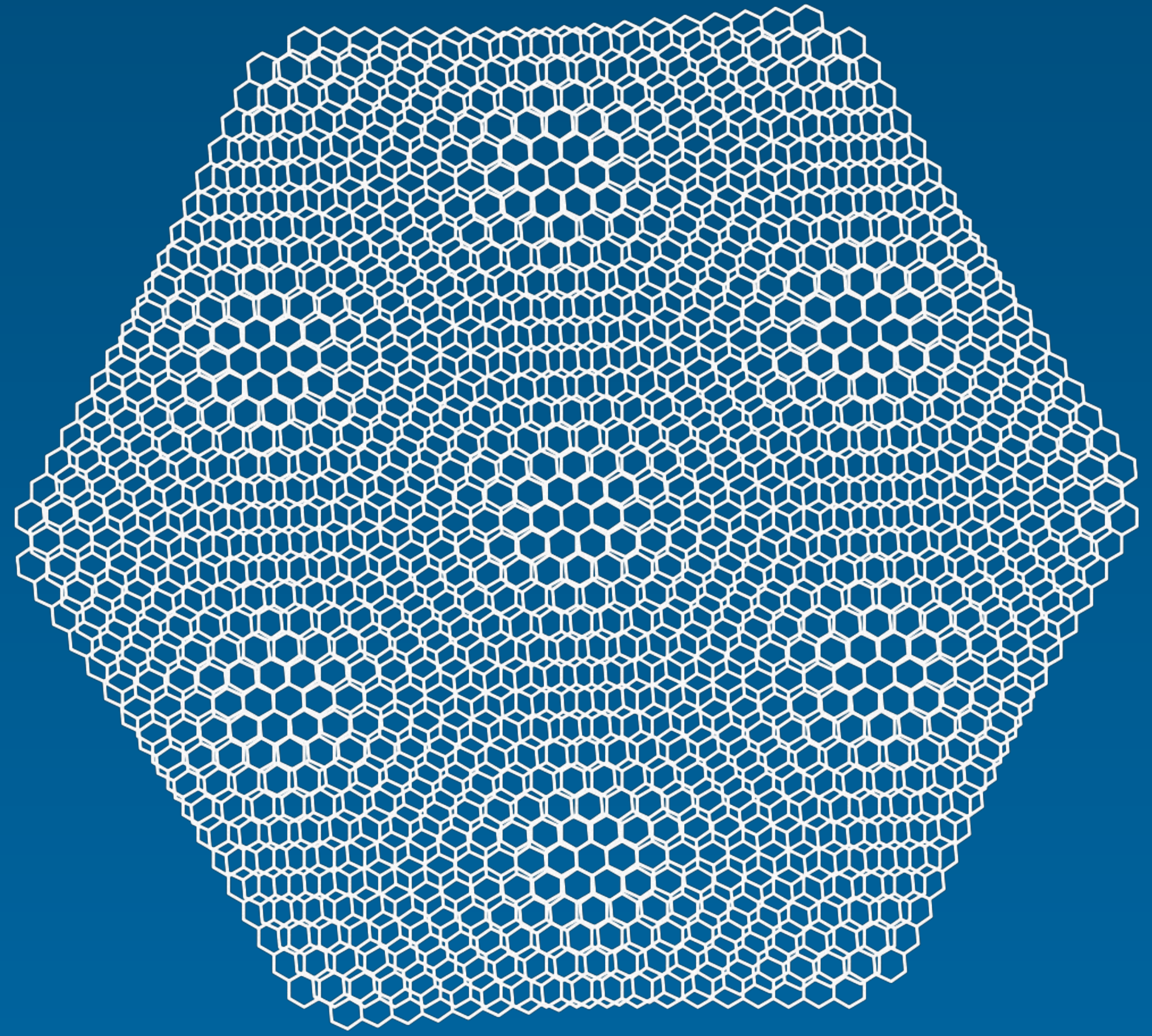
Dresden University of Technology

DRESDEN concept

Dirac quantum criticality in moiré systems



Lukas Janssen

Jan Biedermann

Emmy Noether-Programm

DFG Deutsche Forschungsgemeinschaft

ct.qmat Complexity and Topology in Quantum Matter

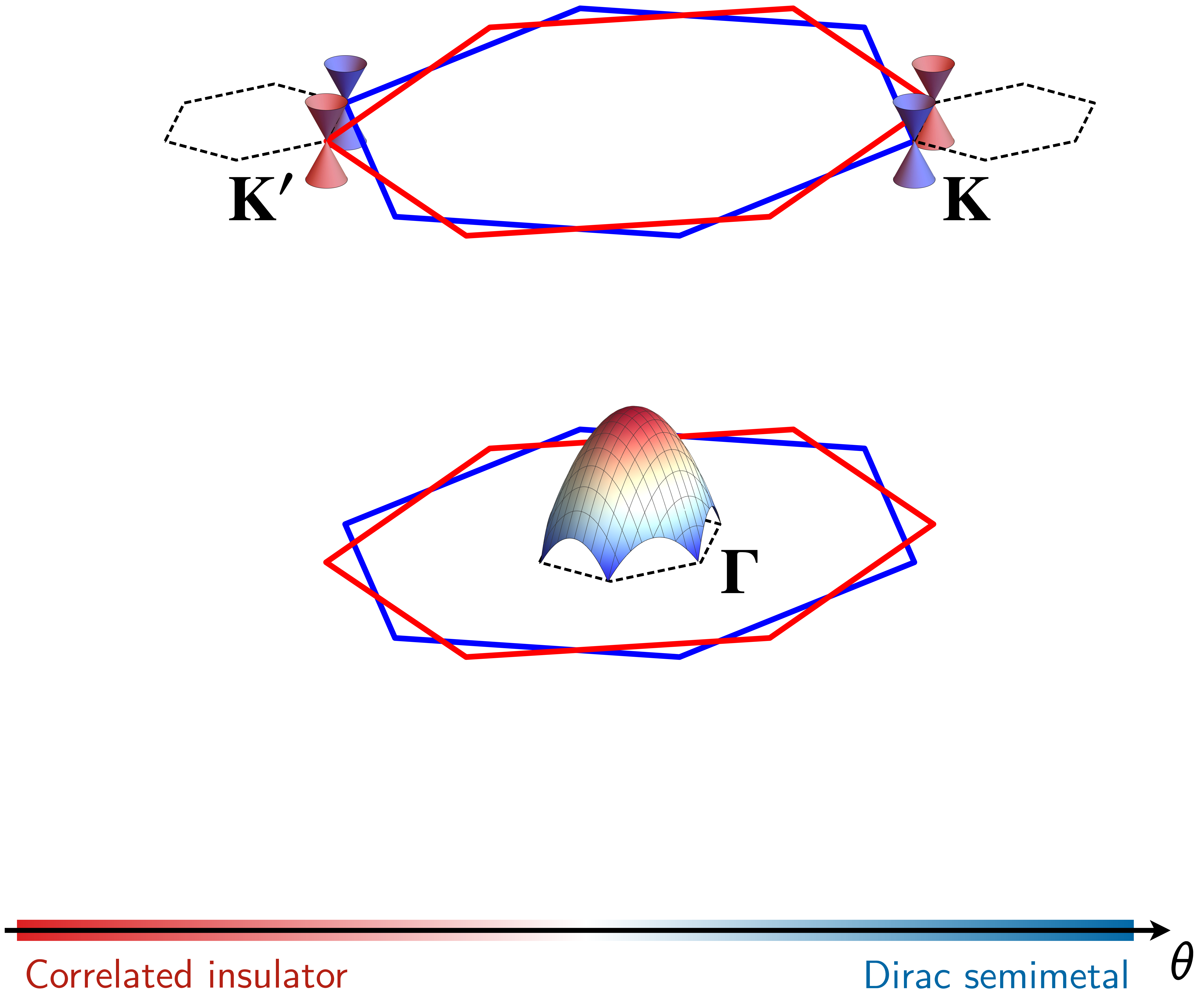
Outline

(1) Introduction

(2) Twisted bilayer graphene

(3) Twisted double bilayer TMDs

(4) Conclusions



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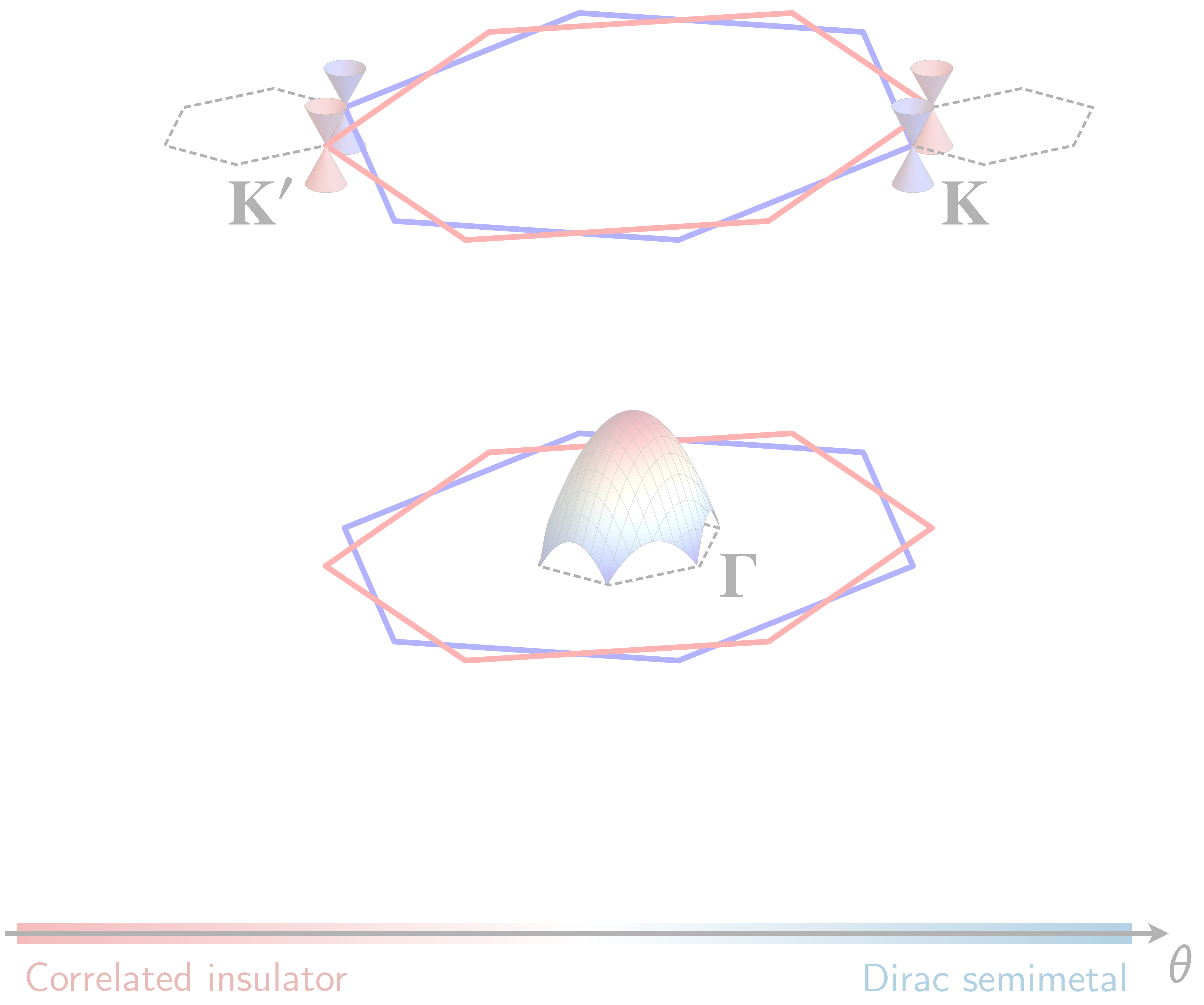
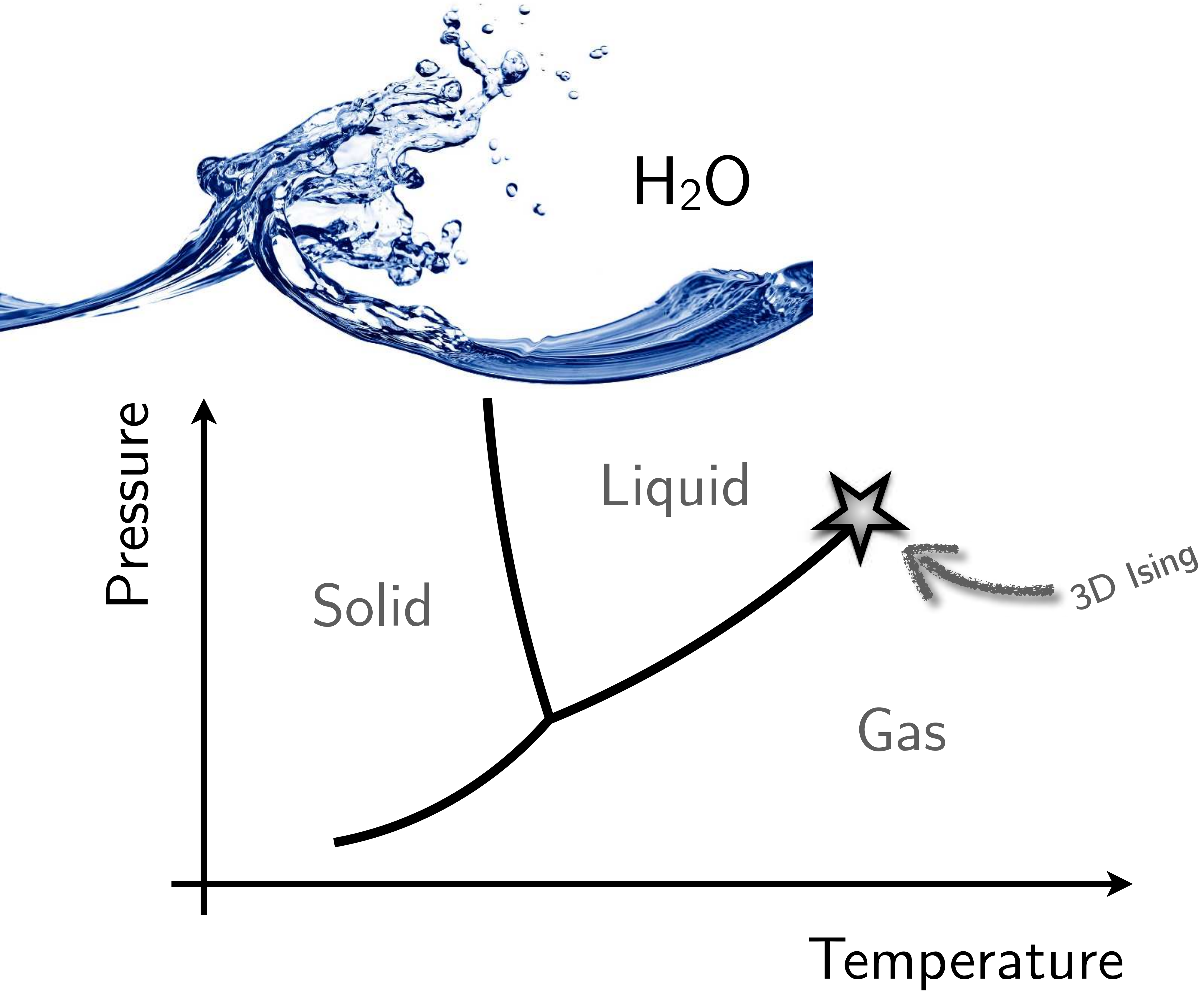
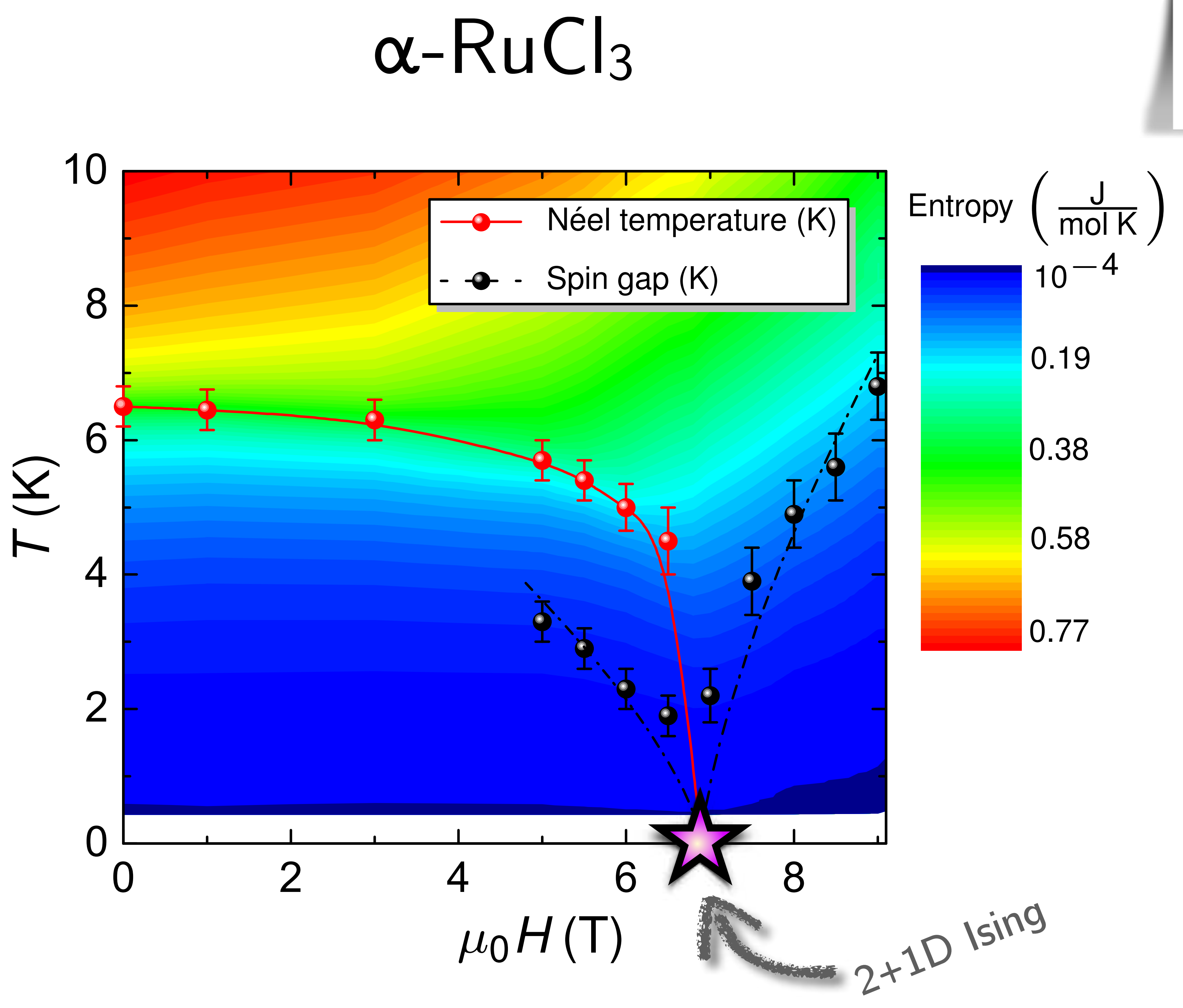
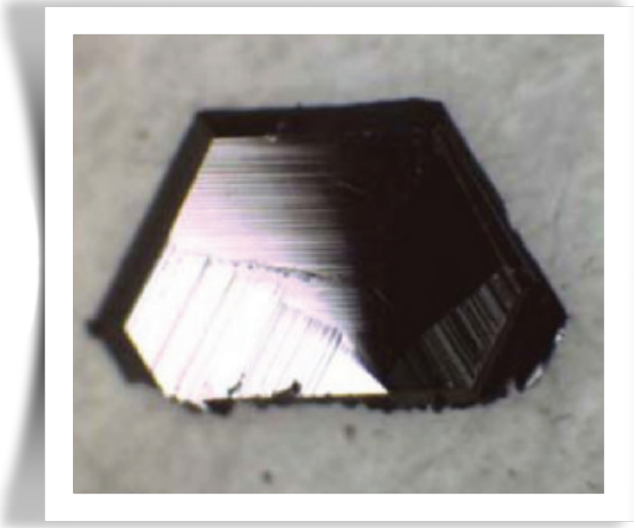


Classical vs quantum criticality





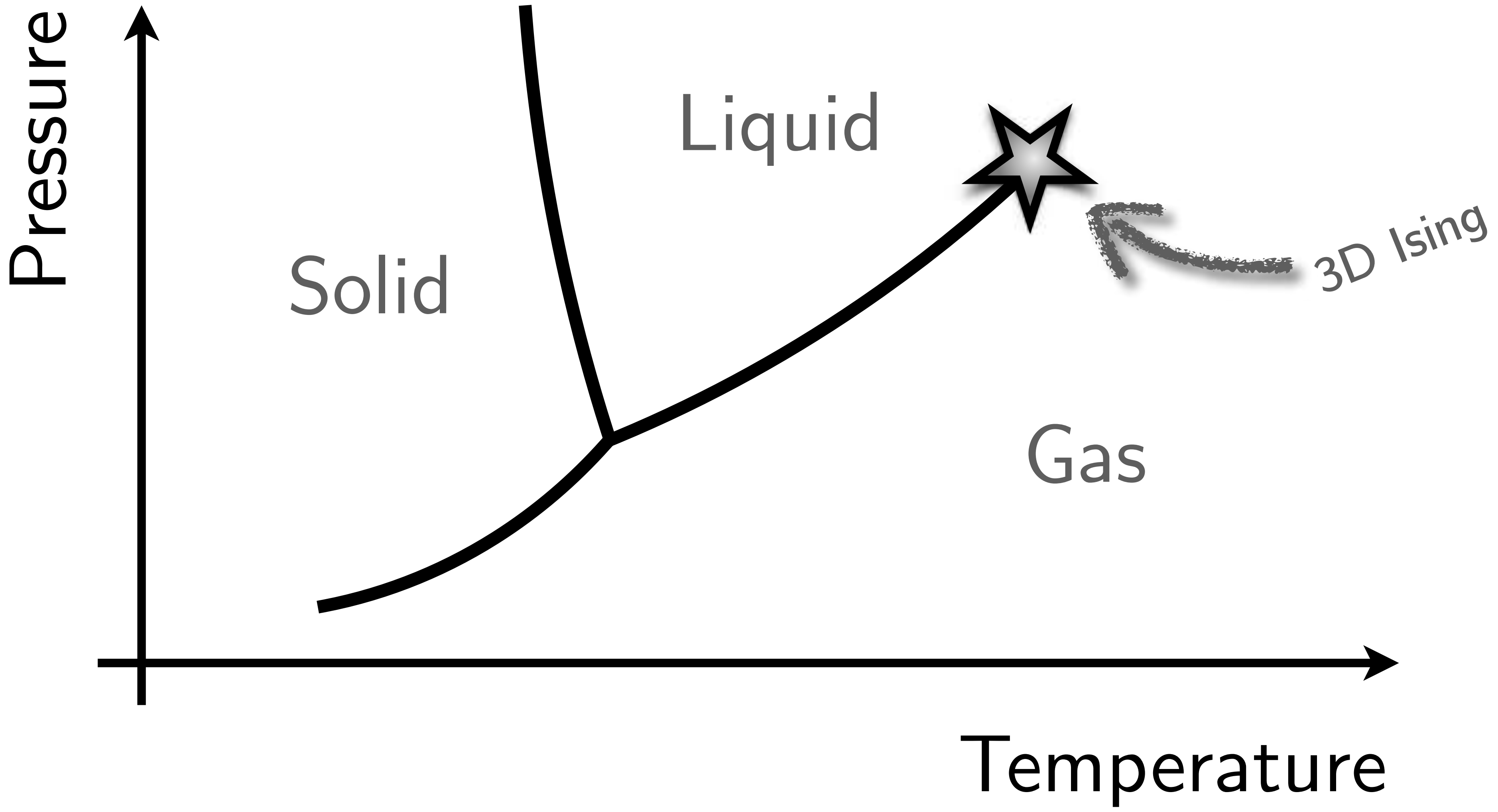


Credit: Jennifer Sears

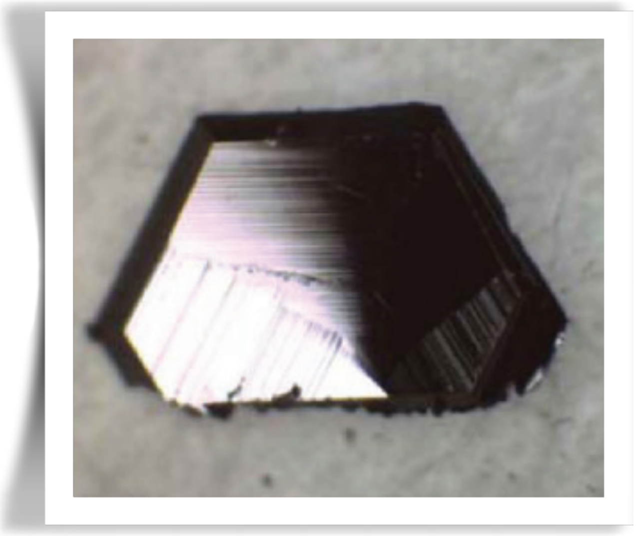
[Wolter, Corredor, LJ, *et al.*, PRB ’17]

Classical vs quantum criticality

H_2O



α-$RuCl_3$



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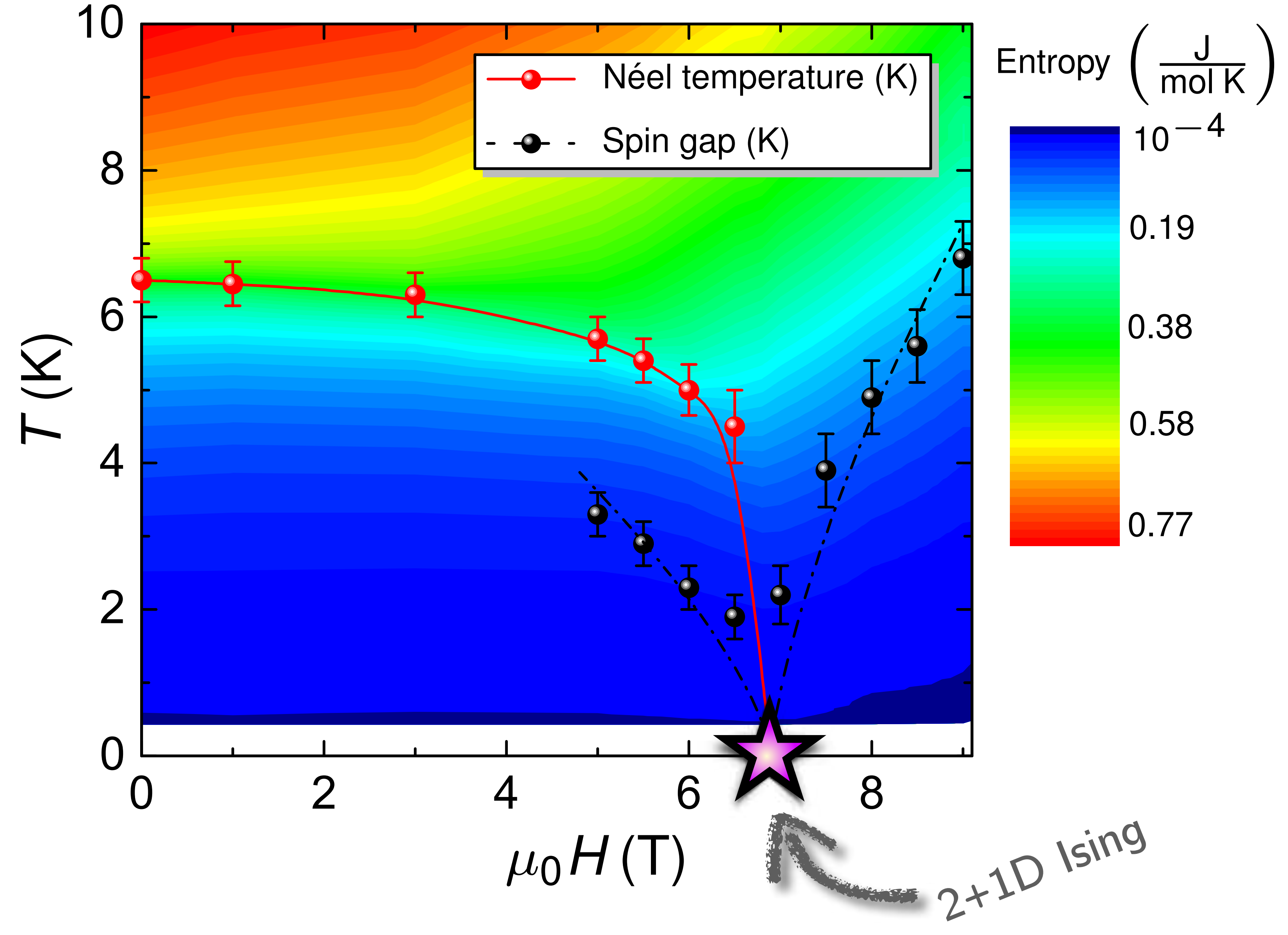
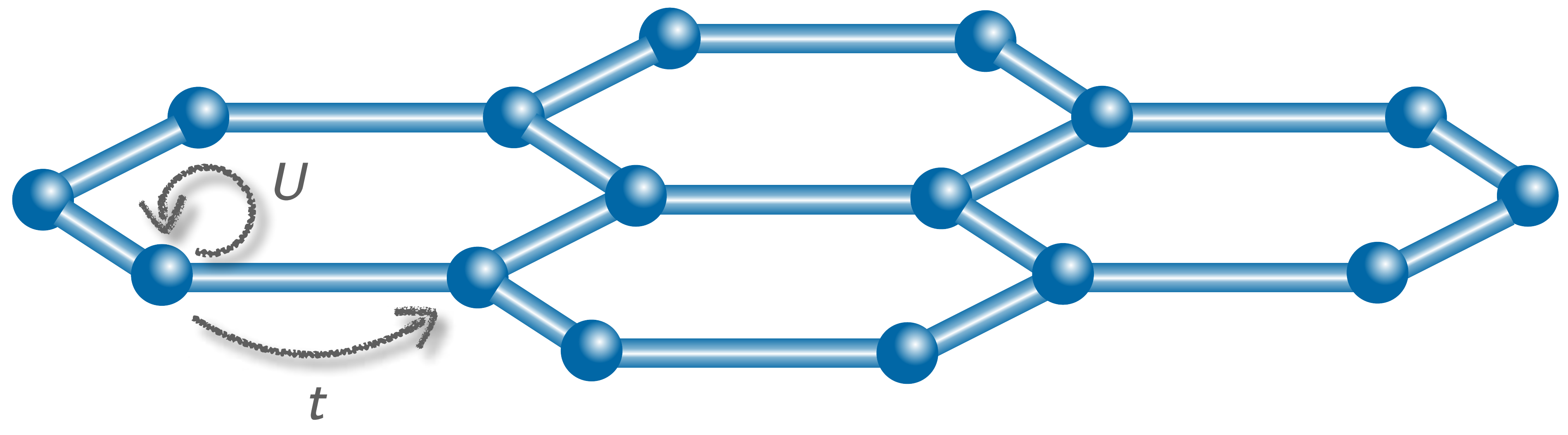


[Wolter, Corredor, LJ, *et al.*, PRB '17]

Universal field theory:

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \varphi)^2 + \frac{r}{2}\varphi^2 + \lambda\varphi^4 + \dots$$

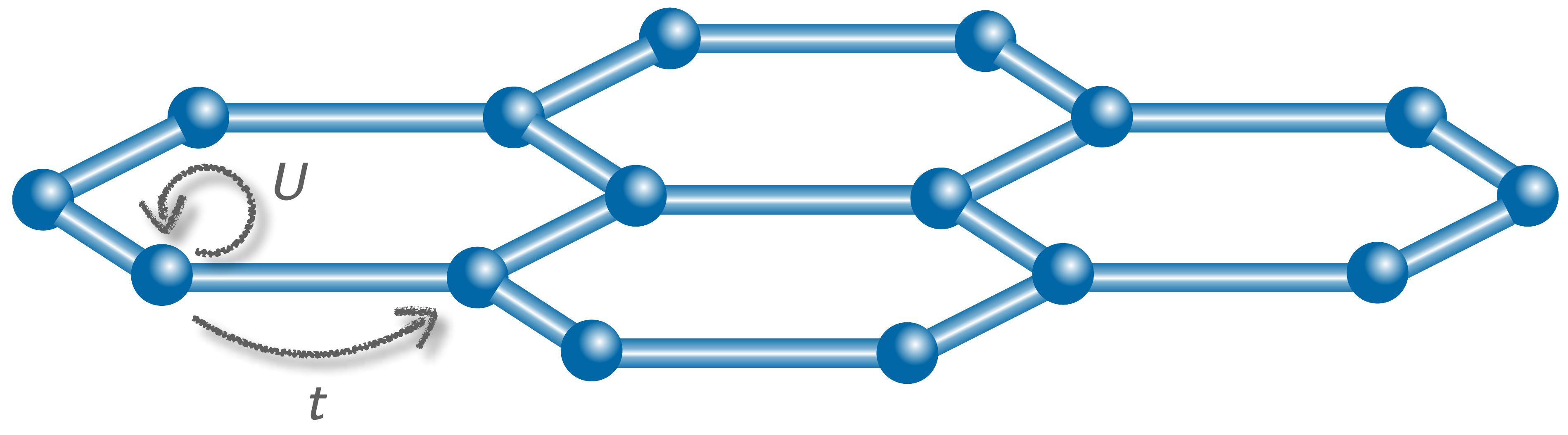
Fermionic quantum criticality



Honeycomb-lattice Hubbard model:

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Fermionic quantum criticality



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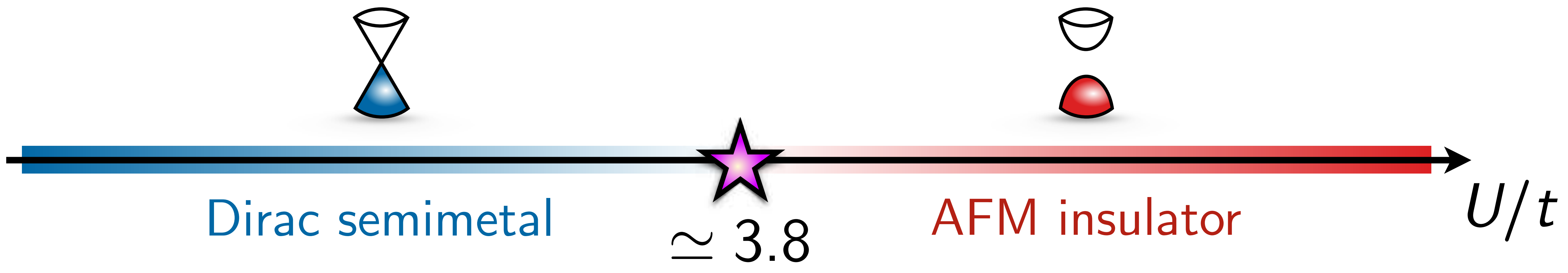
Quantum phase diagram:



[Assaad & Herbut, PRX '13]
[Lang *et al.*, PRL '13]
[Otsuka, Yunoki, Sorella, PRX '16]
[Lang & Läuchli, arXiv:2503.15000]
...

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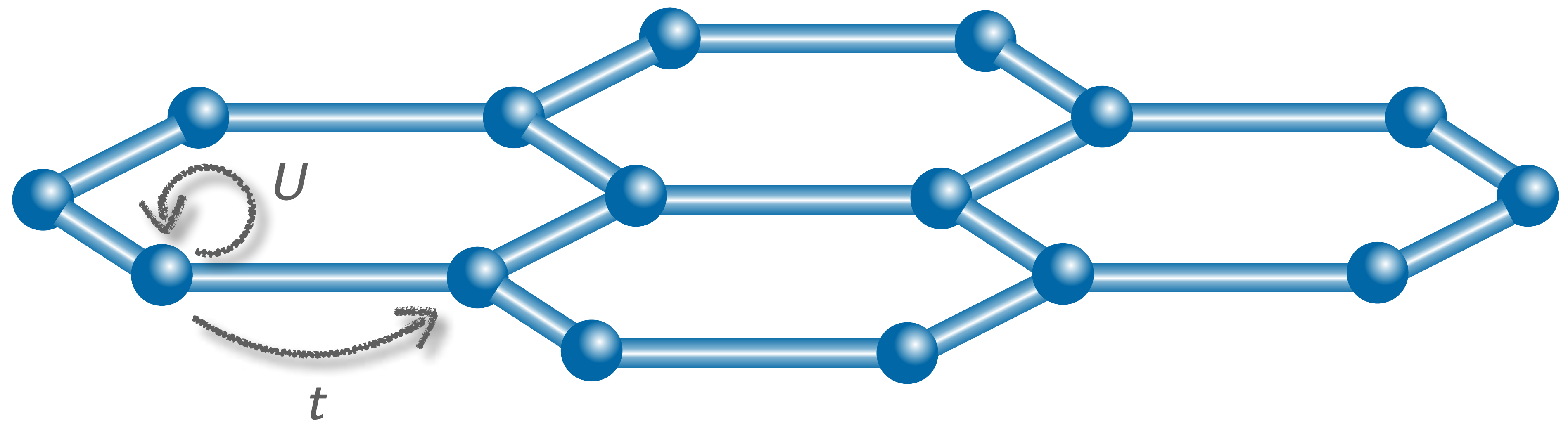

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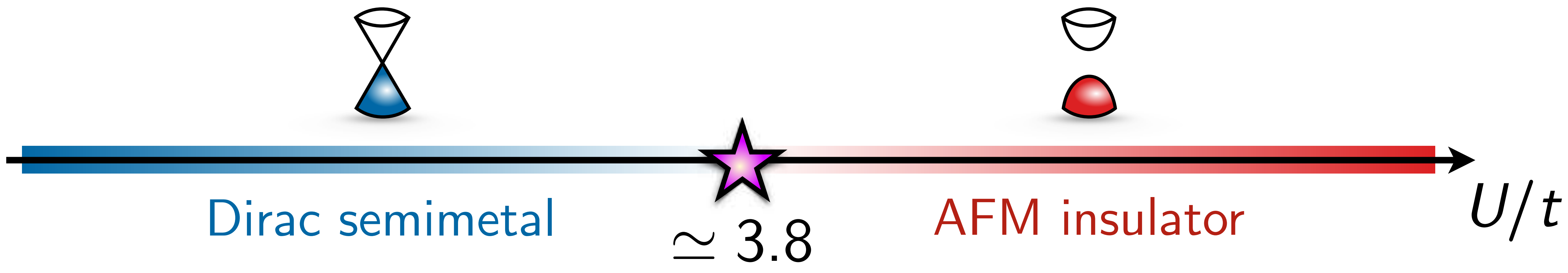


[Assaad & Herbut, PRX '13]
[Lang *et al.*, PRL '13]
[Otsuka, Yunoki, Sorella, PRX '16]
[Lang & Läuchli, arXiv:2503.15000]
...

→ **Talk by T. Lang**

Gross-Neveu-Heisenberg field theory:

$$\mathcal{L} = \bar{\psi}\gamma^\mu \partial_\mu \psi + g(\bar{\psi}\vec{\sigma}\psi)\cdot\vec{\varphi} + \dots$$

[Herbut, Juričić, Vafek, PRB '09]
[LJ & Herbut, PRB '14]
[Zerf *et al.*, PRD '17]
[Ladovrechis, Ray, Meng, LJ, PRB '23]
...

Experimental realization?

week ending
16 JANUARY 2009

PHYSICAL REVIEW LETTERS

026802 (2009)

Is Graphene in Vacuum an Insulator?

Joaquín E. Drut[1] and Timo A. Lähde[2]

[1]Department of Physics, The Ohio State University, Columbus, Ohio 43210-1117, USA
[2]Department of Physics, University of Washington, Seattle, Washington 98195-1560, USA

(Received 11 July 2008; published 13 January 2009)

We present evidence, from lattice Monte Carlo simulations of the phase diagram of graphene as a function of the Coulomb coupling between quasiparticles, that graphene in vacuum is likely to be an insulator. We find a semimetal-insulator transition at $\alpha_g^{\rm crit} = 1.11 \pm 0.06$, where $\alpha_g \simeq 2.16$ in vacuum, and $\alpha_g \simeq 0.79$ on a SiO_2 substrate. Our analysis uses the logarithmic derivative of the order parameter, supplemented by an equation of state. The insulating phase disappears above a critical number of four-component fermion flavors $4 < N_f^{\rm crit} < 6$. Our data are consistent with a second-order transition.

DOI: 10.1103/PhysRevLett.102.026802

PACS numbers: 73.63.Bd, 05.10.Ln, 71.30.+h

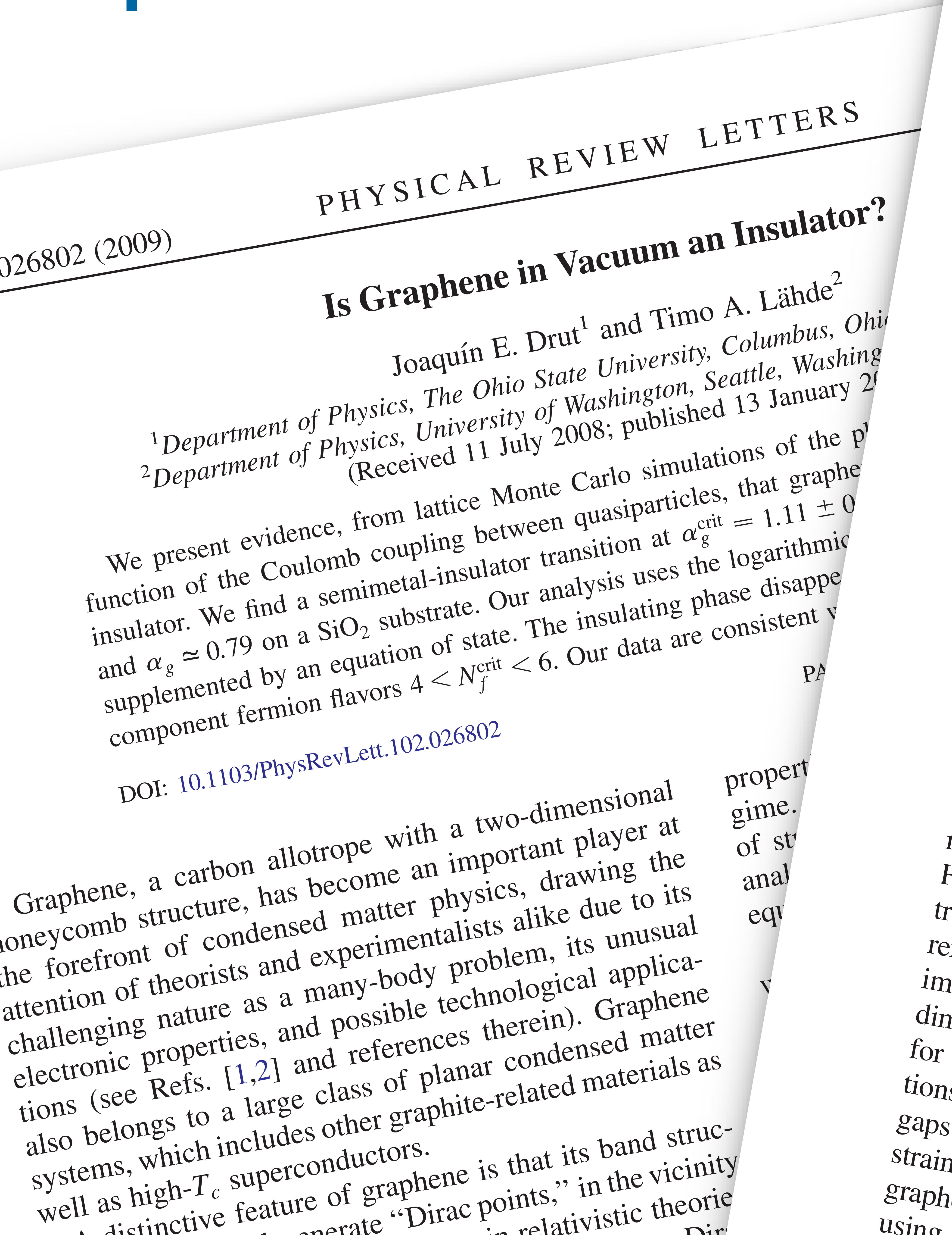
Graphene, a carbon allotrope with a two-dimensional honeycomb structure, has become an important player at the forefront of condensed matter physics, drawing the attention of theorists and experimentalists alike due to its challenging nature as a many-body problem, its unusual electronic properties, and possible technological applications (see Refs. [1,2] and references therein). Graphene also belongs to a large class of planar condensed matter systems, which includes other graphite-related materials as well as high-T_c superconductors.

A distinctive feature of graphene is that its band structure … "Dirac points," in the vicinity … relativistic theories … Dirac

properties resemble QED in a very strongly coupled regime. This provides an exciting opportunity for the study of strongly coupled theories, within a condensed matter analogue that can be experimentally realized with modest equipment.

Notably, Eq. (1) satisfies a chiral $U(2N_f)$ symmetry which can break spontaneously at large enough Coulomb coupling, generating a gap in the quasiparticle spectrum. Whether such an effect occurs in real graphene is an open issue from the experimental point of view (see, however, Ref. [4], where a substrate-induced gap is reported). On the theoretical side, dynamical gap generation is described by a quantum phase transition due to the formation of particle-hole bound states. However, in such a strongly coupled … even a qualitative analysis should be nonperturba… true for graphene in vacuum, where … partially screened

Experimental realization?



PHYSICAL REVIEW LETTERS

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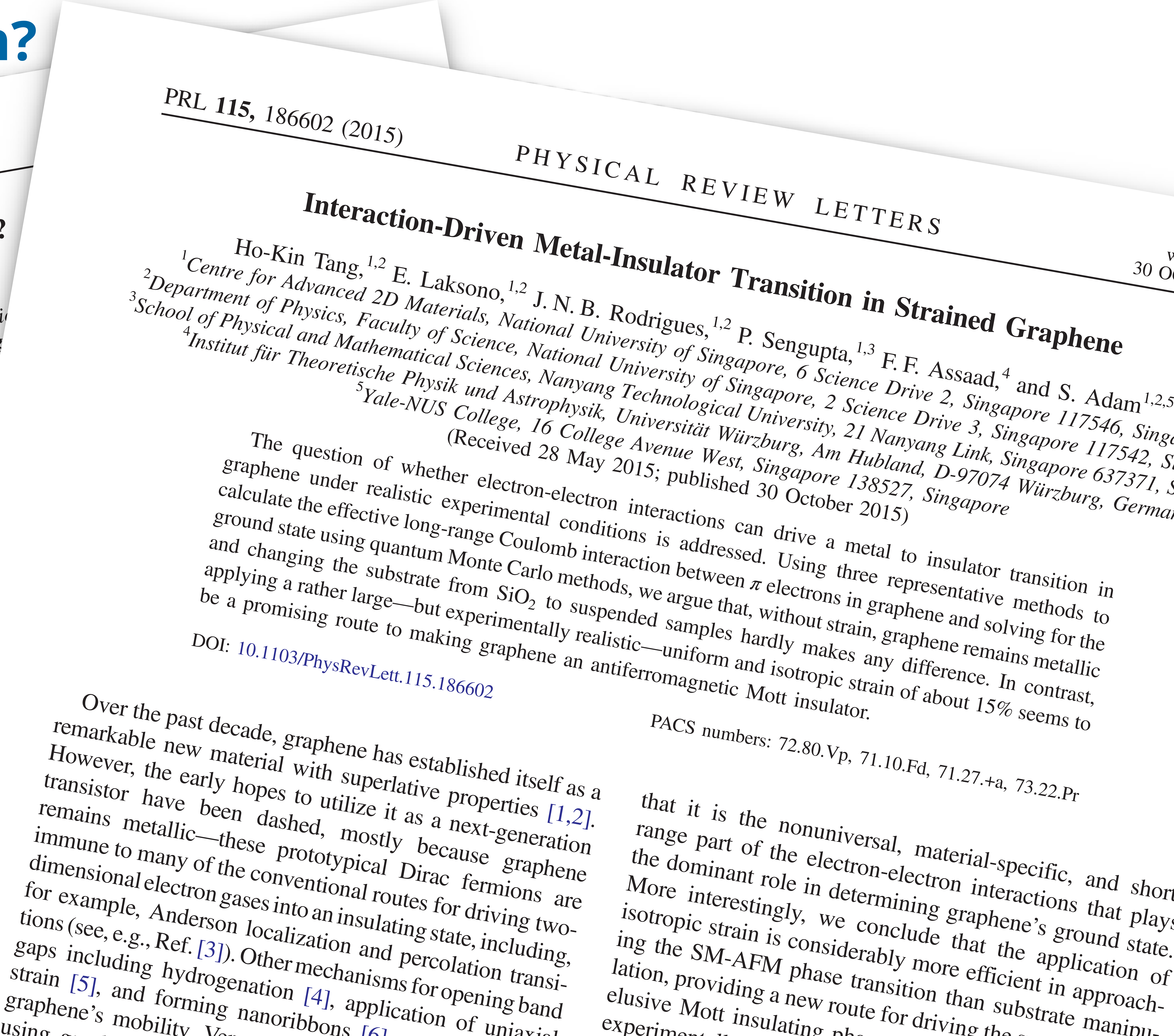


PRL 115, 186602 (2015) PHYSICAL REVIEW LETTERS

30 O

Interaction-Driven Metal-Insulator Transition in Strained Graphene

Ho-Kin Tang,[1,2] E. Laksono,[1,2] J. N. B. Rodrigues,[1,2] P. Sengupta,[1,3] F. F. Assaad,[4] and S. Adam[1,2,5]

[1]Centre for Advanced 2D Materials, National University of Singapore, 6 Science Drive 2, Singapore 117546, Sing

[2]Department of Physics, Faculty of Science, National University of Singapore, 2 Science Drive 3, Singapore 117542, S

[3]School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link, Singapore 637371, S

[4]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germa

[5]Yale-NUS College, 16 College Avenue West, Singapore 138527, Singapore

(Received 28 May 2015; published 30 October 2015)

The question of whether electron-electron interactions can drive a metal to insulator transition in graphene under realistic experimental conditions is addressed. Using three representative methods to calculate the effective long-range Coulomb interaction between π electrons in graphene and solving for the ground state using quantum Monte Carlo methods, we argue that, without strain, graphene remains metallic and changing the substrate from SiO_2 to suspended samples hardly makes any difference. In contrast, applying a rather large—but experimentally realistic—uniform and isotropic strain of about 15% seems to be a promising route to making graphene an antiferromagnetic Mott insulator.

DOI: 10.1103/PhysRevLett.115.186602

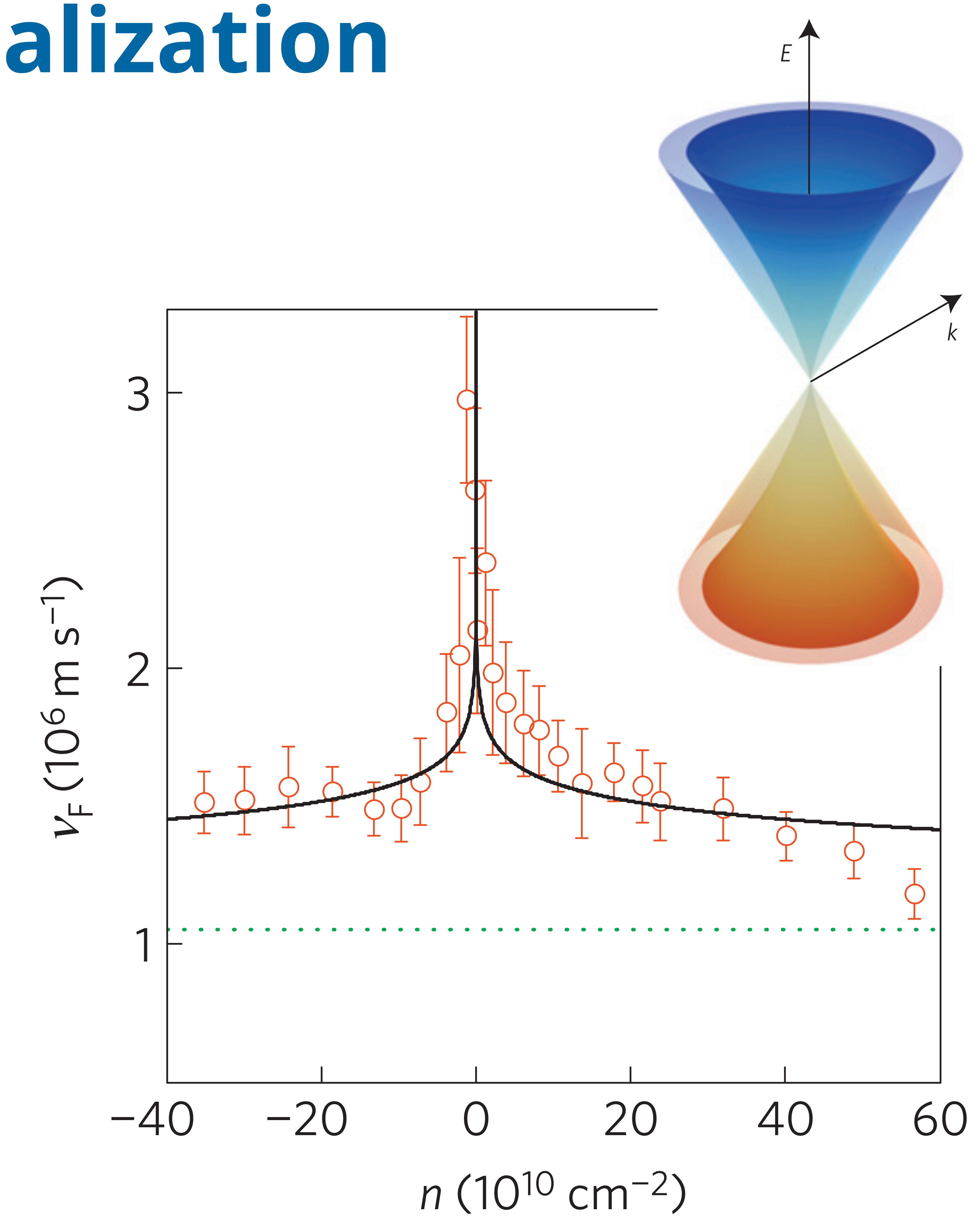
PACS numbers: 72.80.Vp, 71.10.Fd, 71.27.+a, 73.22.Pr

Over the past decade, graphene has established itself as a remarkable new material with superlative properties [1,2]. However, the early hopes to utilize it as a next-generation transistor have been dashed, mostly because graphene remains metallic—these prototypical Dirac fermions are immune to many of the conventional routes for driving two-dimensional electron gases into an insulating state, including, for example, Anderson localization and percolation transitions (see, e.g., Ref. [3]). Other mechanisms for opening band gaps including hydrogenation [4], application of uniaxial strain [5], and forming nanoribbons [6]
graphene's mobility. Ve
using

that it is the nonuniversal, material-specific, and short range part of the electron-electron interactions that plays the dominant role in determining graphene's ground state. More interestingly, we conclude that the application of isotropic strain is considerably more efficient in approaching the SM-AFM phase transition than substrate manipulation, providing a new route for driving the
elusive Mott insulating pha
experiment

Experimental realization?

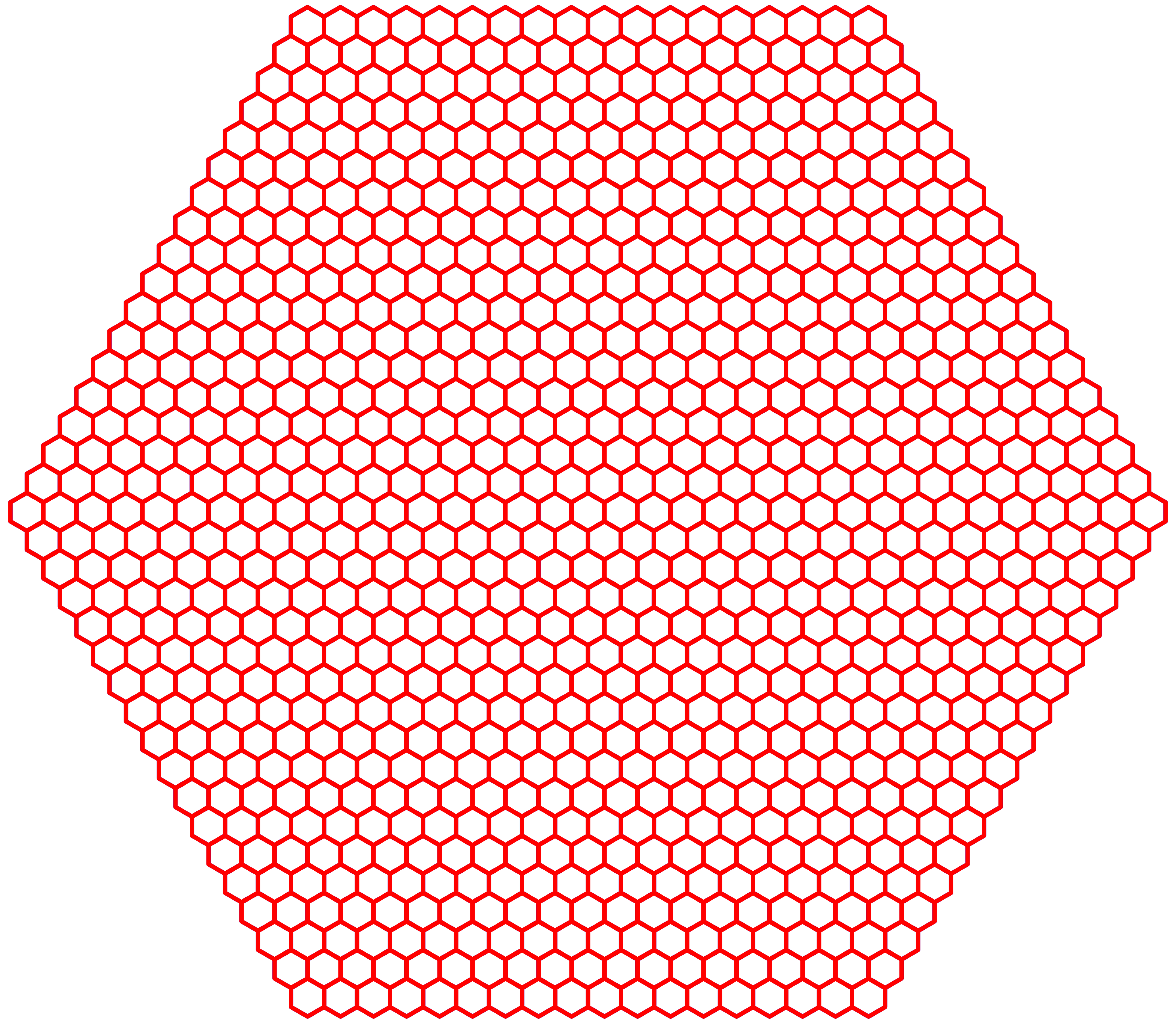
Fermi velocity renormalization



Free-standing graphene remains a Dirac semimetal

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

Twisted bilayer graphene



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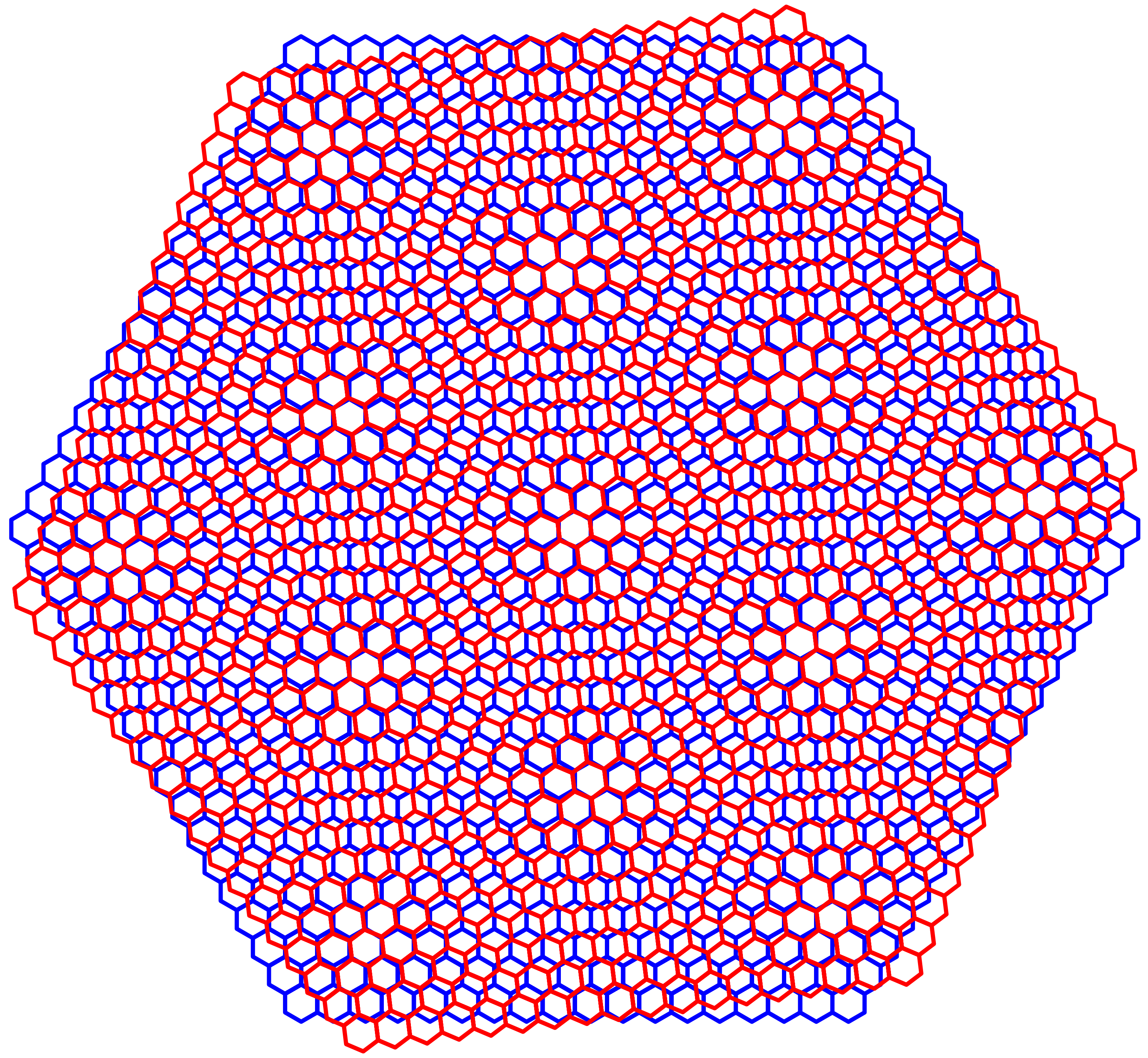
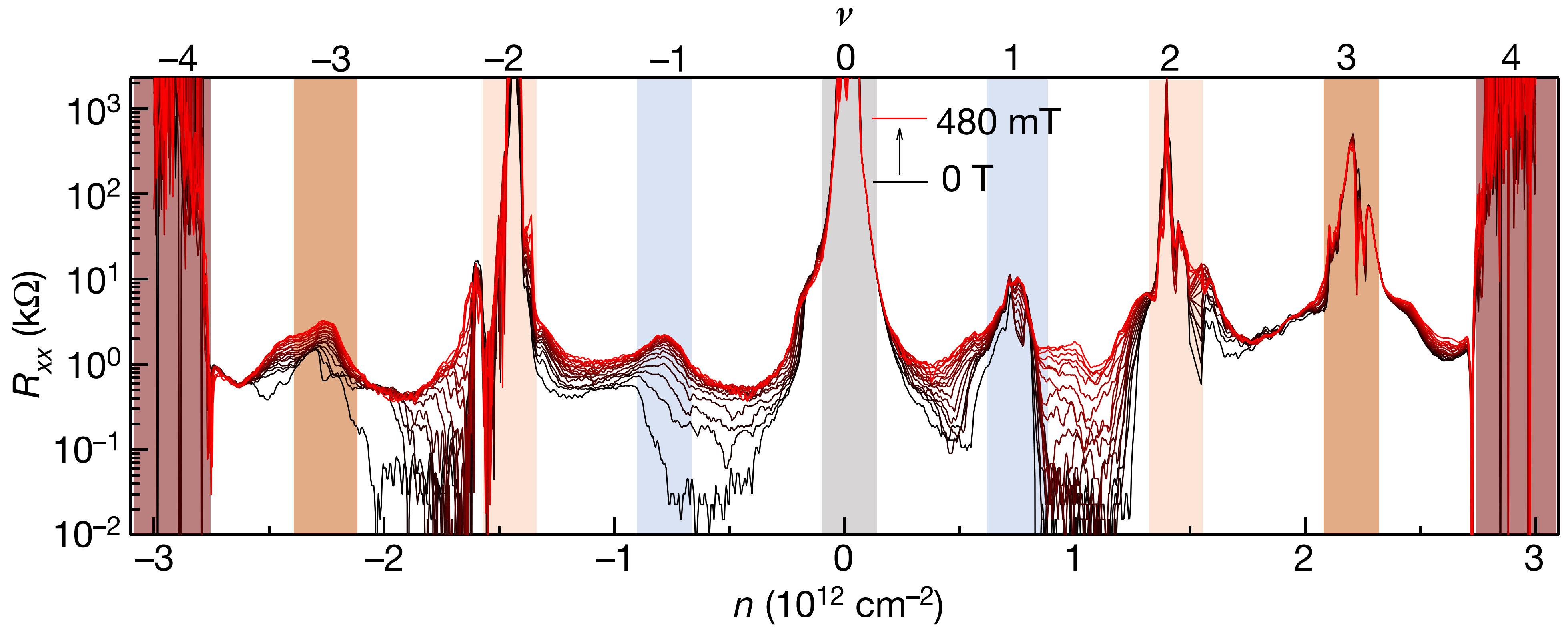
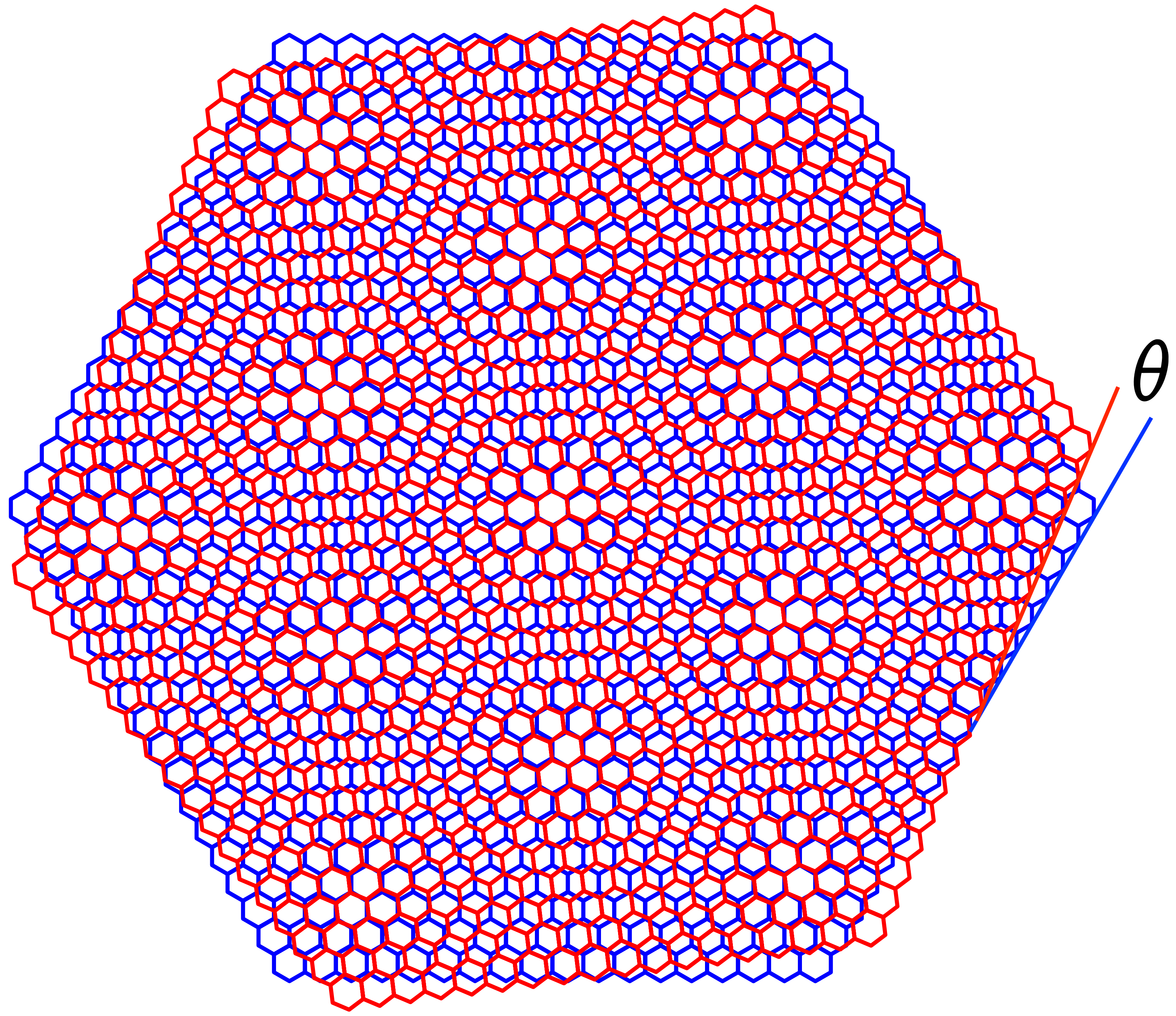


Twisted bilayer graphene

$\theta = 1.16°$



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



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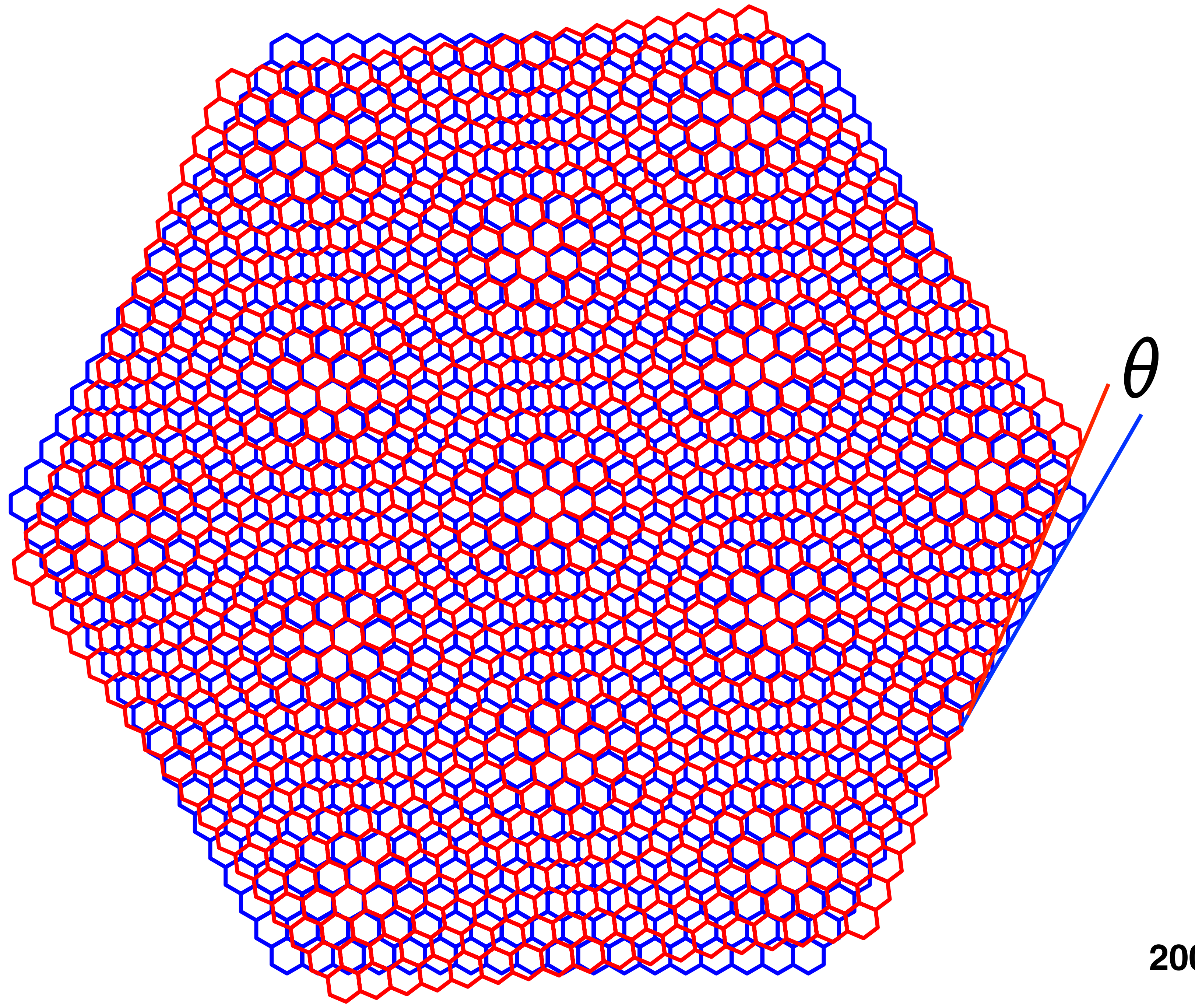

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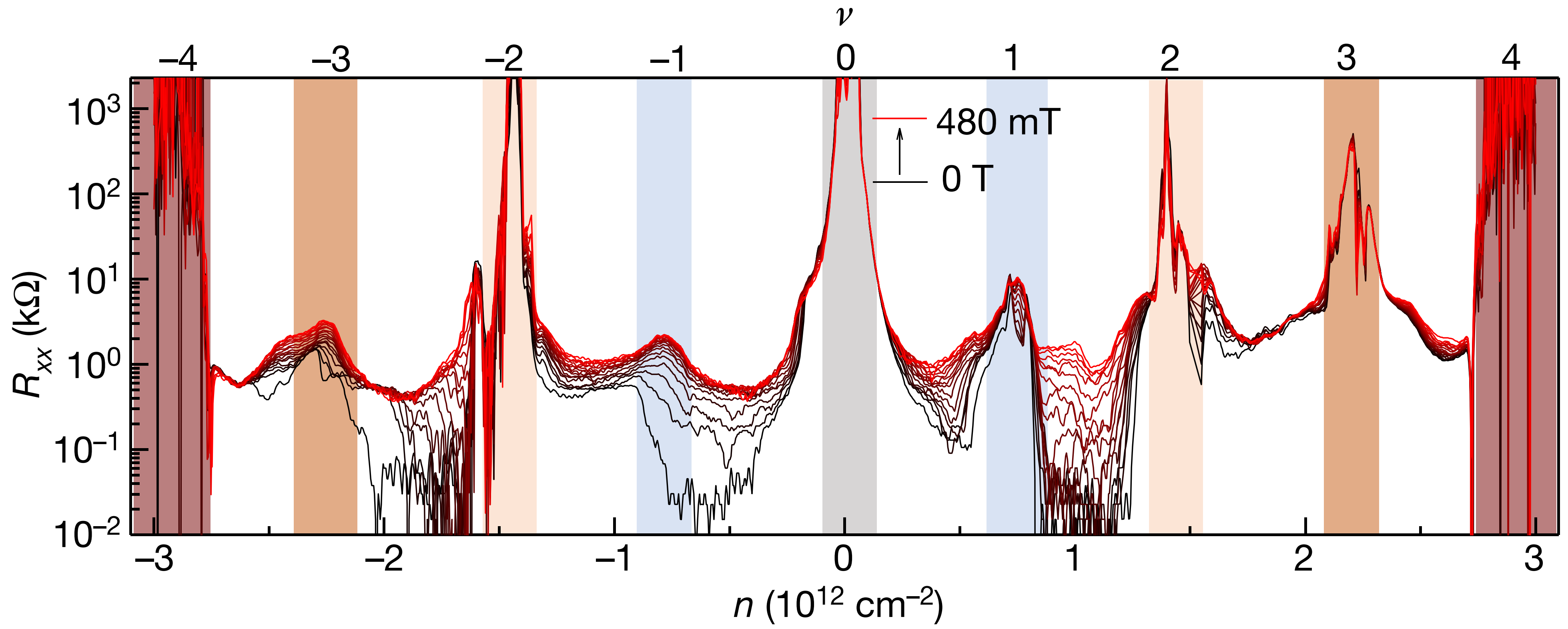
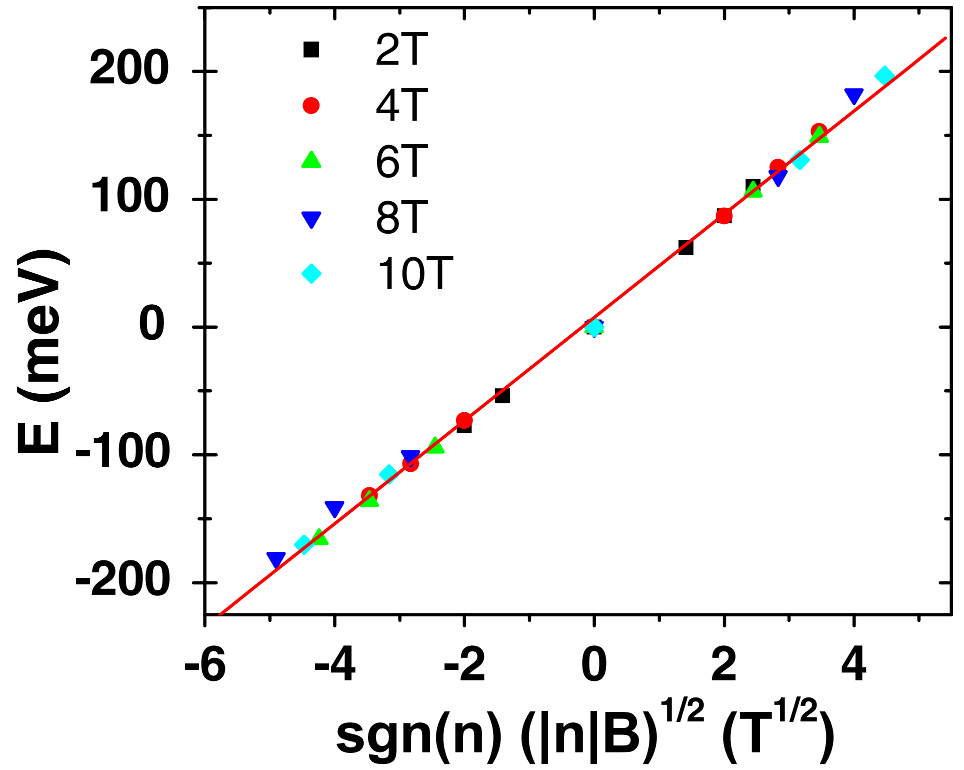


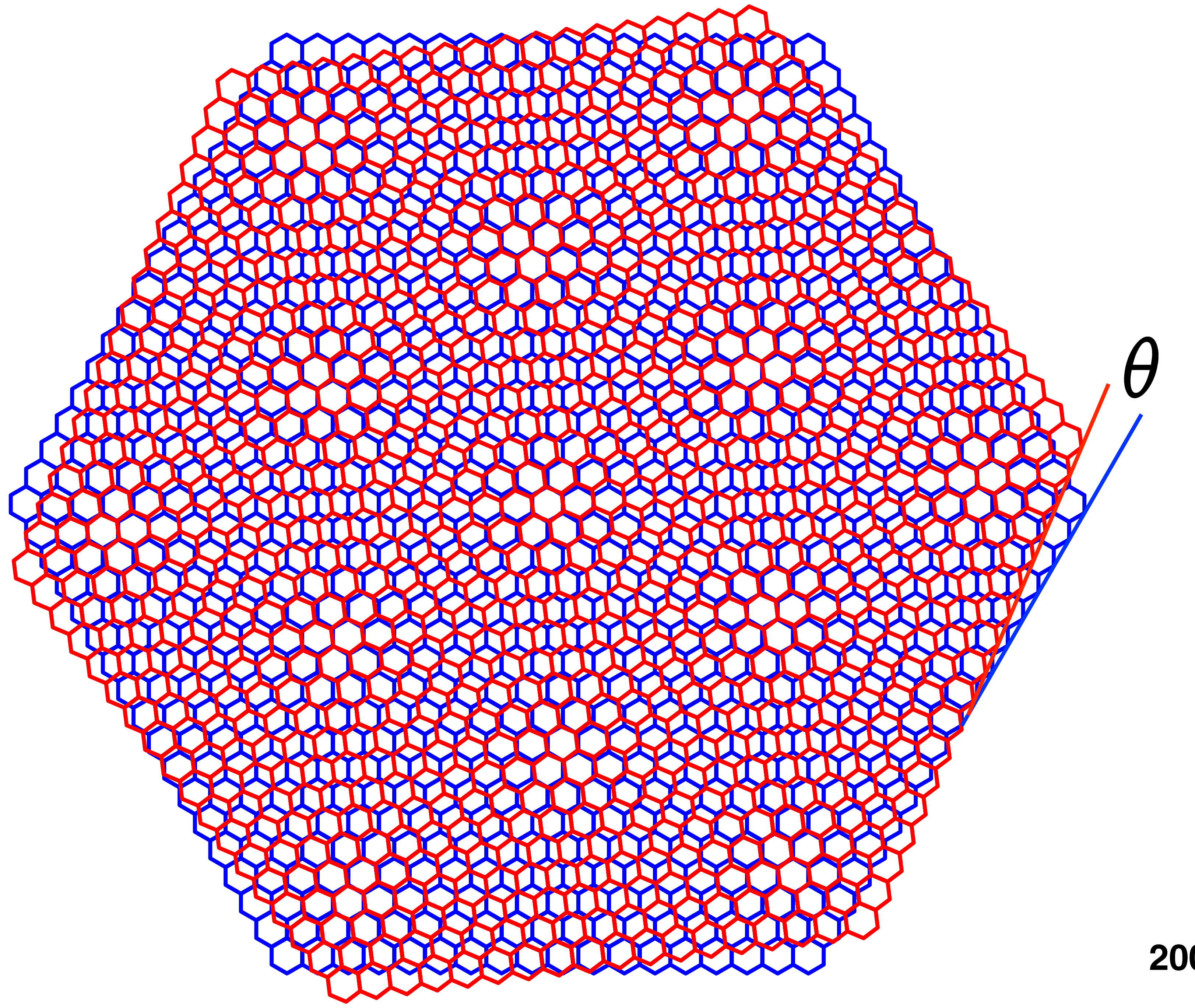
[Lu *et al.*, Nature ’19]

$\theta = 21.8°$



[Luican *et al.*, PRL ’11]

Twisted bilayer graphene



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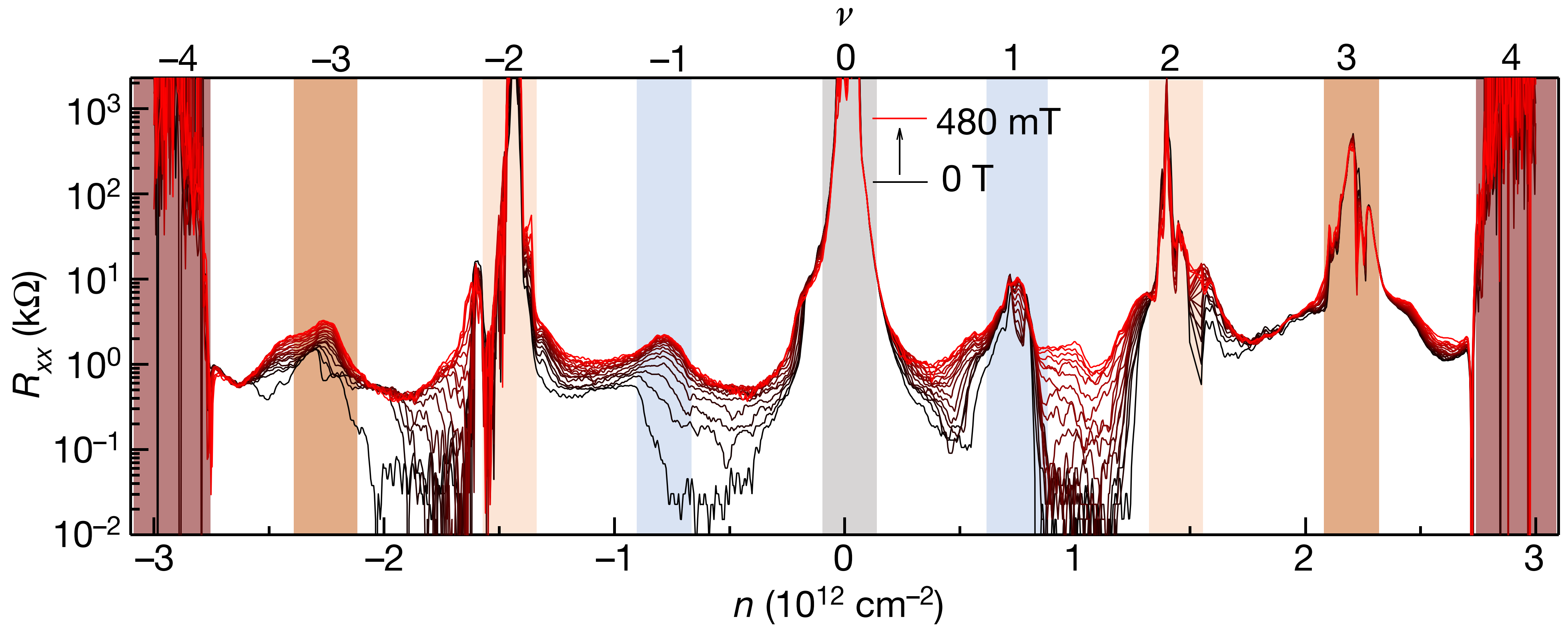

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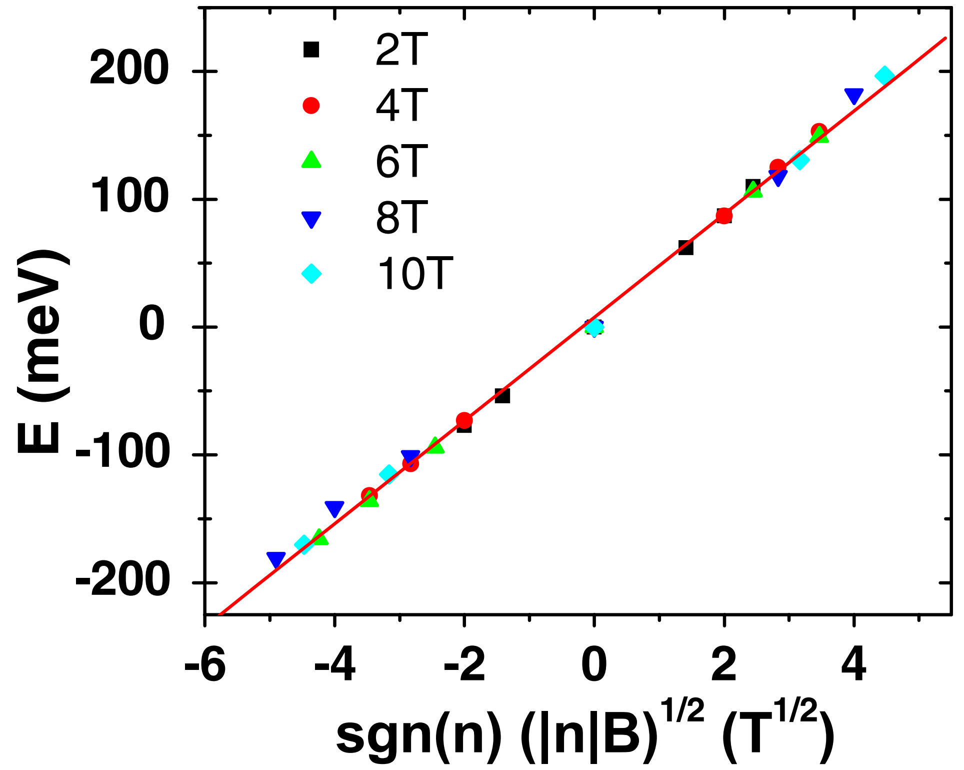


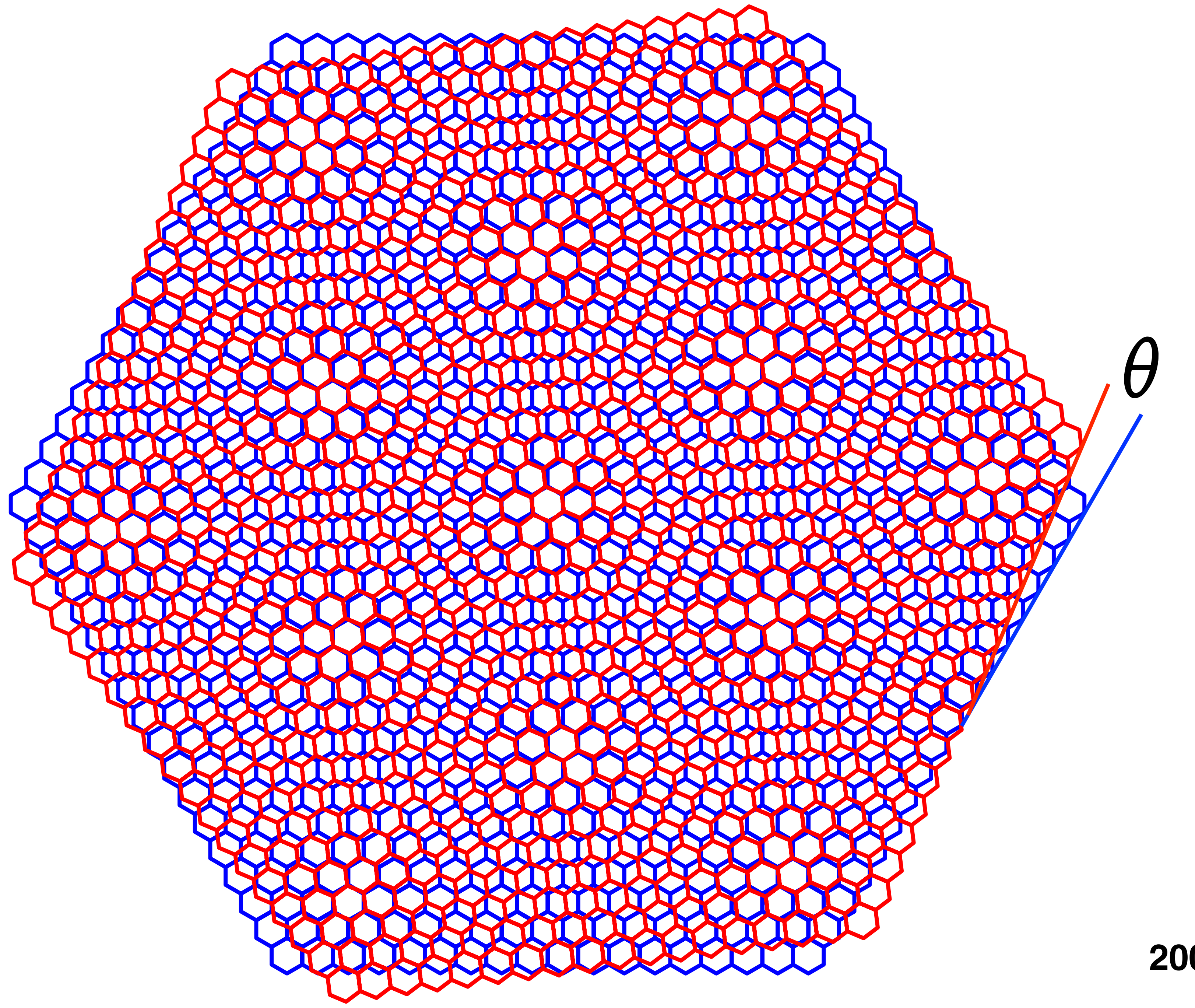
[Luican *et al.*, PRL ’11]

Correlated insulator

Dirac semimetal

... at charge neutrality $\nu = 0$

Twisted bilayer graphene



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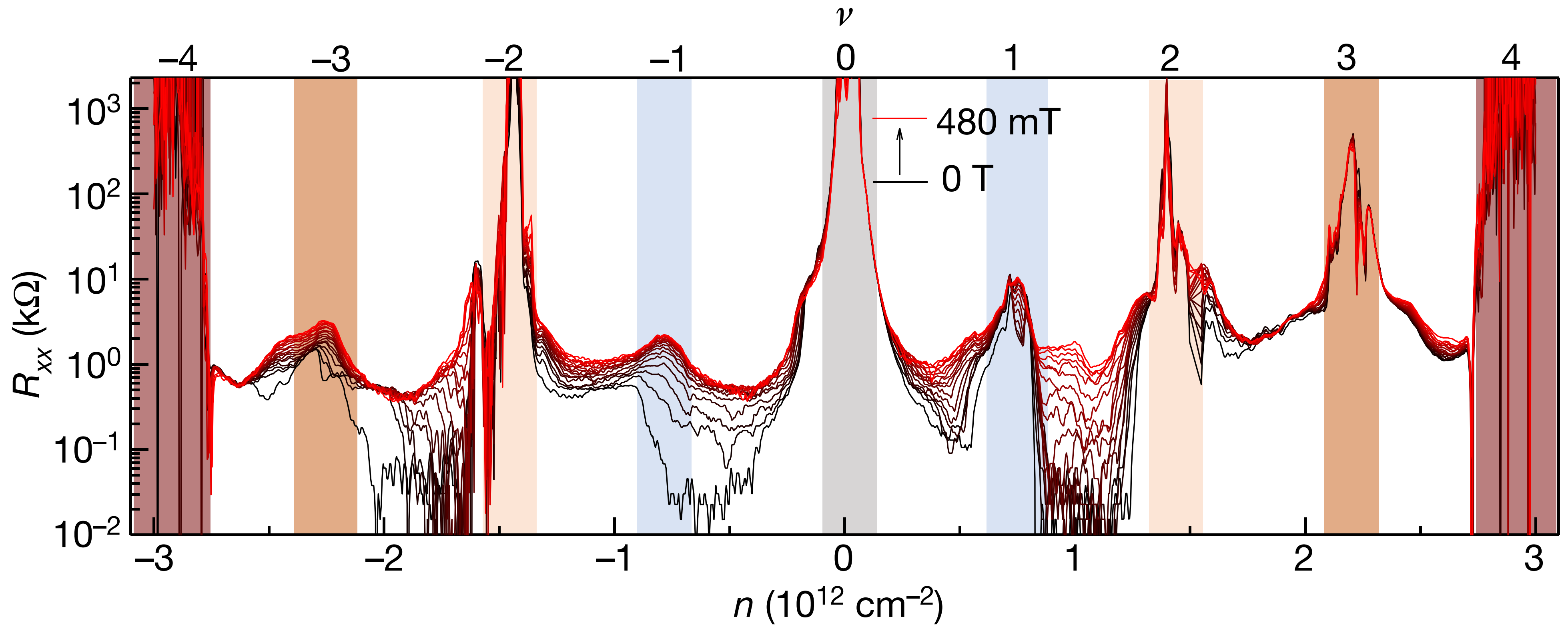

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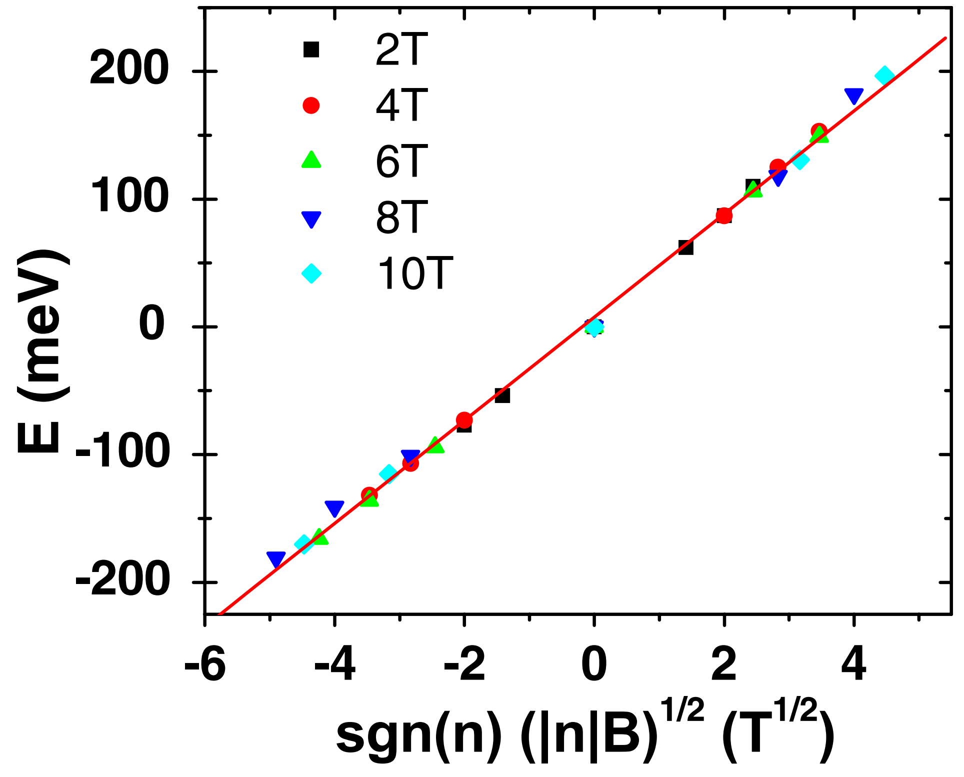

[Luican *et al.*, PRL '11]

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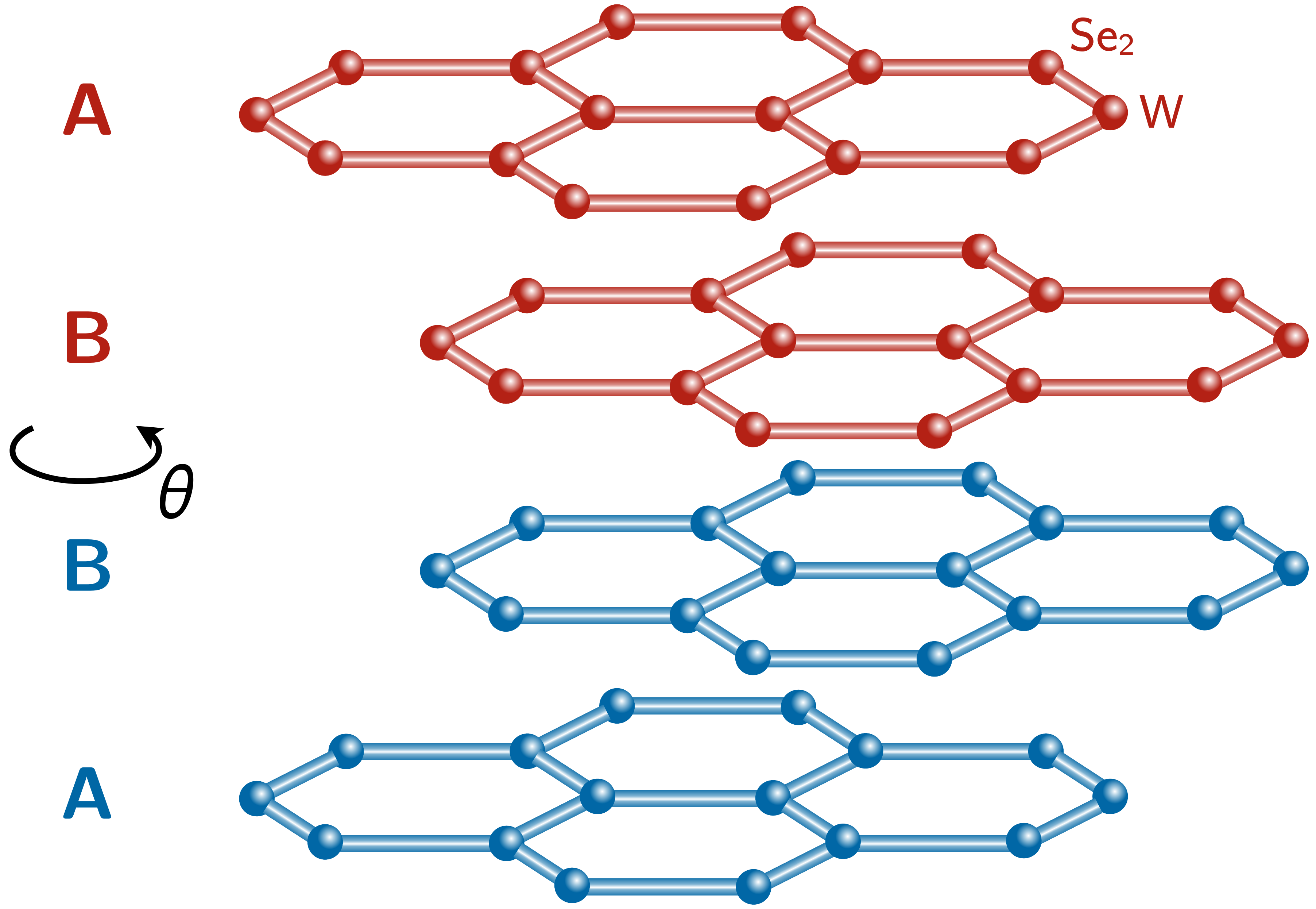
Twisted double bilayer WSe_2



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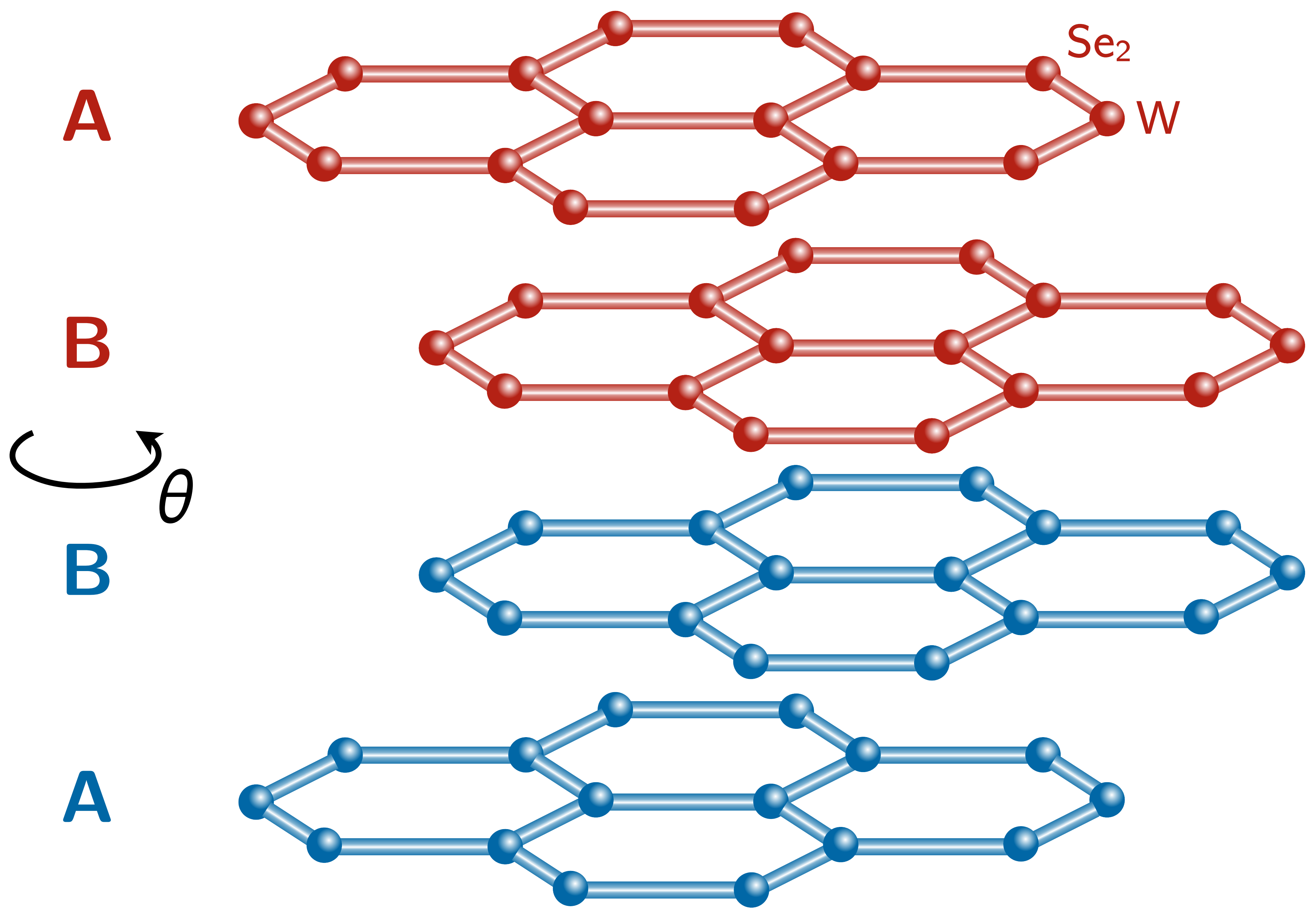
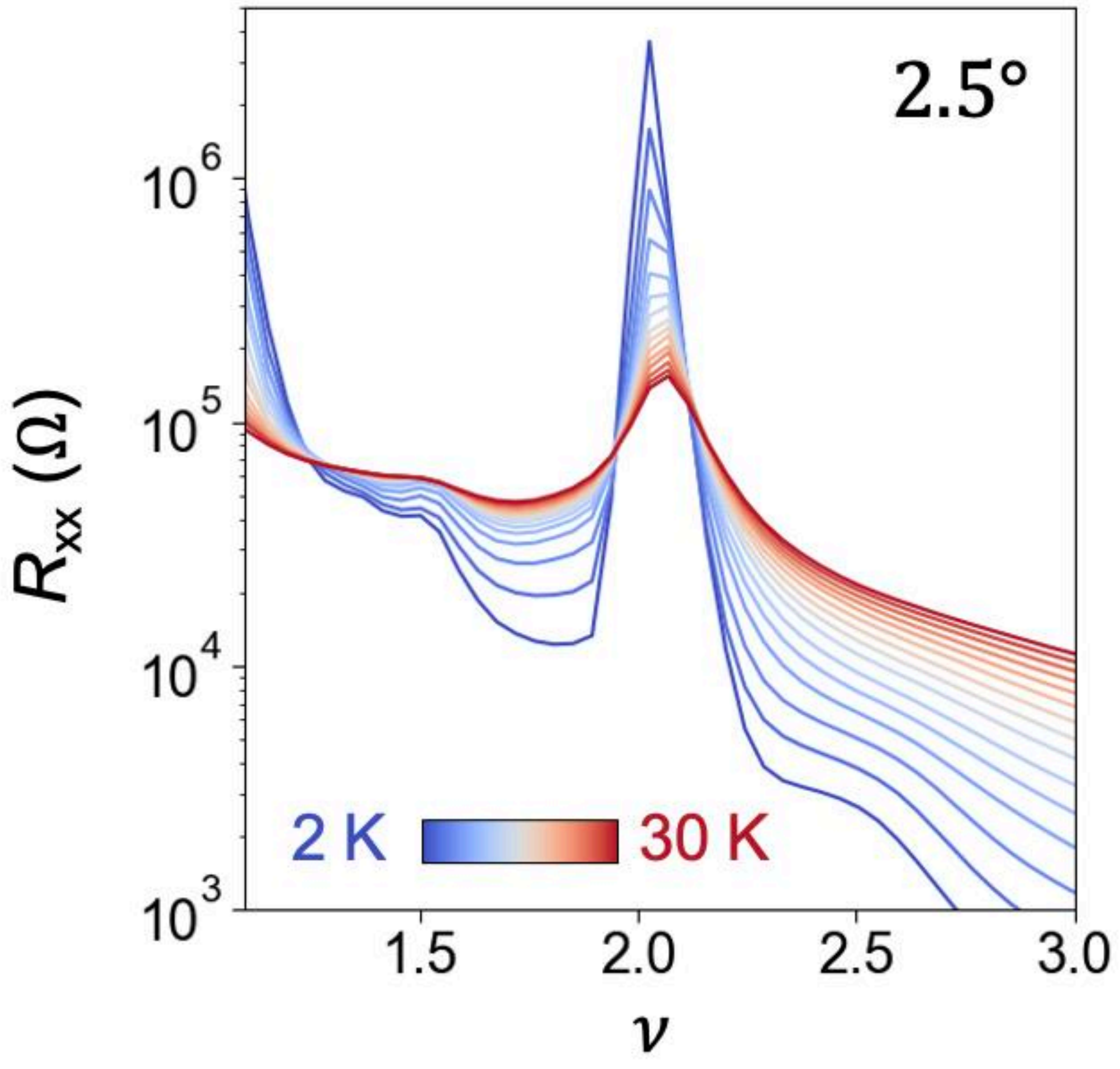
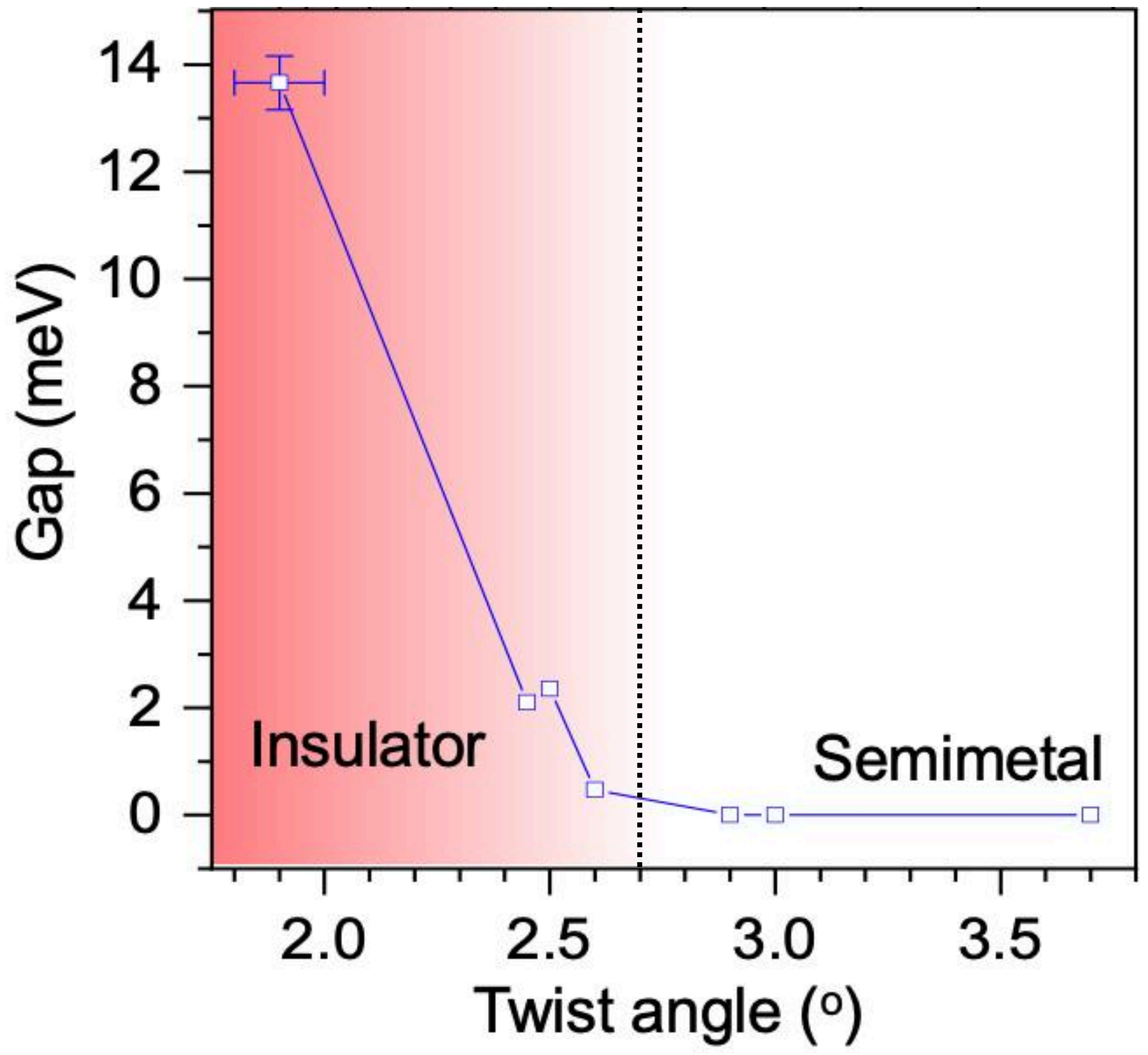


Transport:



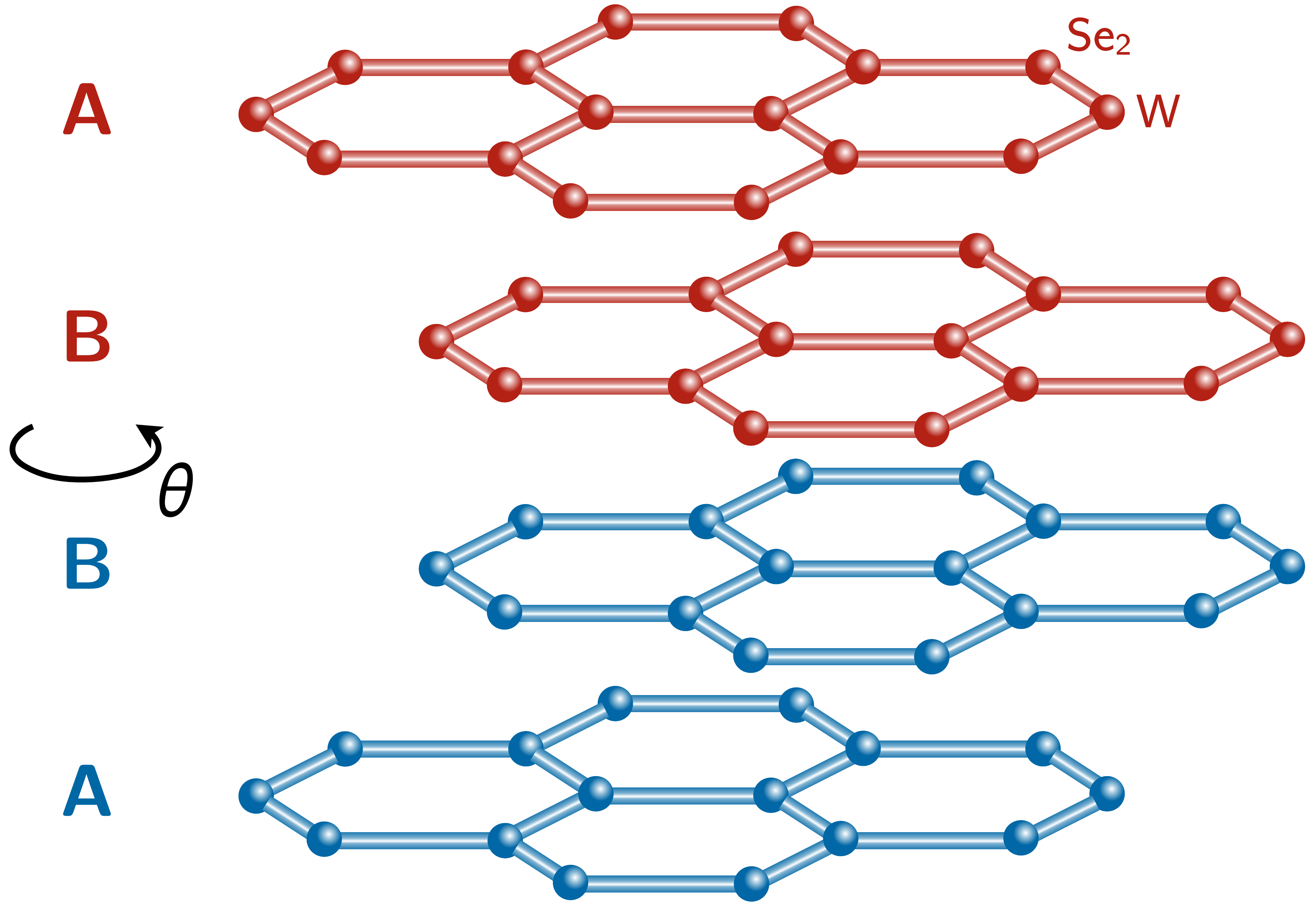
Hole filling



→ **Talk by F. Ihssen**

[Ma *et al.*, arXiv:2412.07150]

Twisted double bilayer WSe_2



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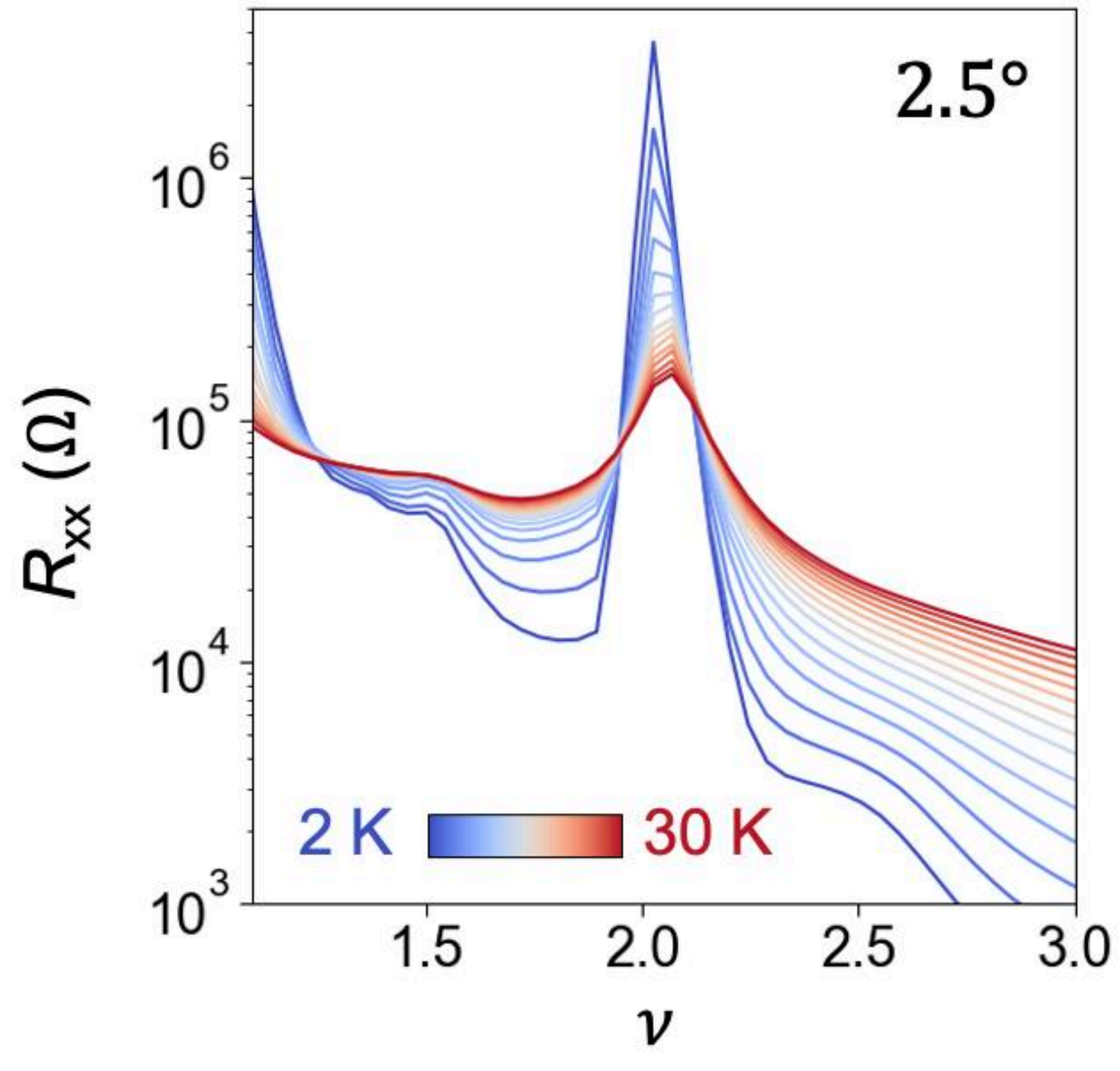

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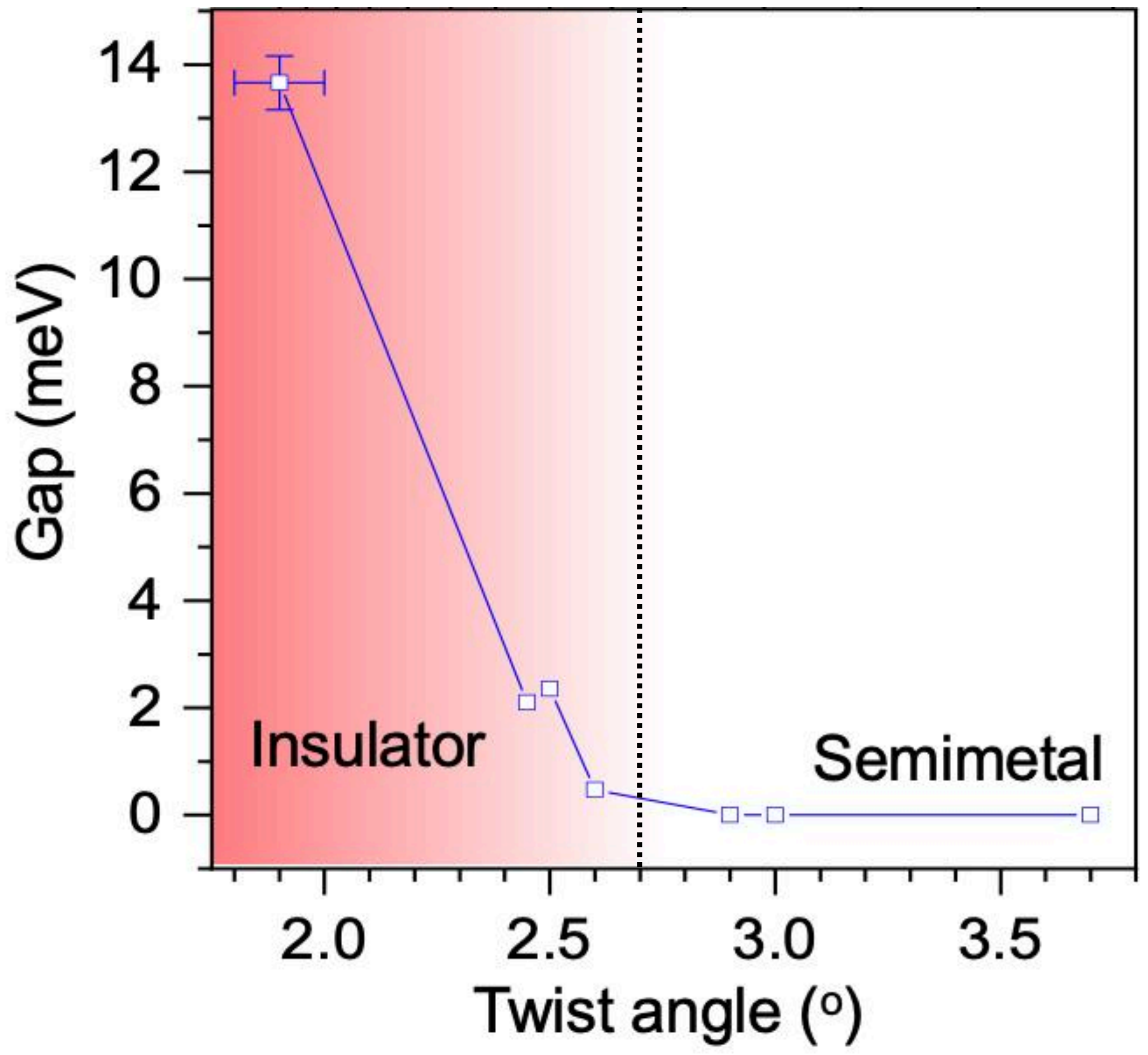

Symmetry of ordered state?
Nature of transition?

→ **Talk by F. Ihssen**

[Ma *et al.*, arXiv:2412.07150]

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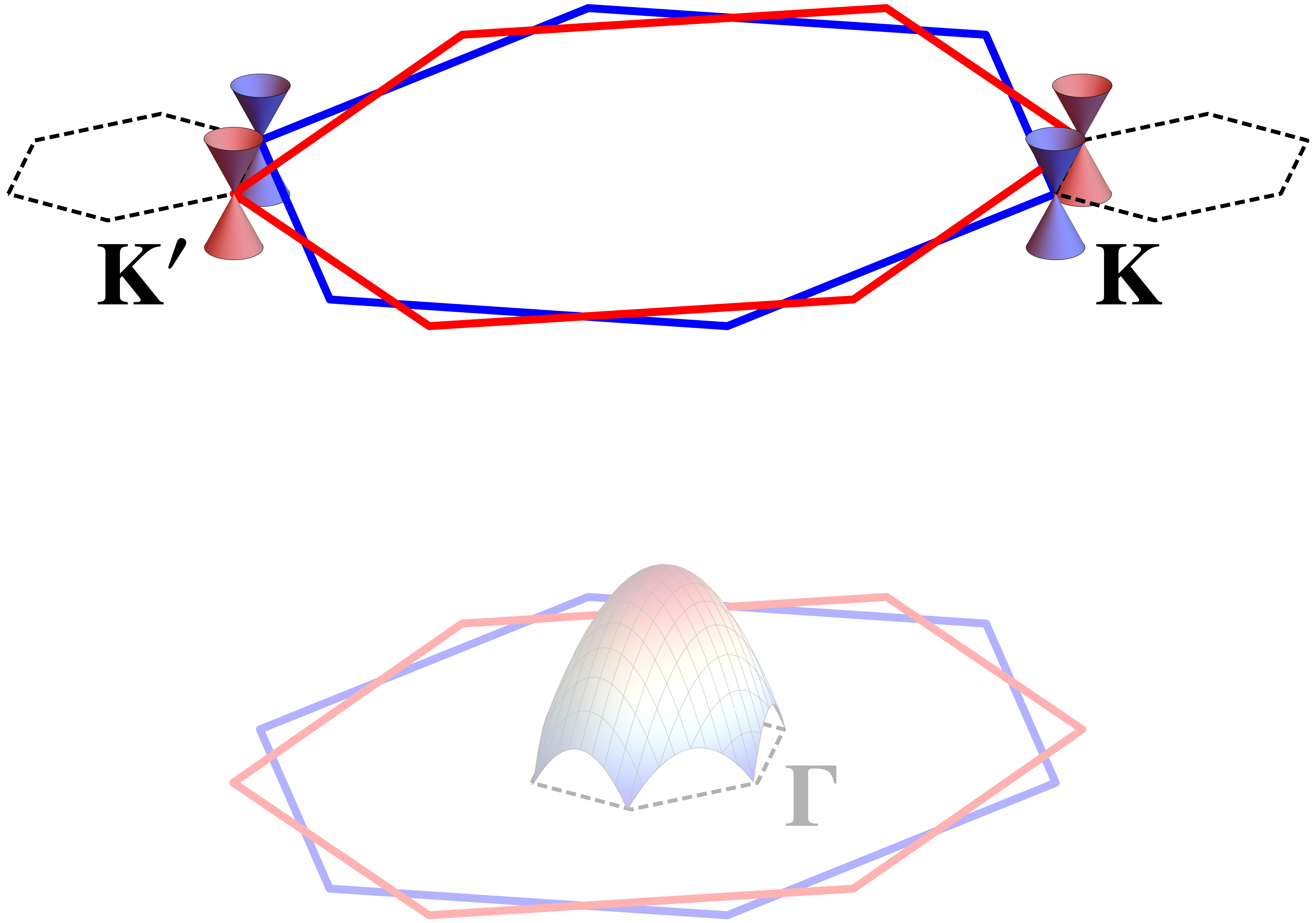
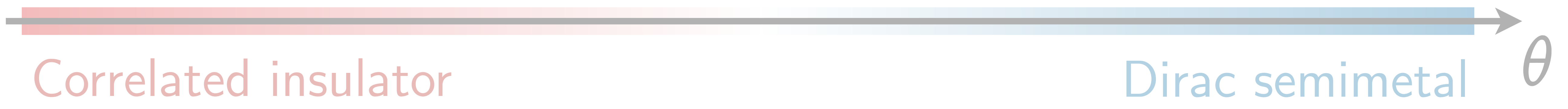
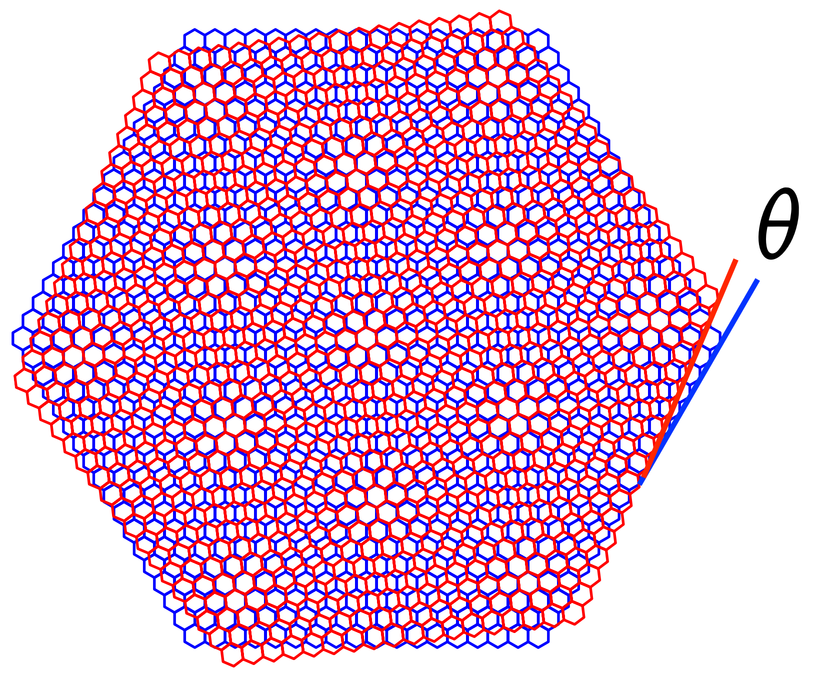


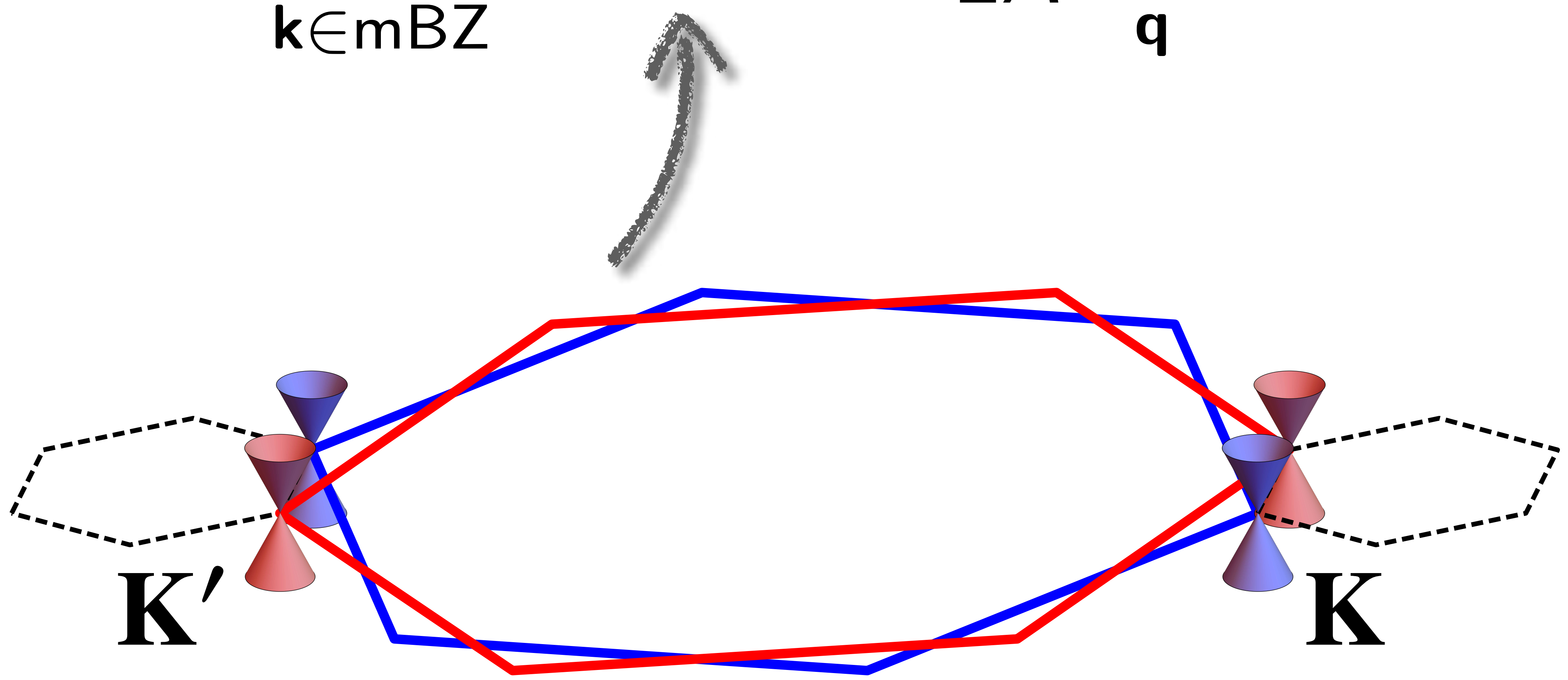


Twisted bilayer graphene: Model



Interacting Bistritzer-MacDonald model:

$$\mathcal{H} = \sum_{\mathbf{k}\in\mathrm{mBZ}} c_{\mathbf{k}}^{\dagger} h(\mathbf{k}) c_{\mathbf{k}} - \frac{1}{2A}\sum_{\mathbf{q}} V_{\mathbf{q}} :\rho_{\mathbf{q}}\rho_{-\mathbf{q}}:$$



[Bistritzer, MacDonald, PNAS '11]
[Bultinck *et al.*, PRX '20]

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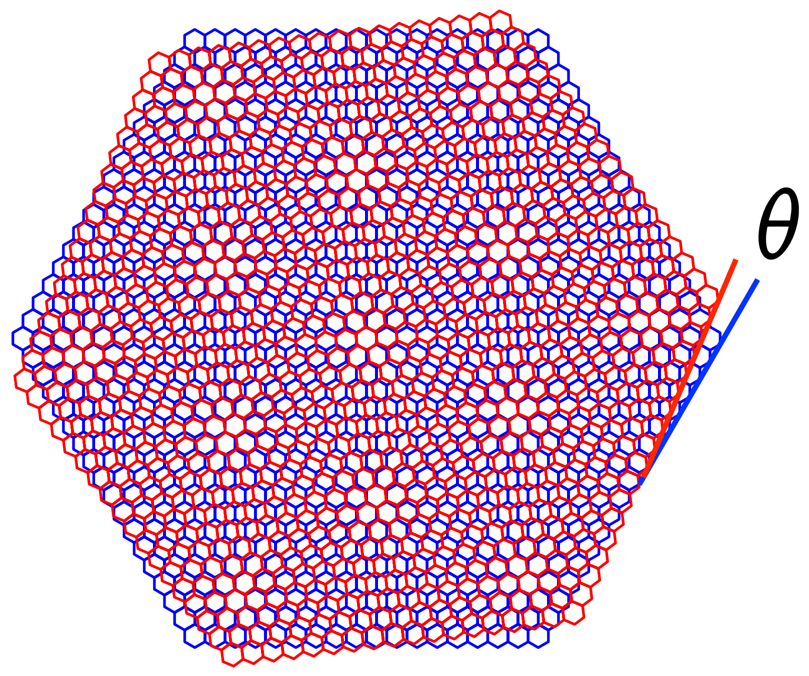

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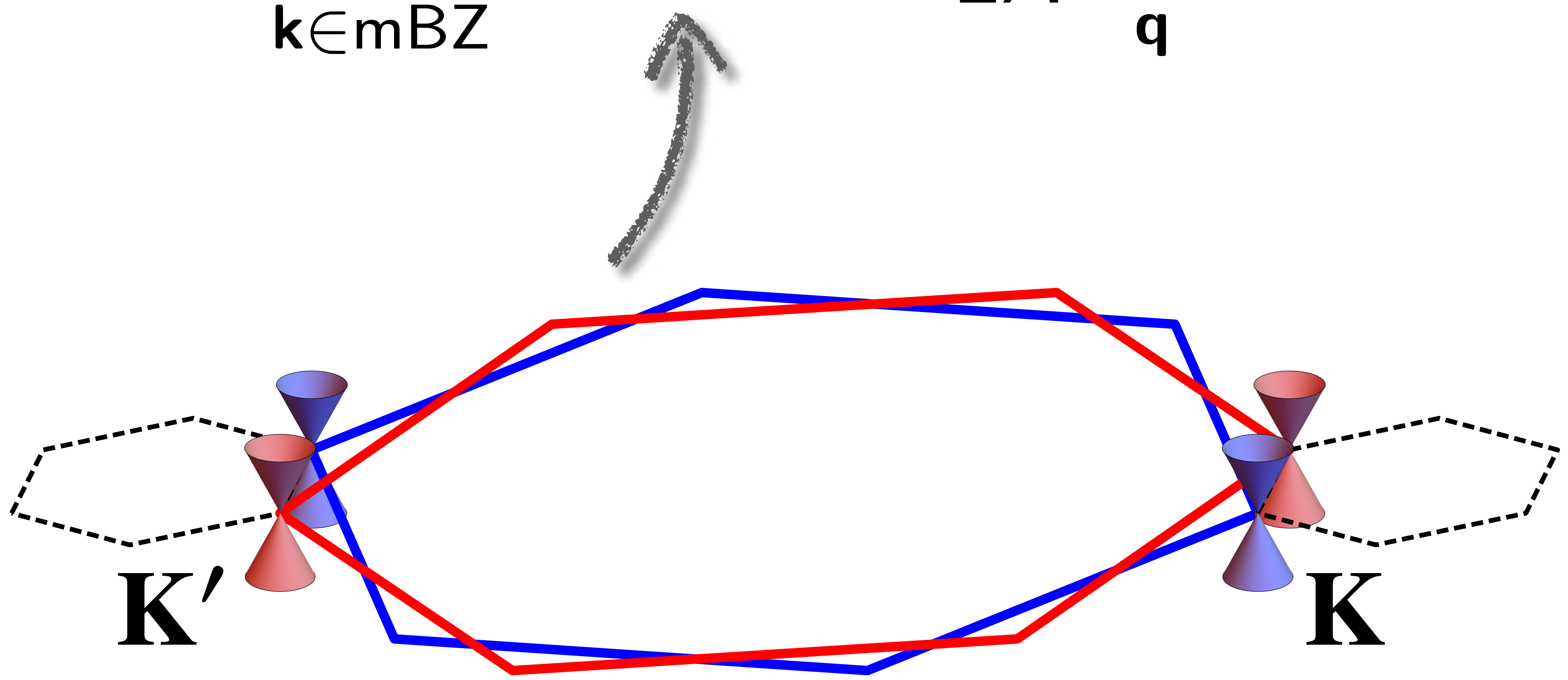
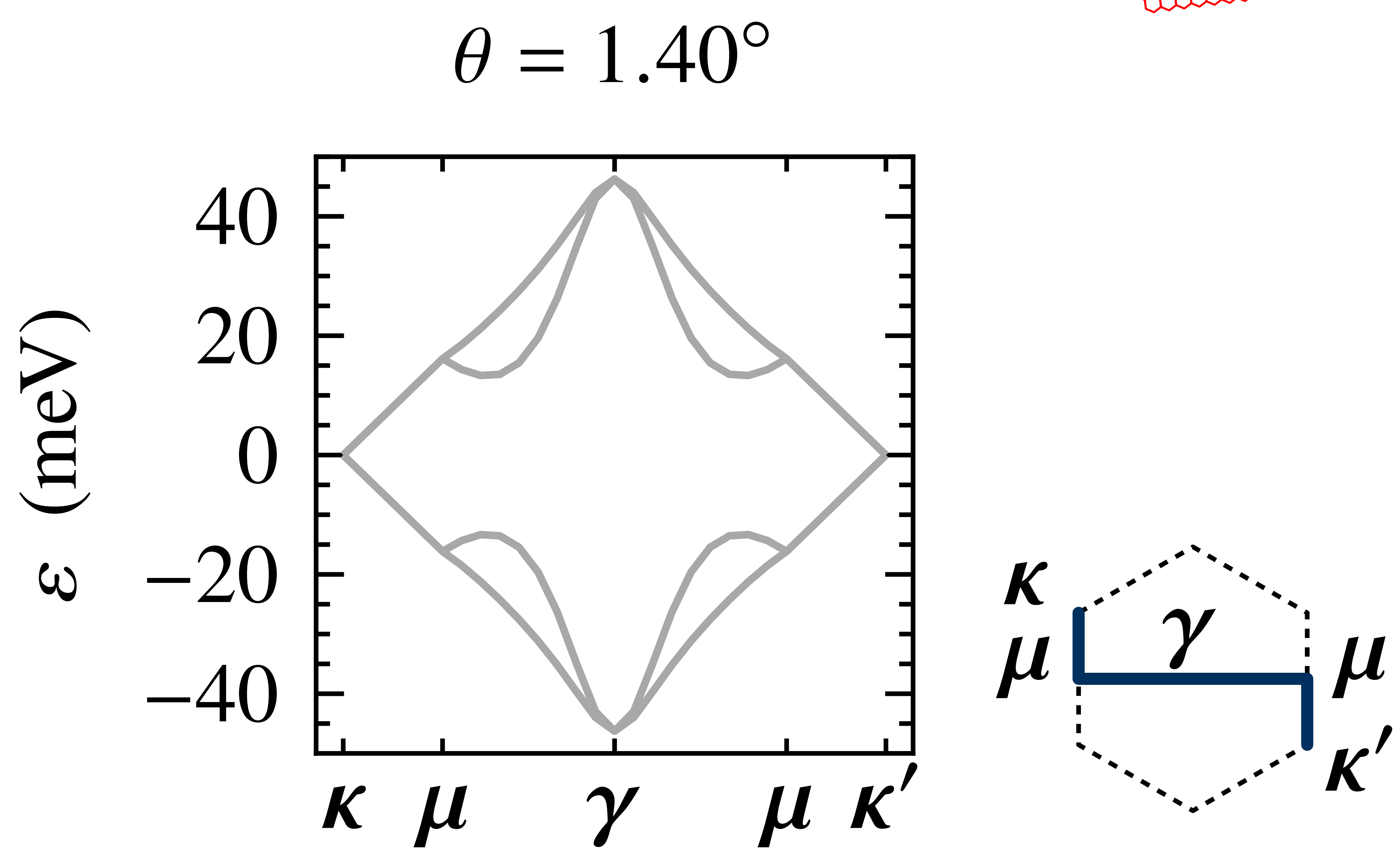
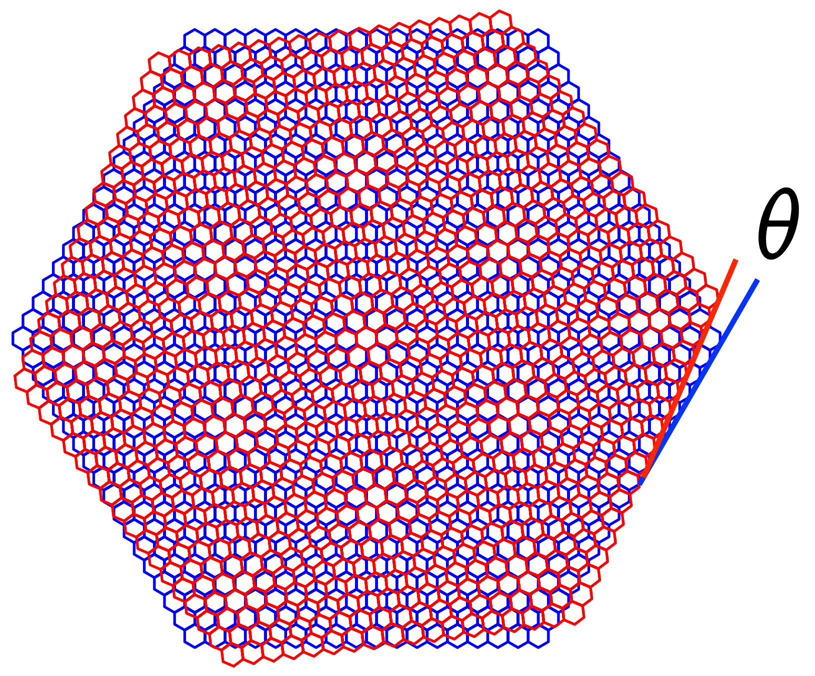


[Bistritzer, MacDonald, PNAS '11]
[Bultinck *et al.*, PRX '20]

Noninteracting spectrum:



Twisted bilayer graphene: Model



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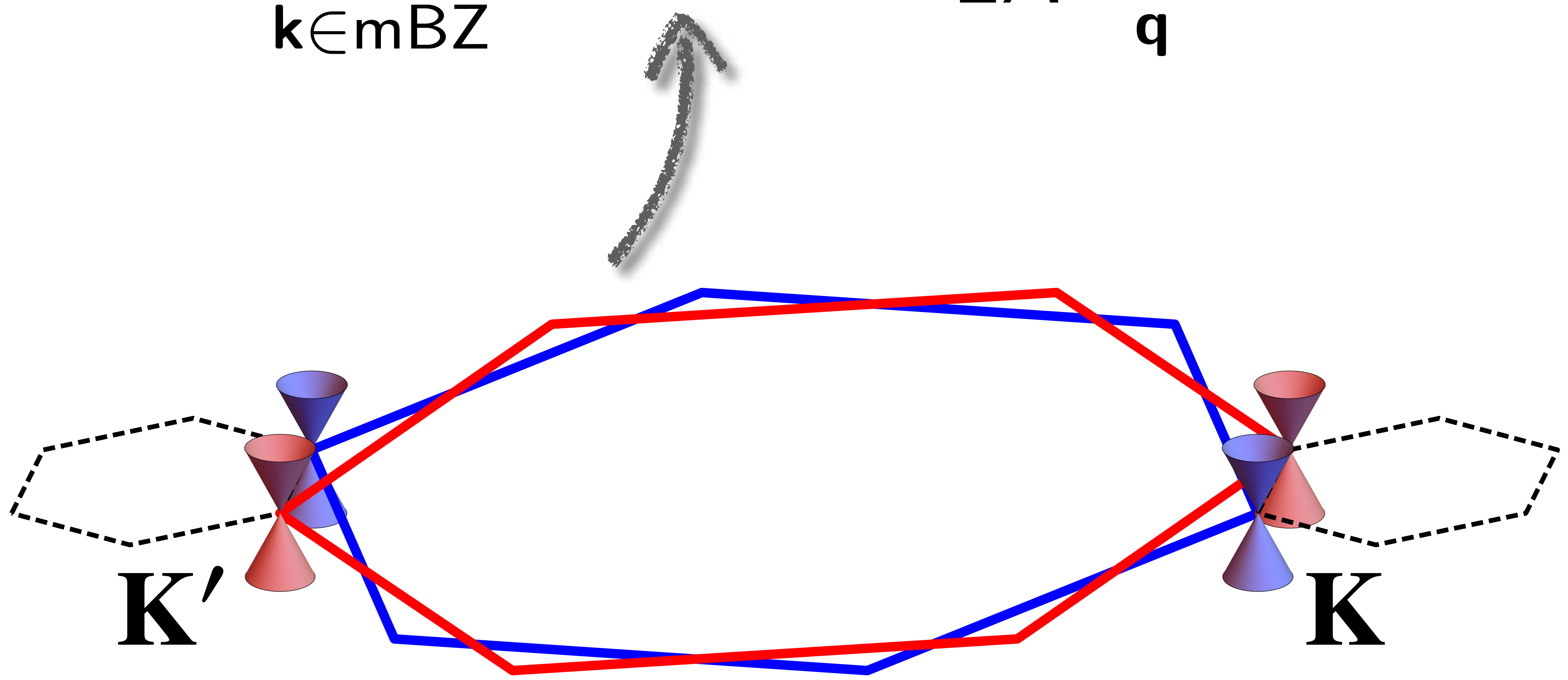

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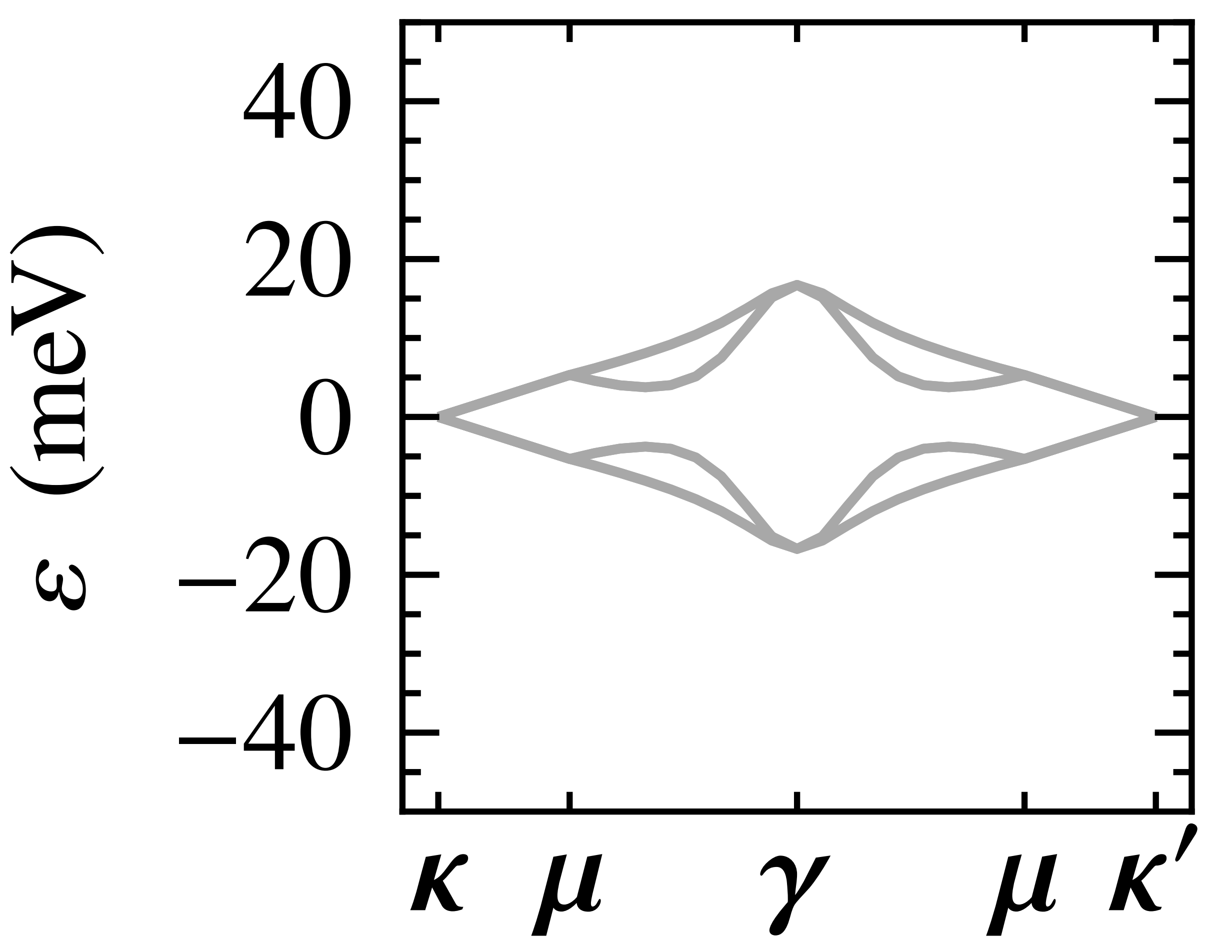
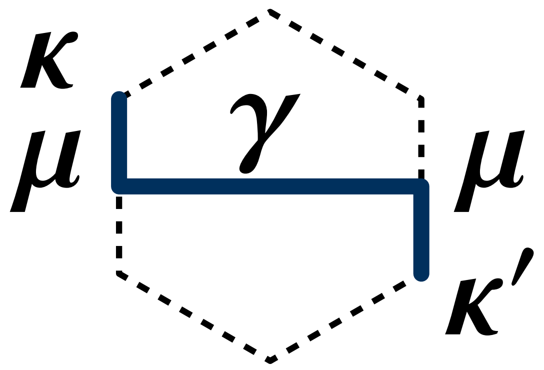
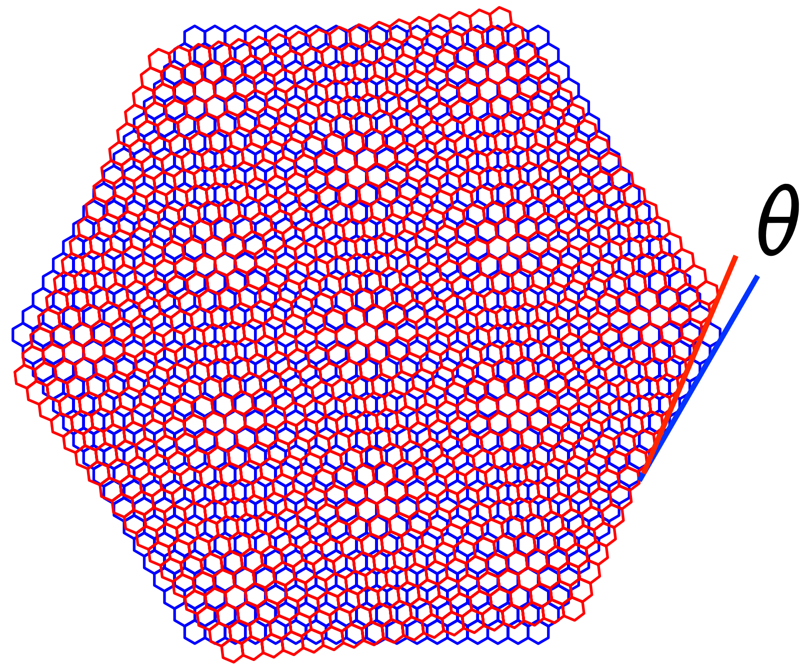
[Bultinck *et al.*, PRX ’20]

Noninteracting spectrum:



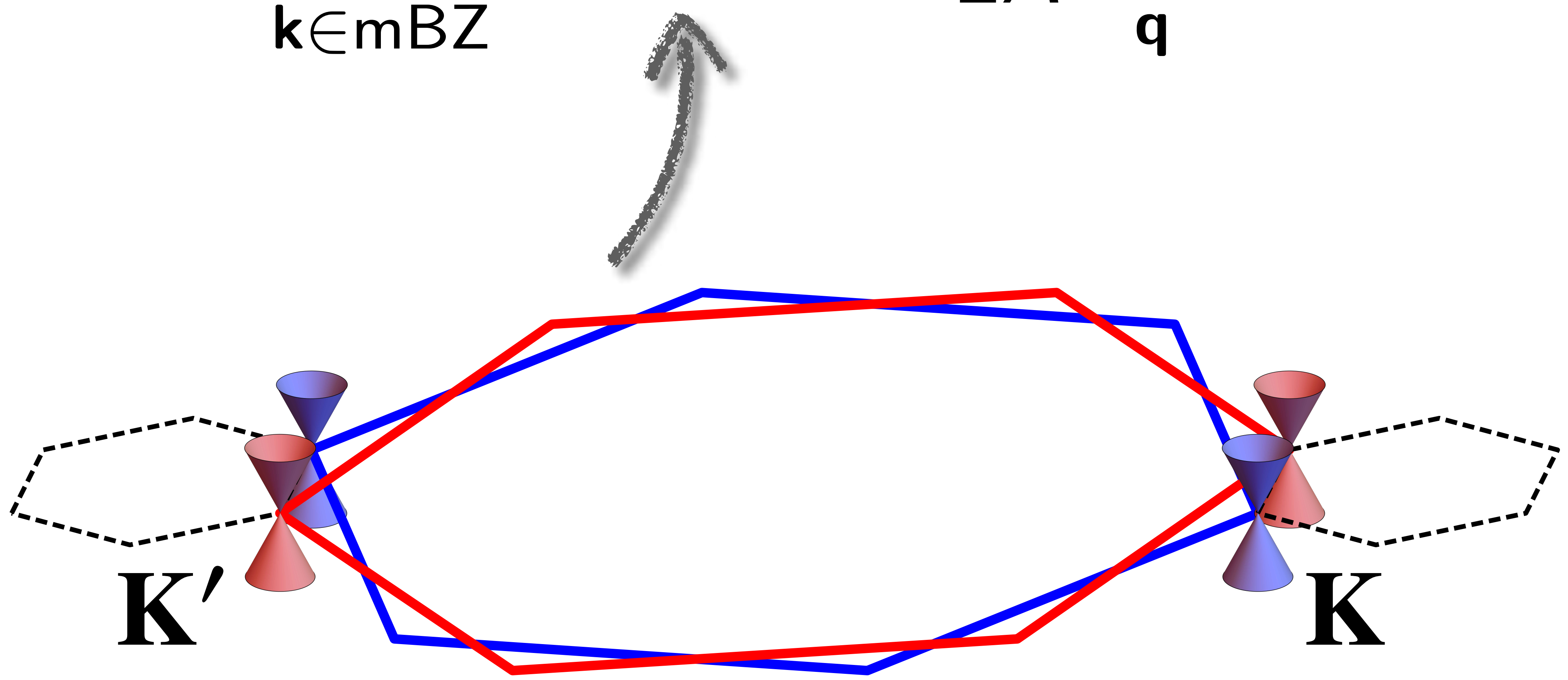


Twisted bilayer graphene: Model



Interacting Bistritzer-MacDonald model:

$$\mathcal{H} = \sum_{\mathbf{k}\in \text{mBZ}} c_{\mathbf{k}}^{\dagger} h(\mathbf{k}) c_{\mathbf{k}} - \frac{1}{2A} \sum_{\mathbf{q}} V_{\mathbf{q}} :\rho_{\mathbf{q}} \rho_{-\mathbf{q}}:$$



[Bistritzer, MacDonald, PNAS '11]
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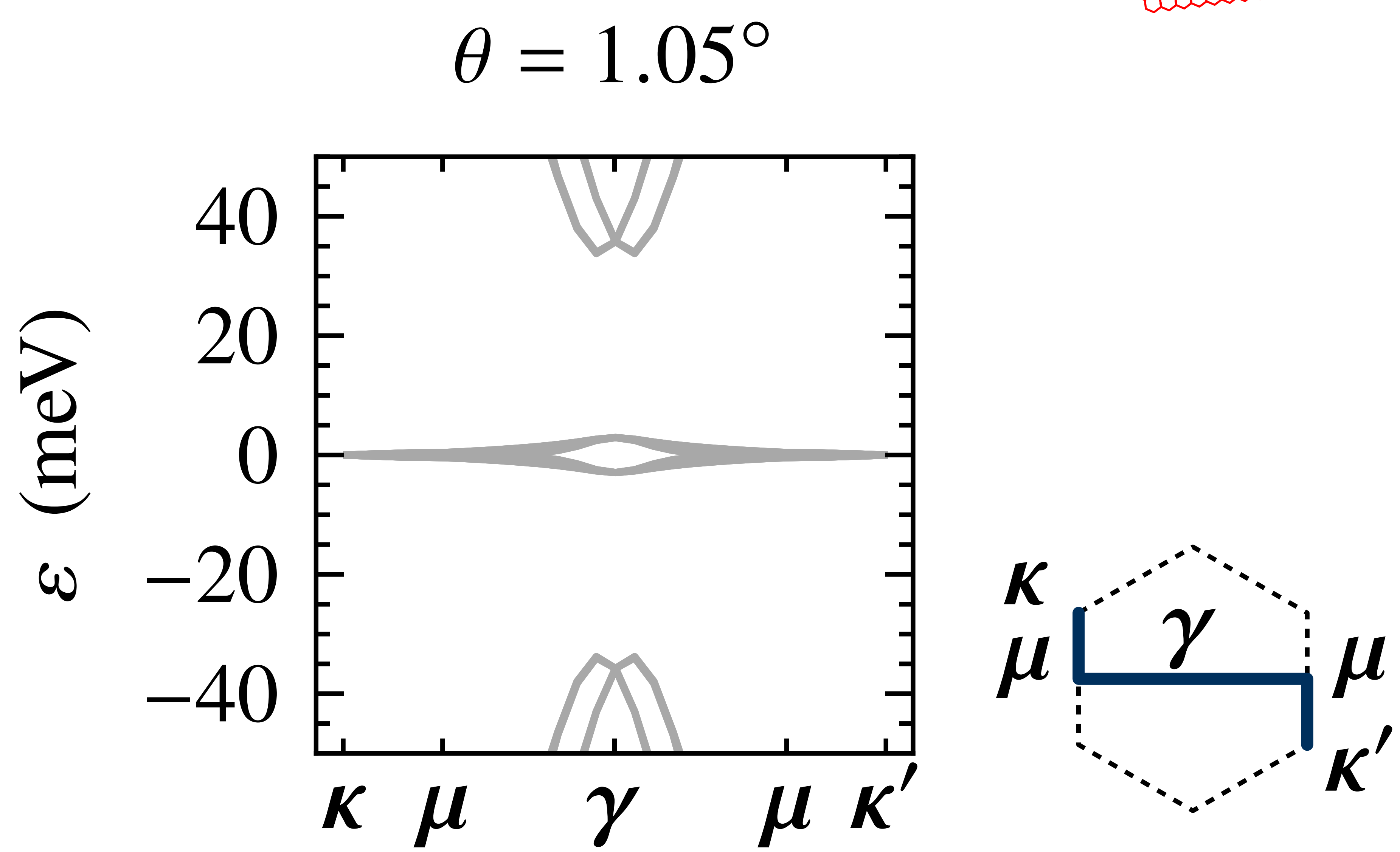

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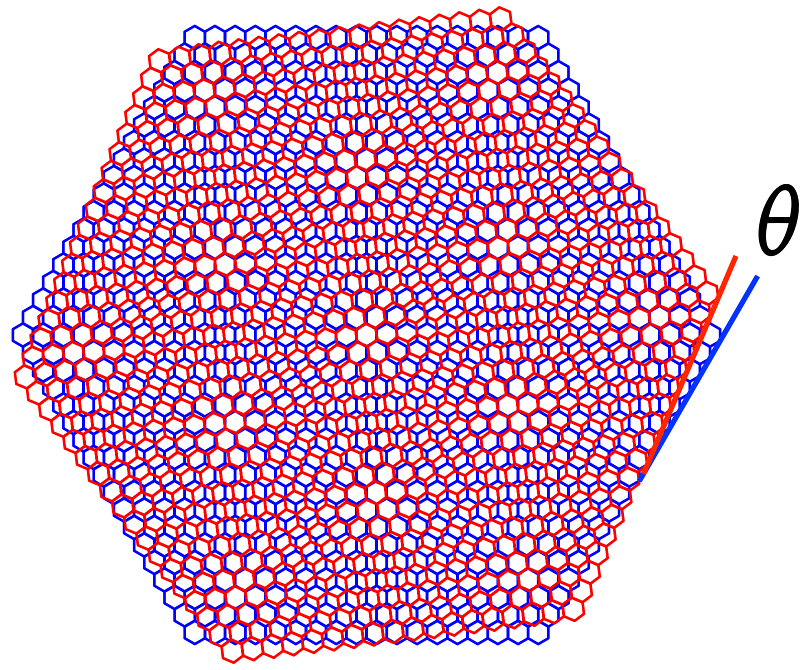

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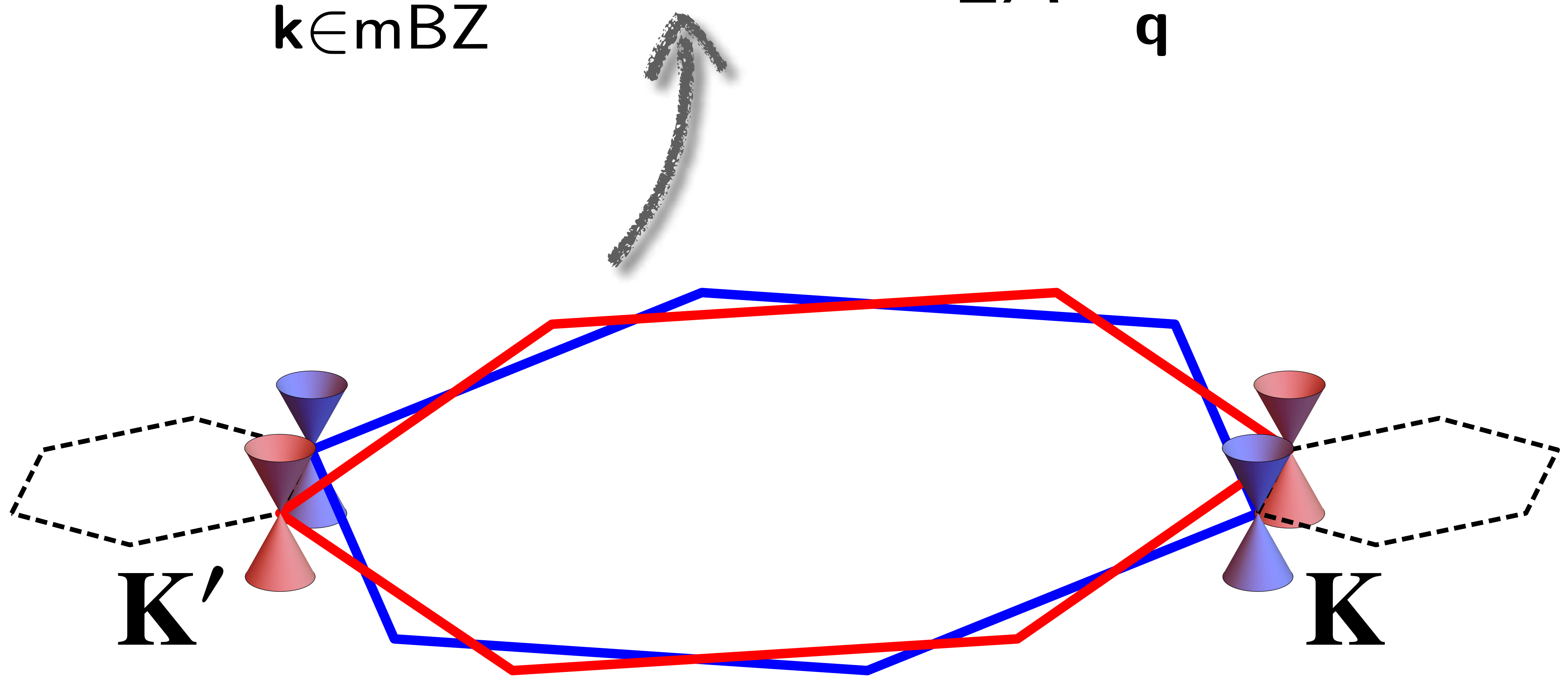

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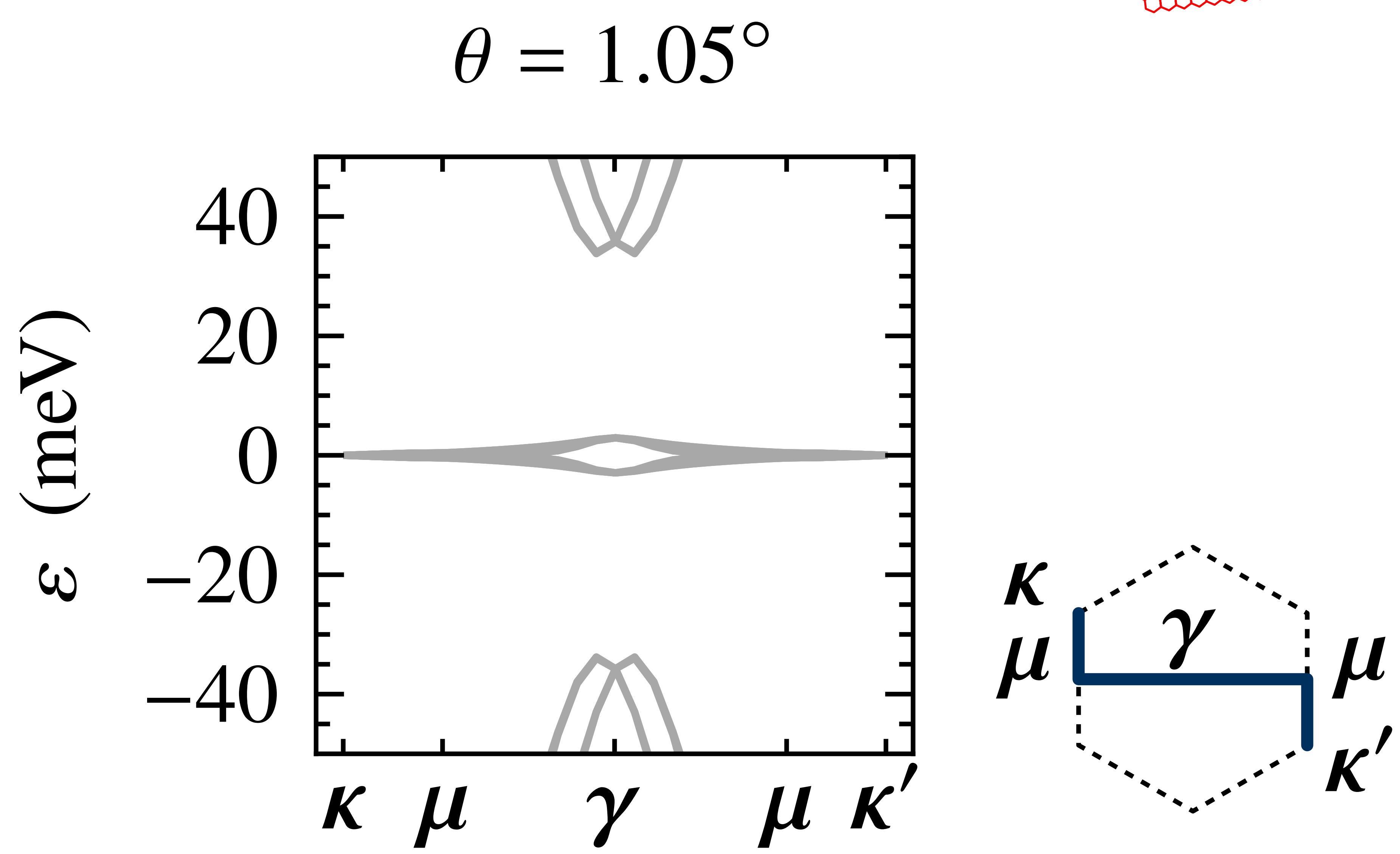
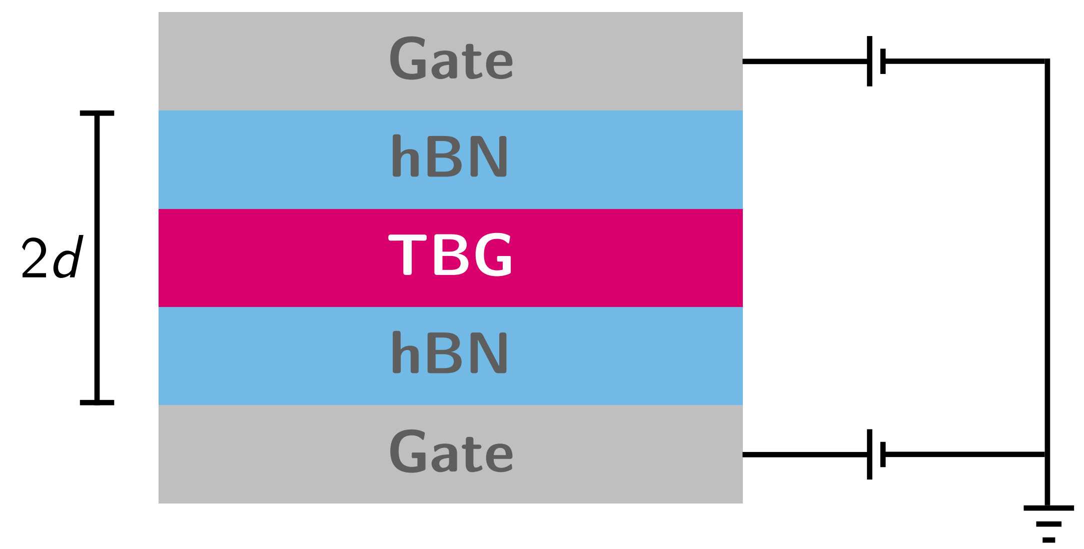


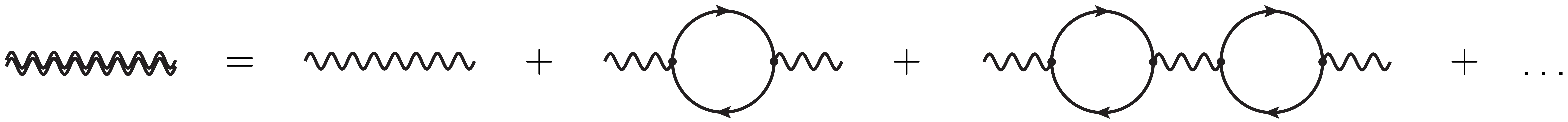
Coulomb interaction:

$$V_{\mathbf{q}} = \frac{e^2}{2\epsilon_0 \epsilon(\theta, \mathbf{q}) |\mathbf{q}|} \tanh(|\mathbf{q}| d)$$



Internal screening

Screened Coulomb interaction:



... RPA in atomistic tight-binding model

[Goodwin *et al.*, PRB '19]

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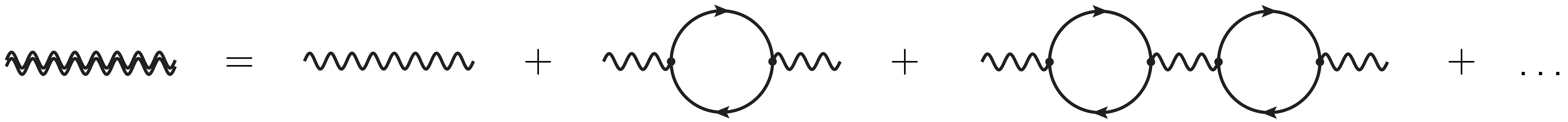

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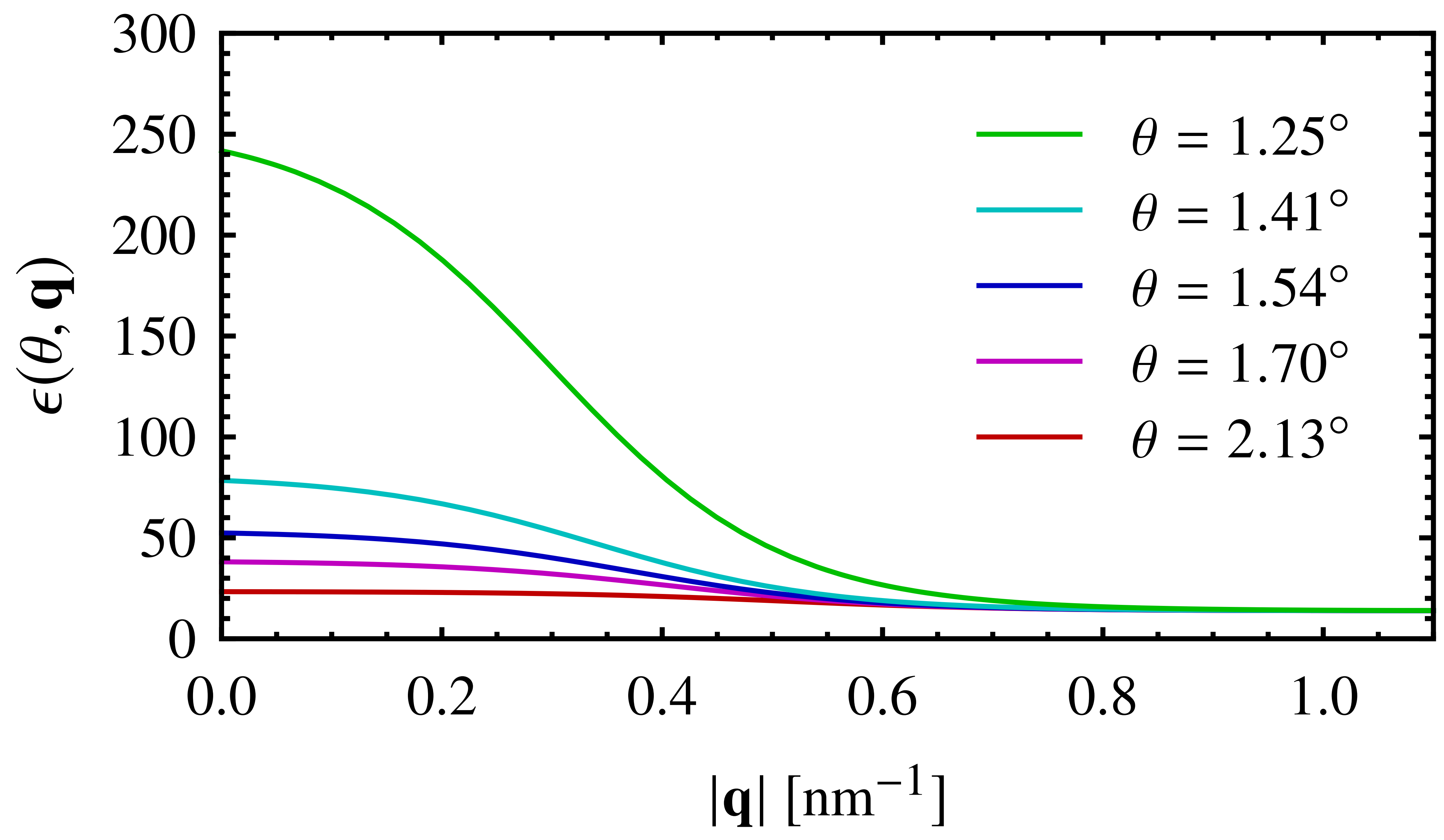
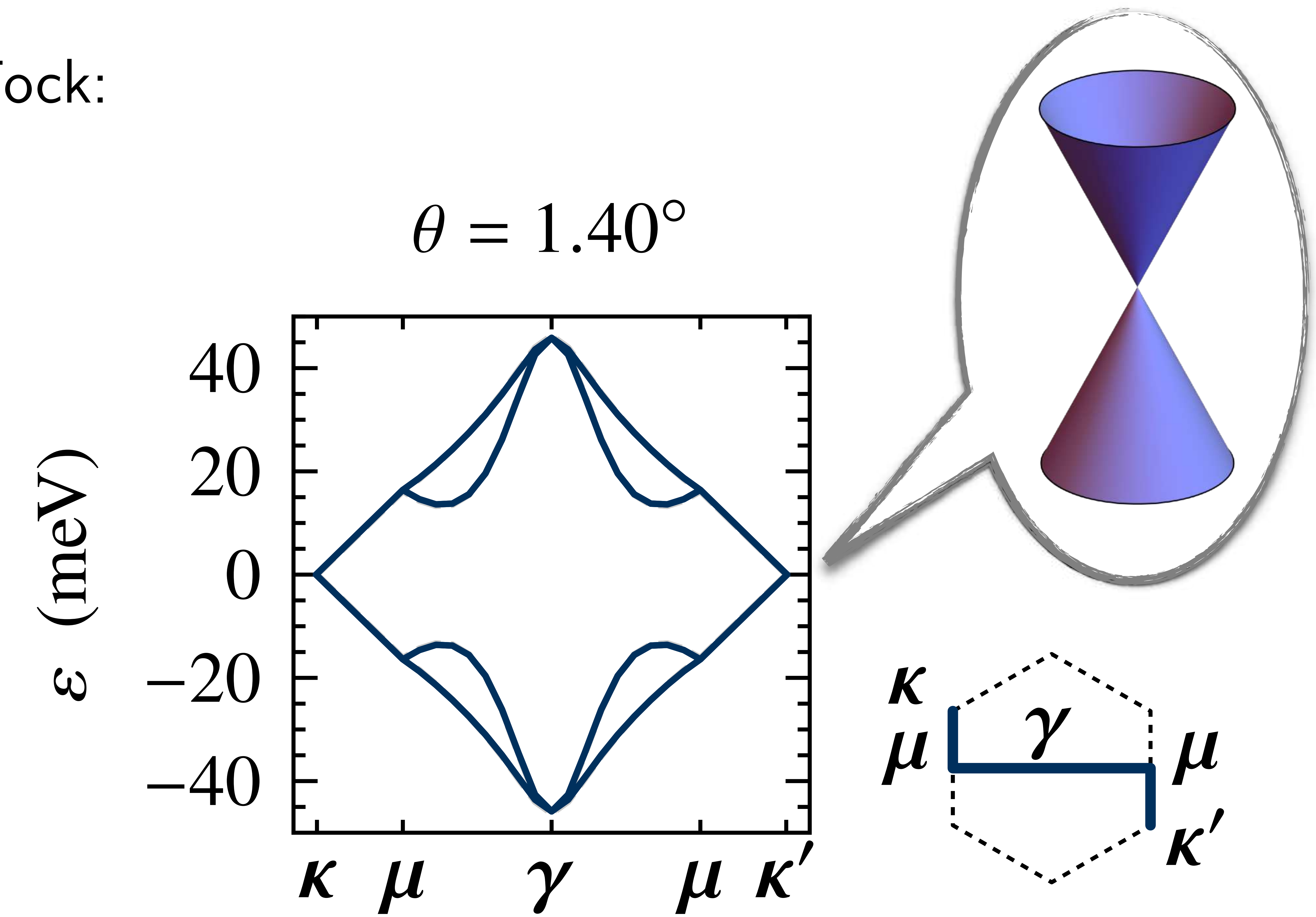
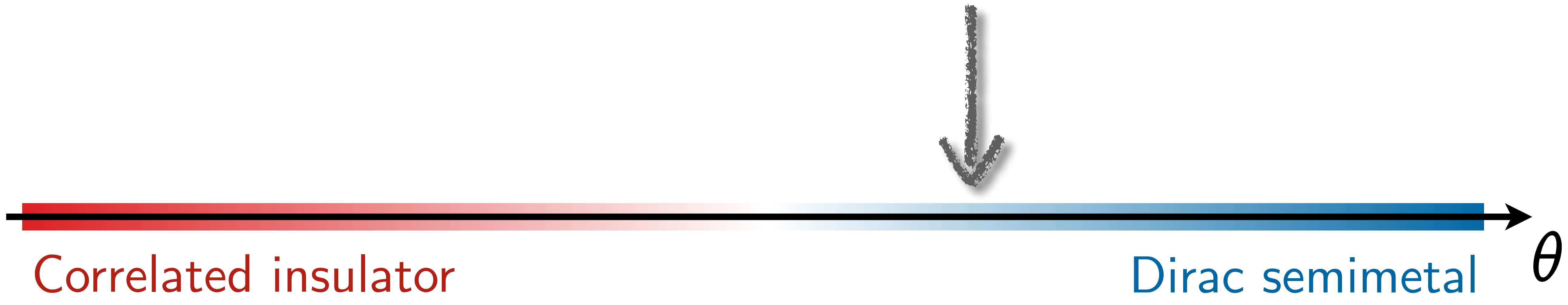
Effective dielectric permittivity:



Twisted bilayer graphene: Interacting spectrum

Selfconsistent Hartree-Fock:





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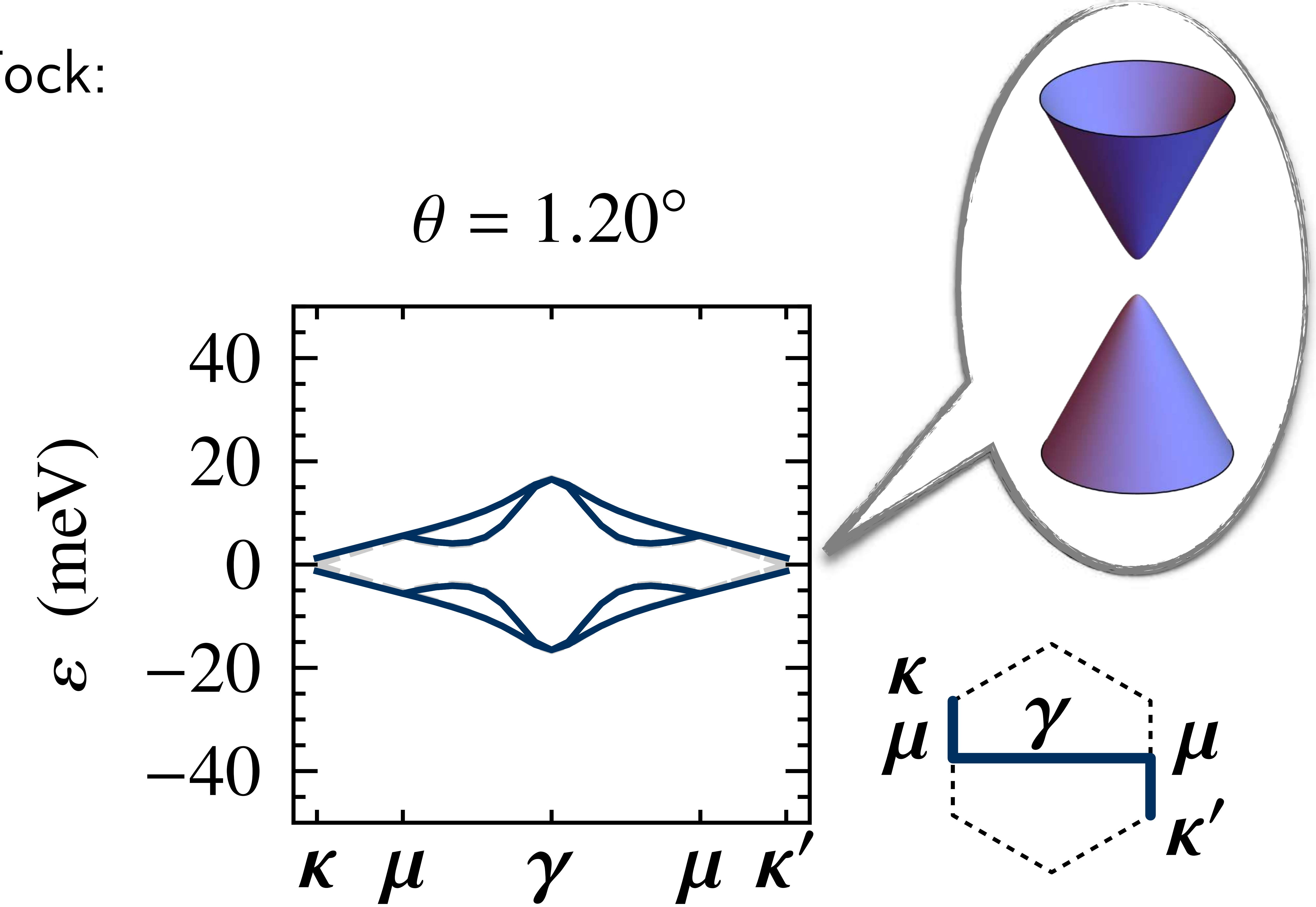

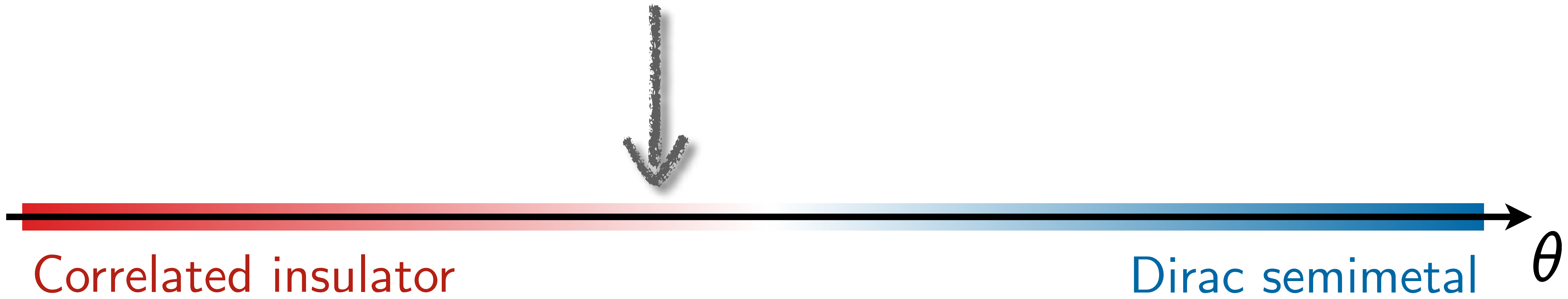

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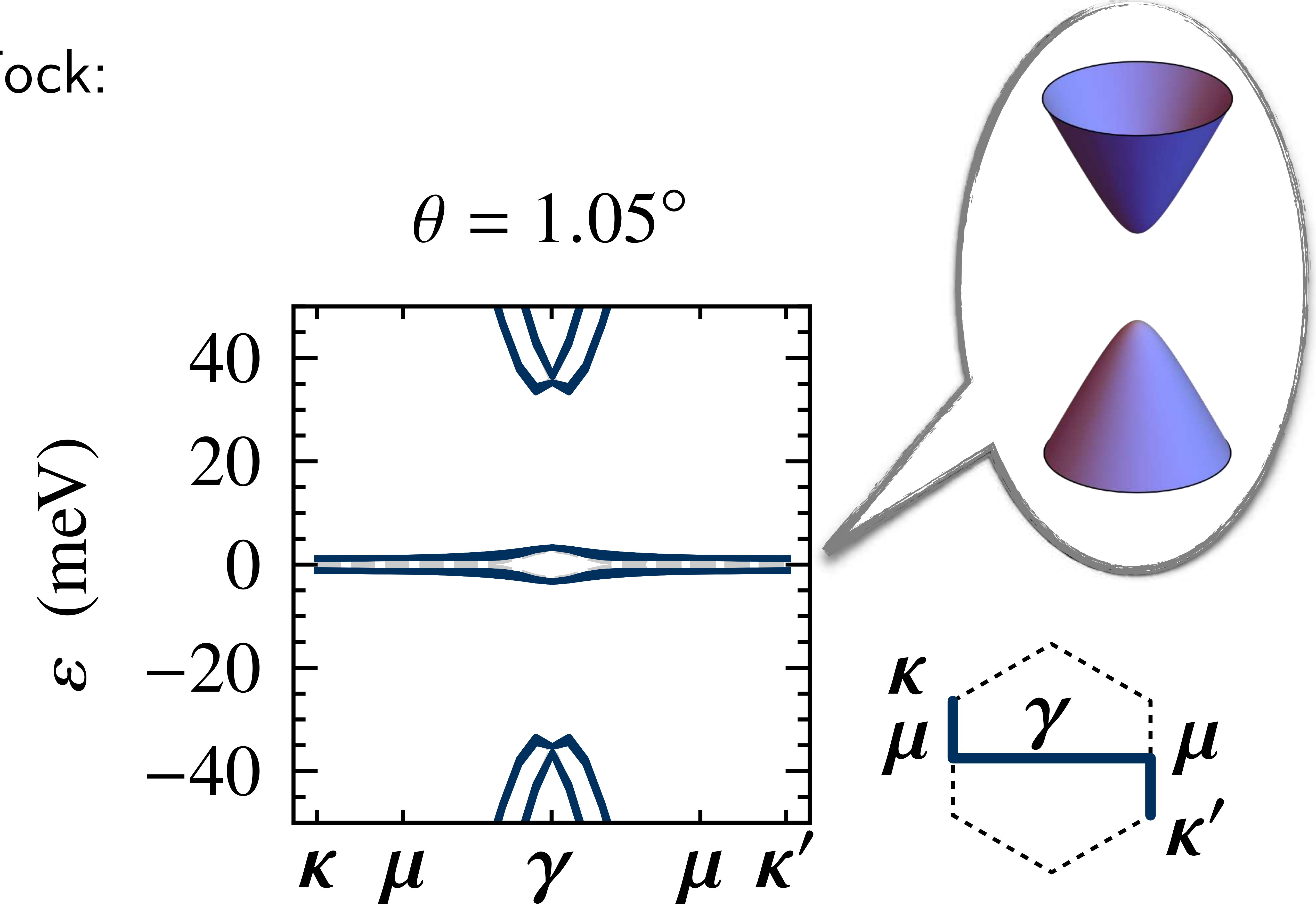
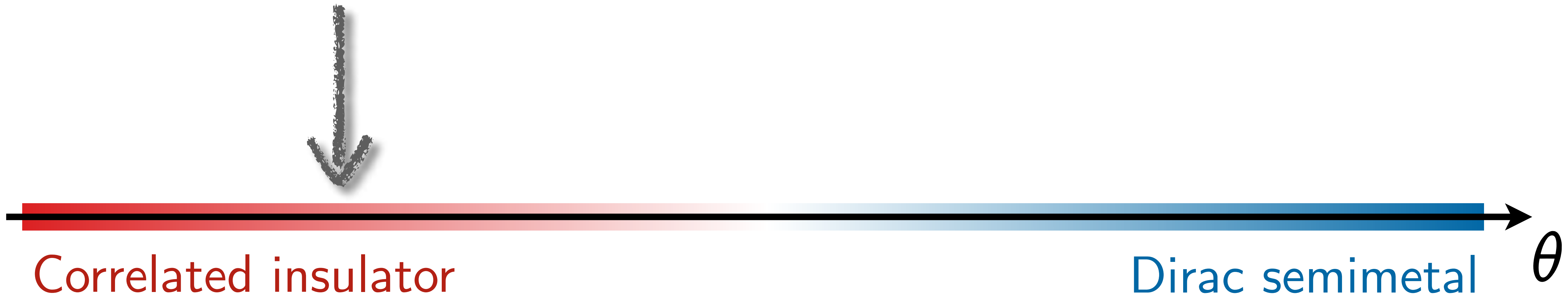




Twisted bilayer graphene: Kramers intervalley-coherent insulator

Density matrix:

$$\langle c^{\dagger}_{\tau\sigma} c_{\tau'\sigma'} \rangle$$

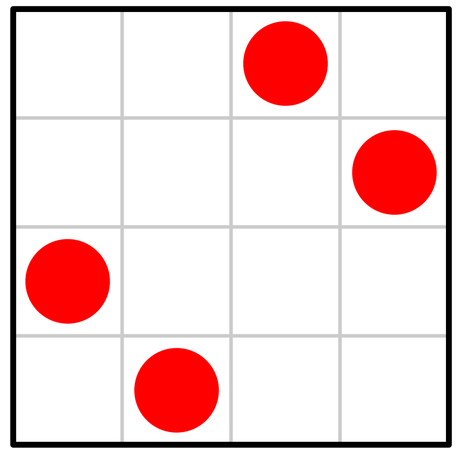
valley

sublattice

Twisted bilayer graphene: Kramers intervalley-coherent insulator

Density matrix:

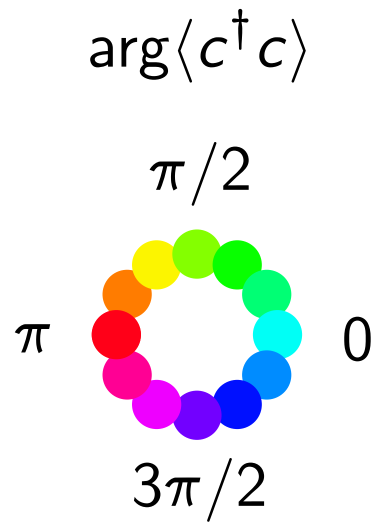
$$\langle c^\dagger_{\tau\sigma} c_{\tau'\sigma'} \rangle \xrightarrow{\mathbf{k}=0} \left\{ \frac{1}{2}\left(\mathbb{1} + \right. \right.$$



$\left.\right)$ Dirac semimetal

valley

sublattice



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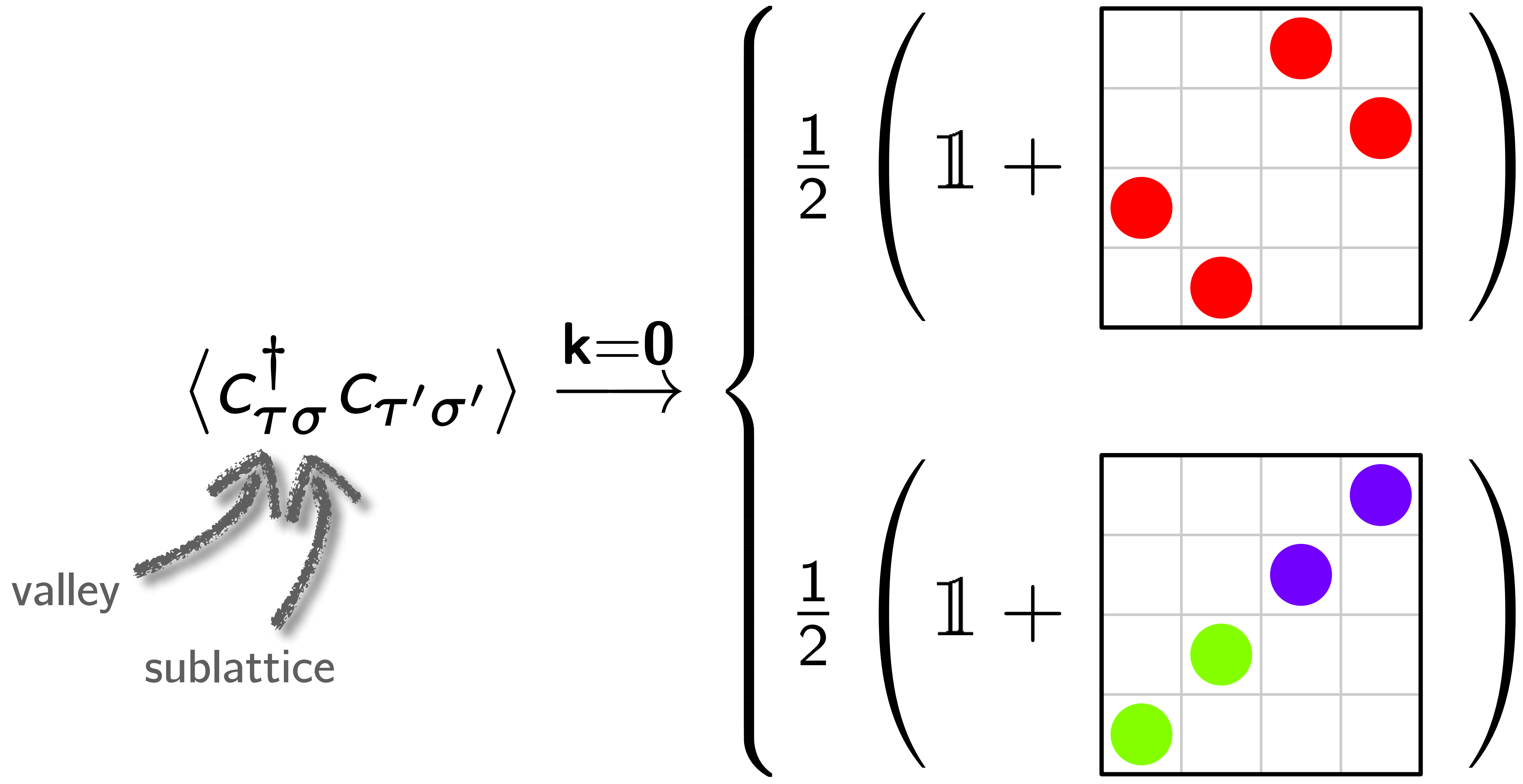
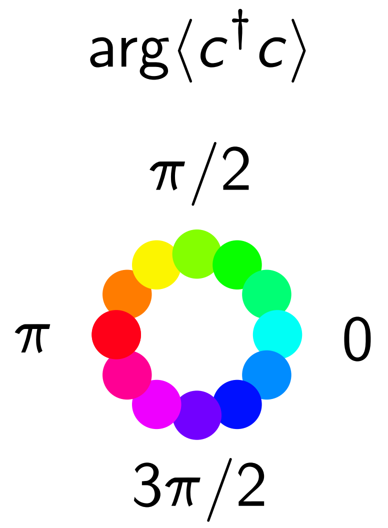


Dirac semimetal

KIVC insulator @ strong coupling



… breaks time reversal $\mathcal{T}$ & $\mathrm{U}(1)_{\mathrm{valley}}$

… preserves combination $(-\mathrm{i})\tau_z\mathcal{T}$

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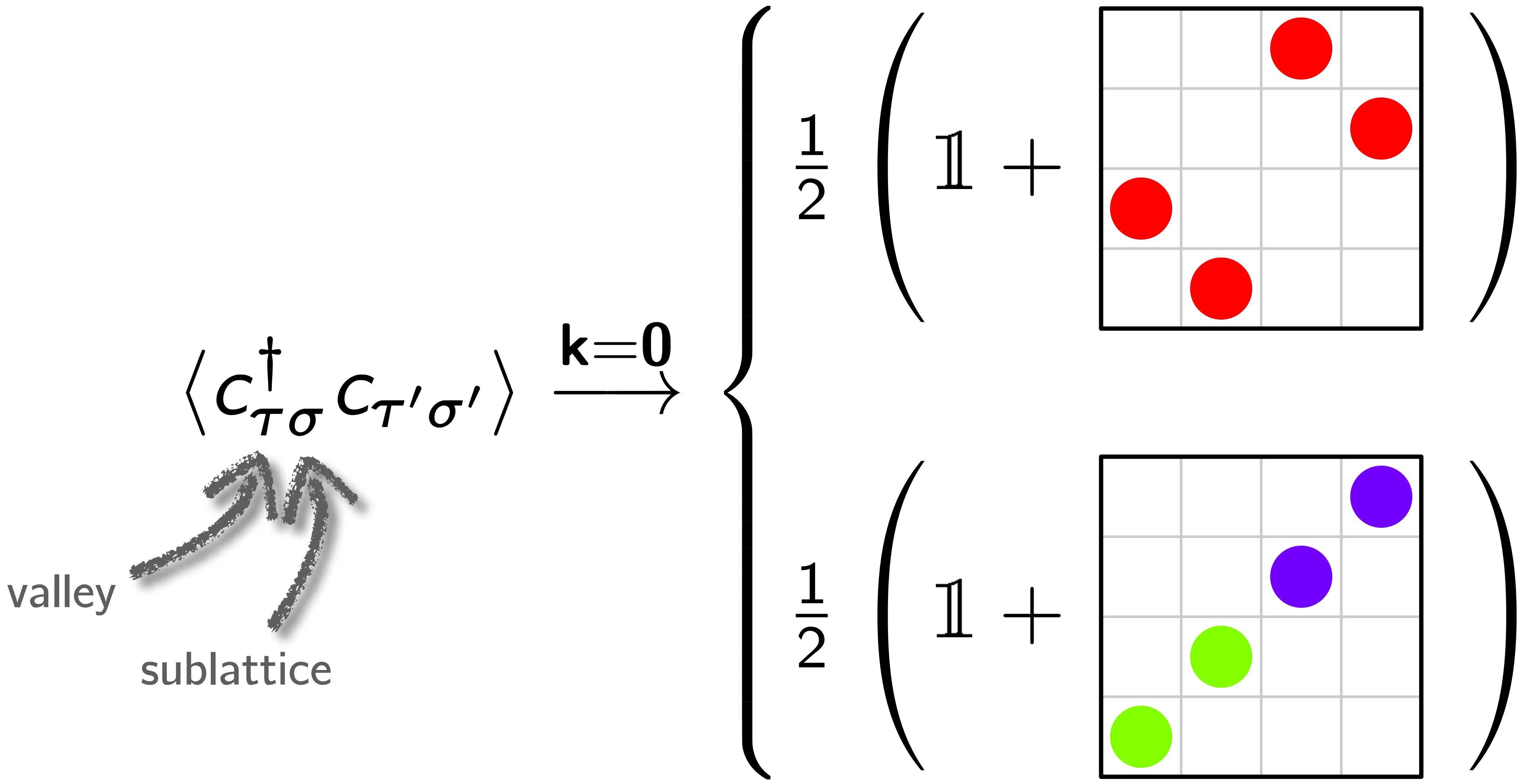

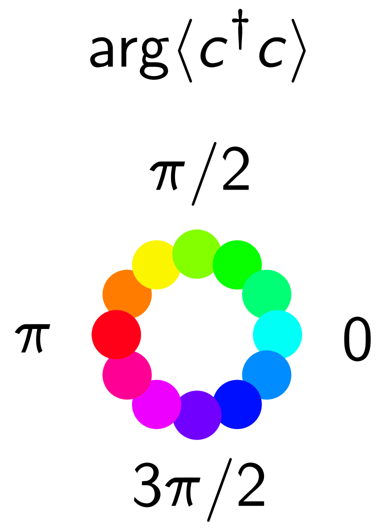

Dirac semimetal

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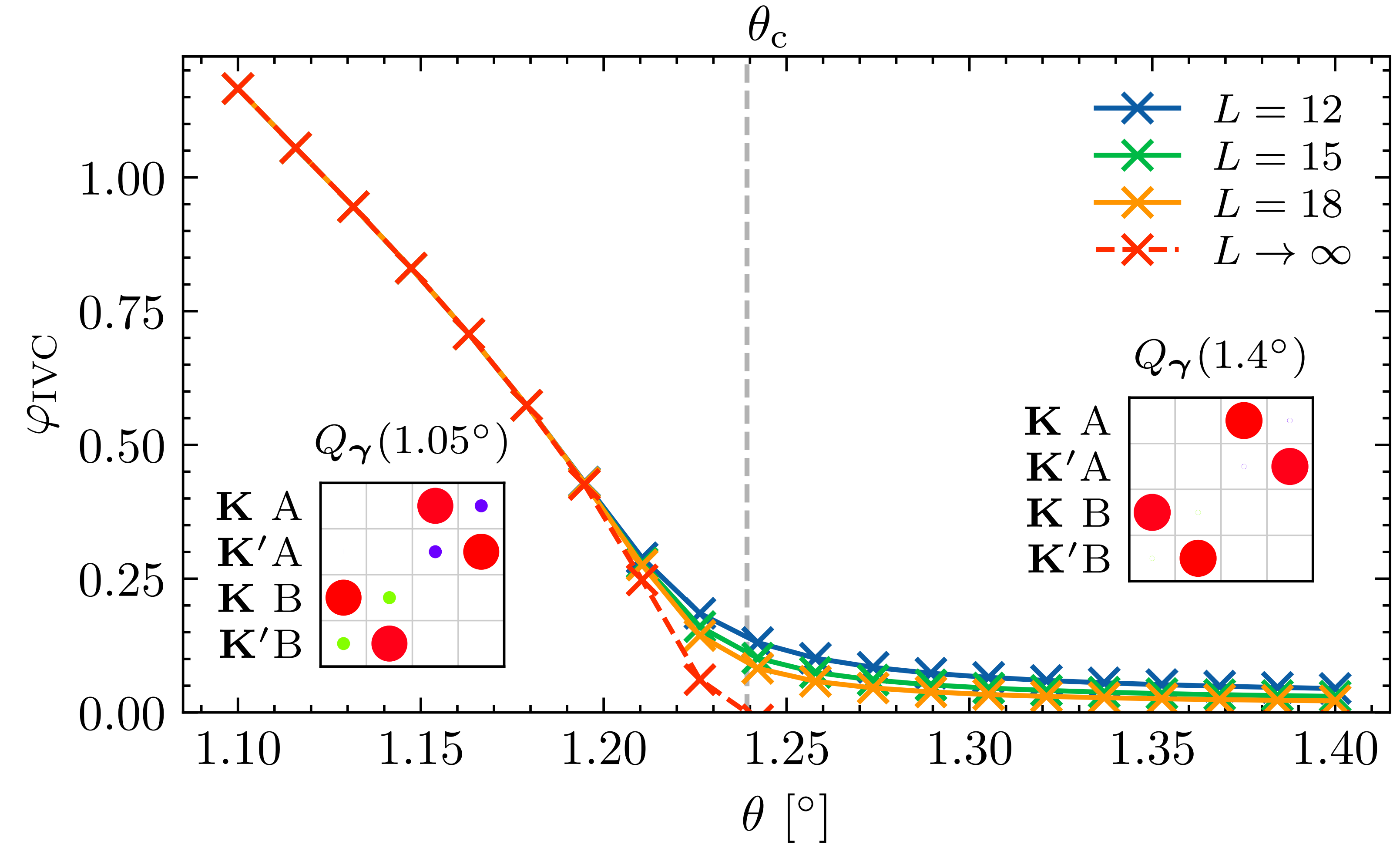
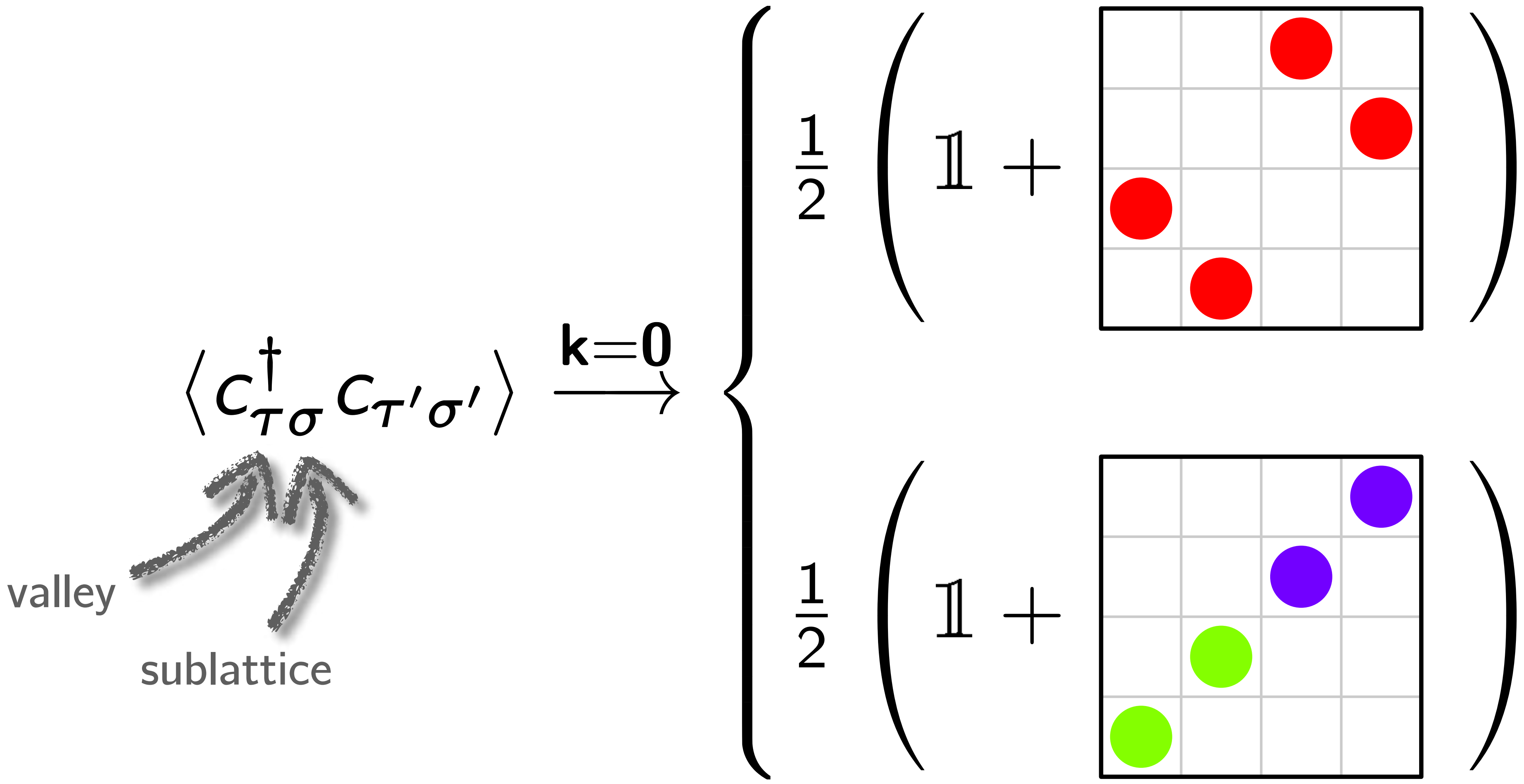
Intervalley-coherence order parameter:



… for d = 20nm

Twisted bilayer graphene: Kramers intervalley-coherent insulator

Density matrix:



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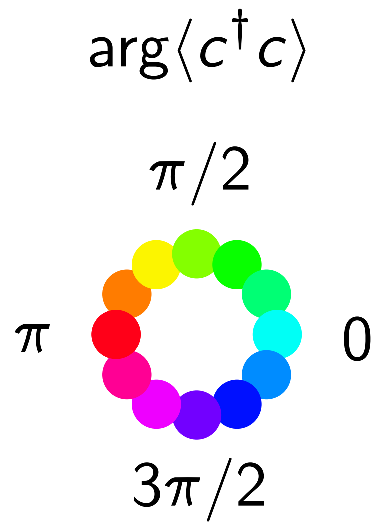

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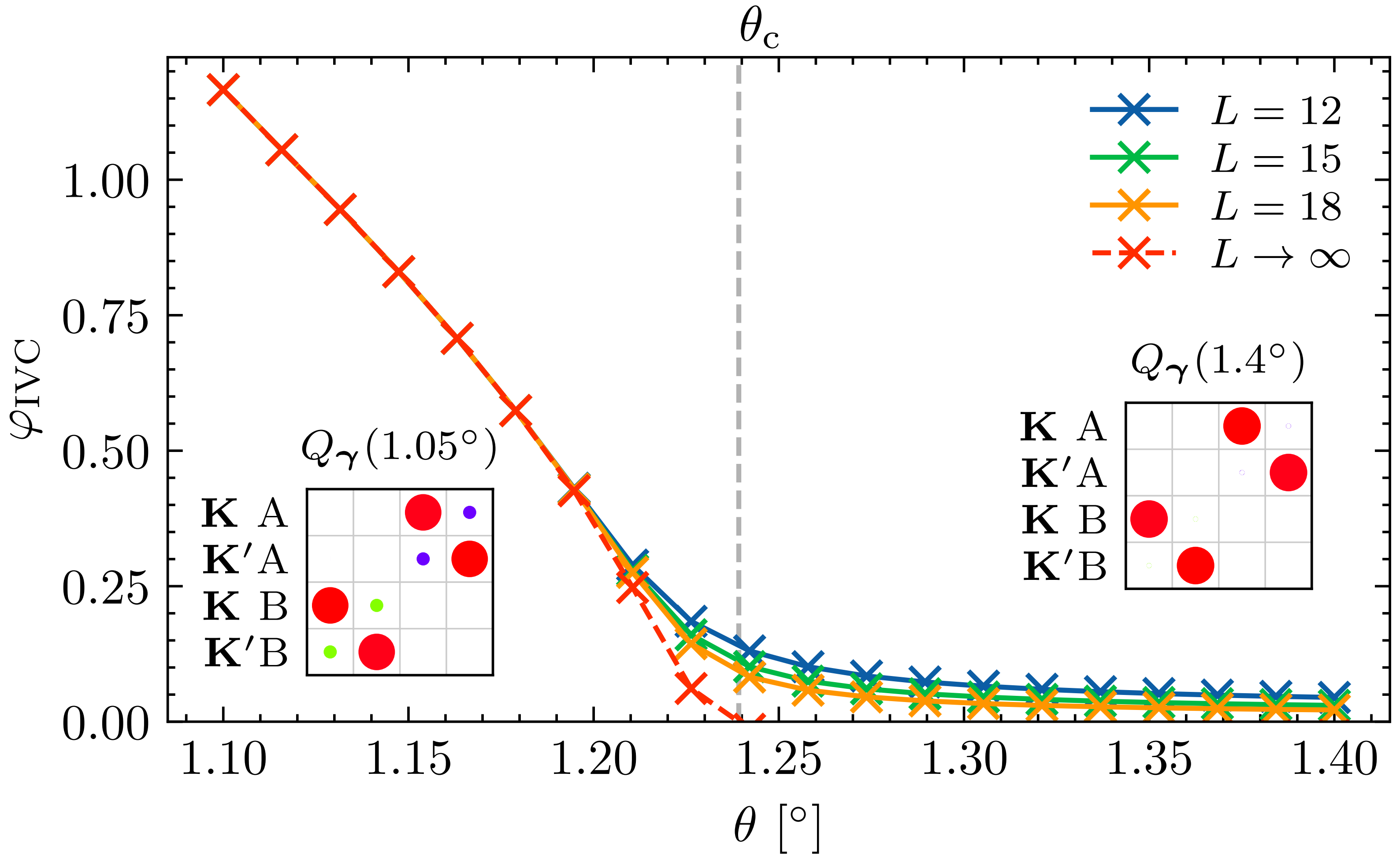
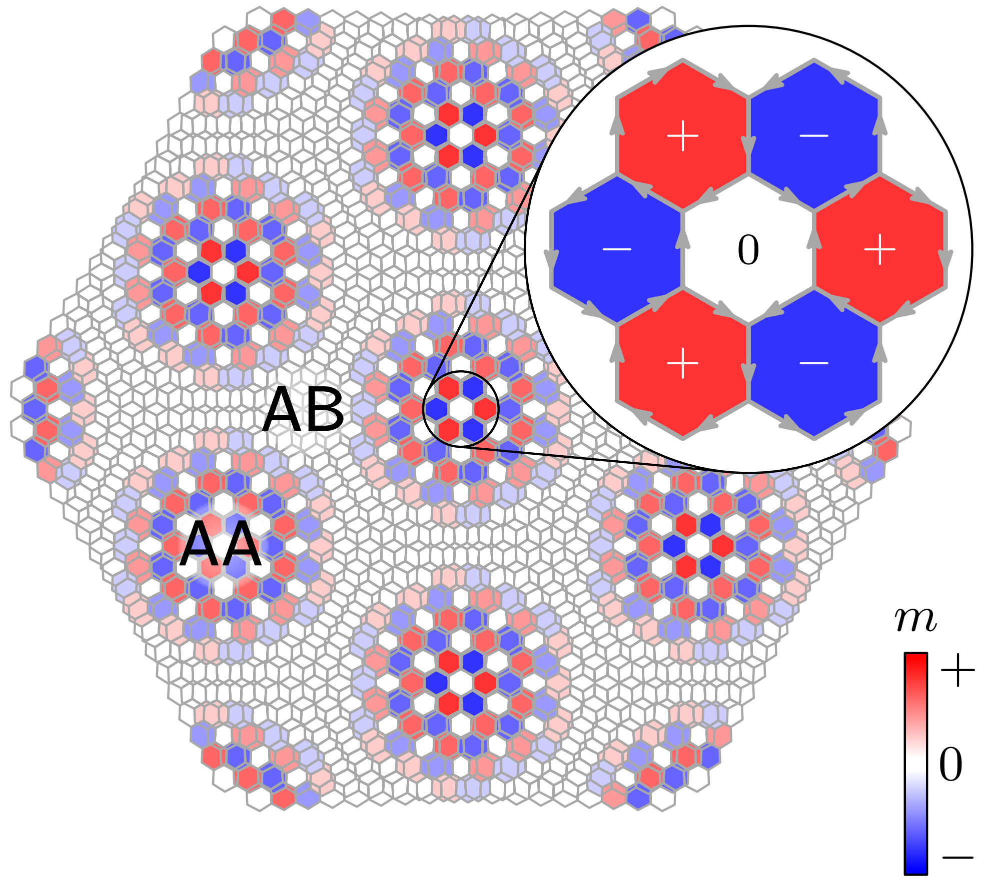


... for d = 20nm

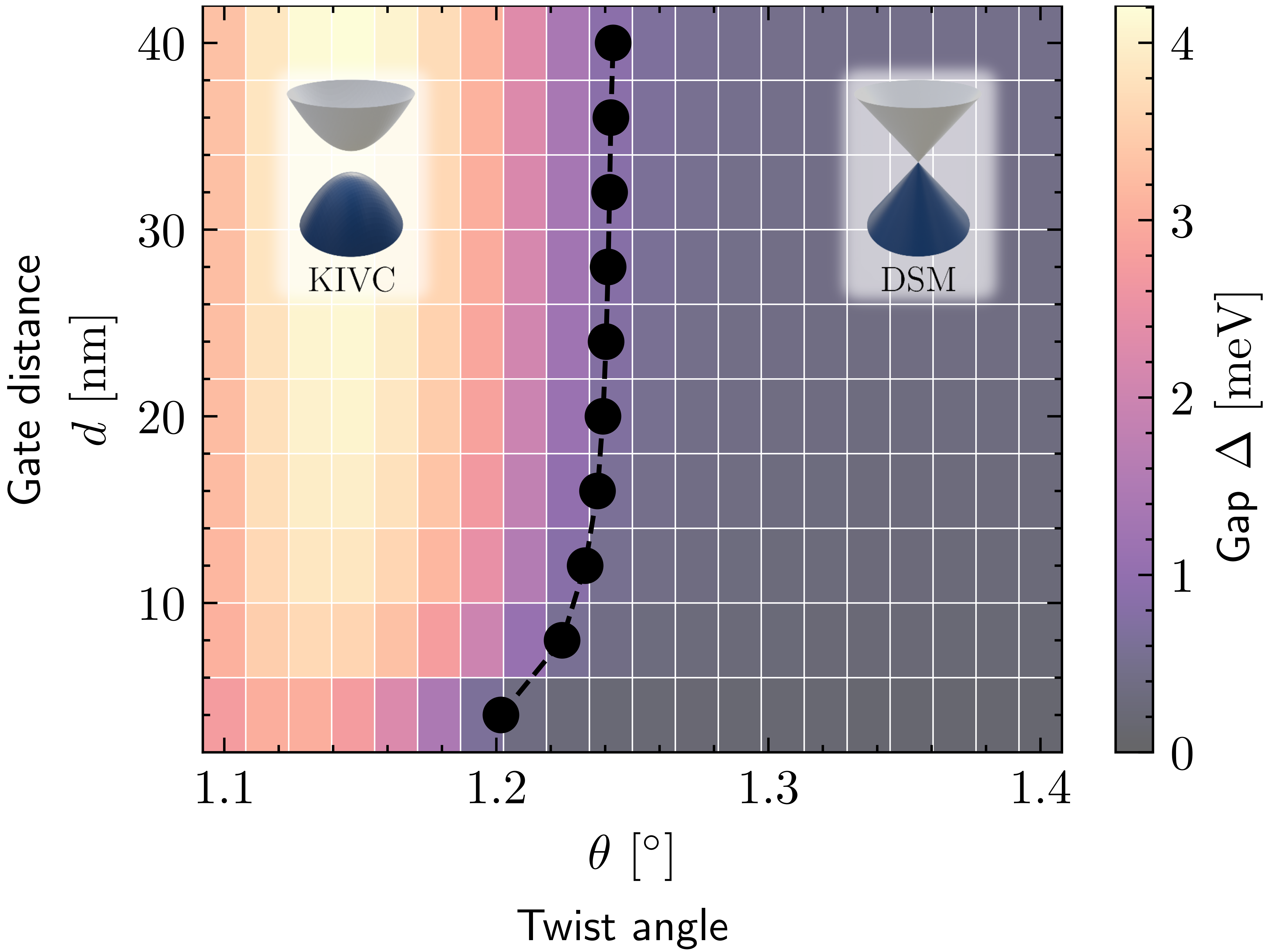
Real-space representation:



... in agreement with
[Bultinck *et al.*, PRX '20]
[Kwan *et al.*, PRX '21]
[Wagner *et al.*, PRL '22]
[Hofmann *et al.*, PRX '22]
[Rai *et al.*, PRX '24]
...

→ **Talk by J. Hofmann**

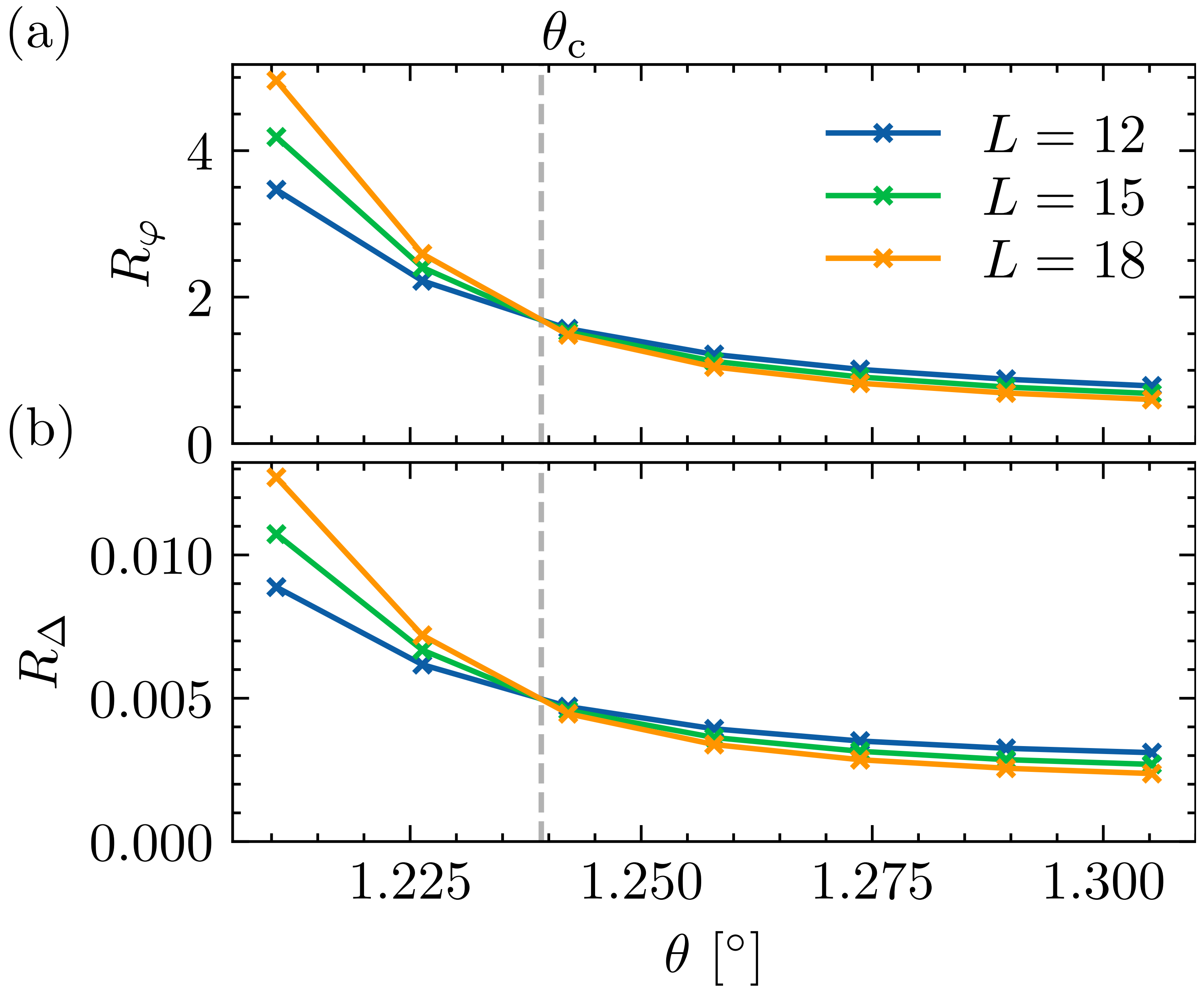
Twisted bilayer graphene: Phase diagram



[Biedermann & LJ, PRB '25]
... see also [Huang *et al.*, Nat. Commun. '25]

Twisted bilayer graphene: Quantum criticality

Crossing-point analysis:



$$R_\varphi = L^{(1+\eta_\varphi)/2}\varphi_{\mathrm{IVC}}$$
$$R_\Delta = L^z \Delta / t_0$$

anomalous dimension

dynamical exponent

nearest-neighbor hopping amplitude

Twisted bilayer graphene: Quantum criticality

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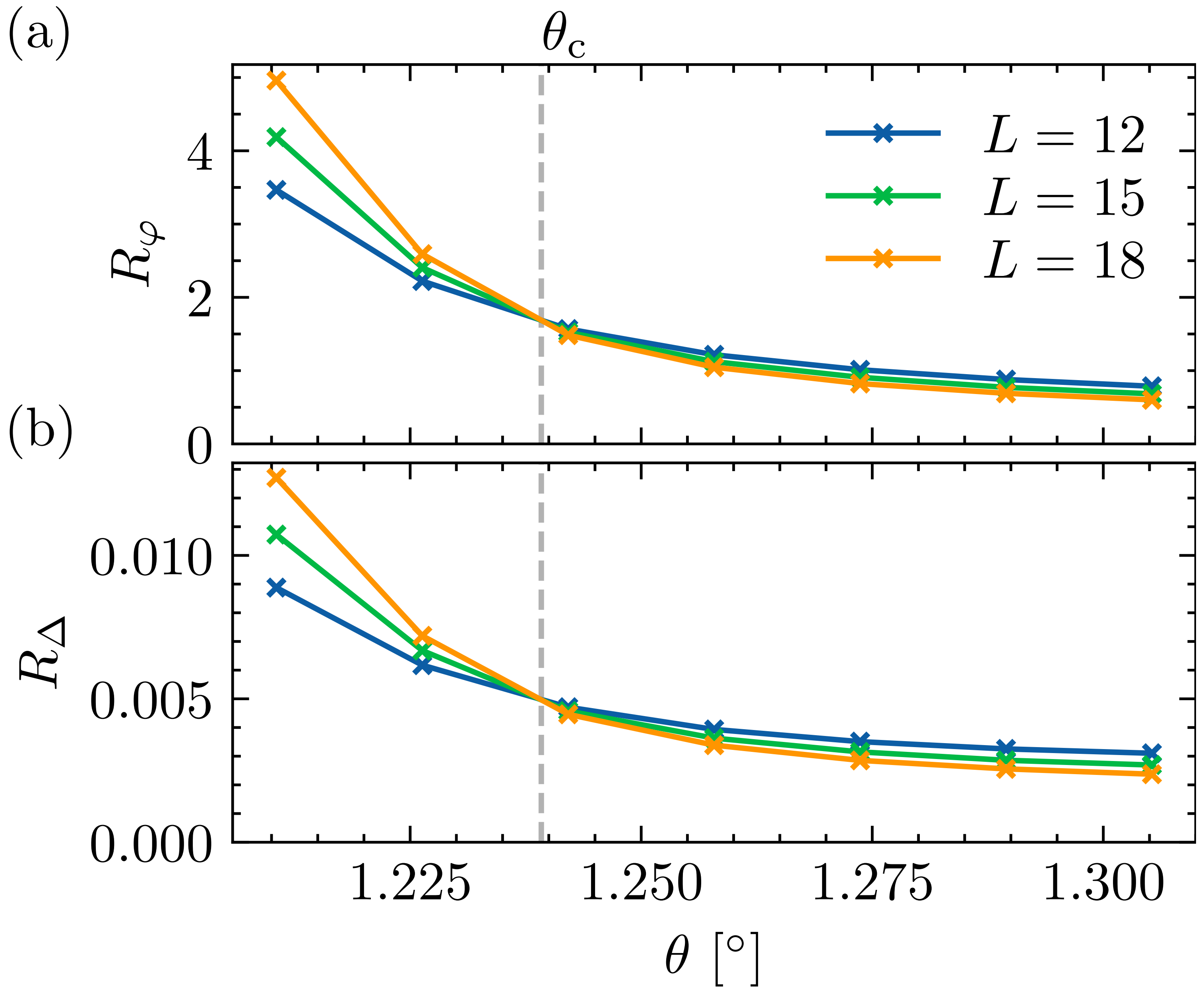

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Gross-Neveu-XY universality class:

$$\mathcal{L} = \bar{\psi}\gamma_\mu\partial_\mu\psi + g\begin{pmatrix}\mathrm{i}\bar{\psi}\gamma_3\psi \\ \mathrm{i}\bar{\psi}\gamma_5\psi\end{pmatrix}\cdot\begin{pmatrix}\varphi_1 \\ \varphi_2\end{pmatrix} + \dots$$

... with emergent relativistic symmetry

[Biedermann & LJ, PRB '25]

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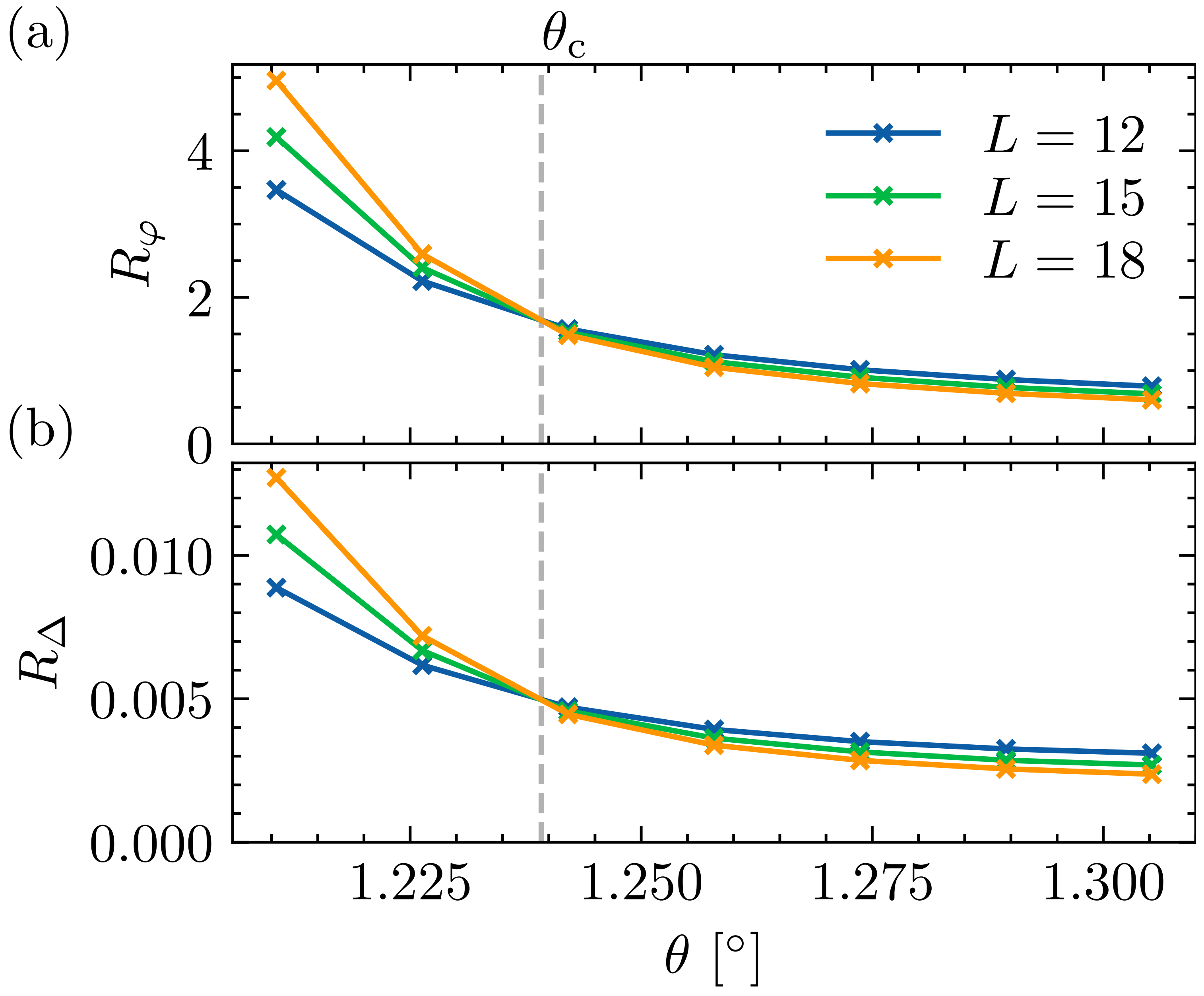

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... with emergent relativistic symmetry

[Biedermann & LJ, PRB '25]

Critical exponents:

$$z = 1$$

$$\eta_\varphi \approx 0.93$$

$$\beta \approx 1.05$$

... from $4 - \epsilon$ and $2 + \epsilon$ expansions

[Hawashin, Scherer, LJ, PRB '25]

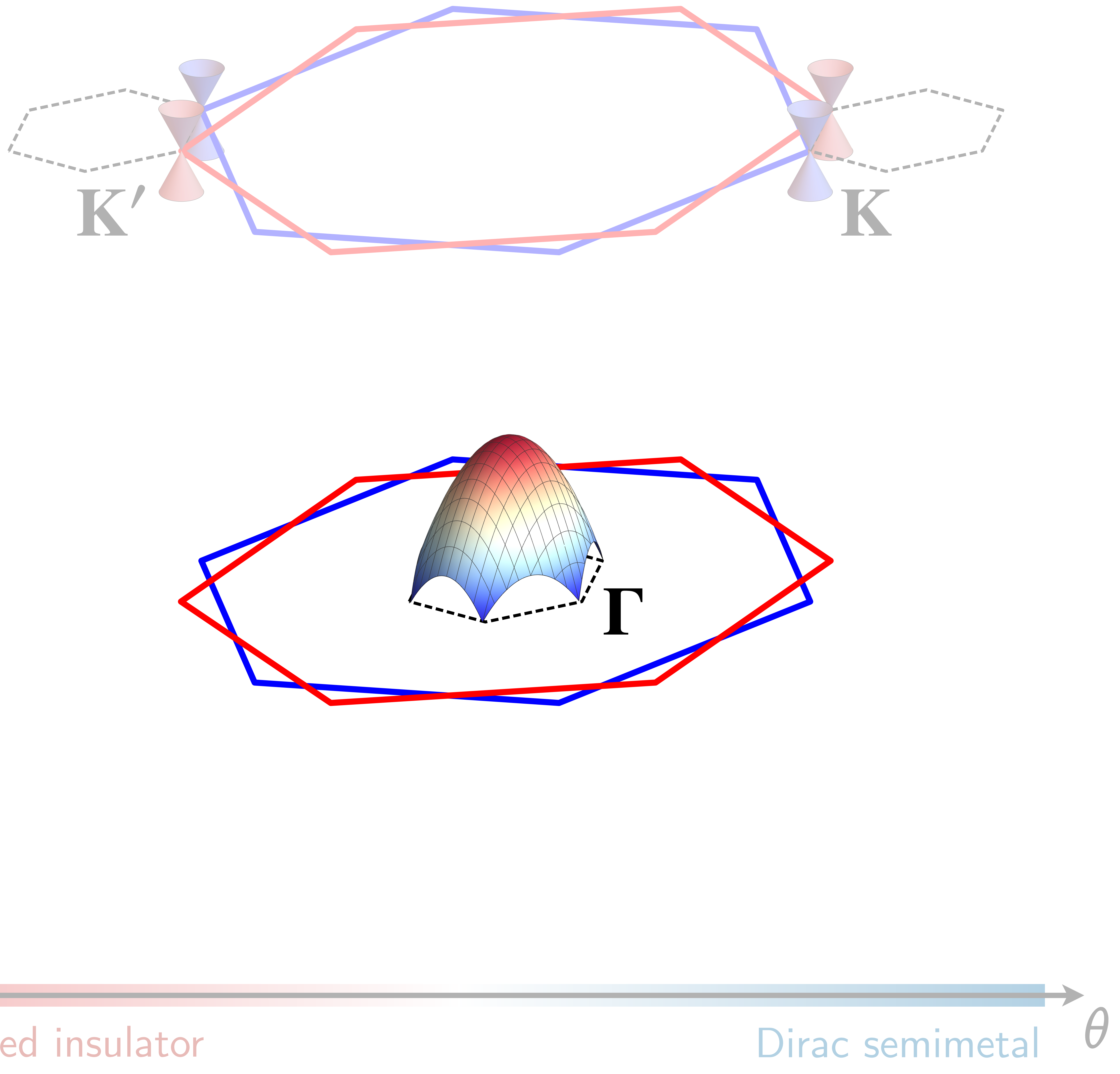
Outline

(1) Introduction

(2) Twisted bilayer graphene

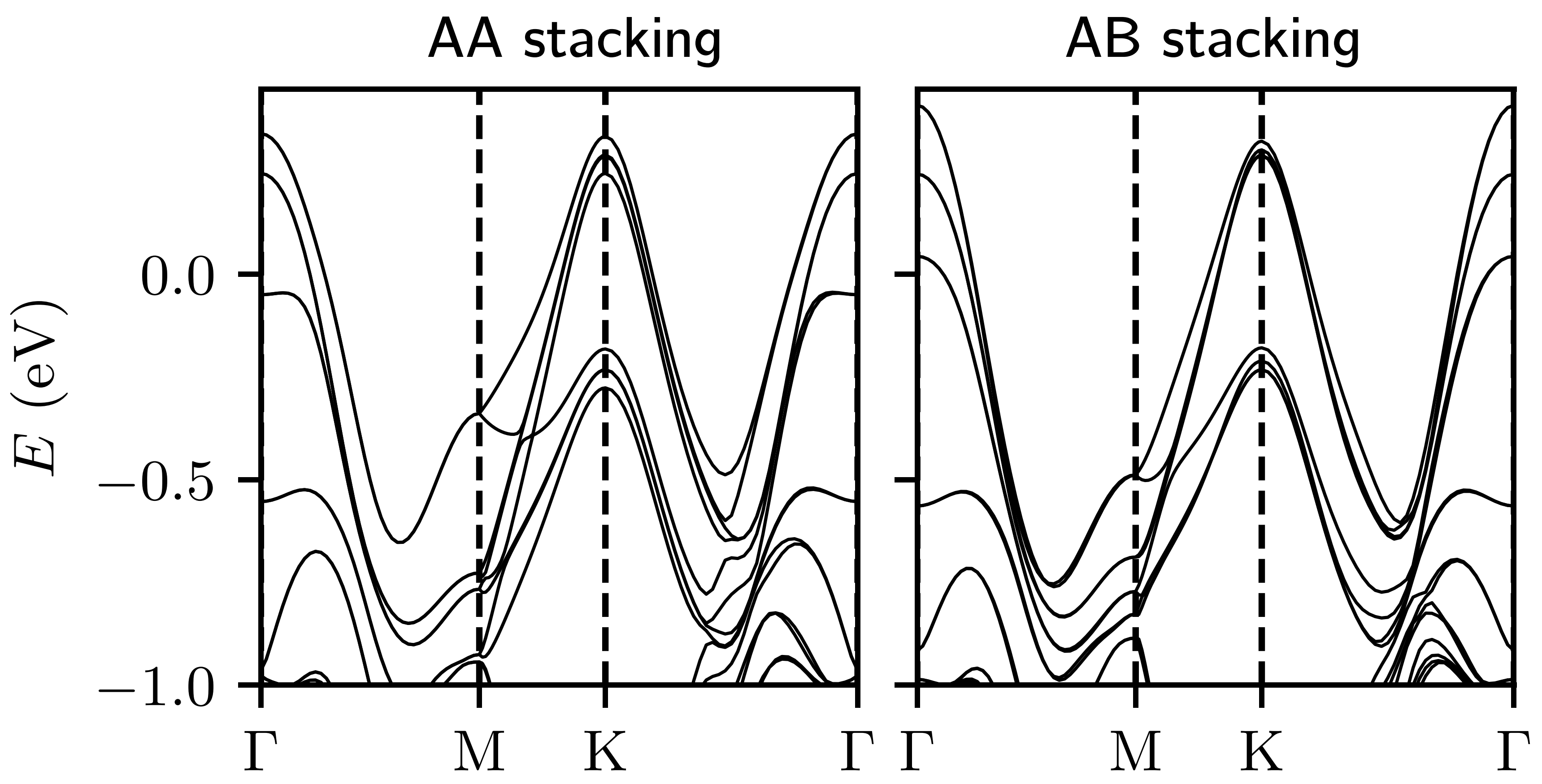
(3) Twisted double bilayer TMDs

(4) Conclusions



Double bilayer transition metal dichalcogenides (TMDs)

Untwisted noninteracting spectrum:



... for double bilayer WSe_2
[Pan *et al.*, PRRes '23]

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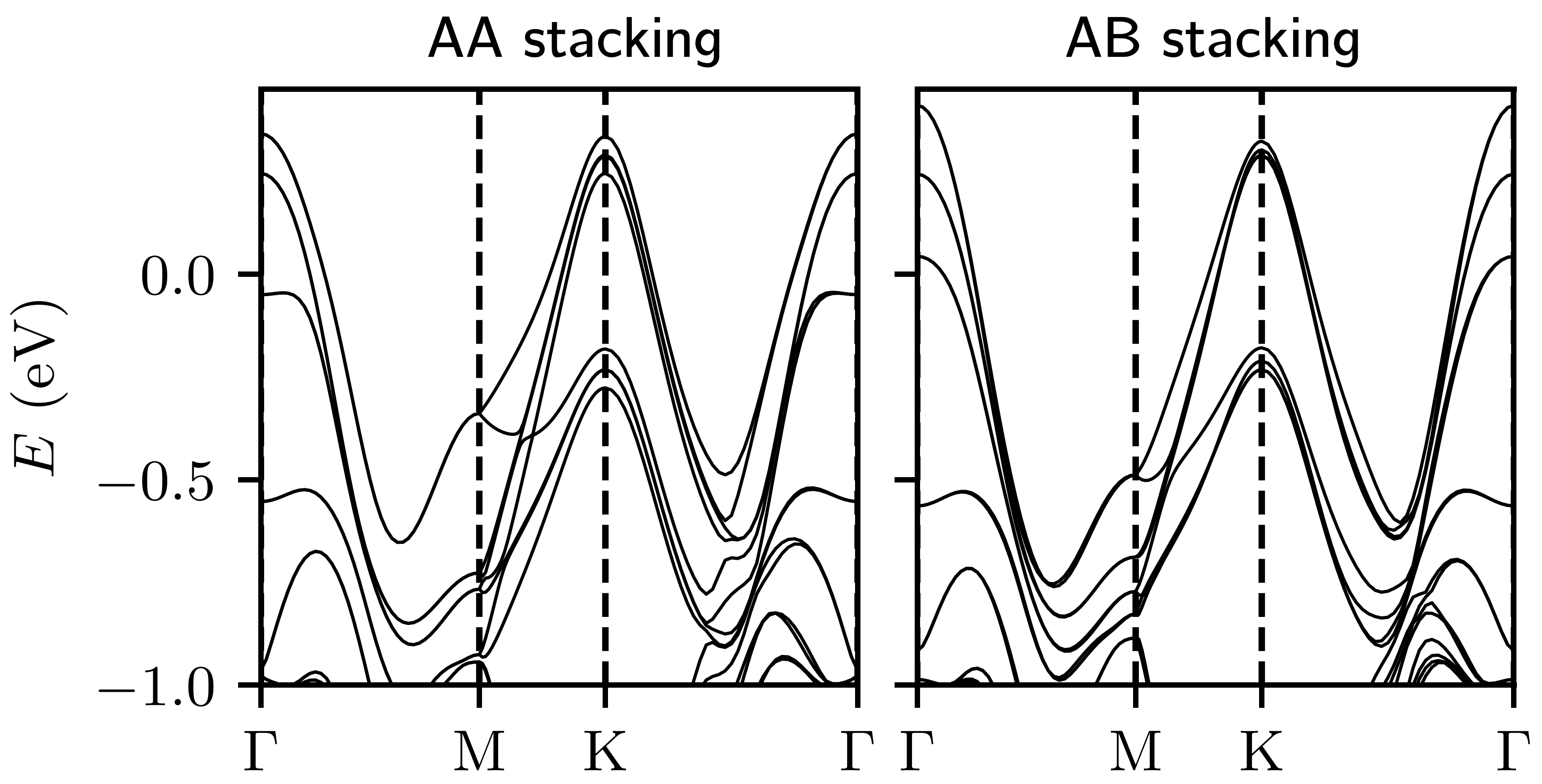

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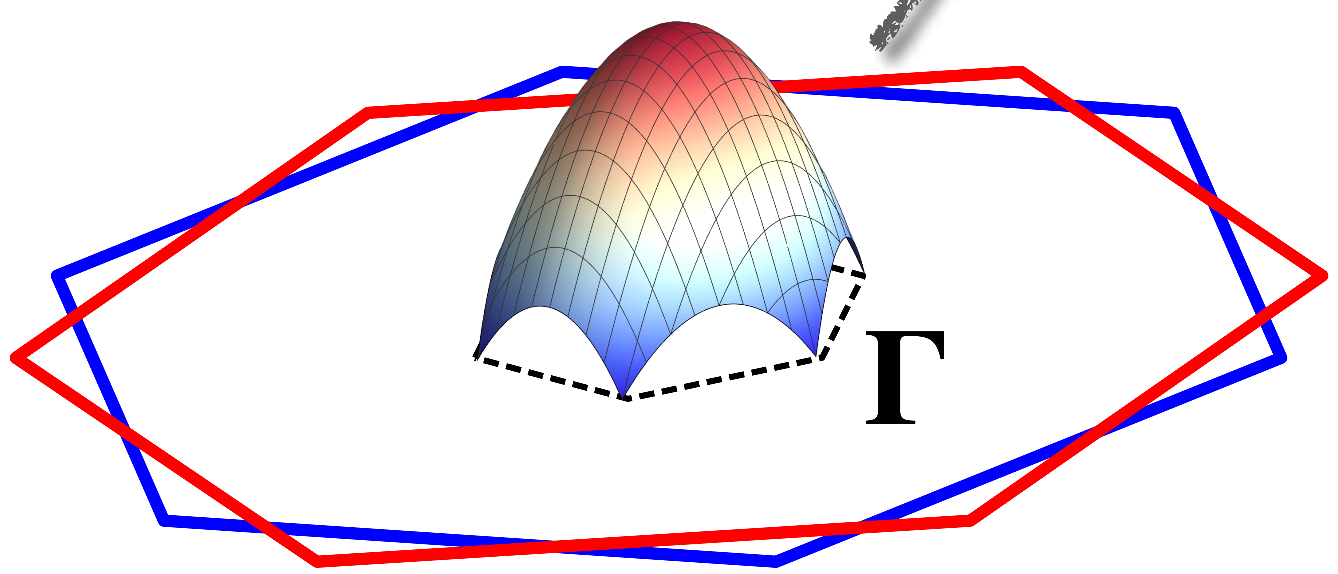

Coulomb interaction with effective permittivity ε_{eff}

[Angeli & MacDonald, PNAS '21]

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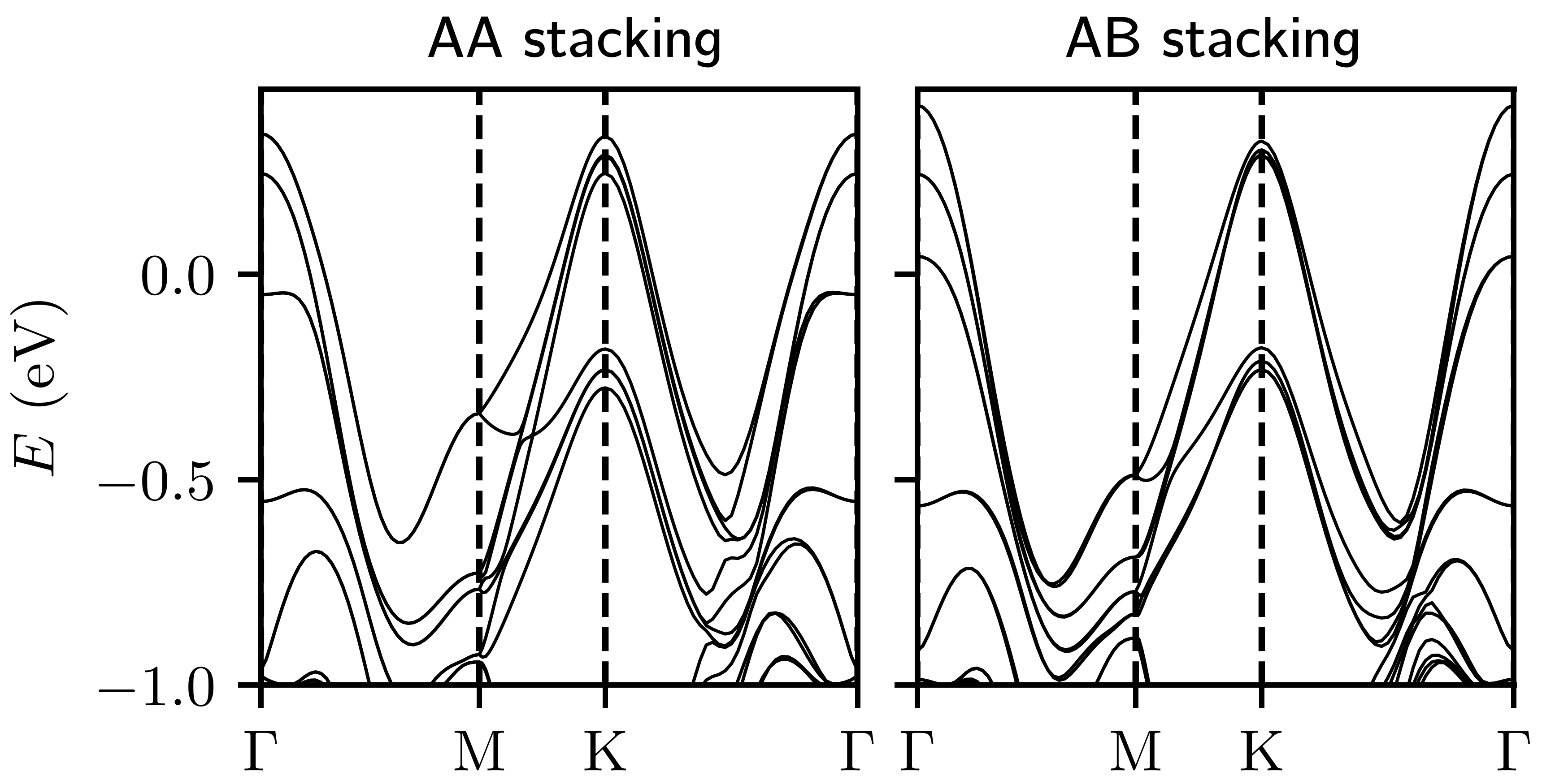

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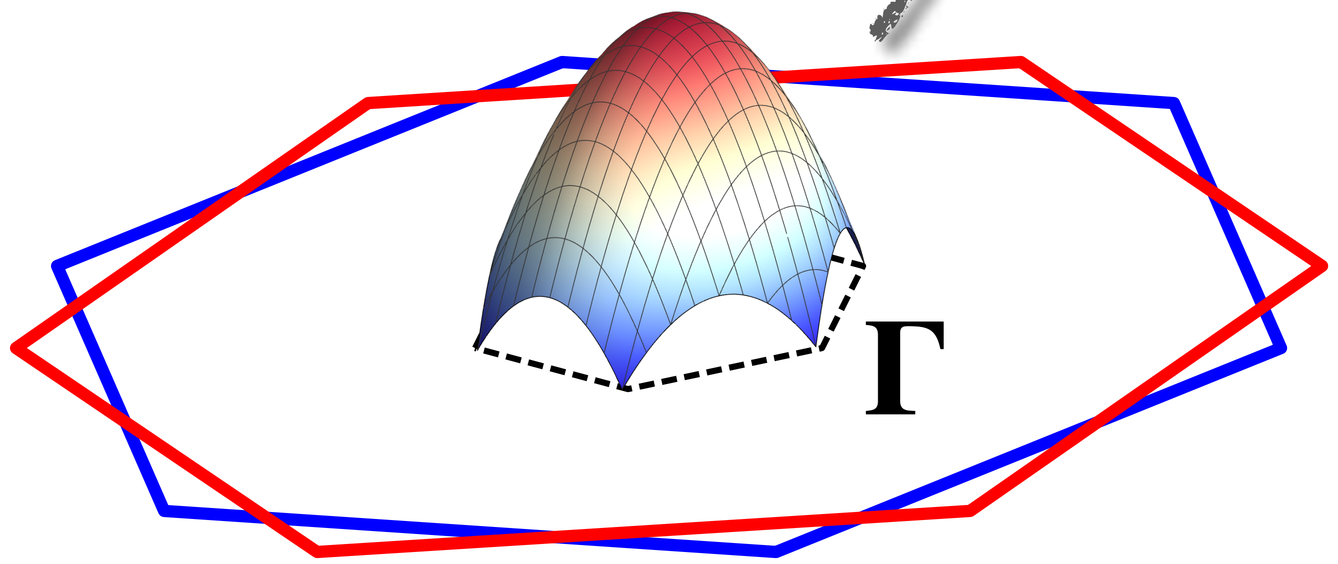

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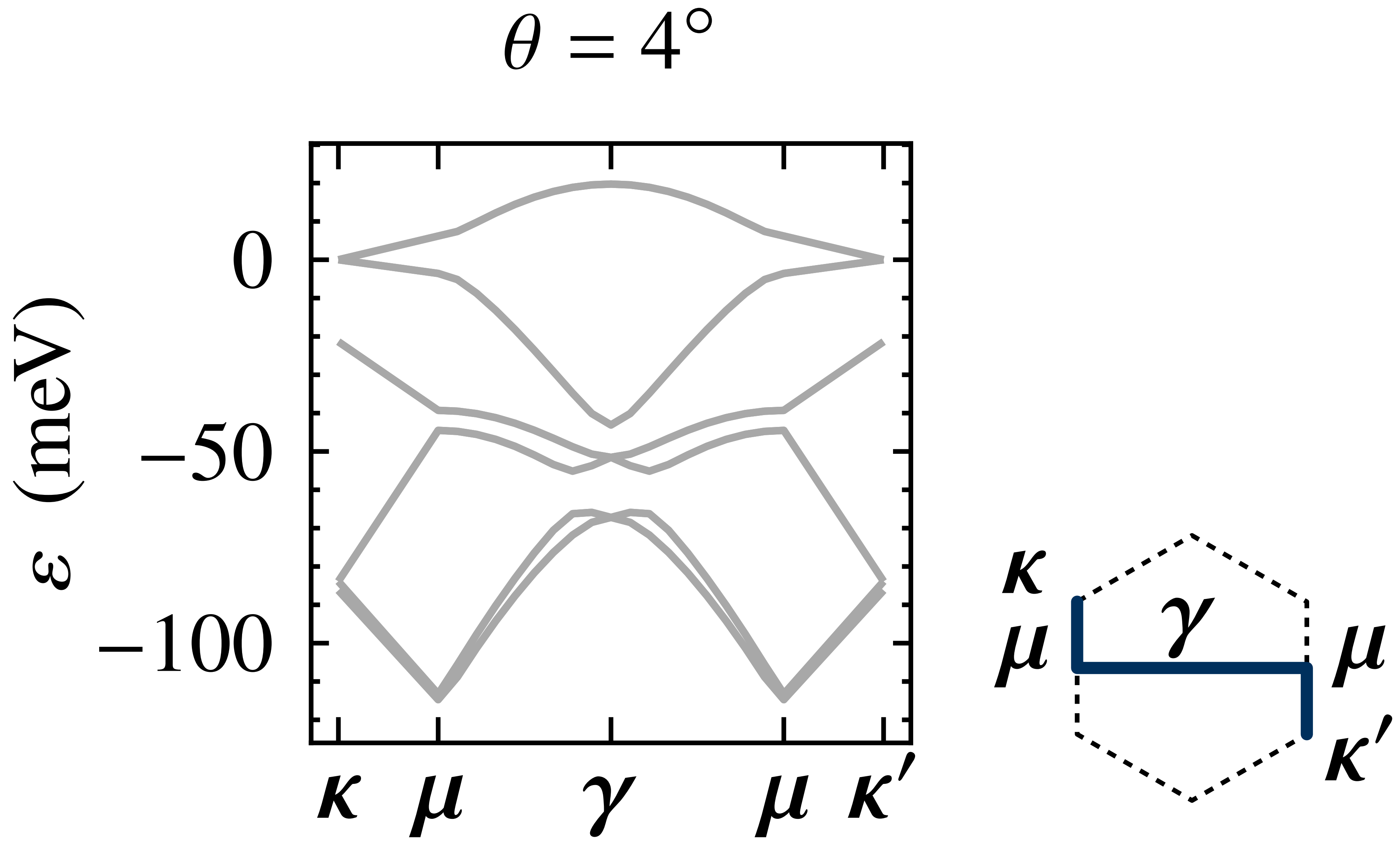

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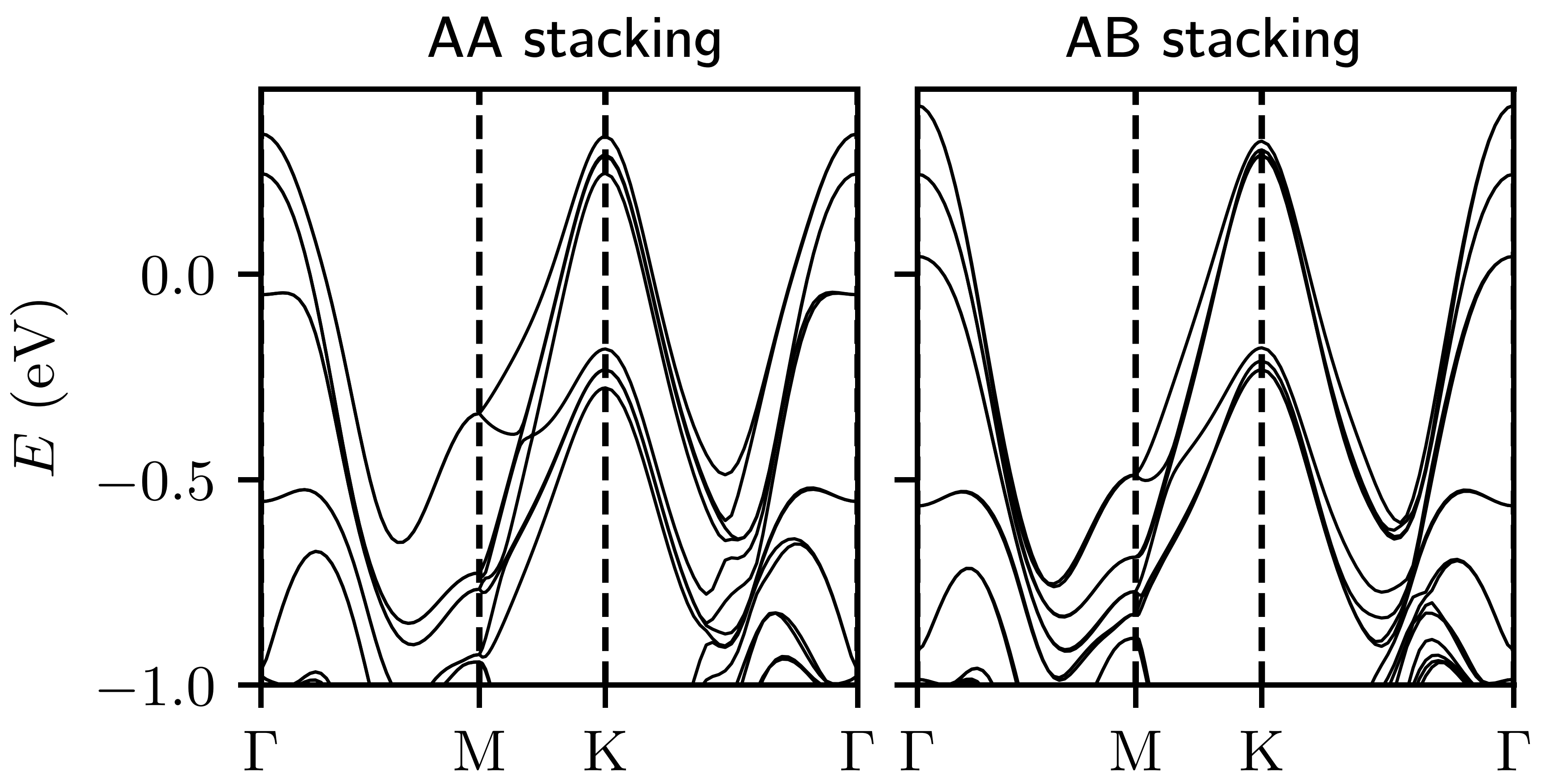

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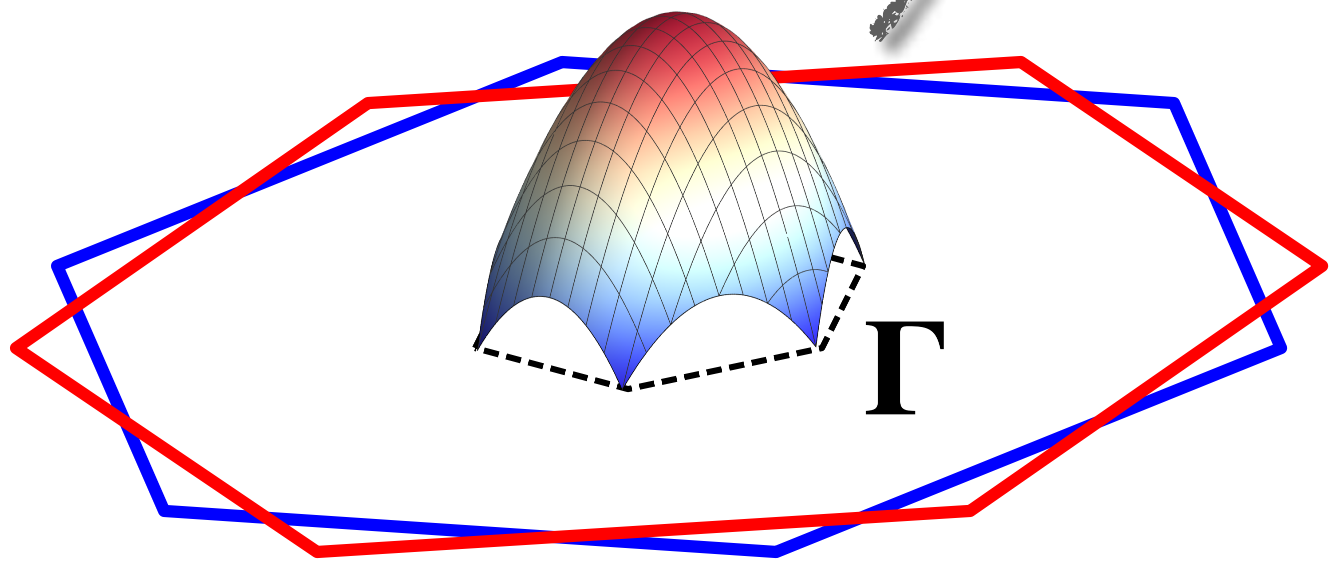

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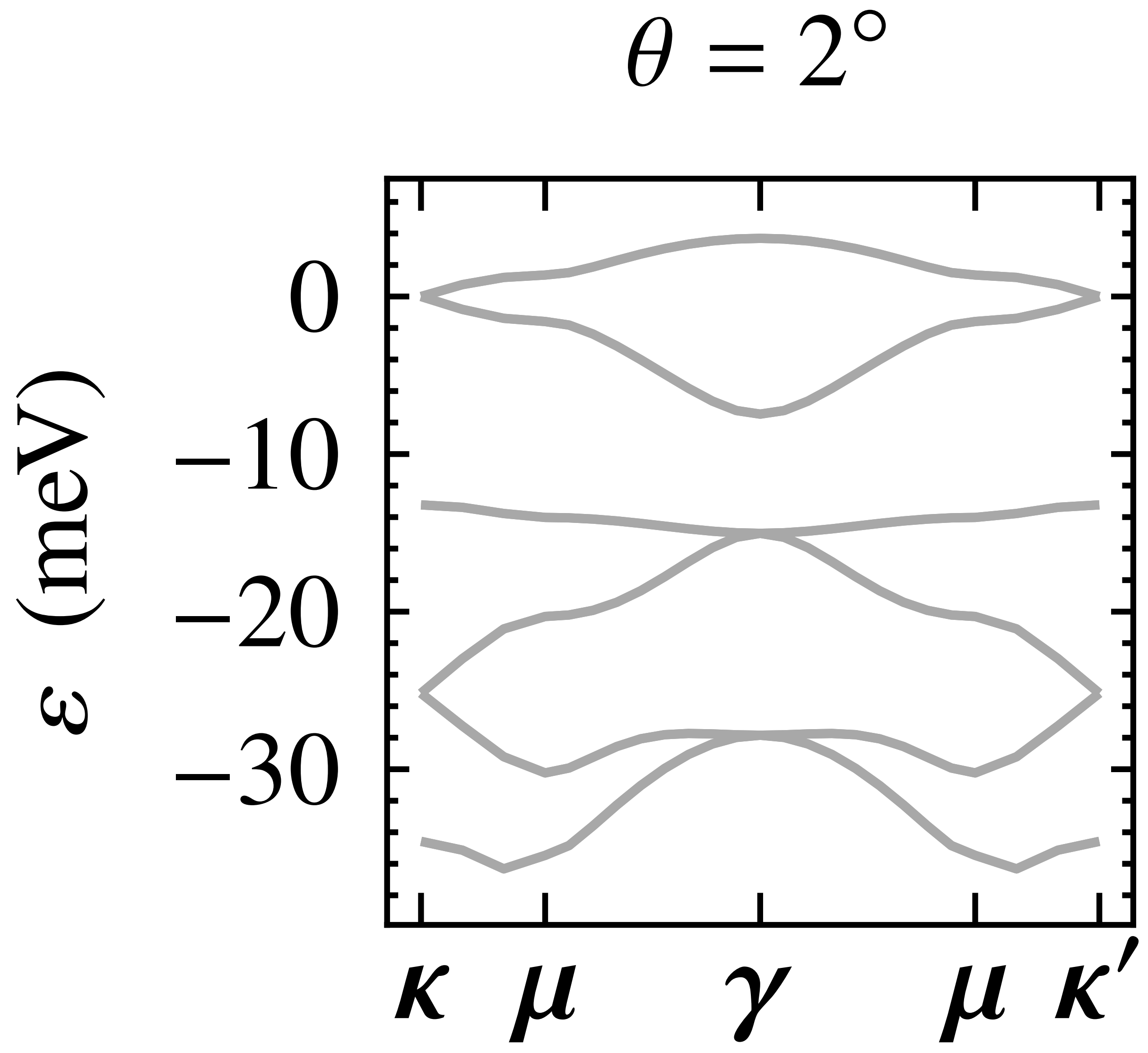

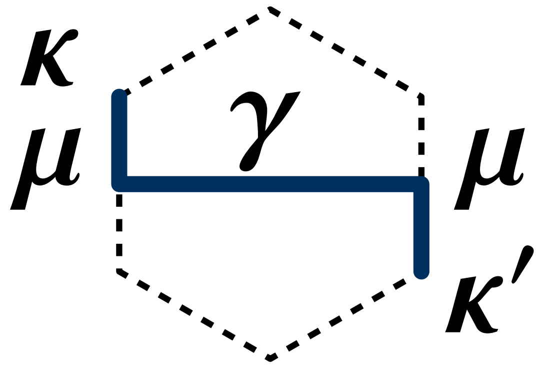

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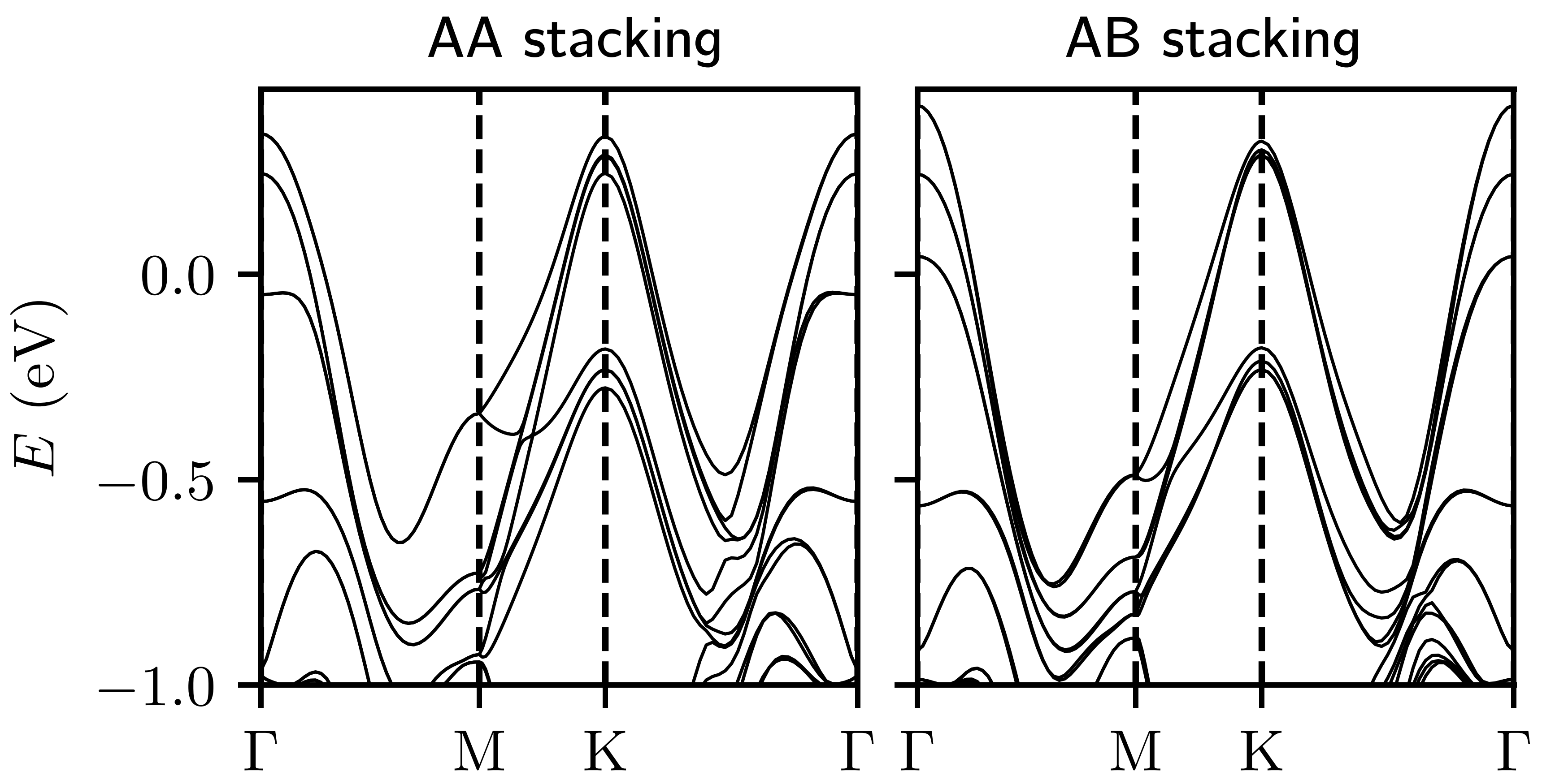

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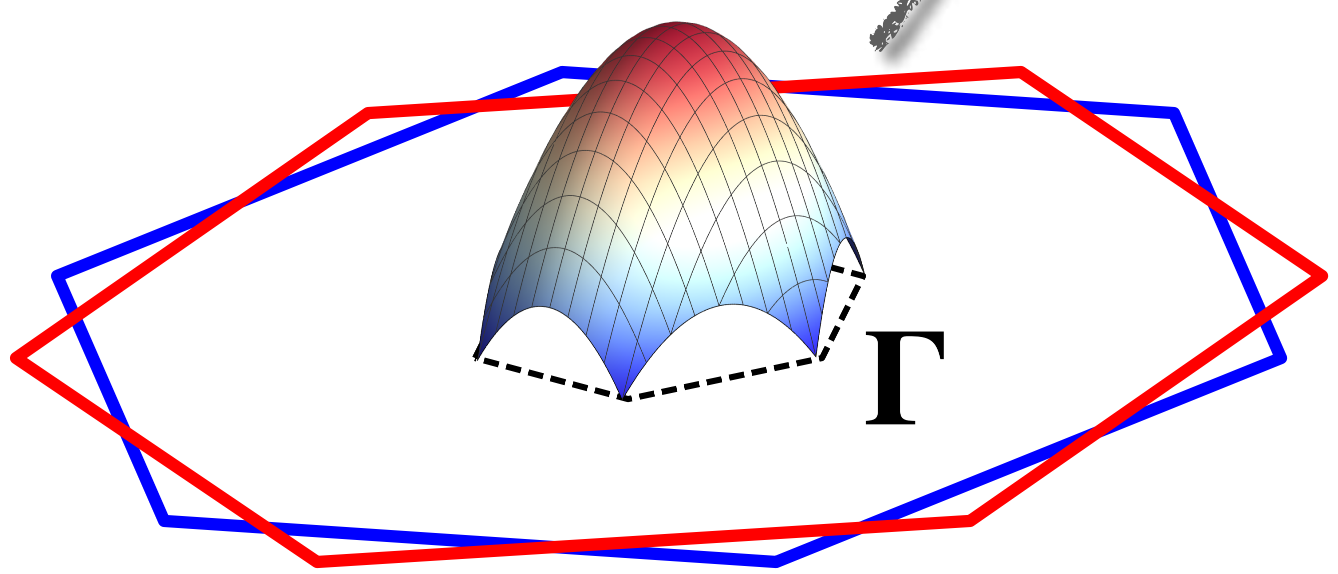

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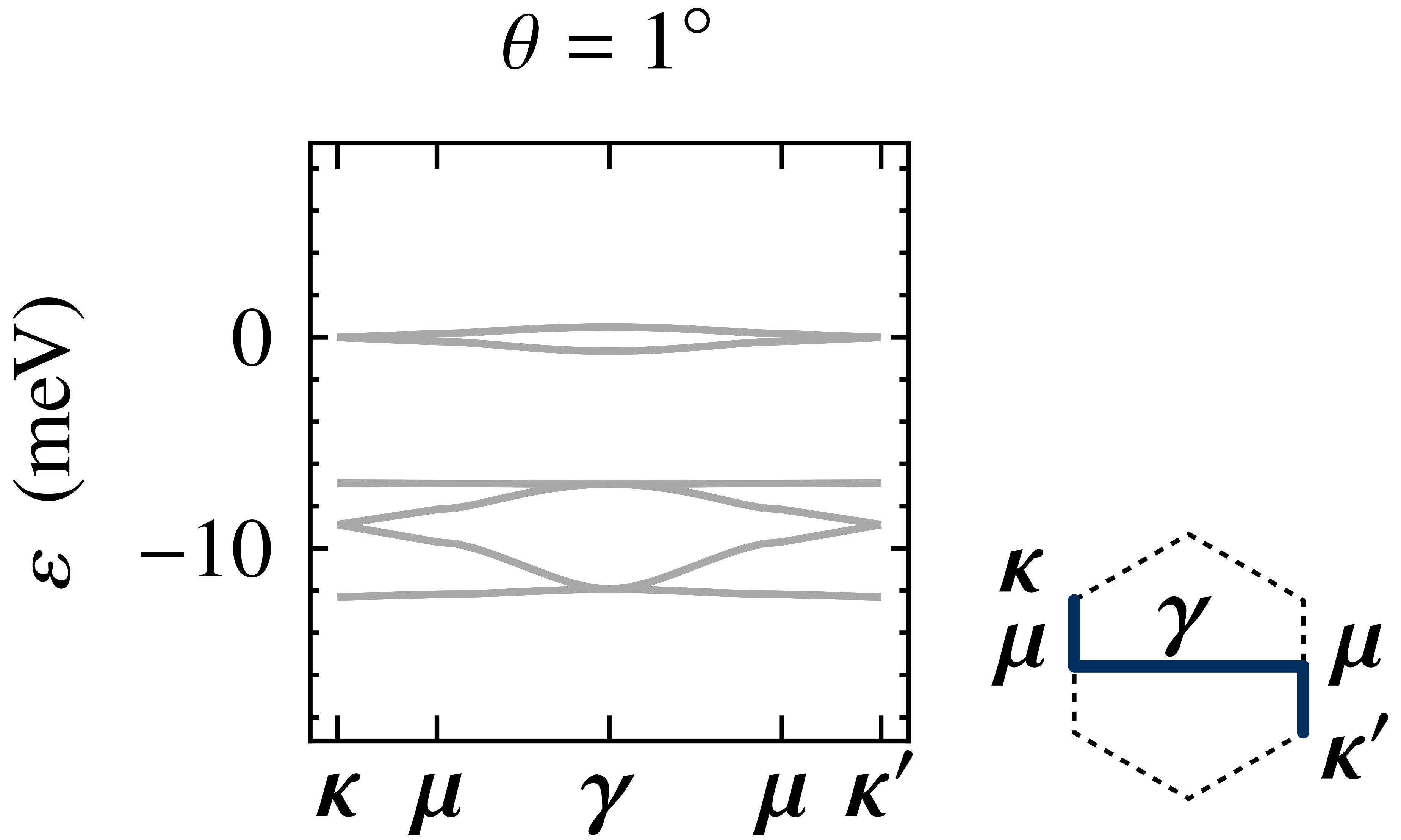
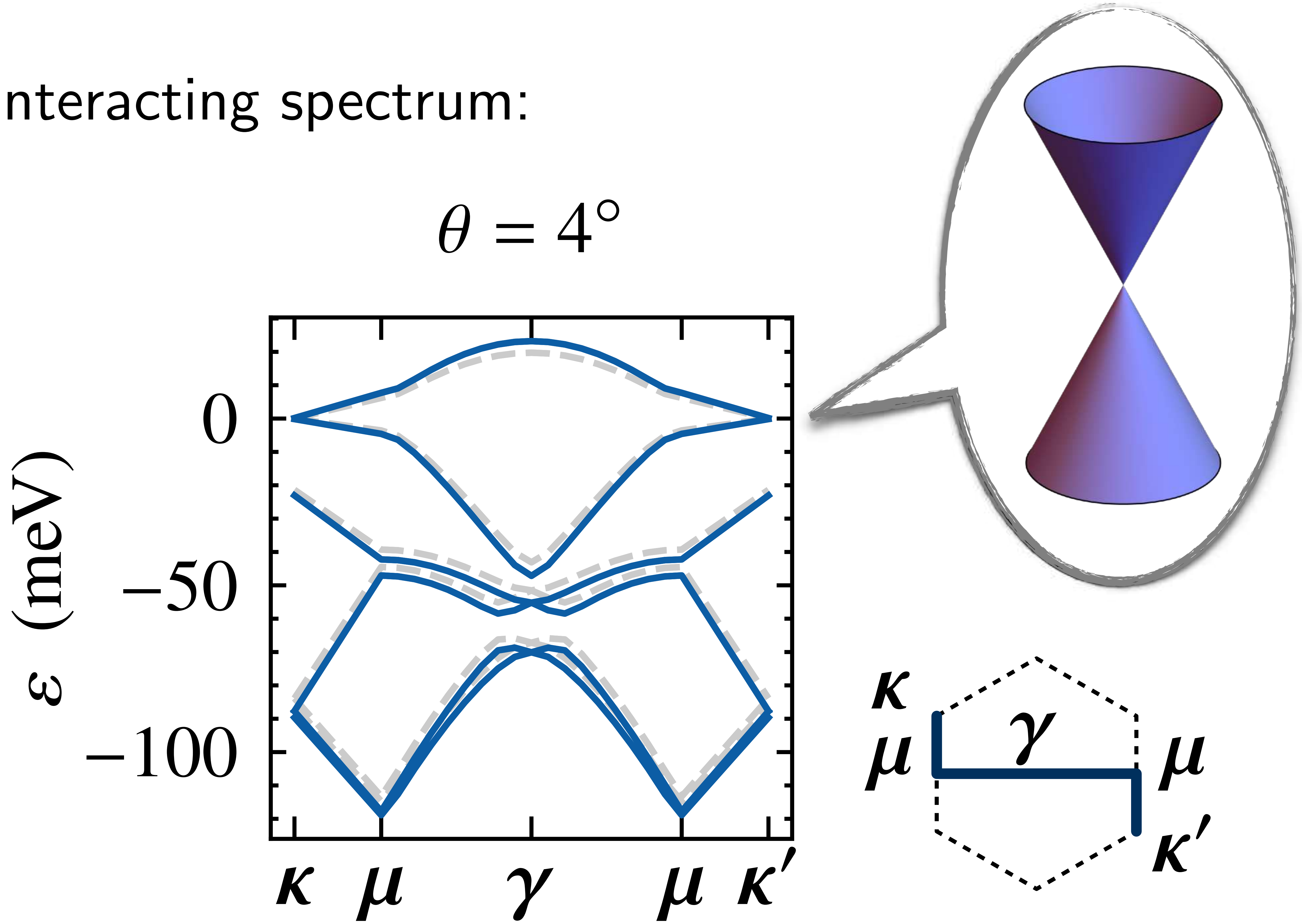
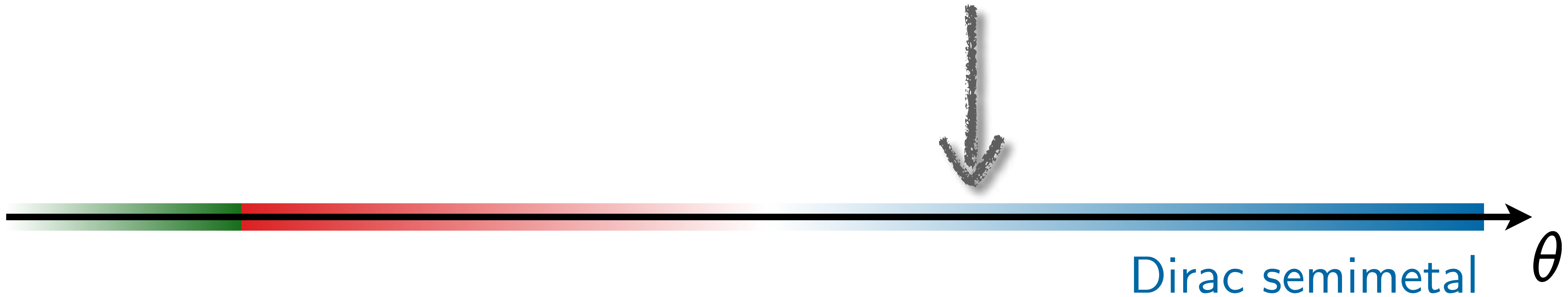


Twisted double bilayer TMDs: Dirac semimetal

Interacting spectrum:





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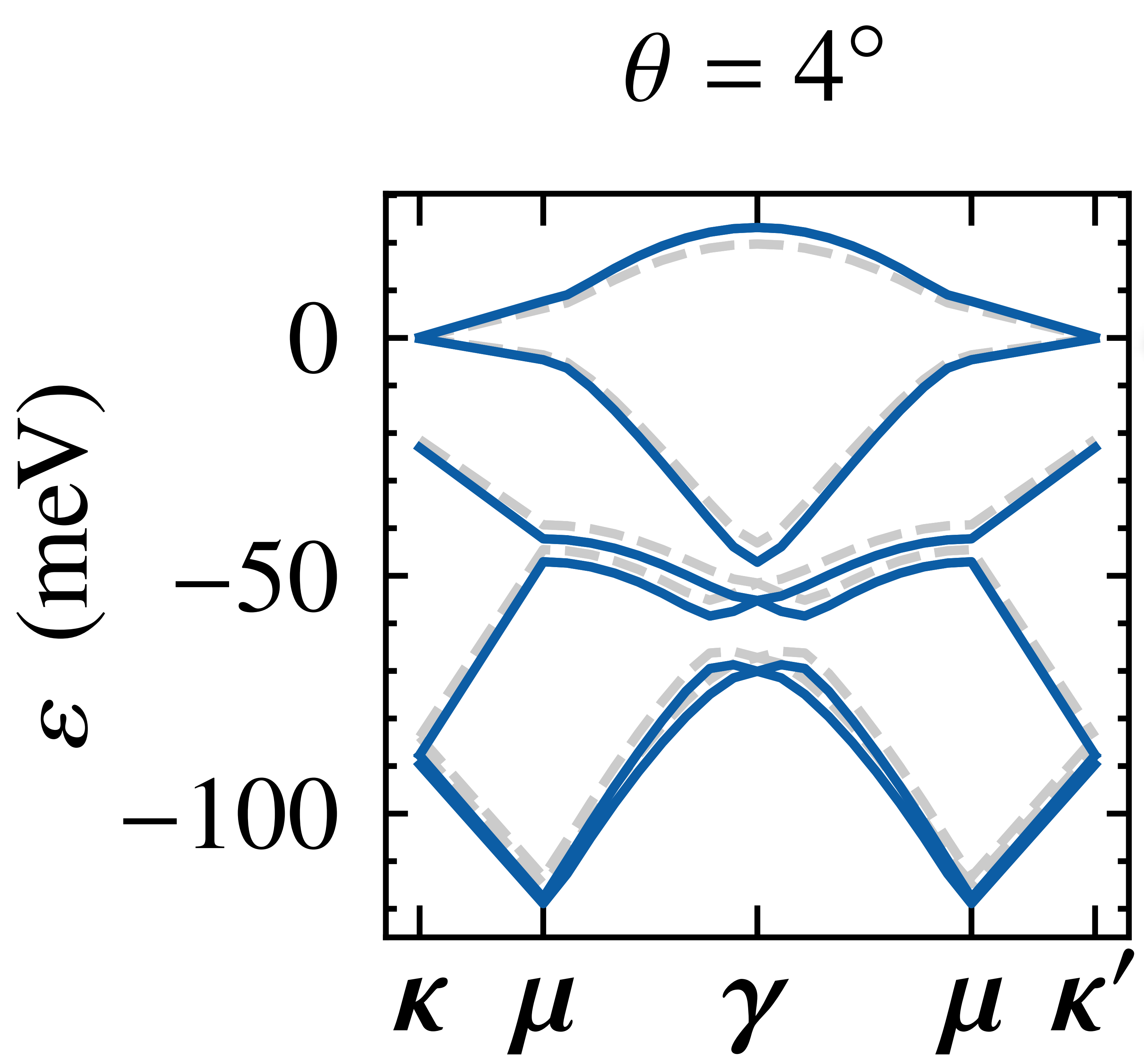
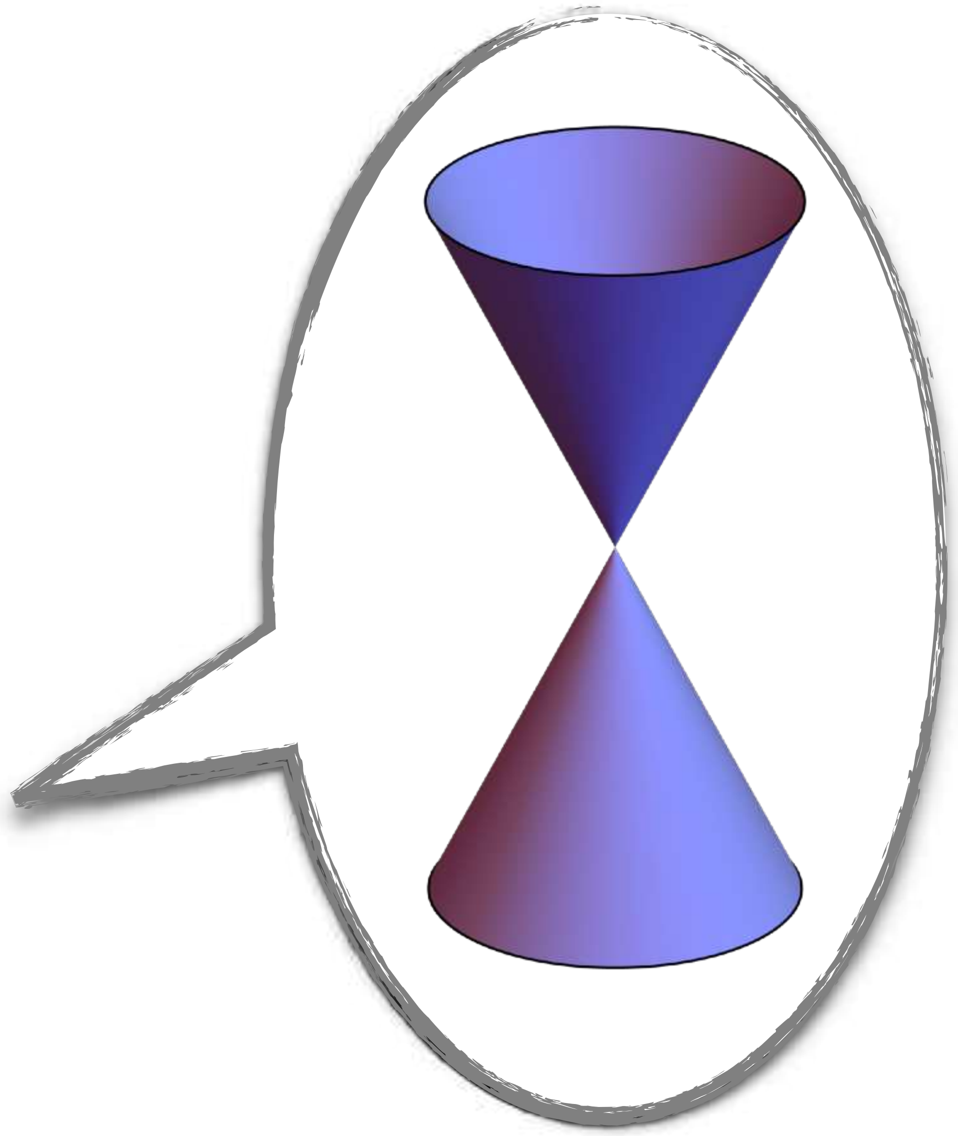
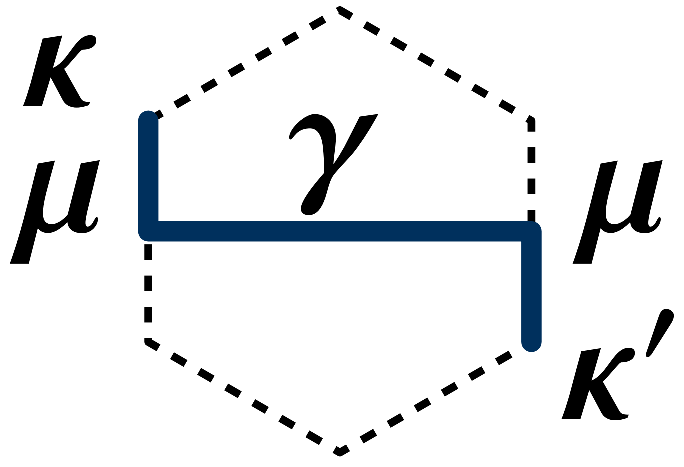
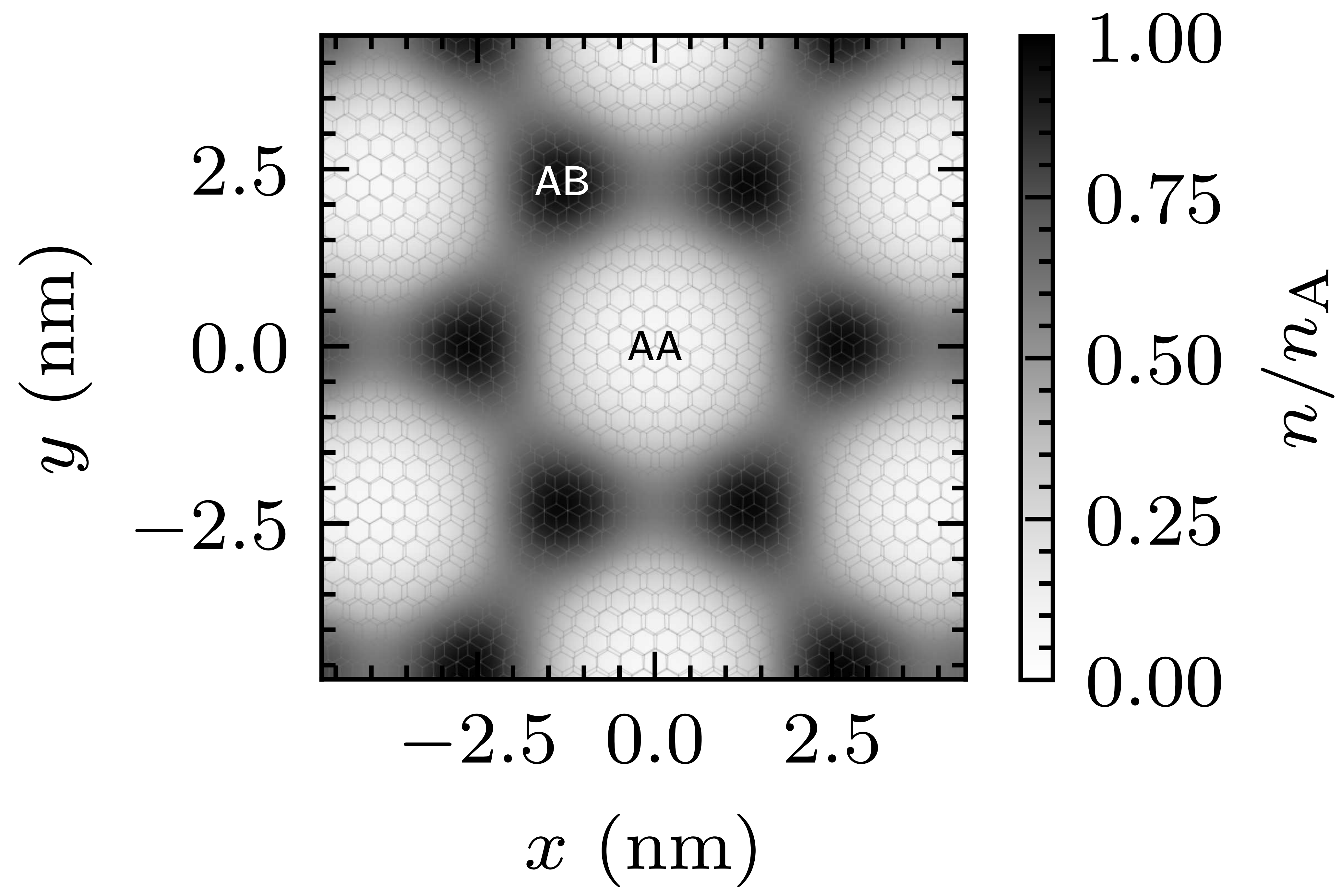
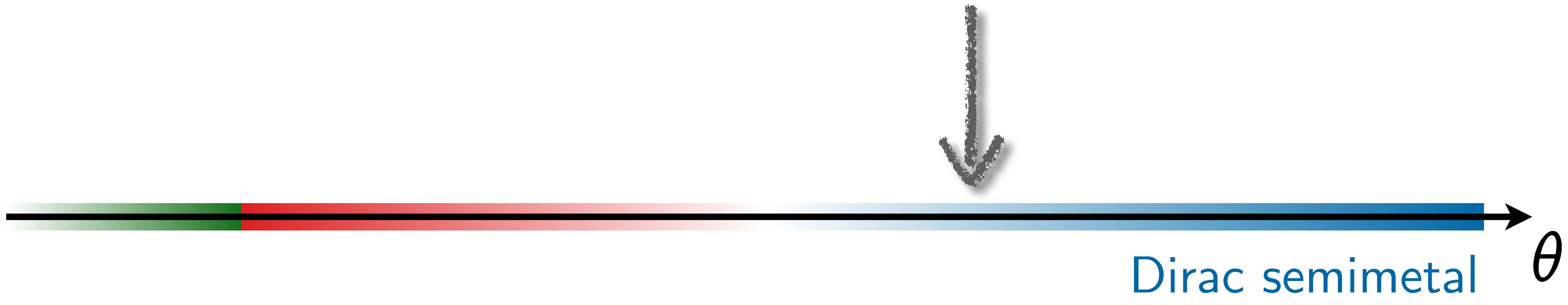






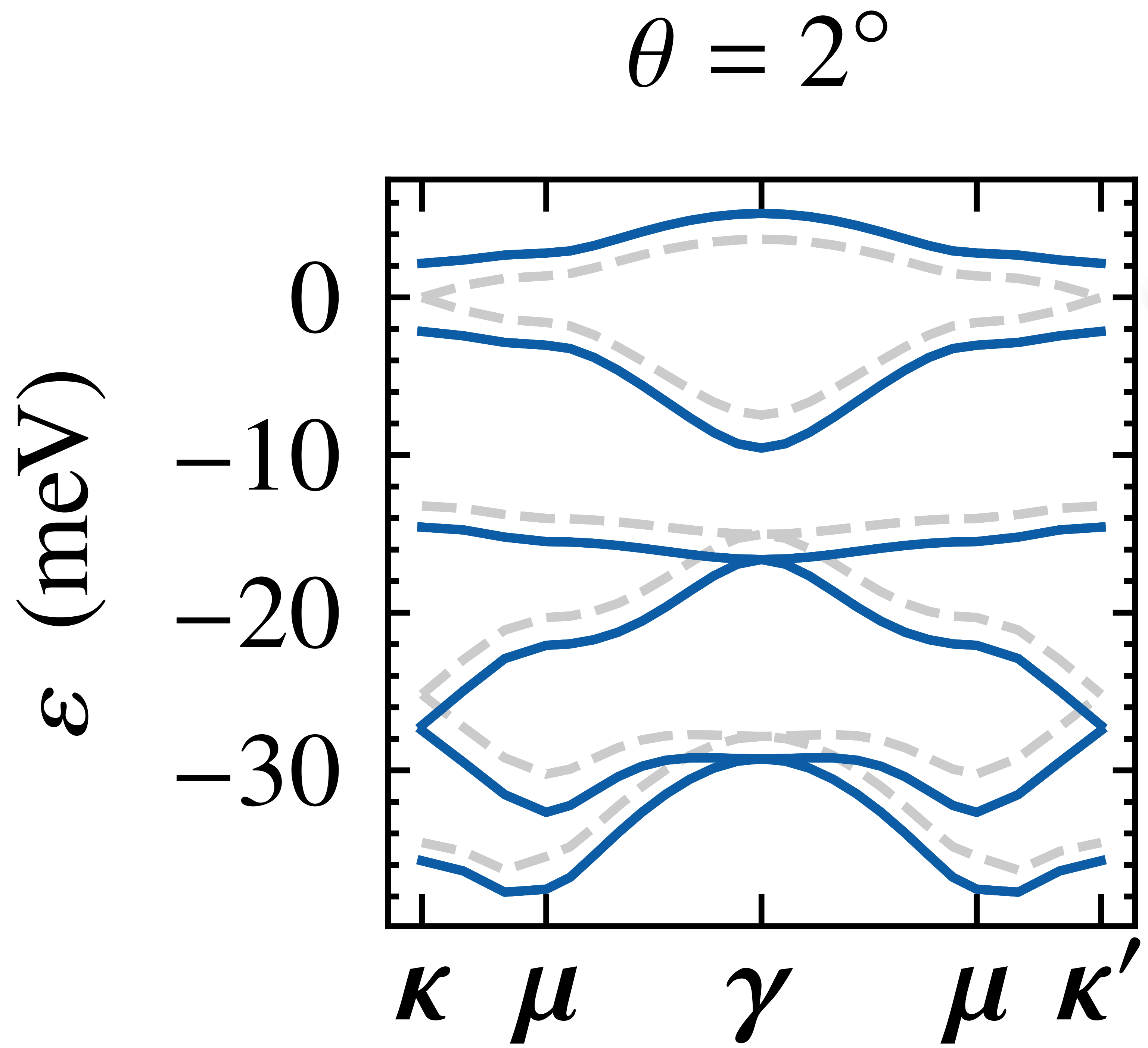
Charge density:

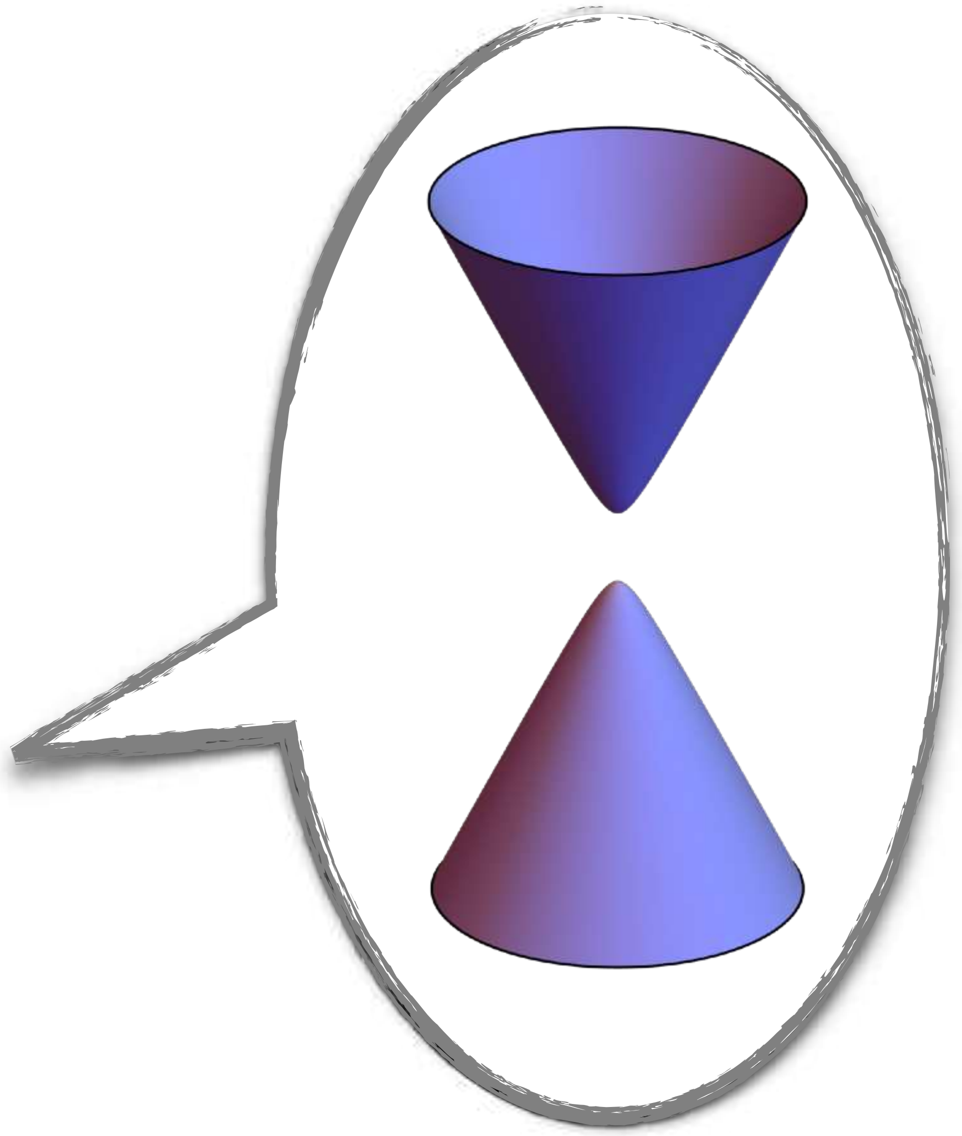


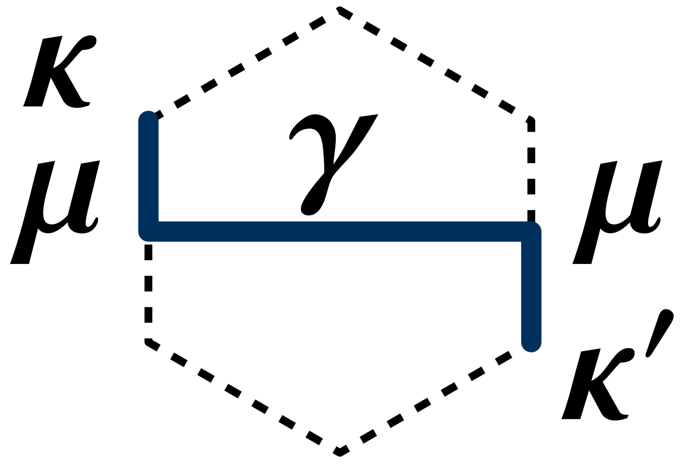


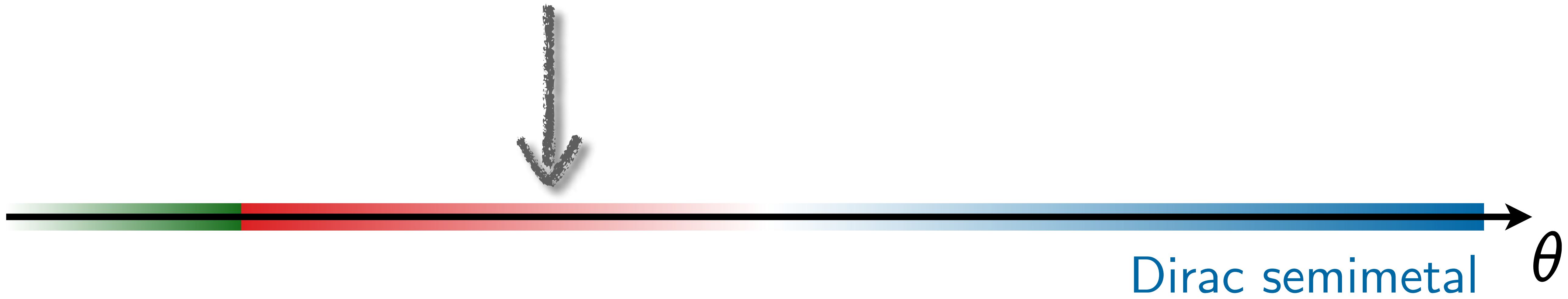
Twisted double bilayer TMDs: Antiferromagnetic insulator

Interacting spectrum:









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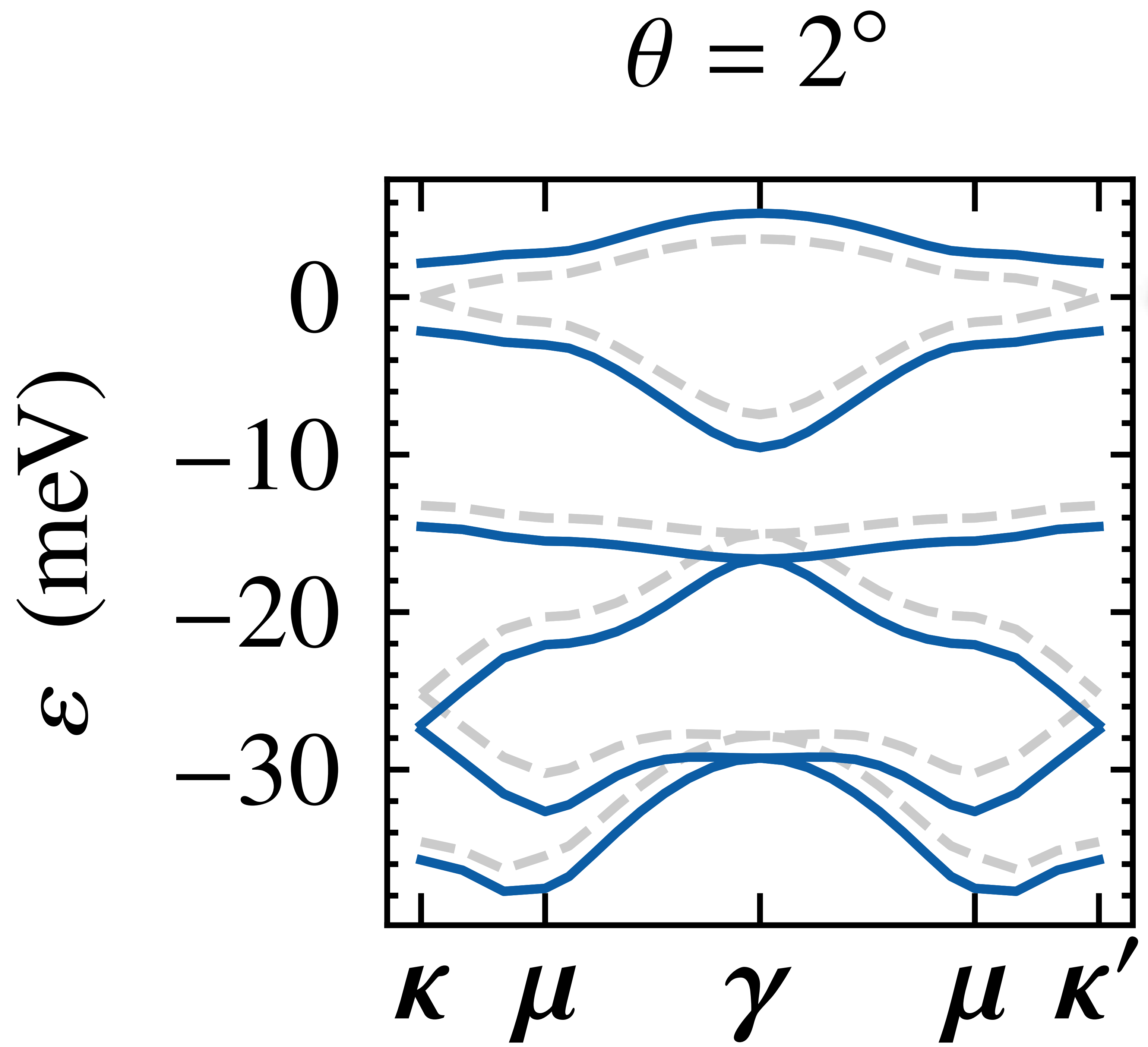
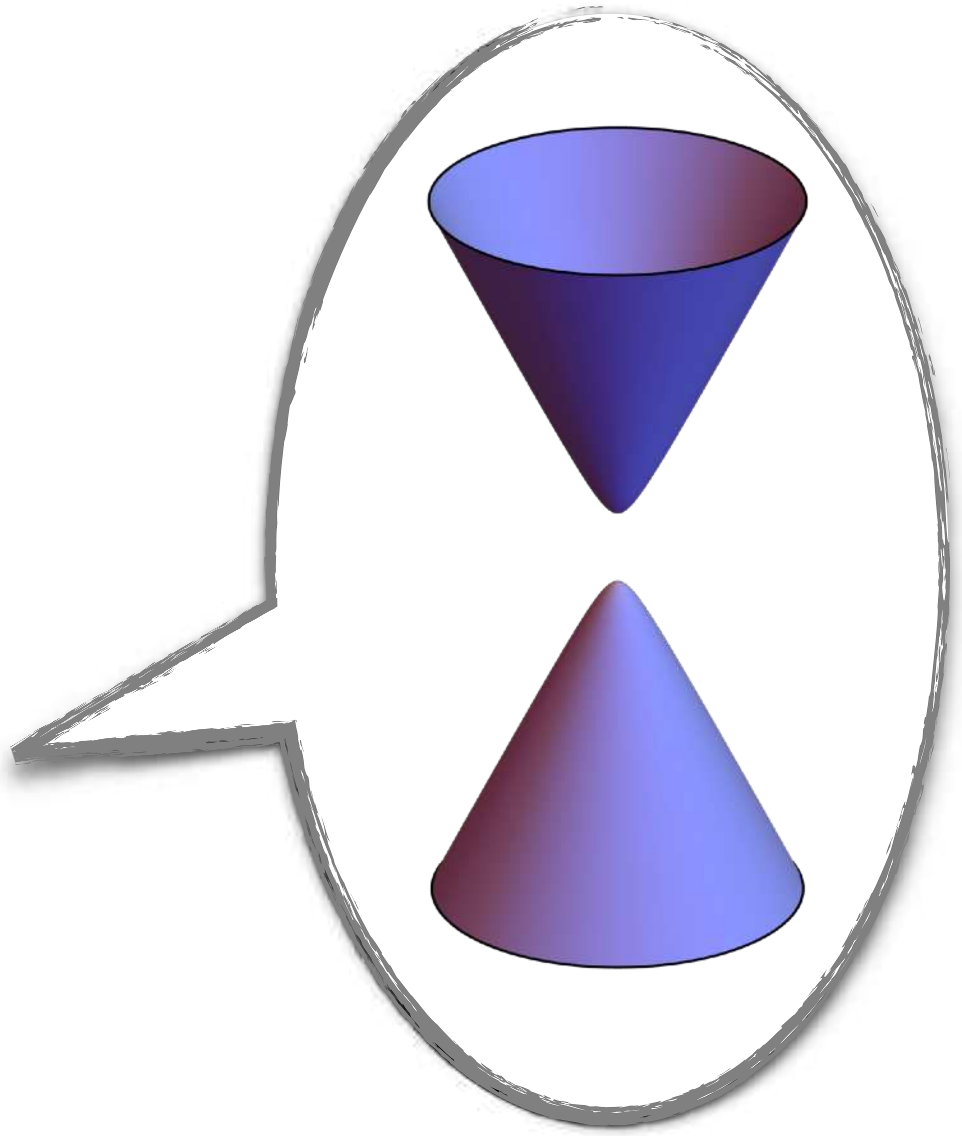
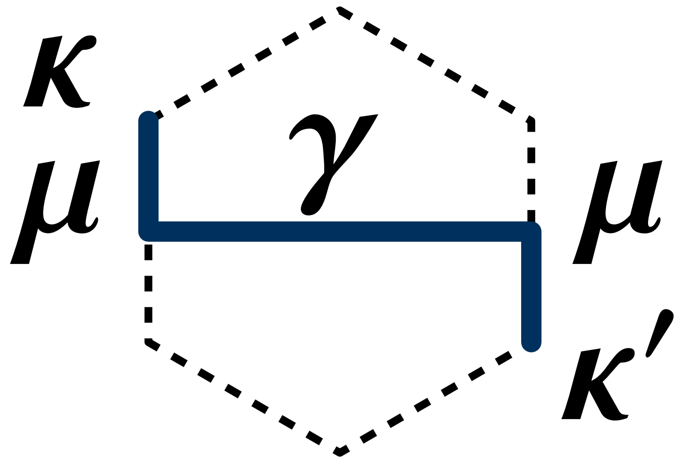
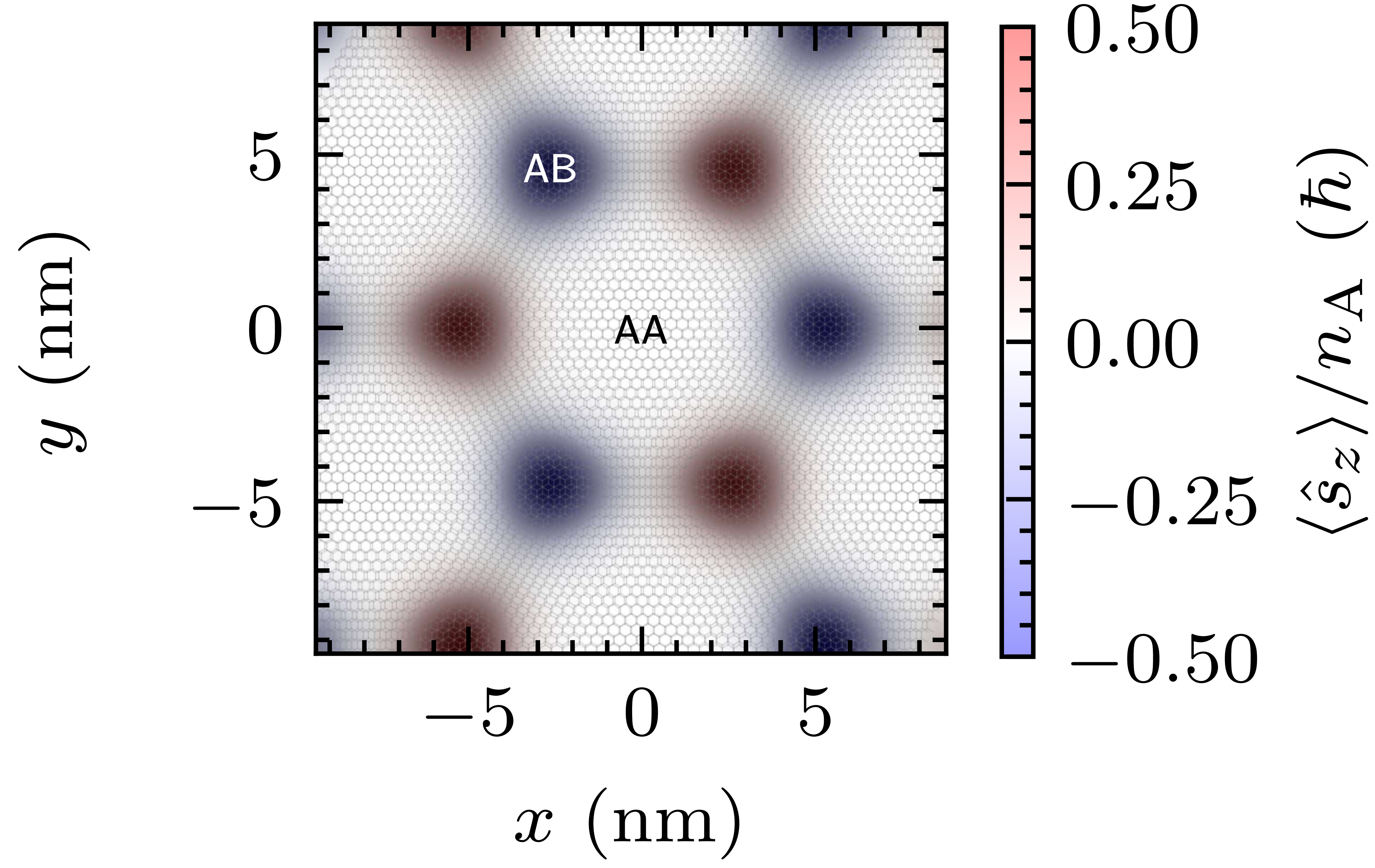






Spin density:



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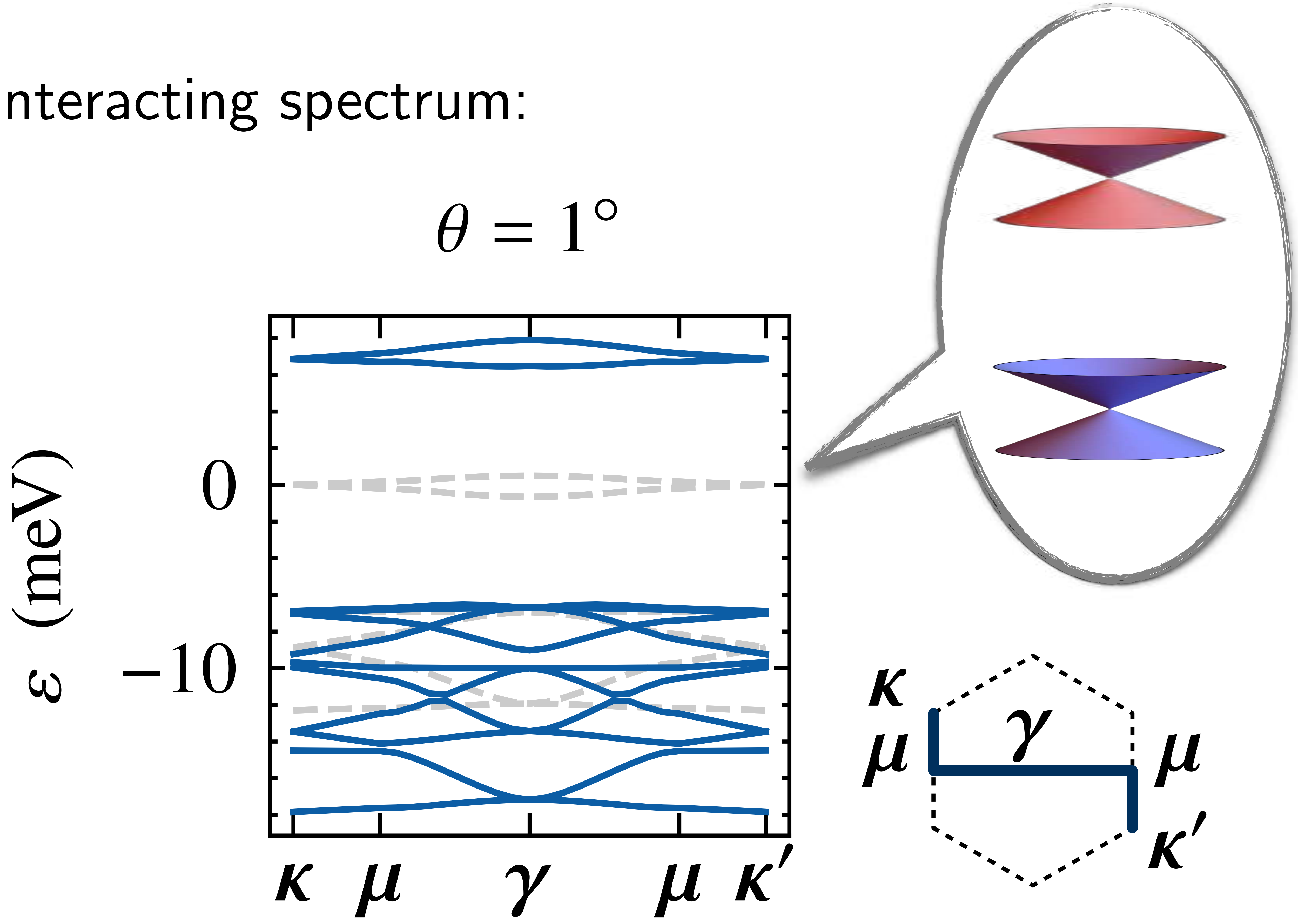

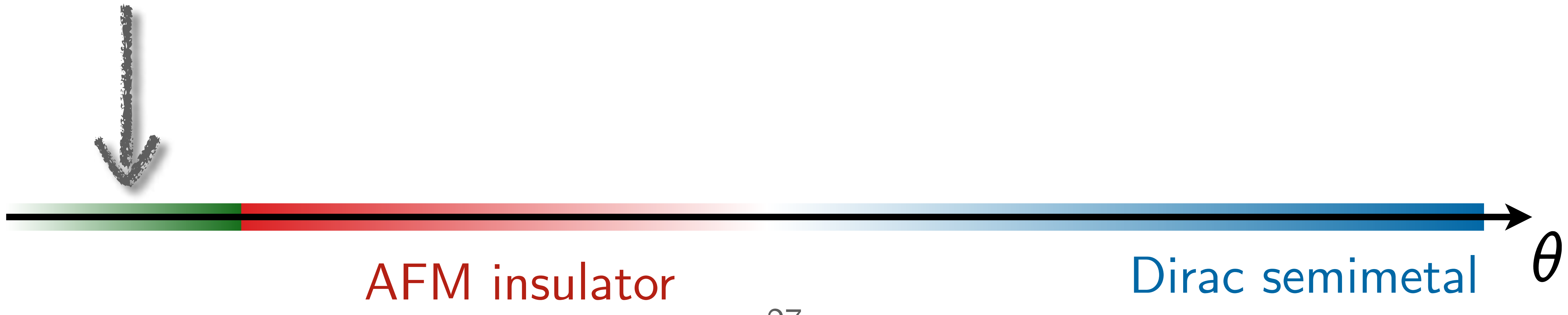

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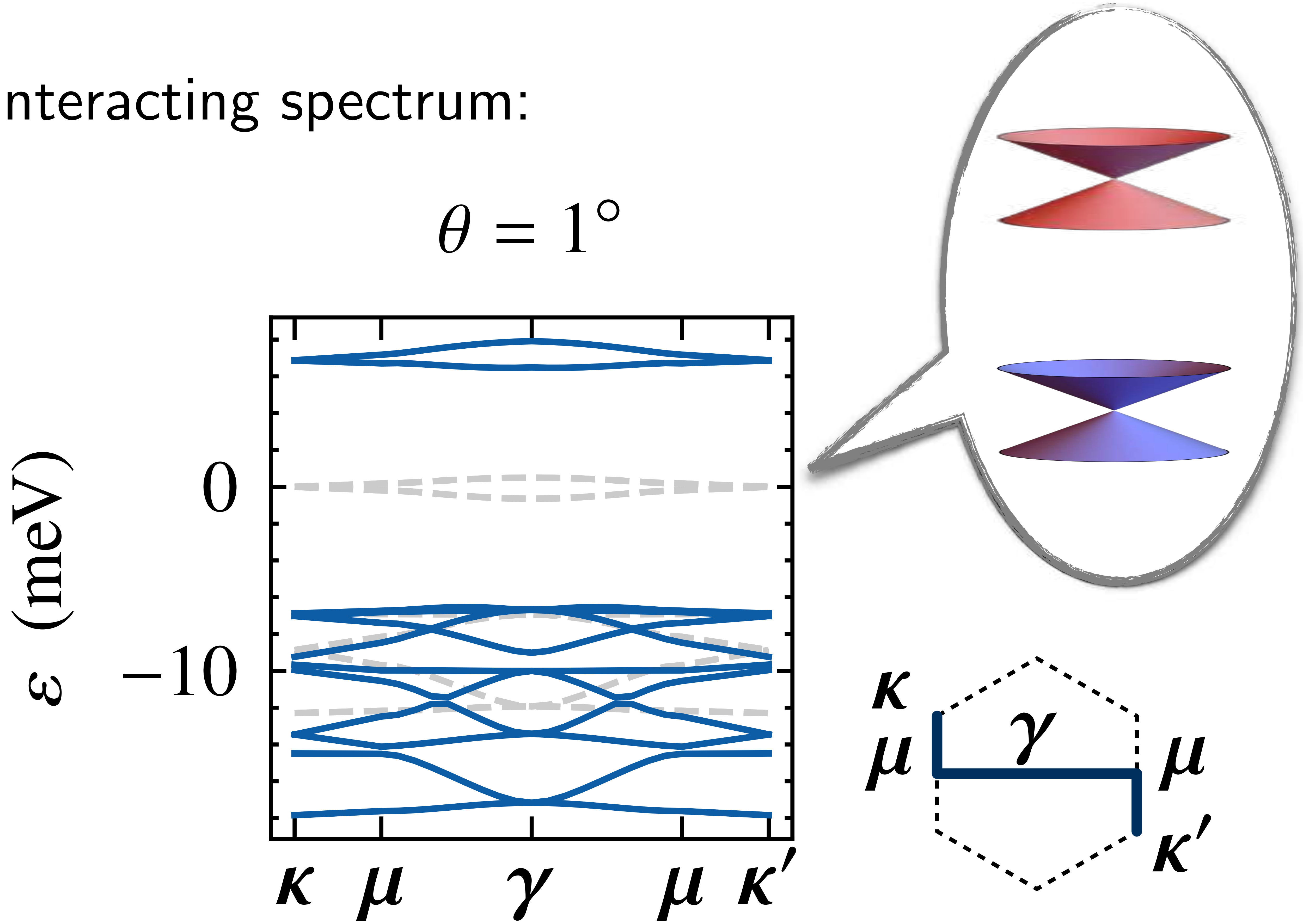

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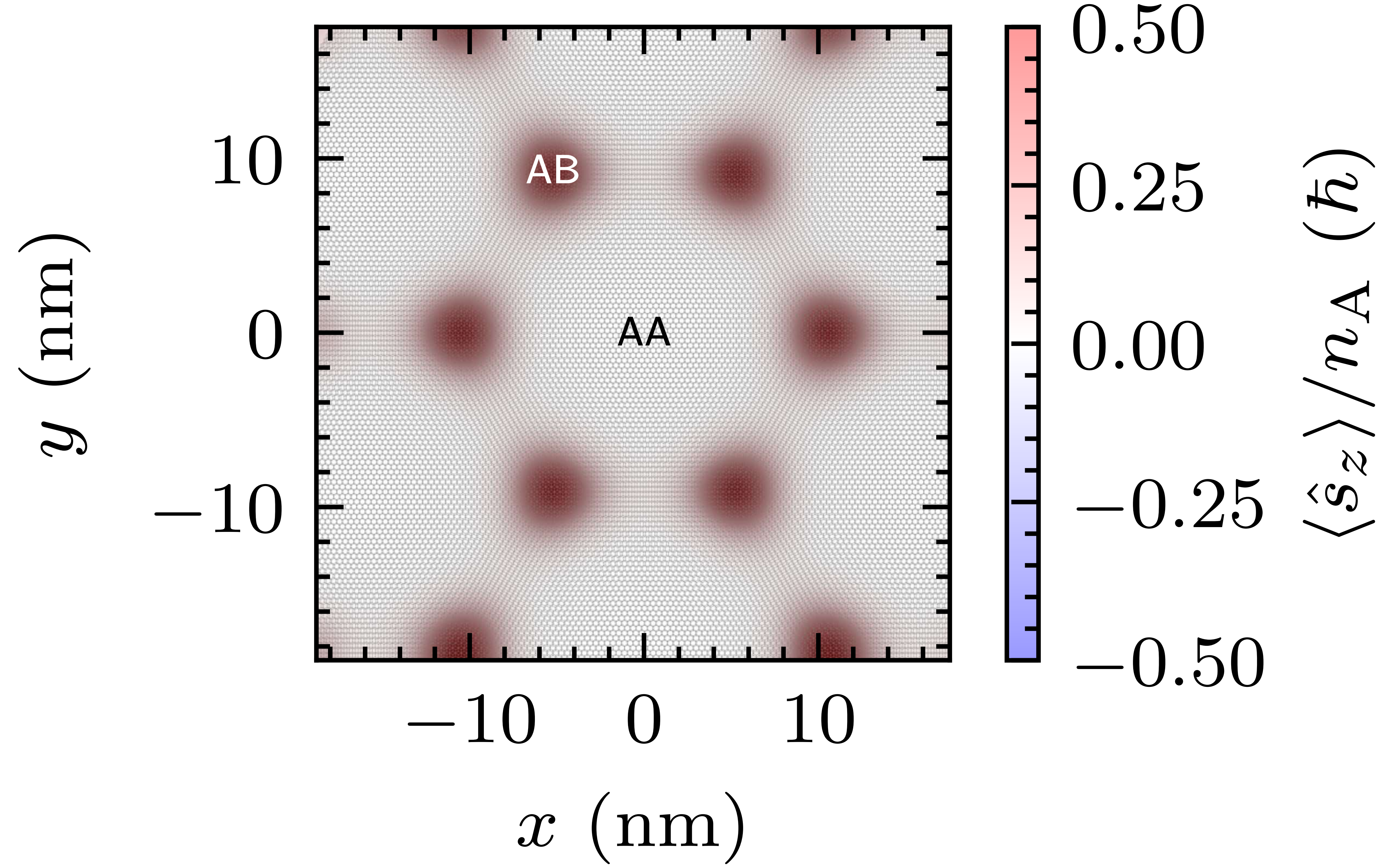
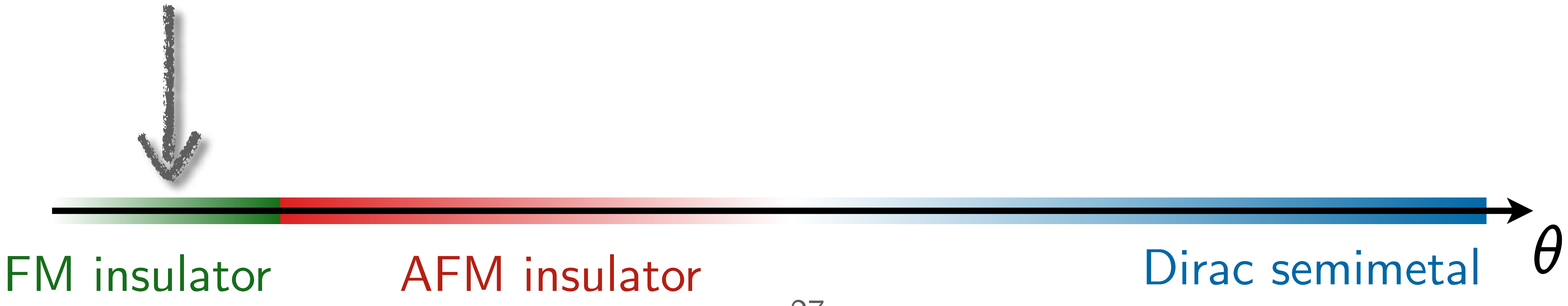
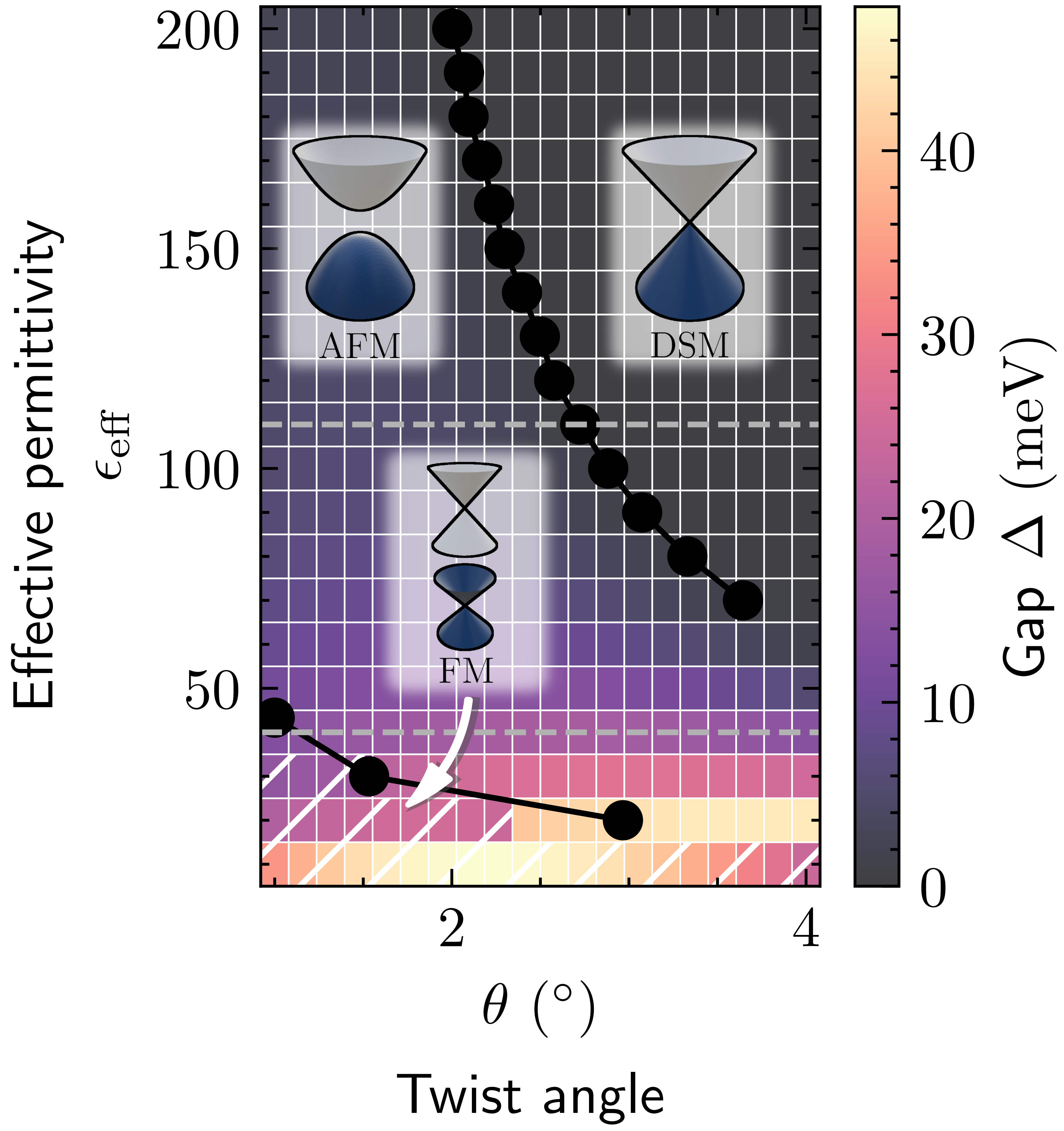




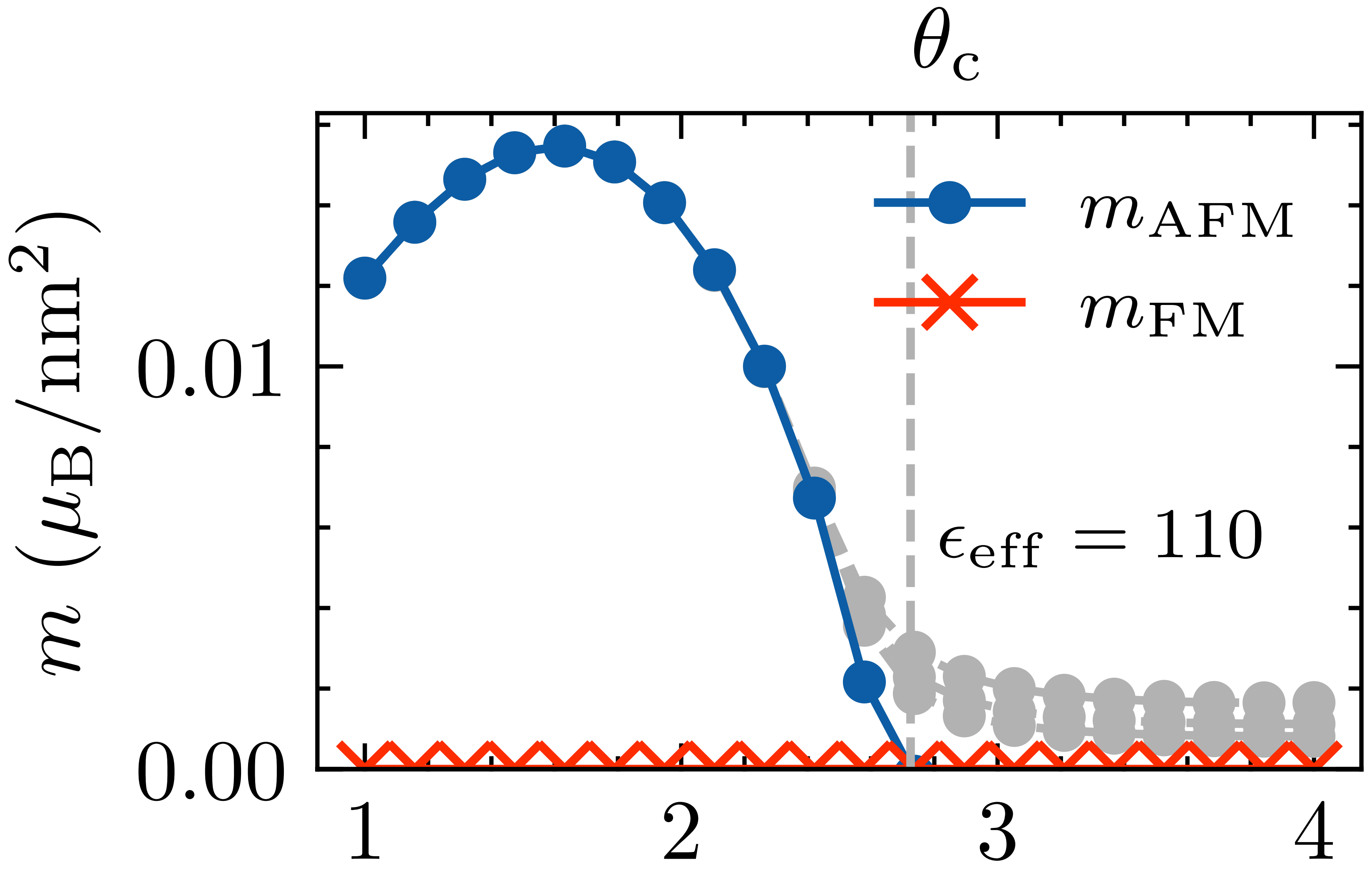
Twisted double bilayer TMDs: Phase diagram



[Biedermann & LJ, arXiv:2509.04561]

Twisted double bilayer TMDs: Quantum criticality

Staggered magnetization:



$$m_{AFM} \propto (\theta_c - \theta)^{\beta}$$

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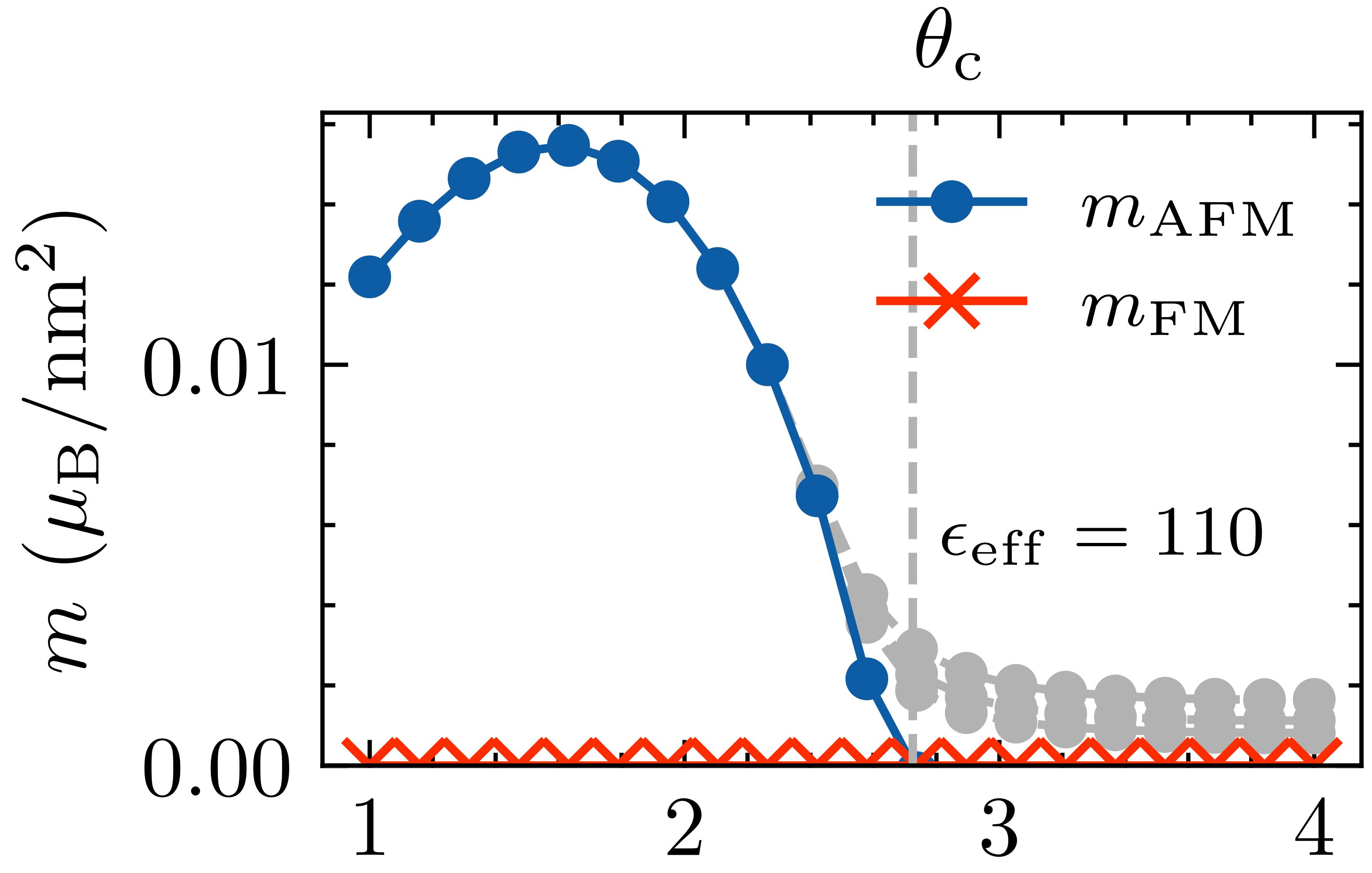

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Gross-Neveu-Heisenberg universality class:

$$\mathcal{L} = \bar{\psi}\gamma^{\mu}\partial_{\mu}\psi + g(\bar{\psi}\vec{\sigma}\psi)\cdot\vec{\varphi} + \ldots$$

... with emergent relativistic symmetry

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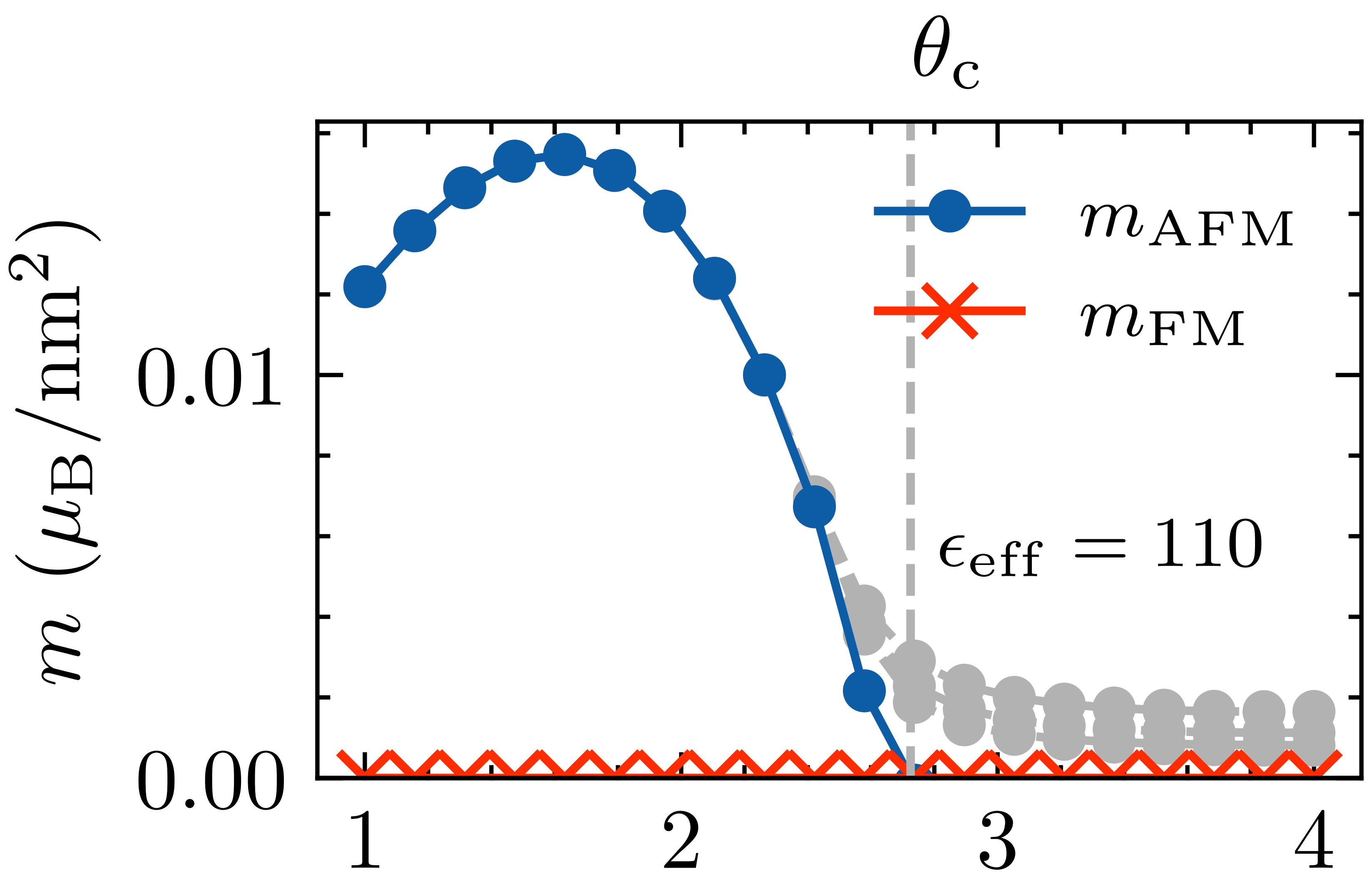

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Critical exponents:

$$z = 1$$
$$\eta_\varphi \approx 1.01$$
$$\beta \approx 1.21$$

... from $4-\epsilon$ and $2+\epsilon$ expansions

[Ladovrechis, Ray, Meng, LJ, PRB '23]

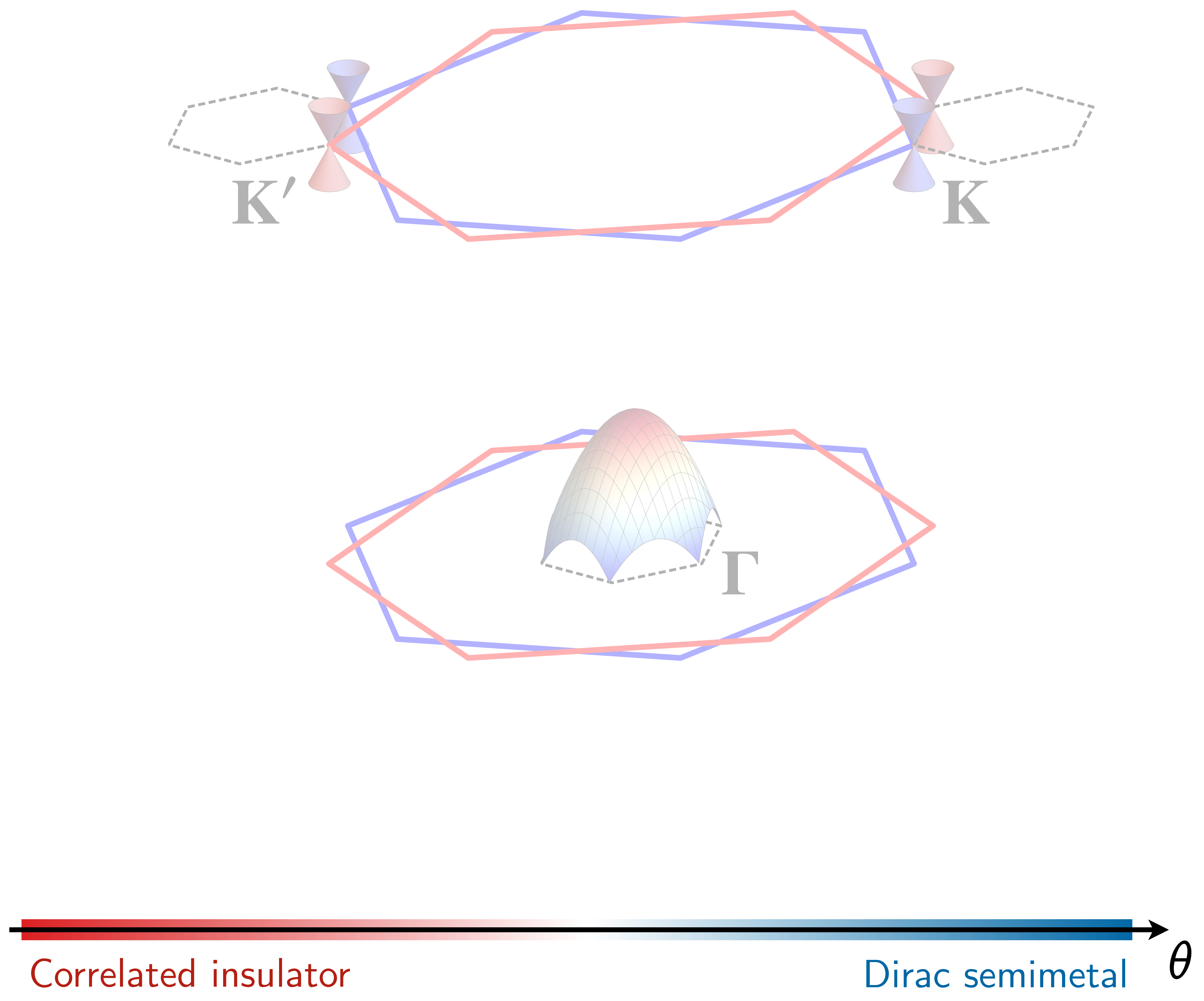
Outline

(1) Introduction

(2) Twisted bilayer graphene

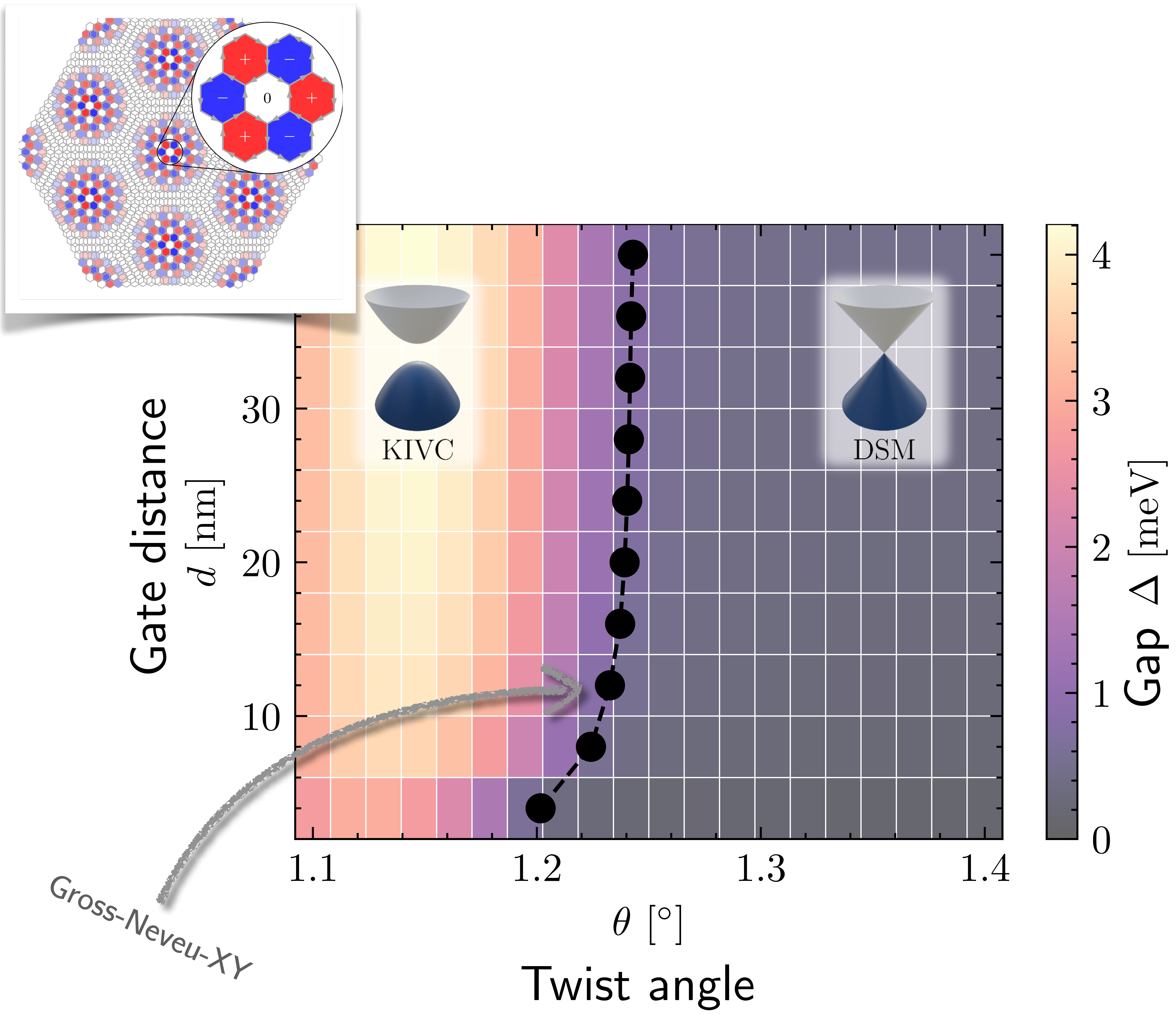
(3) Twisted double bilayer TMDs

(4) Conclusions



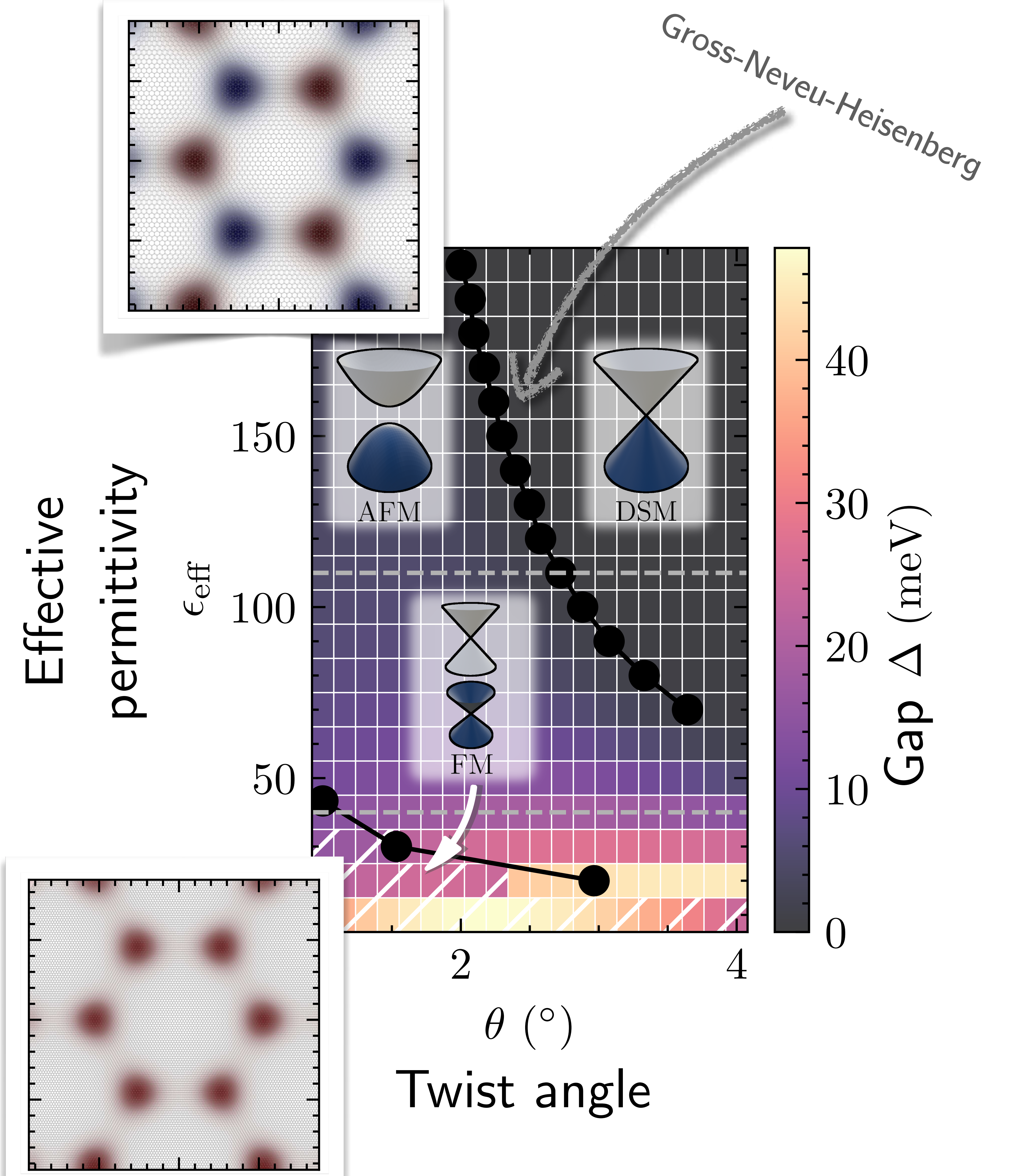
Conclusions

Twisted bilayer graphene:



[Biedermann & LJ, PRB '25]

Twisted double bilayer TMDs:



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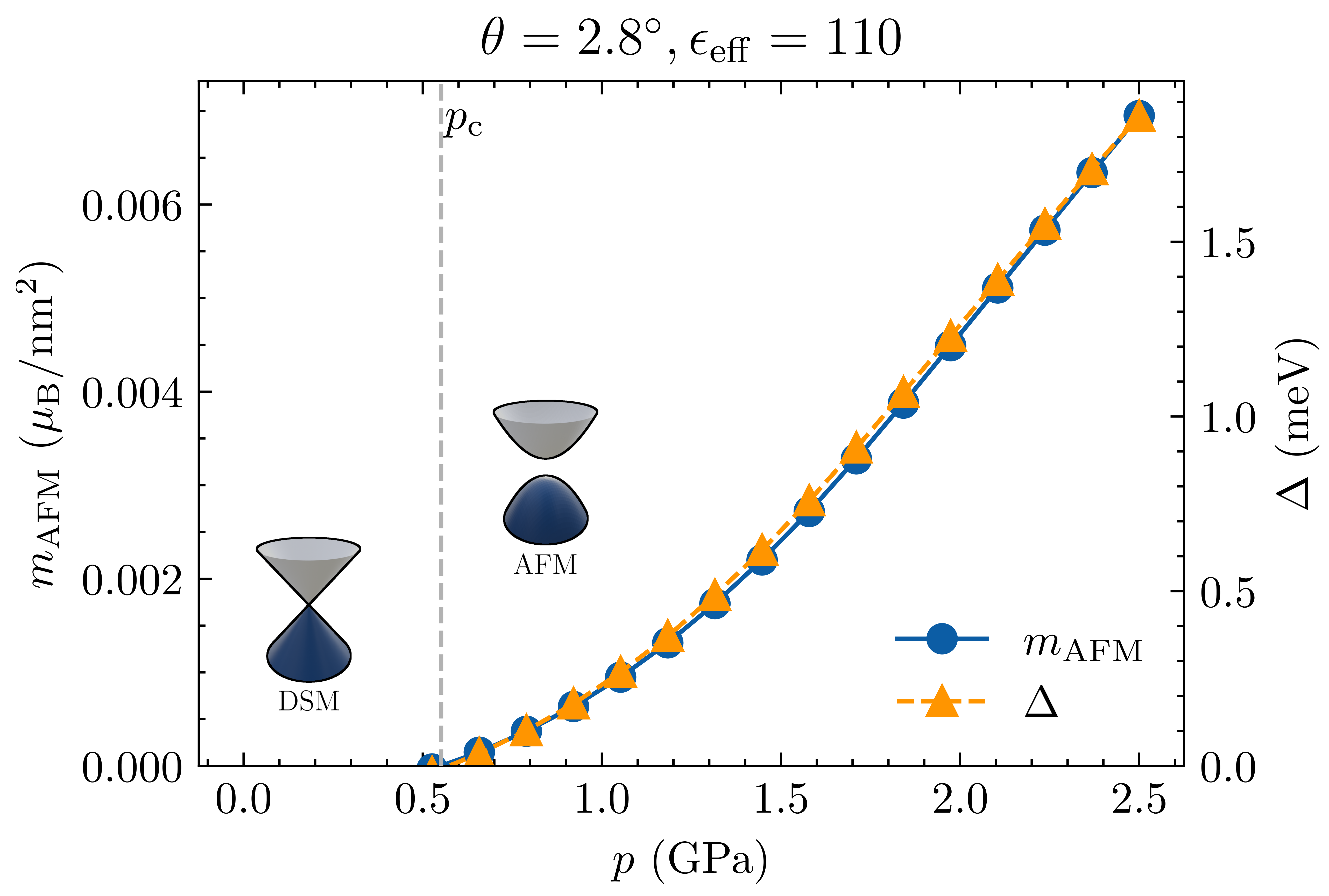
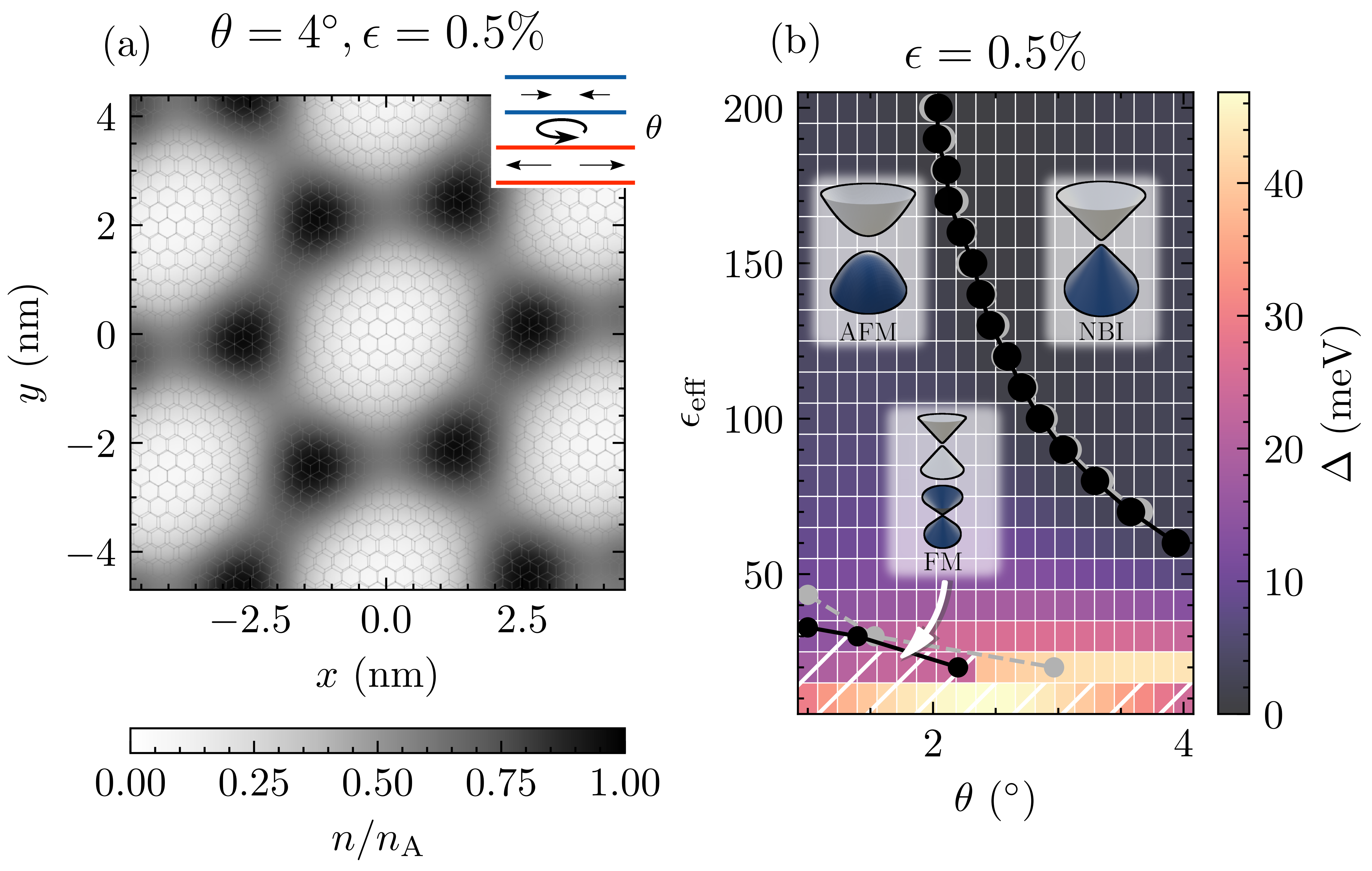
Twisted double bilayer TMDs: Pressure-tuned transition



Twisted double bilayer TMDs: Heterostrain



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