures

– Much interest in using textures in memory devices, as an information carrier

Motivation :

– Much interest in antiferromagnets

– Much interest in topological textures

– Much interest in using textures in memory devices, as an information carrier

– Vital to understand their interplay with carriers

Motivation :

– Much interest in antiferromagnets

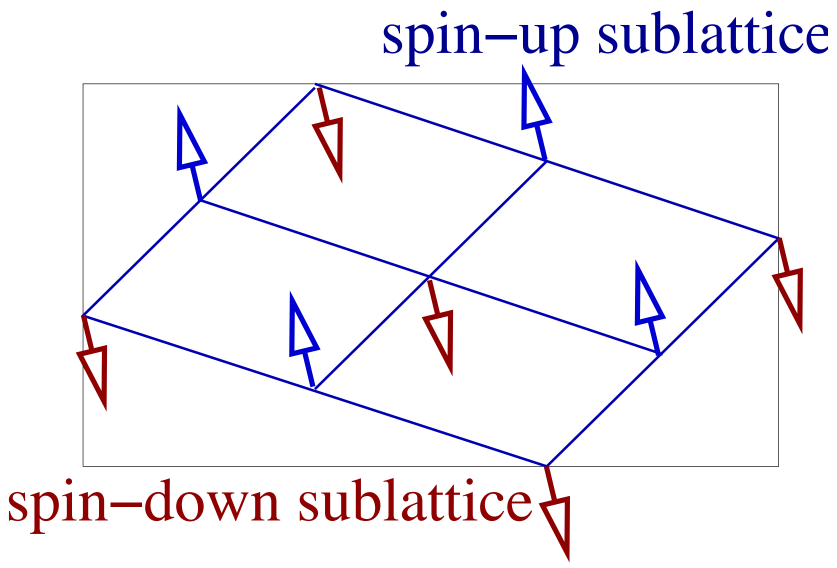
– Much interest in topological textures

– Much interest in using textures in memory devices, as an information carrier

– Vital to understand their interplay with carriers

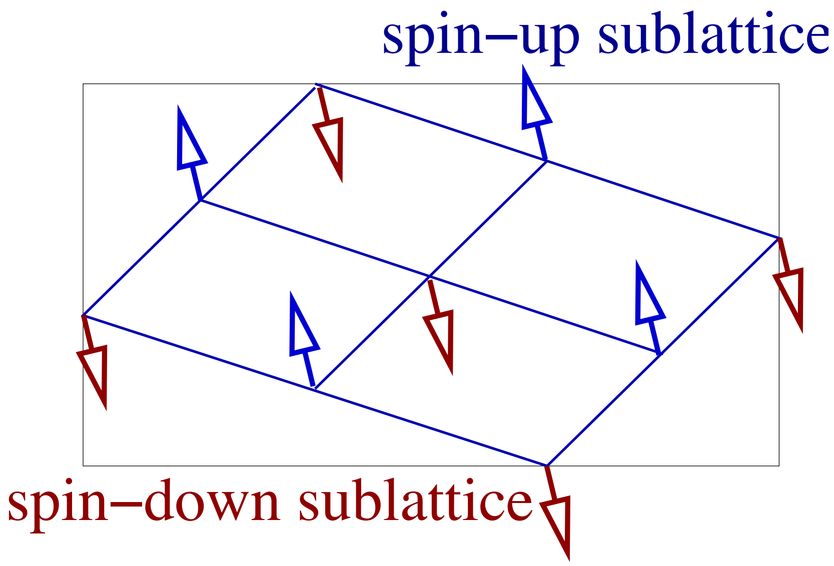
And now, on to the main heroes of our story :

Néel antiferromagnet :



$$\mathbf{M}(\mathbf{r}+\mathbf{a}) = -\mathbf{M}(\mathbf{r})$$

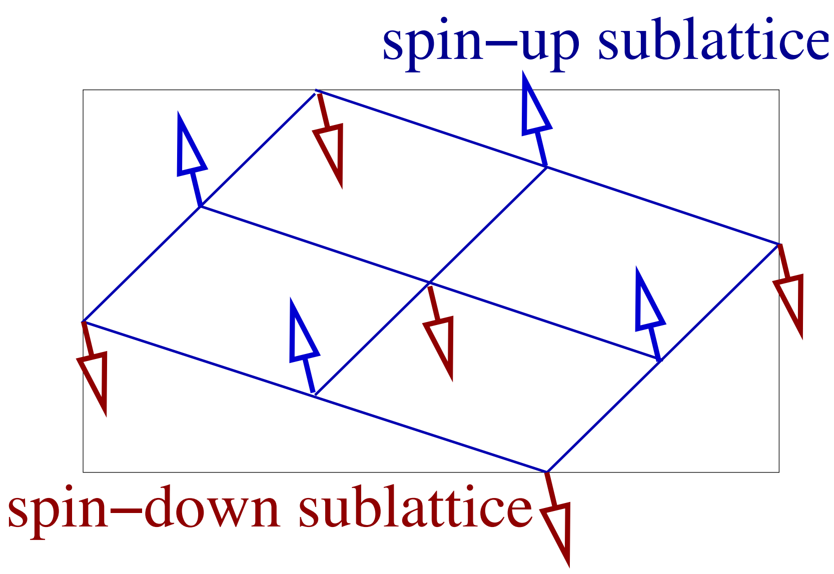
Néel antiferromagnet :



$$\mathbf{M}(\mathbf{r}+\mathbf{a}) = -\mathbf{M}(\mathbf{r})$$

$$\mathbf{M}(\mathbf{r}) = \mathbf{M}_0 \exp[\, i\,(\mathbf{Q}\cdot\mathbf{r})\,]$$

Néel antiferromagnet :

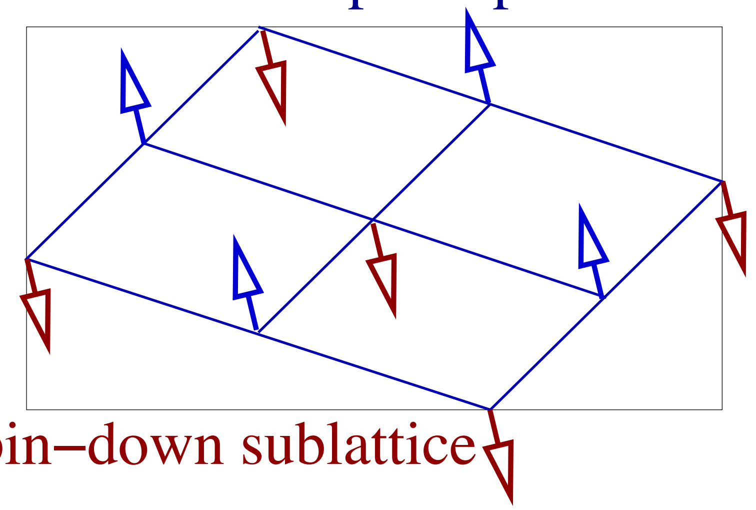


$$\mathbf{M}(\mathbf{r}+\mathbf{a}) = -\mathbf{M}(\mathbf{r})$$

$$\mathbf{M}(\mathbf{r}) = \mathbf{M}_0 \exp[\, i\,(\mathbf{Q}\cdot\mathbf{r})\,]$$

$$\mathbf{Q} = \left(\frac{\pi}{a}\,,\,\frac{\pi}{a}\right)$$

Néel antiferromagnet :



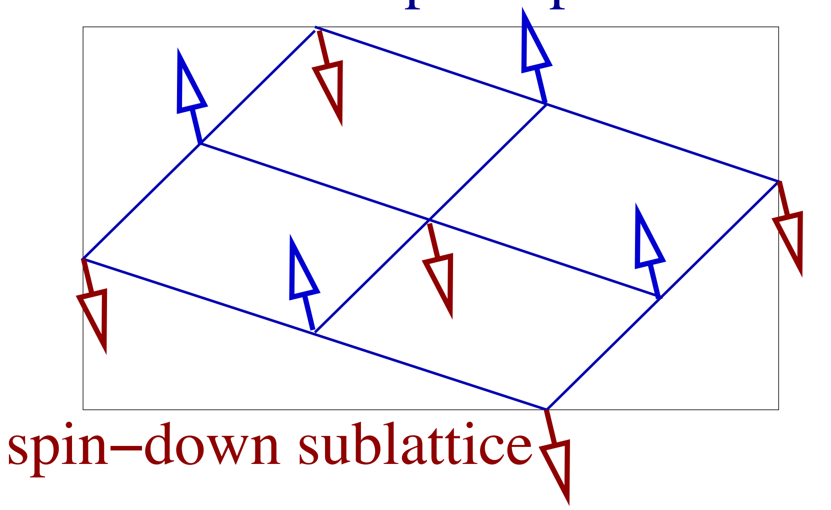
$$\mathbf{M}(\mathbf{r}+\mathbf{a}) = -\mathbf{M}(\mathbf{r})$$

$$\mathbf{M}(\mathbf{r}) = \mathbf{M}_0 \exp[\, i\,(\mathbf{Q}\cdot\mathbf{r})\,]$$

$$\mathbf{Q} = \left(\frac{\pi}{a}\,,\,\frac{\pi}{a}\right)$$

$\mathbf{M}(\mathbf{r})$ couples to conduction electron spin σ :

Néel antiferromagnet :



$$\mathbf{M}(\mathbf{r}+\mathbf{a}) = -\mathbf{M}(\mathbf{r})$$

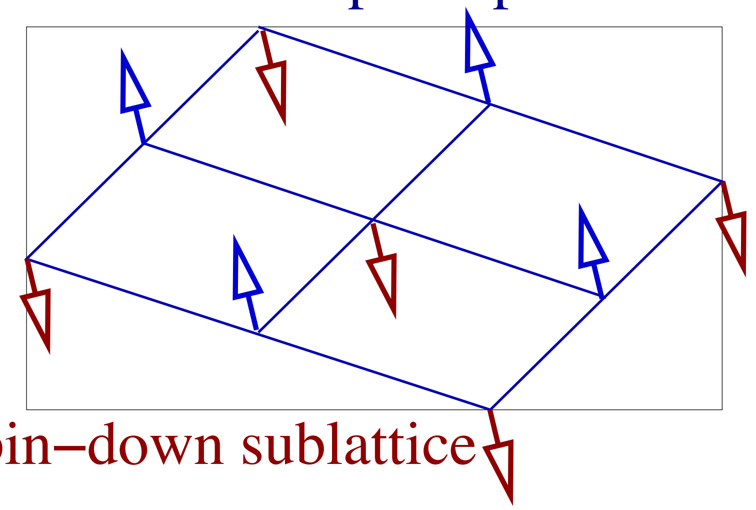
$$\mathbf{M}(\mathbf{r}) = \mathbf{M}_0 \exp[\, i\,(\mathbf{Q}\cdot\mathbf{r})\,]$$

$$\mathbf{Q} = \left(\frac{\pi}{a}\,,\,\frac{\pi}{a}\right)$$

$\mathbf{M}(\mathbf{r})$ couples to conduction electron spin σ :

$$J\,(\mathbf{M}(\mathbf{r})\cdot\sigma) \sim J\,(\mathbf{M}_0\cdot\sigma)\,e^{i\mathbf{Q}\cdot\mathbf{r}} = (\mathbf{\Delta}\cdot\sigma)e^{i\mathbf{Q}\cdot\mathbf{r}}$$

Néel antiferromagnet :



$$\mathbf{M}(\mathbf{r}+\mathbf{a}) = -\mathbf{M}(\mathbf{r})$$

$$\mathbf{M}(\mathbf{r}) = \mathbf{M}_0 \exp[\, i\,(\mathbf{Q}\cdot\mathbf{r})\,]$$

$$\mathbf{Q} = \left(\frac{\pi}{a}\,,\ \frac{\pi}{a}\right)$$

$\mathbf{M}(\mathbf{r})$ couples to conduction electron spin σ :

$$J\,(\mathbf{M}(\mathbf{r})\cdot\sigma) \sim J\,(\mathbf{M}_0\cdot\sigma)\,e^{i\mathbf{Q}\cdot\mathbf{r}} = (\mathbf{\Delta}\cdot\sigma)e^{i\mathbf{Q}\cdot\mathbf{r}}$$

… that is, couples any momentum $\mathbf{p}$ to $\mathbf{p}+\mathbf{Q}$.

Bispinor

$$\Psi = (\psi_{\mathbf{p}}\,, \psi_{\mathbf{p}+\mathbf{Q}})$$

Bispinor $\Psi = (\psi_{\mathbf{p}}\,, \psi_{\mathbf{p}+\mathbf{Q}})$

The Hamiltonian : $\mathcal{H} = \begin{bmatrix} \varepsilon(\mathbf{p}) & (\mathbf{\Delta}\cdot\sigma) \\ (\mathbf{\Delta}\cdot\sigma) & \varepsilon(\mathbf{p}+\mathbf{Q}) \end{bmatrix}$

Bispinor $\Psi = (\psi_{\mathbf{p}}\,, \psi_{\mathbf{p}+\mathbf{Q}})$

The Hamiltonian : $\mathcal{H} = \begin{bmatrix} \varepsilon(\mathbf{p}) & (\mathbf{\Delta}\cdot\sigma) \\ (\mathbf{\Delta}\cdot\sigma) & \varepsilon(\mathbf{p}+\mathbf{Q}) \end{bmatrix}$

The spectrum $E_{\mathbf{p}} = \varepsilon_+(\mathbf{p}) \pm \sqrt{|\mathbf{\Delta}|^2 + \varepsilon_-^2(\mathbf{p})}$,

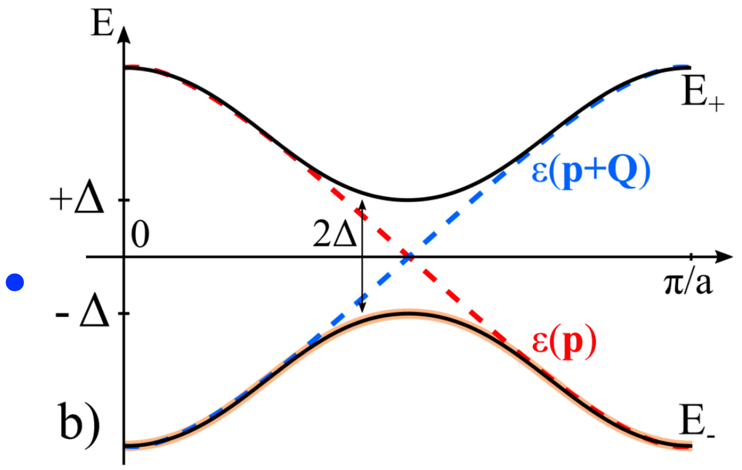
where $\varepsilon_\pm(\mathbf{p}) \equiv \frac{1}{2}\left[\varepsilon(\mathbf{p}) \pm \varepsilon(\mathbf{p}+\mathbf{Q})\right]$.

Bispinor $\Psi = (\psi_{\mathbf{p}}\,, \psi_{\mathbf{p}+\mathbf{Q}})$

The Hamiltonian : $\mathcal{H} = \begin{bmatrix} \varepsilon(\mathbf{p}) & (\mathbf{\Delta}\cdot\sigma) \\ (\mathbf{\Delta}\cdot\sigma) & \varepsilon(\mathbf{p}+\mathbf{Q}) \end{bmatrix}$

The spectrum $E_{\mathbf{p}} = \varepsilon_{+}(\mathbf{p}) \pm \sqrt{|\mathbf{\Delta}|^2 + \varepsilon_{-}^2(\mathbf{p})}$,

where $\varepsilon_{\pm}(\mathbf{p}) \equiv \frac{1}{2}\left[\varepsilon(\mathbf{p}) \pm \varepsilon(\mathbf{p}+\mathbf{Q})\right]$.

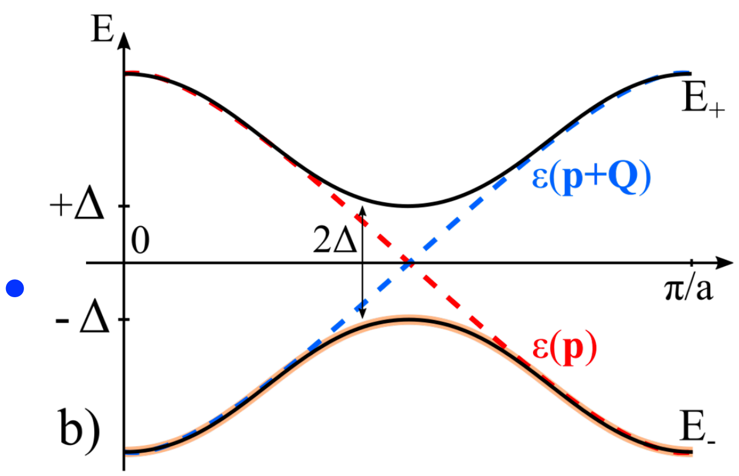


Bispinor $\Psi = (\psi_{\mathbf{p}}\,, \psi_{\mathbf{p}+\mathbf{Q}})$

The Hamiltonian : $\mathcal{H} = \begin{bmatrix} \varepsilon(\mathbf{p}) & (\boldsymbol{\Delta}\cdot\sigma) \\ (\boldsymbol{\Delta}\cdot\sigma) & \varepsilon(\mathbf{p}+\mathbf{Q}) \end{bmatrix}$

The spectrum $E_{\mathbf{p}} = \varepsilon_{+}(\mathbf{p}) \pm \sqrt{|\boldsymbol{\Delta}|^2 + \varepsilon_{-}^2(\mathbf{p})}$,

where $\varepsilon_{\pm}(\mathbf{p}) \equiv \frac{1}{2}\left[\varepsilon(\mathbf{p}) \pm \varepsilon(\mathbf{p}+\mathbf{Q})\right]$.



Generalisation for a non-uniform $\boldsymbol{\Delta}_{\mathbf{r}} = \hat{\mathbf{n}}_{\mathbf{r}}\Delta$?

Hamiltonian for a non-uniform $\boldsymbol{\Delta}_{\mathbf{r}} = \hat{\mathbf{n}}_{\mathbf{r}} \Delta$?

Hamiltonian for a non-uniform $\mathbf{\Delta_r} = \hat{\mathbf{n}}_\mathbf{r}\Delta$?

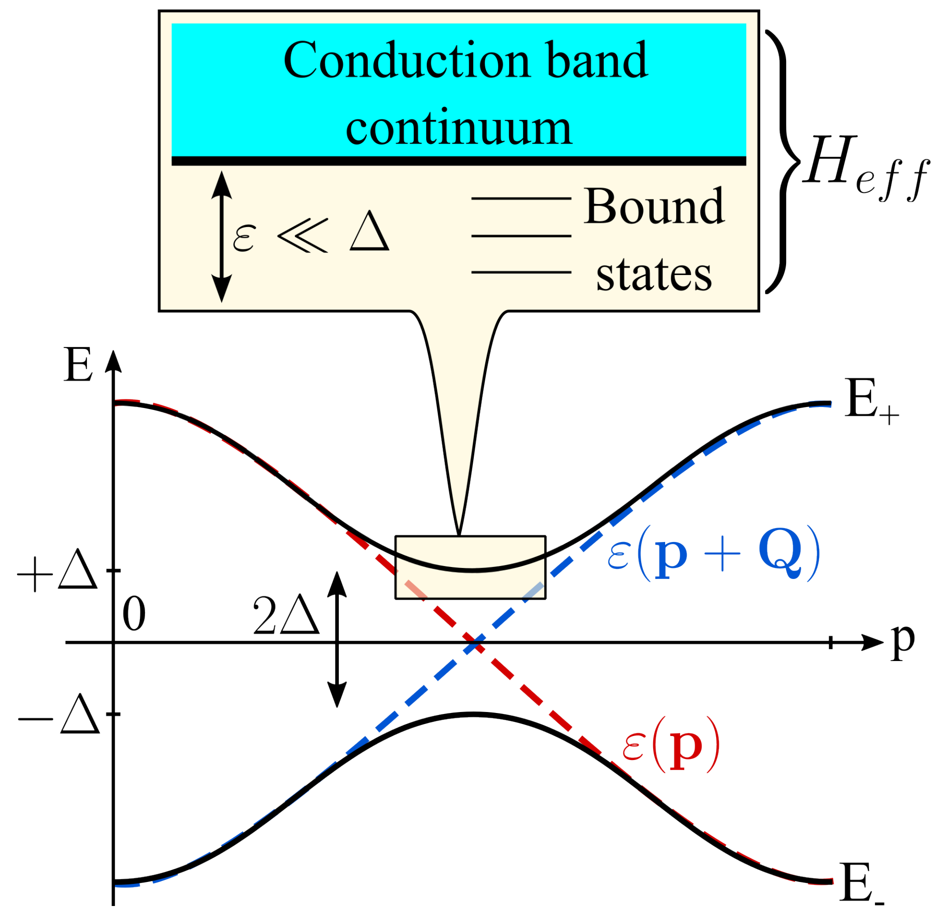
Stay close to the gap edge ($\frac{E-\Delta}{\Delta} \ll 1$)

and go from "Dirac" to "Schrödinger" :

Hamiltonian for a non-uniform $\mathbf{\Delta_r} = \hat{\mathbf{n}}_\mathbf{r}\Delta$?

Stay close to the gap edge ($\frac{E-\Delta}{\Delta} \ll 1$)

and go from “Dirac” to “Schrödinger” :



Hamiltonian for a non-uniform $\mathbf{\Delta}_{\mathbf{r}} = \hat{\mathbf{n}}_{\mathbf{r}} \Delta$?

Hamiltonian for a non-uniform $\mathbf{\Delta_r} = \hat{\mathbf{n}}_\mathbf{r} \Delta$?

Effective-mass theory near band extrema:

Hamiltonian for a non-uniform $\mathbf{\Delta}_\mathbf{r} = \hat{\mathbf{n}}_\mathbf{r}\Delta$?

Effective-mass theory near band extrema:

Undo $(\mathbf{\Delta}_\mathbf{r} \cdot \sigma)$ by spin rotation: $U^\dagger_\mathbf{r}(\hat{\mathbf{n}}_\mathbf{r} \cdot \sigma)U_\mathbf{r} = \sigma^z$

Hamiltonian for a non-uniform $\boldsymbol{\Delta}_{\mathbf{r}} = \hat{\mathbf{n}}_{\mathbf{r}} \Delta$?

Effective-mass theory near band extrema:

Undo $(\boldsymbol{\Delta}_{\mathbf{r}} \cdot \sigma)$ by spin rotation: $U^{\dagger}_{\mathbf{r}} (\hat{\mathbf{n}}_{\mathbf{r}} \cdot \sigma) U_{\mathbf{r}} = \sigma^z$

Off diagonal – uniform $\boldsymbol{\Delta}$: $\mathcal{H} = \begin{bmatrix} \varepsilon(\mathbf{p}) & \sigma^z \Delta \\ \sigma^z \Delta & \varepsilon(\mathbf{p} + \mathbf{Q}) \end{bmatrix}$

Hamiltonian for a non-uniform $\mathbf{\Delta}_{\mathbf{r}} = \hat{\mathbf{n}}_{\mathbf{r}}\Delta$?

Effective-mass theory near band extrema:

Undo $(\mathbf{\Delta}_{\mathbf{r}} \cdot \sigma)$ by spin rotation: $U^{\dagger}_{\mathbf{r}}(\hat{\mathbf{n}}_{\mathbf{r}} \cdot \sigma)U_{\mathbf{r}} = \sigma^z$

Off diagonal – uniform $\mathbf{\Delta}$: $\mathcal{H} = \begin{bmatrix} \varepsilon(\mathbf{p}) & \sigma^z\Delta \\ \sigma^z\Delta & \varepsilon(\mathbf{p}+\mathbf{Q}) \end{bmatrix}$

On the diagonal – a Peierls substitution:

Hamiltonian for a non-uniform $\mathbf{\Delta_r} = \hat{\mathbf{n}}_\mathbf{r}\Delta$?

Effective-mass theory near band extrema:

Undo $(\mathbf{\Delta_r} \cdot \sigma)$ by spin rotation: $U_\mathbf{r}^\dagger(\hat{\mathbf{n}}_\mathbf{r} \cdot \sigma)U_\mathbf{r} = \sigma^z$

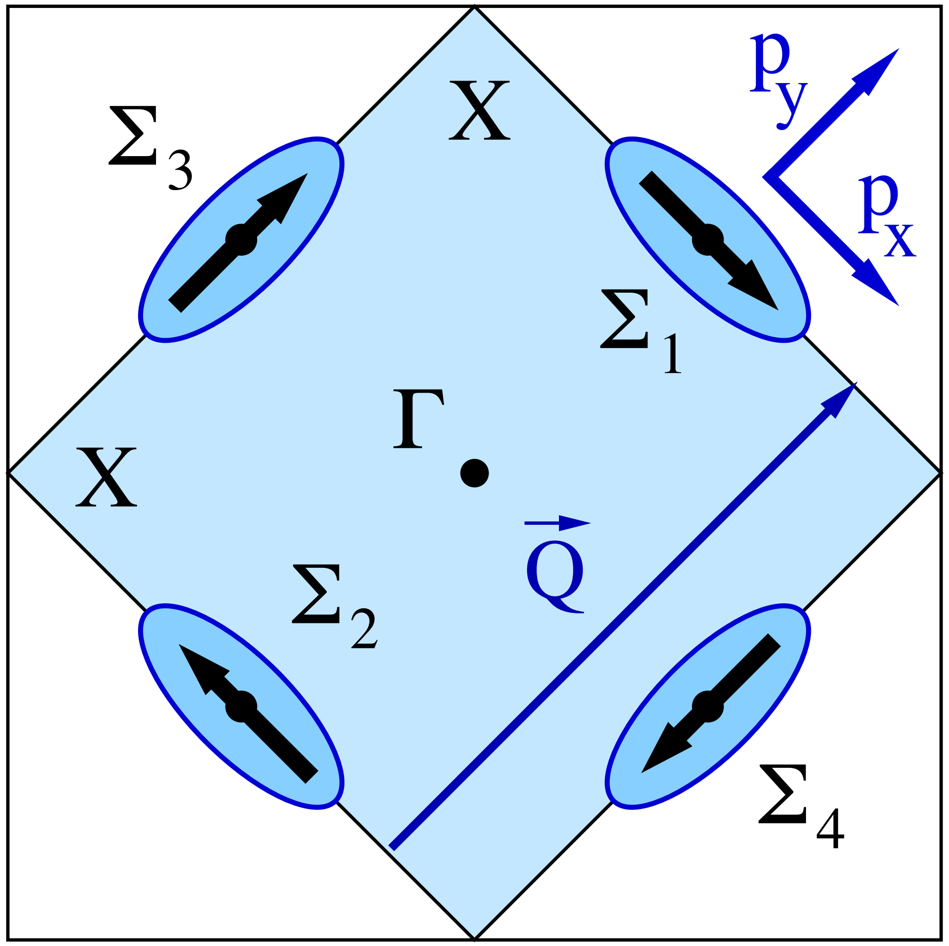
Off diagonal – uniform $\mathbf{\Delta}$: $\mathcal{H} = \begin{bmatrix} \varepsilon(\mathbf{p}) & \sigma^z\Delta \\ \sigma^z\Delta & \varepsilon(\mathbf{p}+\mathbf{Q}) \end{bmatrix}$

On the diagonal – a Peierls substitution:

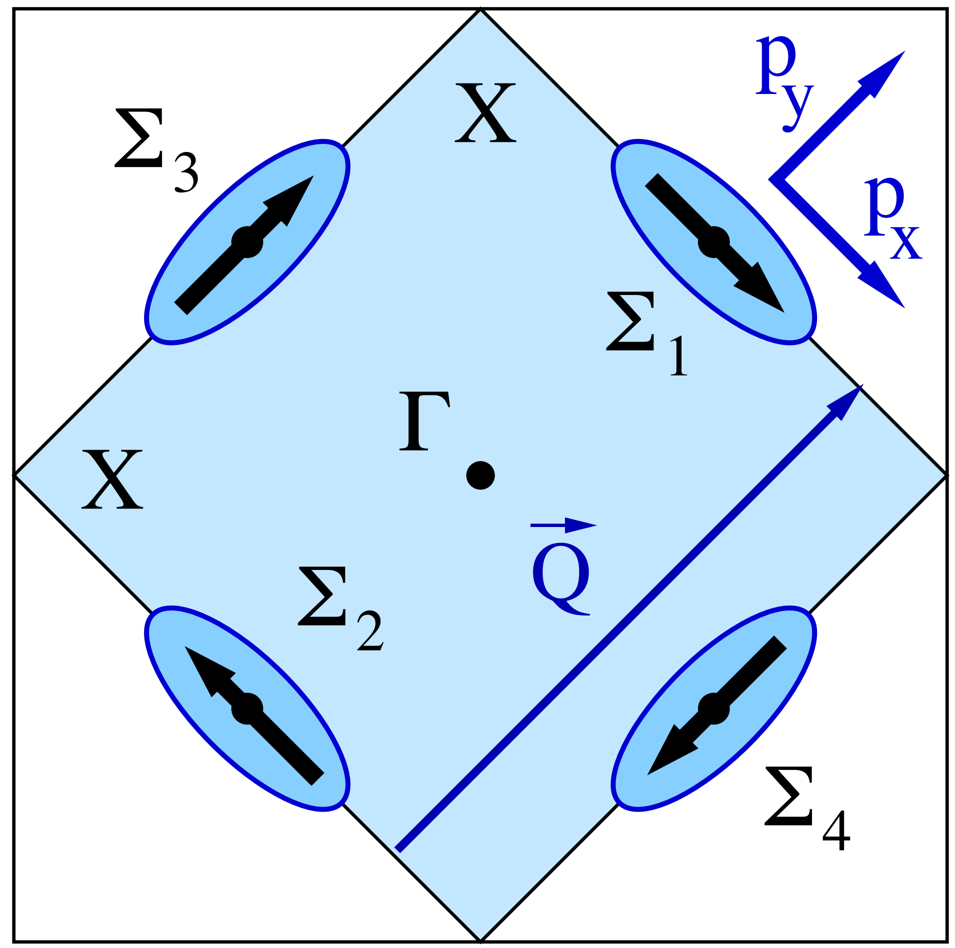
$\hat{p}_i \to \hat{p}_i + (\mathbf{A}_i \cdot \sigma)$ with $(\mathbf{A}_i \cdot \sigma) = A_i^\alpha \sigma^\alpha = -i\hbar U_\mathbf{r}^\dagger \partial_i U_\mathbf{r}$

Where are our band extrema ?

Where are our band extrema ?



Where are our band extrema ?

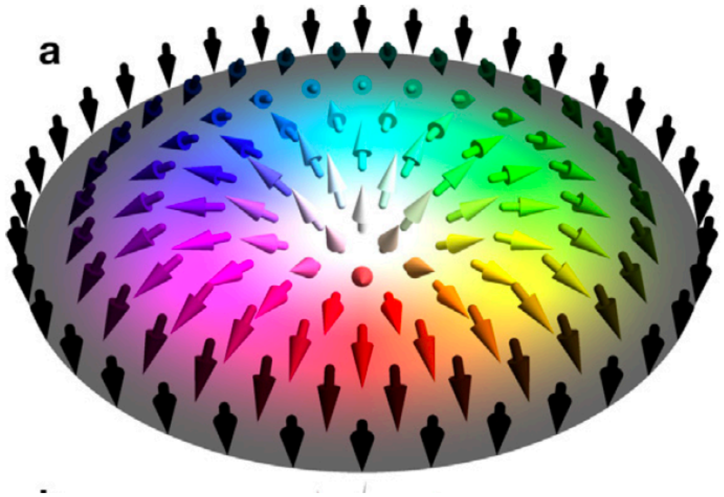


… and $\mathcal{H}_\Sigma = \frac{(\hat{p}_i + A_i^z \sigma_z)^2}{2m_i^*} + \frac{\left(A_i^\parallel\right)^2}{2m_i} + v\left(\mathbf{A}_y^\parallel \cdot \sigma\right)$

Now, on to our Skyrmion :

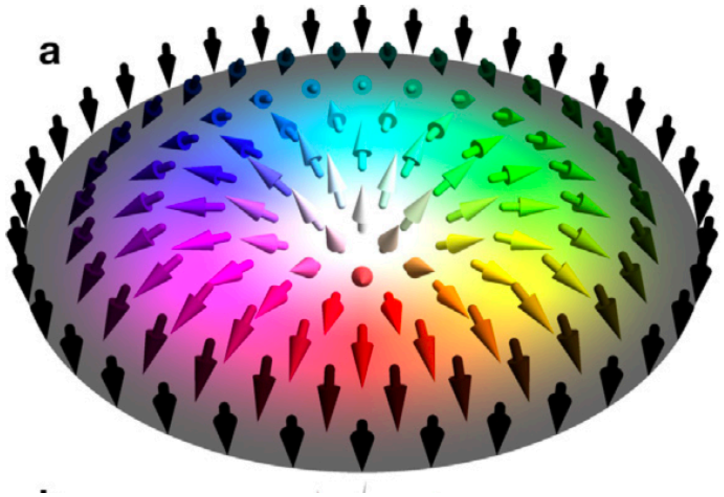
Now, on to our Skyrmion :

The 'Néel' profile :



Now, on to our Skyrmion :

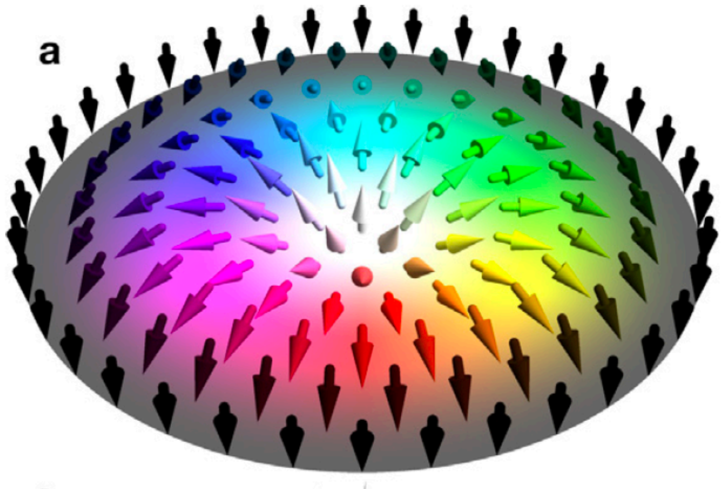
The 'Néel' profile :



$$\hat{\mathbf{n}}_{\mathbf{r}} = (\sin\theta_r \cos\phi, \sin\theta_r \sin\phi, \cos\theta_r),\ r = \sqrt{x^2 + y^2},\ \phi = \arctan\frac{y}{x}$$

Now, on to our Skyrmion :

The 'Néel' profile :

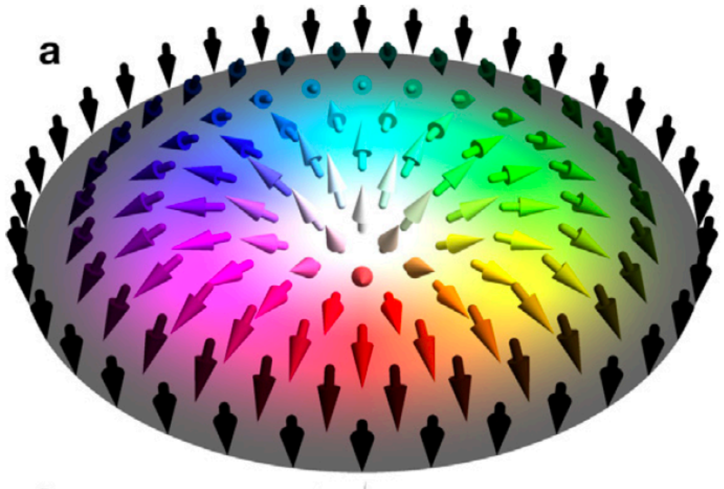


$$\hat{\mathbf{n}}_{\mathbf{r}} = (\sin\theta_r \cos\phi, \sin\theta_r \sin\phi, \cos\theta_r),\ r = \sqrt{x^2 + y^2},\ \phi = \arctan\frac{y}{x}$$

Topological charge (winding number) $Q = 1$

Now, on to our Skyrmion :

The 'Néel' profile :



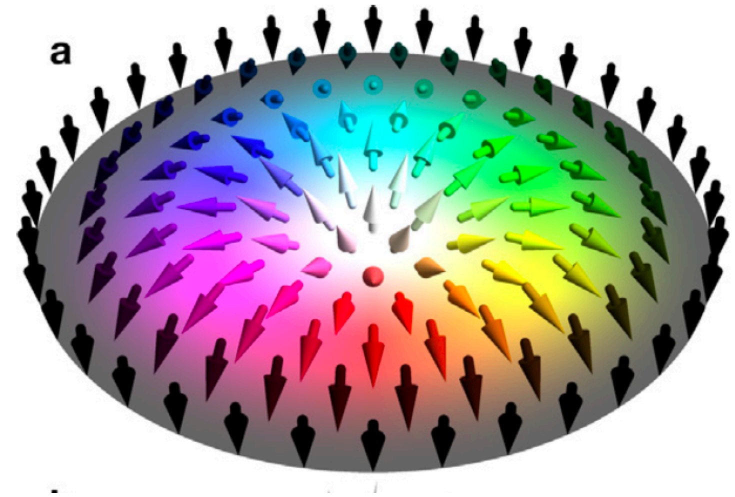
$$\hat{\mathbf{n}}_{\mathbf{r}} = (\sin\theta_r\cos\phi, \sin\theta_r\sin\phi, \cos\theta_r),\ r = \sqrt{x^2+y^2},\ \phi = \arctan\frac{y}{x}$$

Topological charge (winding number) $Q = 1$

A single length, radius R : $\sin\theta = \dfrac{2z}{1+z^2},\ z = \dfrac{r}{R}$

Now, on to our Skyrmion :

The 'Néel' profile :



$$\hat{\mathbf{n}}_{\mathbf{r}} = (\sin\theta_r \cos\phi, \sin\theta_r \sin\phi, \cos\theta_r),\ r = \sqrt{x^2+y^2},\ \phi = \arctan\frac{y}{x}$$

Topological charge (winding number) $Q = 1$

A single length, radius R : $\sin\theta = \dfrac{2z}{1+z^2},\ z = \dfrac{r}{R}$

Now, back to the Hamiltonian, term by term :

$$\mathcal{H}_{\Sigma} = \frac{\left(\hat{p}_i + A_i^z \sigma_z\right)^2}{2m_i^*} + \frac{\left(A_i^{\|}\right)^2}{2m_i} + v\left(\mathbf{A}_y^{\|} \cdot \sigma\right)$$

$$\mathcal{H}_\Sigma = \frac{\left(\hat{p}_i + A_i^z \sigma_z\right)^2}{2m_i^*} + \frac{\left(A_i^{\parallel}\right)^2}{2m_i} + v\left(\mathbf{A}_y^{\parallel} \cdot \sigma\right)$$

I: $\frac{\left(\hat{p}_i + A_i^z \sigma_z\right)^2}{2m_i^*}$, where $A_x^z = \frac{-\hbar y}{R^2 + r^2}$, $A_y^z = \frac{\hbar x}{R^2 + r^2}$

$$\mathcal{H}_\Sigma = \frac{\left(\hat{p}_i + A_i^z \sigma_z\right)^2}{2m_i^*} + \frac{\left(A_i^{\parallel}\right)^2}{2m_i} + v\left(\mathbf{A}_y^{\parallel} \cdot \sigma\right)$$

I: $\frac{\left(\hat{p}_i + A_i^z \sigma_z\right)^2}{2m_i^*}$, where $A_x^z = \frac{-\hbar y}{R^2 + r^2}$, $A_y^z = \frac{\hbar x}{R^2 + r^2}$

A_i^z produces geometric flux $\pm 2\pi\hbar$.

$$\mathcal{H}_\Sigma = \frac{\left(\hat{p}_i + A_i^z \sigma_z\right)^2}{2m_i^*} + \frac{\left(A_i^{\parallel}\right)^2}{2m_i} + v\left(\mathbf{A}_y^{\parallel} \cdot \sigma\right)$$

1: $\frac{\left(\hat{p}_i + A_i^z \sigma_z\right)^2}{2m_i^*}$, where $A_x^z = \frac{-\hbar y}{R^2 + r^2}$, $A_y^z = \frac{\hbar x}{R^2 + r^2}$

A_i^z produces geometric flux $\pm 2\pi\hbar$.

2: $\frac{\left(A_i^{\parallel}\right)^2}{2m_i} = \frac{\hbar^2}{2R^2}\left[\frac{1}{m_x} + \frac{1}{m_y}\right]\frac{1}{(1+z^2)^2}$ repulsive potential.

$$\mathcal{H}_\Sigma = \frac{\left(\hat{p}_i + A_i^z \sigma_z\right)^2}{2m_i^*} + \frac{\left(A_i^{\|}\right)^2}{2m_i} + v\left(\mathbf{A}_y^{\|} \cdot \sigma\right)$$

1: $\frac{\left(\hat{p}_i + A_i^z \sigma_z\right)^2}{2m_i^*}$, where $A_x^z = \frac{-\hbar y}{R^2 + r^2}$, $A_y^z = \frac{\hbar x}{R^2 + r^2}$

A_i^z produces geometric flux $\pm 2\pi\hbar$.

2: $\frac{\left(A_i^{\|}\right)^2}{2m_i} = \frac{\hbar^2}{2R^2}\left[\frac{1}{m_x} + \frac{1}{m_y}\right]\frac{1}{(1+z^2)^2}$ repulsive potential.

3: $v\left(\mathbf{A}_y^{\|} \cdot \sigma\right) = -\frac{\hbar v}{R}\frac{\sigma^x}{1+z^2}$ – attraction !

Large Skyrmion ($R \gg \xi = \frac{\hbar v}{\Delta}$)

Large Skyrmion ($R \gg \xi = \frac{\hbar v}{\Delta}$)

Attraction $-\Delta \frac{\xi}{R} \frac{\sigma^x}{1+z^2}$ dominates :

Large Skyrmion ($R \gg \xi = \dfrac{\hbar v}{\Delta}$)

Attraction $-\Delta \dfrac{\xi}{R} \dfrac{\sigma^x}{1+z^2}$ dominates :

$$\epsilon_0^c(R) \approx -\Delta \frac{\xi}{R} \left[1 - 2\sqrt{\frac{\xi}{R}} \left(n + \frac{1}{2} \right) + \ldots \right]$$

Large Skyrmion ($R \gg \xi = \dfrac{\hbar v}{\Delta}$)

Attraction $-\Delta \dfrac{\xi}{R} \dfrac{\sigma^x}{1+z^2}$ dominates :

$$\epsilon_0^c(R) \approx -\Delta \frac{\xi}{R}\left[1 - 2\sqrt{\frac{\xi}{R}}\left(n+\frac{1}{2}\right) + \ldots\right]$$

– For $R \gg \xi$, the bound states remain shallow.

Large Skyrmion ($R \gg \xi = \dfrac{\hbar v}{\Delta}$)

Attraction $-\Delta \dfrac{\xi}{R} \dfrac{\sigma^x}{1+z^2}$ dominates :

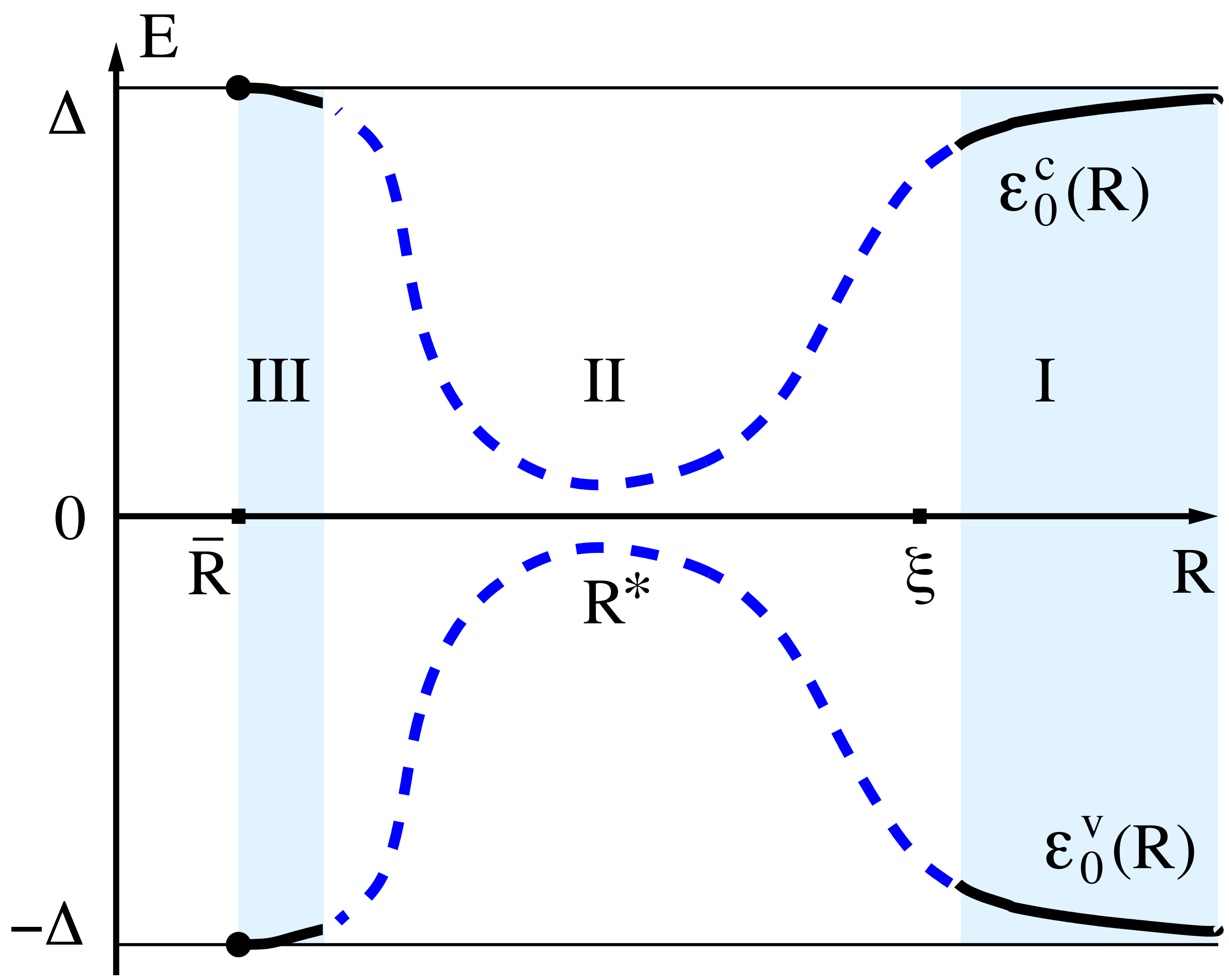
$$\epsilon_0^c(R) \approx -\Delta \frac{\xi}{R} \left[1 - 2\sqrt{\frac{\xi}{R}} \left(n + \frac{1}{2} \right) + \ldots \right]$$

– For $R \gg \xi$, the bound states remain shallow.

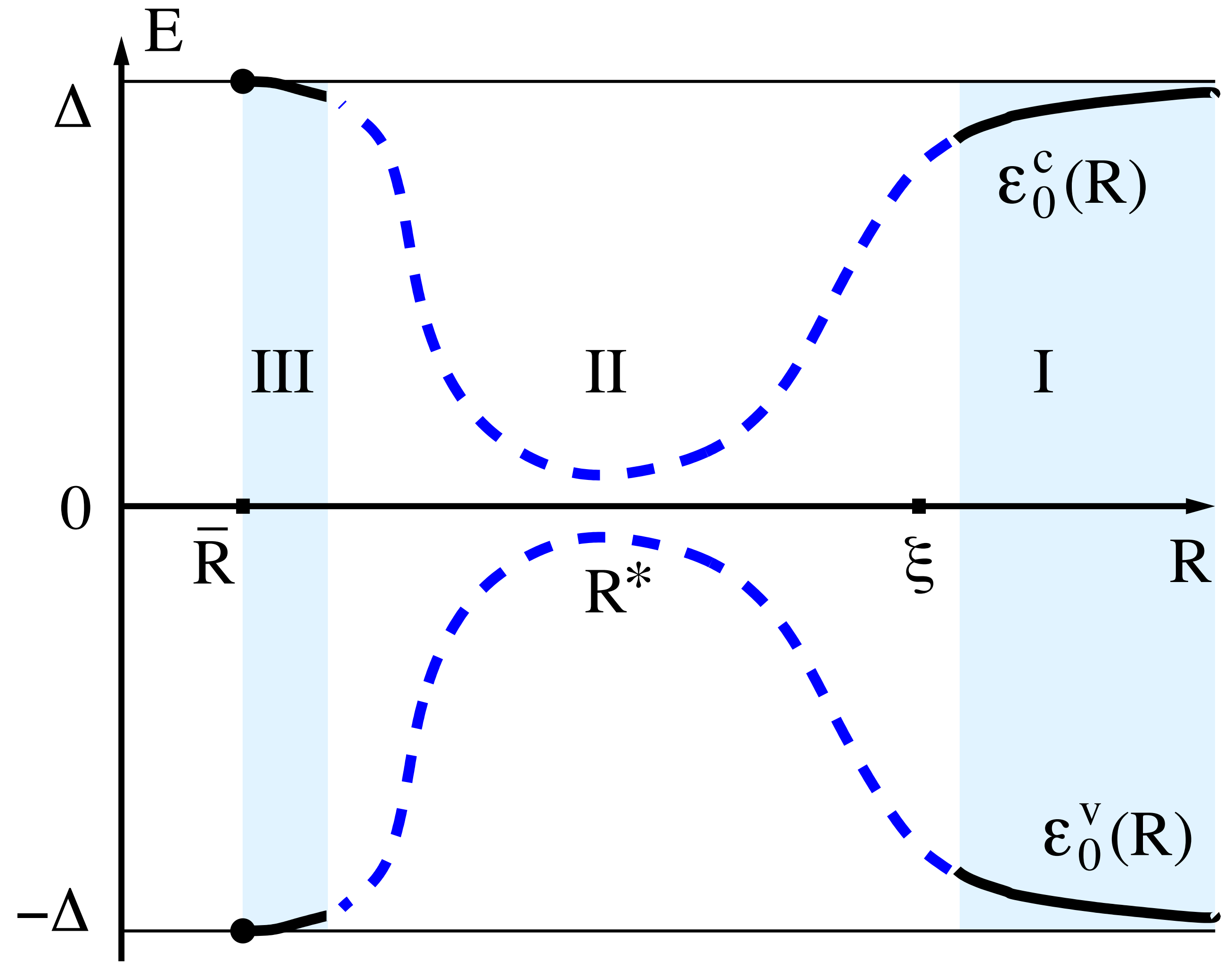
– $R \sim \xi$: low-energy approximation breakdown.

Toy problem, full picture :

Toy problem, full picture :

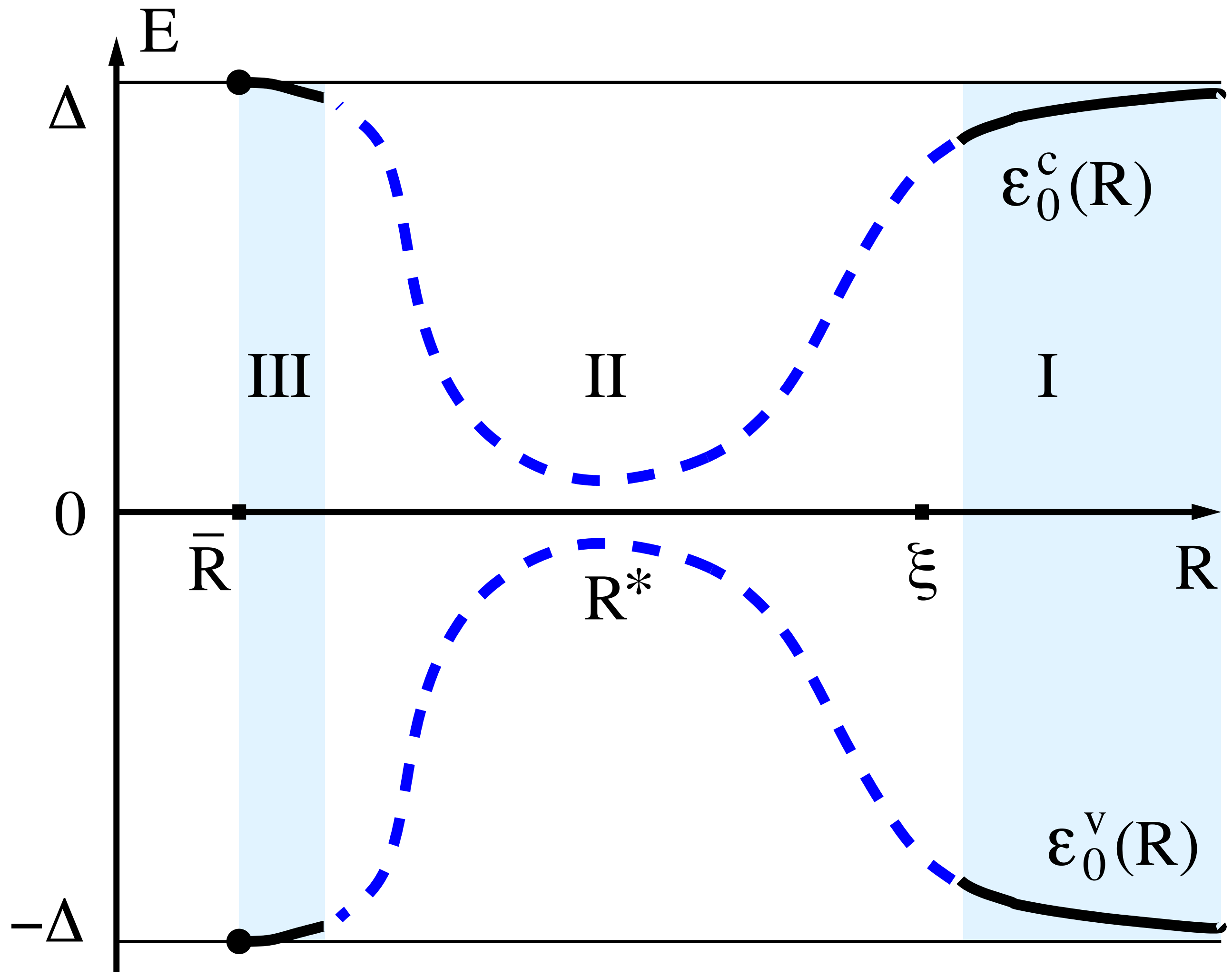


Toy problem, full picture :



$$\epsilon_0^c(R) \approx -\Delta \frac{\xi}{R}$$

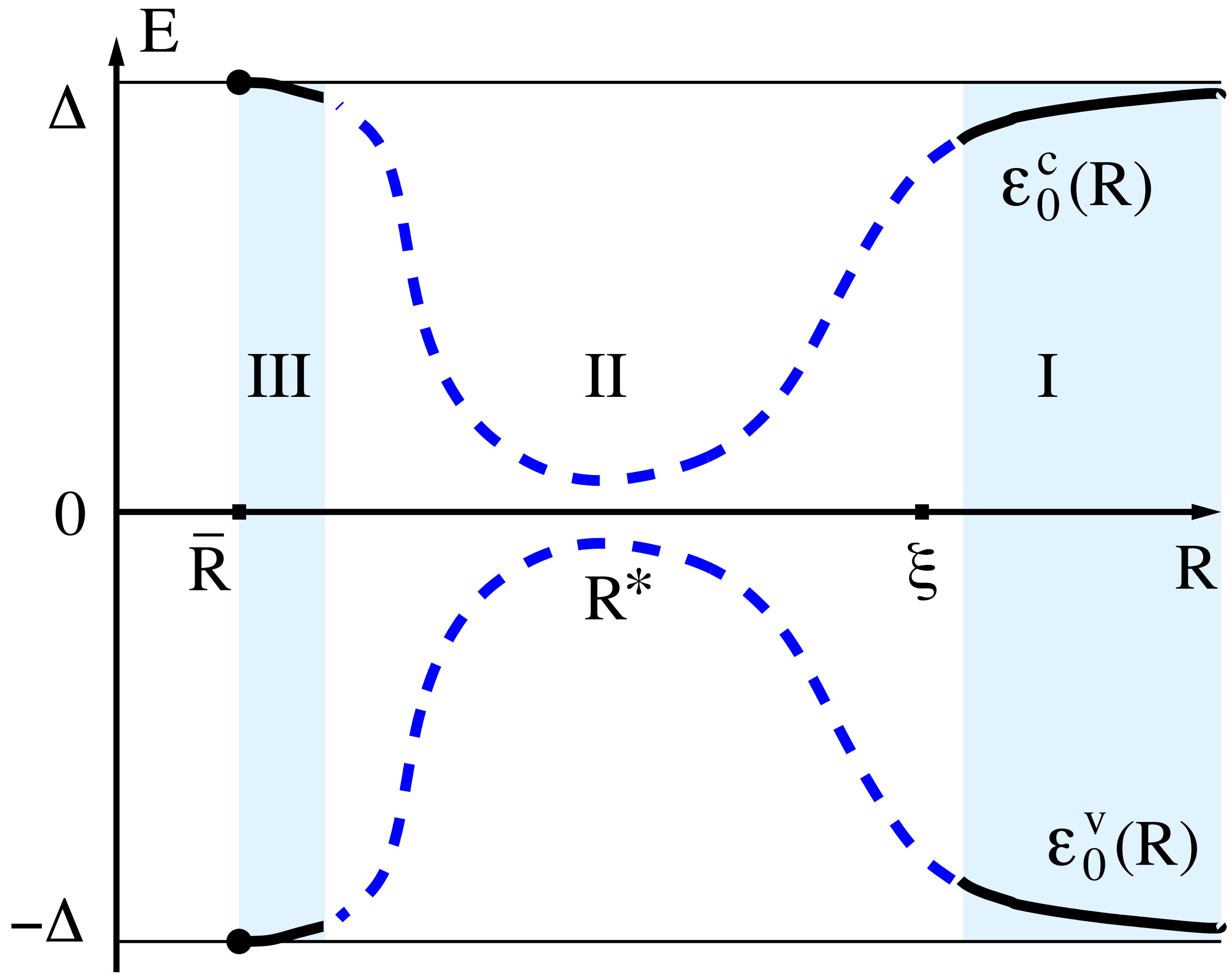
Toy problem, full picture :



$$\epsilon_0^c(R) \approx -\Delta \frac{\xi}{R}$$

The scales :

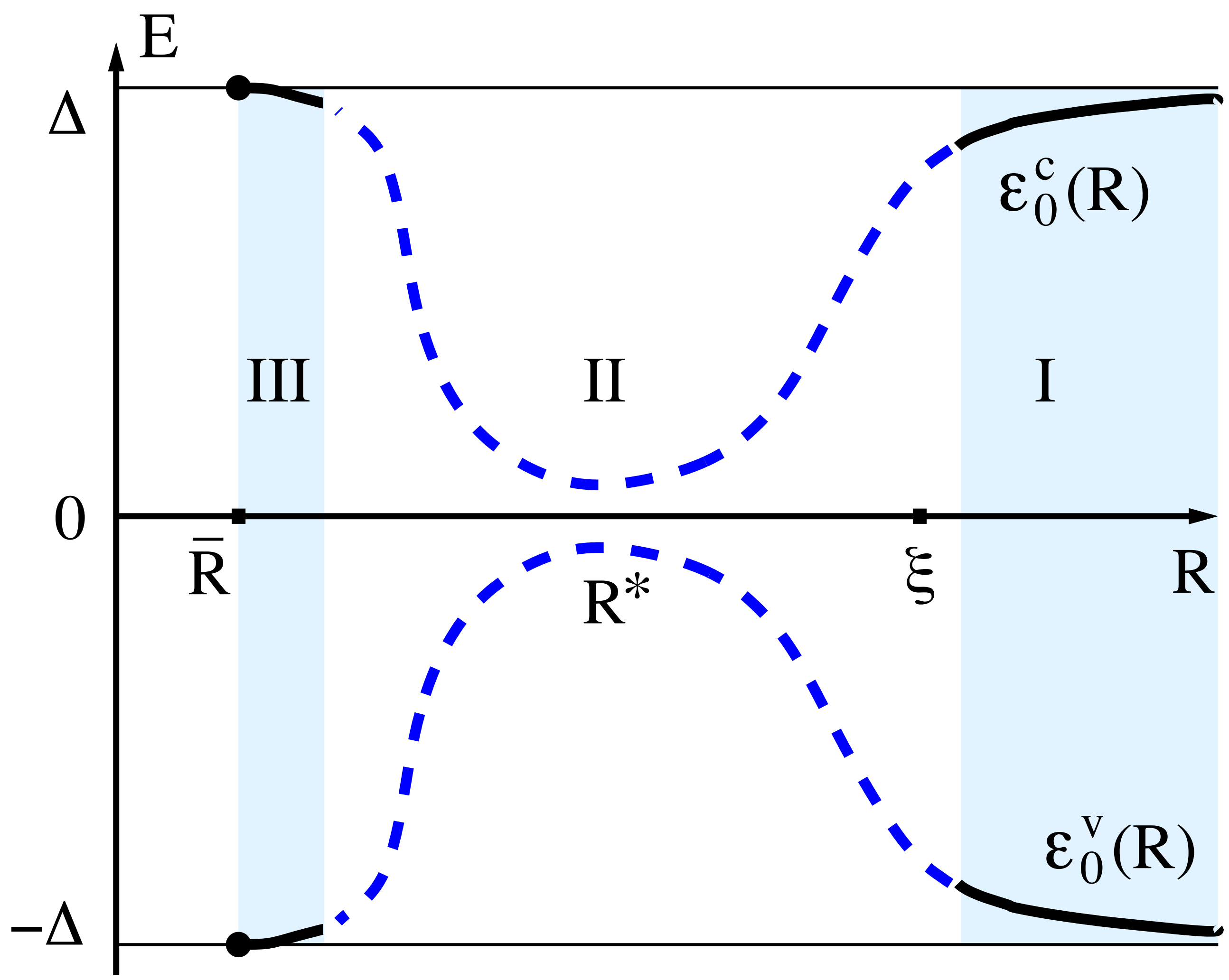
Toy problem, full picture :



$$\epsilon_0^c(R) \approx -\Delta \frac{\xi}{R}$$

The scales : $\bar{R} \sim \sqrt{\frac{m_y}{m_x}} \sqrt{\xi a},$

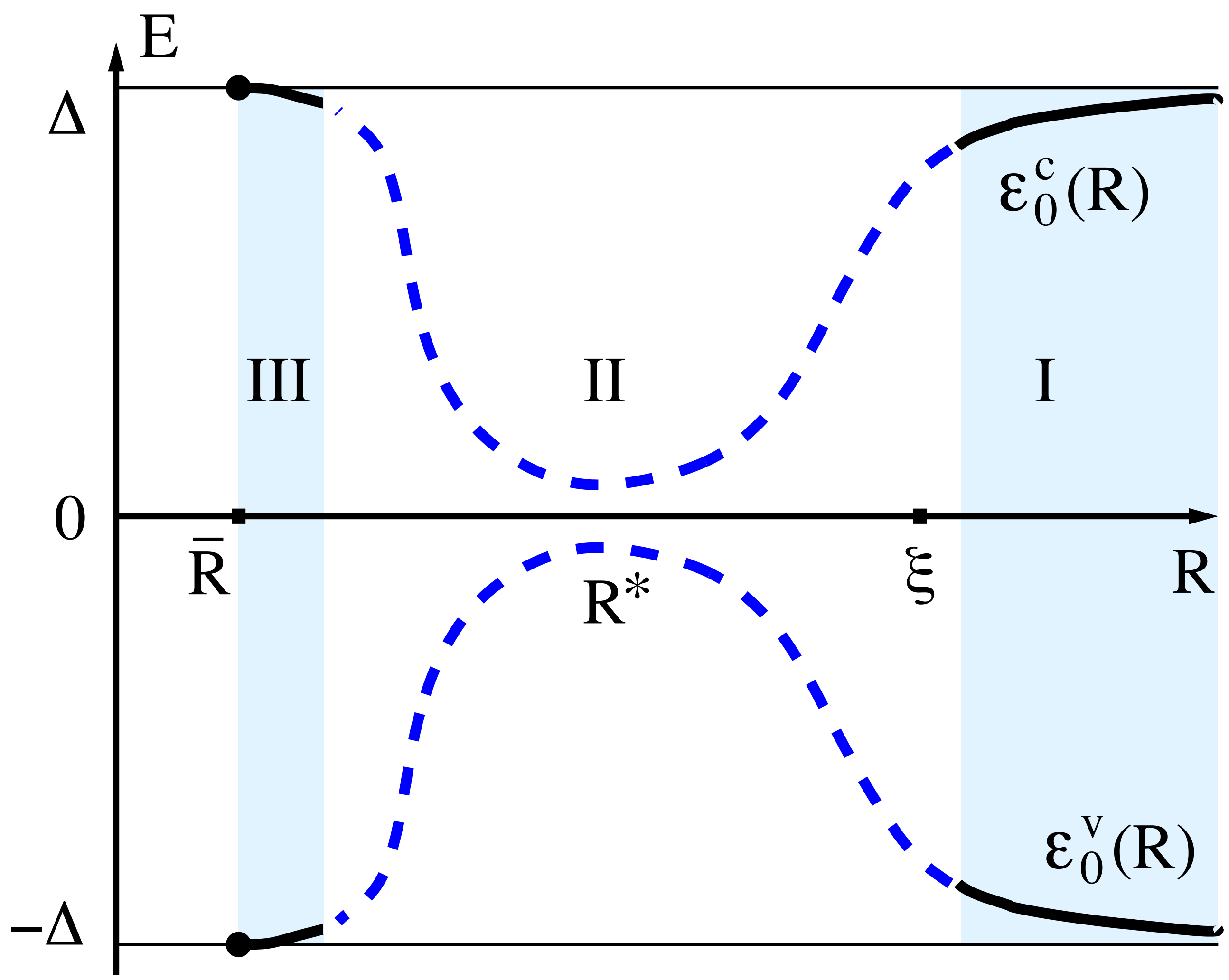
Toy problem, full picture :



$$\epsilon_0^c(R) \approx -\Delta\frac{\xi}{R}$$

The scales : $\bar{R} \sim \sqrt{\frac{m_y}{m_x}}\sqrt{\xi a},\ \ a \ll \bar{R} \ll \xi\,;$

Toy problem, full picture :



$$\epsilon_0^c(R) \approx -\Delta \frac{\xi}{R}$$

$$R^* \sim \xi \; :$$

$$\varepsilon_0^c(R^*) \sim \Delta$$

The scales : $\bar{R} \sim \sqrt{\frac{m_y}{m_x}}\sqrt{\xi a}, \;\; a \ll \bar{R} \ll \xi \, ;$

Summary :

[PRB **107**, 114406 (2023) and **109**, 224425 (2024)]

Summary :

[PRB **107**, 114406 (2023) and **109**, 224425 (2024)]

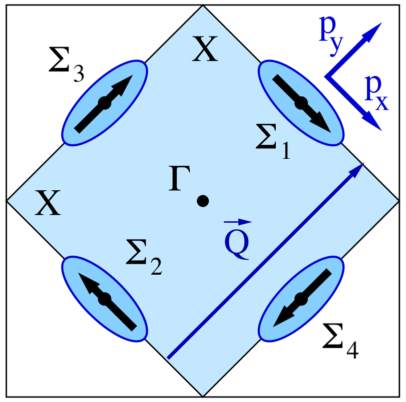
– texture-induced spin-orbit coupling $v(A_y^{\parallel} \cdot \sigma) \sim \frac{\hbar v}{L}$

Summary :

[PRB **107**, 114406 (2023) and **109**, 224425 (2024)]

– texture-induced spin-orbit coupling $v(A_y^{\|} \cdot \sigma) \sim \frac{\hbar v}{L}$

– hinges on lower symmetry of Σ points



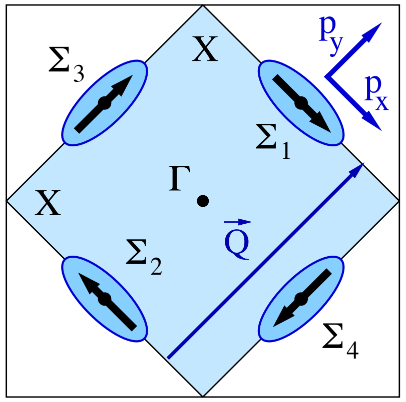
Summary :

[PRB **107**, 114406 (2023) and **109**, 224425 (2024)]

– texture-induced spin-orbit coupling $v(A_y^{\|} \cdot \sigma) \sim \dfrac{\hbar v}{L}$

– hinges on lower symmetry of Σ points

– skyrmion-electron bound states

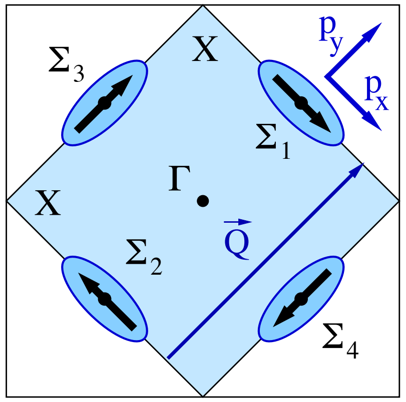


Summary :

[PRB **107**, 114406 (2023) and **109**, 224425 (2024)]

– texture-induced spin-orbit coupling $v(A_y^{\parallel} \cdot \sigma) \sim \frac{\hbar v}{L}$

– hinges on lower symmetry of Σ points



– skyrmion-electron bound states

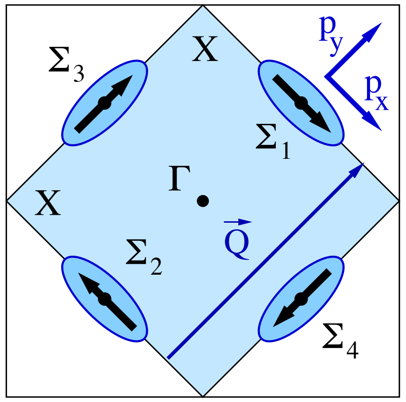
– with doping, the skyrmion becomes charged

Summary :

[PRB **107**, 114406 (2023) and **109**, 224425 (2024)]

– texture-induced spin-orbit coupling $v(A_y^{||} \cdot \sigma) \sim \dfrac{\hbar v}{L}$

– hinges on lower symmetry of $\sum$ points



– skyrmion-electron bound states

– with doping, the skyrmion becomes charged

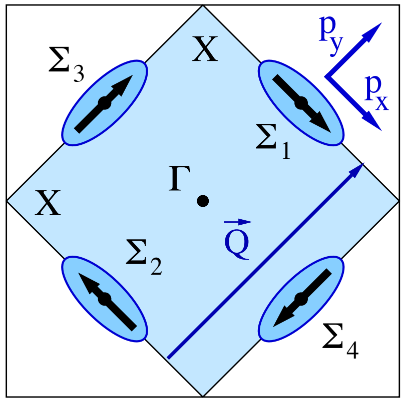
– and can be manipulated by electric field.

Summary :

[PRB **107**, 114406 (2023) and **109**, 224425 (2024)]

– texture-induced spin-orbit coupling $v(A_y^{\|} \cdot \sigma) \sim \frac{\hbar v}{L}$

– hinges on lower symmetry of Σ points



– skyrmion-electron bound states

– with doping, the skyrmion becomes charged

– and can be manipulated by electric field.

Thank you !