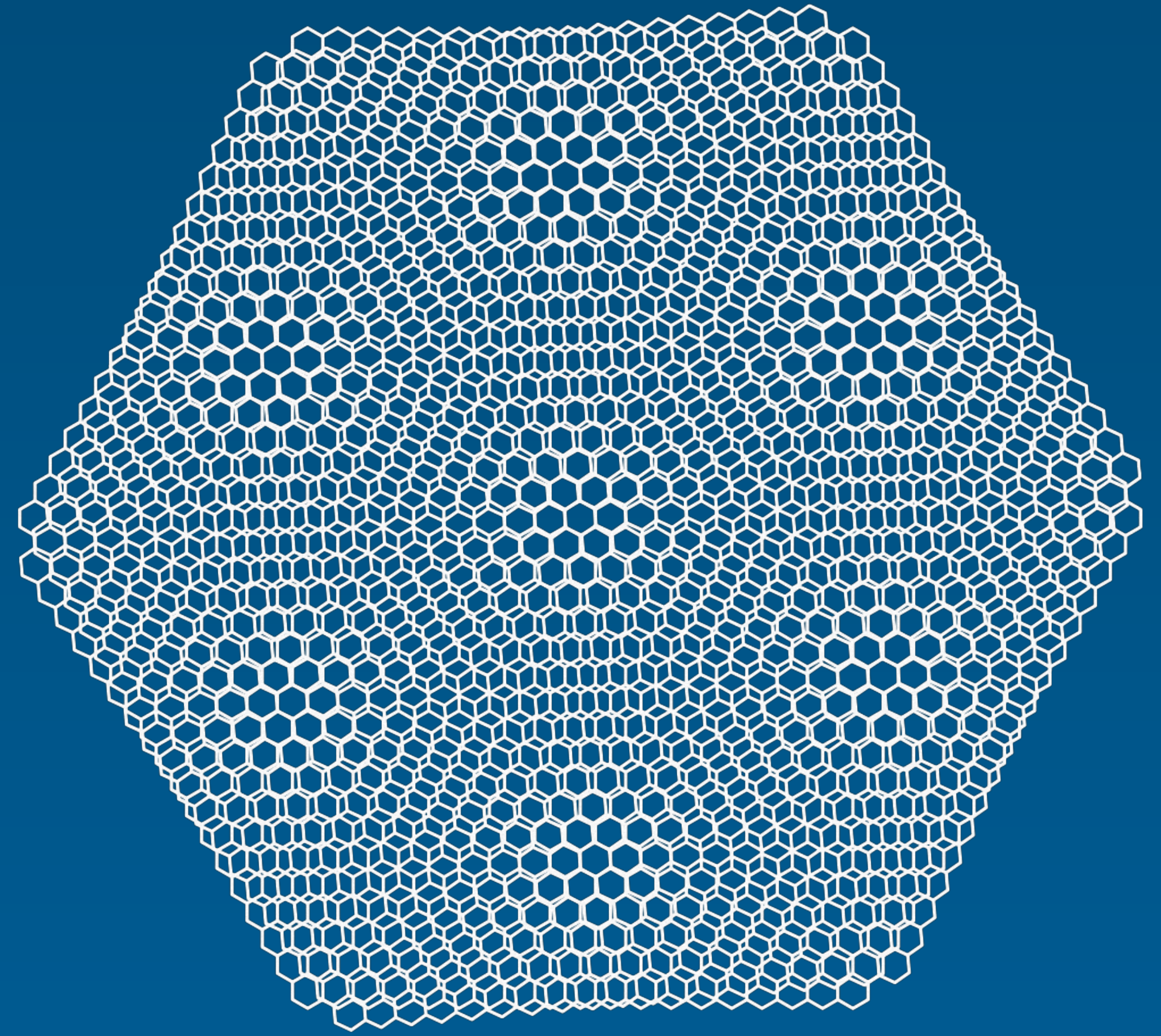
TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

Interaction effects in Bernal and twisted bilayer graphene



Lukas Janssen

Shouryya Ray

Jan Biedermann

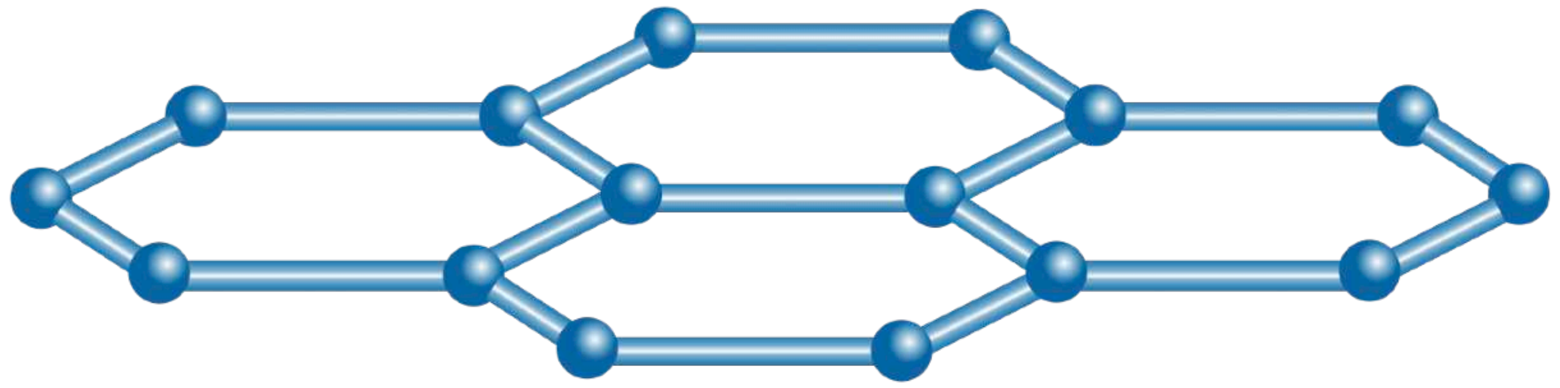
Emmy Noether-Programm

DFG Deutsche Forschungsgemeinschaft

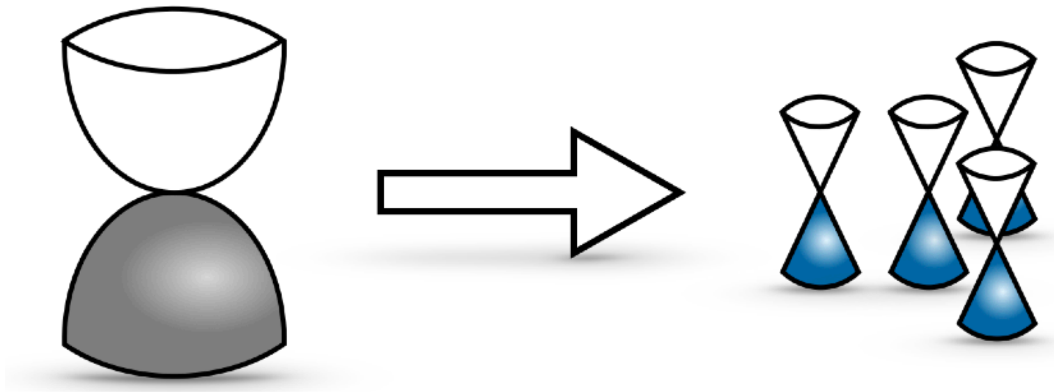
ct.qmat Complexity and Topology in Quantum Matter

Outline

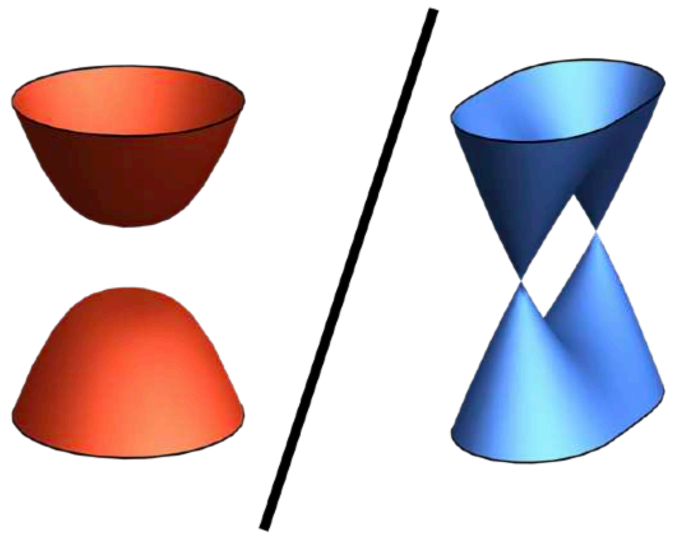
(1) Introduction



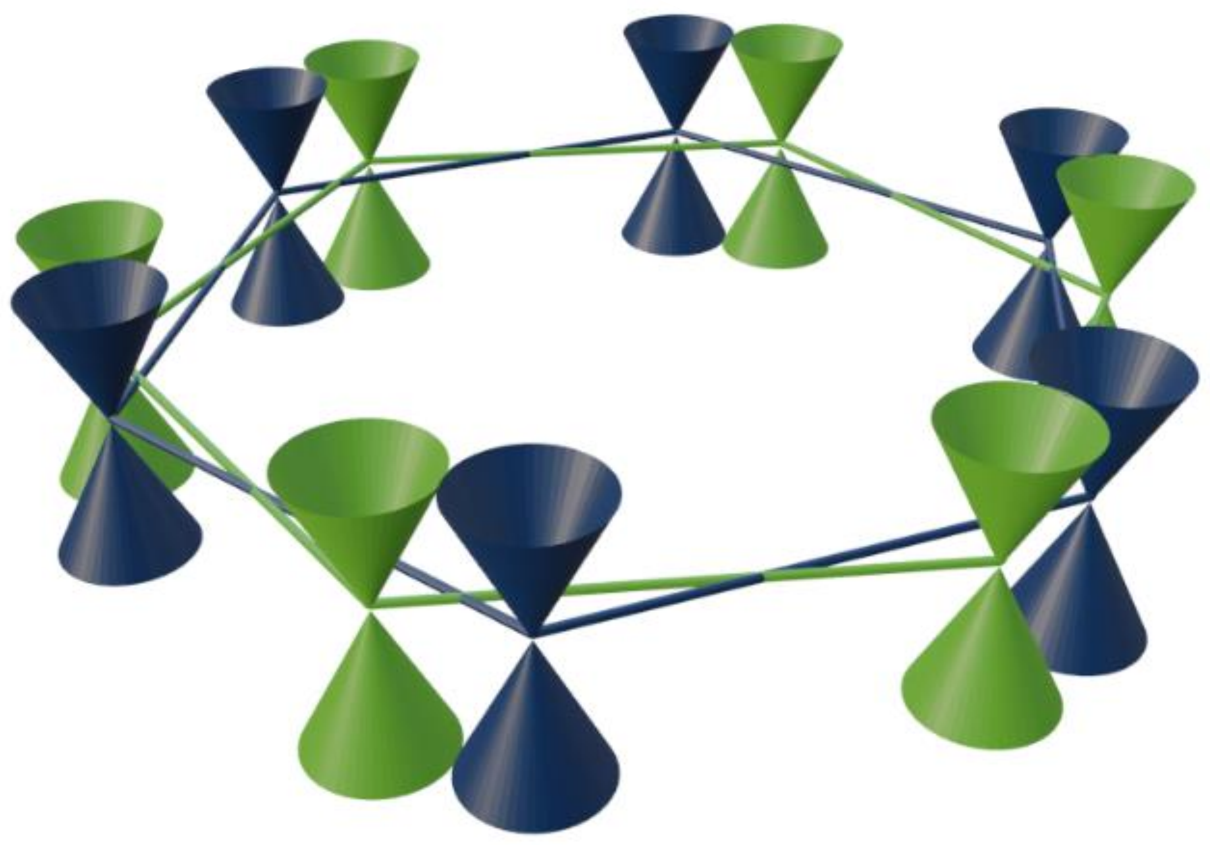
(2) Interaction-induced Dirac cones



(3) Competing nematic & antiferromagnetic orders



(4) Twist-tuned quantum criticality



(5) Conclusions

Outline

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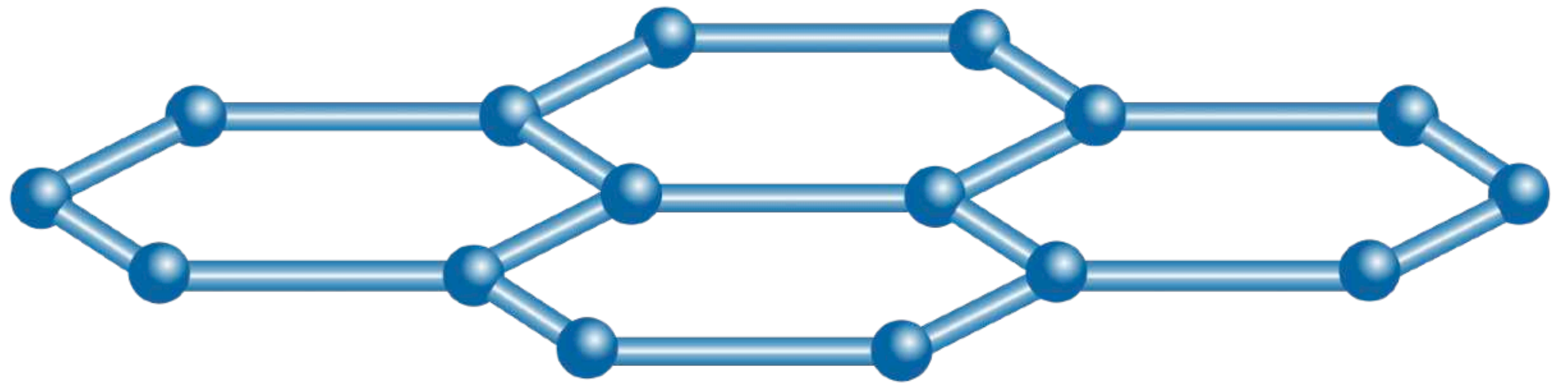

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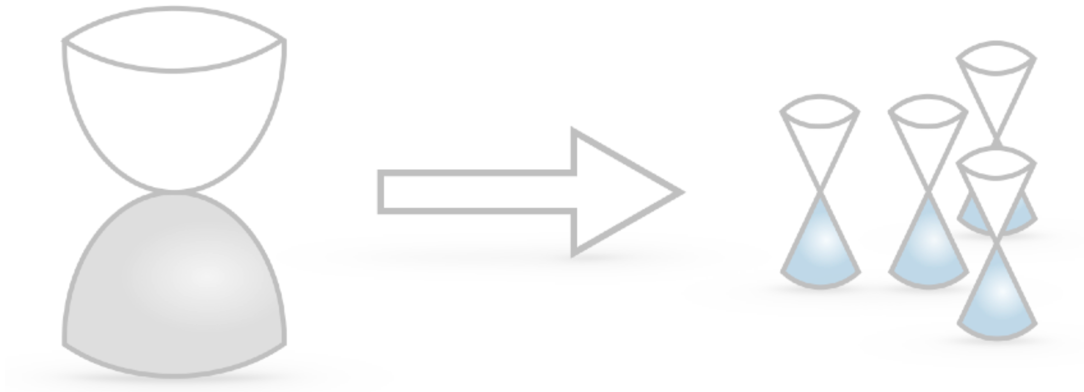

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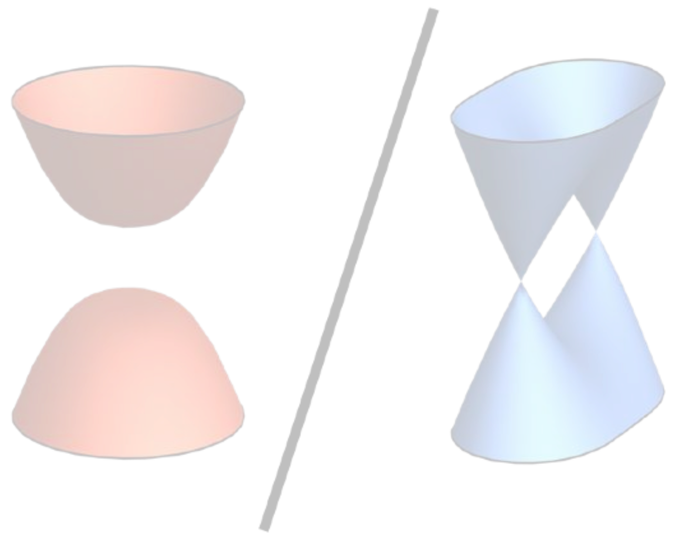

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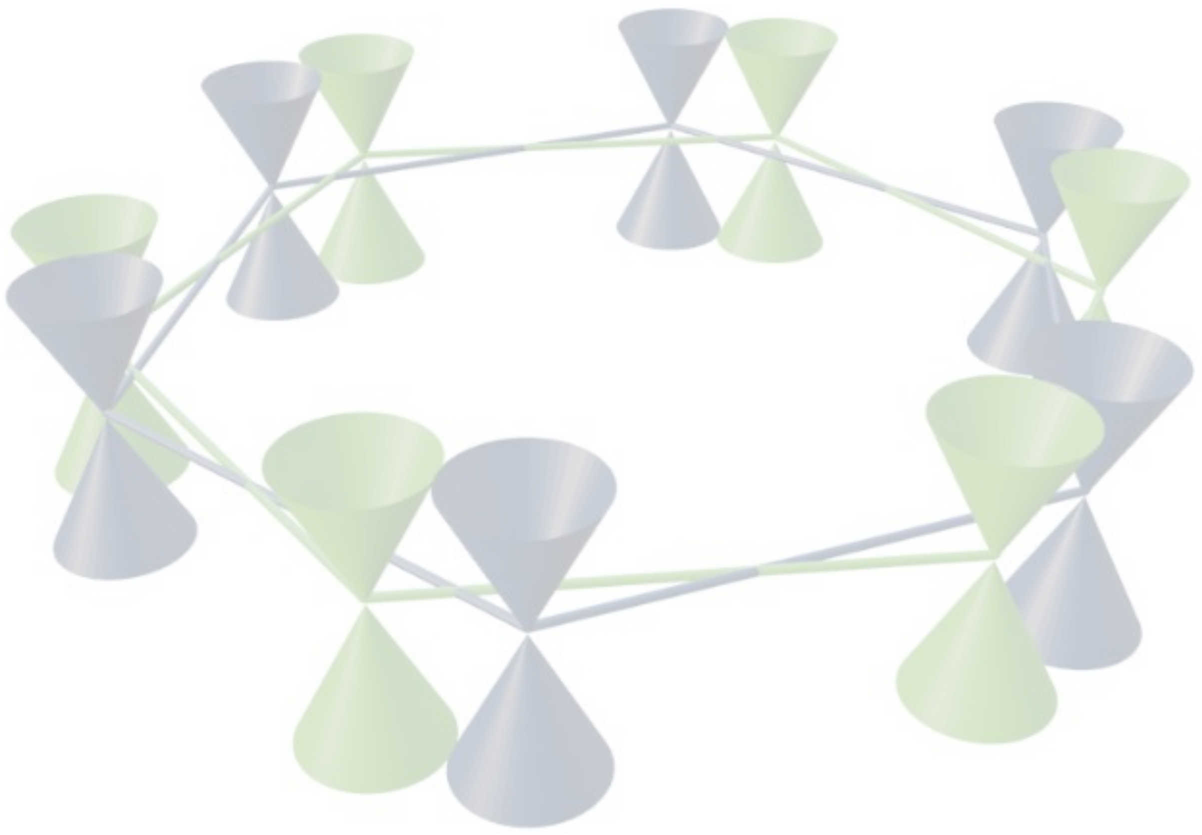
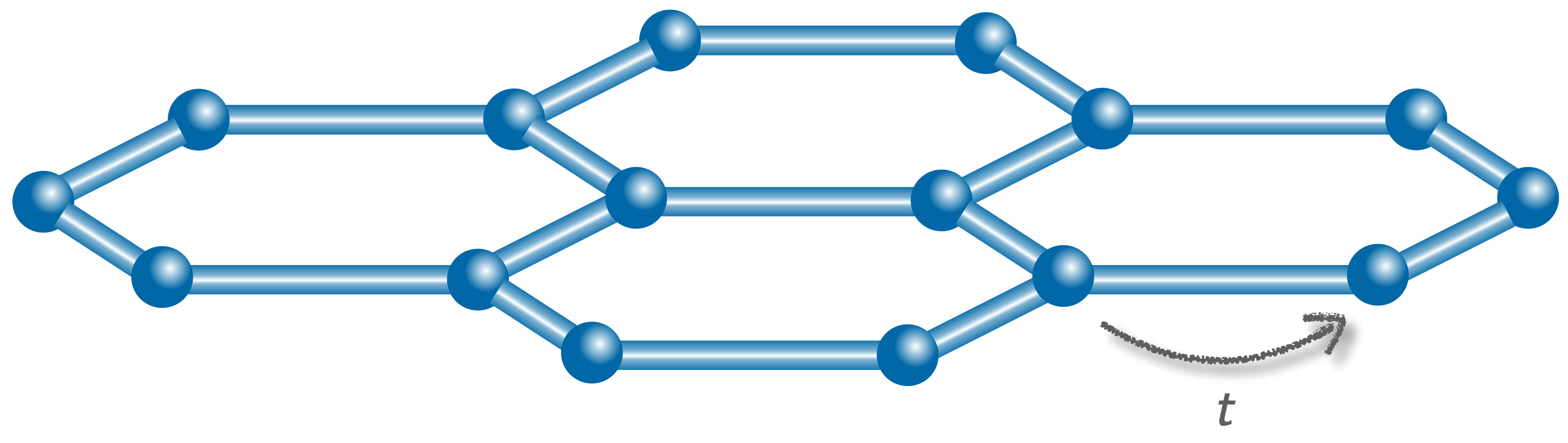
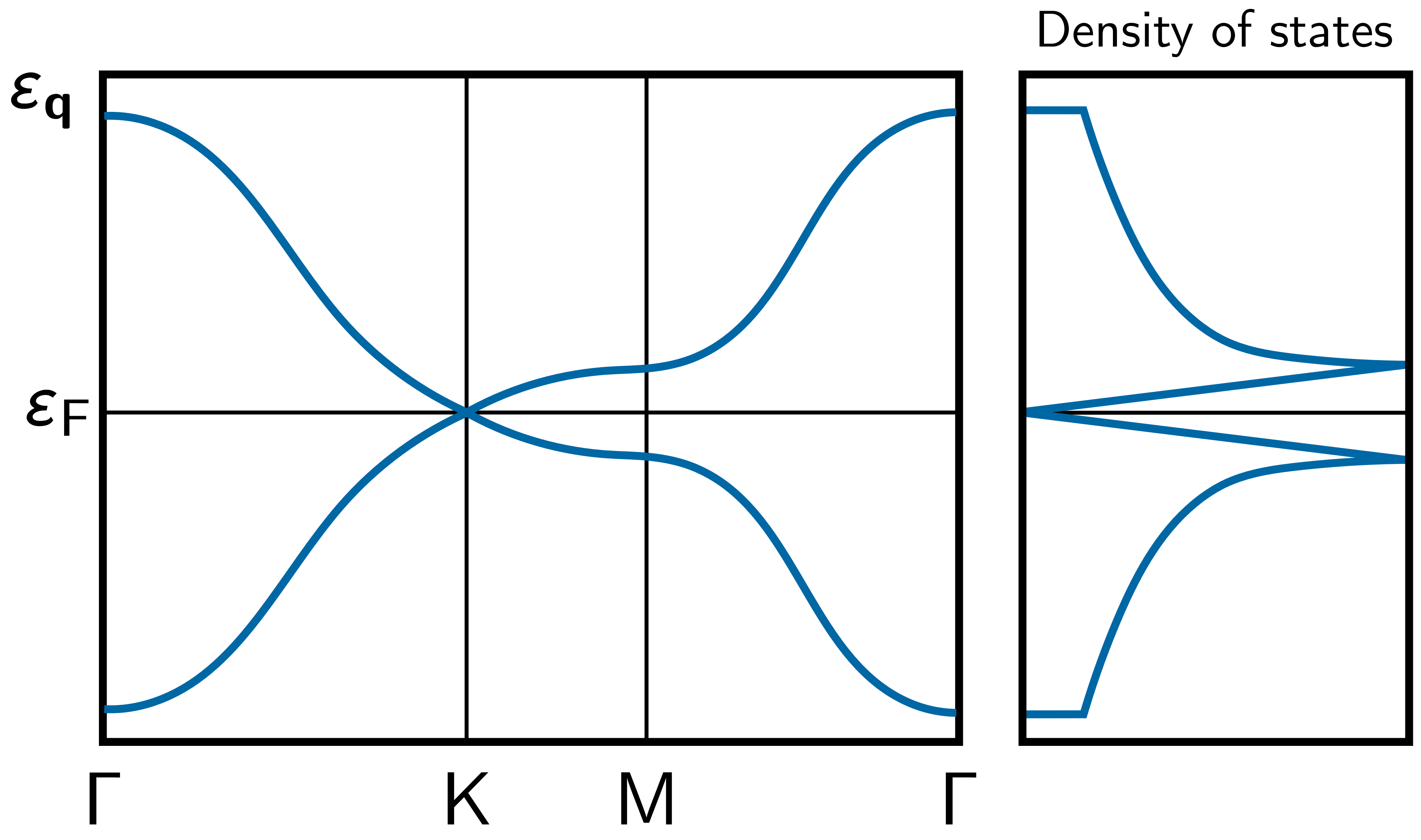


(5) Conclusions

Graphene





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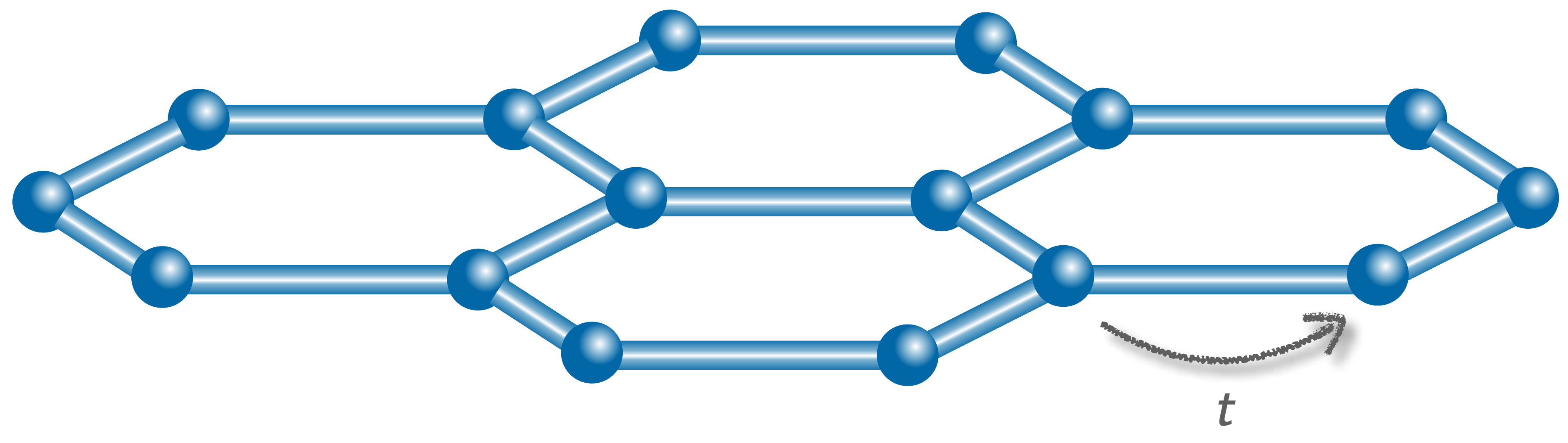
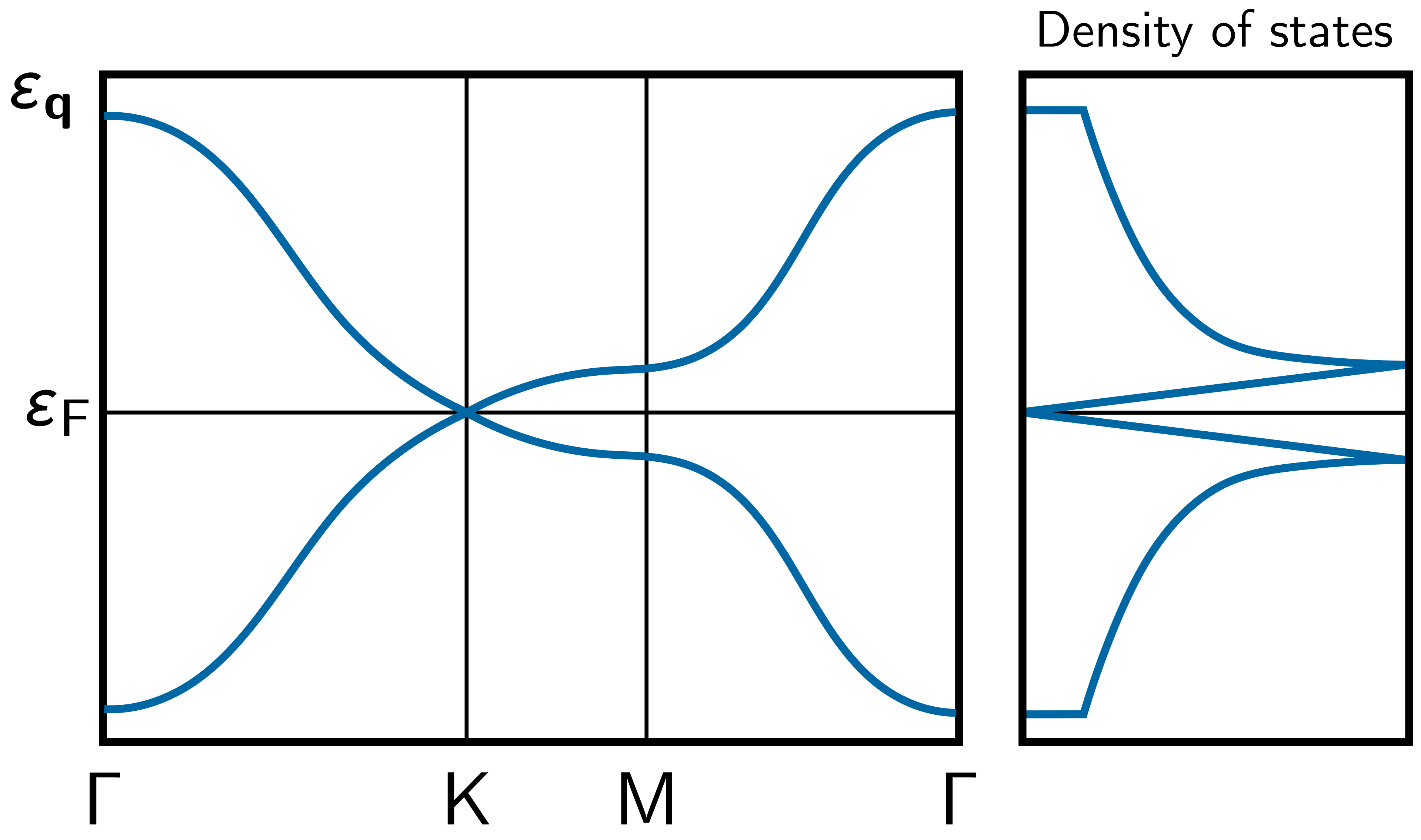




Low-energy spectrum:

$$\varepsilon_{\mathbf{K}+\mathbf{q}} = \pm f_1 q + \mathcal{O}(q^2)$$

"Dirac cone"

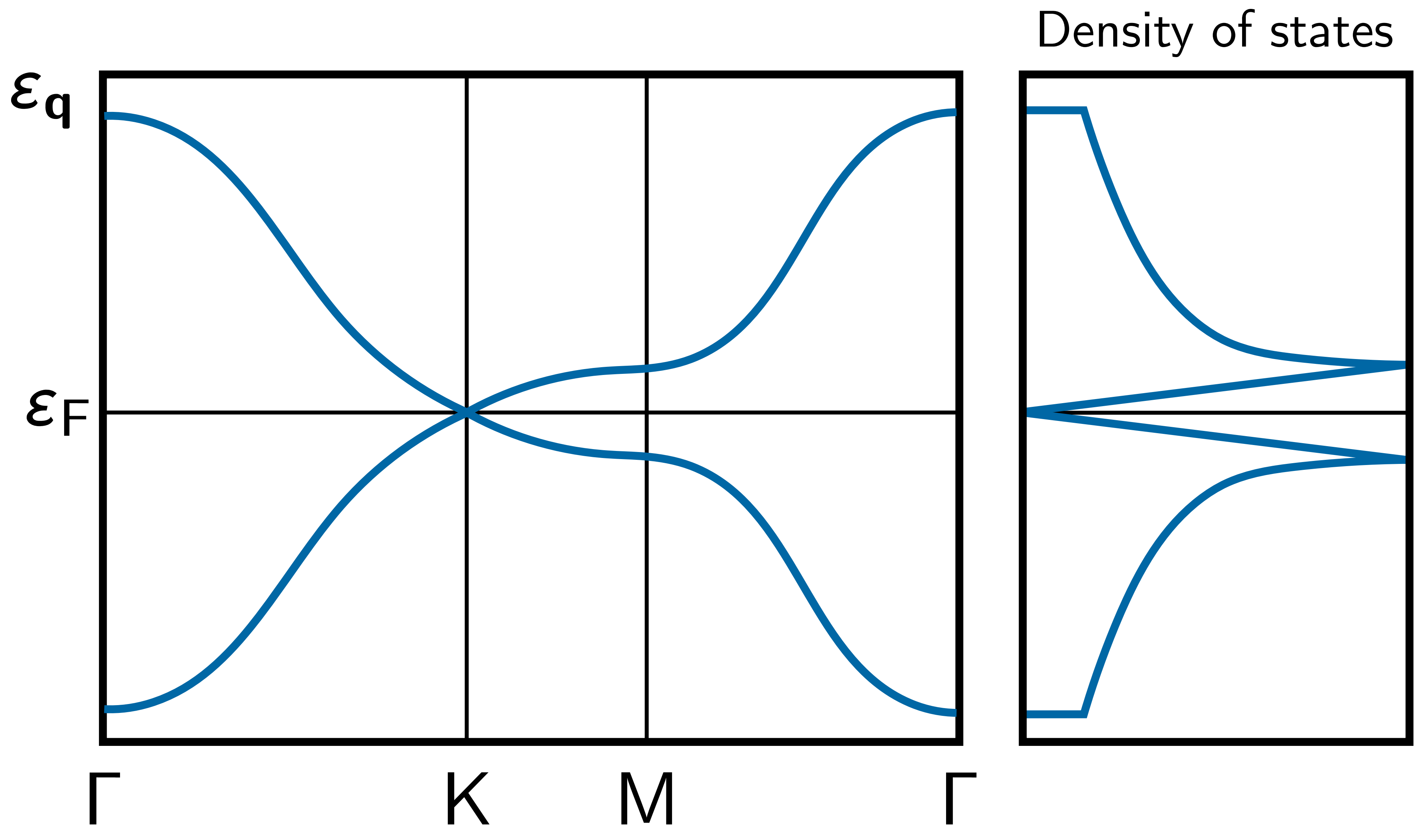
with $f_1/a_0 = v_F \hbar/a_0 = 3t/2 \simeq 4\,\mathrm{eV}$

... for $a_0 \simeq 0.142\,\mathrm{nm}$, $t \simeq 2.7\,\mathrm{eV}$

Interactions

Coulomb repulsion:

$$V(r) \propto \frac{e^2}{r} \qquad \text{unscreened}$$



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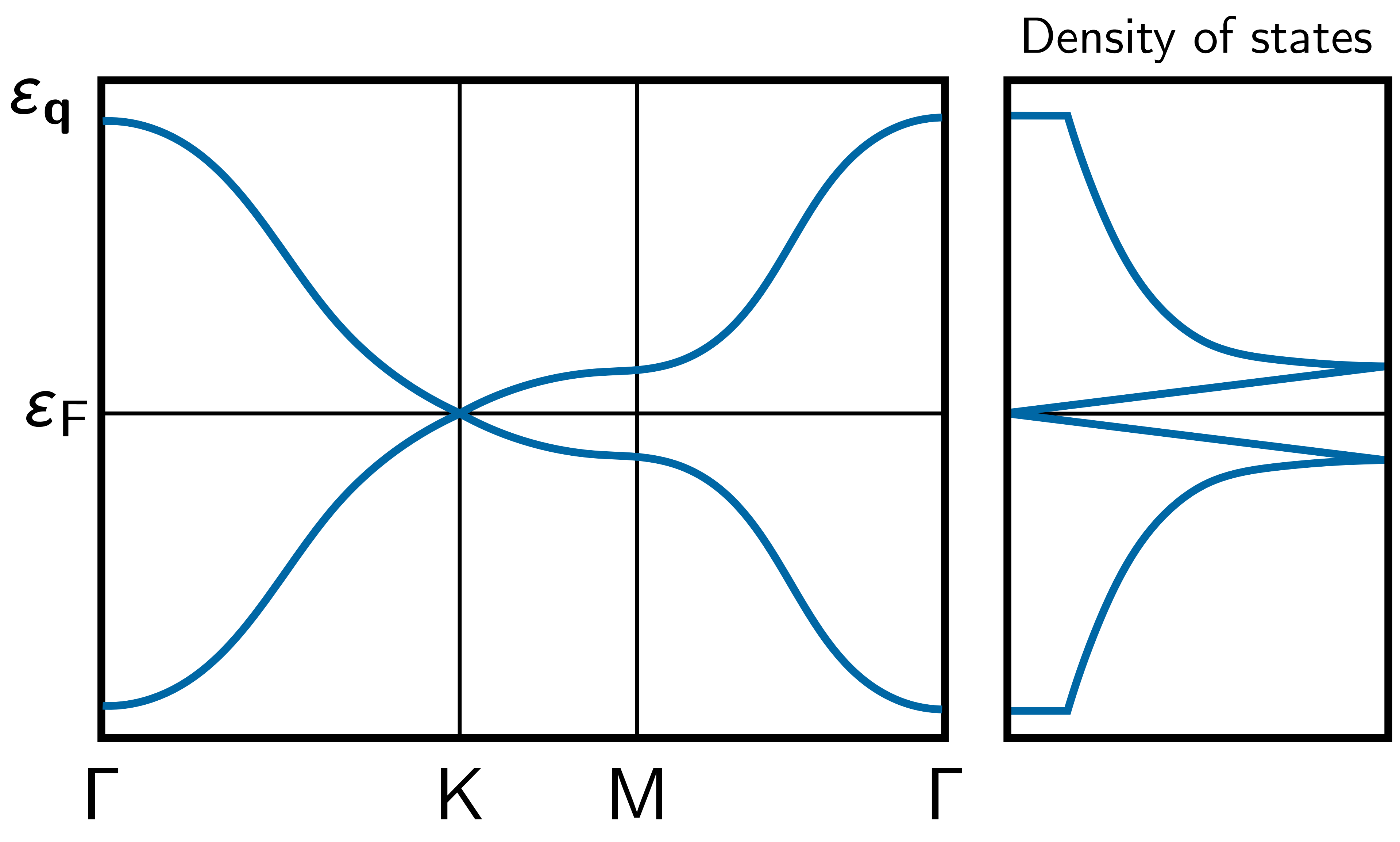

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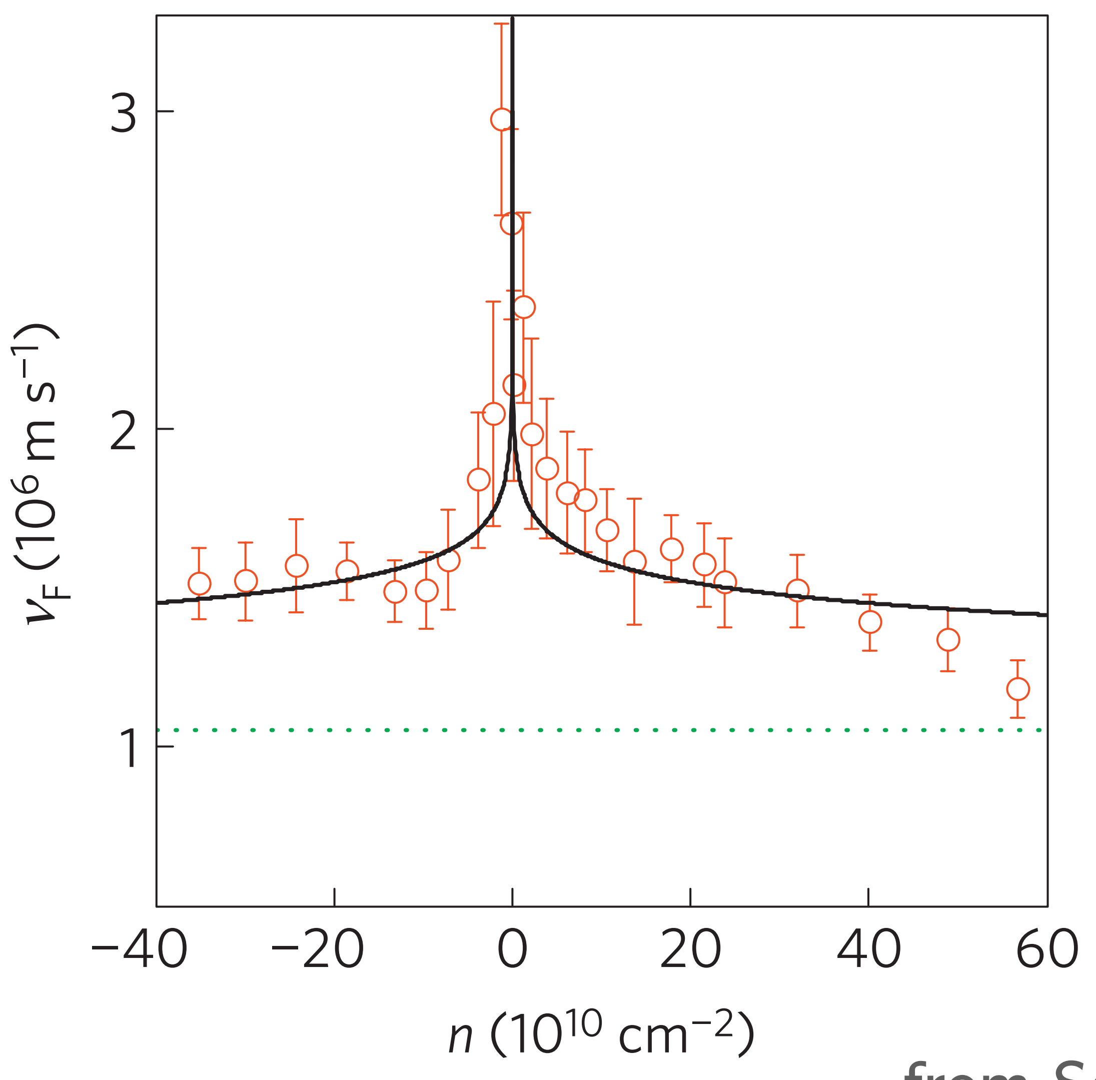
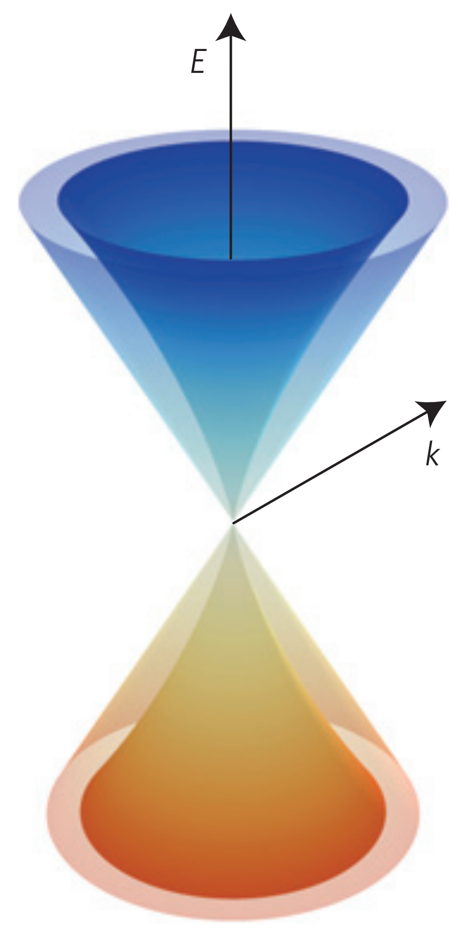
Fermi velocity renormalization:





... from SdH oscillations

[Elias *et al.*, Nat. Phys. '11]

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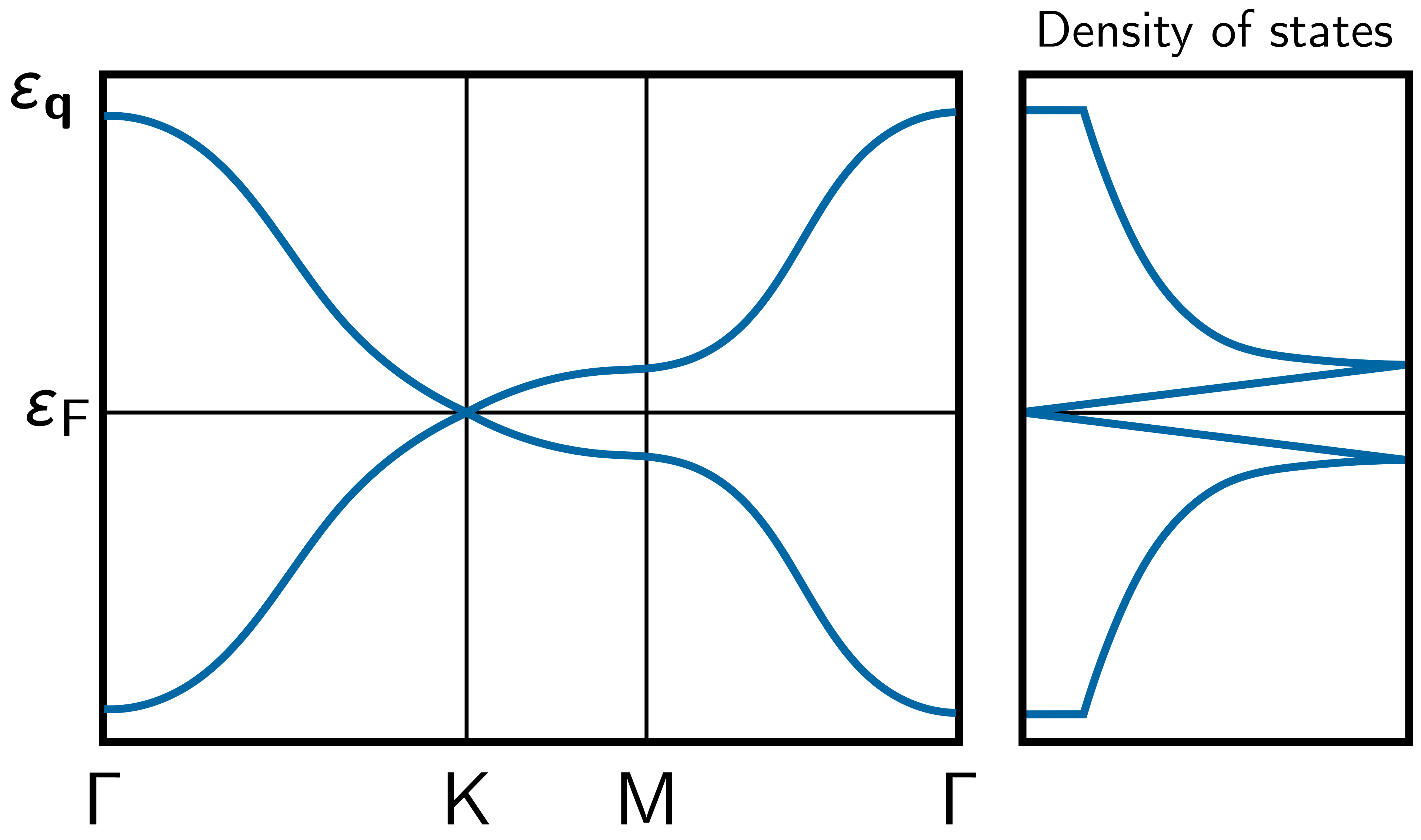

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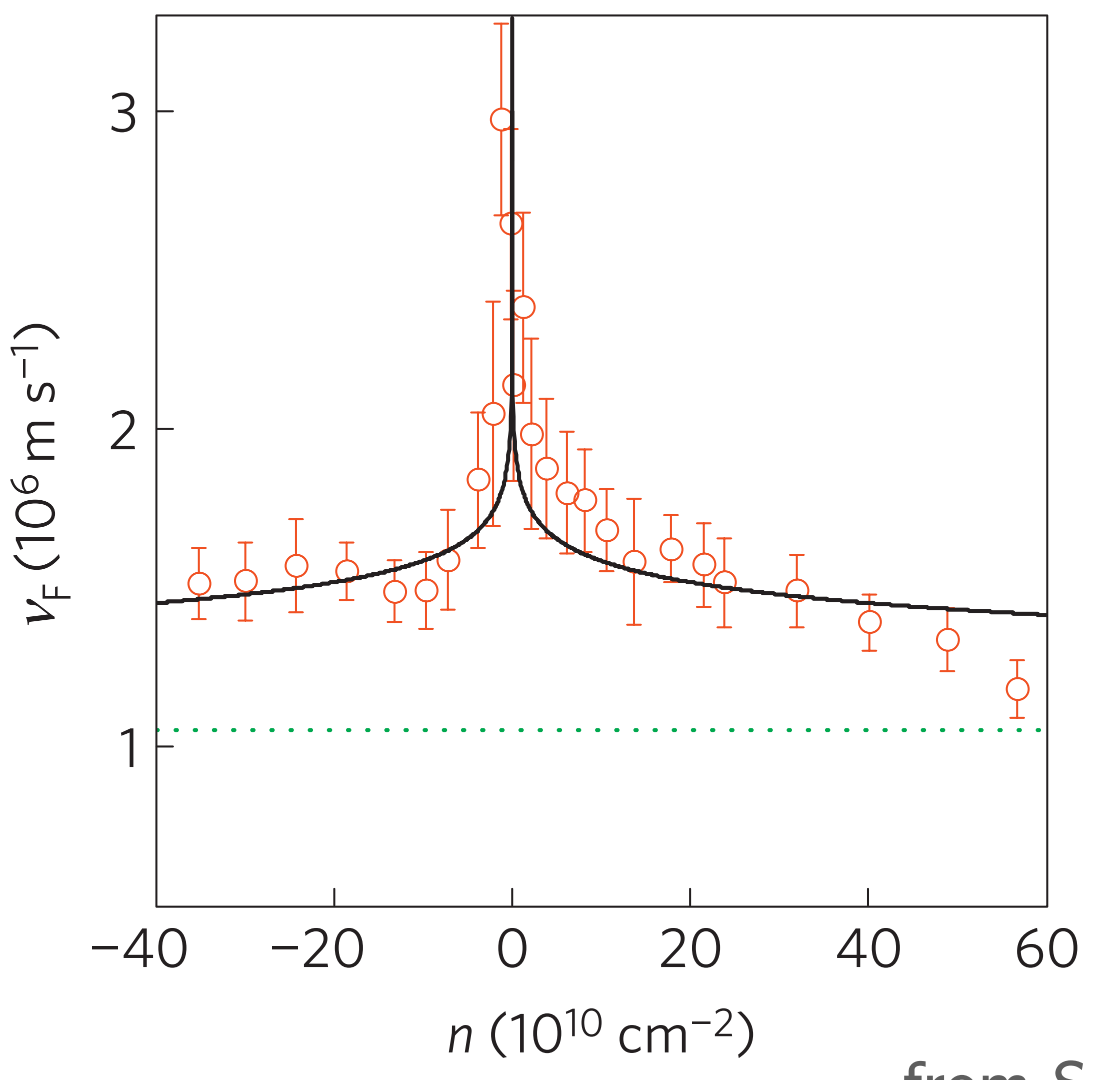

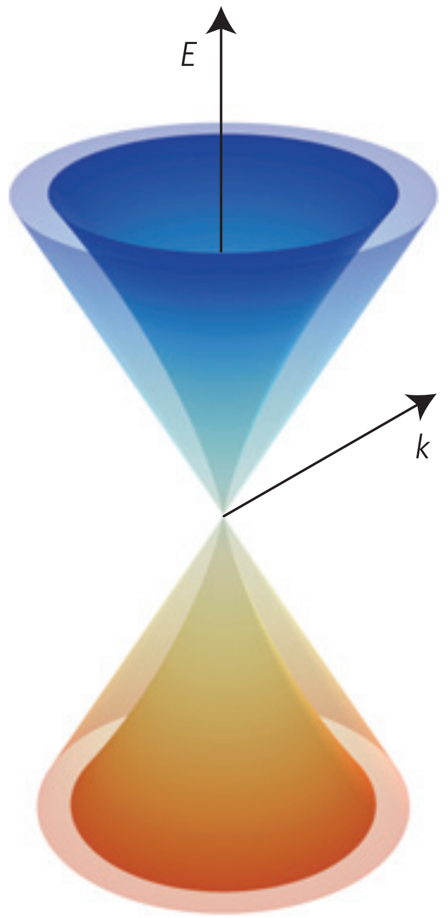

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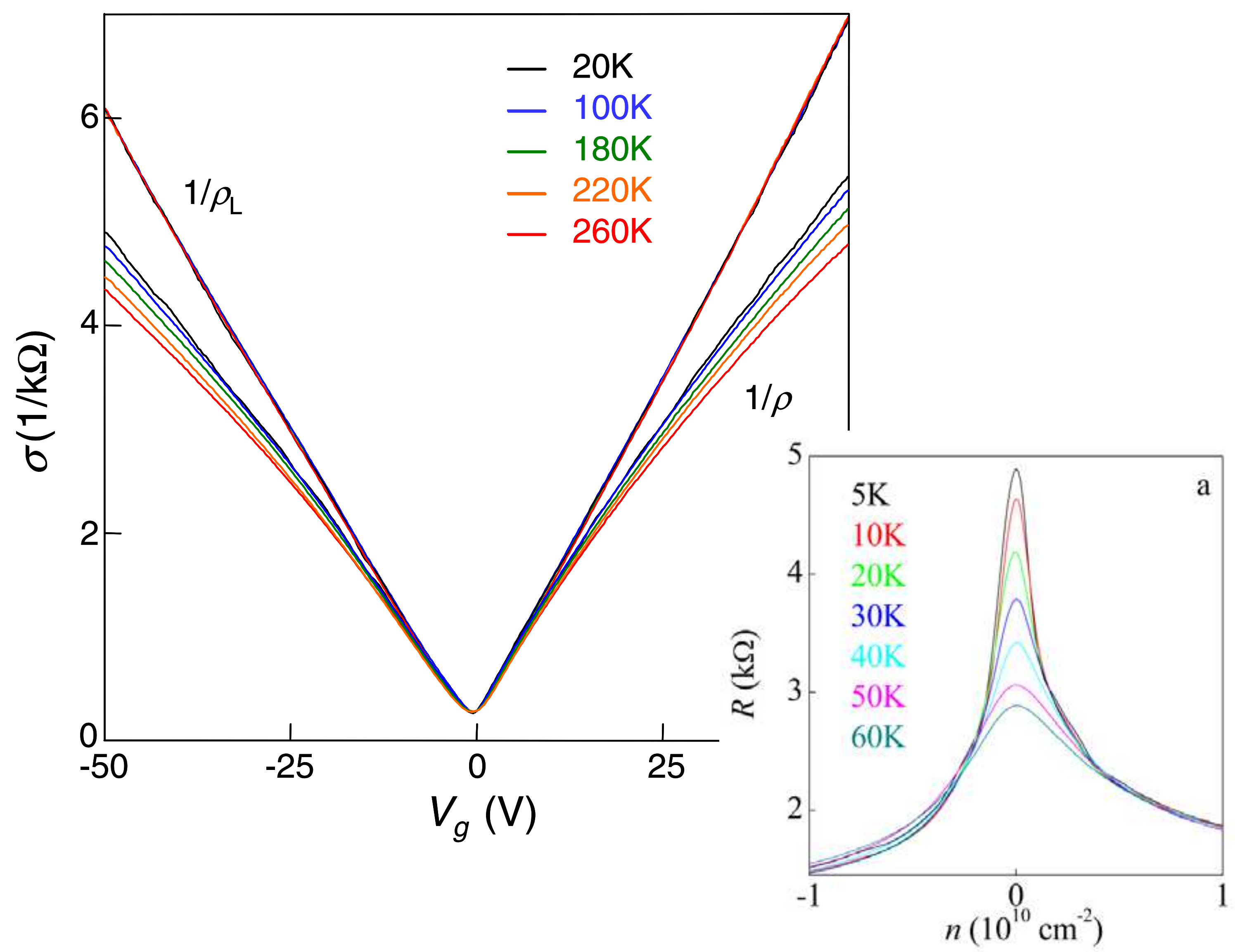
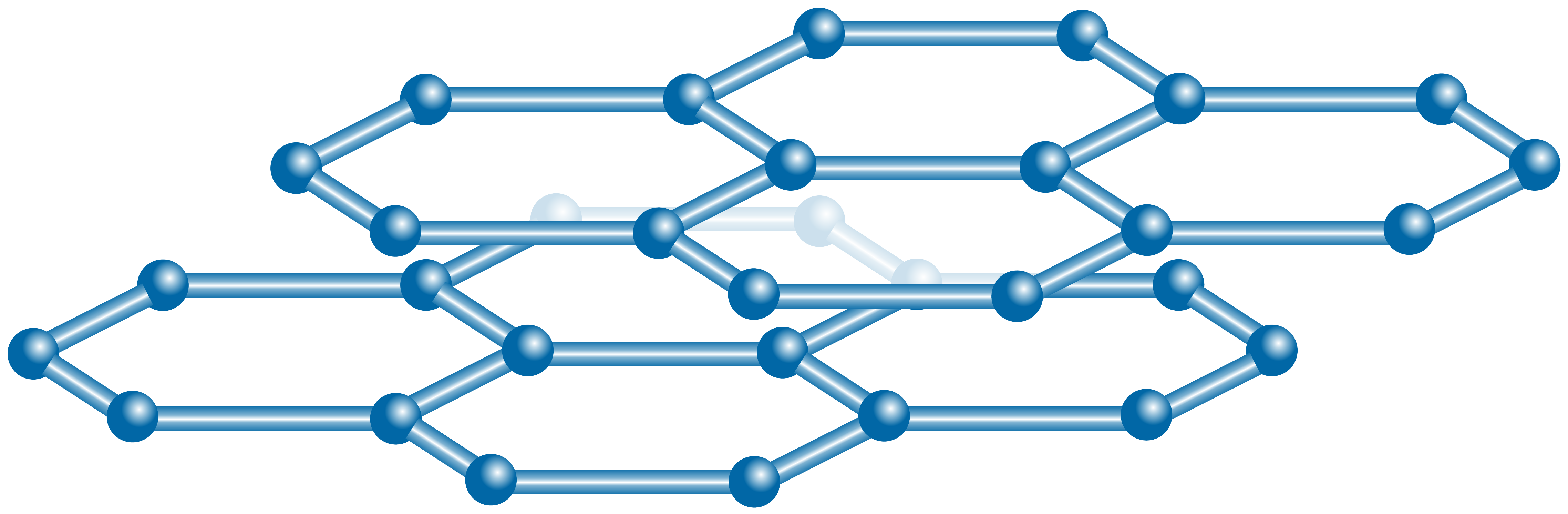
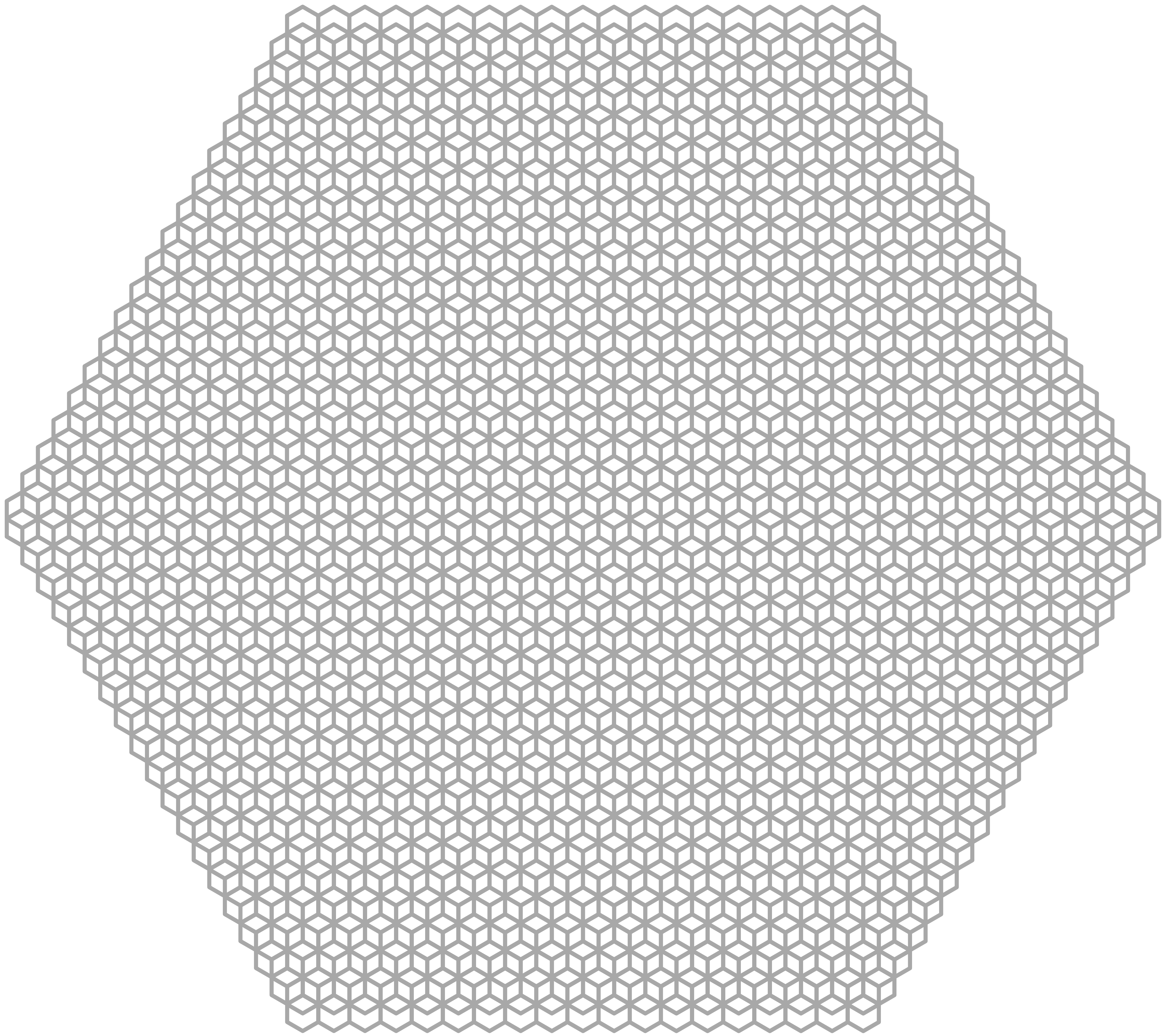
Transport:



[Morozov *et al.*, PRL '08]

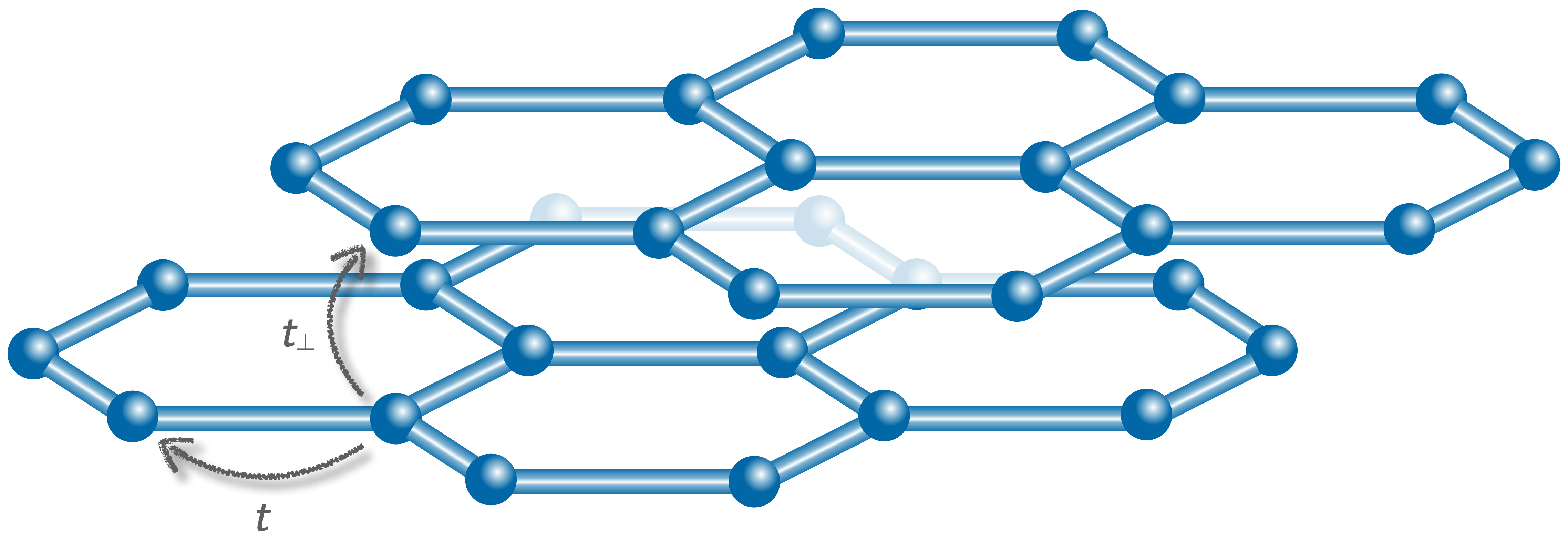
Bernal bilayer graphene

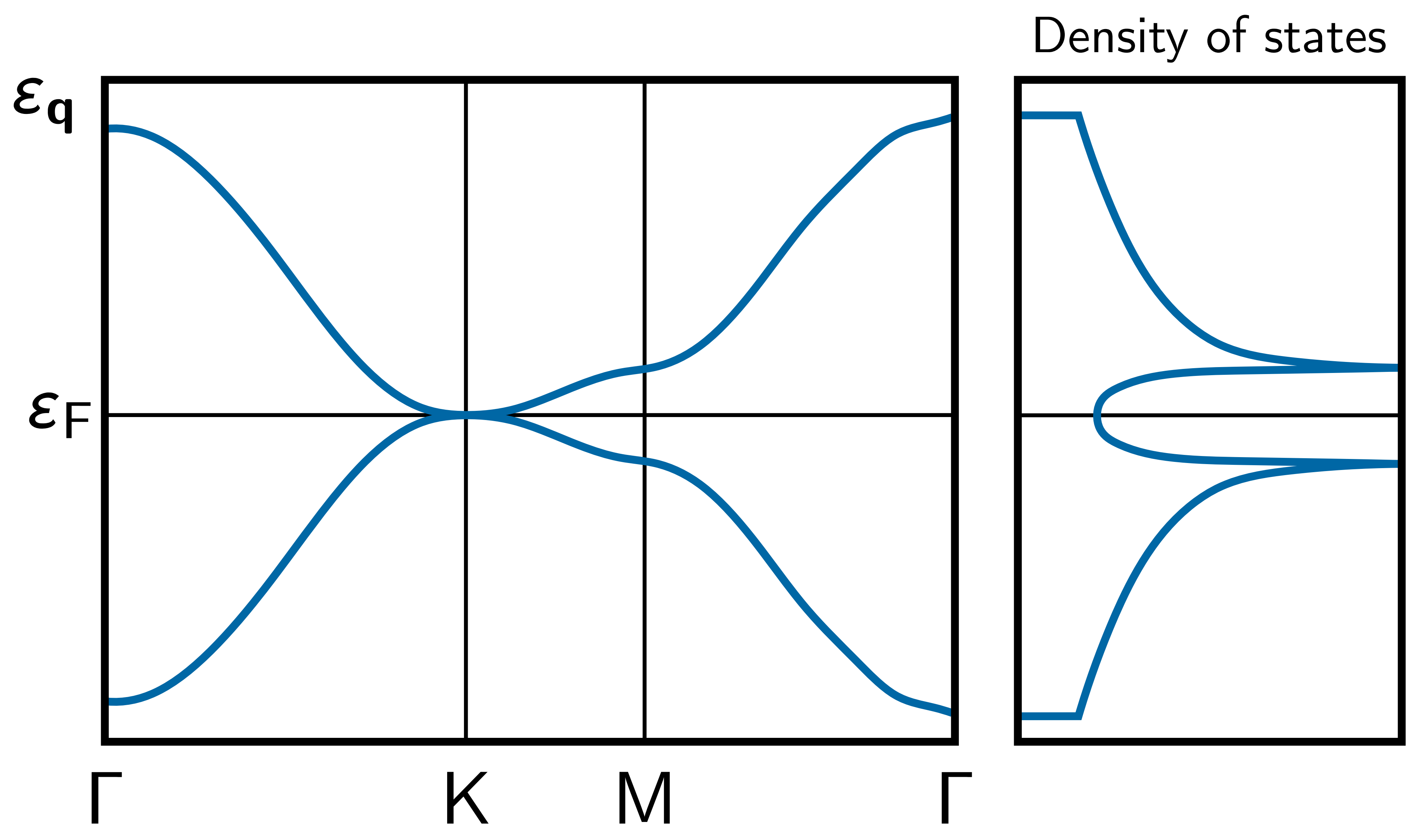




AB stacking

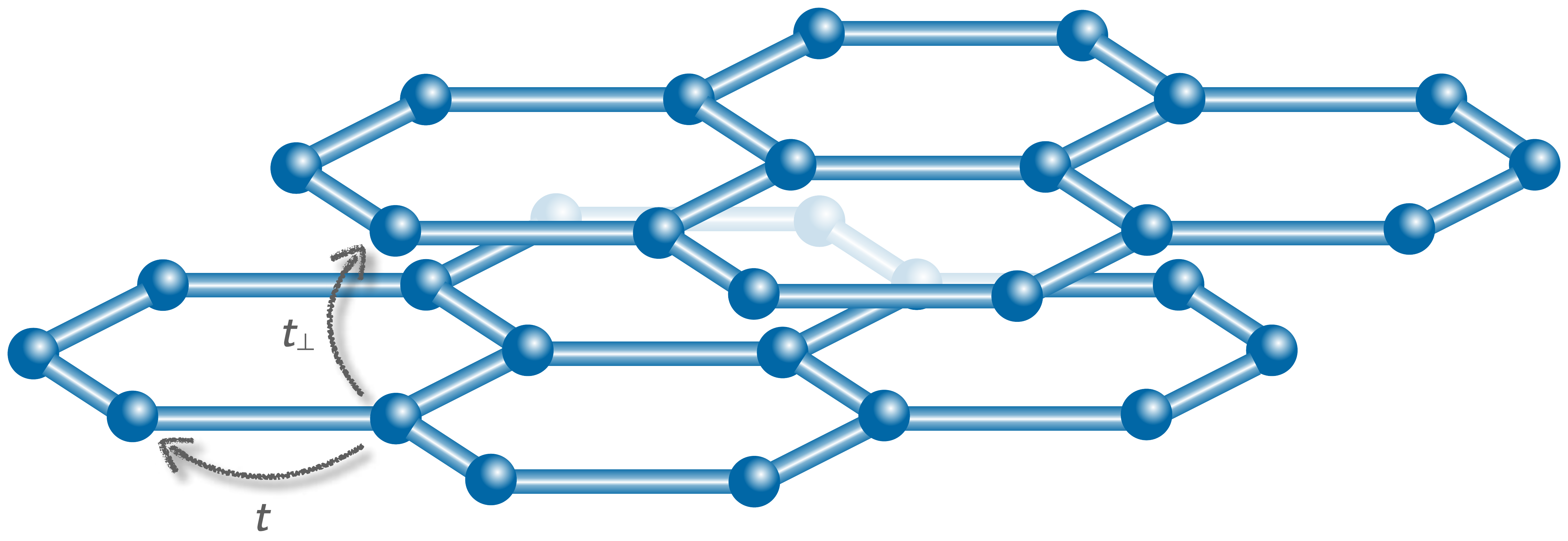
Bernal bilayer graphene

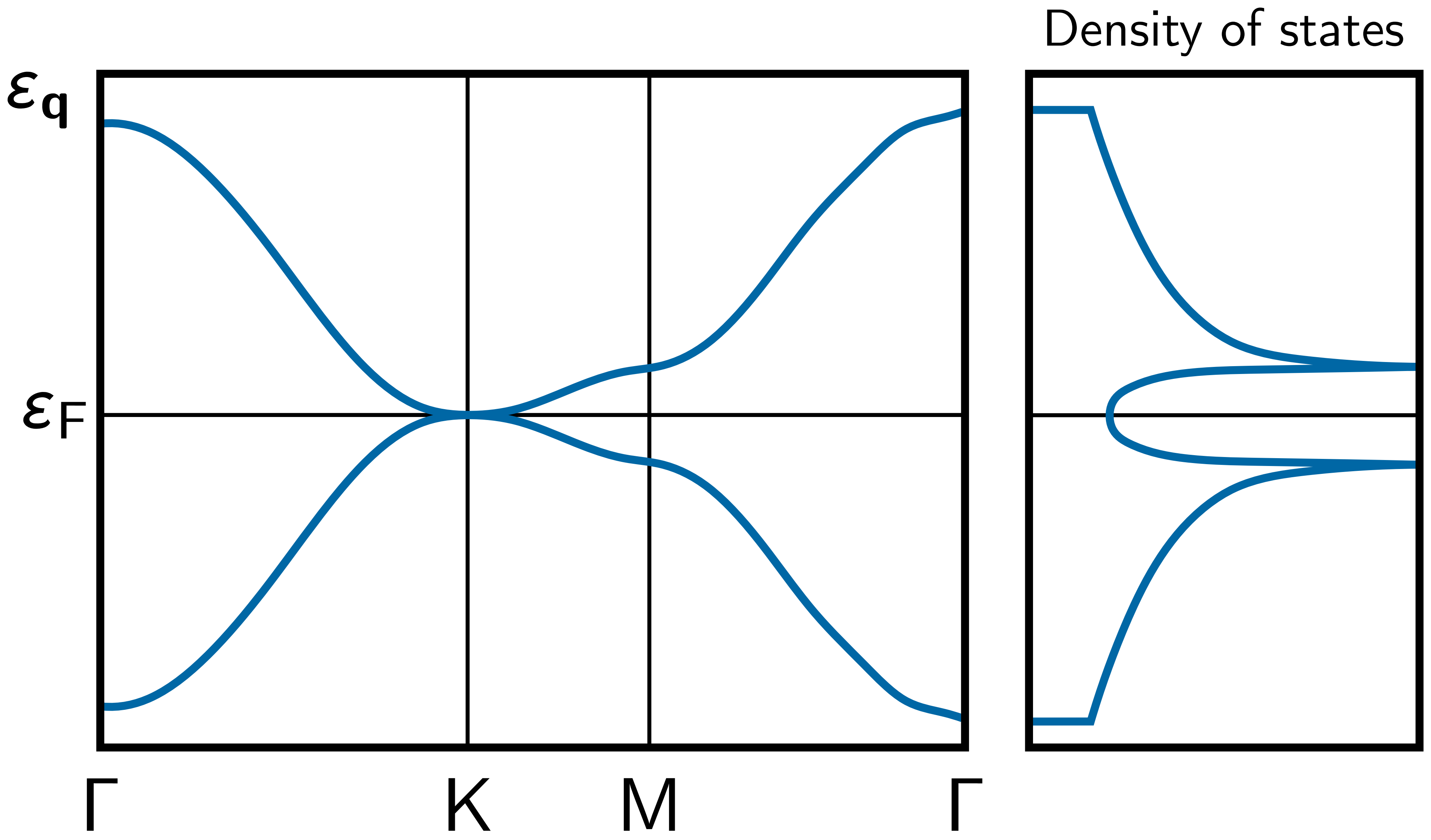




[McCann & Fal'ko, PRL '06]

Bernal bilayer graphene

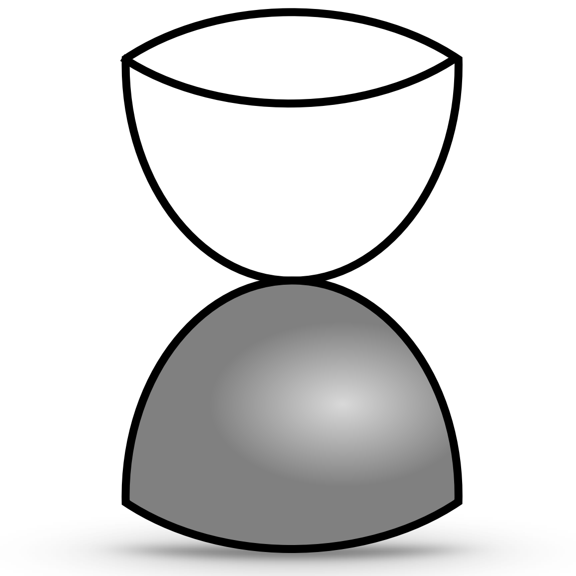




[McCann & Fal'ko, PRL '06]

Low-energy spectrum:

$$\varepsilon_{\mathbf{K}+\mathbf{q}} = \pm f_2 q^2 + \mathcal{O}(q^3)$$



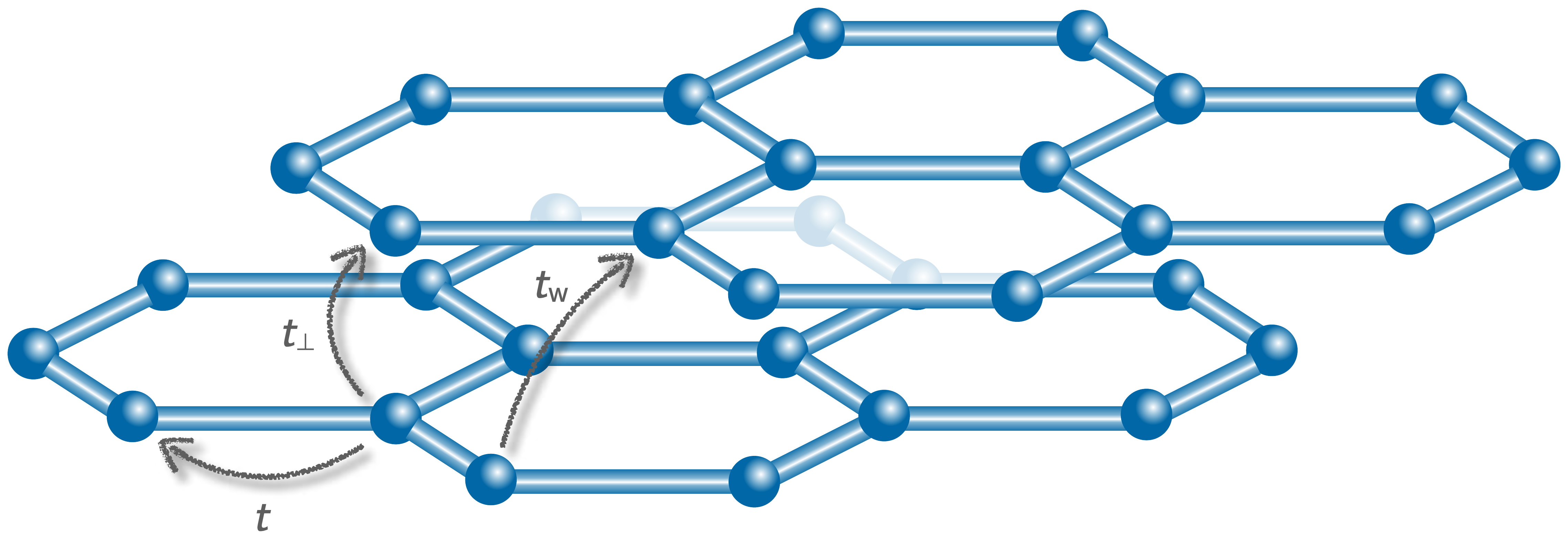
"Quadratic band touching"

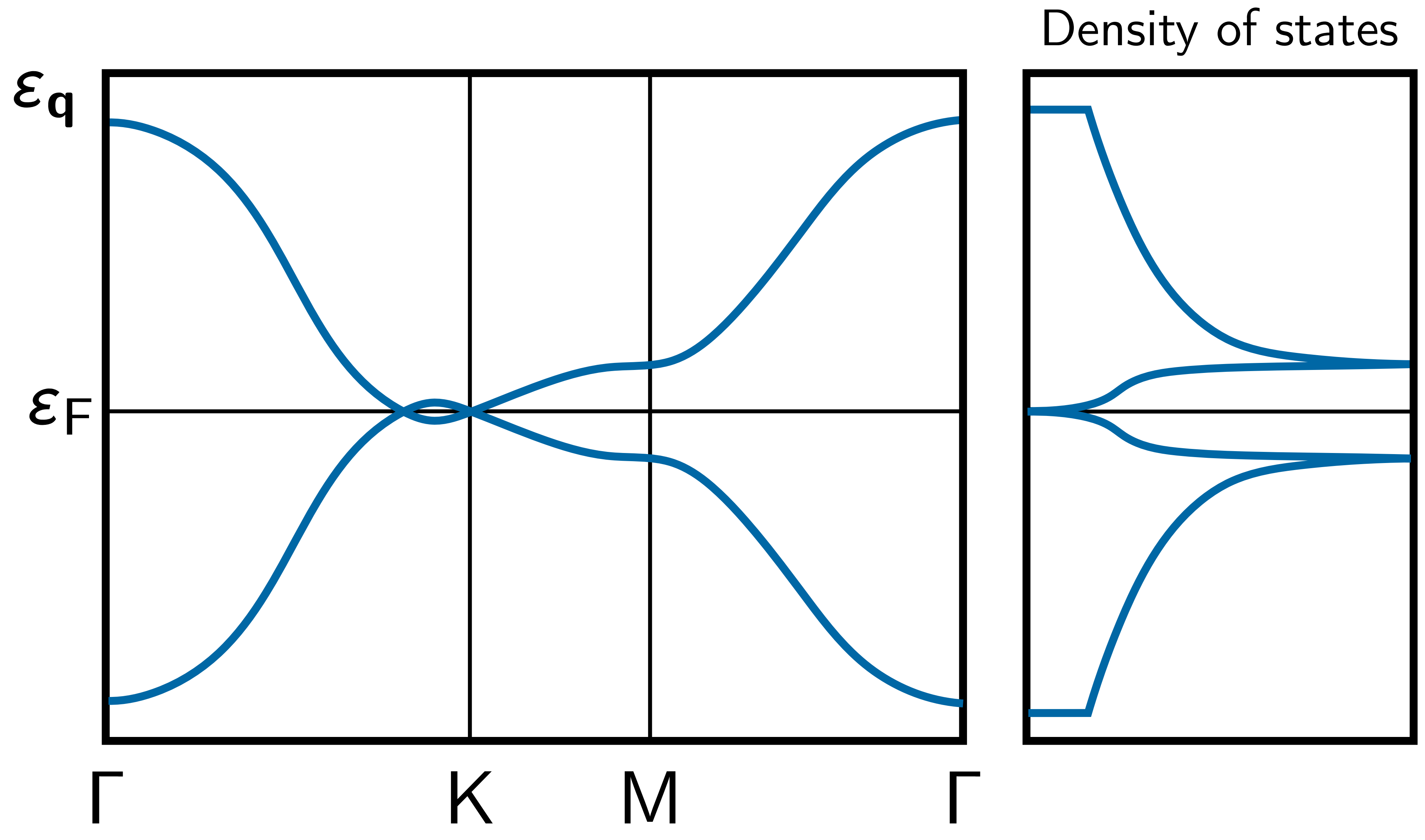
with $f_2/a_0^2 = 3t^2/(4t_\perp) \simeq 20\,\text{eV}$

... for $t \simeq 3\,\text{eV}$, $t_\perp \simeq 0.3\,\text{eV}$

[Malard *et al.*, PRB '07]
[Zhang *et al.*, PRB '08]

Trigonal warping





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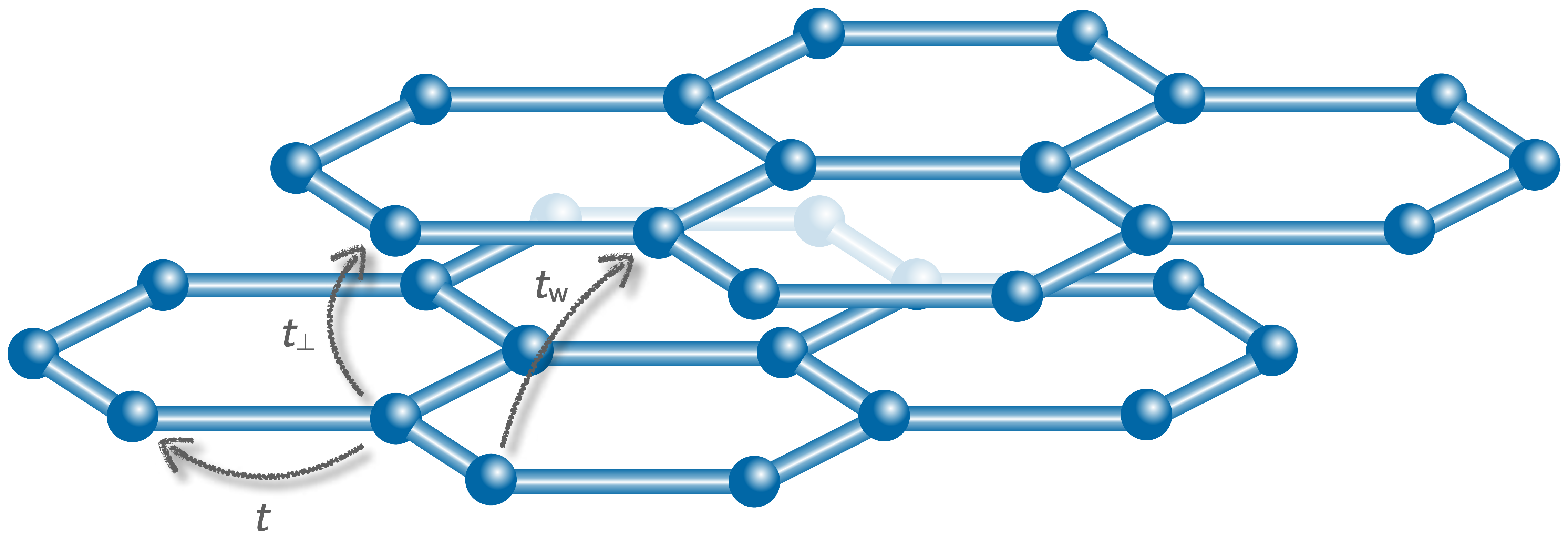
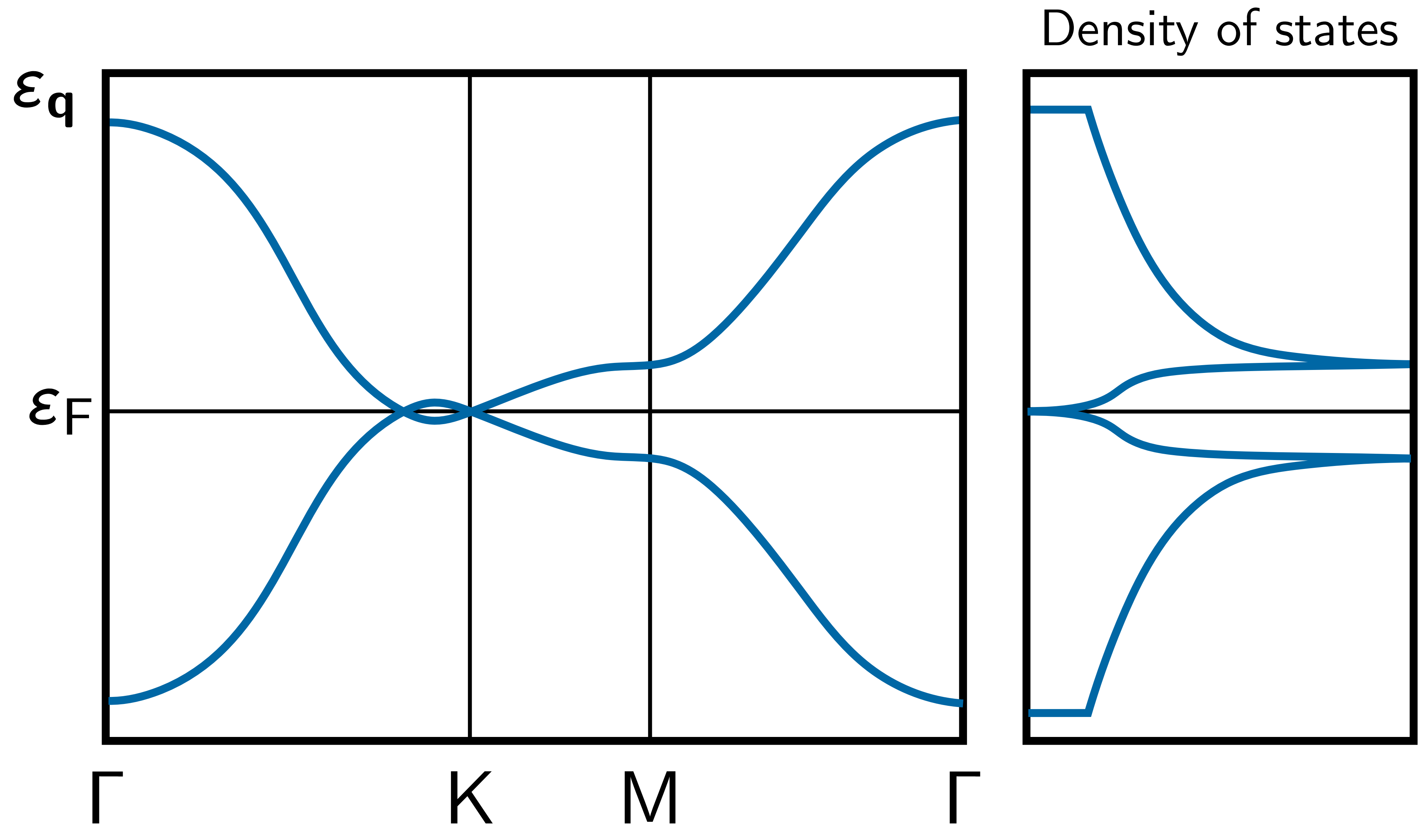
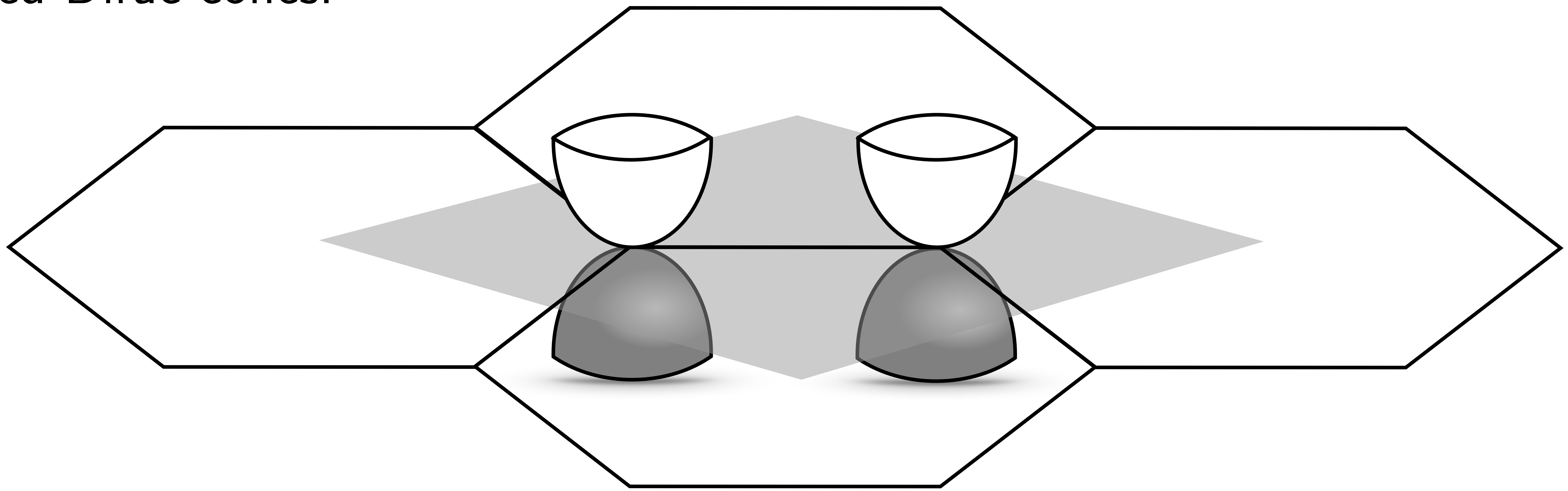




Warping-induced Dirac cones:



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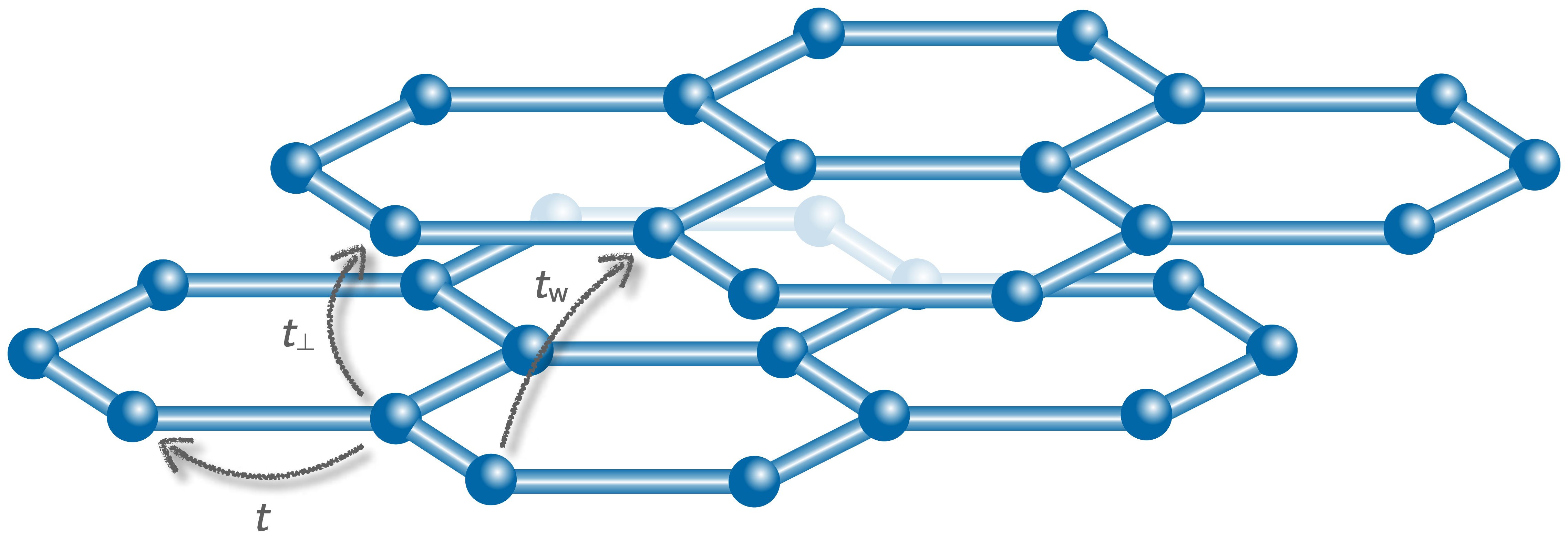

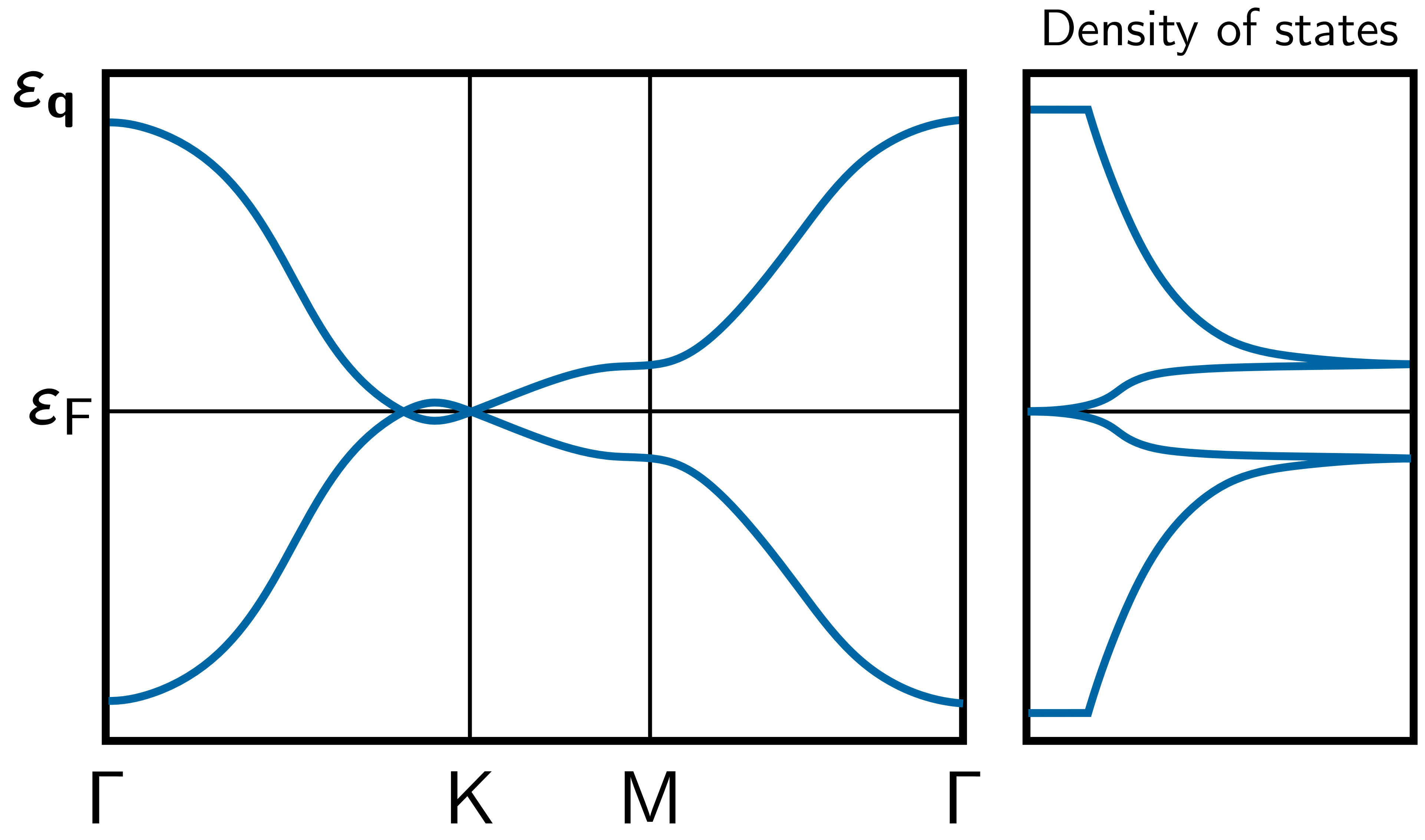

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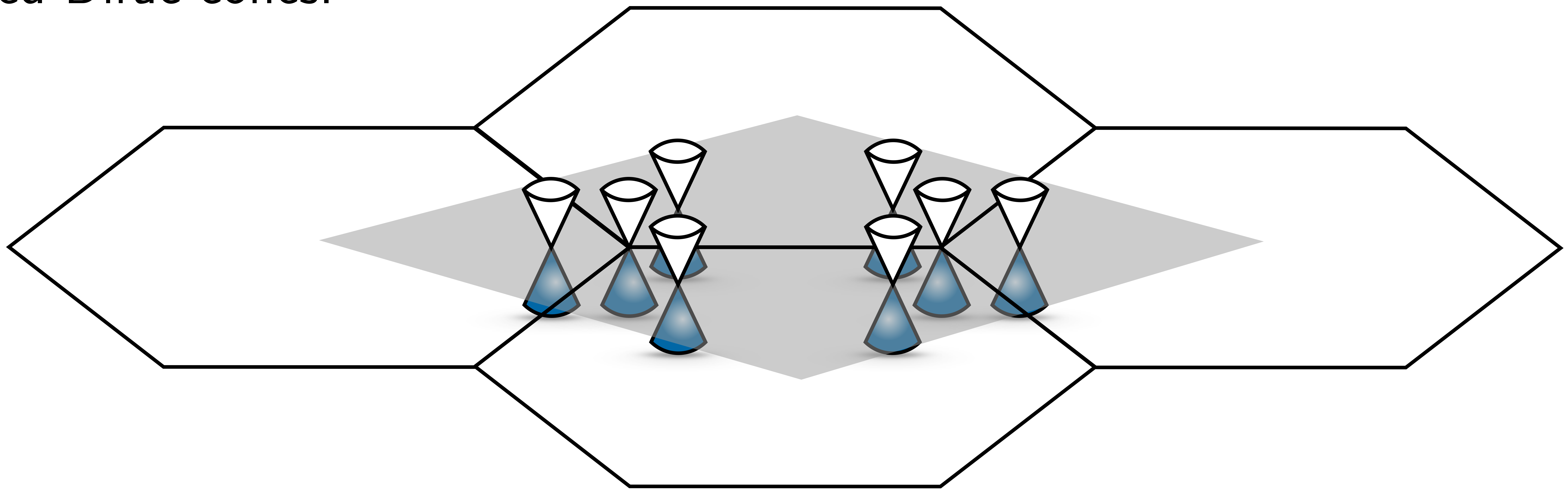

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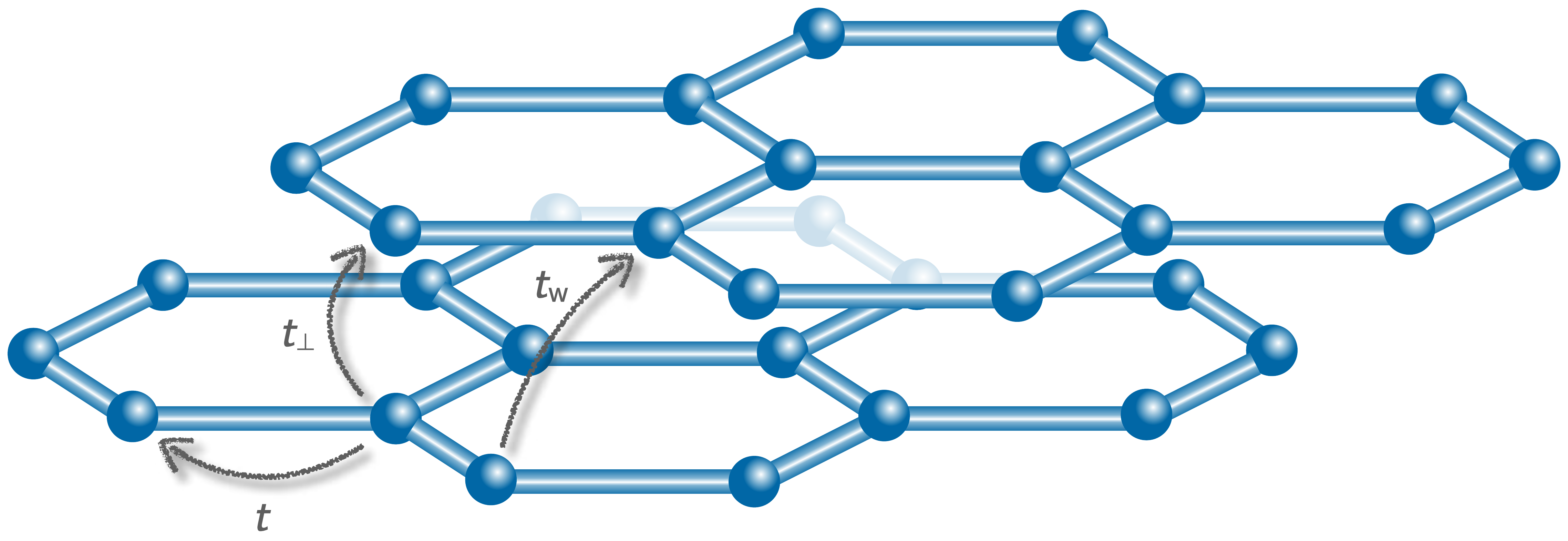
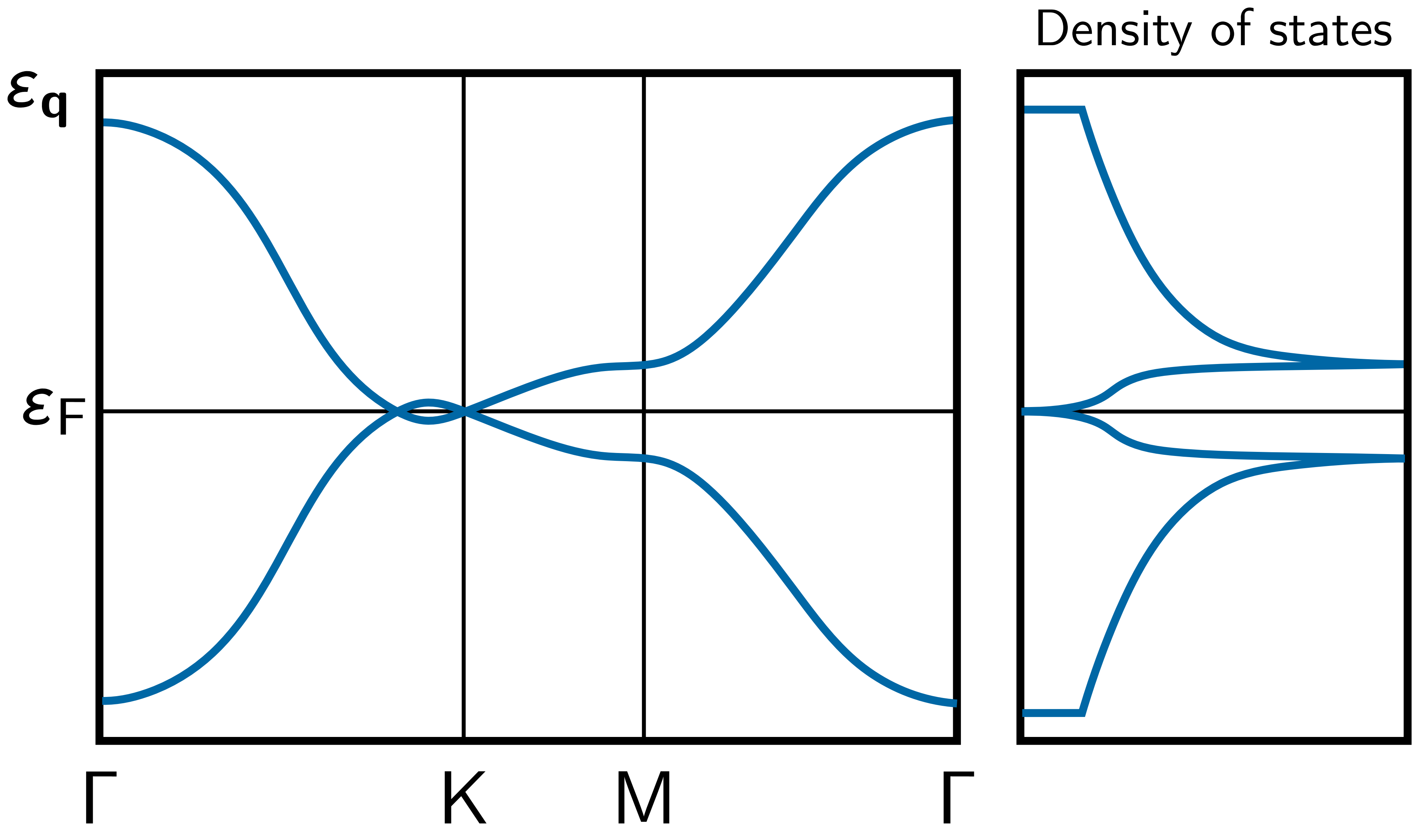




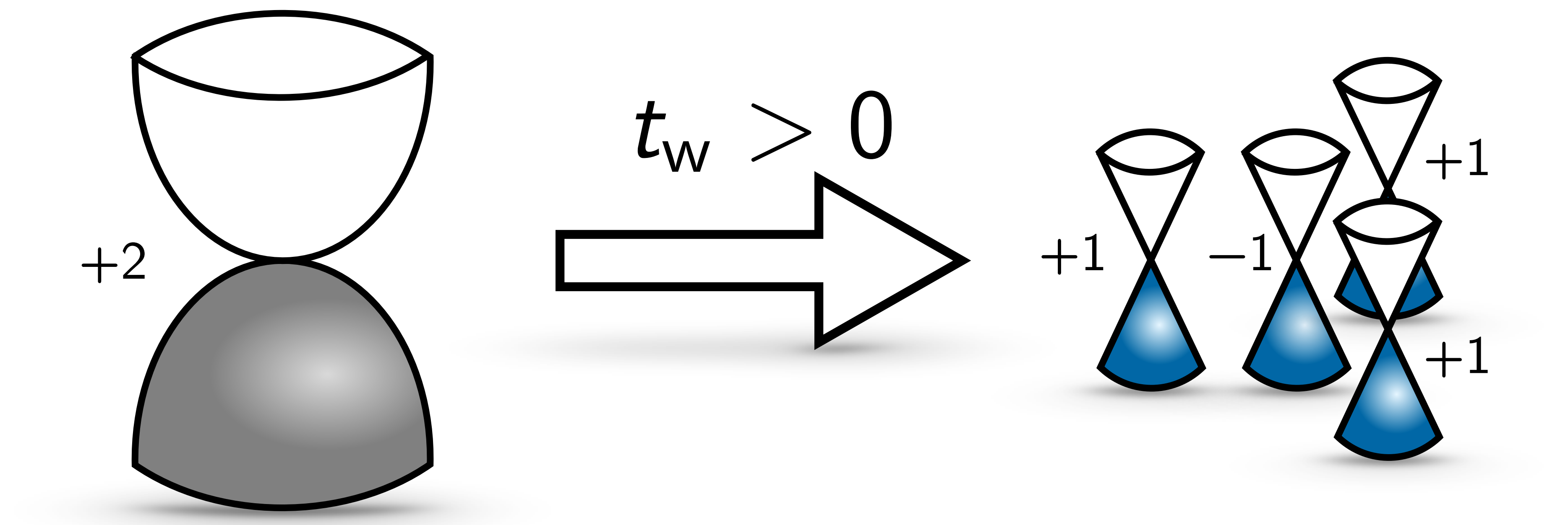
Low-energy spectrum:

$$\varepsilon_{\mathbf{K}+\mathbf{q}} = f_1 q \pm f_2 q^2 \cos 3\varphi + \mathcal{O}(q^3)$$

... for $q \ll f_1/f_2 \simeq 0.004 a_0^{-1}$

with $f_1/a_0 = \sqrt{3} t_{\mathrm{w}}/2 \simeq 0.09\,\mathrm{eV} \ll f_2/a_0^2 \approx 20\,\mathrm{eV}$

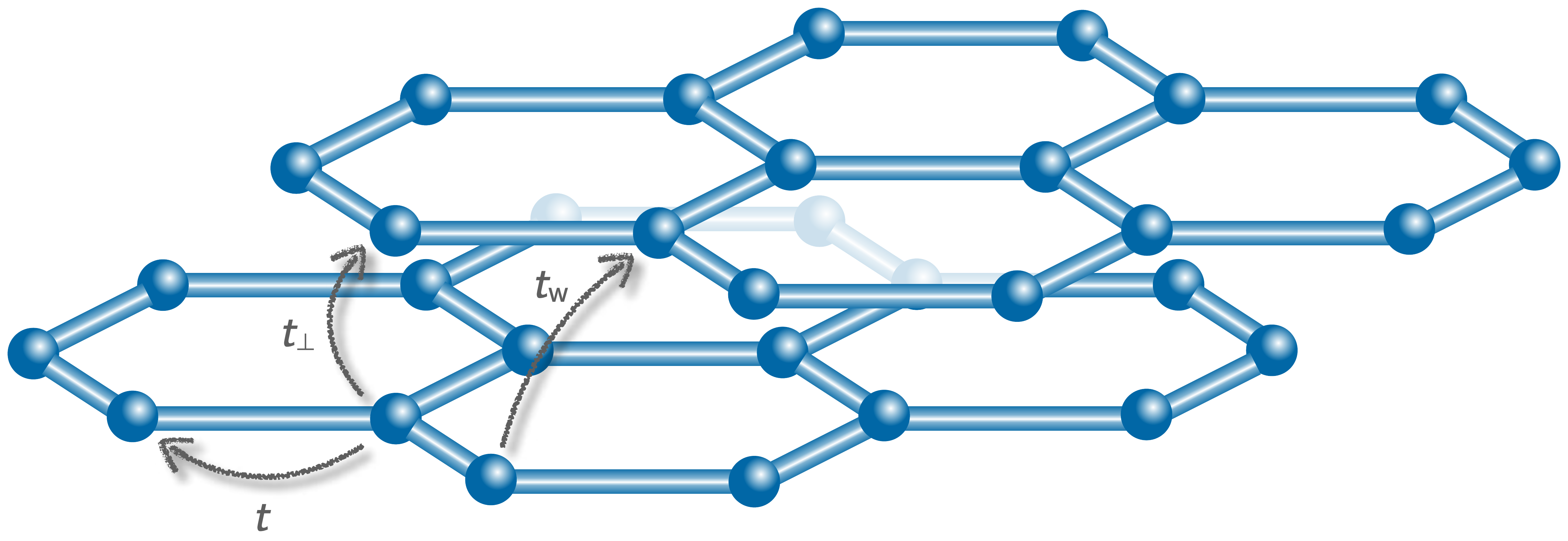
... for $t_{\mathrm{w}} \simeq 0.1\,\mathrm{eV}$

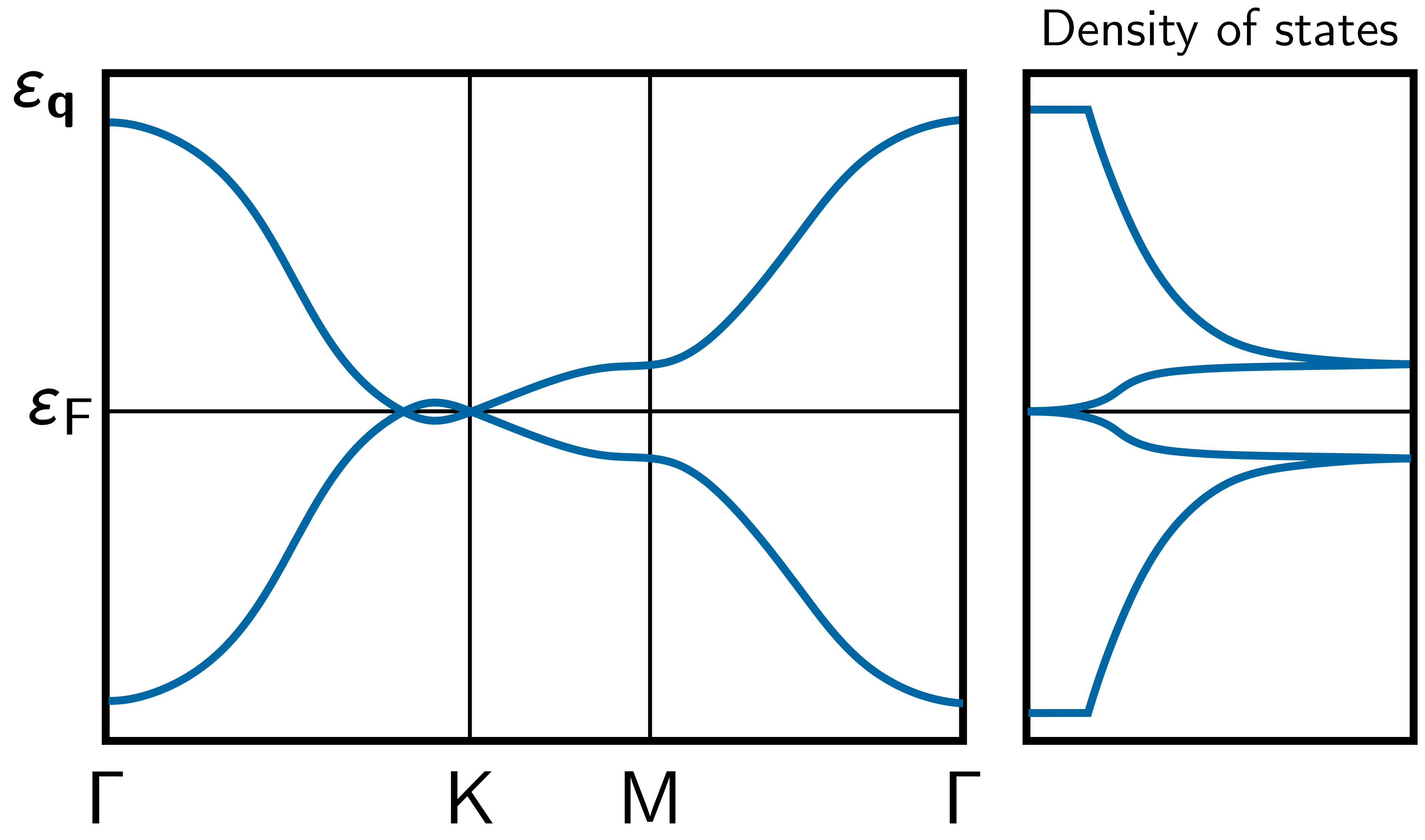


Berry charge
$Q = +2$

Berry charges
$Q = -1 + 3\times(+1)$

Trigonal warping





Low-energy spectrum:

Experimentally accessible?

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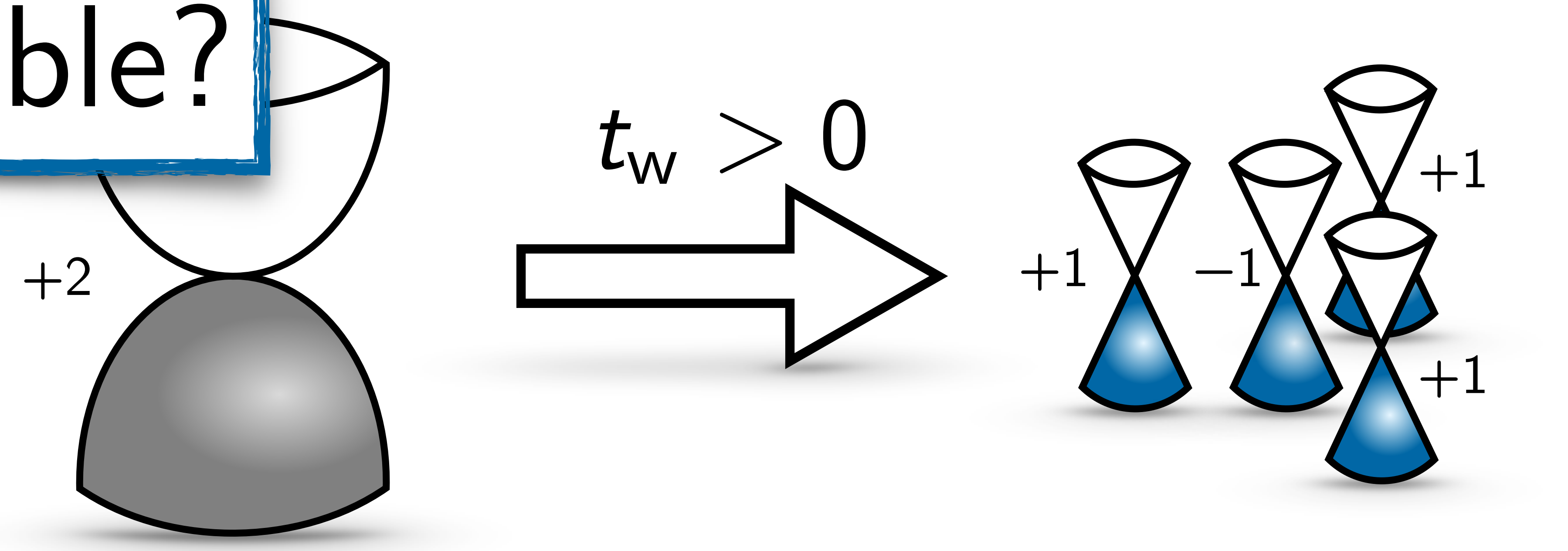

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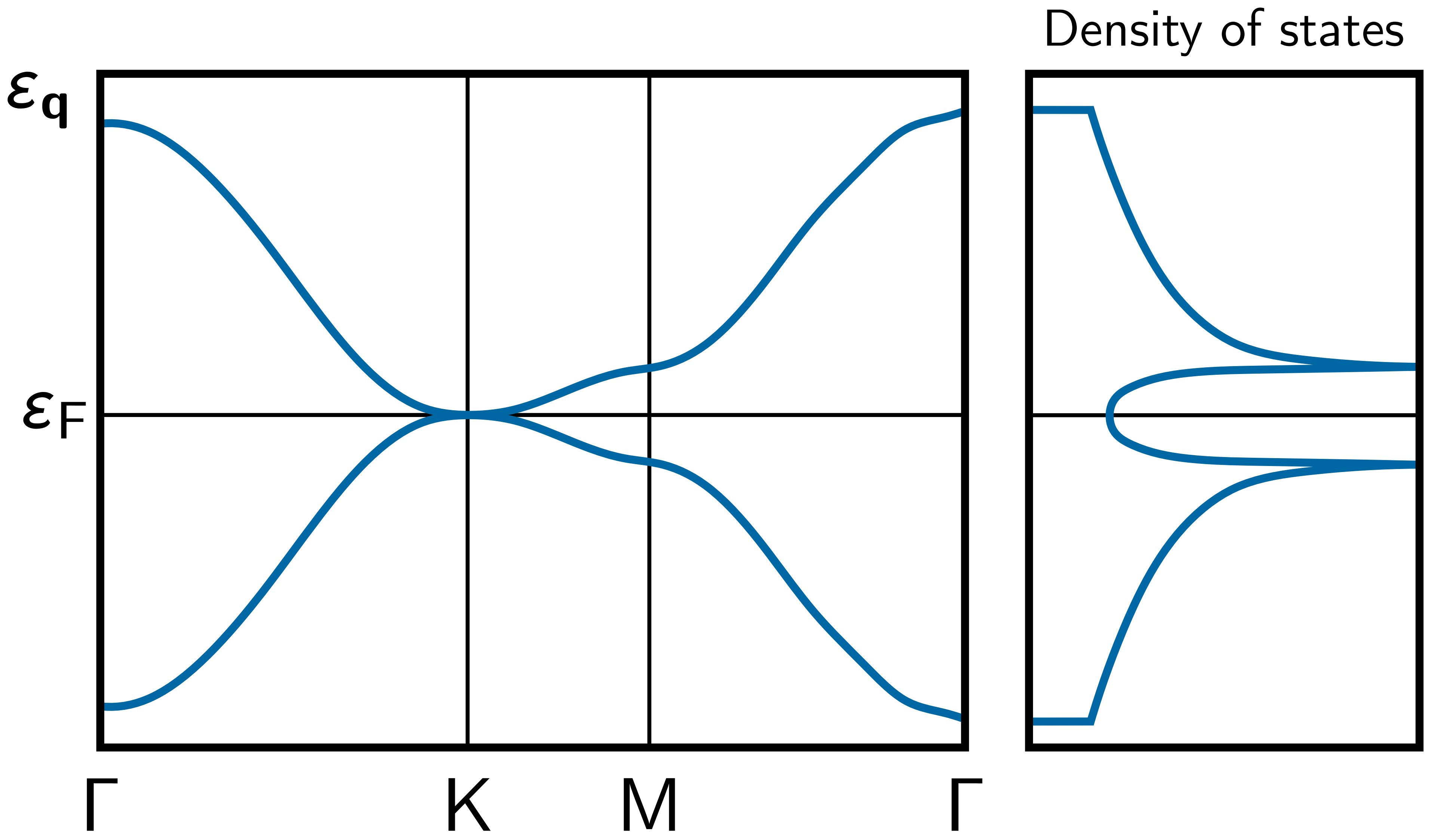
... for $t_w \simeq 0.1\,\text{eV}$

Interactions:

Coulomb repulsion:

$$V(r) \propto \frac{e^2}{r} \mathrm{e}^{-r/r_0} \qquad \text{screened}$$



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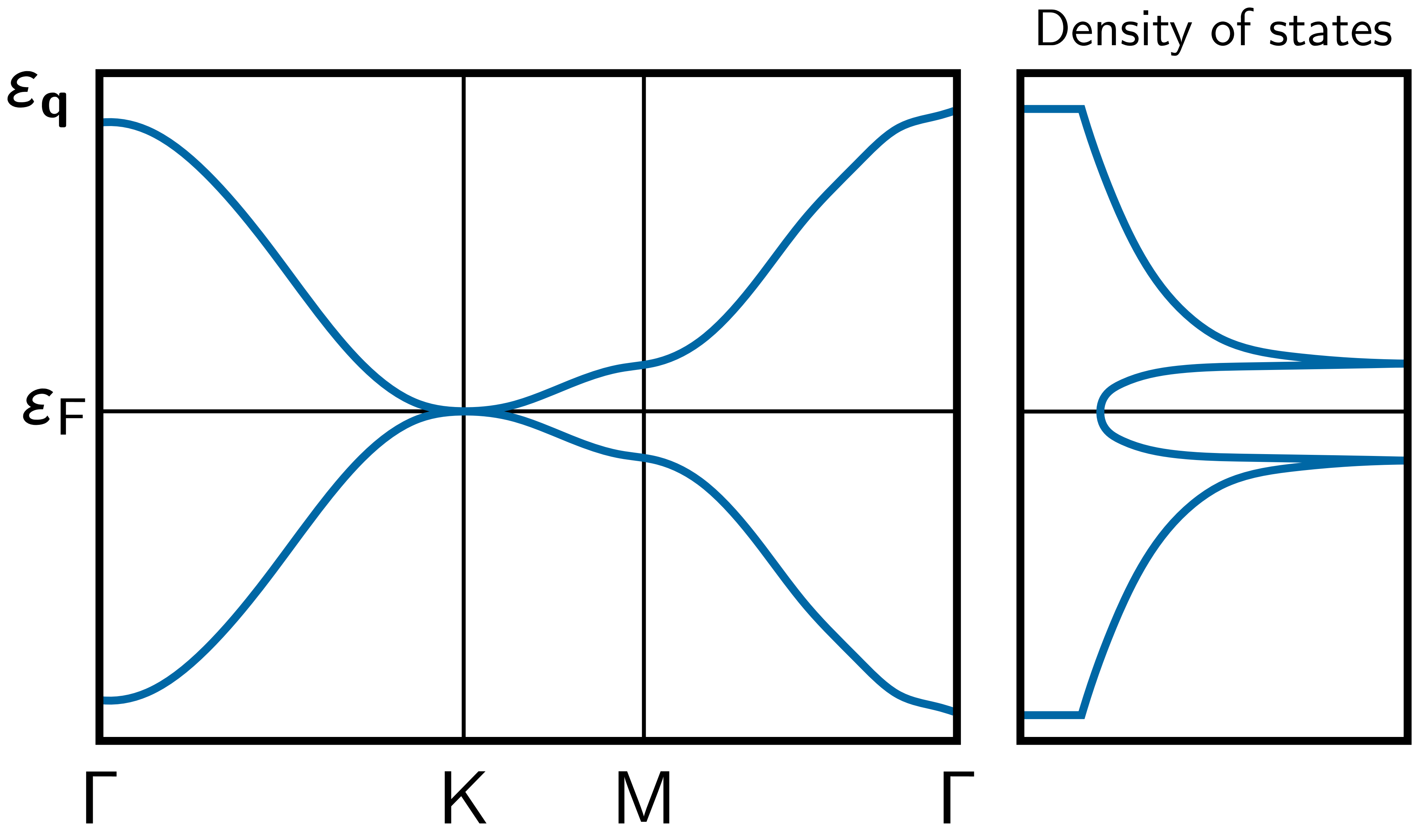

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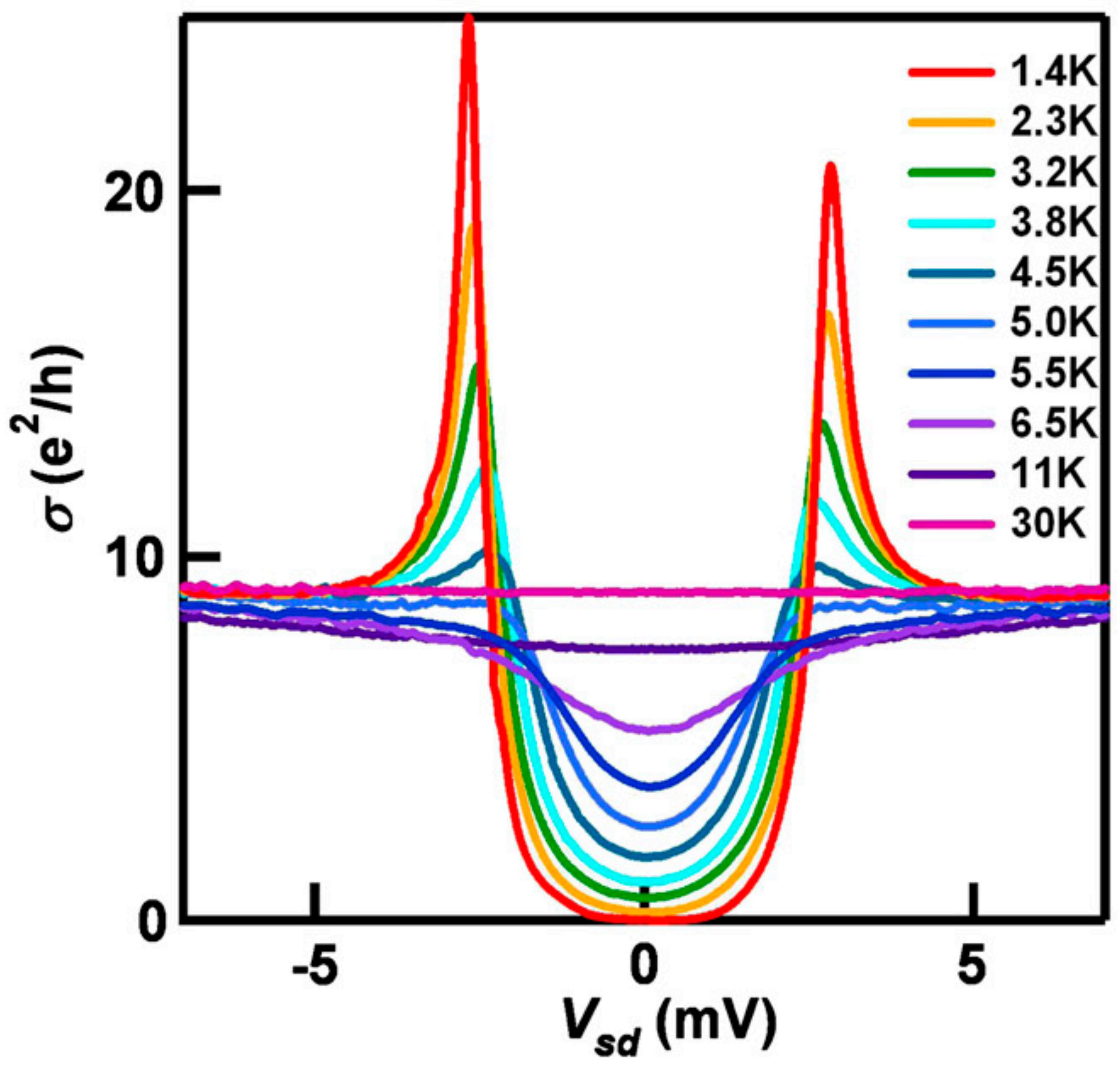

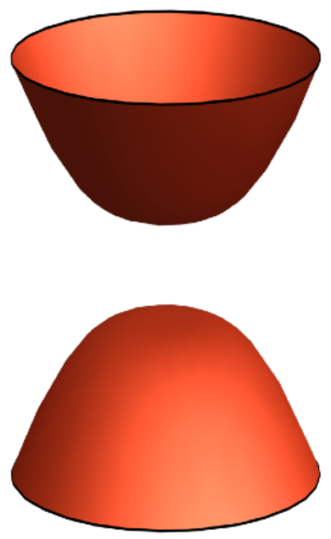

Full gap?

[Bao *et al.*, PNAS '12]

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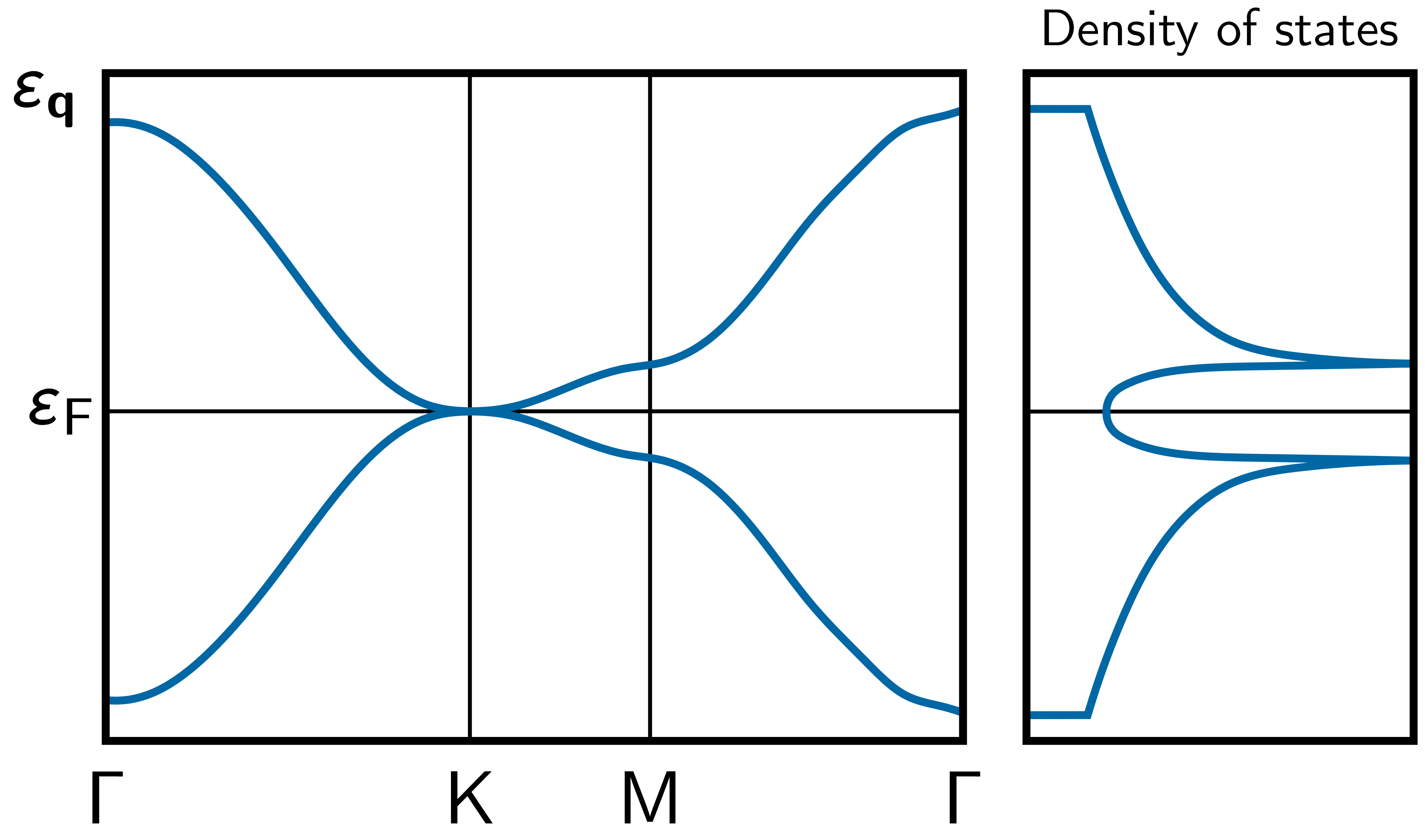

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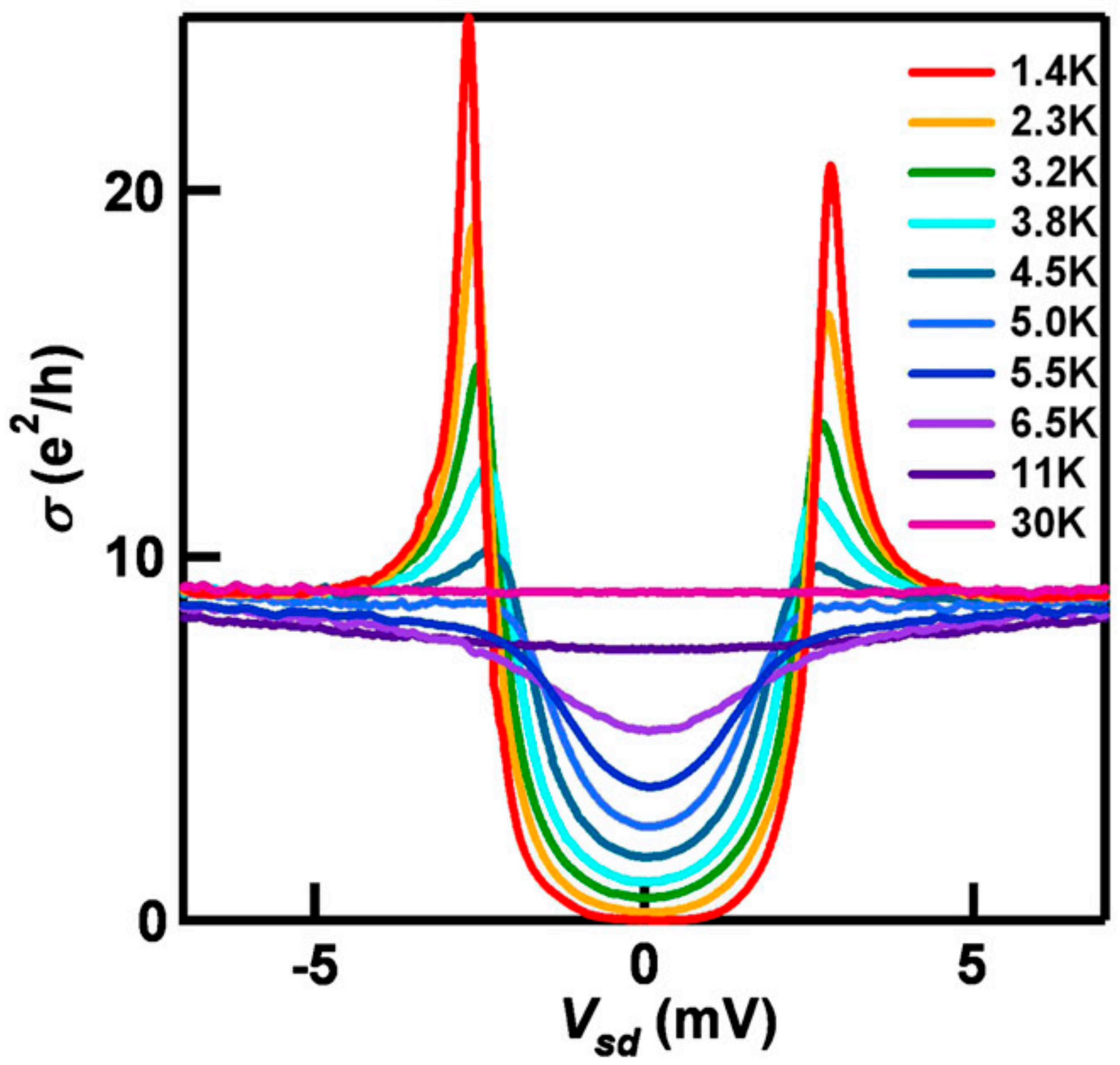
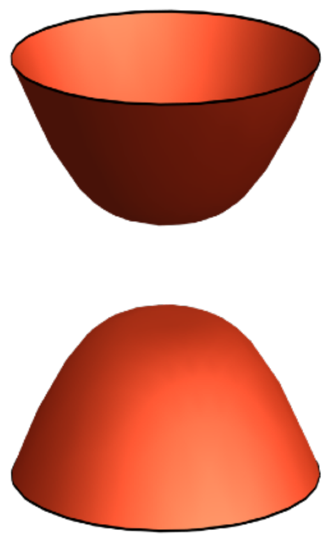
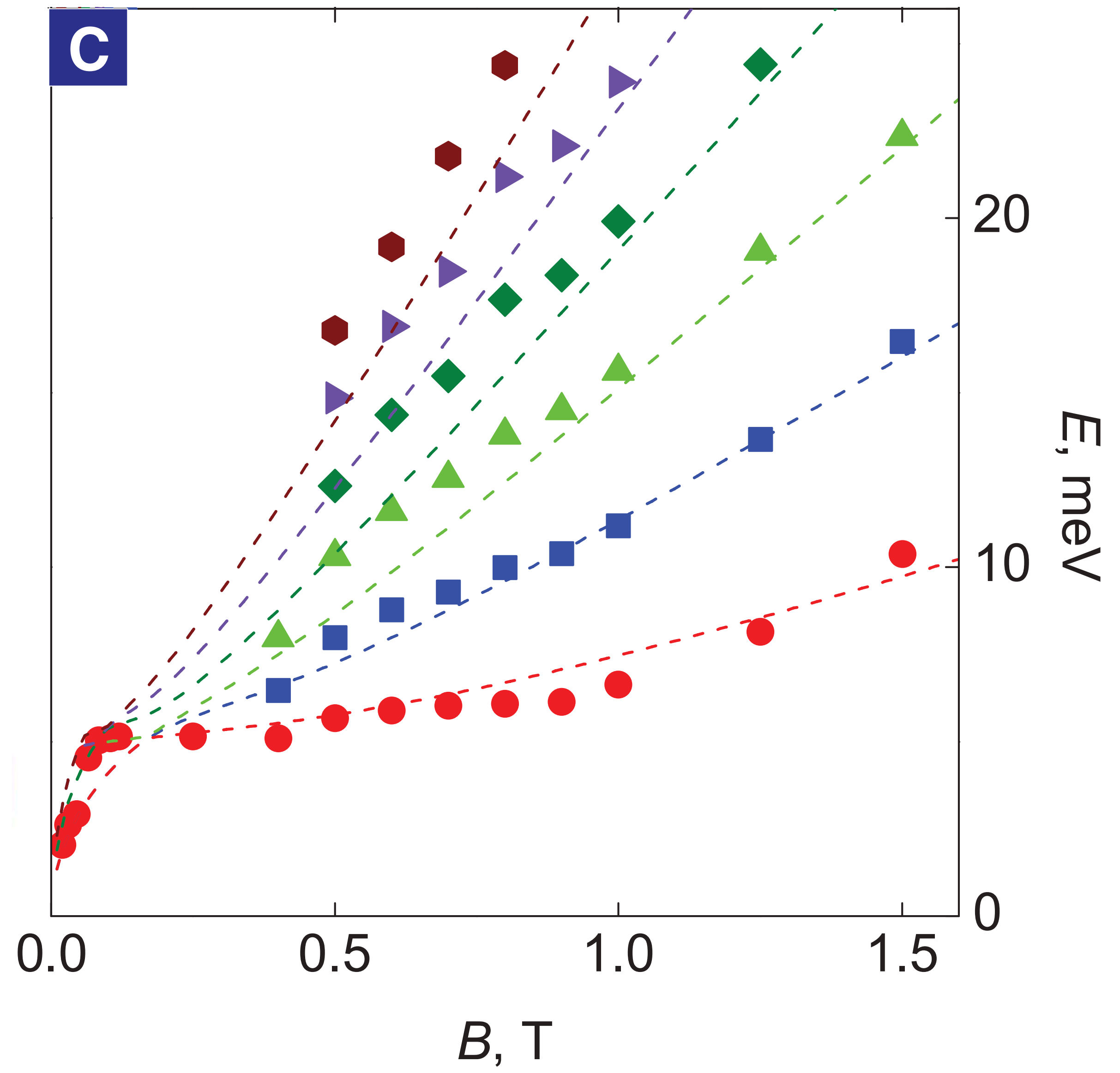




Full gap?

[Bao *et al.*, PNAS '12]

Landau levels:



Partial gap?

[Mayorov *et al.*, Science '11]

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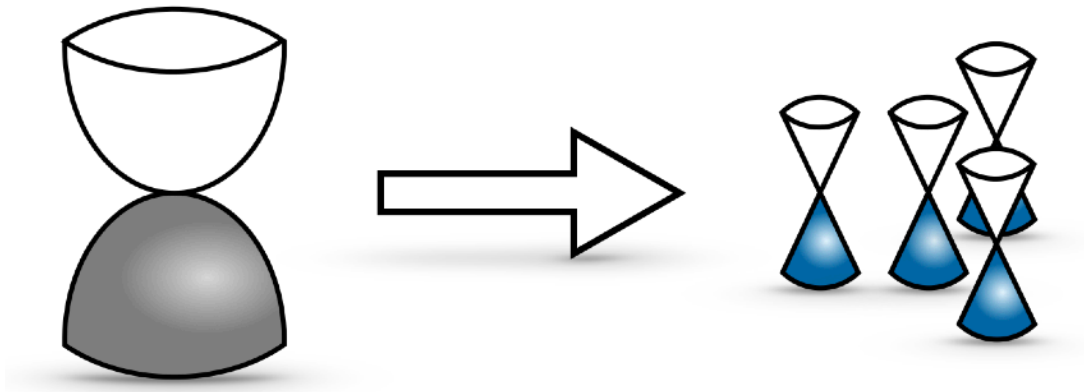
(2) **Interaction-induced Dirac cones**



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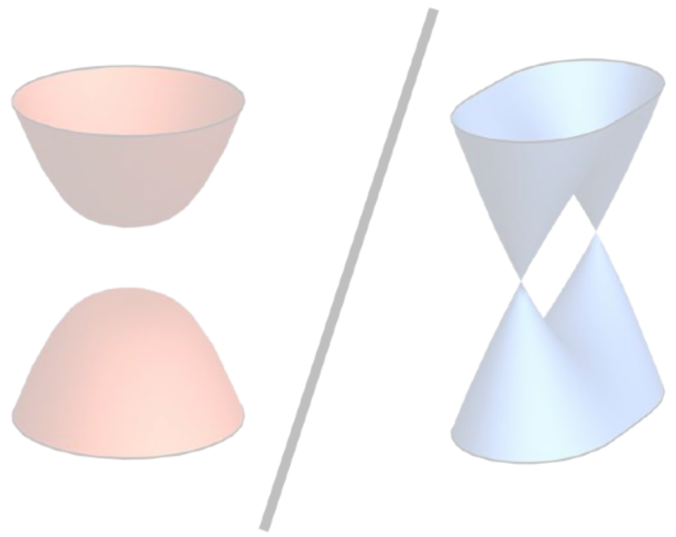

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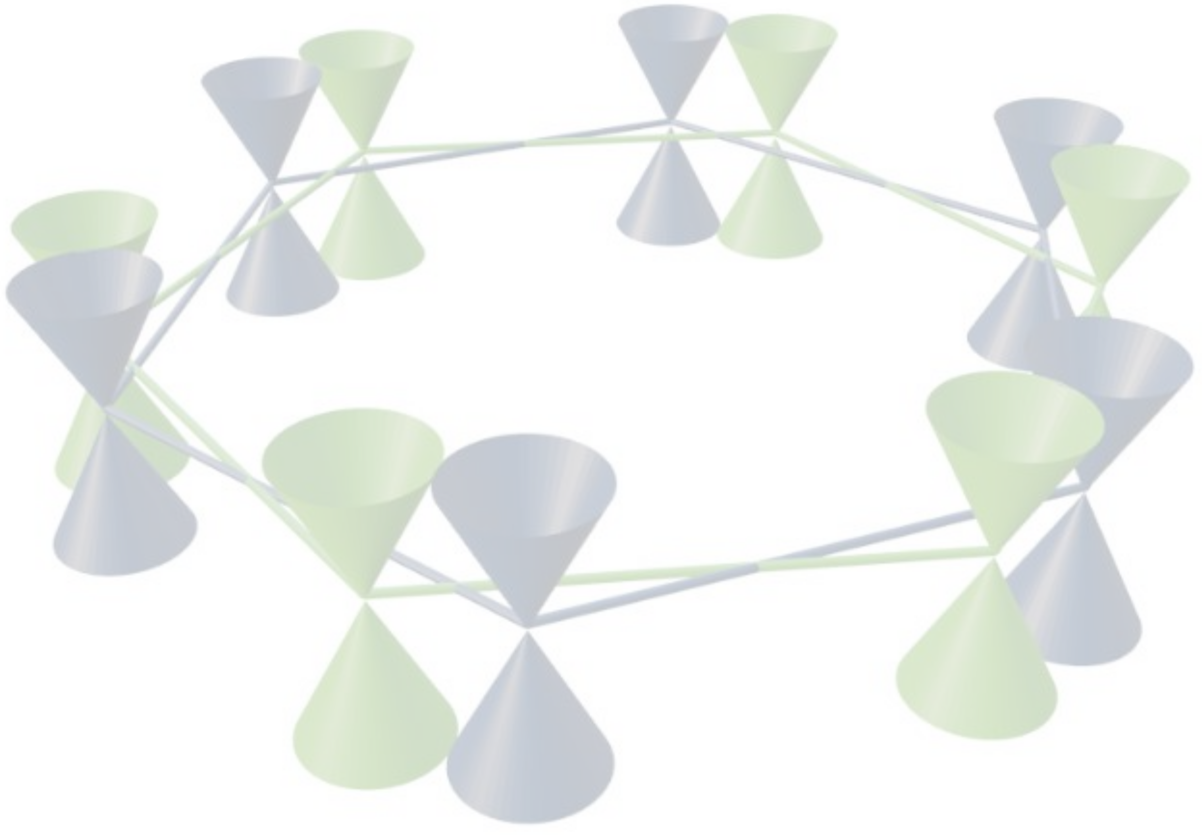
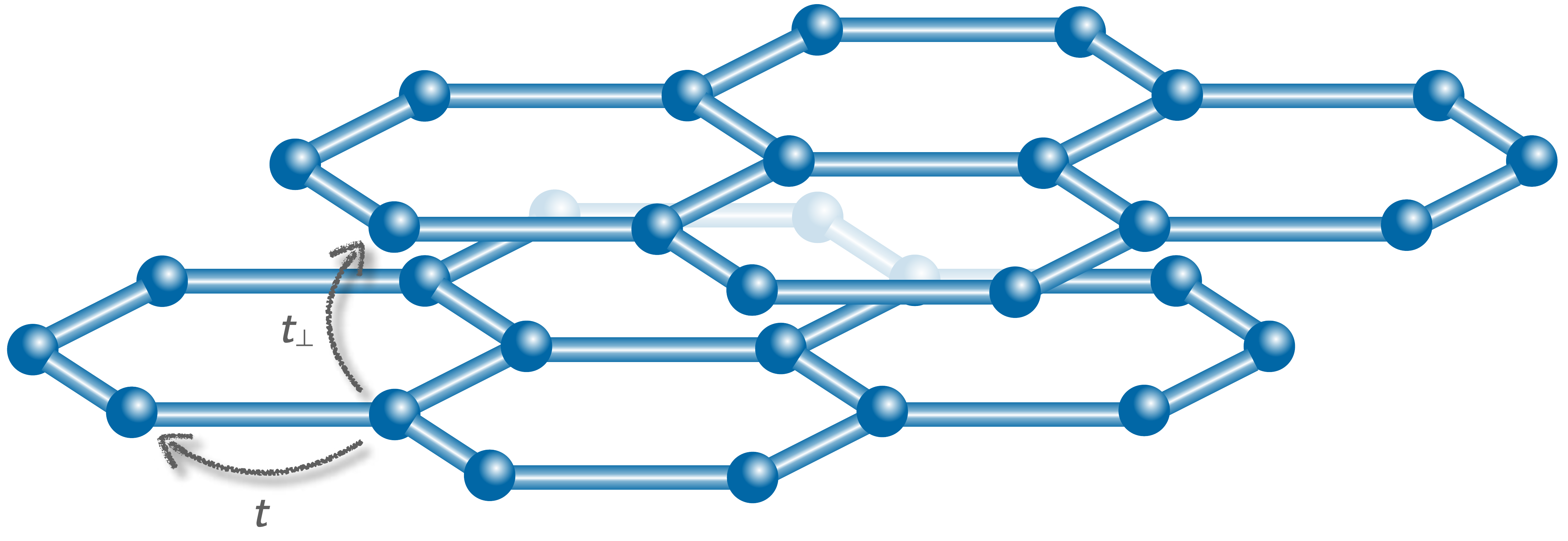


(5) Conclusions

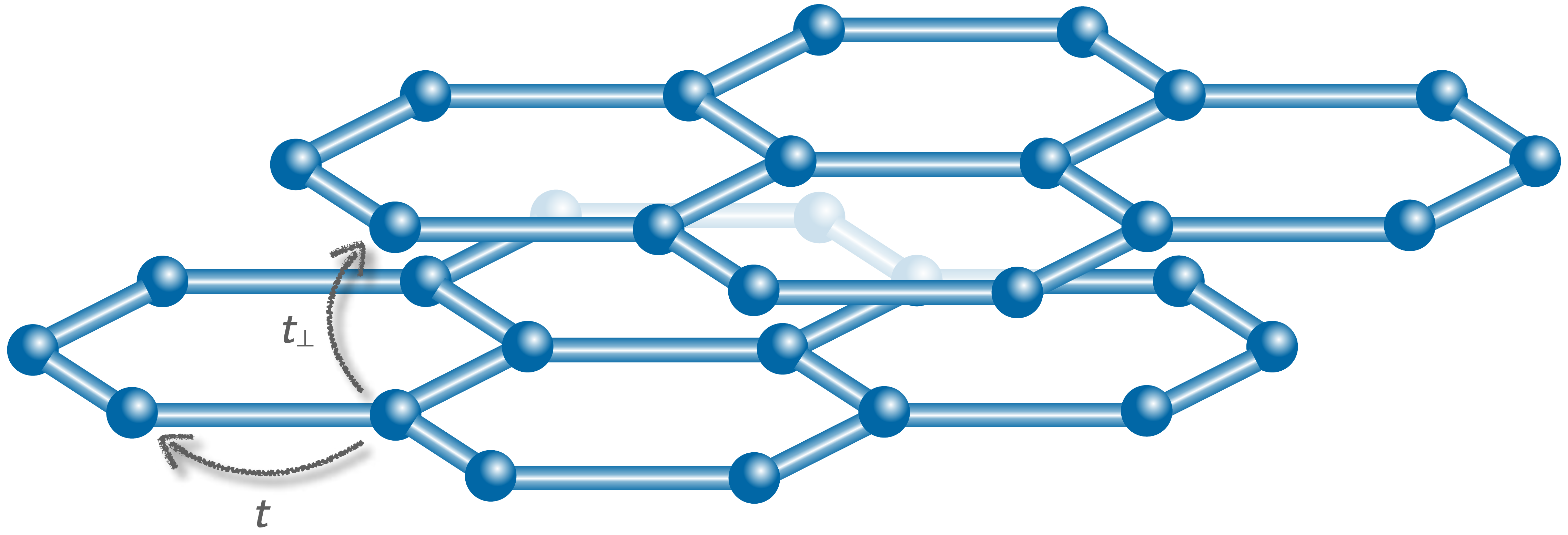
Spinless fermions on Bernal bilayer



Hamiltonian:

$$H_0 = -t \sum_{\langle ij \rangle} \sum_{\ell=1}^{2} a^\dagger_{i\ell} b_{j\ell} - t_\perp \sum_i a^\dagger_{i1} b_{i2} + \text{h.c.}$$

Spinless fermions on Bernal bilayer



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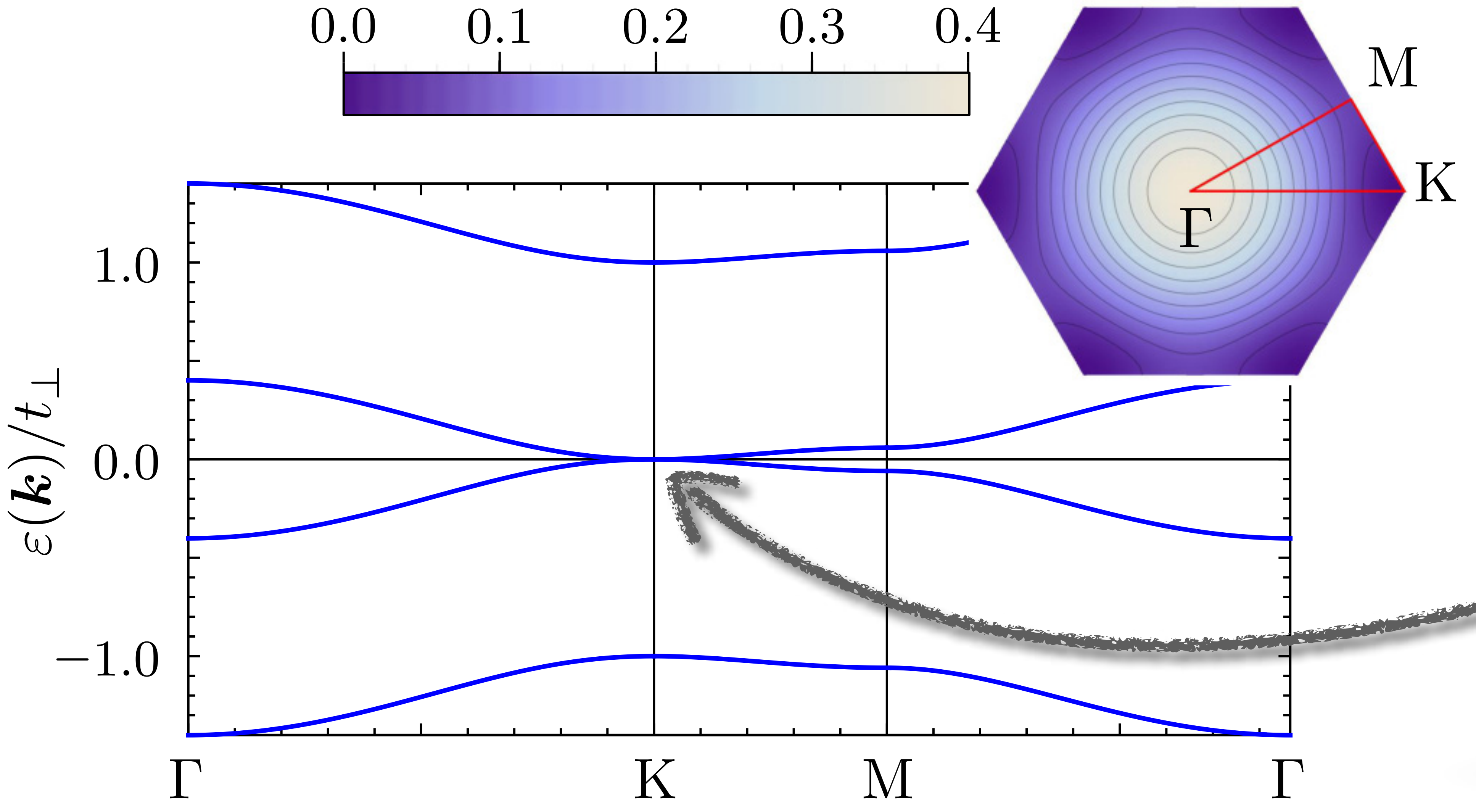
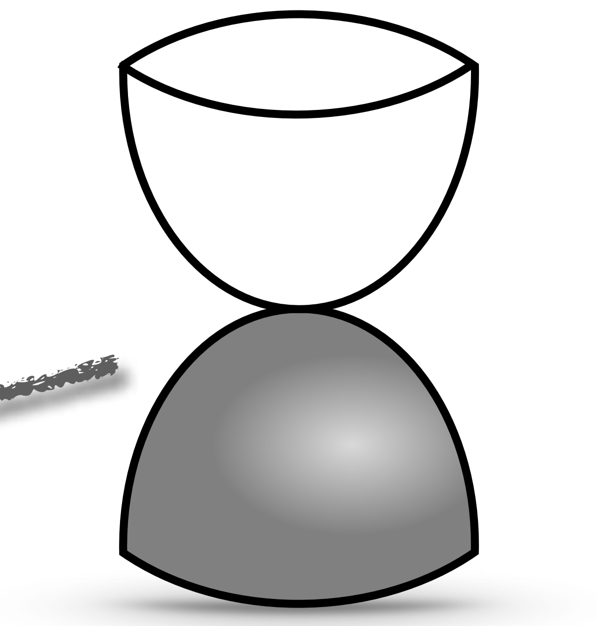
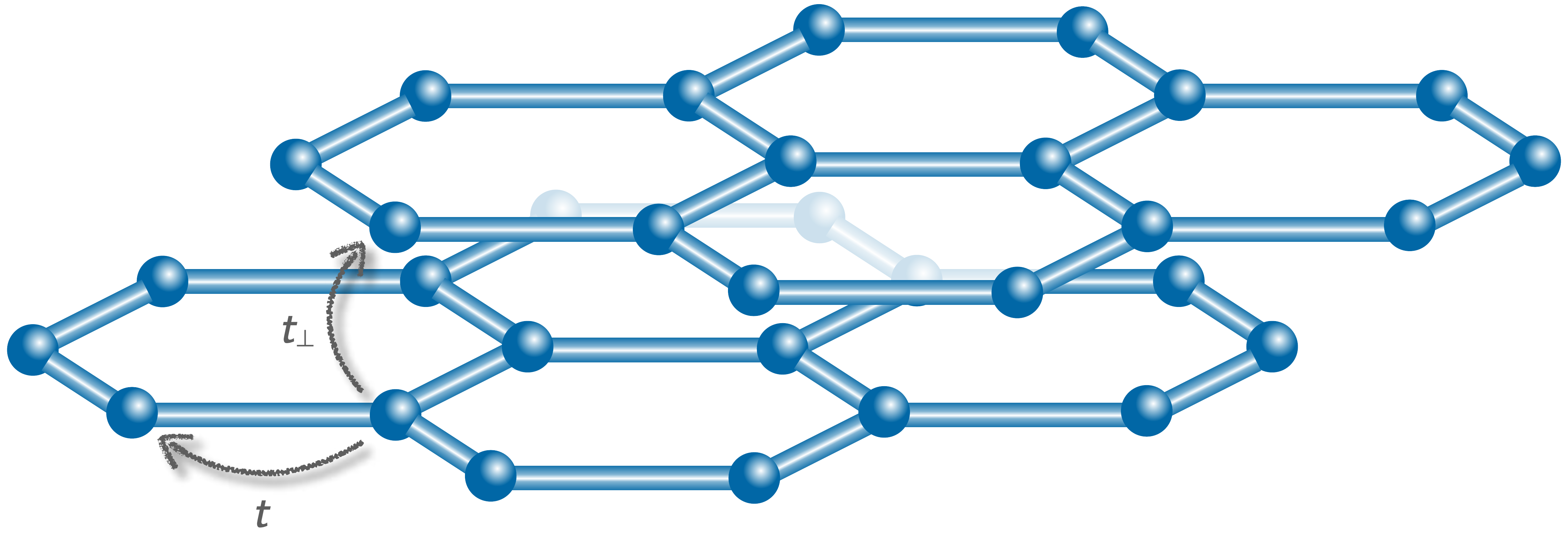
Spectrum:





Spinless fermions on Bernal bilayer



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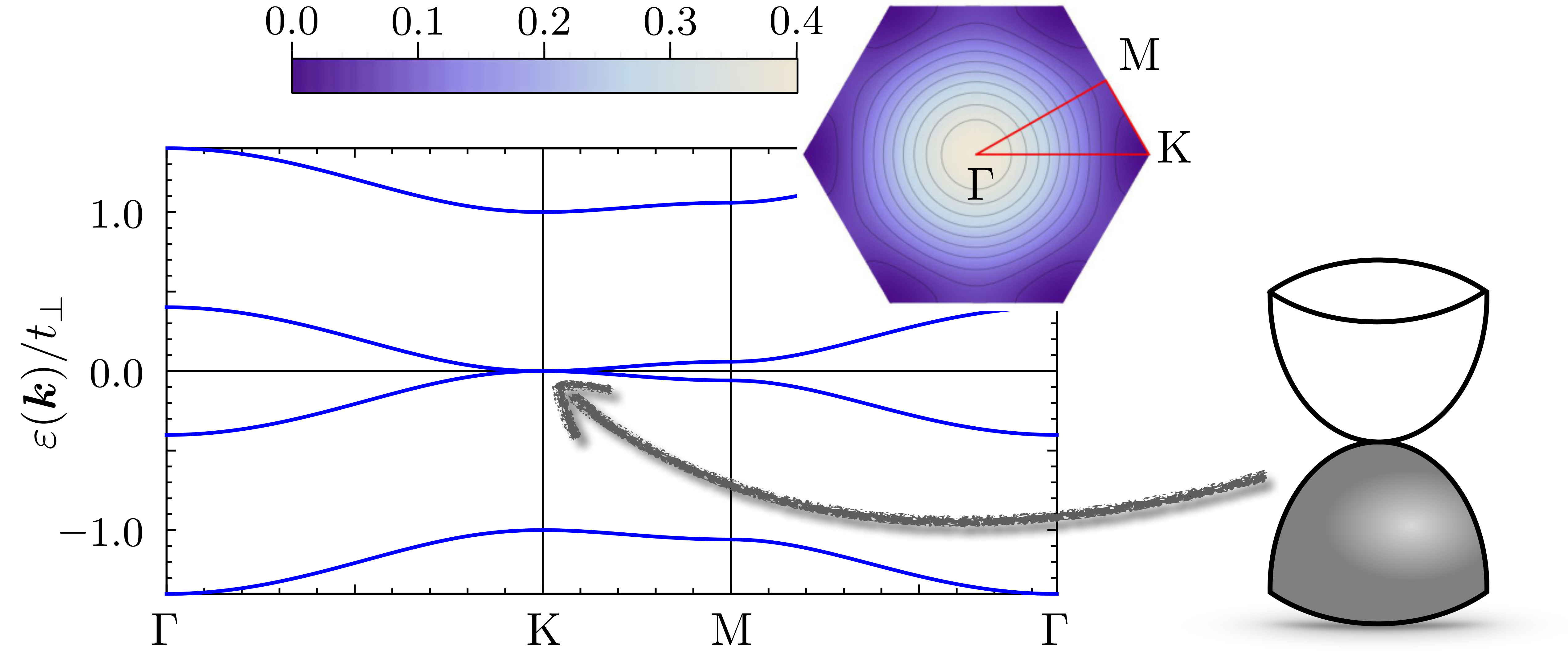

Low energy:

$$\varepsilon_{\mathbf{K}+\mathbf{q}} = \pm f_2 q^2 + f_3 q^3 \cos 3\varphi + \mathcal{O}(q^3)$$

with $f_3/a_0^3 = f_2/(2\sqrt{3}a_0^2) \simeq 6\,\text{eV}$

... significantly larger than f_1/a_0

Interactions

Coulomb repulsion:

$$H_{\text{int}} = V \sum_{\langle ij \rangle} \sum_{\ell=1}^{2} (n_{i\ell} - \tfrac{1}{2})(n_{j\ell} - \tfrac{1}{2})$$

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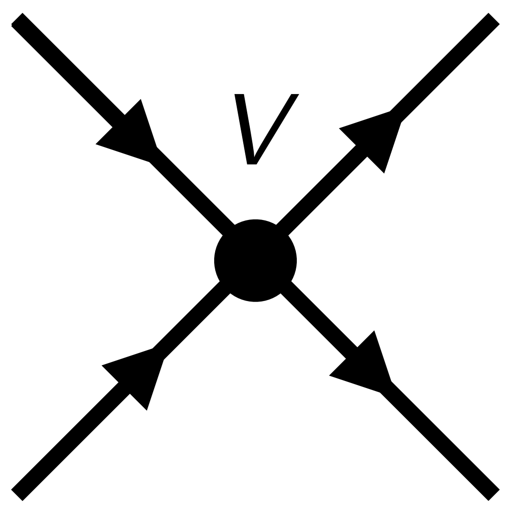
Feynman diagram:

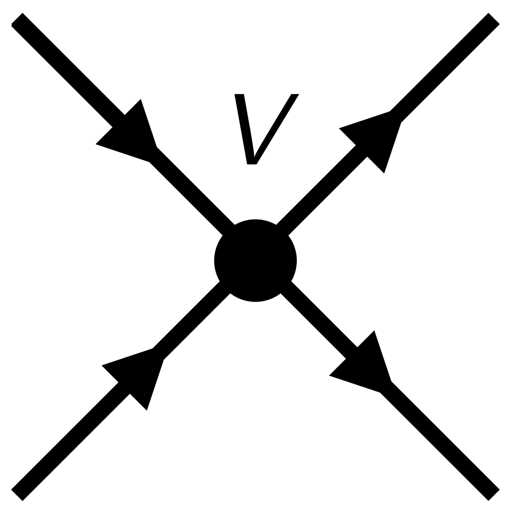


Interactions

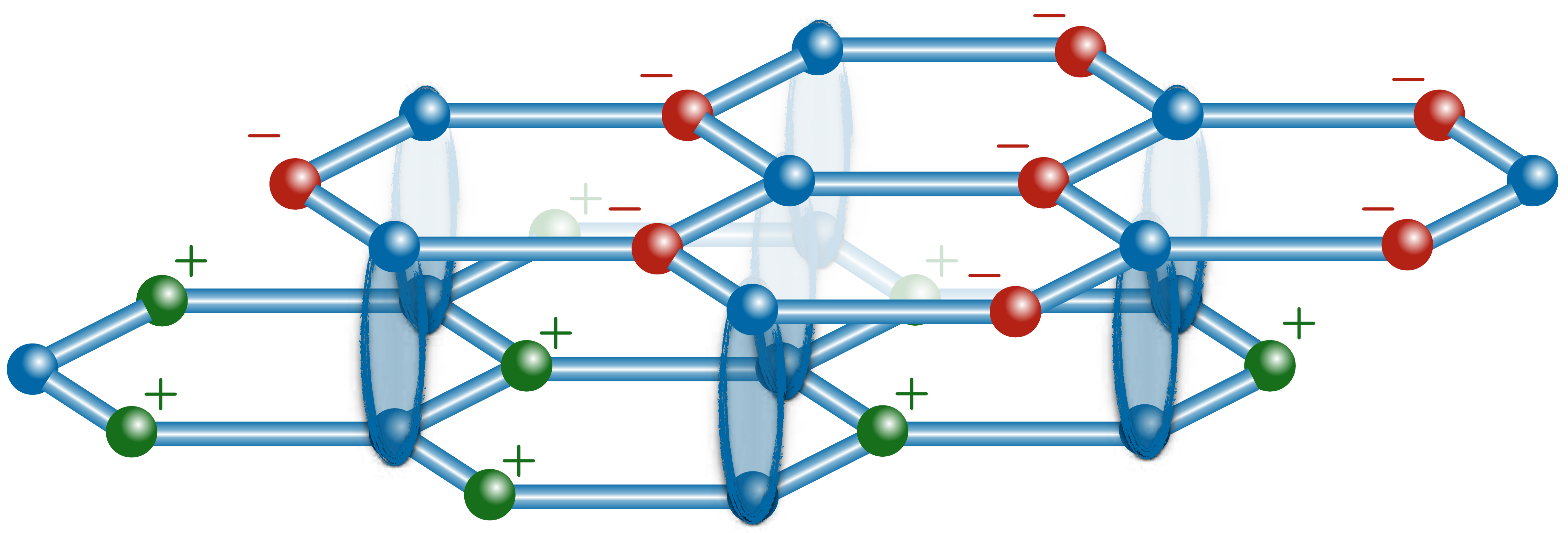
Coulomb repulsion:

$$H_{\text{int}} = V \sum_{\langle ij \rangle} \sum_{\ell=1}^{2} (n_{i\ell} - \tfrac{1}{2})(n_{j\ell} - \tfrac{1}{2})$$

Feynman diagram:



Strong-coupling limit:



Charge-layer polarization

Interactions

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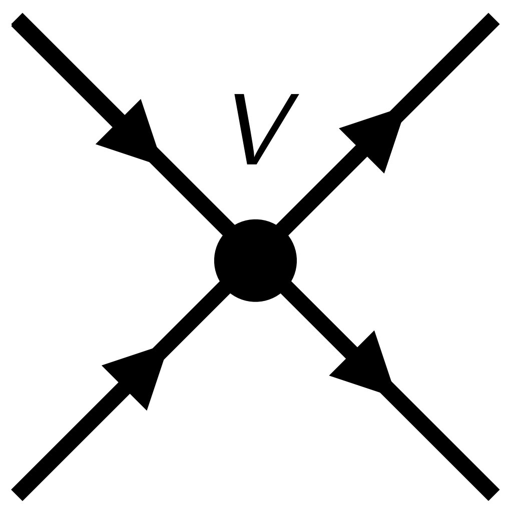

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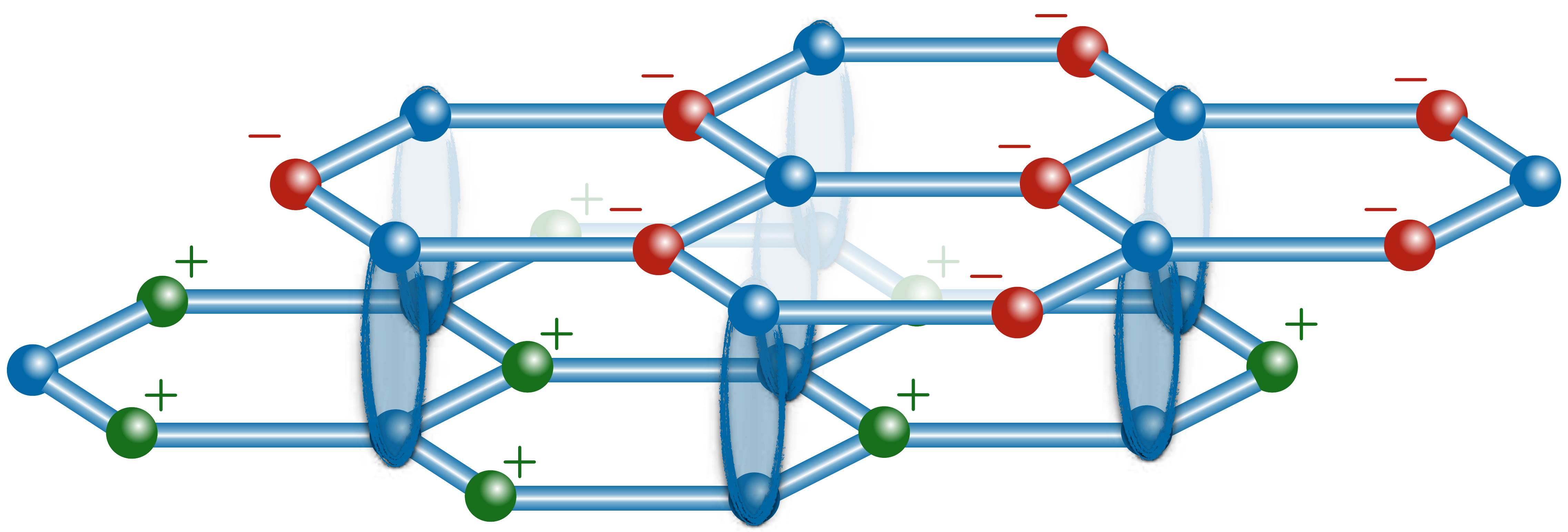
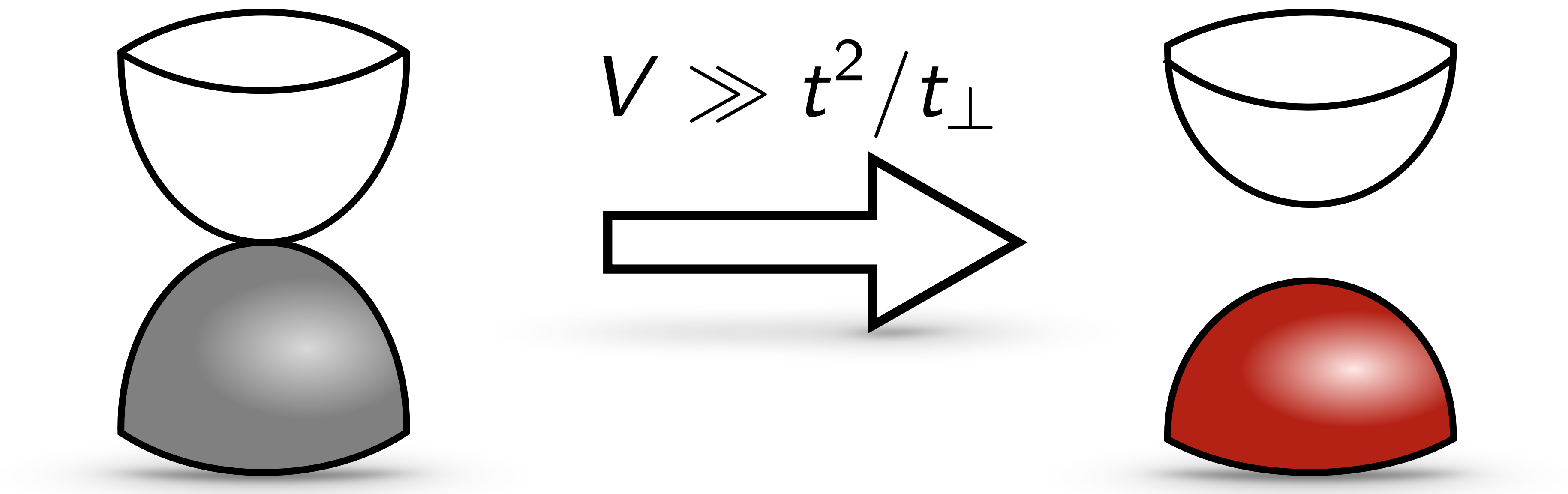


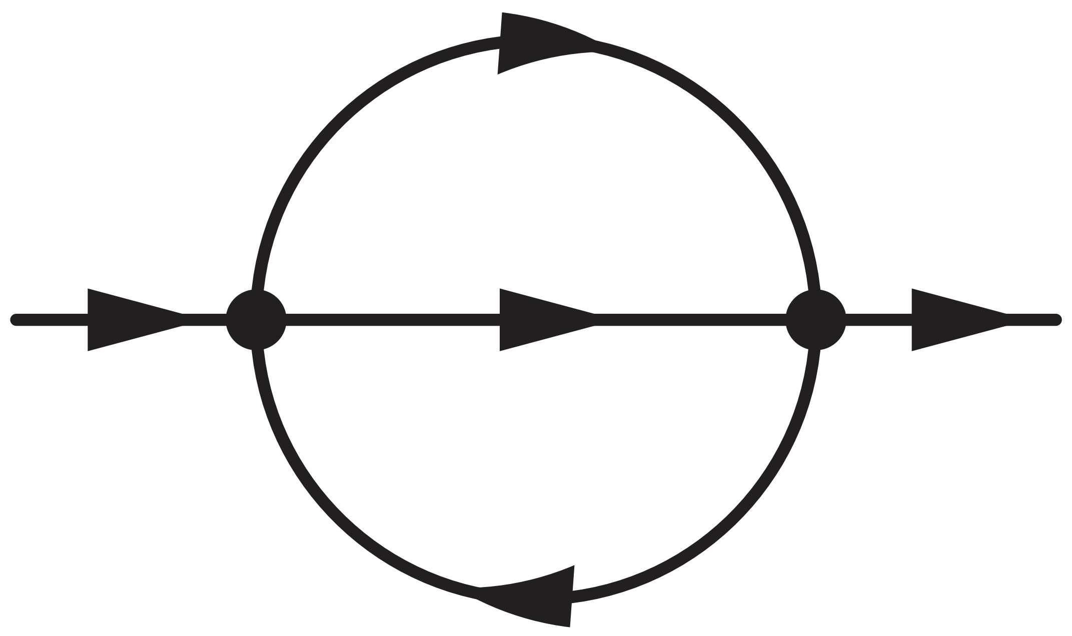
Charge-layer polarization



Full gap opening

Intermediate coupling

Self-energy corrections:



... technical obstacles: two-loop, nonrelativistic & anisotropic propagator

... trick: real-space evaluation [Groote *et al.*, NPB '99]

[Ray, Vojta, LJ, PRB '18]

Intermediate coupling

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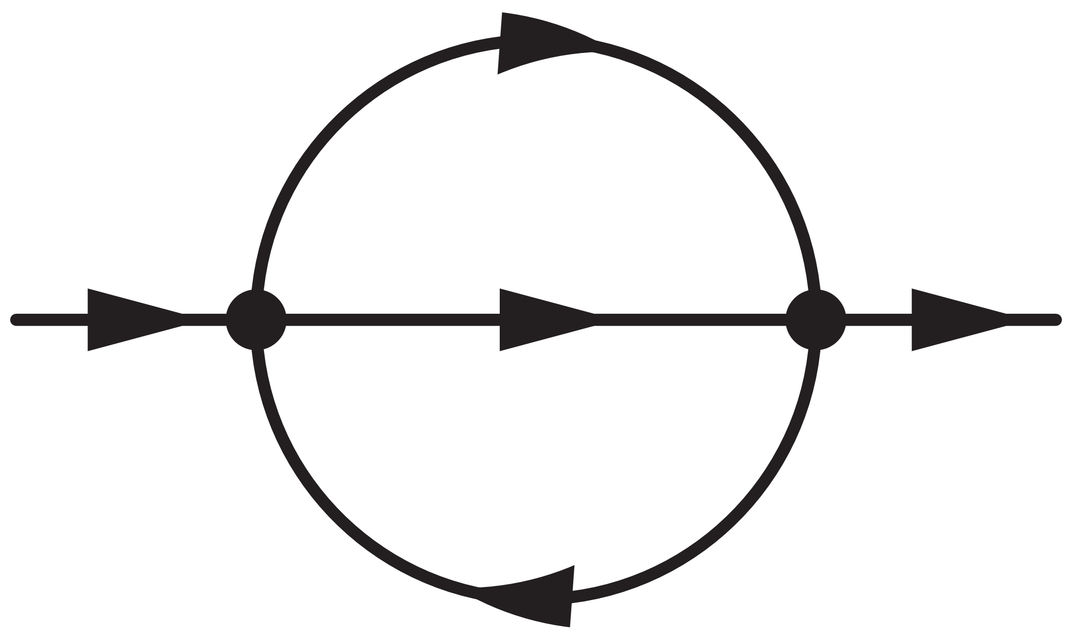

$\propto (f_3/f_2)V^2\mathcal{O}(q)$ linear in q !

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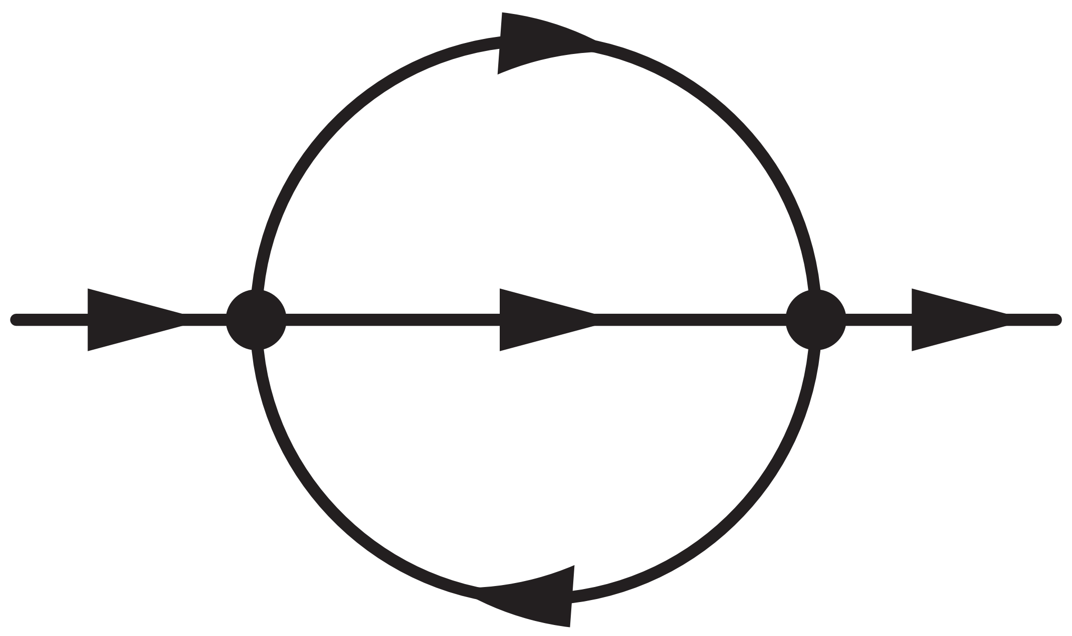

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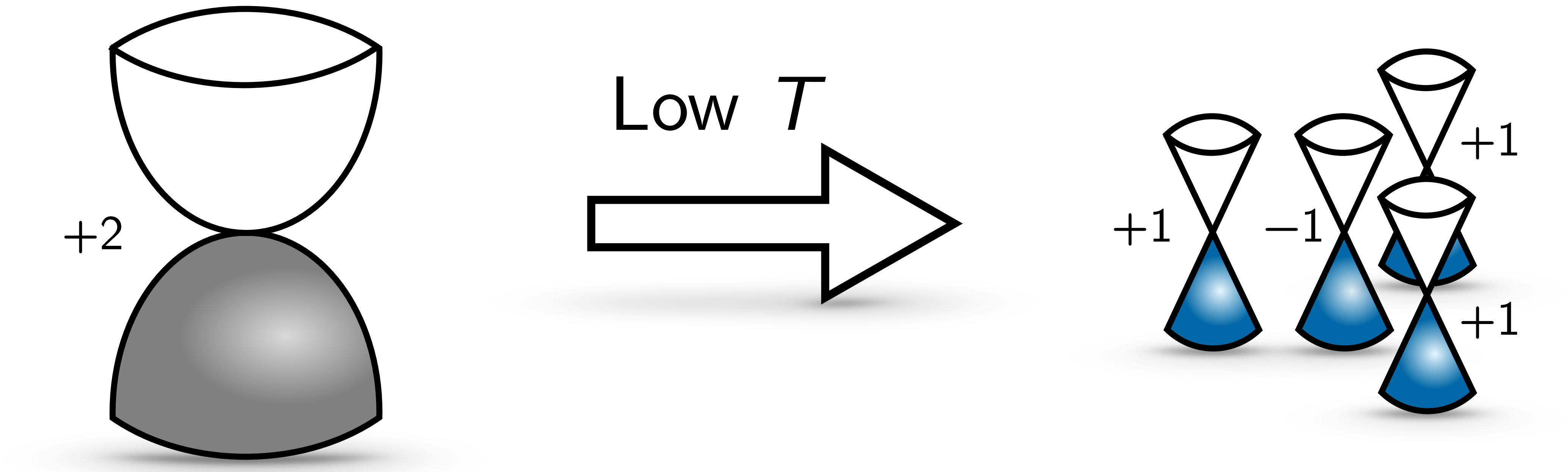
Effective spectrum:



[Ray, Vojta, LJ, PRB '18]

Intermediate coupling

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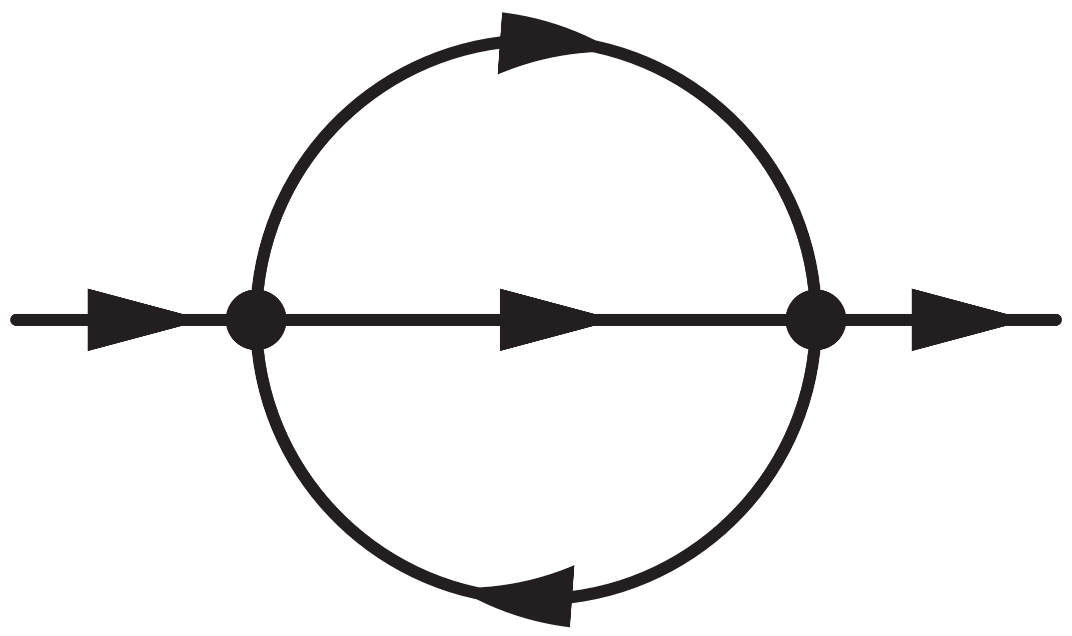

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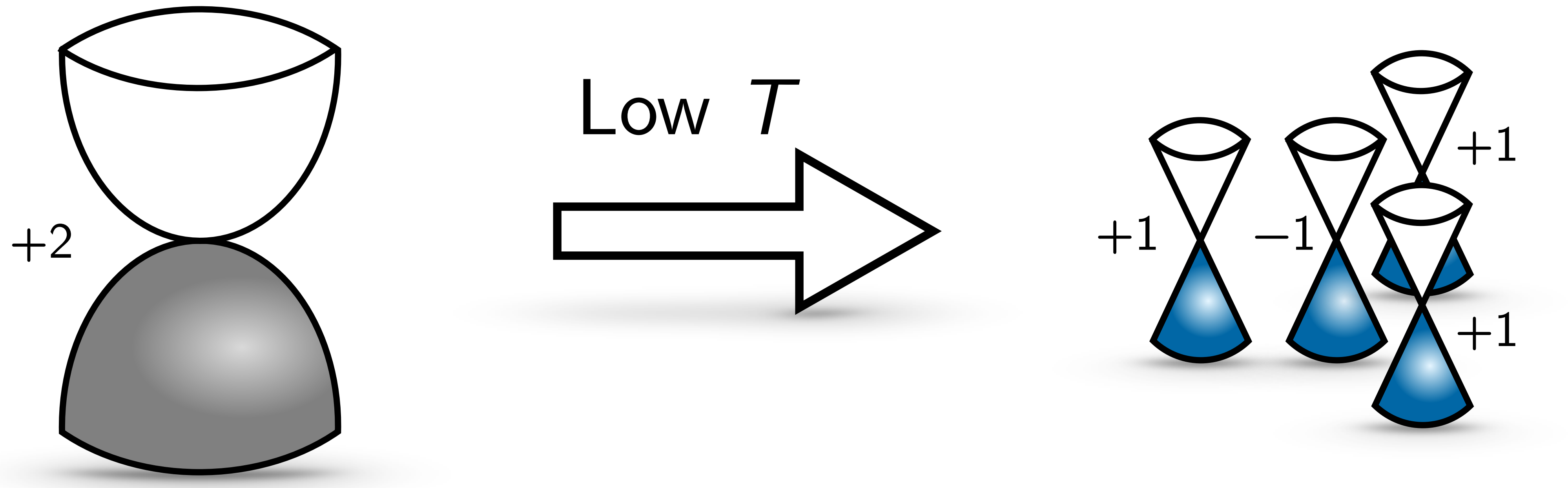
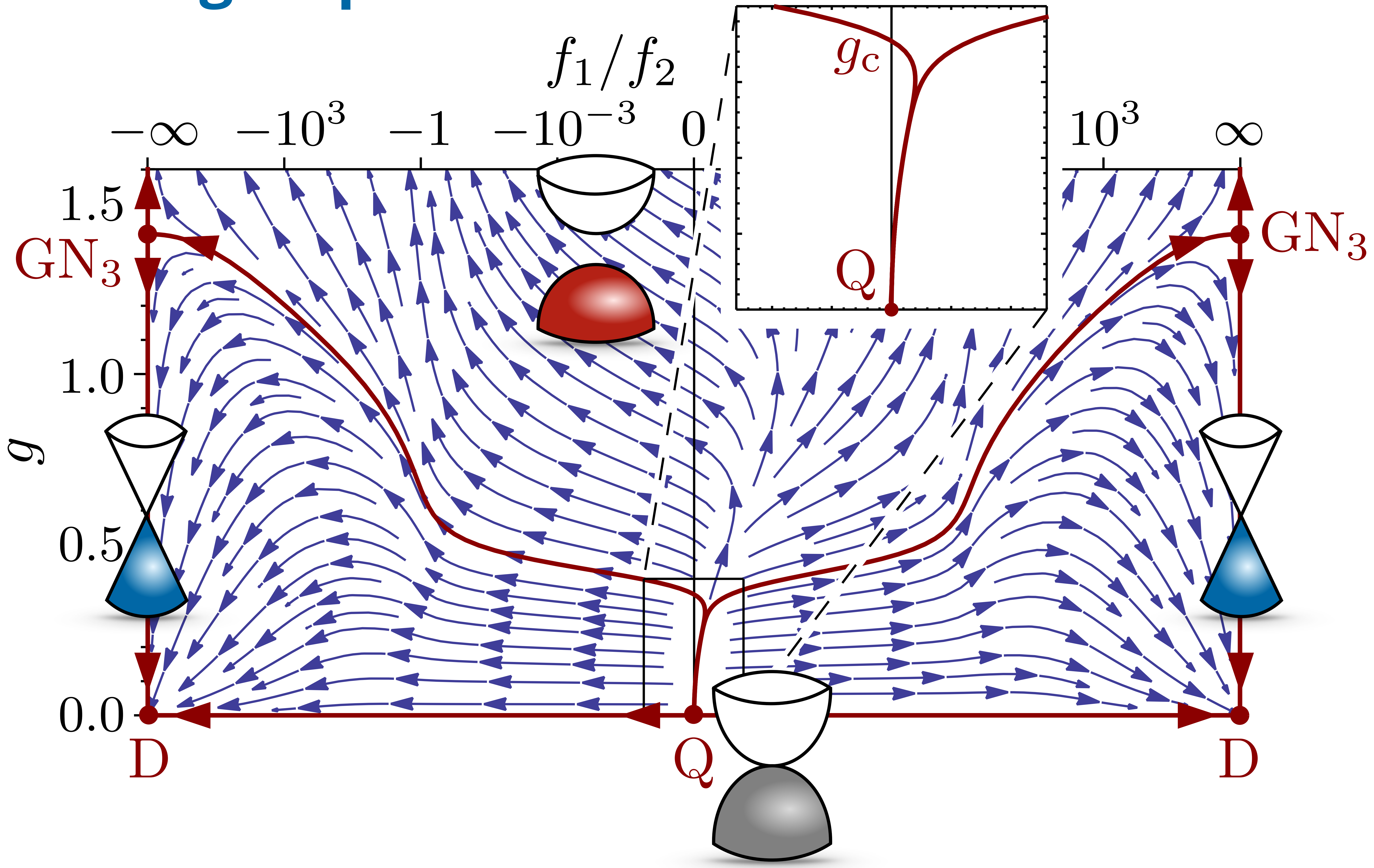


$$f_1^{\mathrm{eff}}/a_0 \sim V^2/(t^2/t_\perp) \sim \mathcal{O}(1\,\mathrm{eV}) \gg t_\mathrm{w}$$

[Ray, Vojta, LJ, PRB '18]

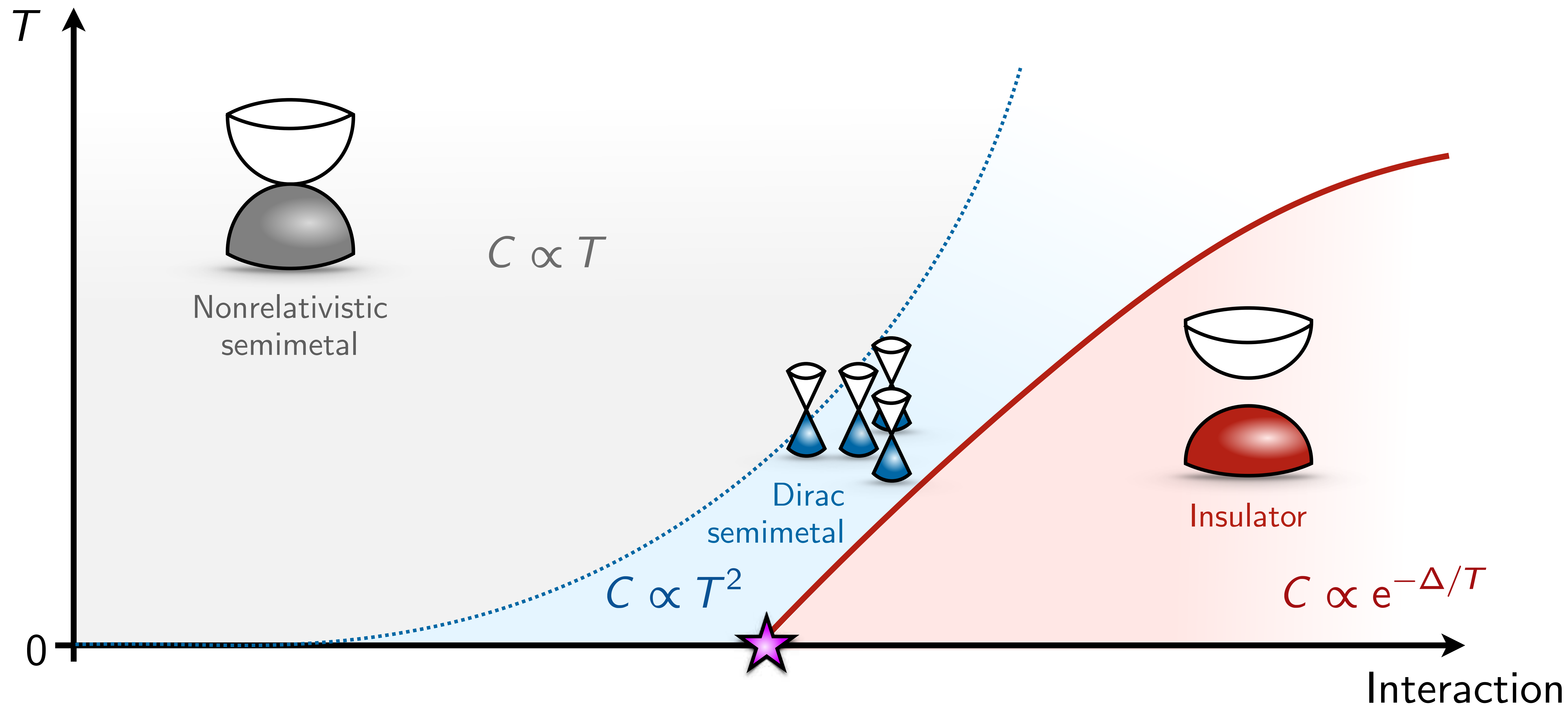
Renormalization group flow



Effective Hamiltonian: $H_0 \propto f_1^{\mathrm{eff}} \mathcal{O}(q) + f_2 \mathcal{O}(q^2) + f_3 \mathcal{O}(q^3)$

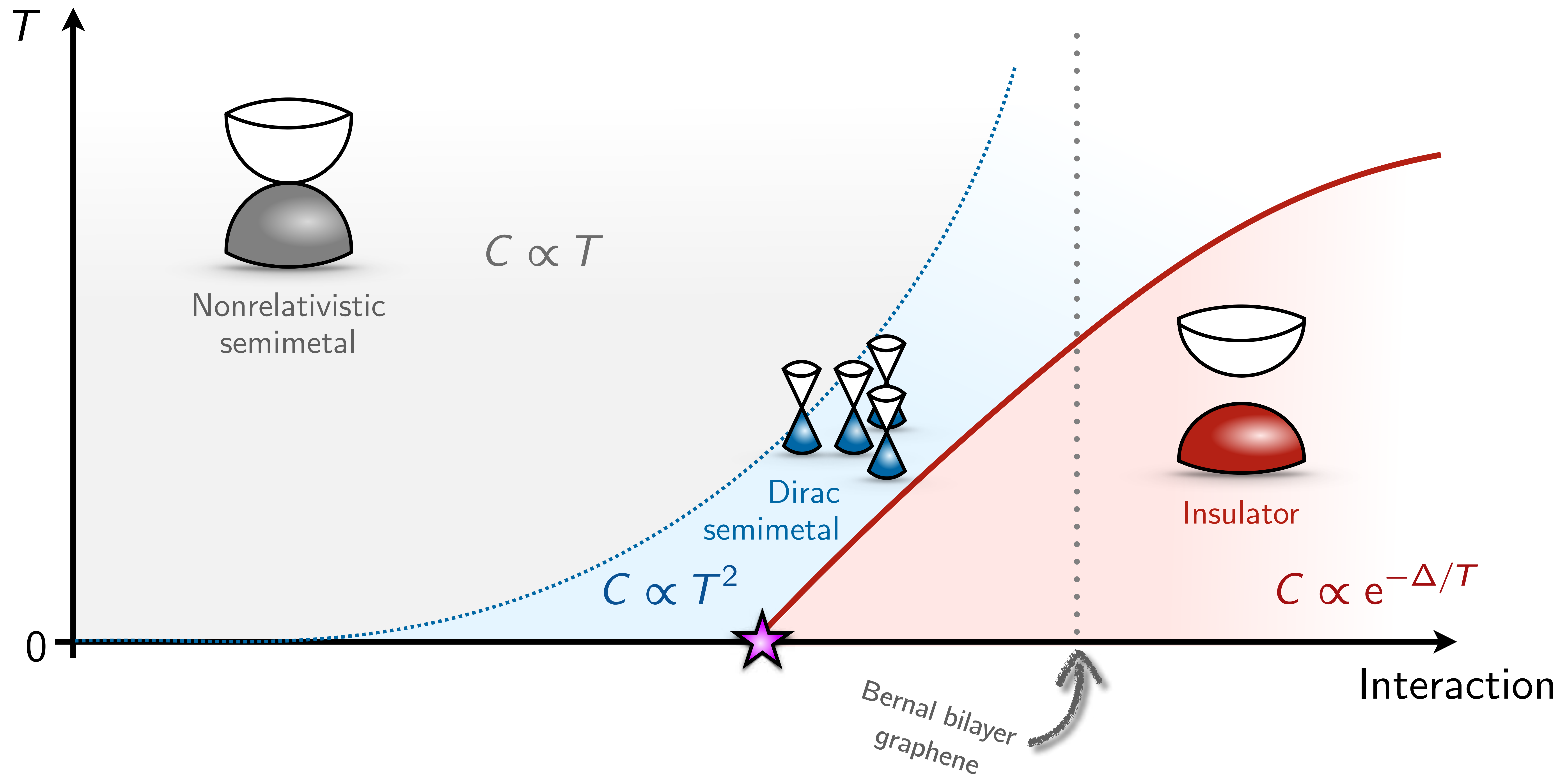
[Ray, Vojta, LJ, PRB '18]

Phase diagram



[Ray, Vojta, LJ, PRB '18]

Phase diagram

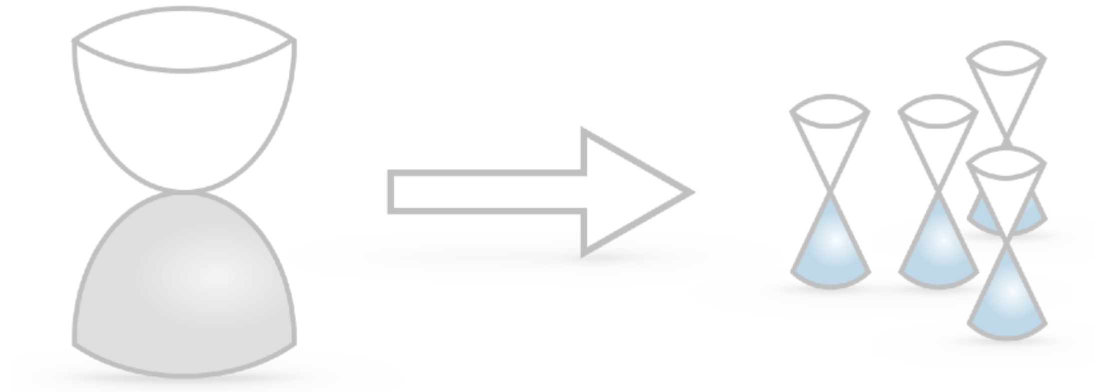


[Ray, Vojta, LJ, PRB '18]

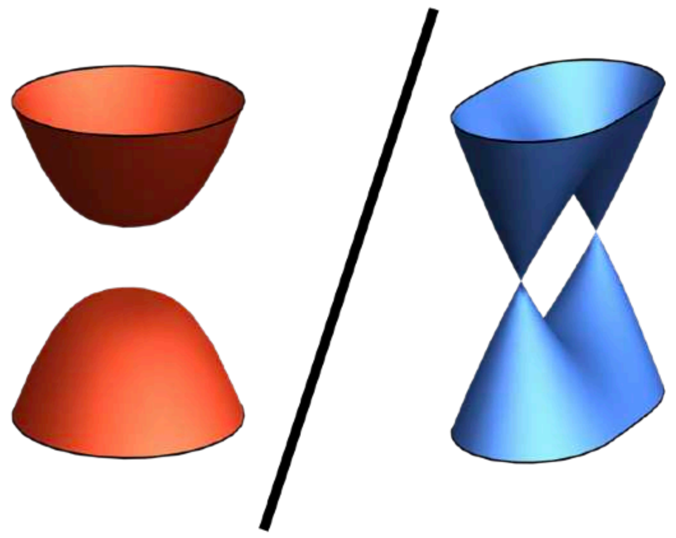
Outline

(1) Introduction

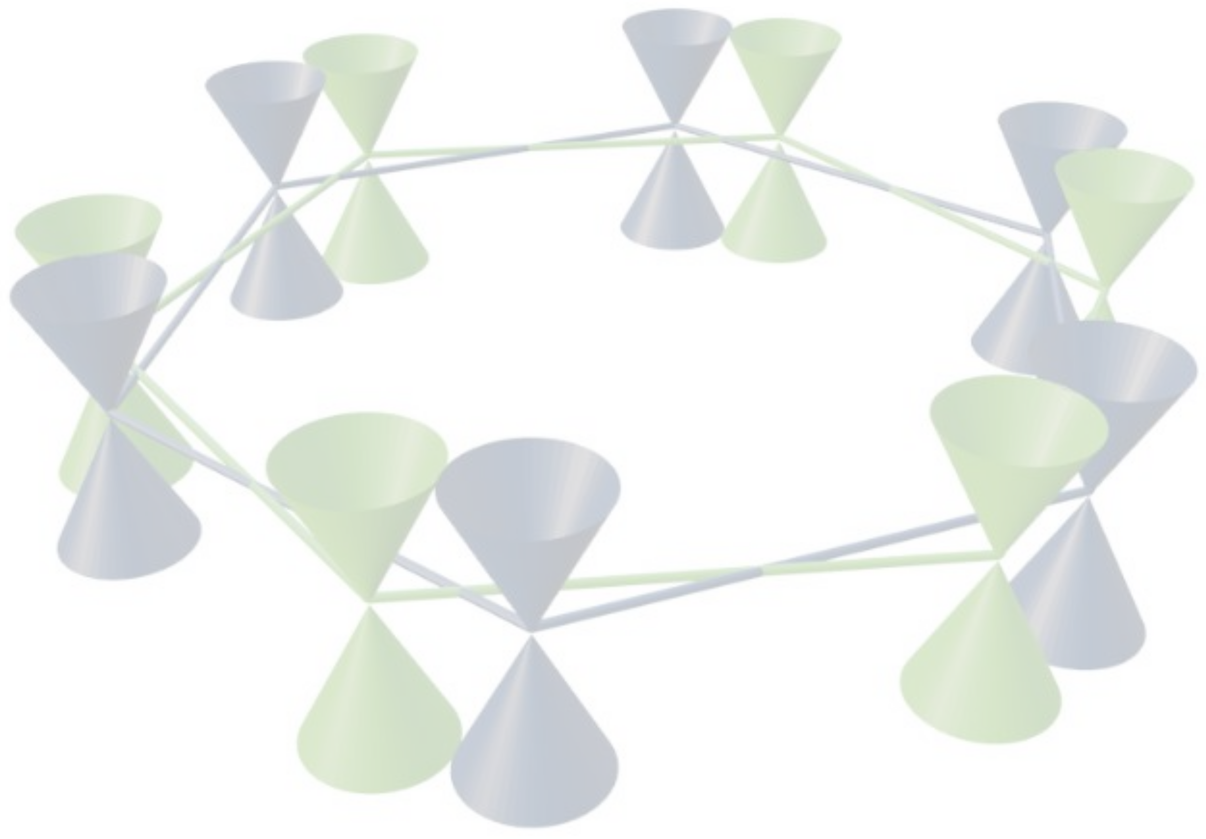
(2) Interaction-induced Dirac cones



(3) **Competing nematic & antiferromagnetic orders**



(4) Twist-tuned quantum criticality



(5) Conclusions

Spin-1/2 fermions on Bernal bilayer

Toy Hamiltonian:

$$H_{\text{int}} = U \sum_i \sum_{\ell=1}^{2} (n_{i\ell\uparrow} - \tfrac{1}{2})(n_{i\ell\downarrow} - \tfrac{1}{2}) + V \sum_{\langle ij \rangle} \sum_{\ell=1}^{2} (n_{i\ell} - \tfrac{1}{2})(n_{j\ell} - \tfrac{1}{2}) + \ldots$$

... with parameters chosen to stabilize antiferromagnetic and/or nematic orders

[Ray, LJ, PRB '21]

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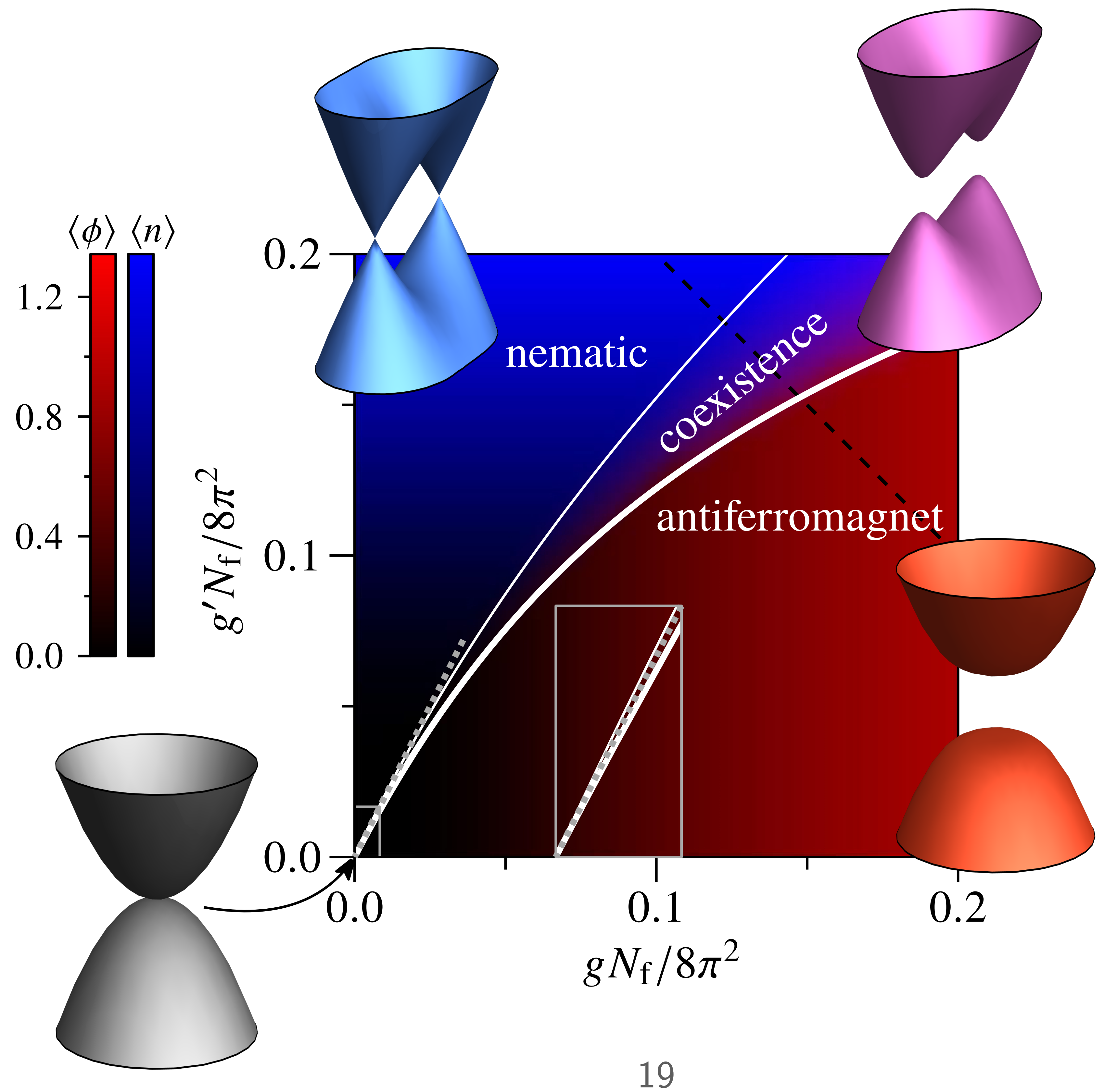
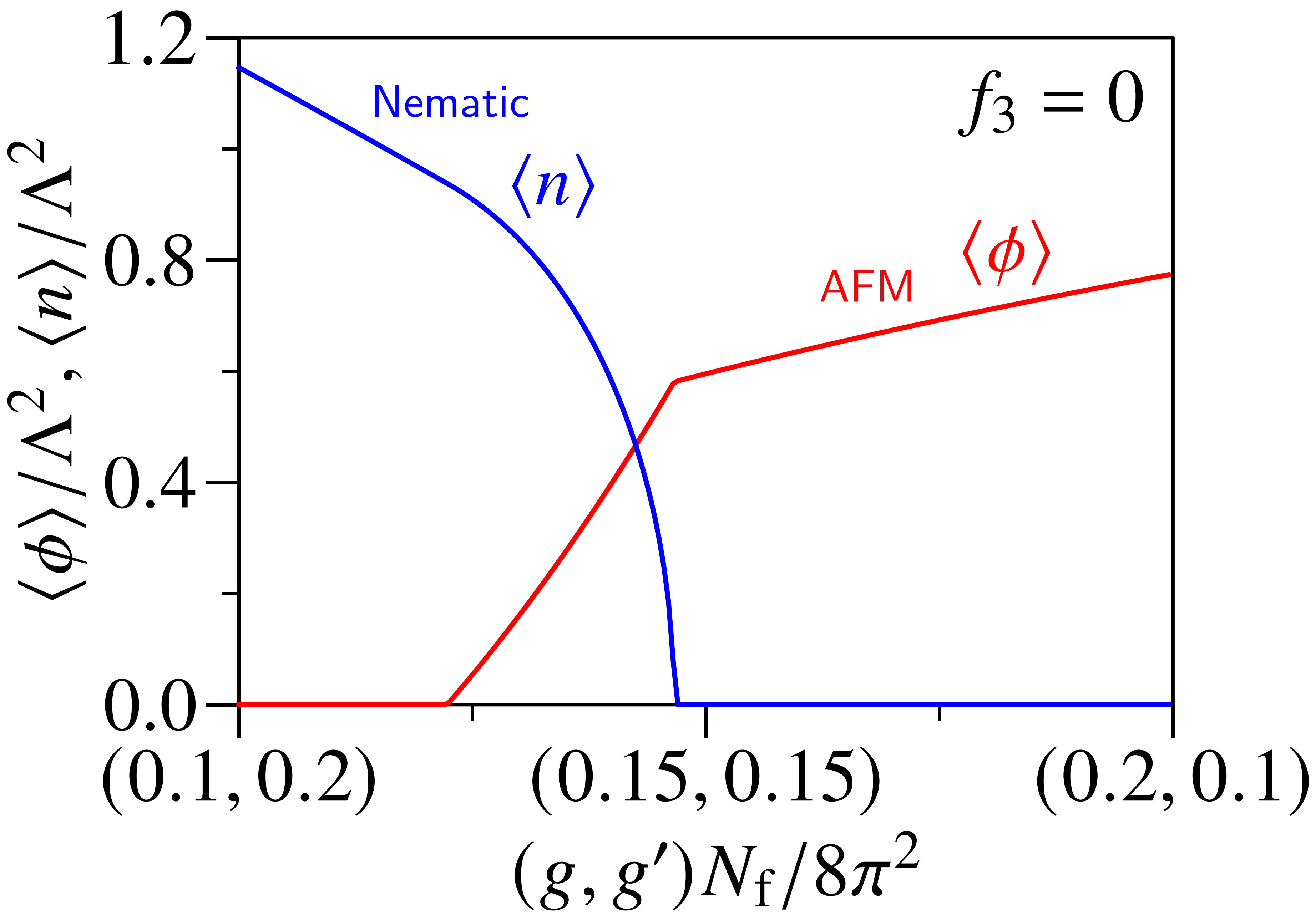
Mean-field phase diagram:



[Ray, LJ, PRB '21]

Quantum phase transitions

Order parameters:



[Ray, LJ, PRB '21]

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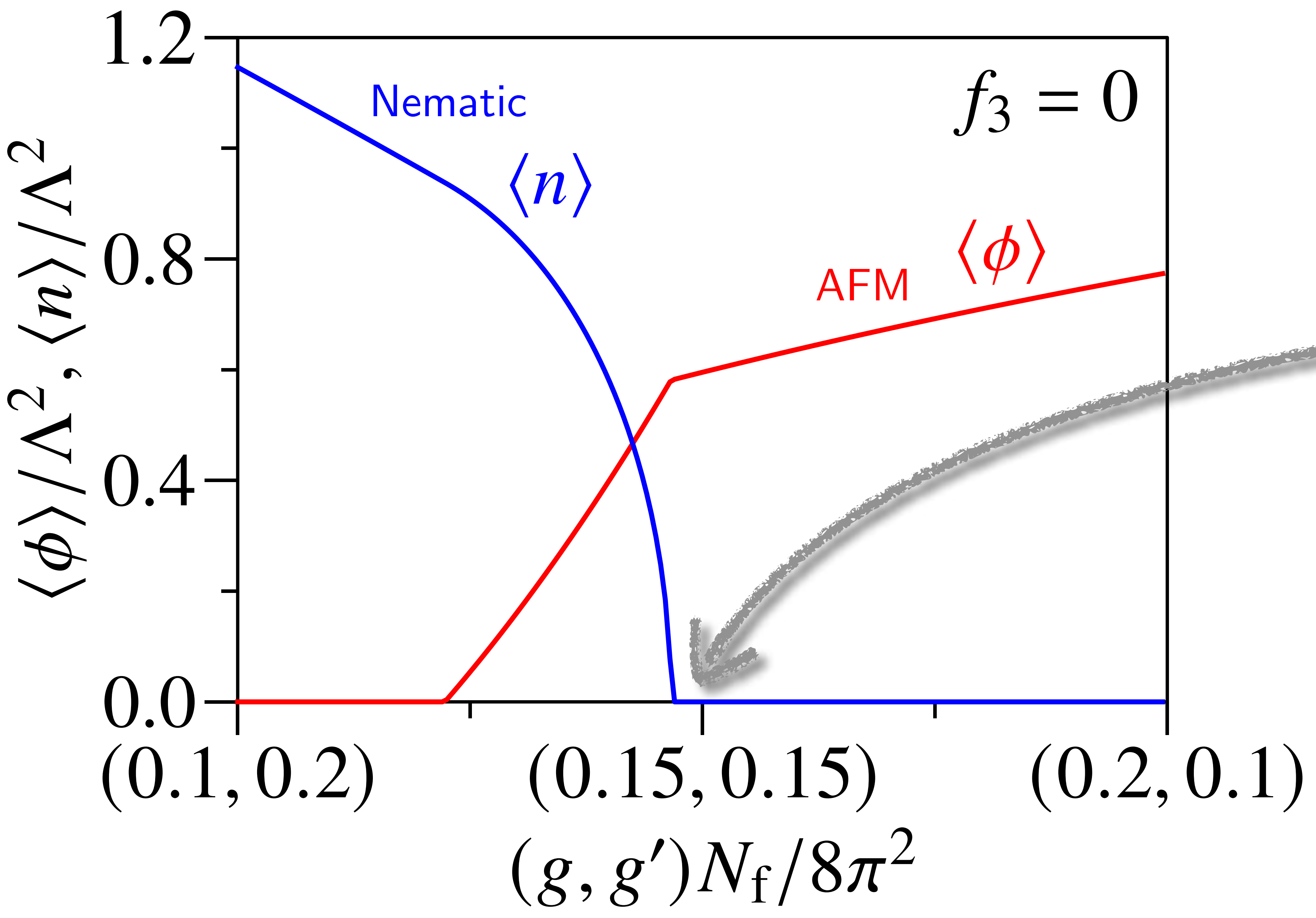
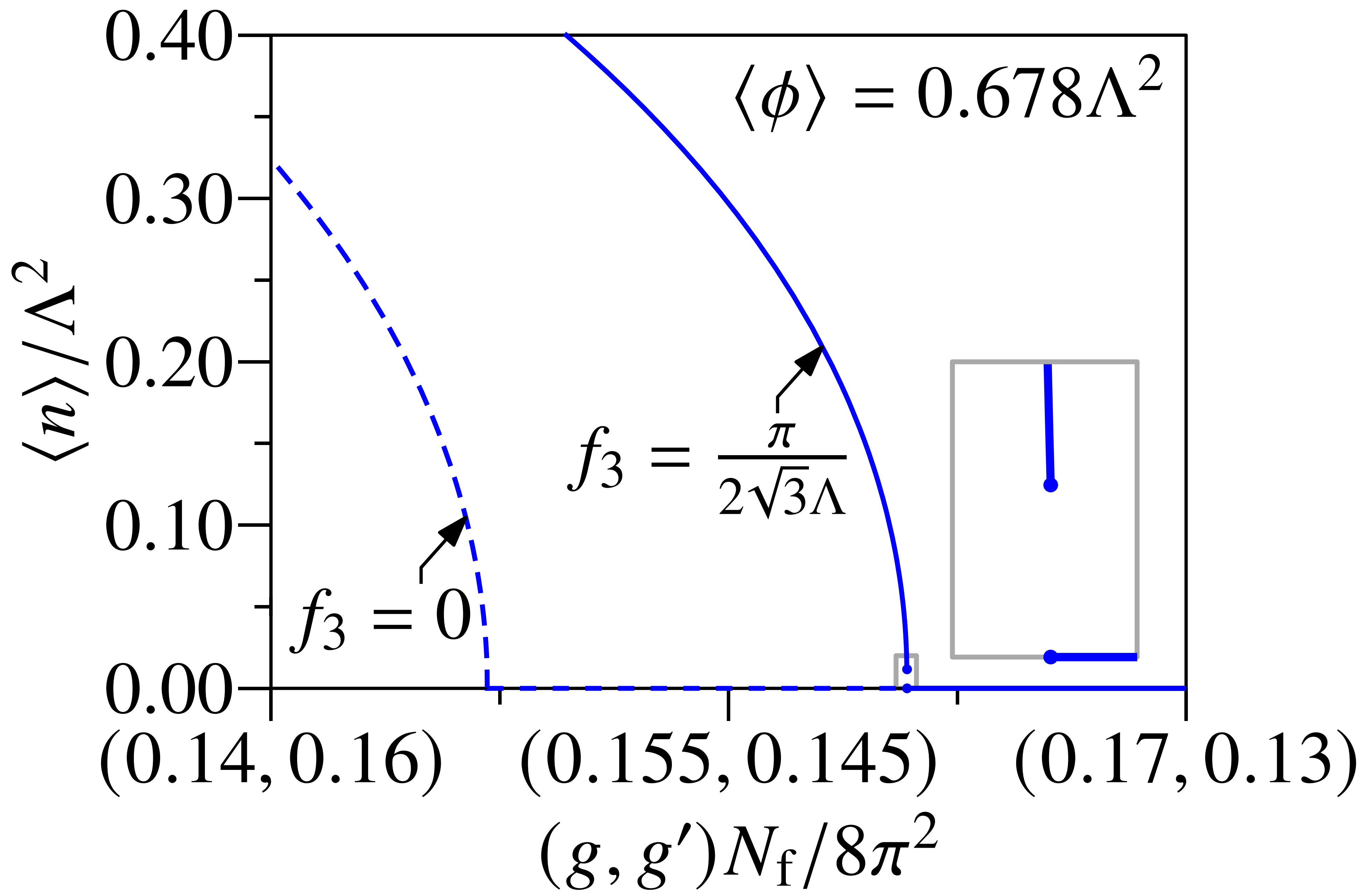


Coexistence-to-AFM transition:



[Ray, LJ, PRB '21]

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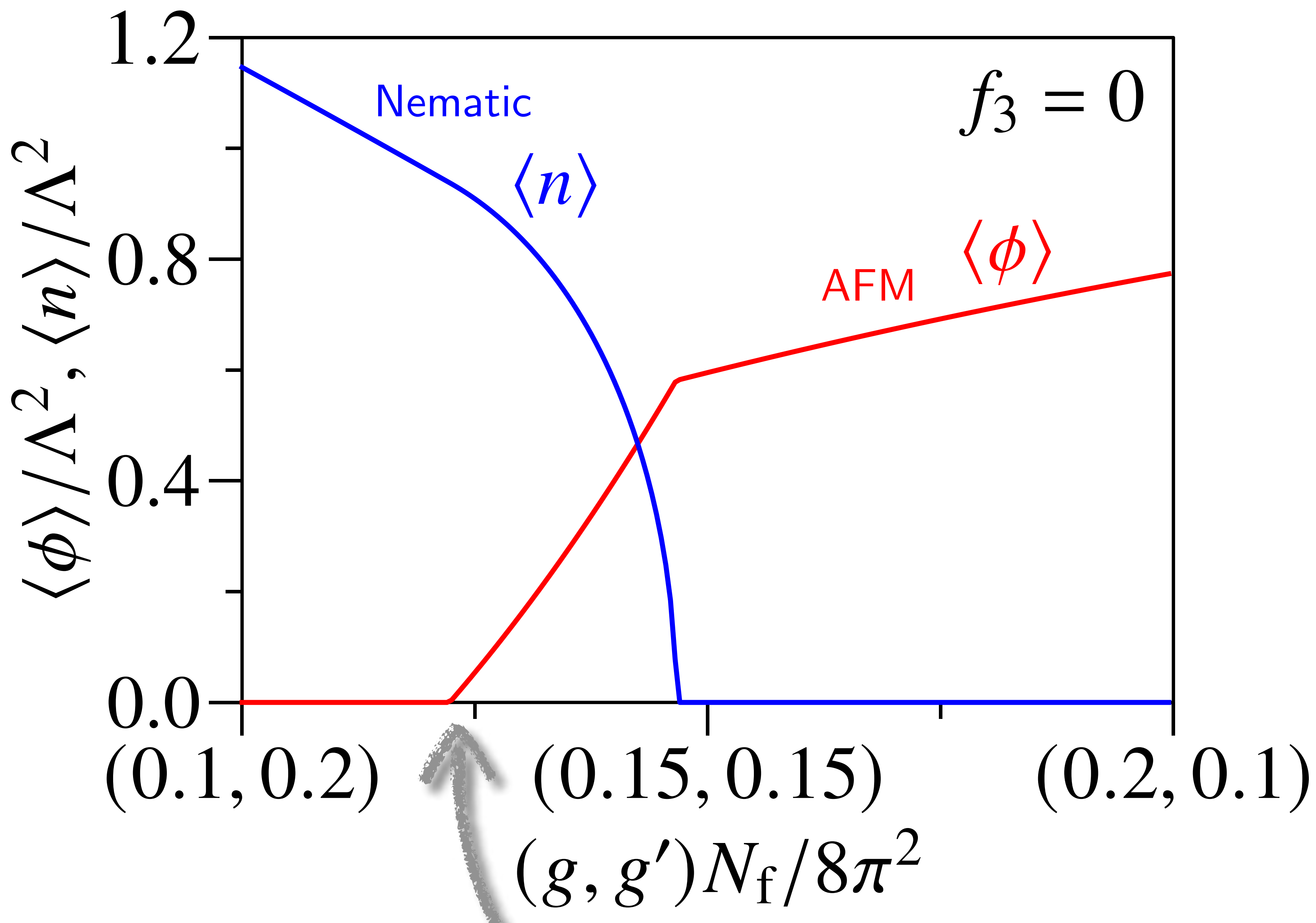
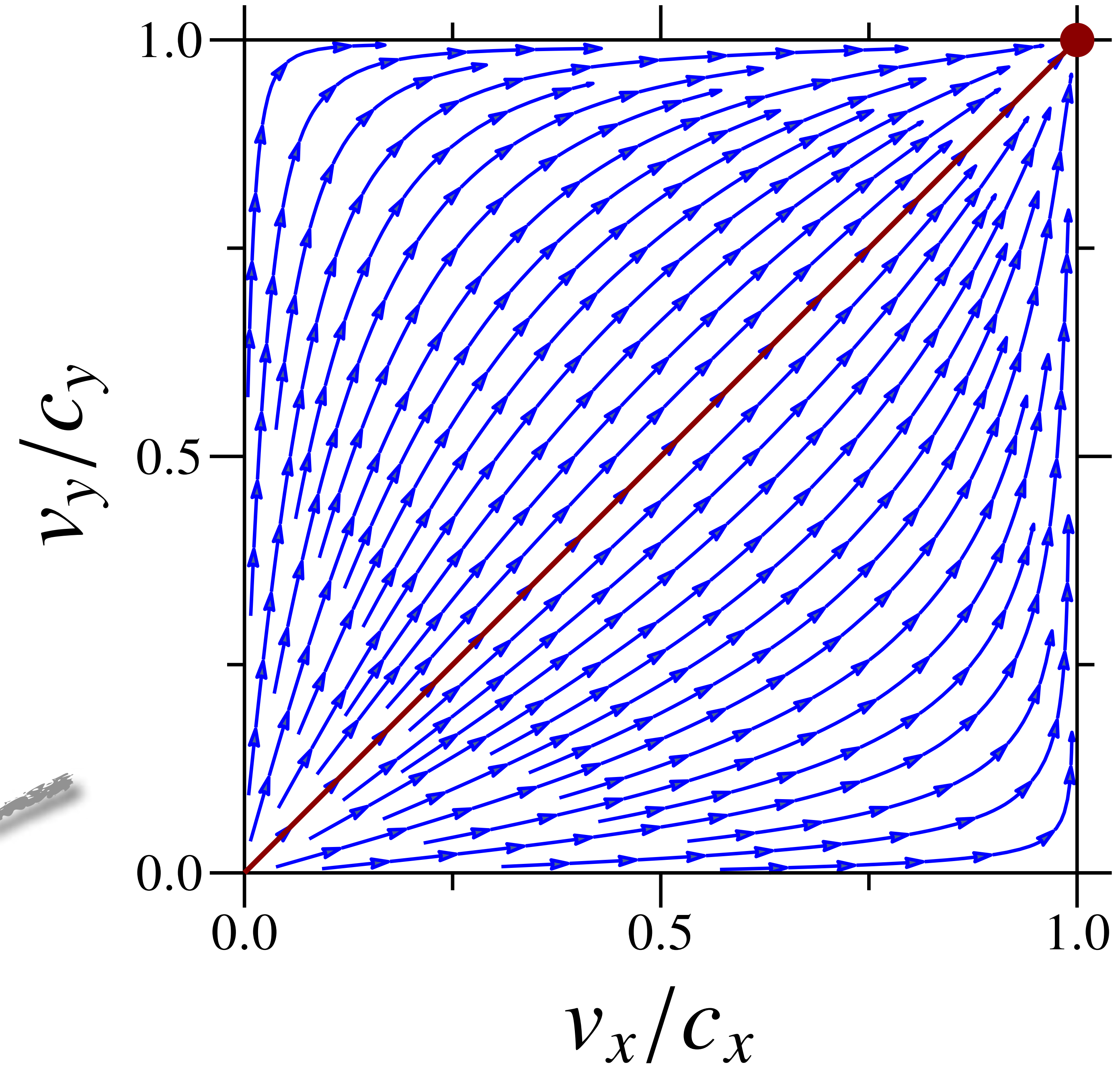


Nematic-to-coexistence transition:



[Ray, LJ, PRB '21]

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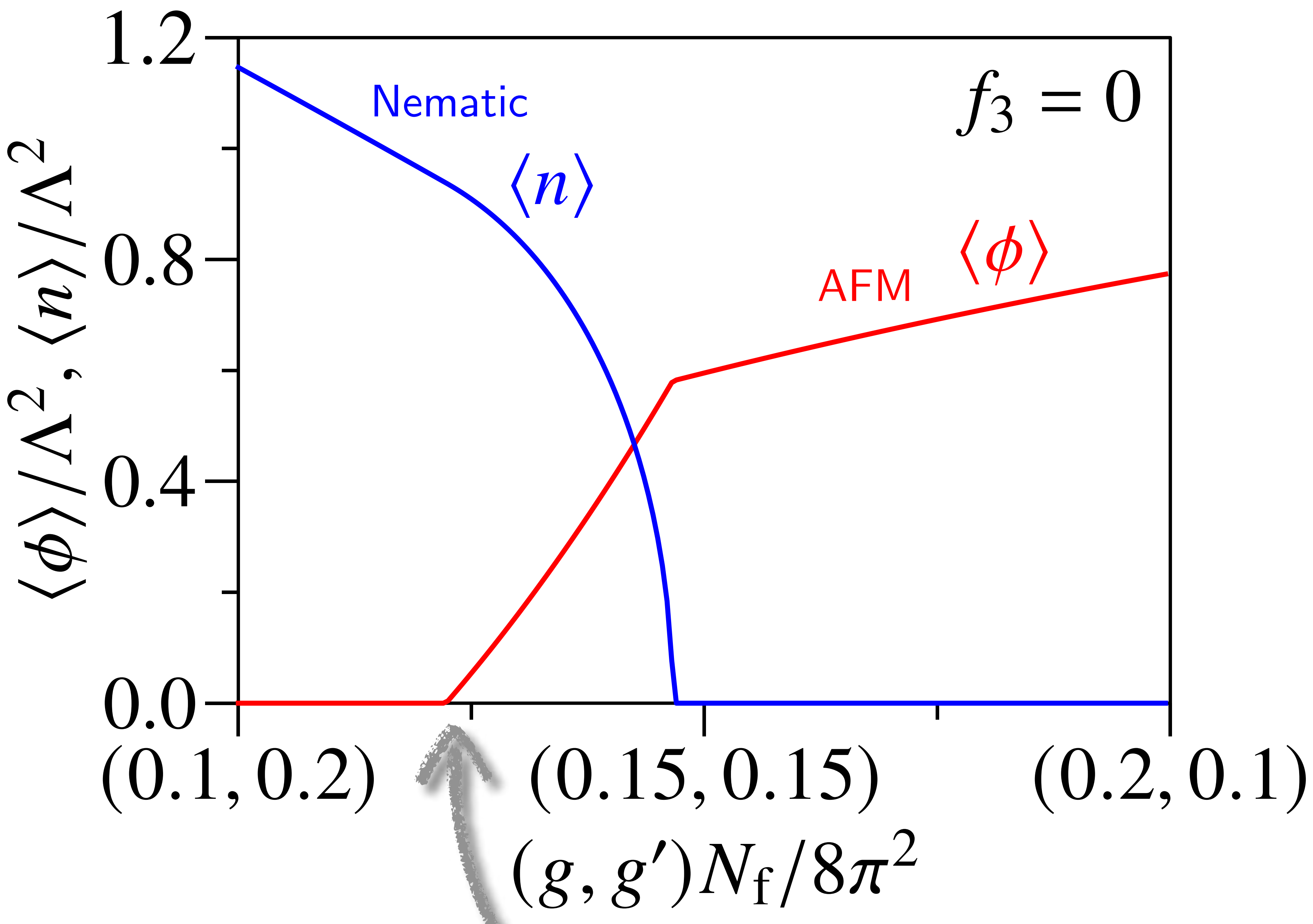

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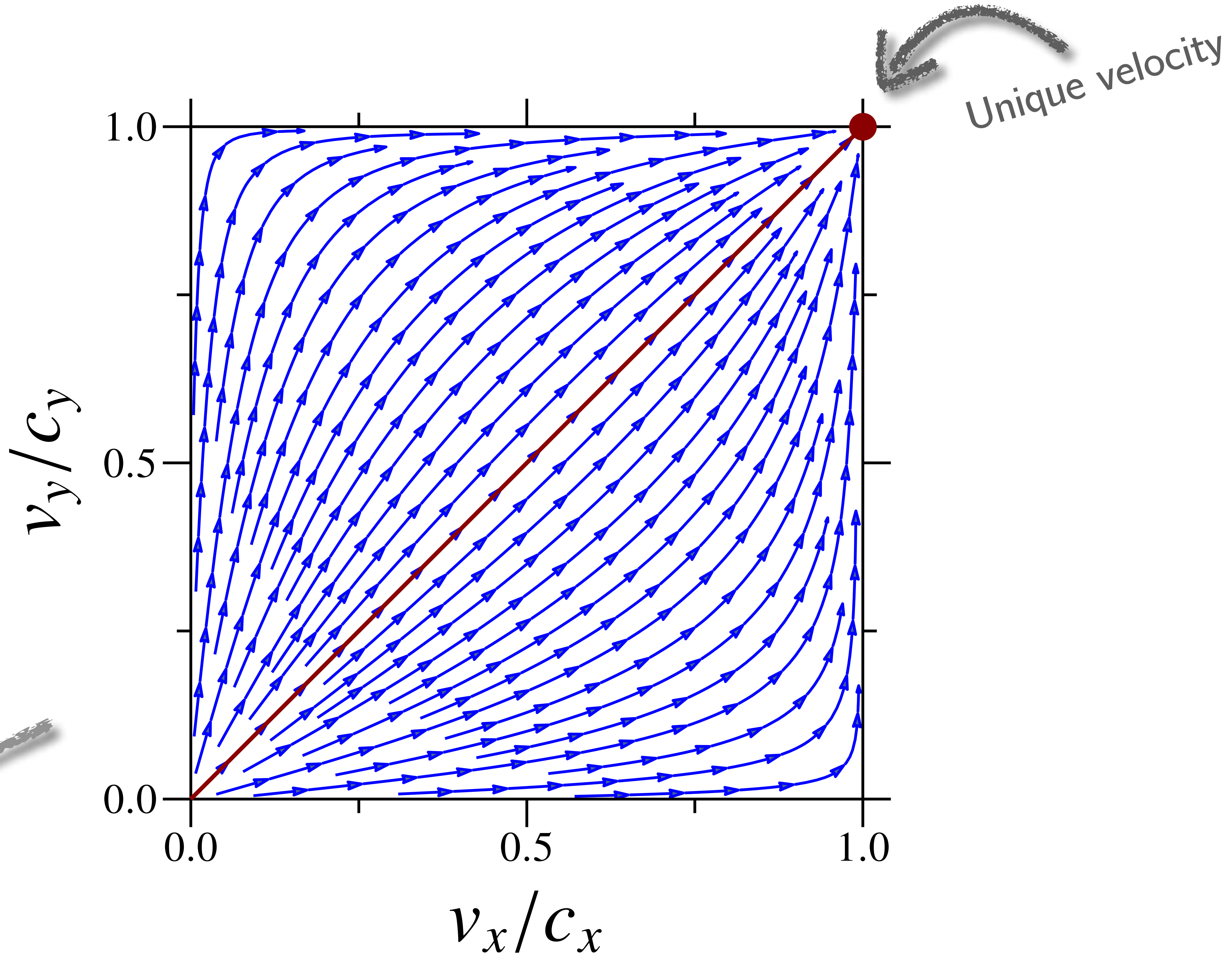

Emergent Lorentz symmetry!

[Ray, LJ, PRB '21]

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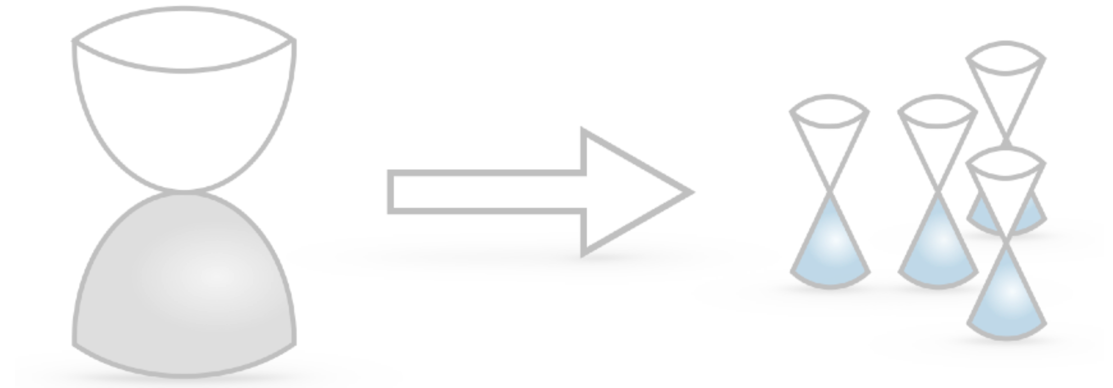

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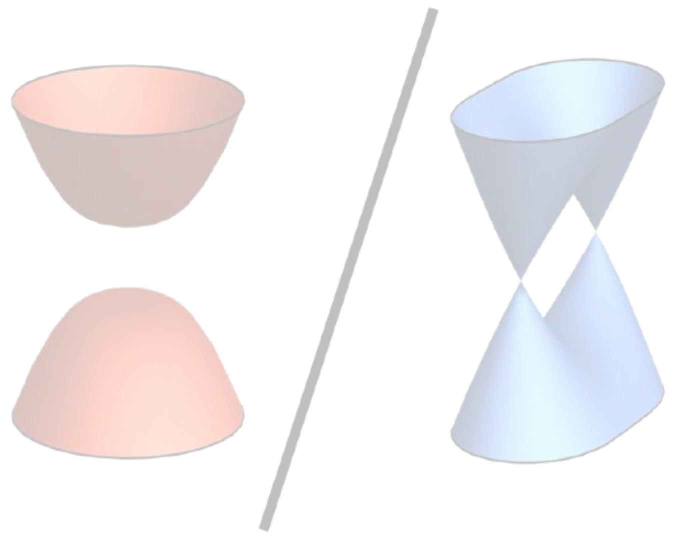

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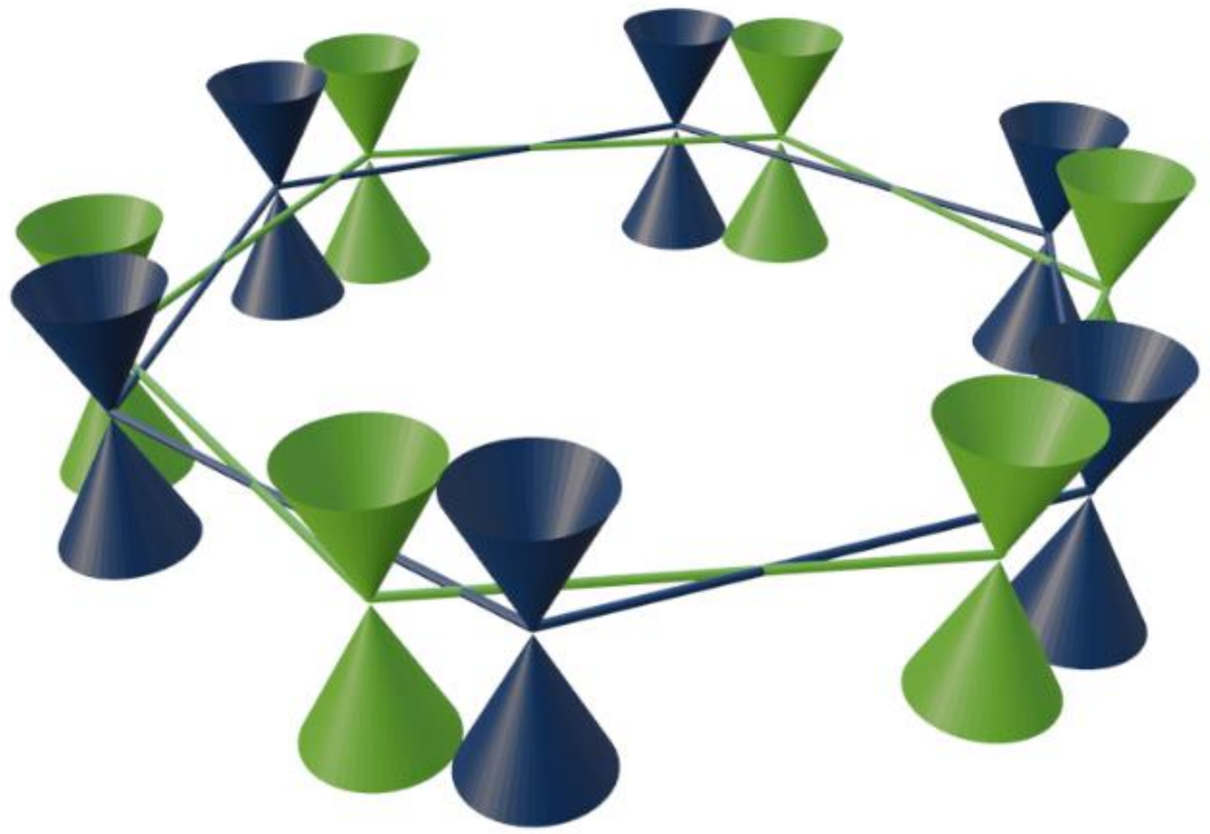
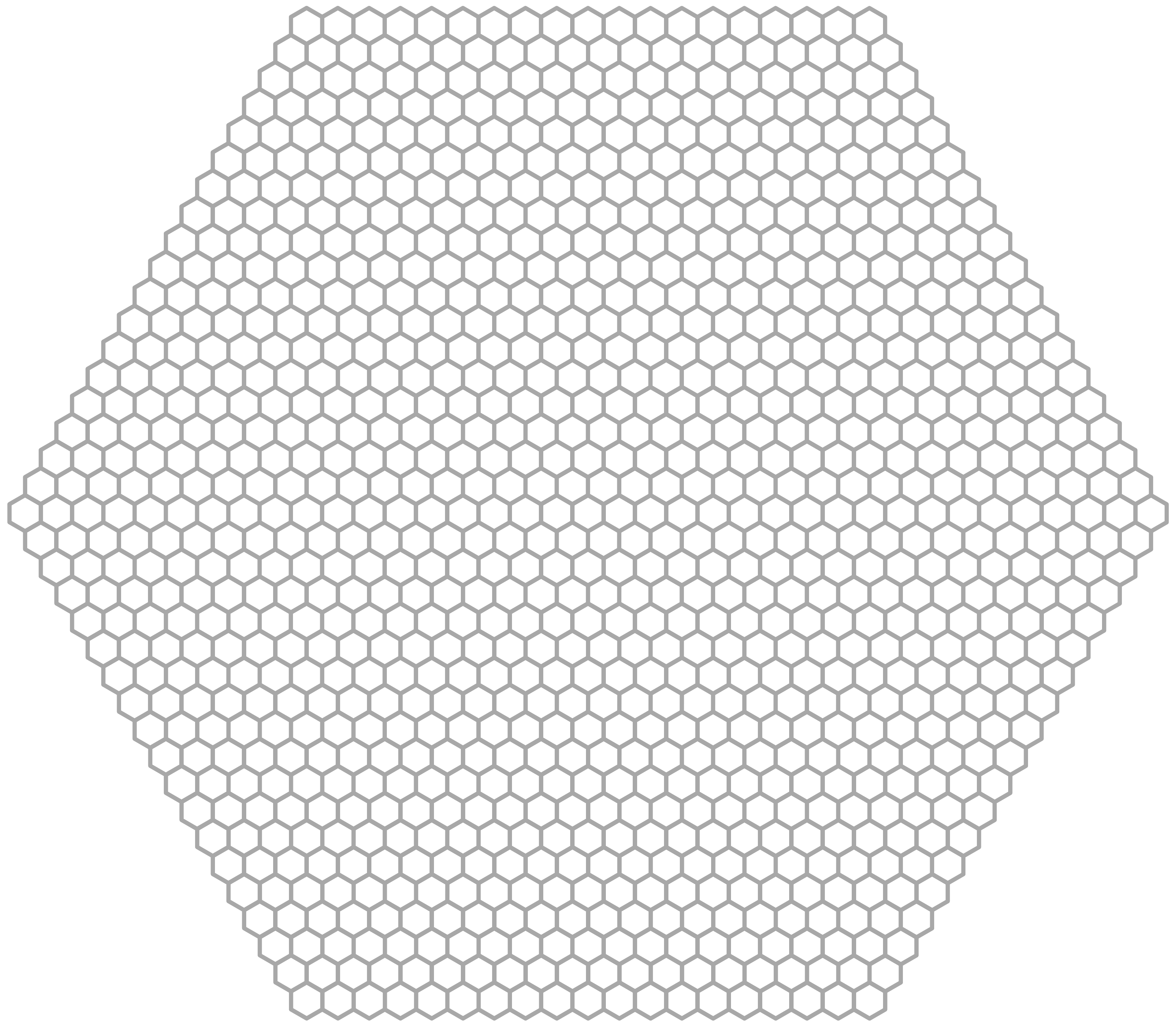


(5) Conclusions

Twisted bilayer graphene



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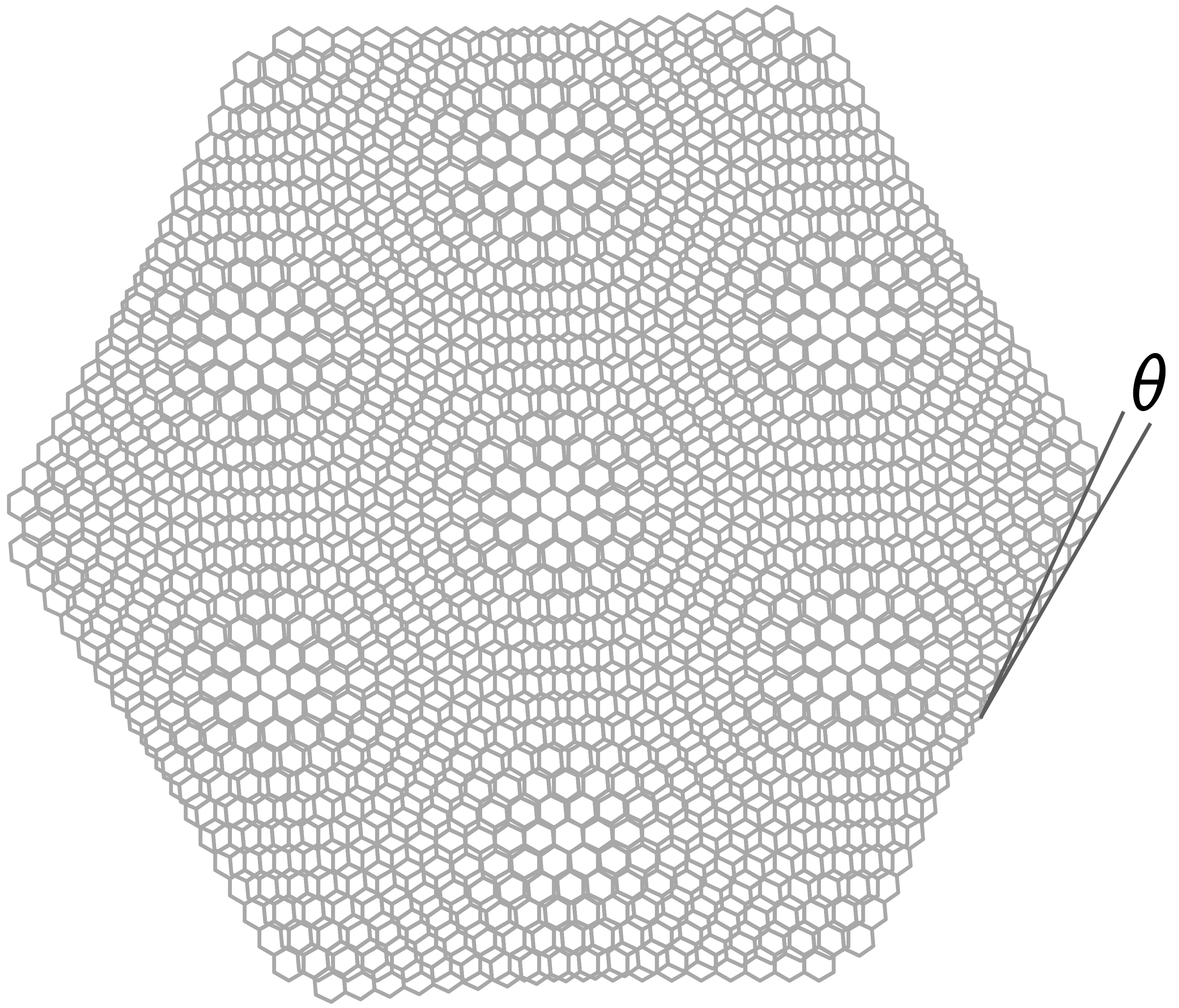
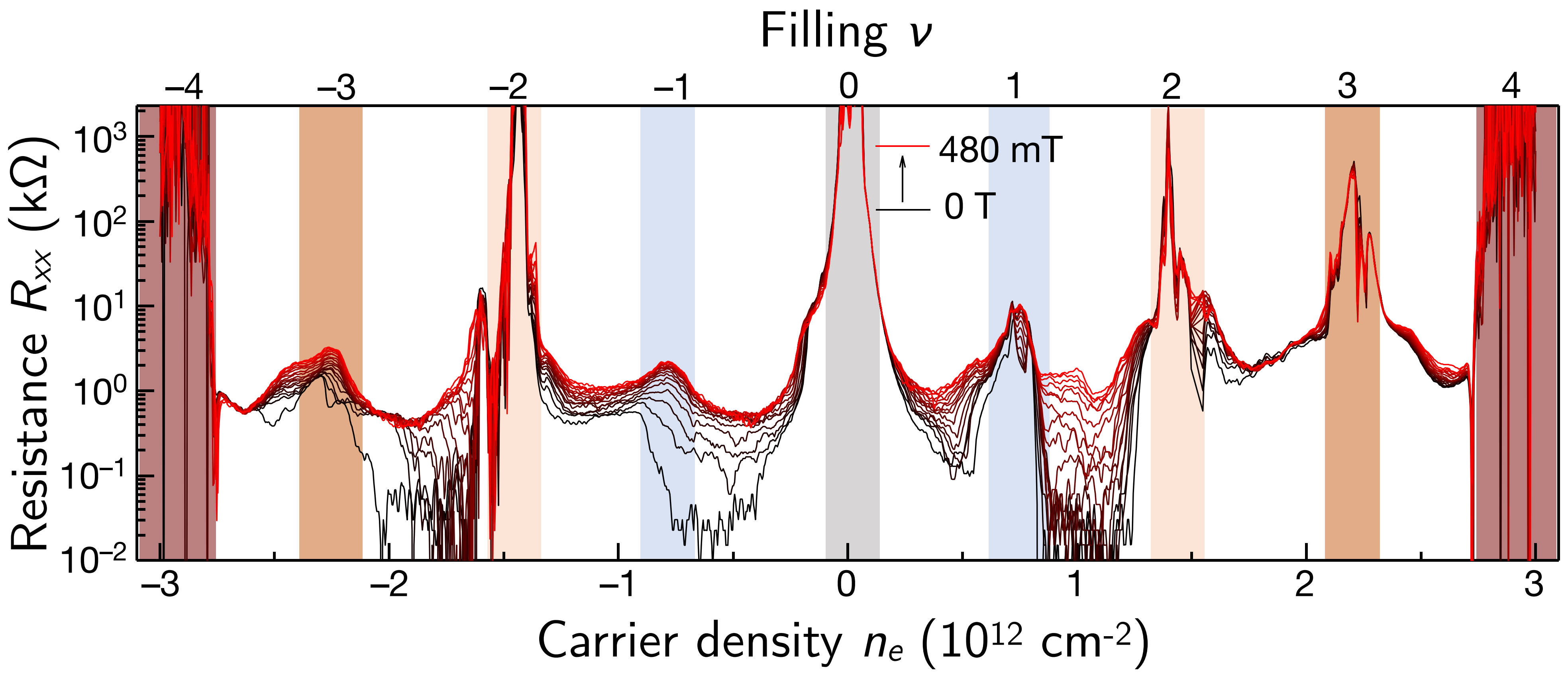
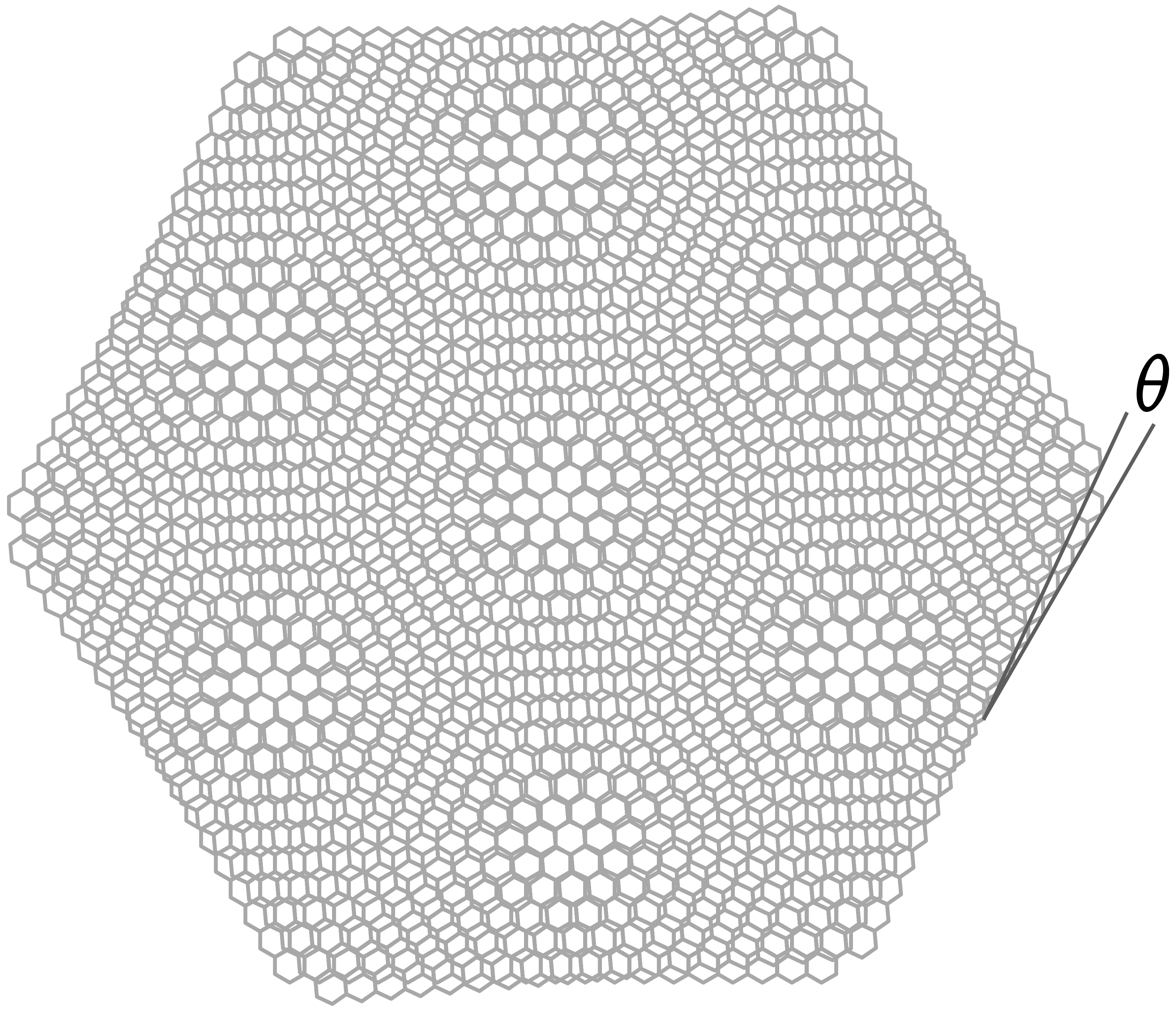


Twisted bilayer graphene

$$\theta = 1.16^\circ$$



[Lu *et al.*, Nature '19]



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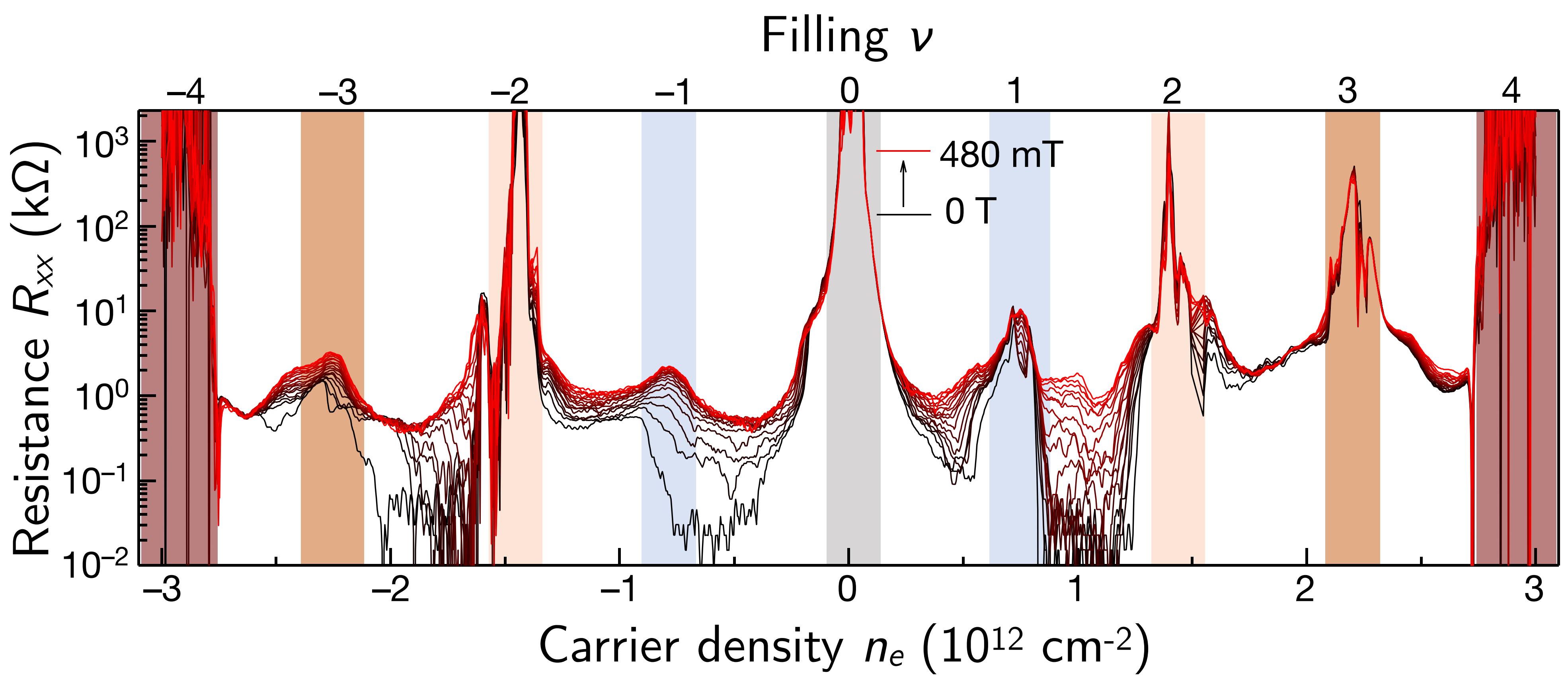

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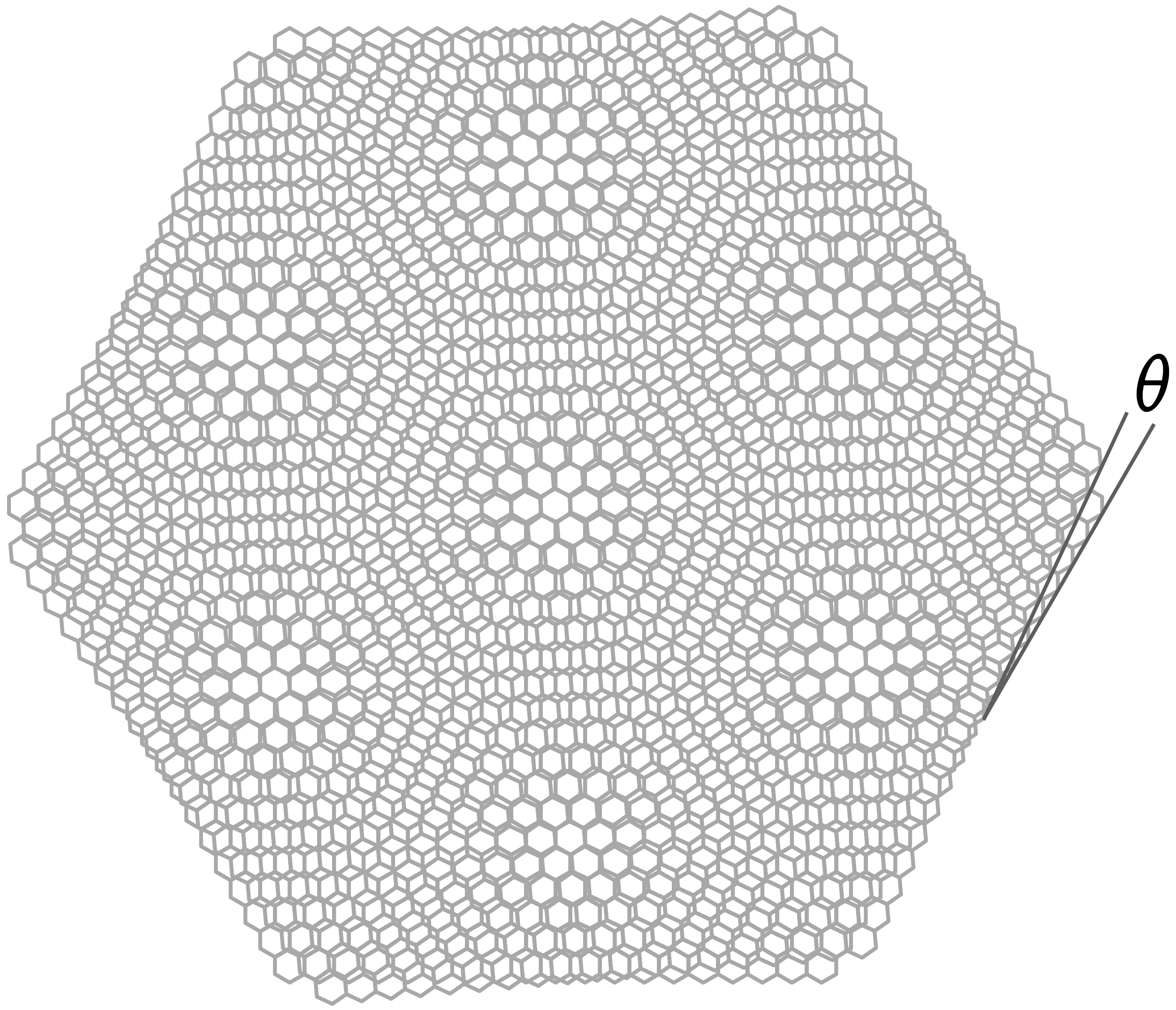

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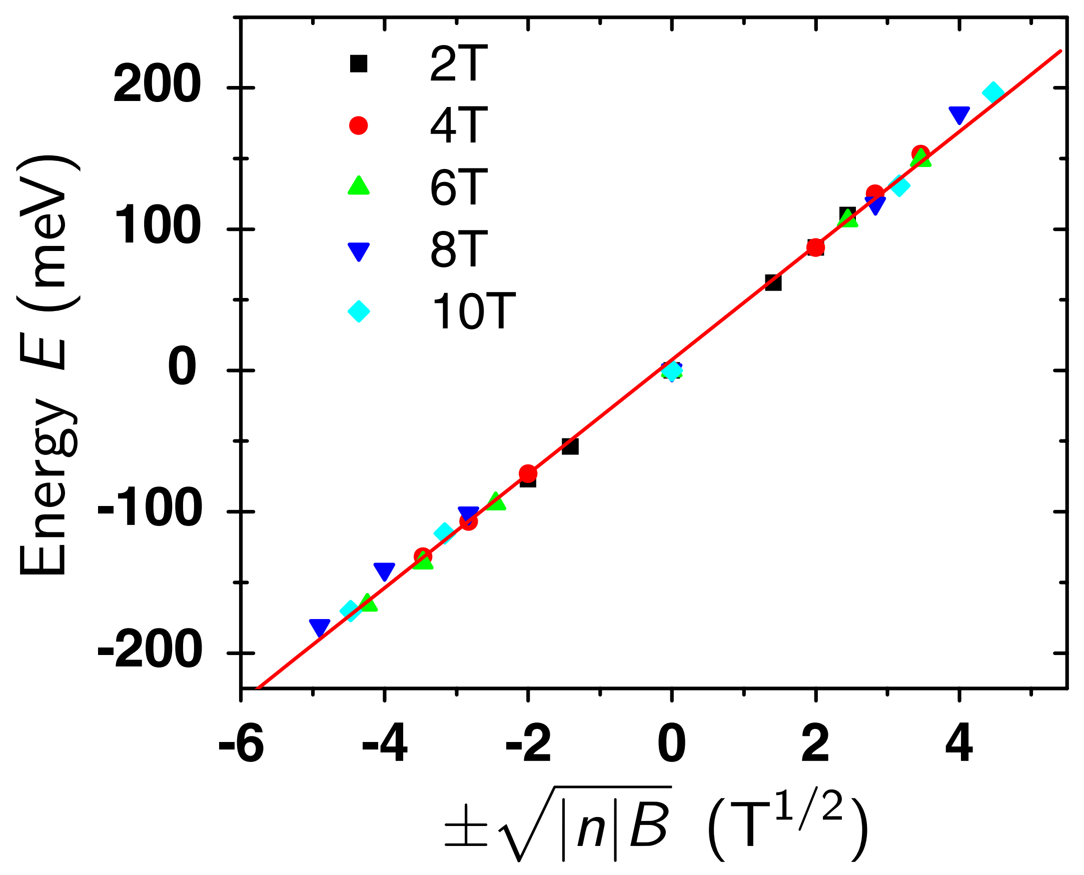

[Luican *et al.*, PRL '11]

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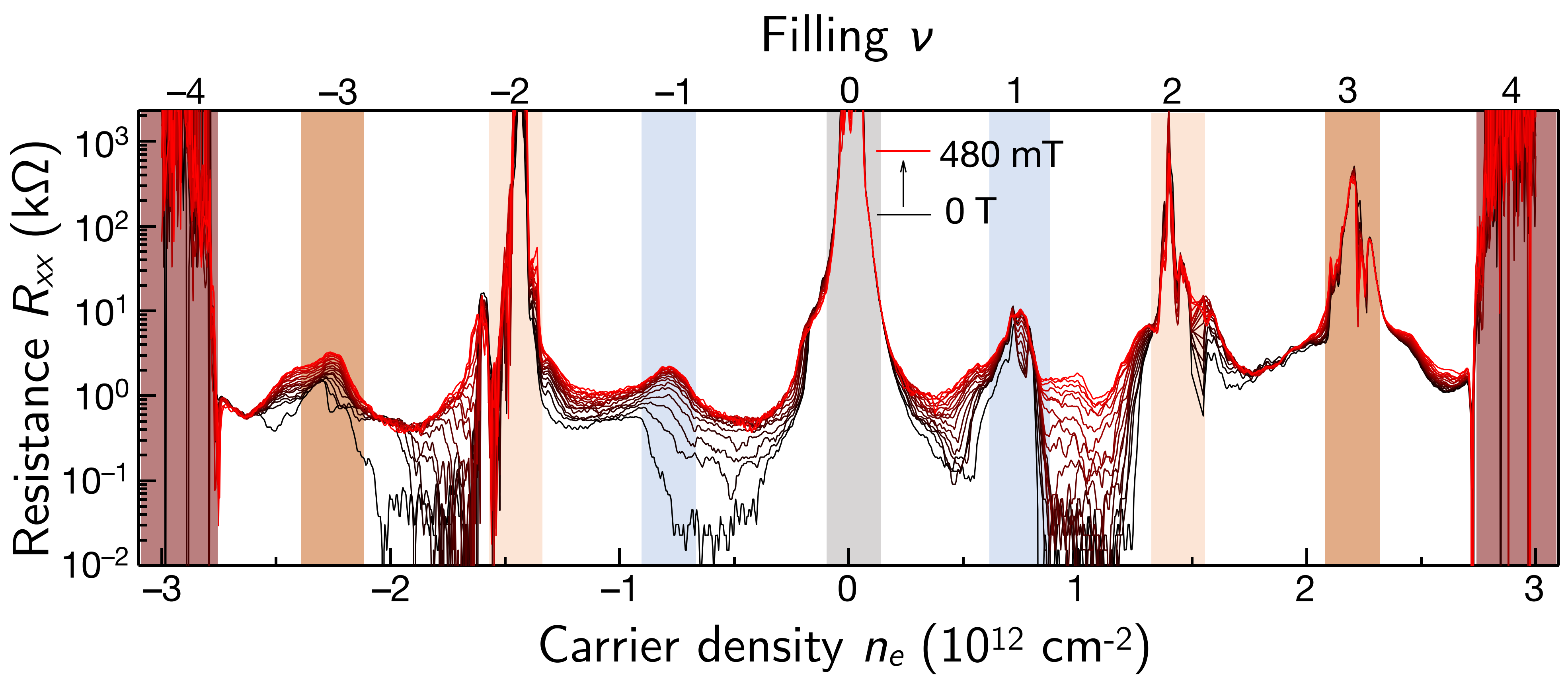

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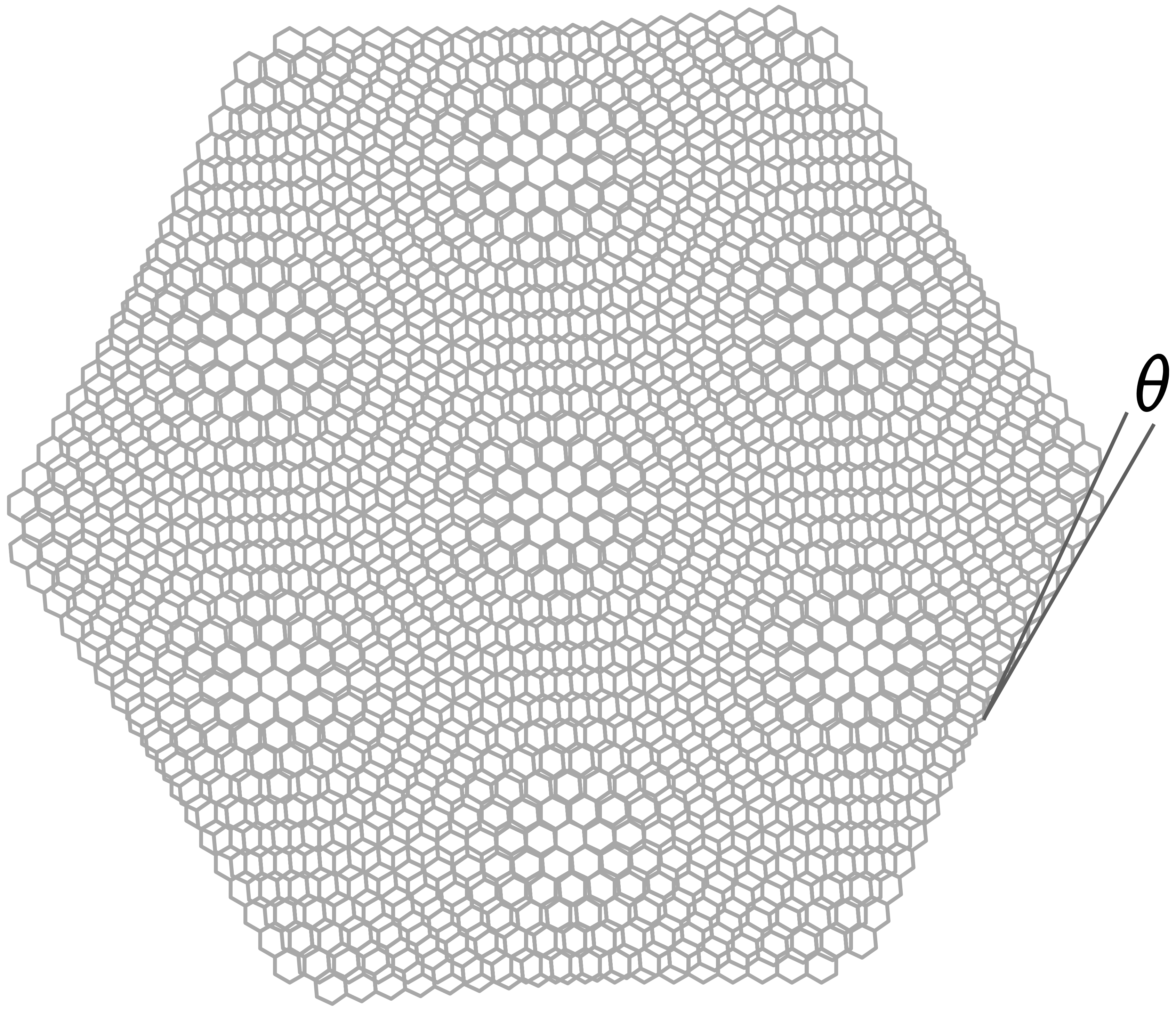

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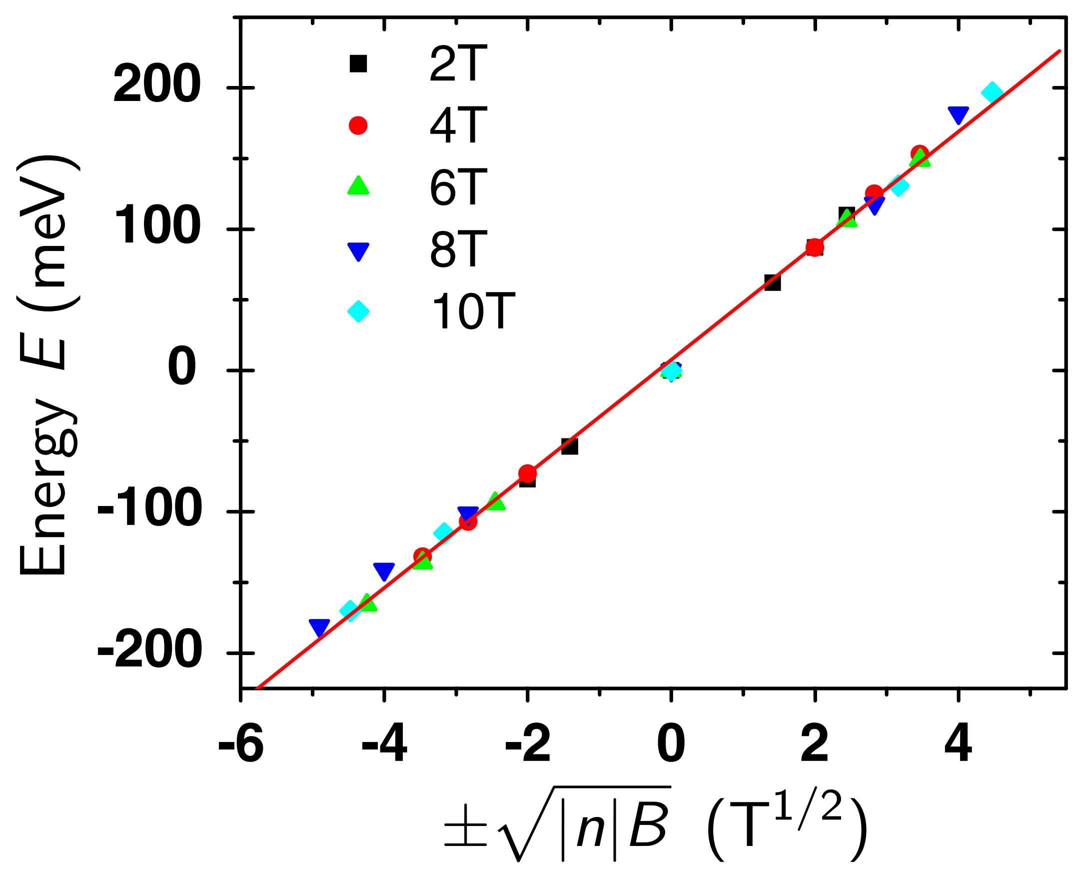
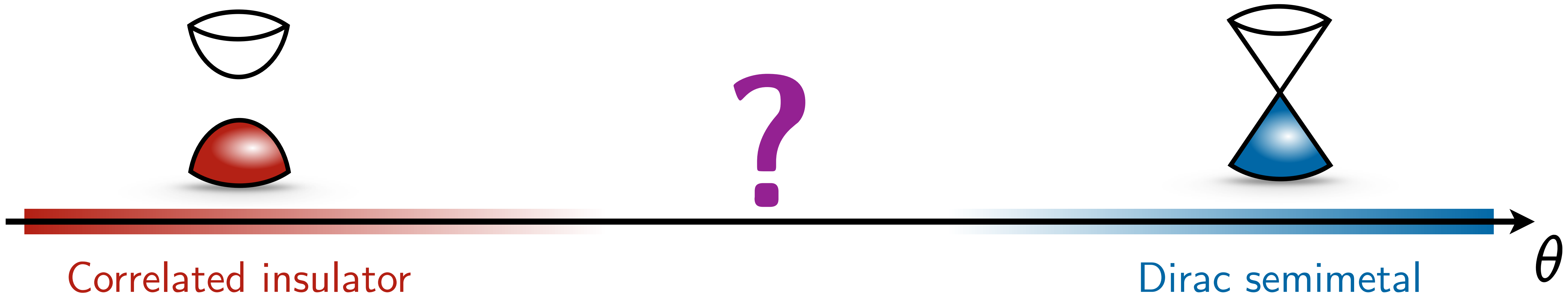
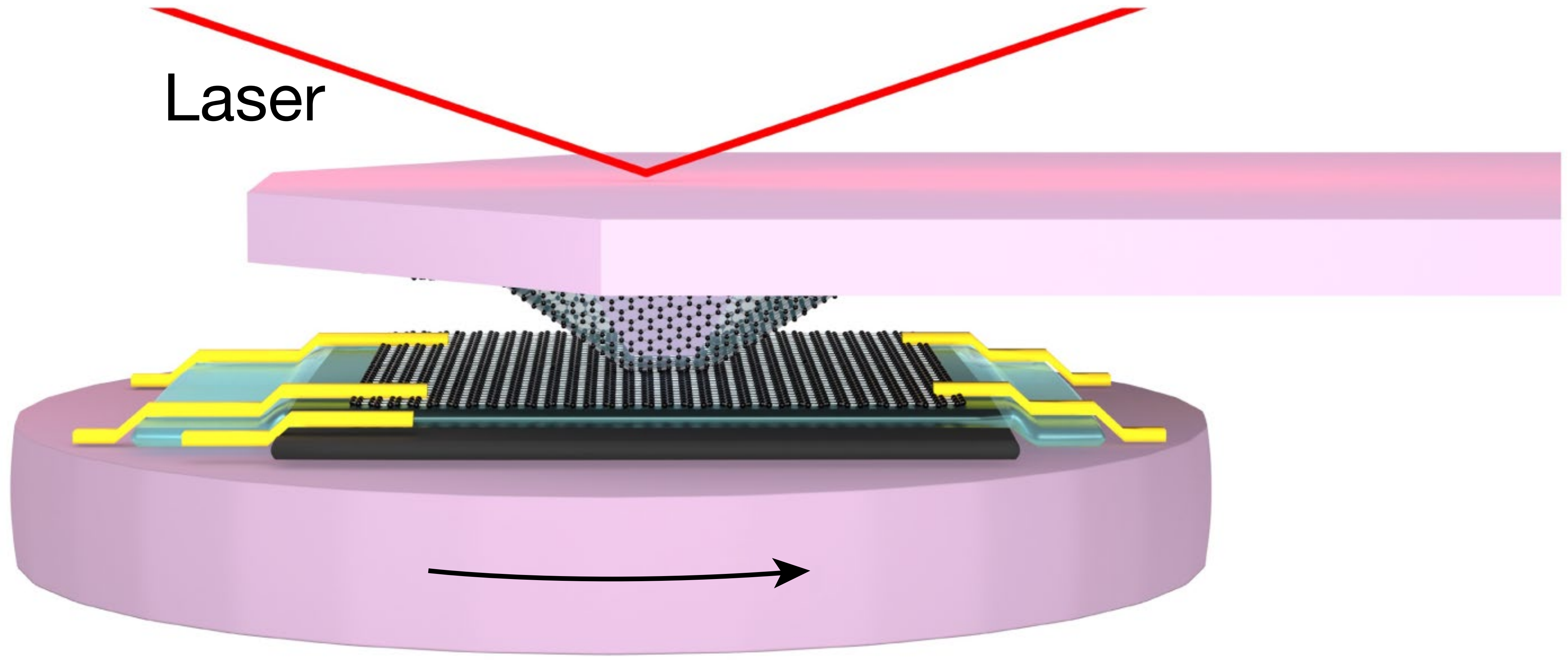


[Luican *et al.*, PRL '11]

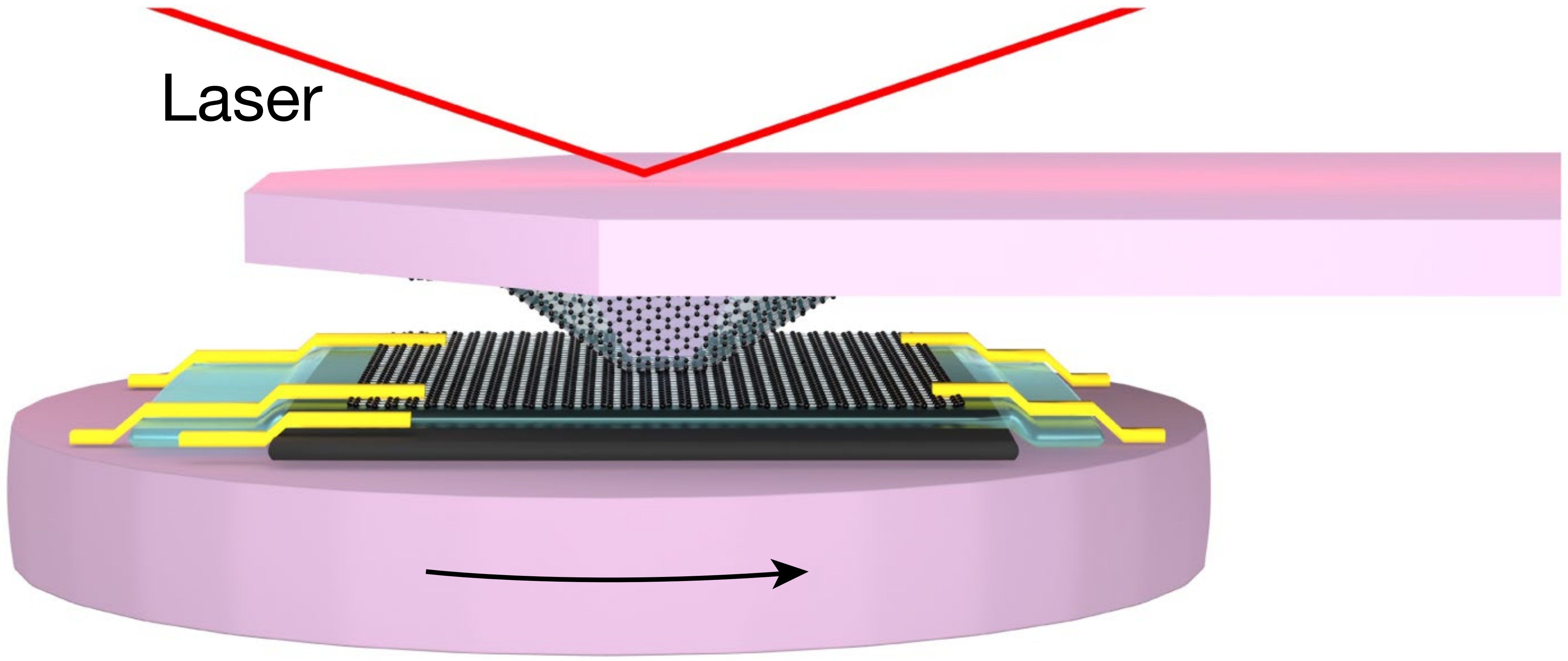


Quantum twisting microscope

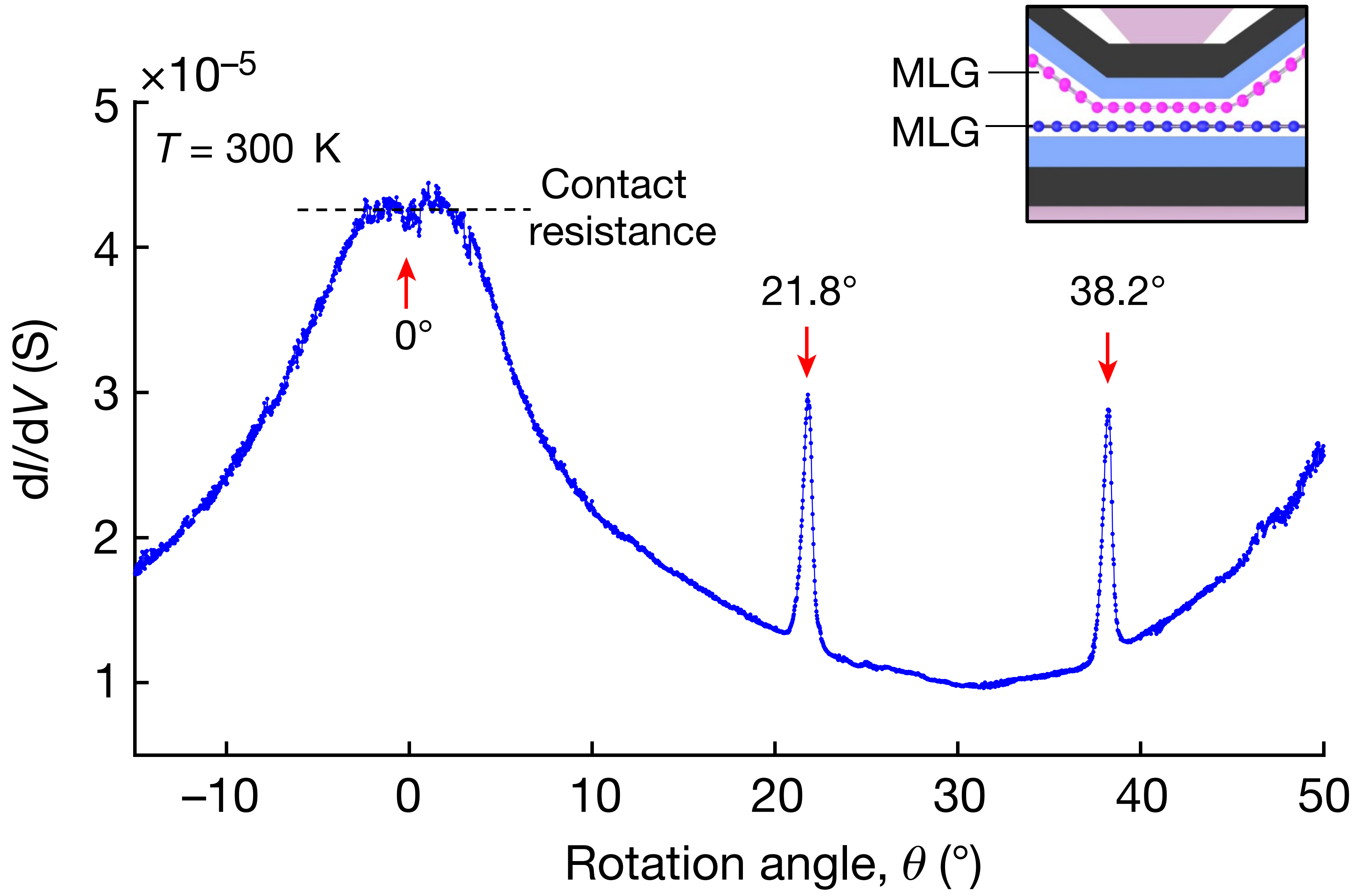


[Inbar *et al.*, Nature '23]

Quantum twisting microscope

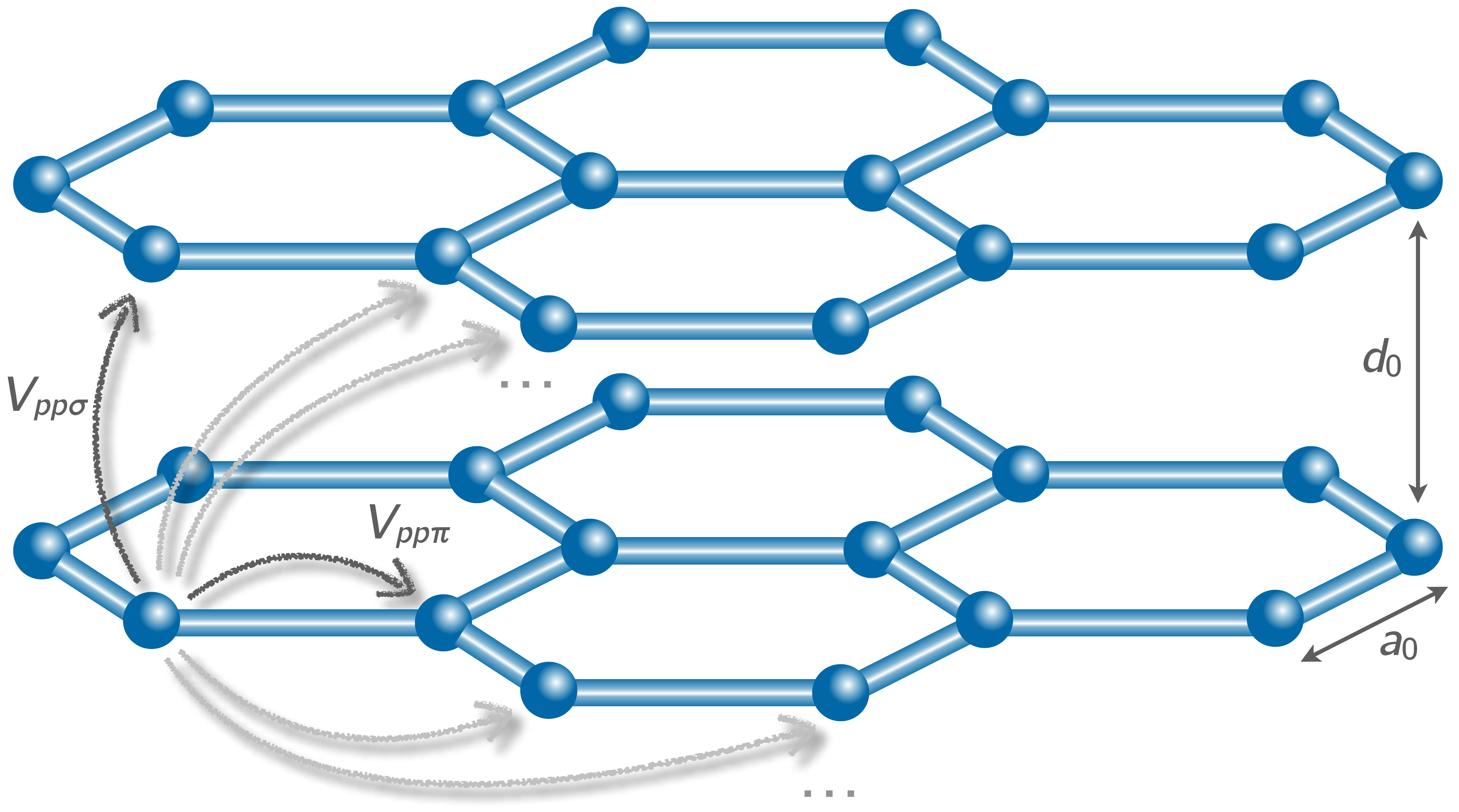


$T = 300$ K



[Inbar *et al.*, Nature '23]

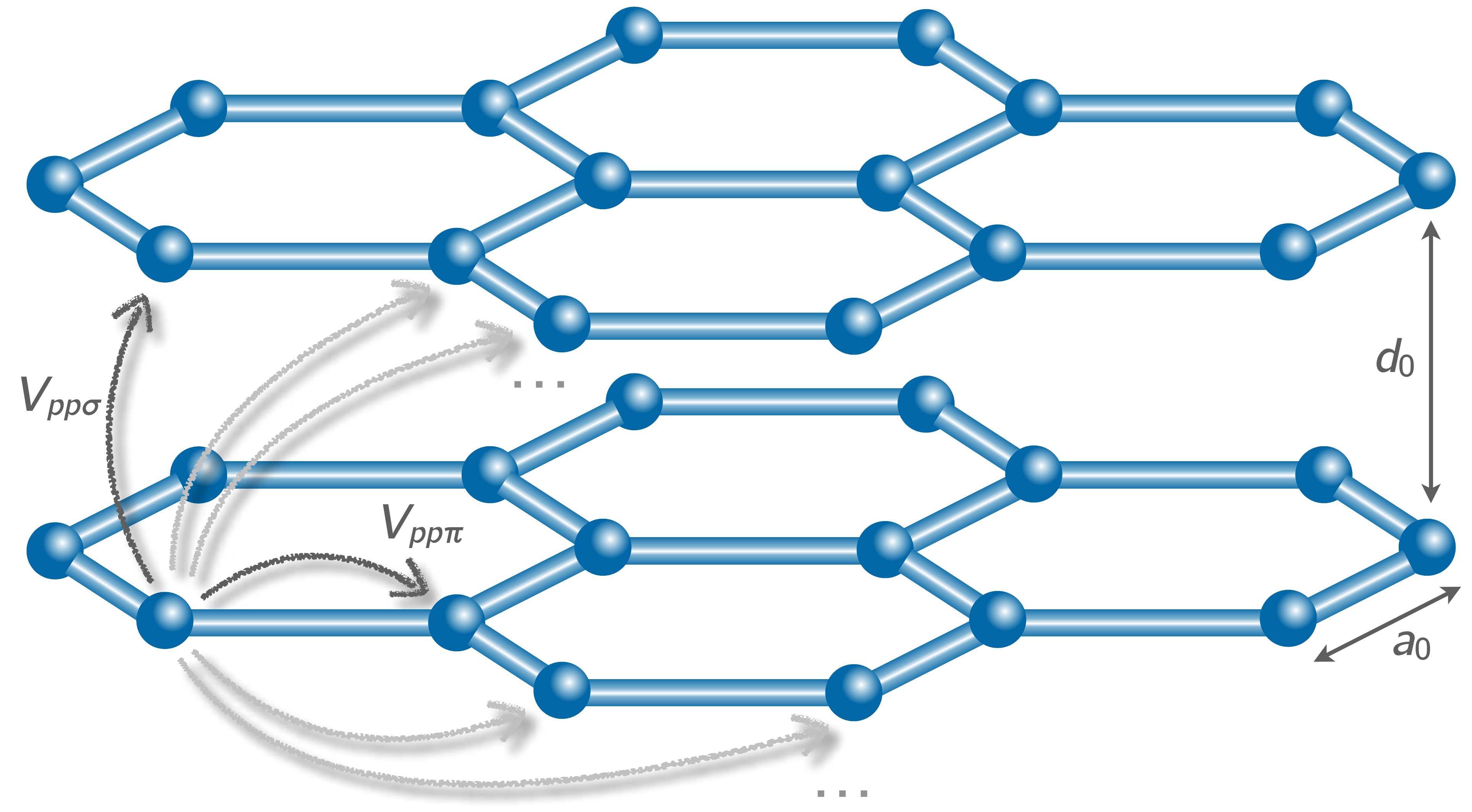
Lattice model



Hamiltonian:

$$H_0 = \sum_{i \neq j} t(\mathbf{R}_i - \mathbf{R}_j)\, c_i^\dagger c_j$$

Lattice model



Hamiltonian:

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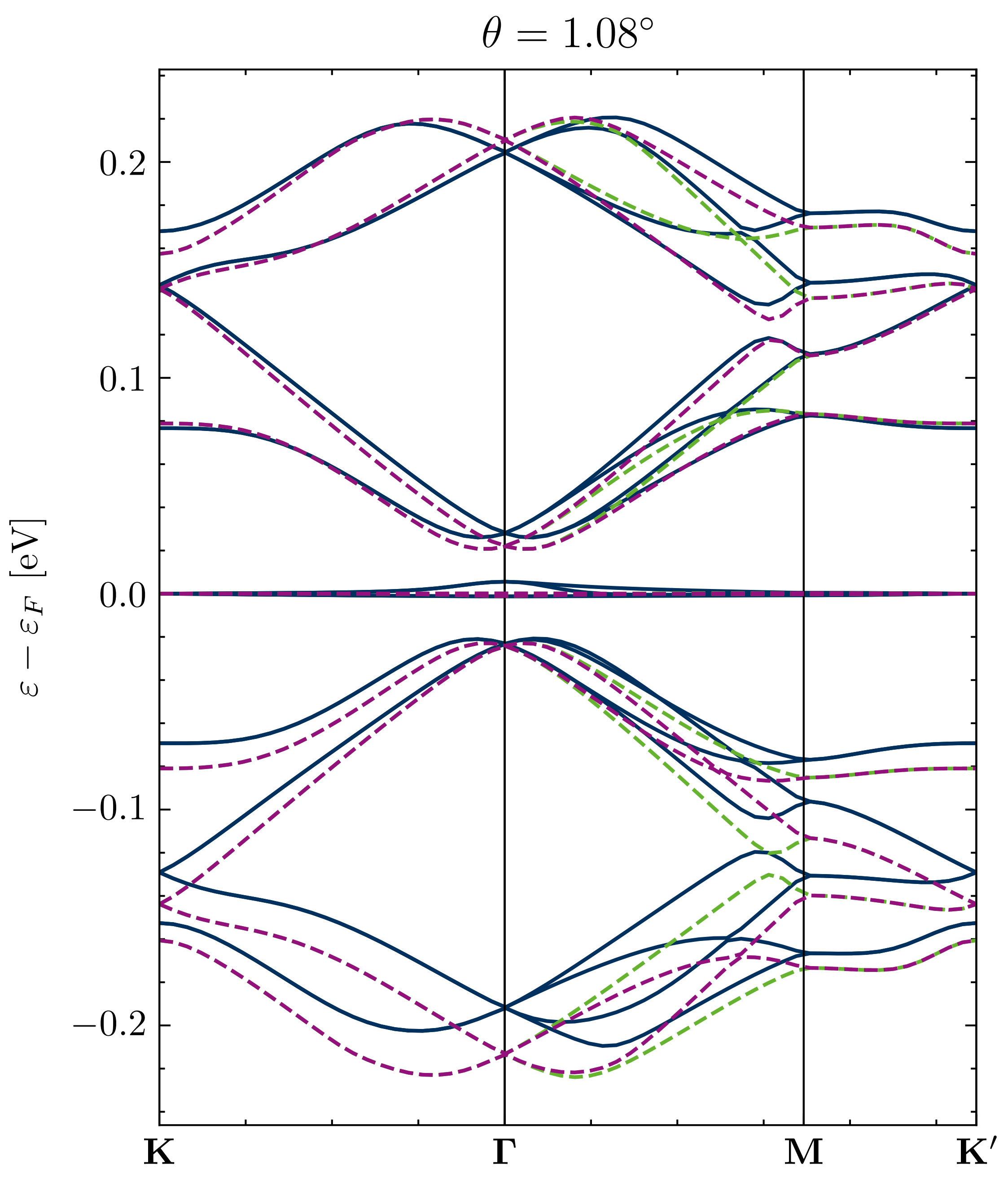
Slater-Koster hopping:

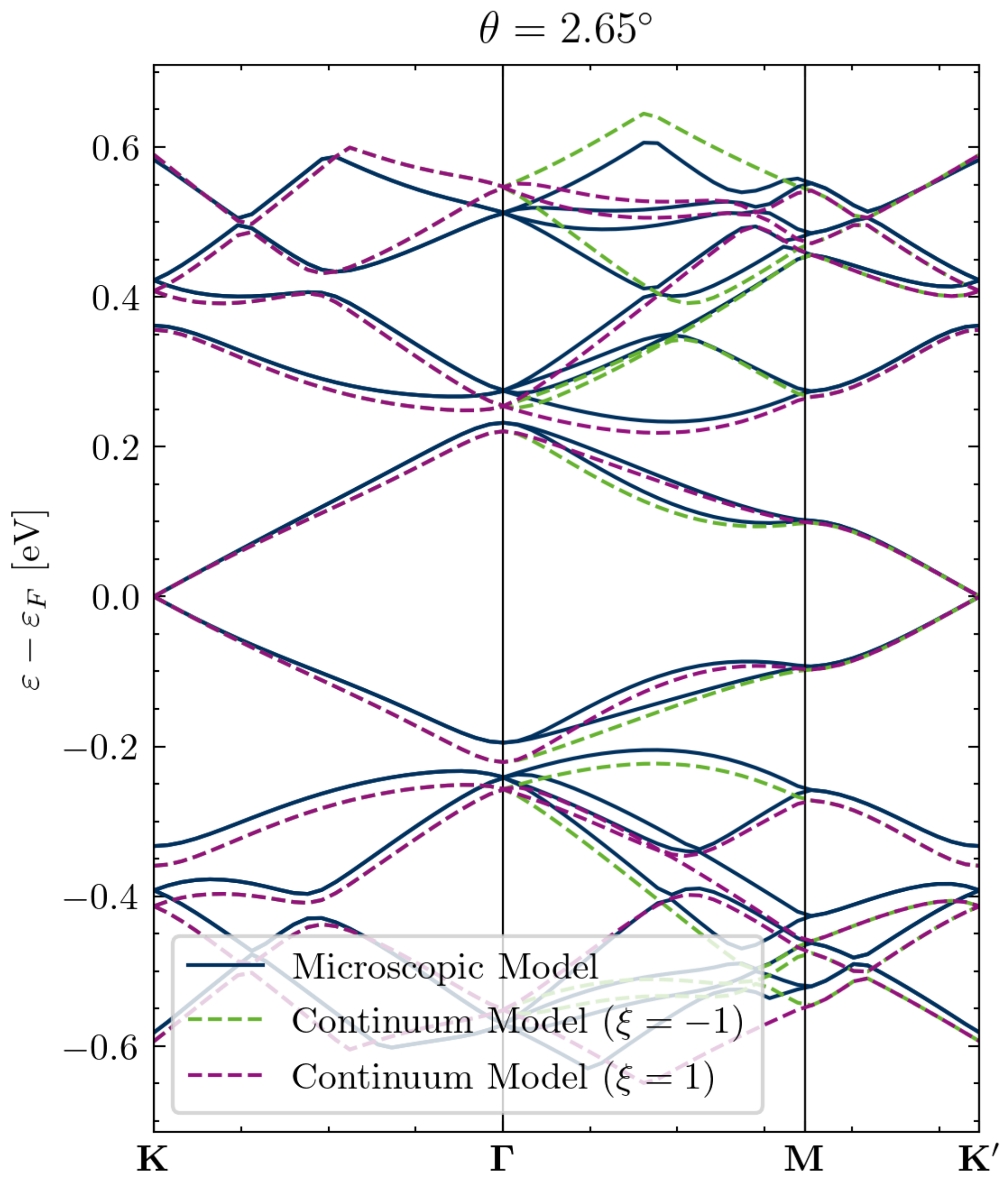
[Moon & Koshino, PRB '13]
[Koshino *et al.*, PRX '18]

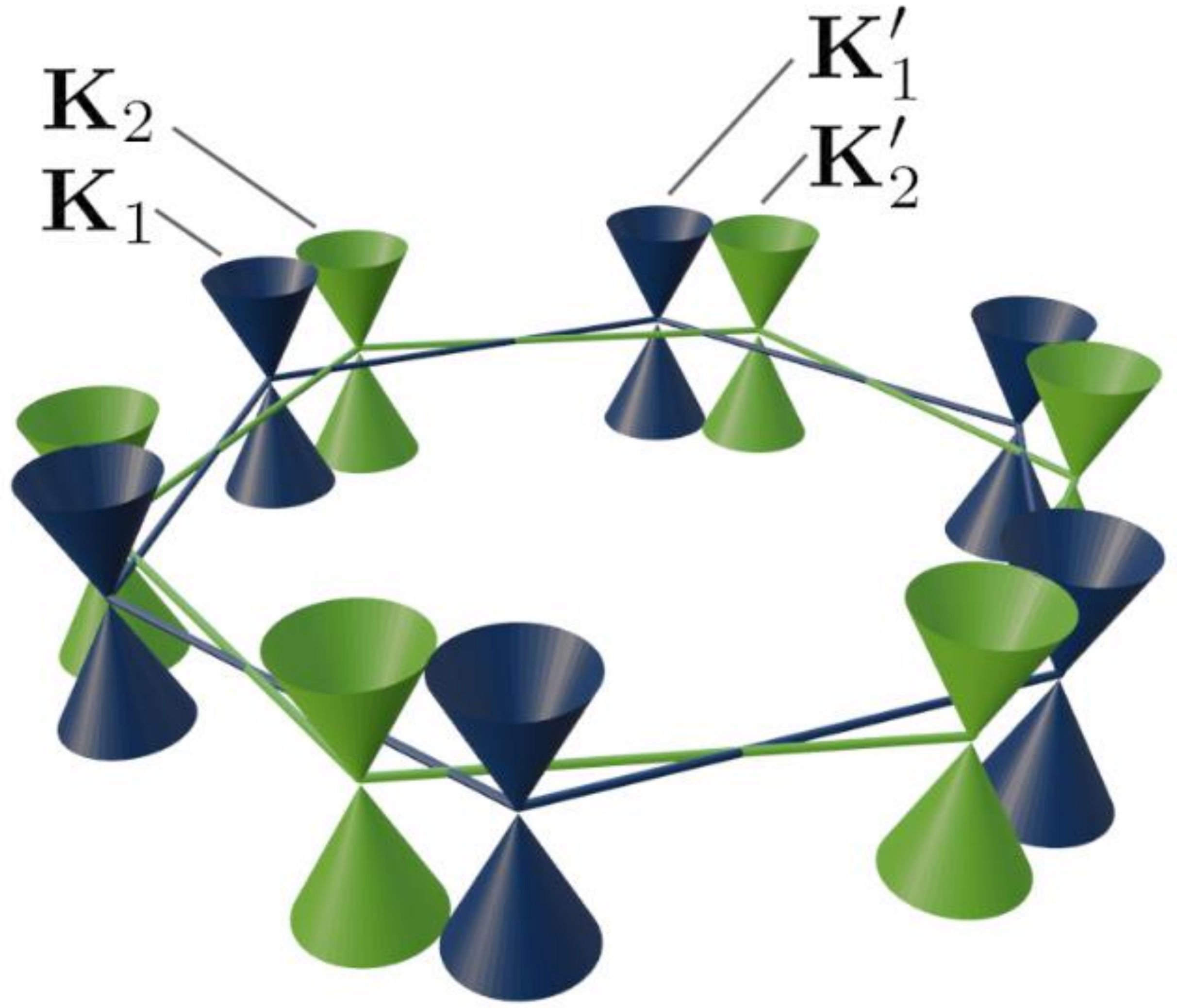
$$t(\mathbf{r}) = \begin{cases} -V_{pp\pi} \frac{x^2+y^2}{r^2} e^{-\frac{r-a_0}{r_0}} - V_{pp\sigma} \frac{z^2}{r^2} e^{-\frac{r-d_0}{r_0}} & \text{for } a_0 \leq r \leq 6a_0 \\ 0 & \text{for } r > 6a_0 \end{cases}$$

... with $V_{pp\pi} \approx -2.7\,\mathrm{eV}$, $V_{pp\sigma} \approx 0.48\,\mathrm{eV}$, and decay length $r_0 \approx 0.319 a_0$

Electronic band structure







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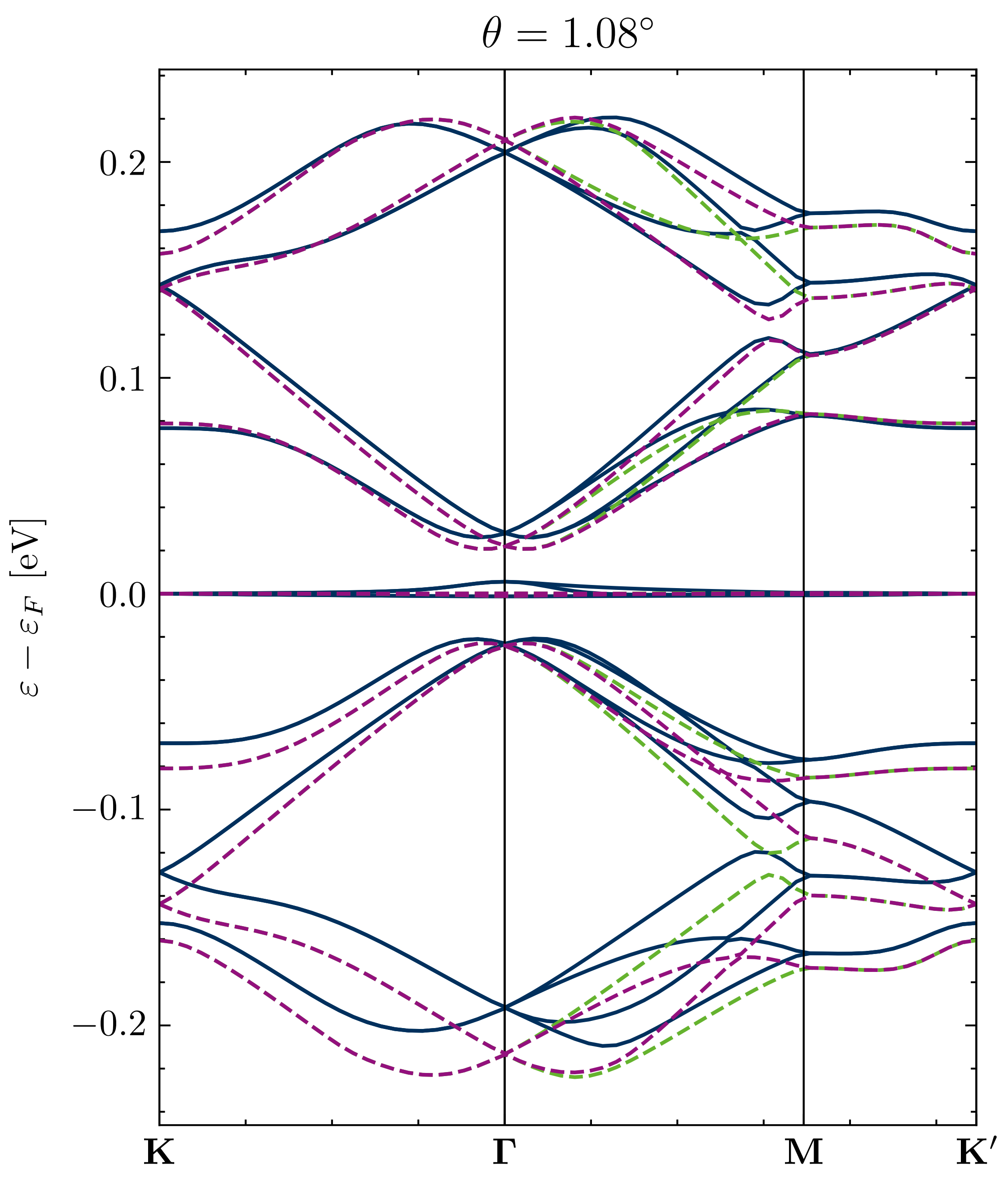
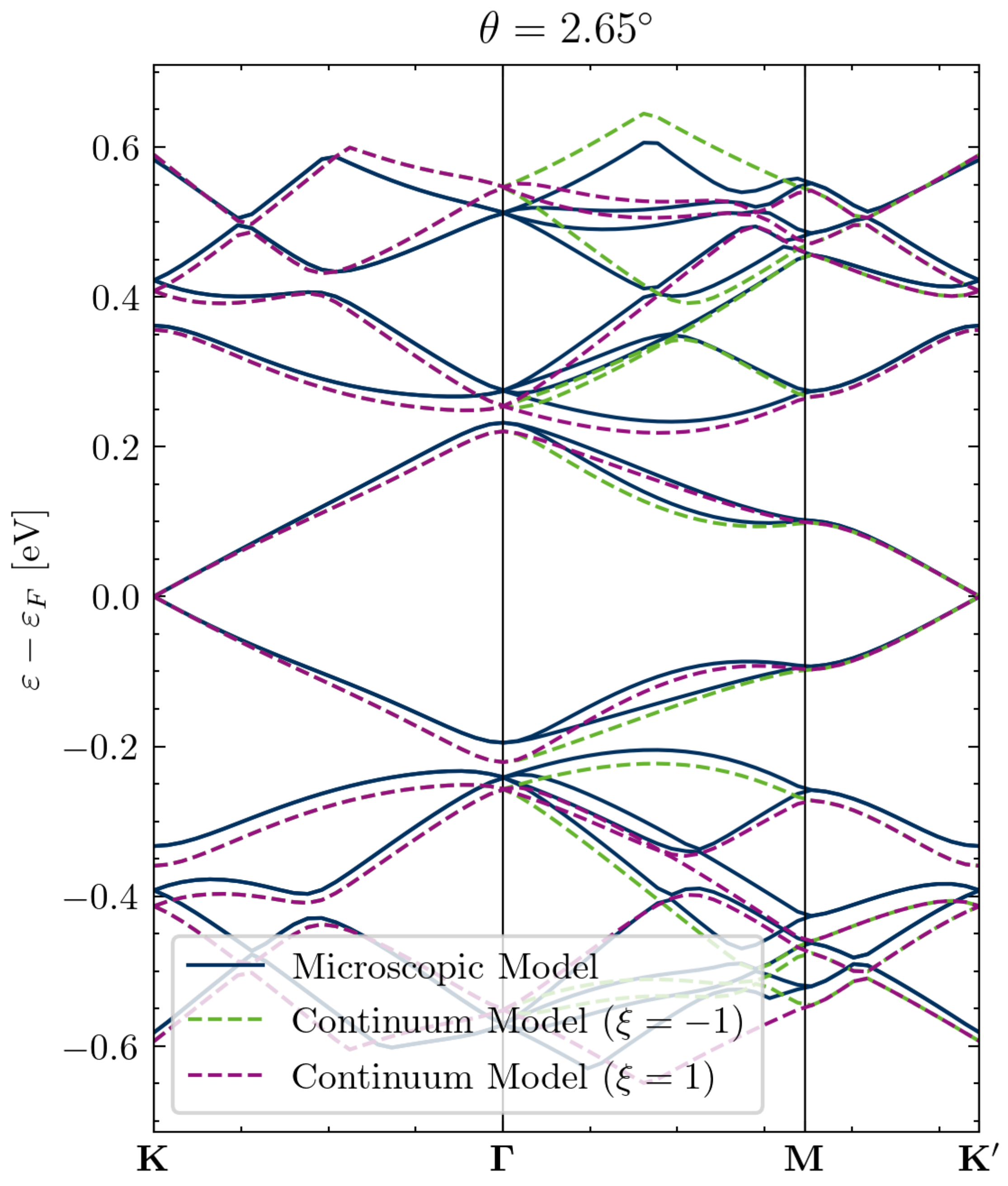
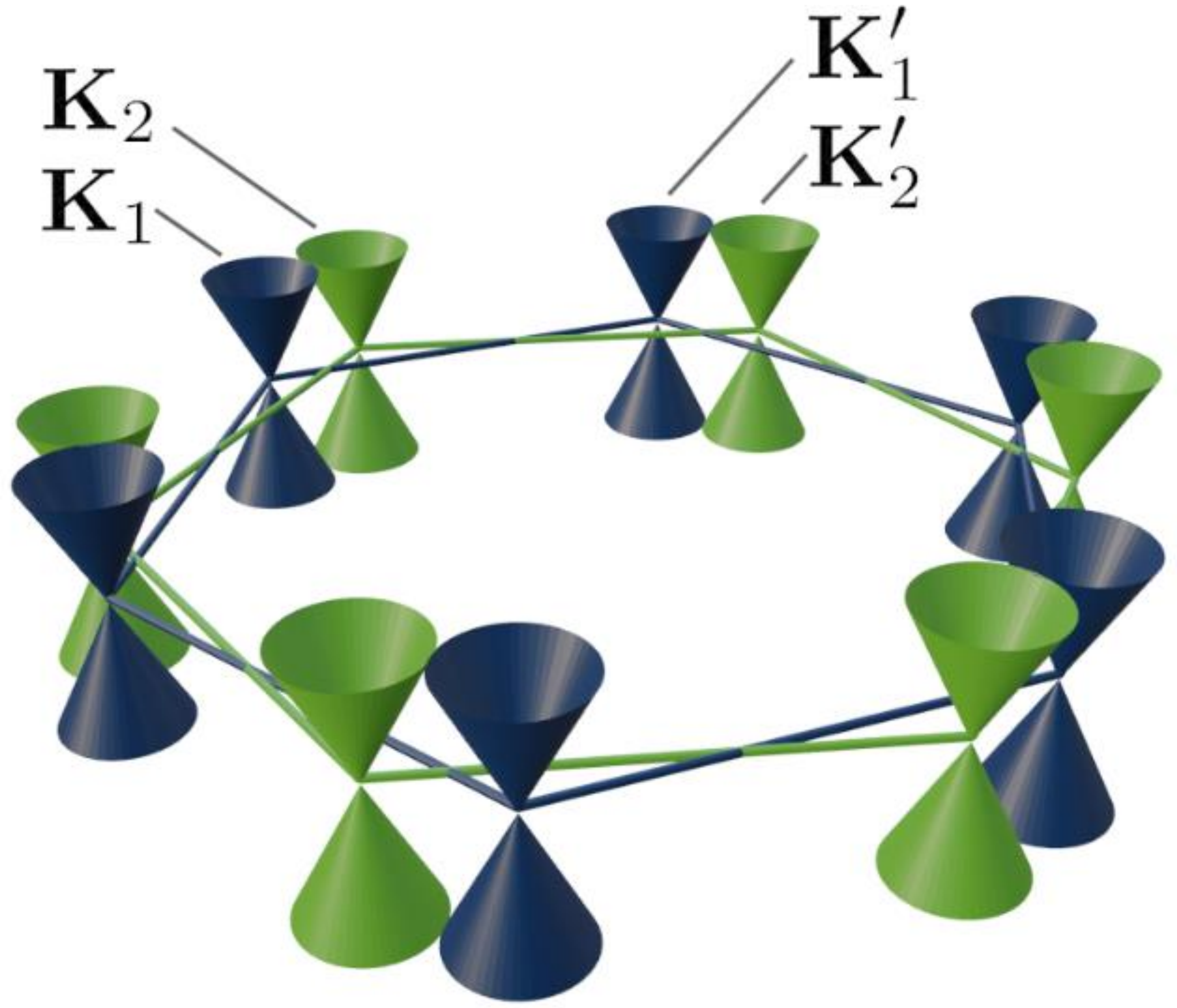
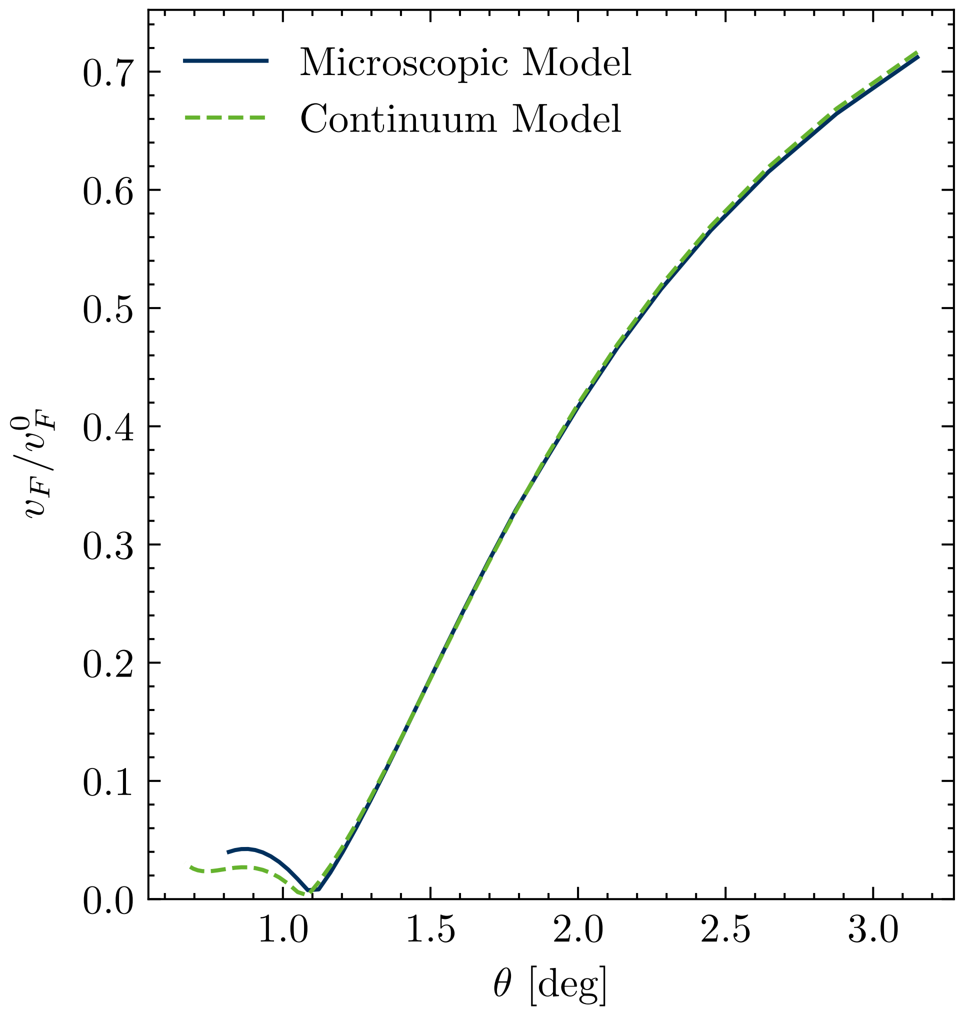


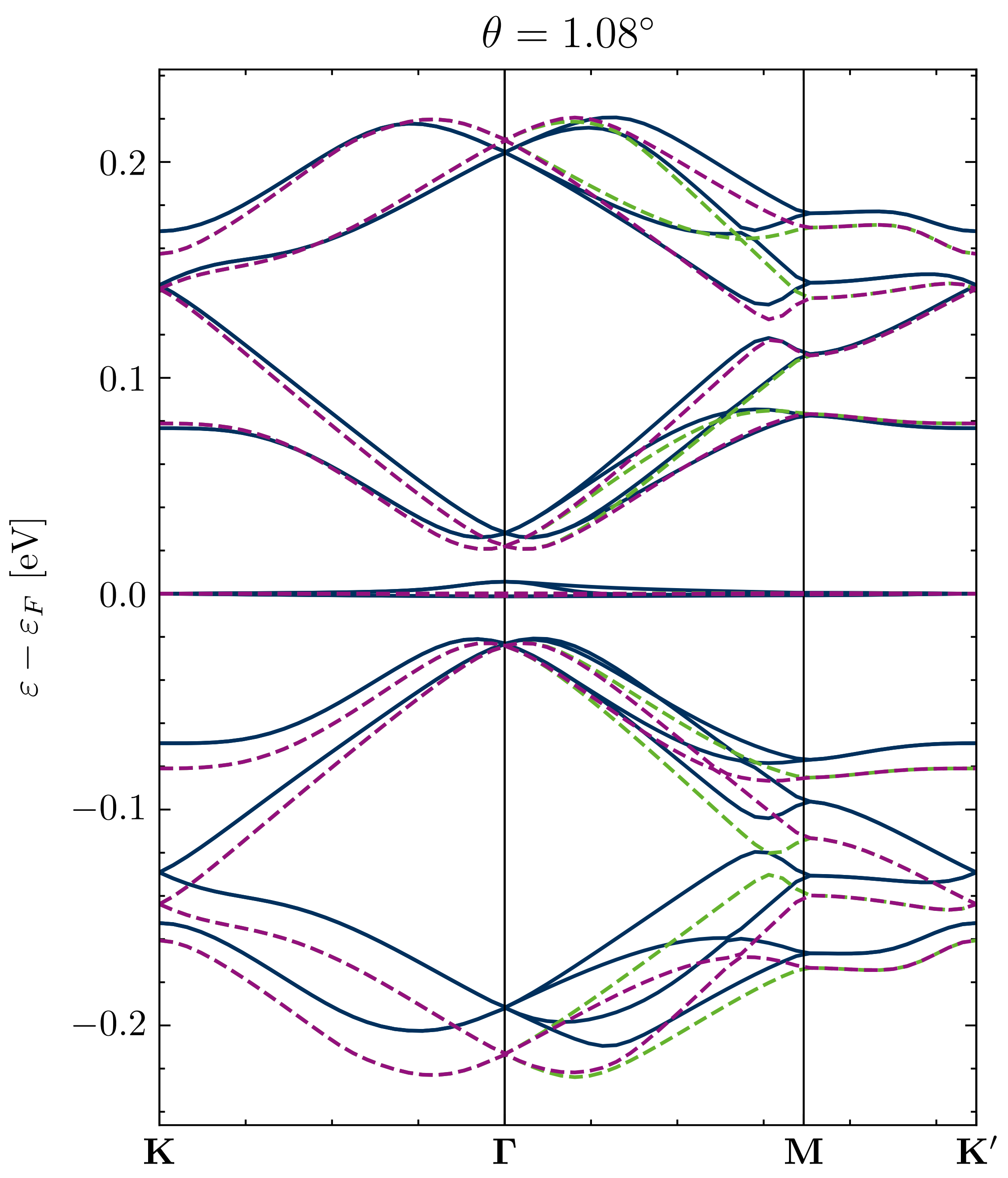


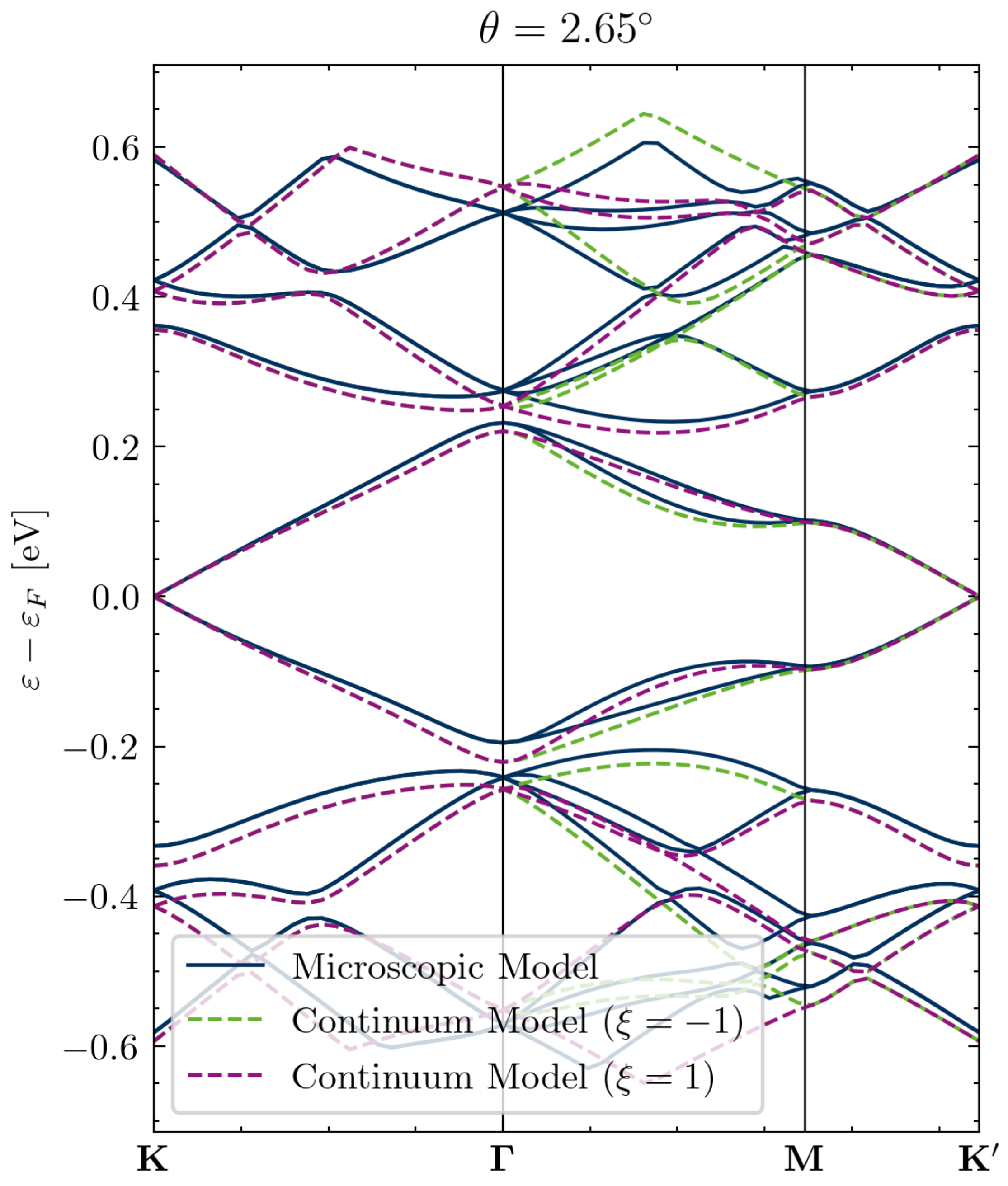


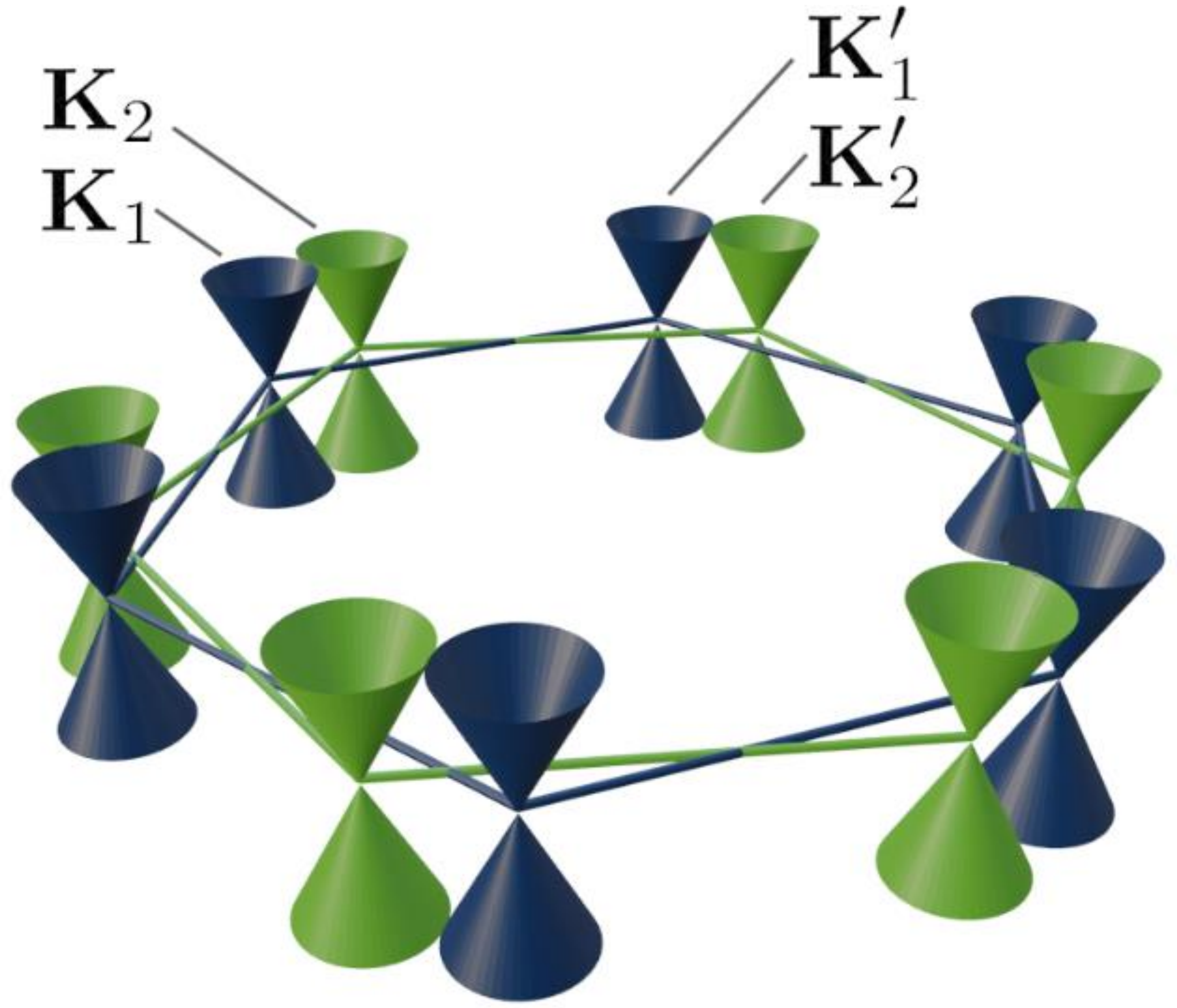
Fermi velocity:



Electronic band structure







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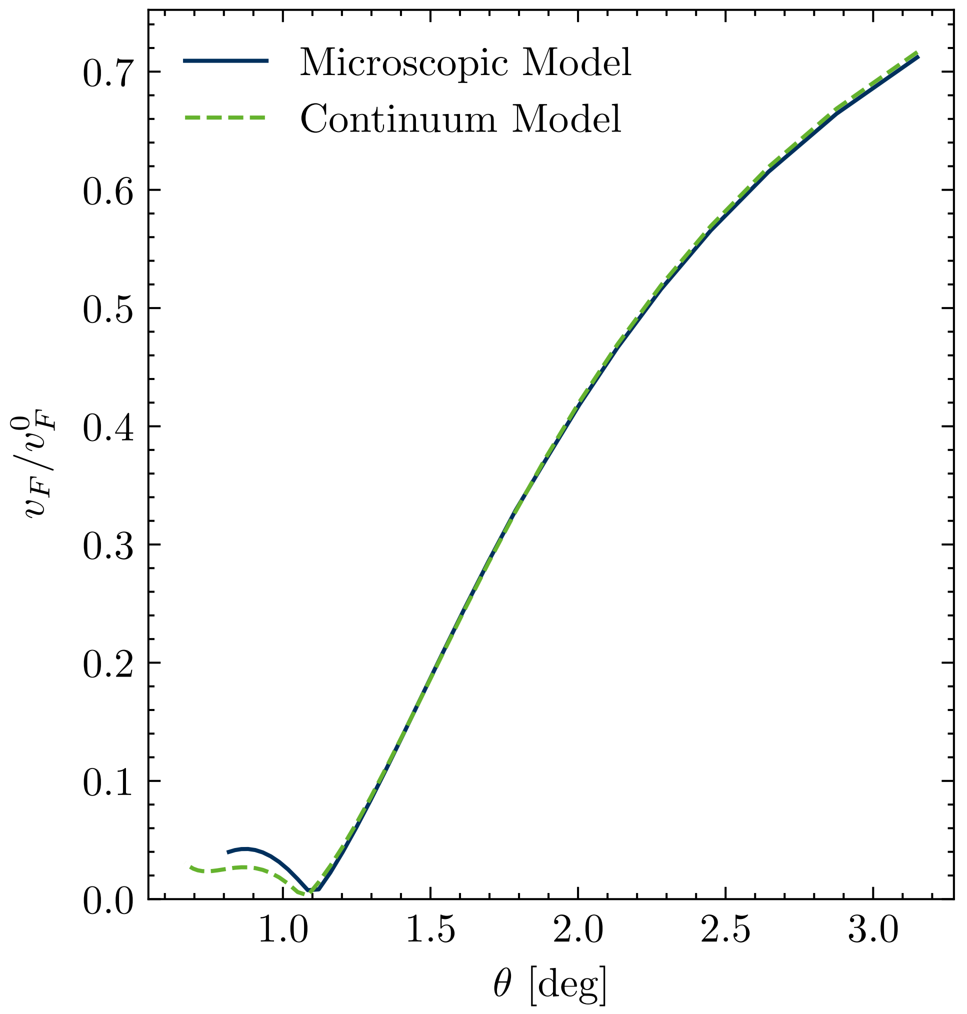
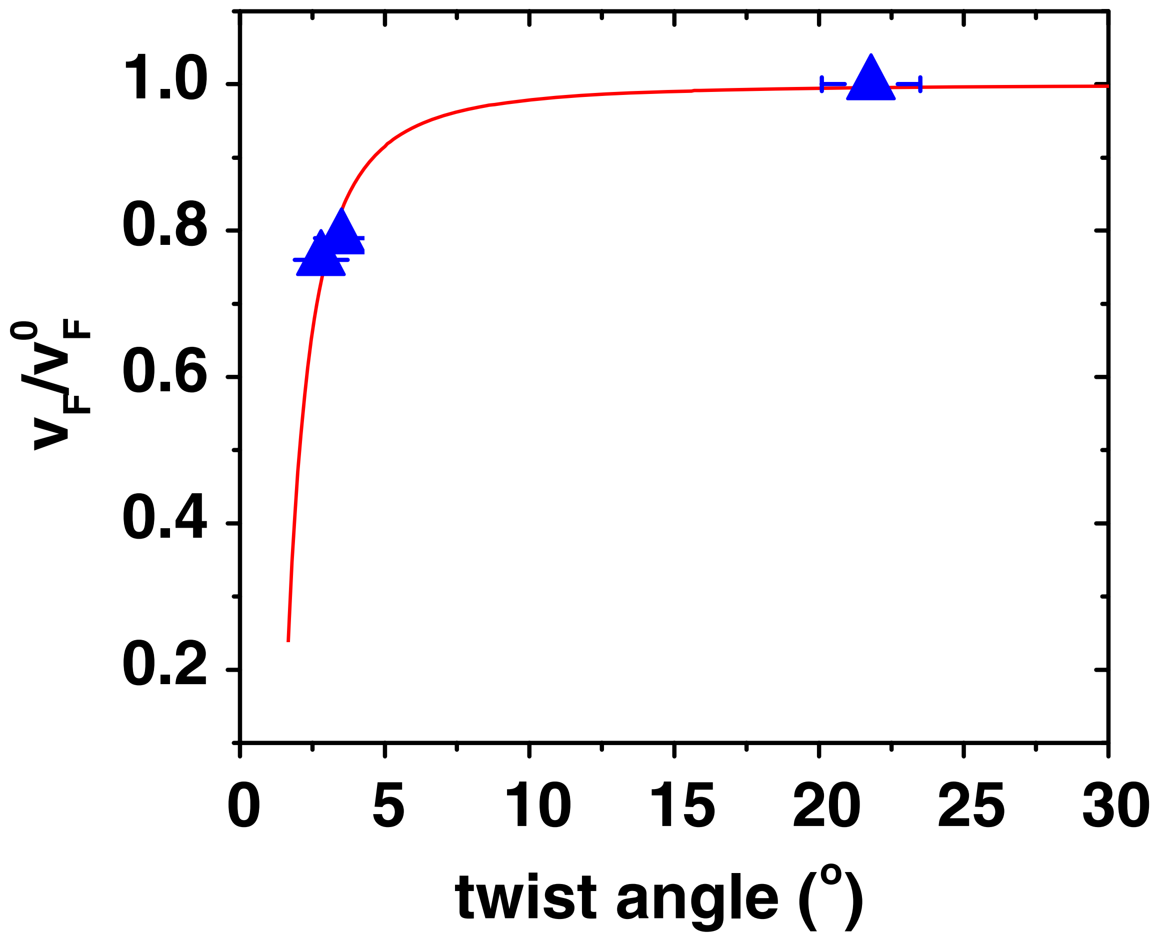


Experiment:

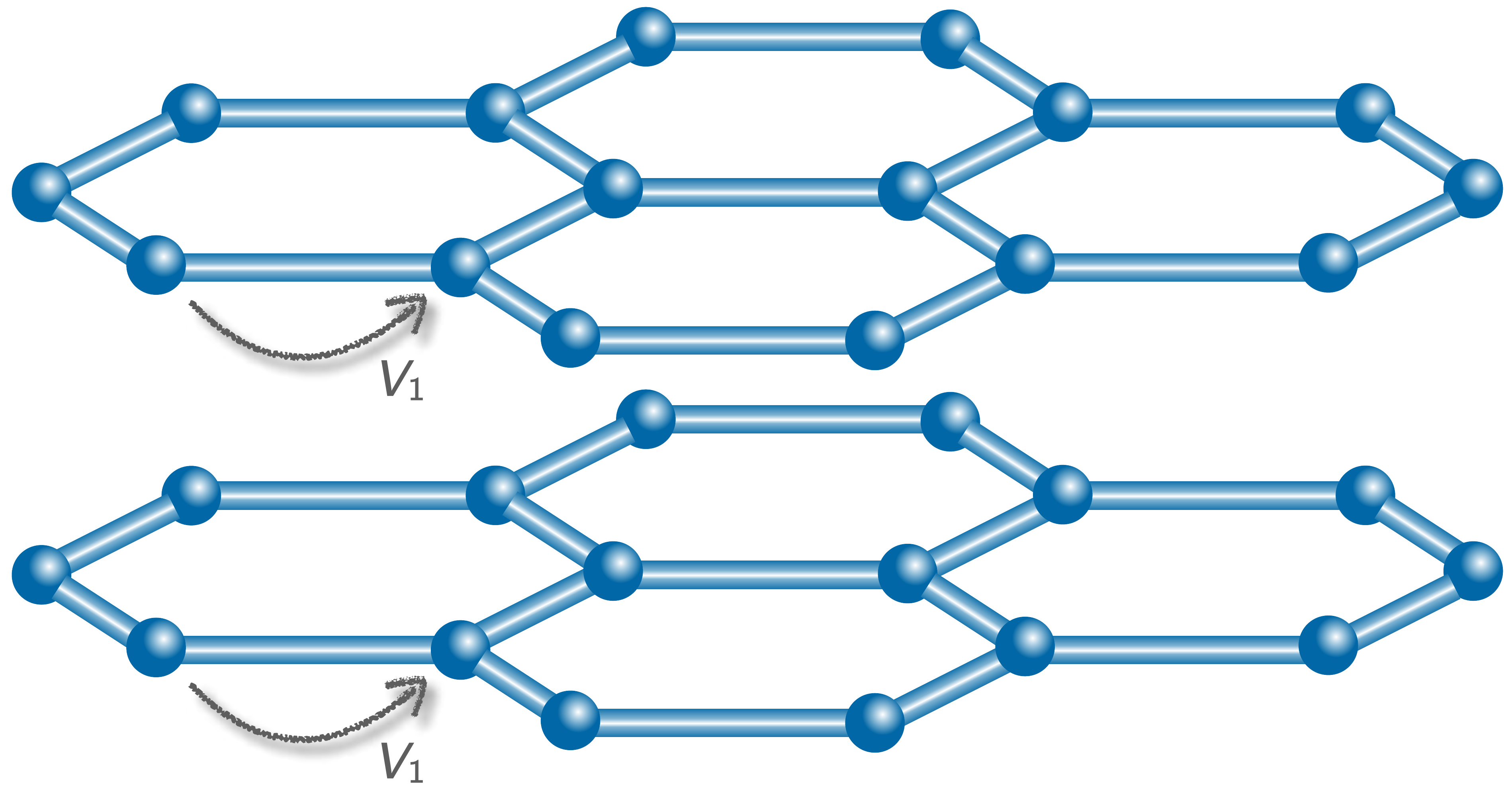


[Luican *et al.*, PRL '11]

Interactions

Toy lattice model:

$$H = \sum_{i \neq j} t(\mathbf{R}_i - \mathbf{R}_j)\, c_i^\dagger c_j + V_1 \sum_{\langle ij \rangle} n_i n_j$$



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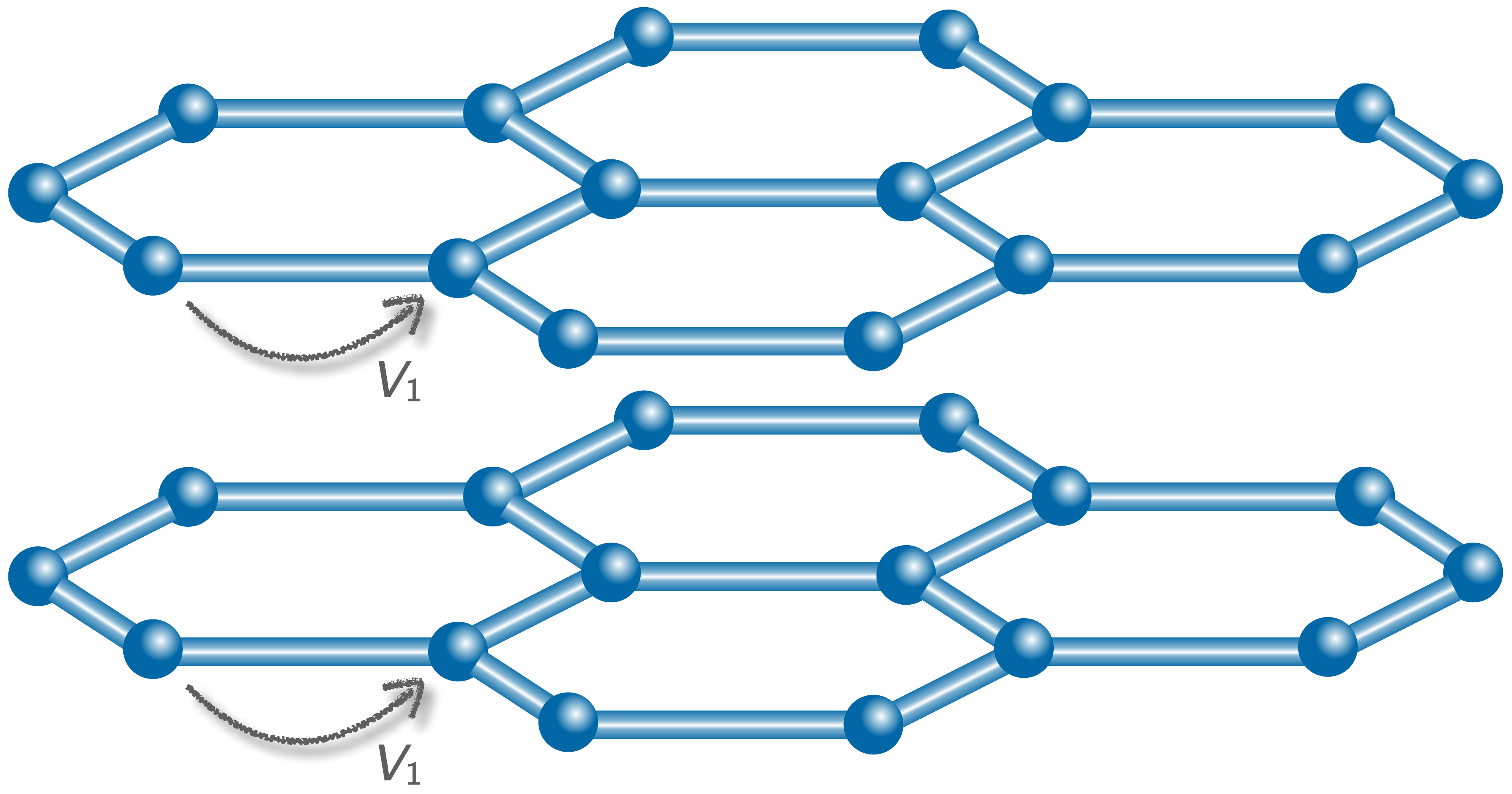
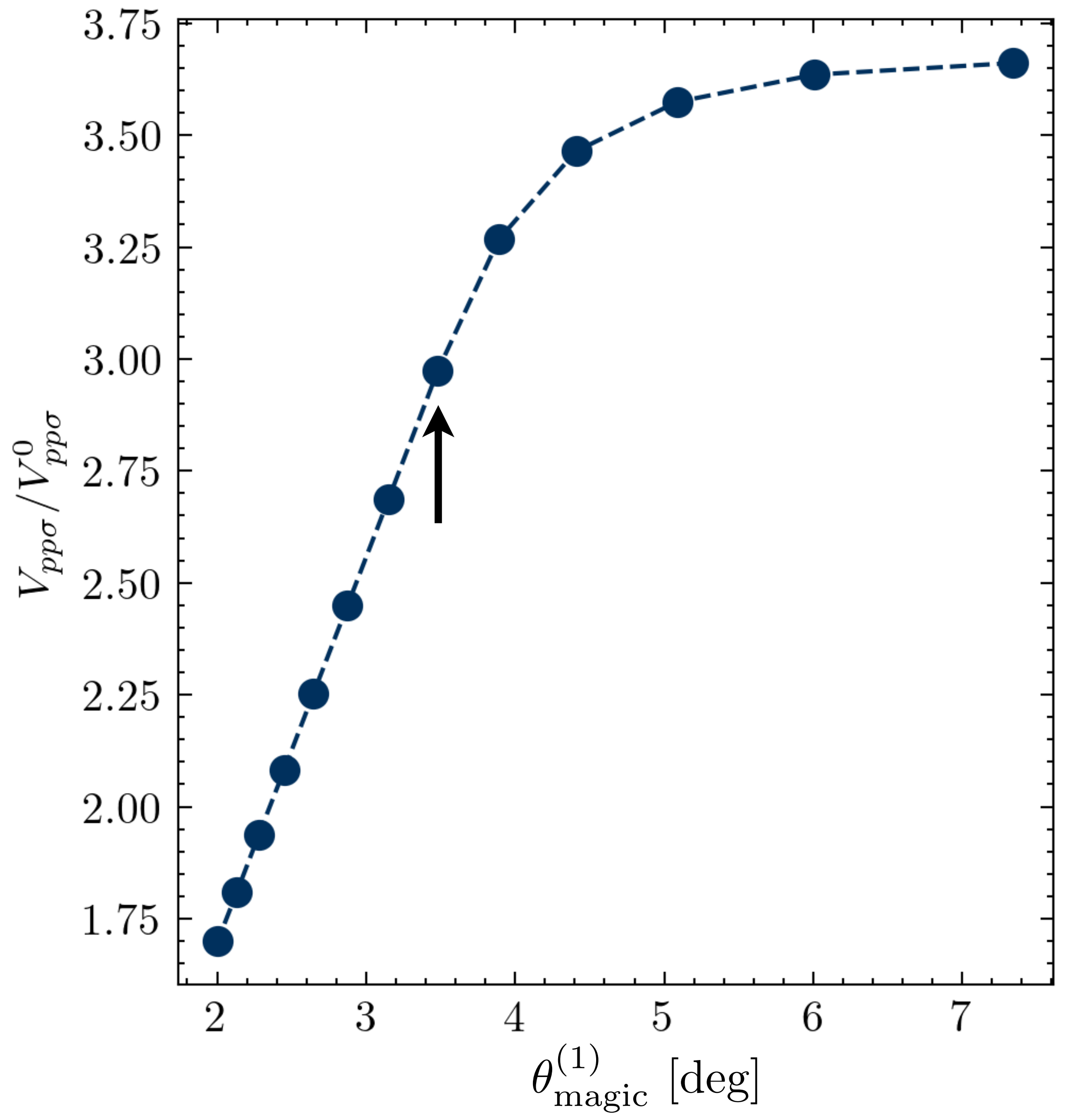


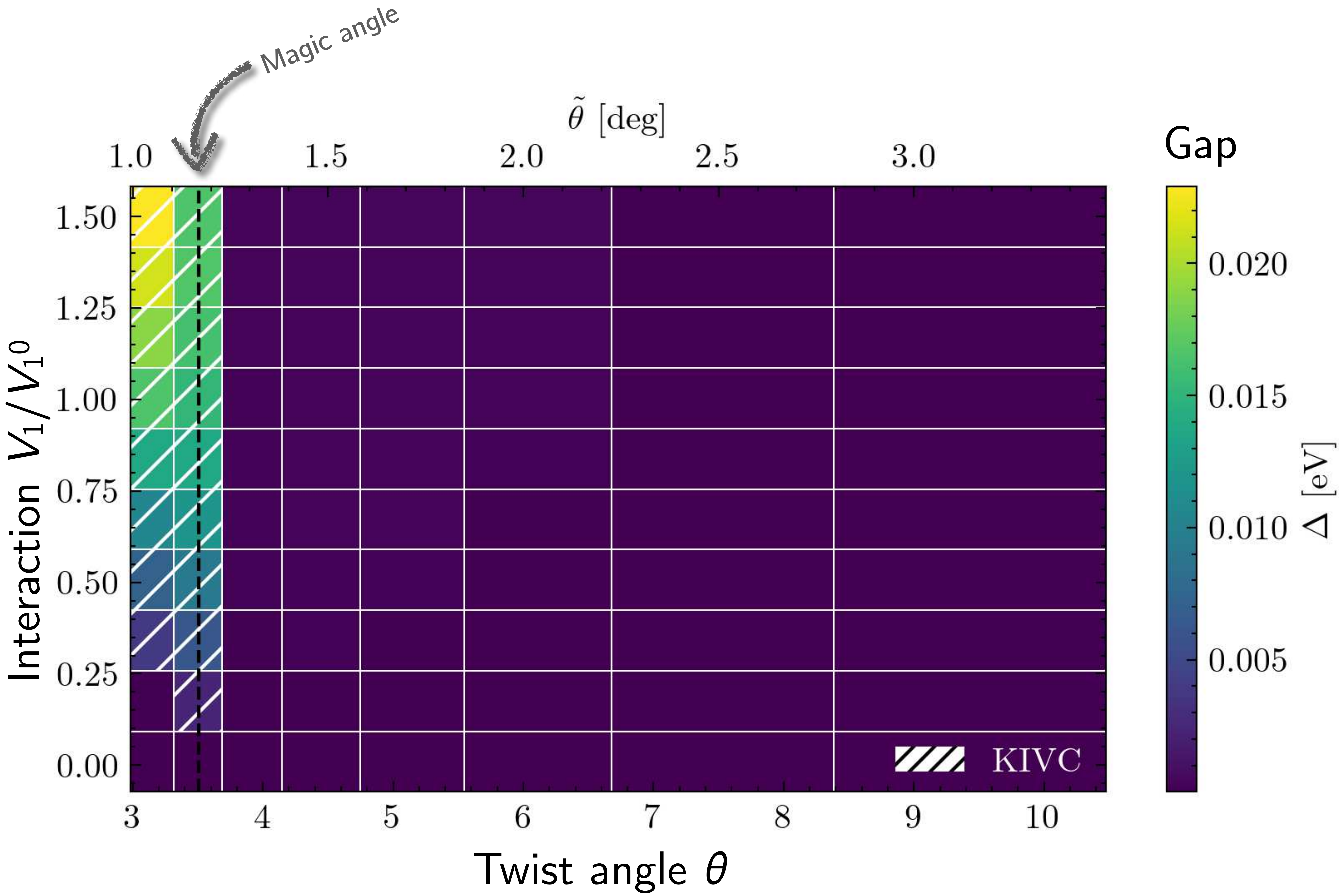
$$H = \sum_{i \neq j} t(\mathbf{R}_i - \mathbf{R}_j)\, c_i^\dagger c_j + V_1 \sum_{\langle ij \rangle} n_i n_j$$

Simplifications:

- Spinless fermions
- Nearest-neighbor intralayer interactions only
- Neglect corrugation effects
- Increased interlayer hopping $V_{pp\sigma}$ … such that $\theta^{(1)}_{\text{magic}} \simeq 3.5°$

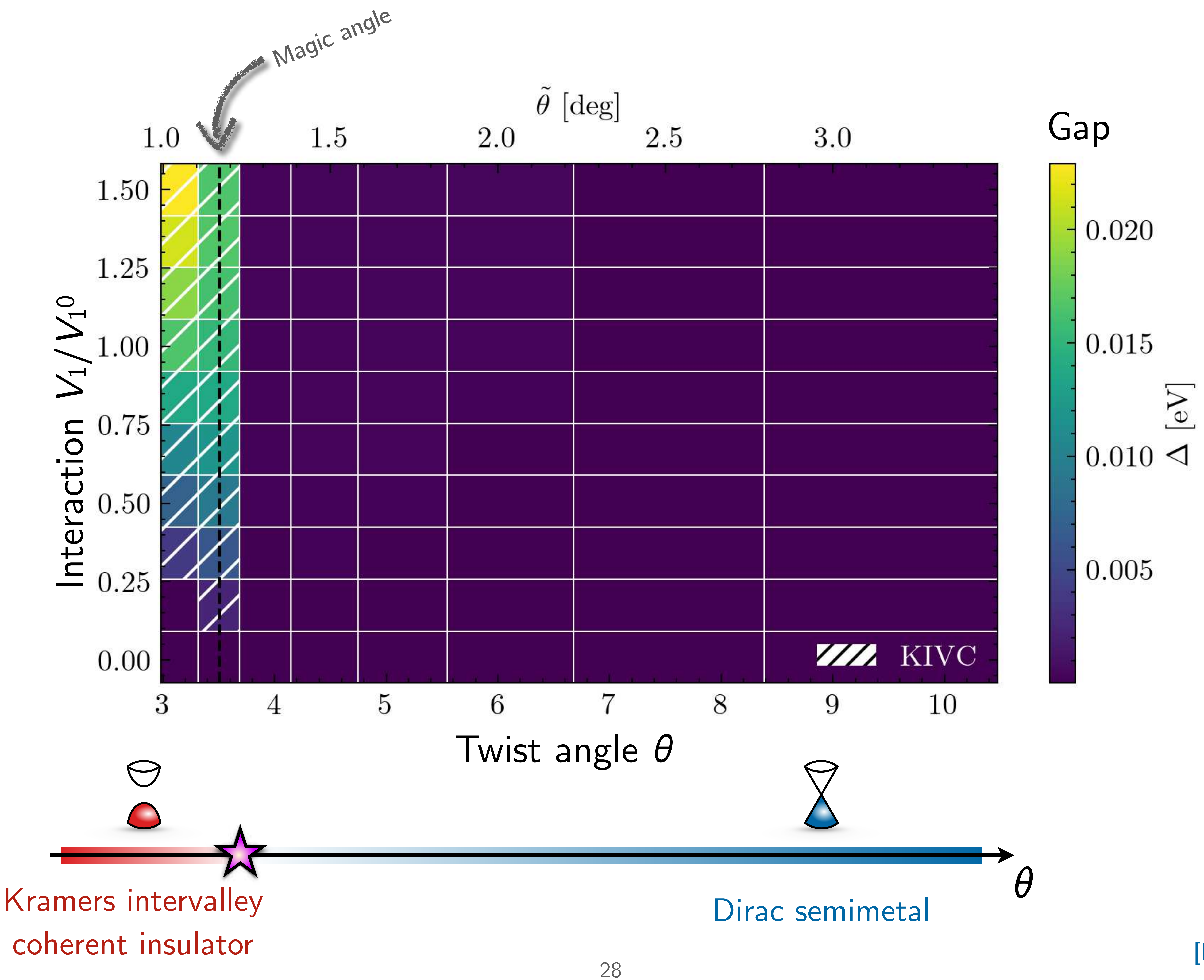


Quantum phase diagram: Mean-field theory



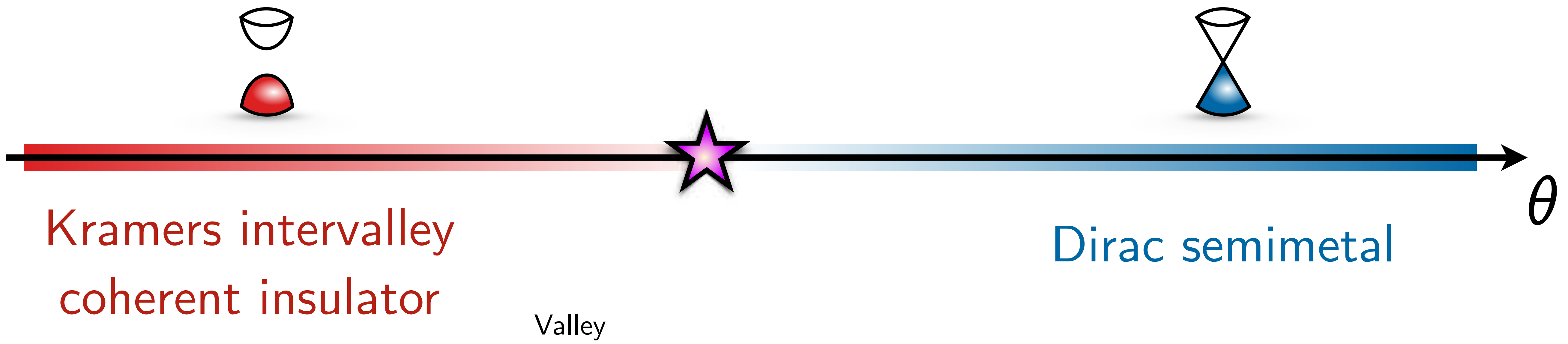
[Biedermann & LJ, *in preparation*]

Quantum phase diagram: Mean-field theory

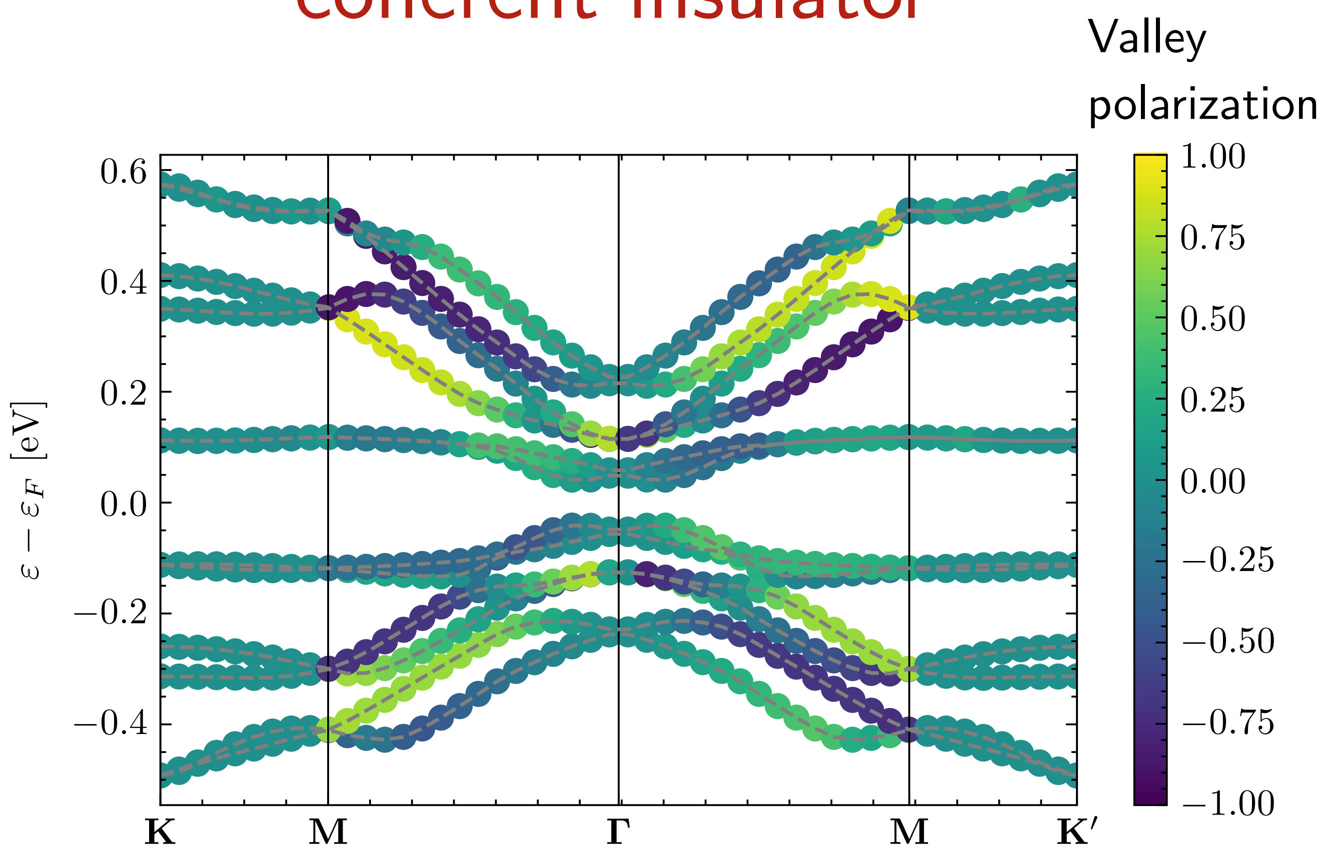


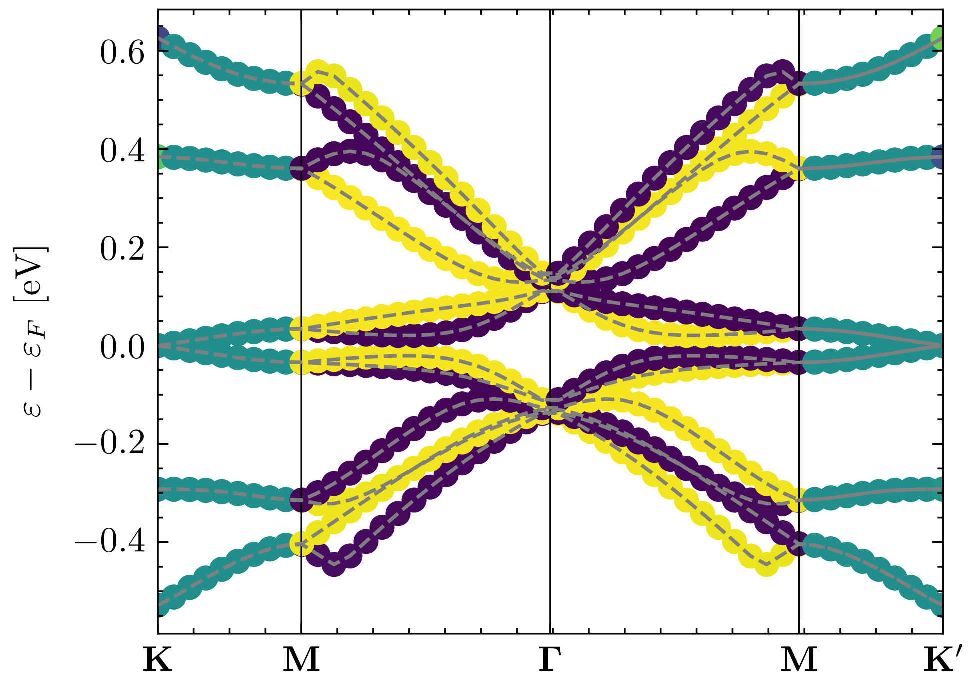
[Biedermann & LJ, *in preparation*]

Twist-tuned transition



Band structure:





[Biedermann & LJ, *in preparation*]

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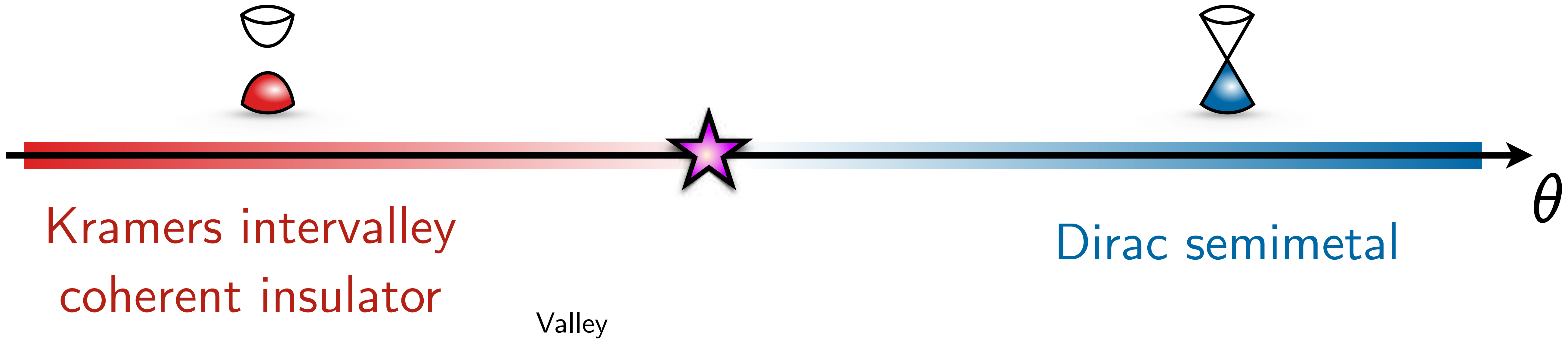

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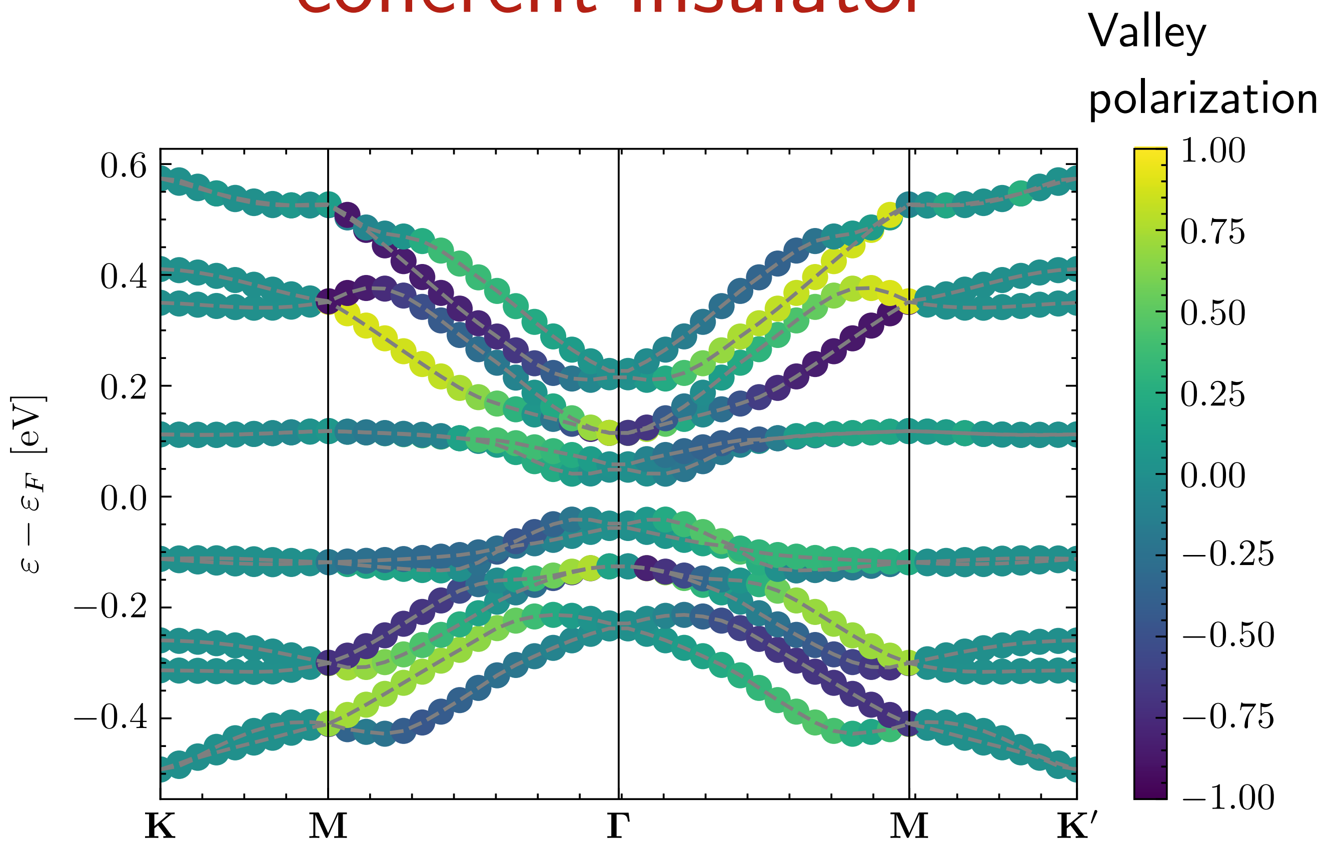
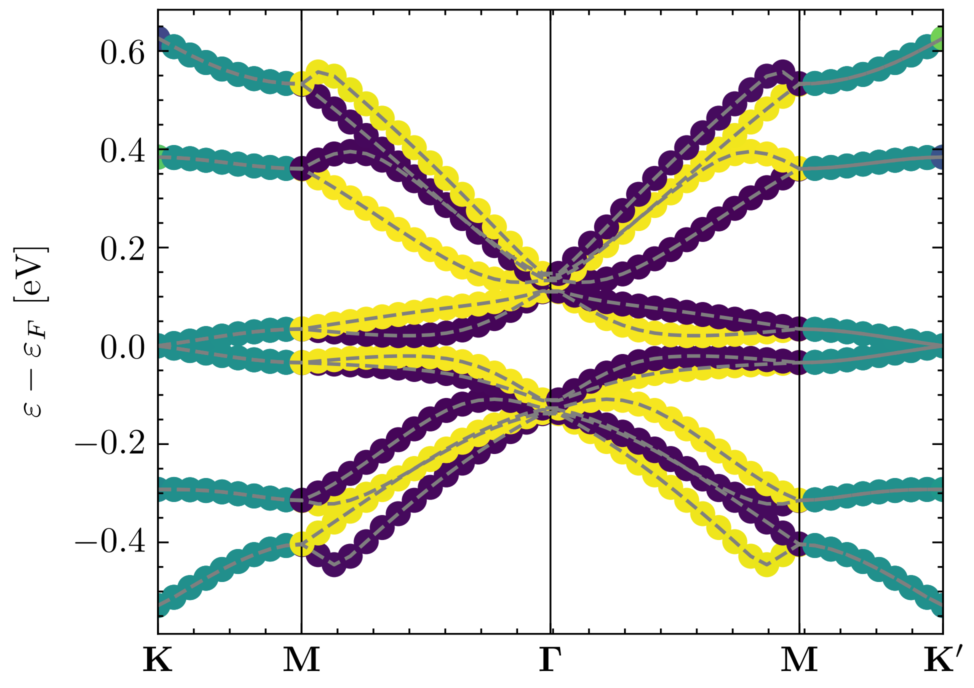
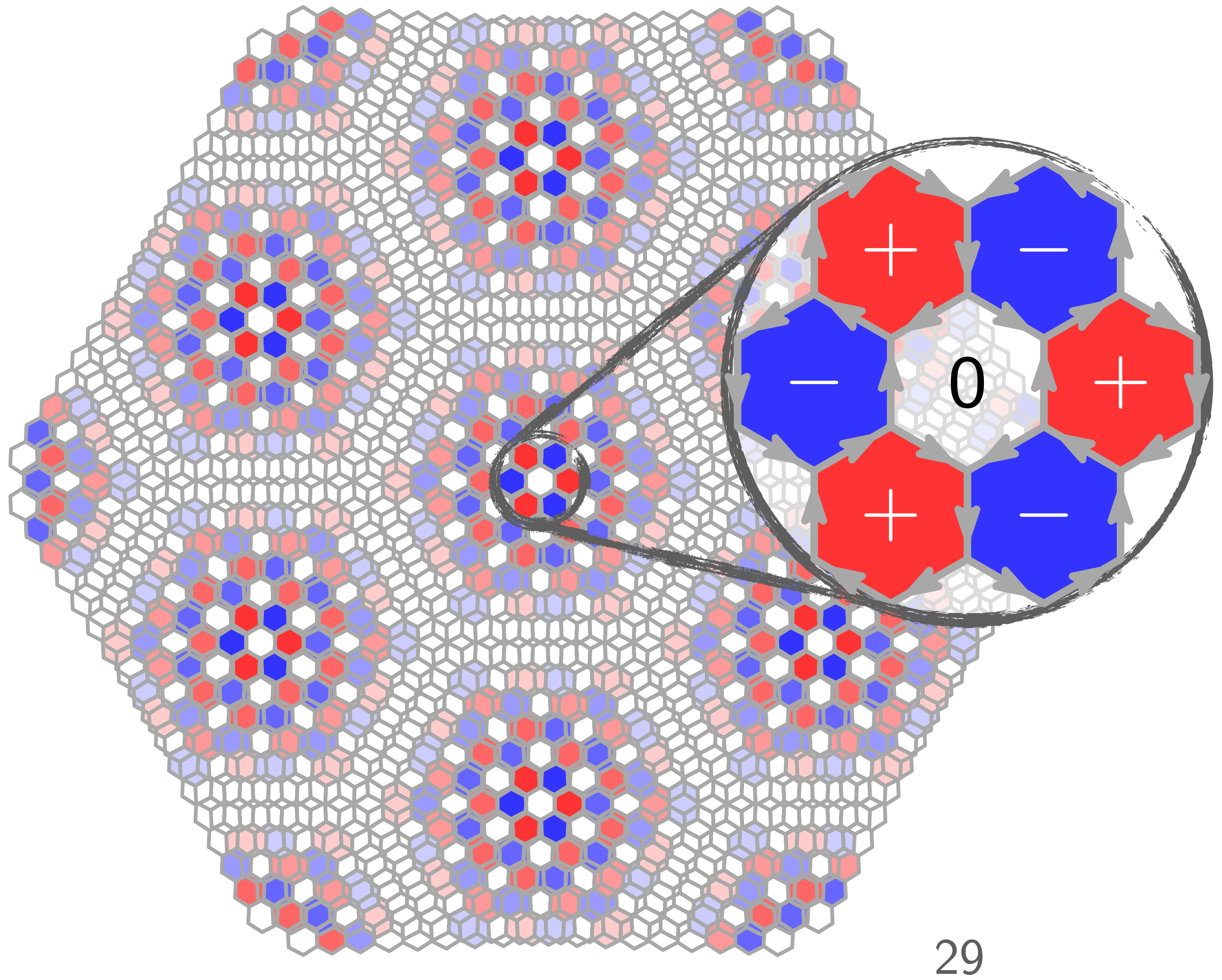




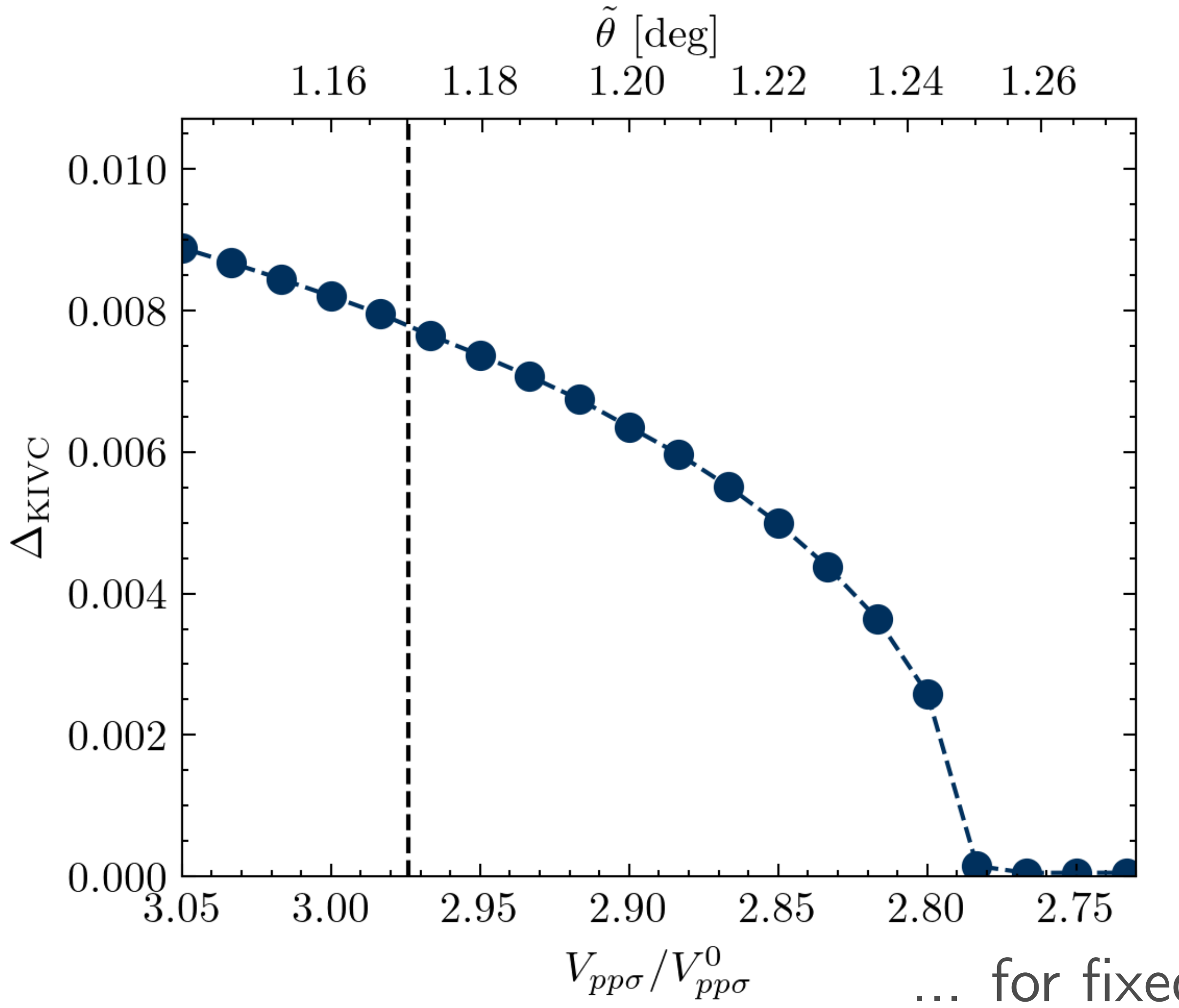
Real-space currents:



[Biedermann & LJ, *in preparation*]

Twist-tuned quantum criticality

KIVC order parameter Δ vs $\tilde{\theta}$:



... for fixed $V_1 = V_1^0 = 1.45\,\mathrm{eV}$

[Biedermann & LJ, *in preparation*]

Twist-tuned quantum criticality

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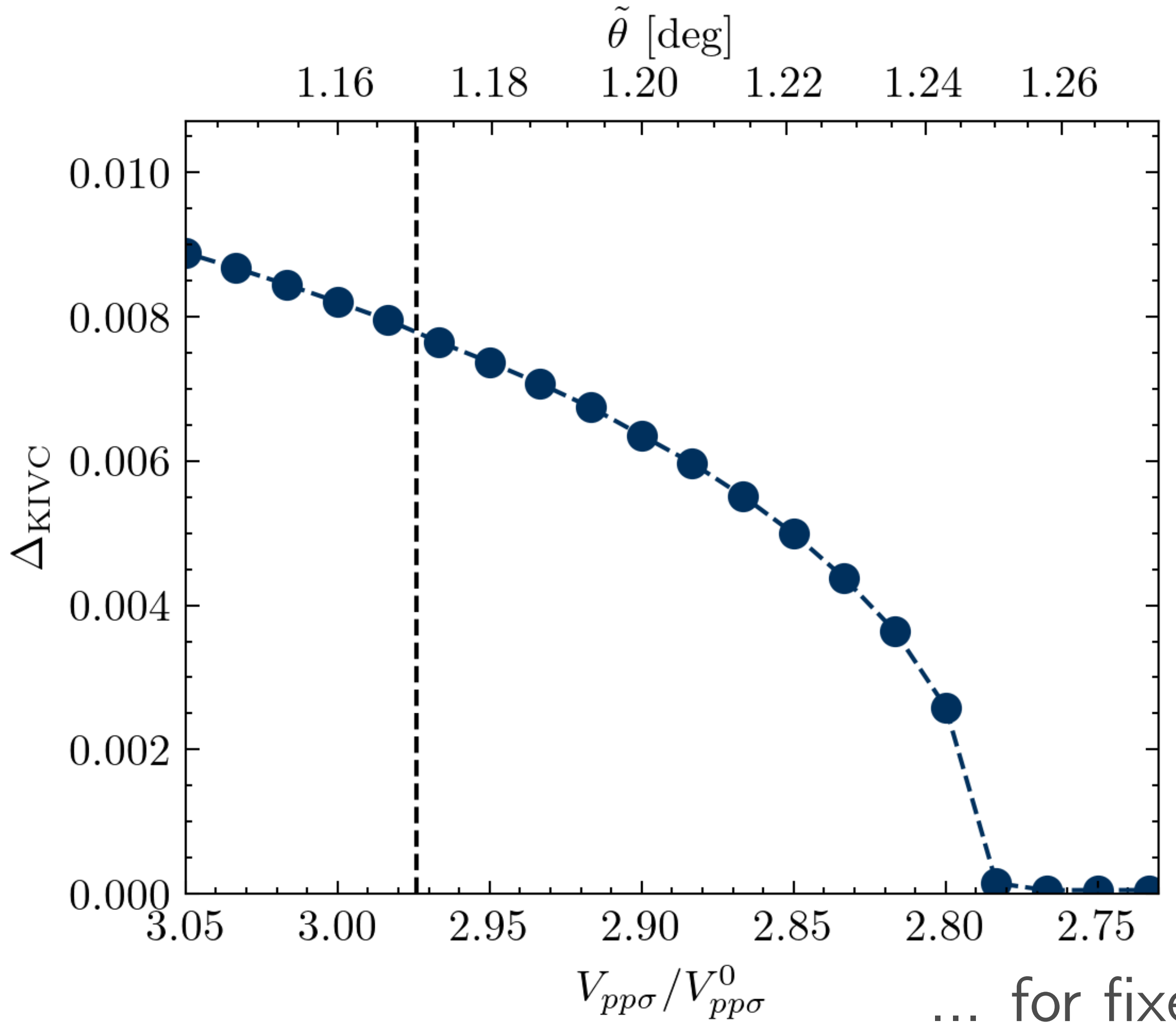

… for fixed $V_1 = V_1^0 = 1.45\,\mathrm{eV}$

Effective field theory:

$$\mathcal{L} = \bar{\psi}\gamma^\mu \partial_\mu \psi + g\left[(\bar{\psi}\gamma_3\psi)^2 + (\bar{\psi}\gamma_5\psi)^2\right]$$

… Gross-Neveu-XY

with emergent Lorentz invariance

[Biedermann & LJ, *in preparation*]

Twist-tuned quantum criticality

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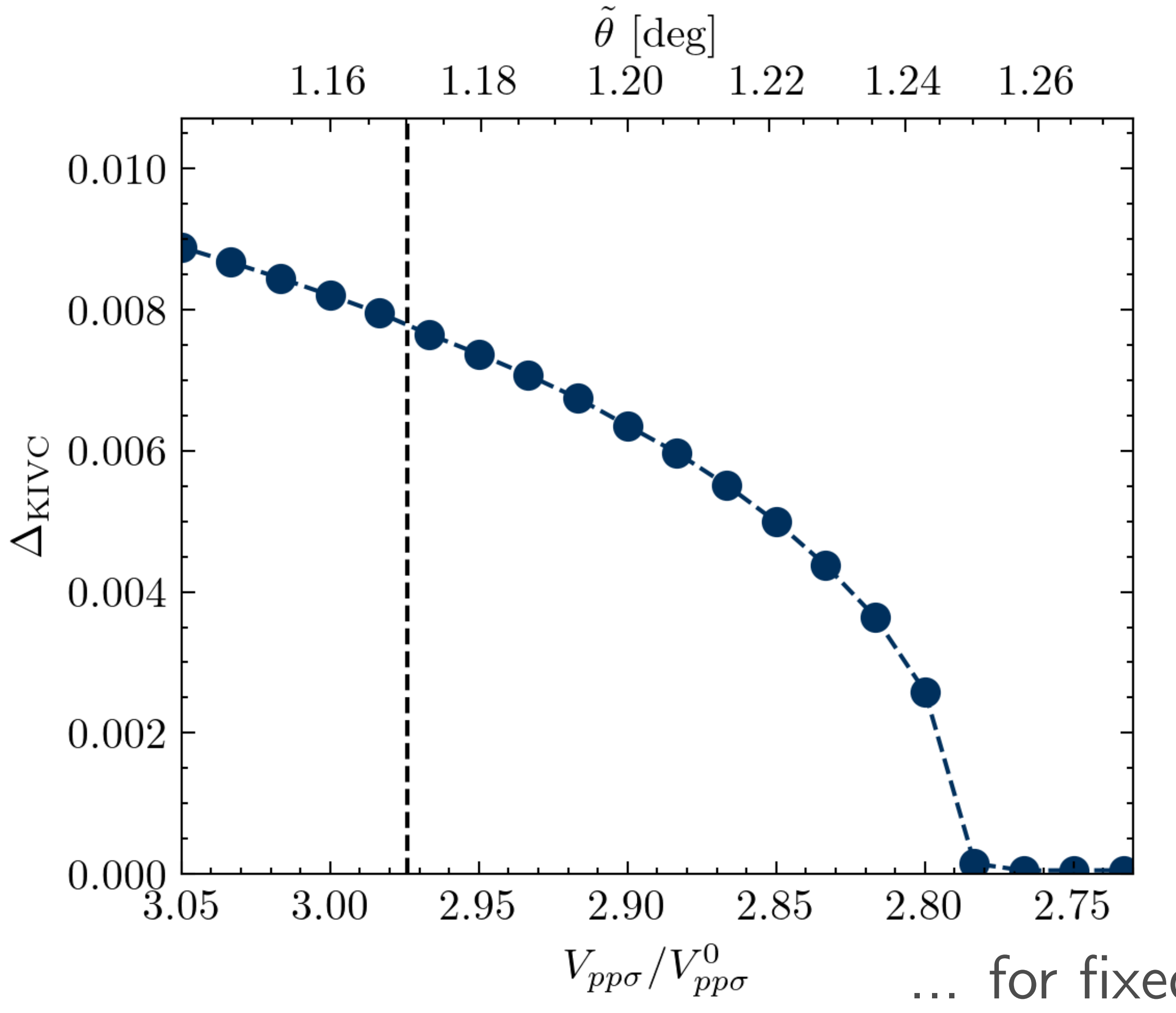

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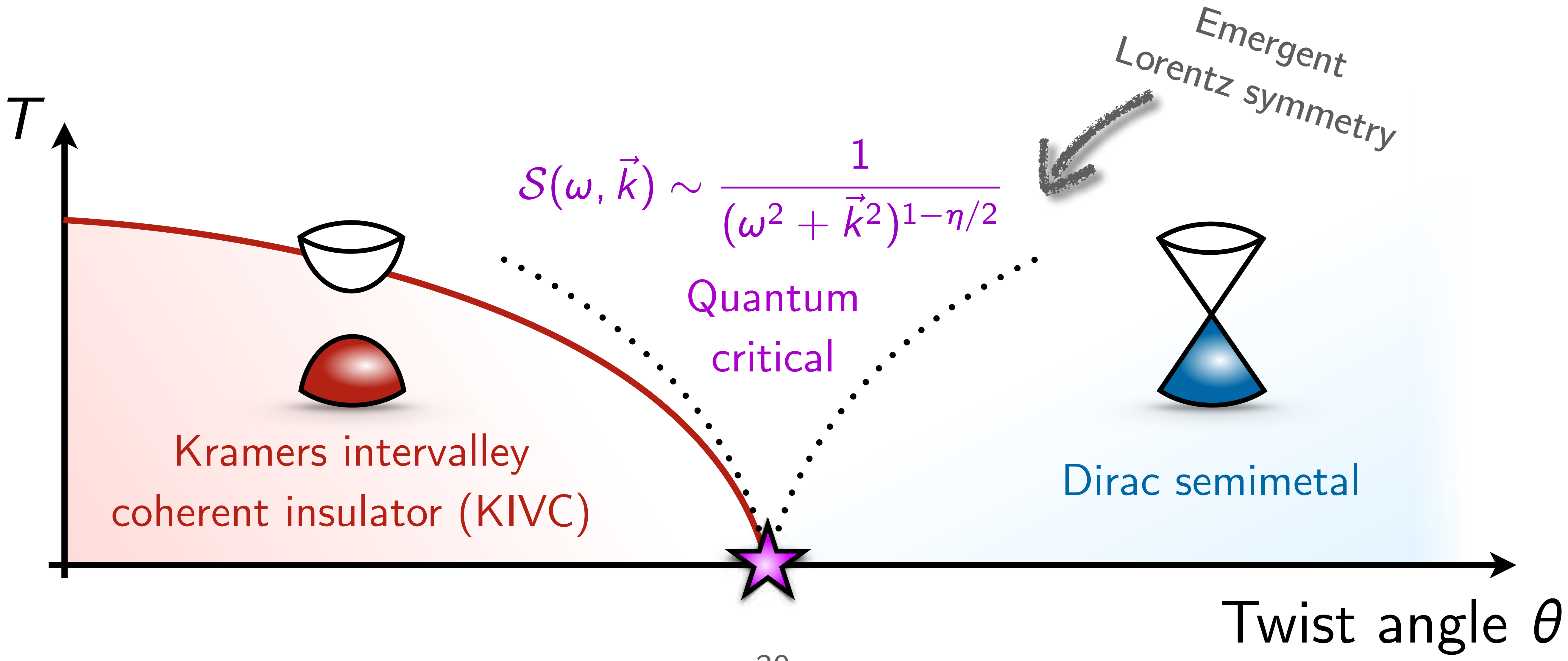
Phase diagram:

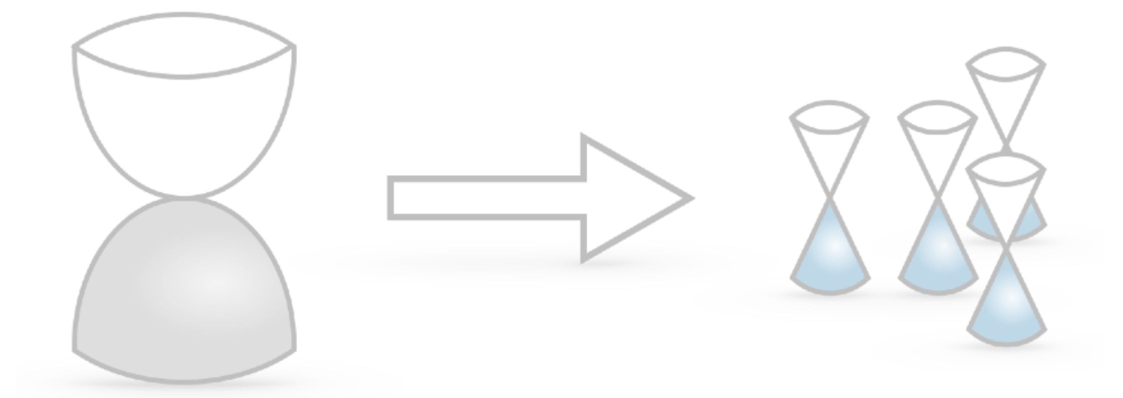


[Biedermann & LJ, *in preparation*]

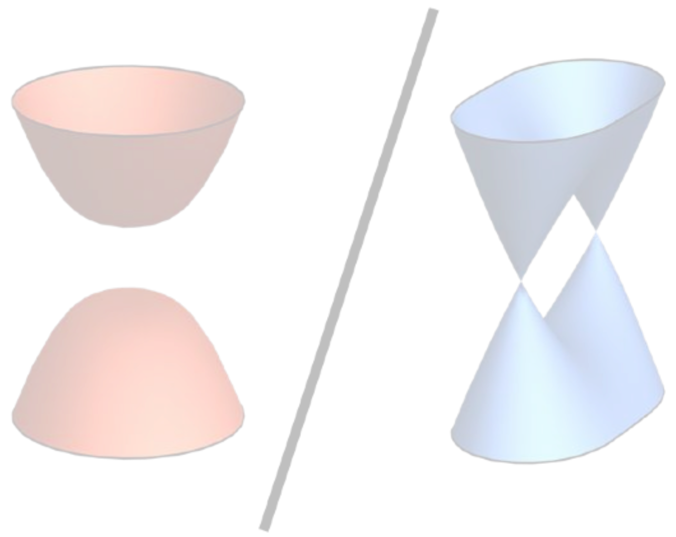
Outline

(1) Introduction

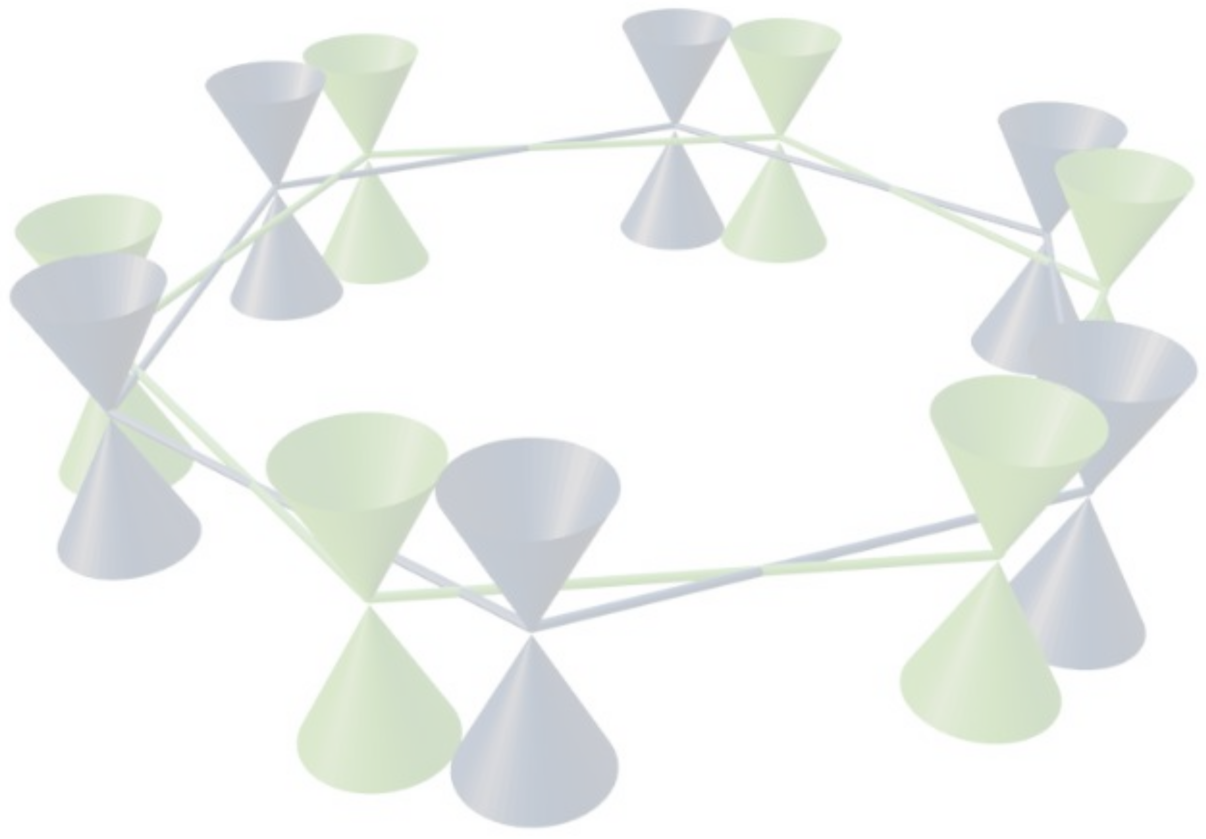
(2) Interaction-induced Dirac cones



(3) Competing nematic & antiferromagnetic orders

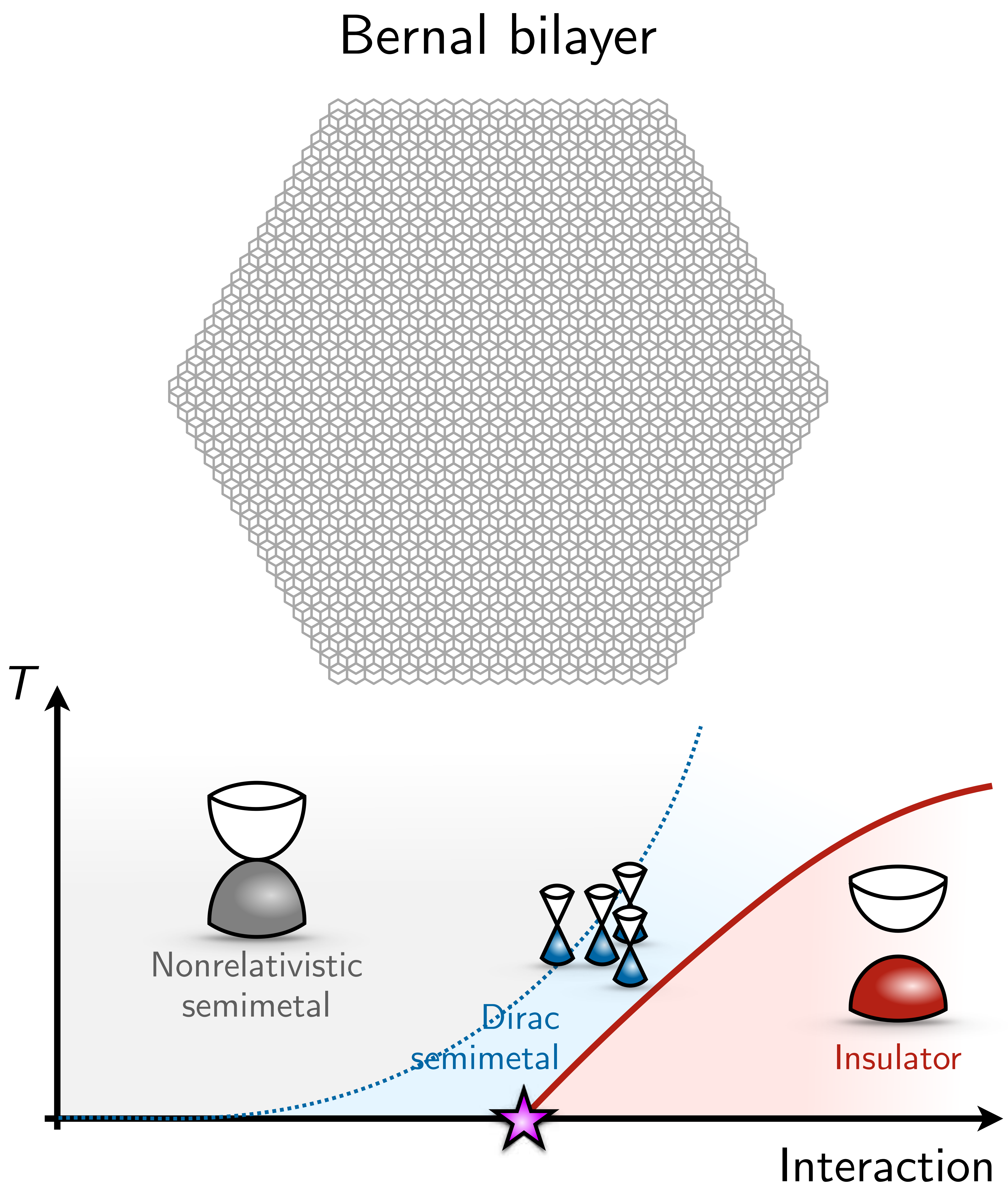


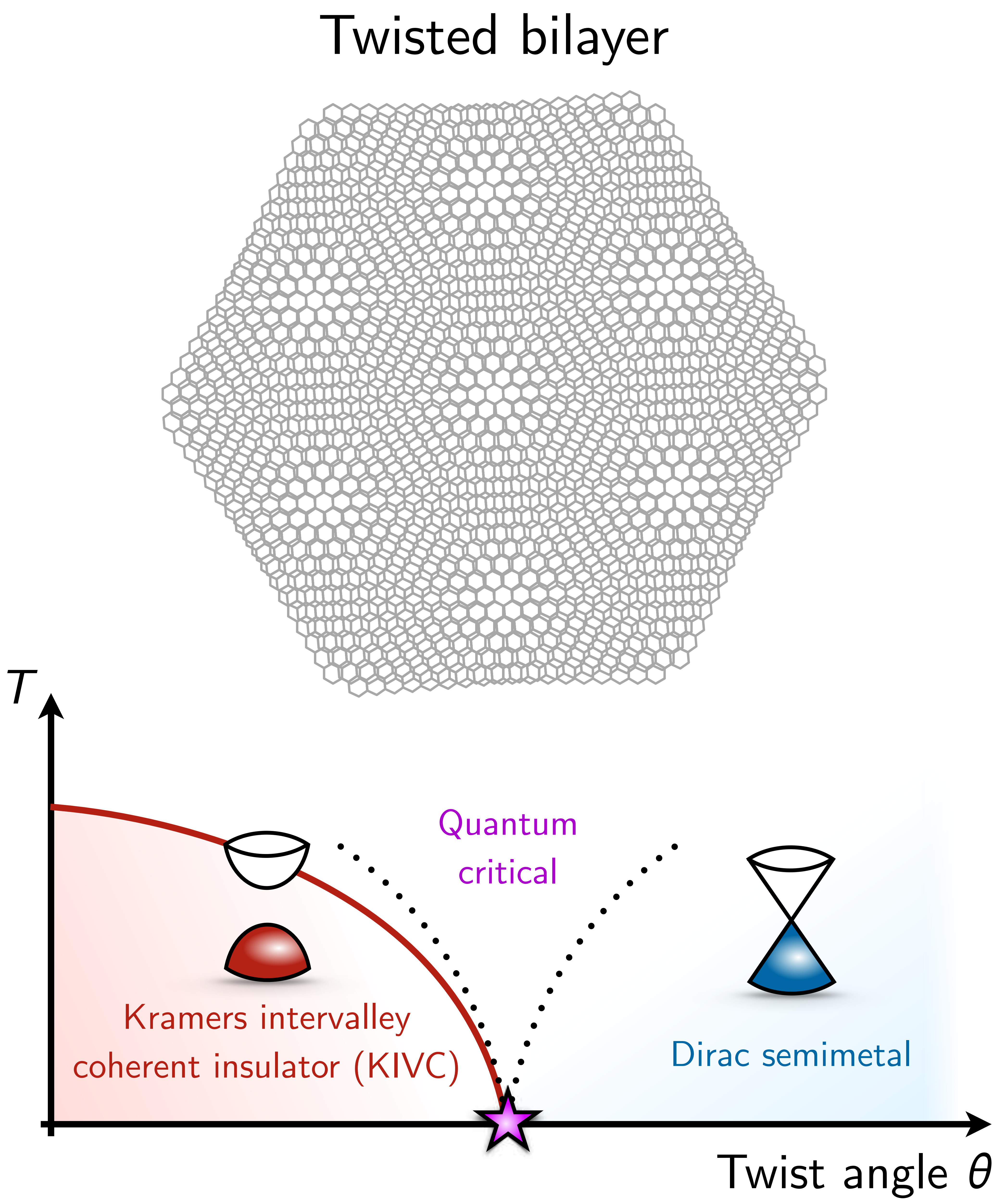
(4) Twist-tuned quantum criticality



(5) Conclusions

Conclusions





Candidate ground states

State of Matter	C_2	$\mathcal{T}$	$C_2\mathcal{T}$	$U_V(1)$
Semimetallic (SM)	✓	✓	✓	✓
Valley-Hall (VH)	✗	✓	✗	✓
Quantum Anomalous Hall (QAH)	✓	✗	✗	✓
Valley-Polarized (VP)	✗	✗	✓	✓
Kramers Intervalley-Coherent (KIVC)	✗	✗	✓	✗

Valley polarization

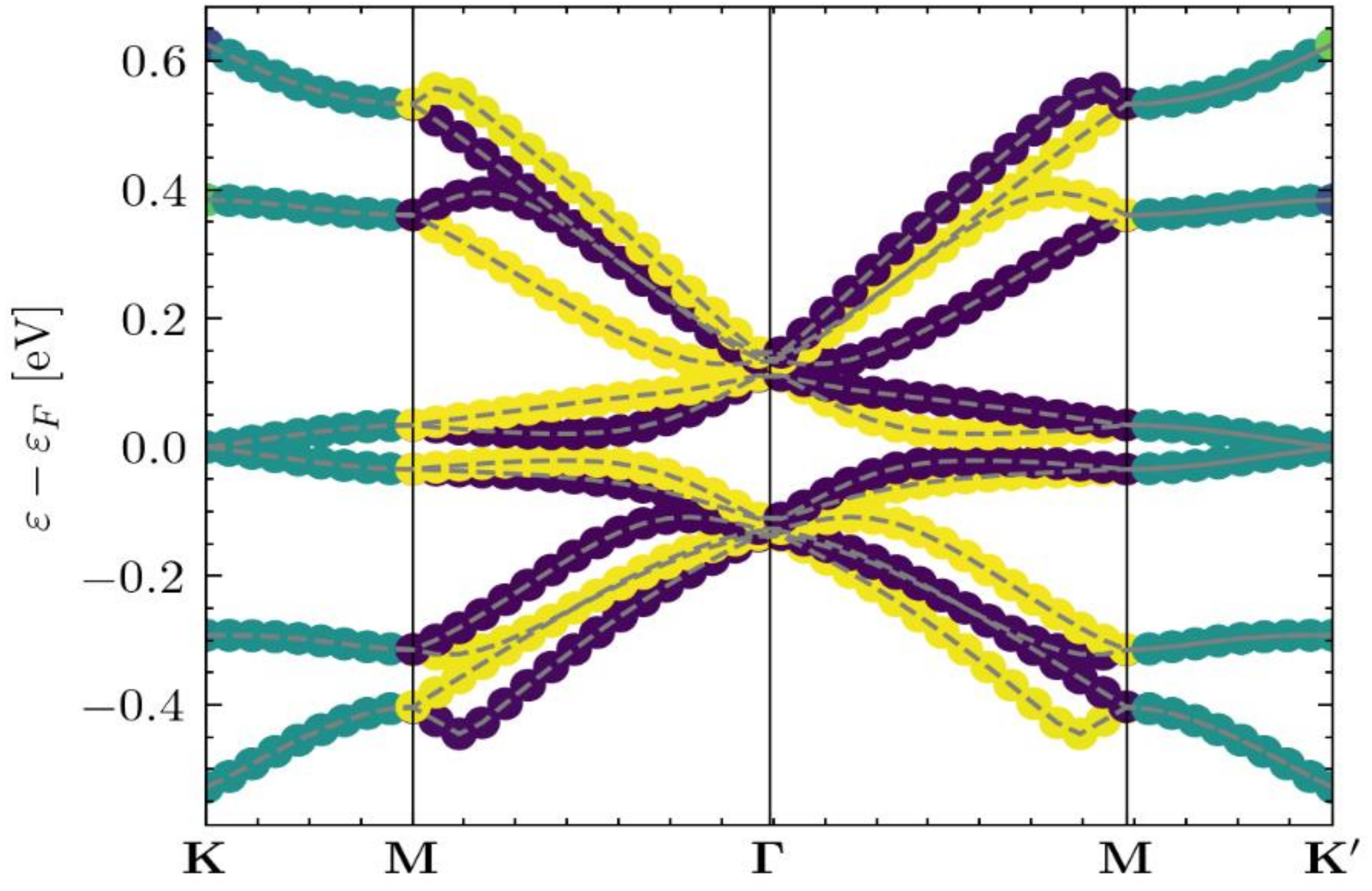
Valley polarization operator:

$$V_\ell = \frac{\mathrm{i}}{3\sqrt{3}} \sum_{\langle\langle ij \rangle\rangle \in \ell} \eta_{ij} \sigma_z^{ij} c_i^\dagger c_j$$

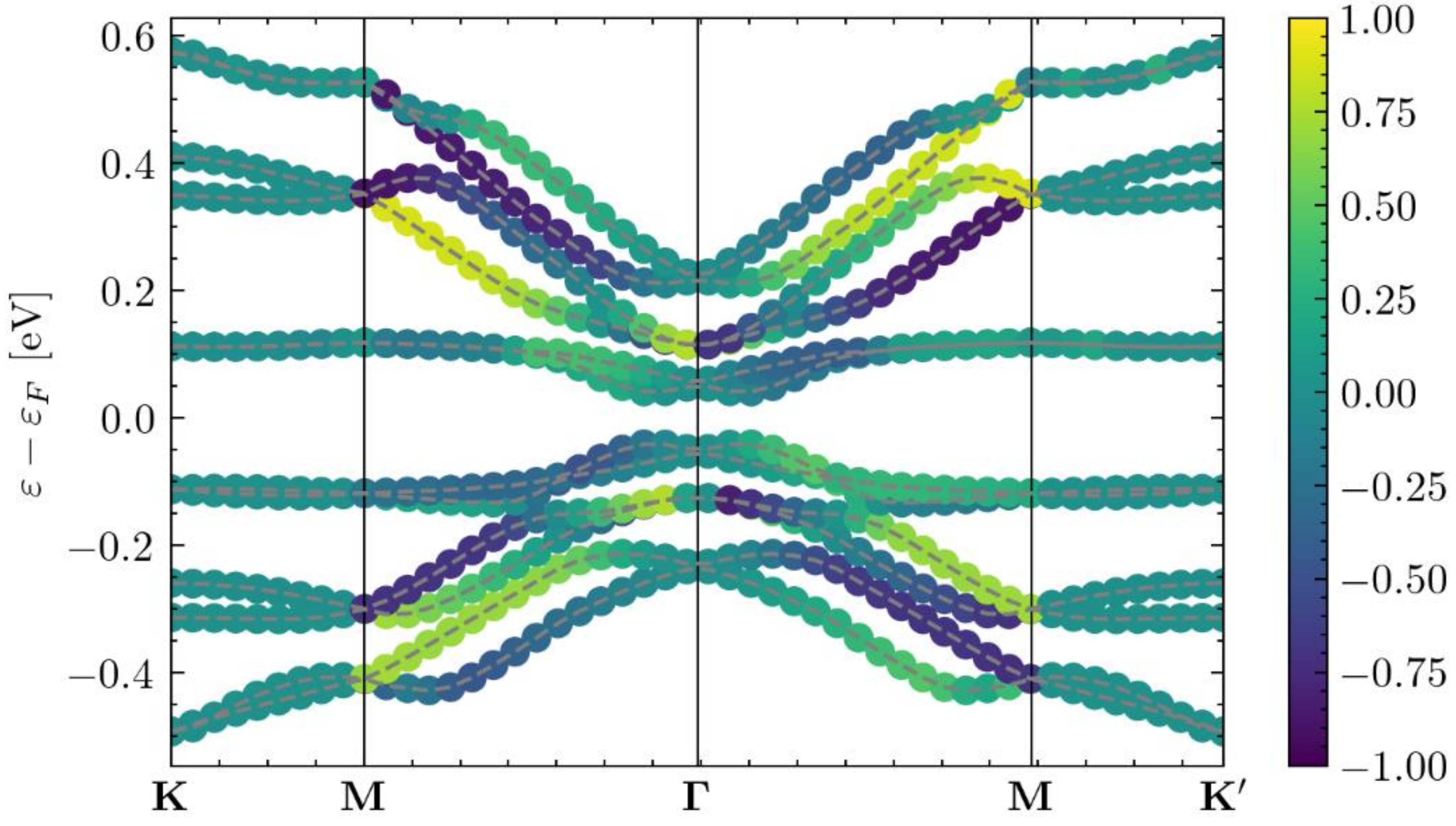
... with $\eta_{ij} = \pm 1$ for clockwise (counterclockwise) hopping

[Ramires & Lado, PRB '19]

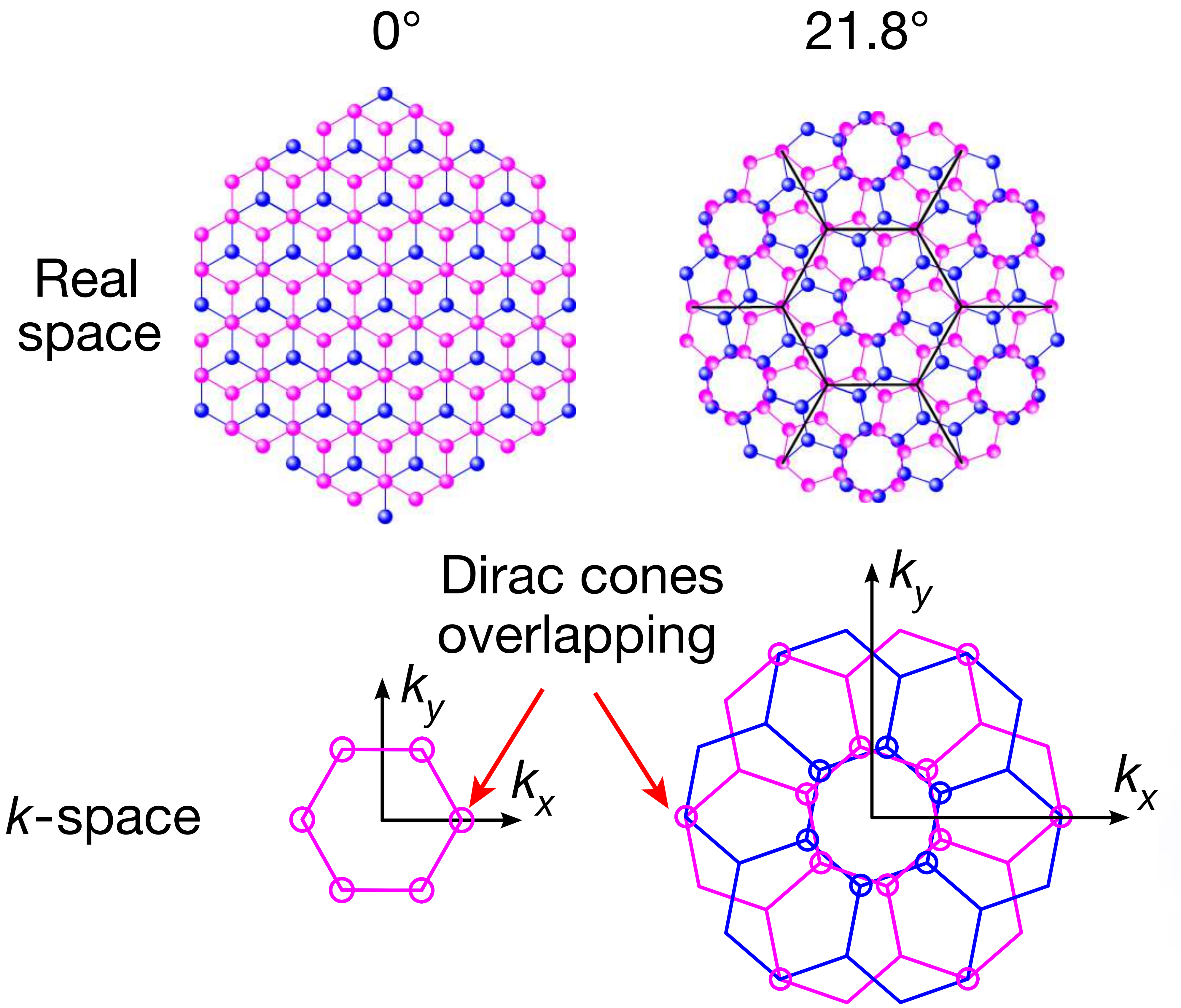
Dirac semimetal



KIVC insulator



Overlapping Dirac cones



Overlapping Dirac cones

$T = 300$ K