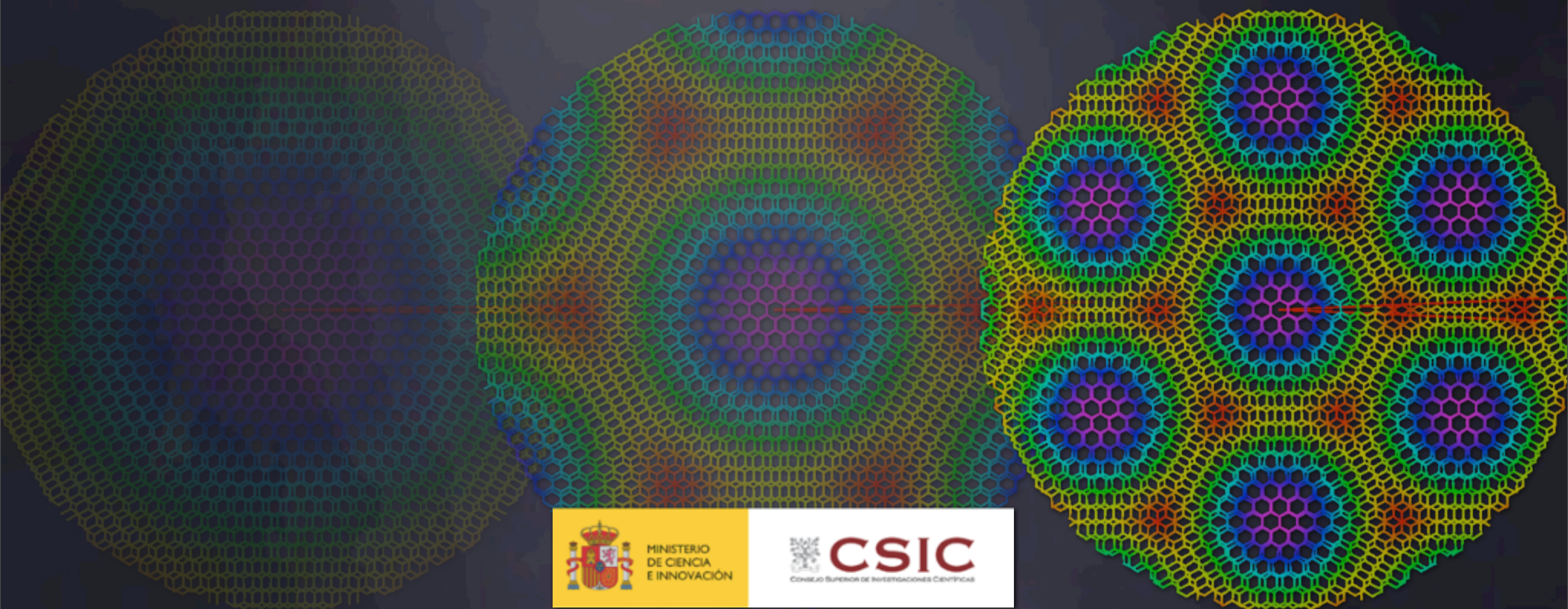
Twisted graphene bilayers

KITP - Graphene 2012

Pablo San José
IEM-CSIC (Madrid)



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Collaborators

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IEM-CSIC (Madrid)

Paco Guinea
ICMM-CSIC (Madrid)

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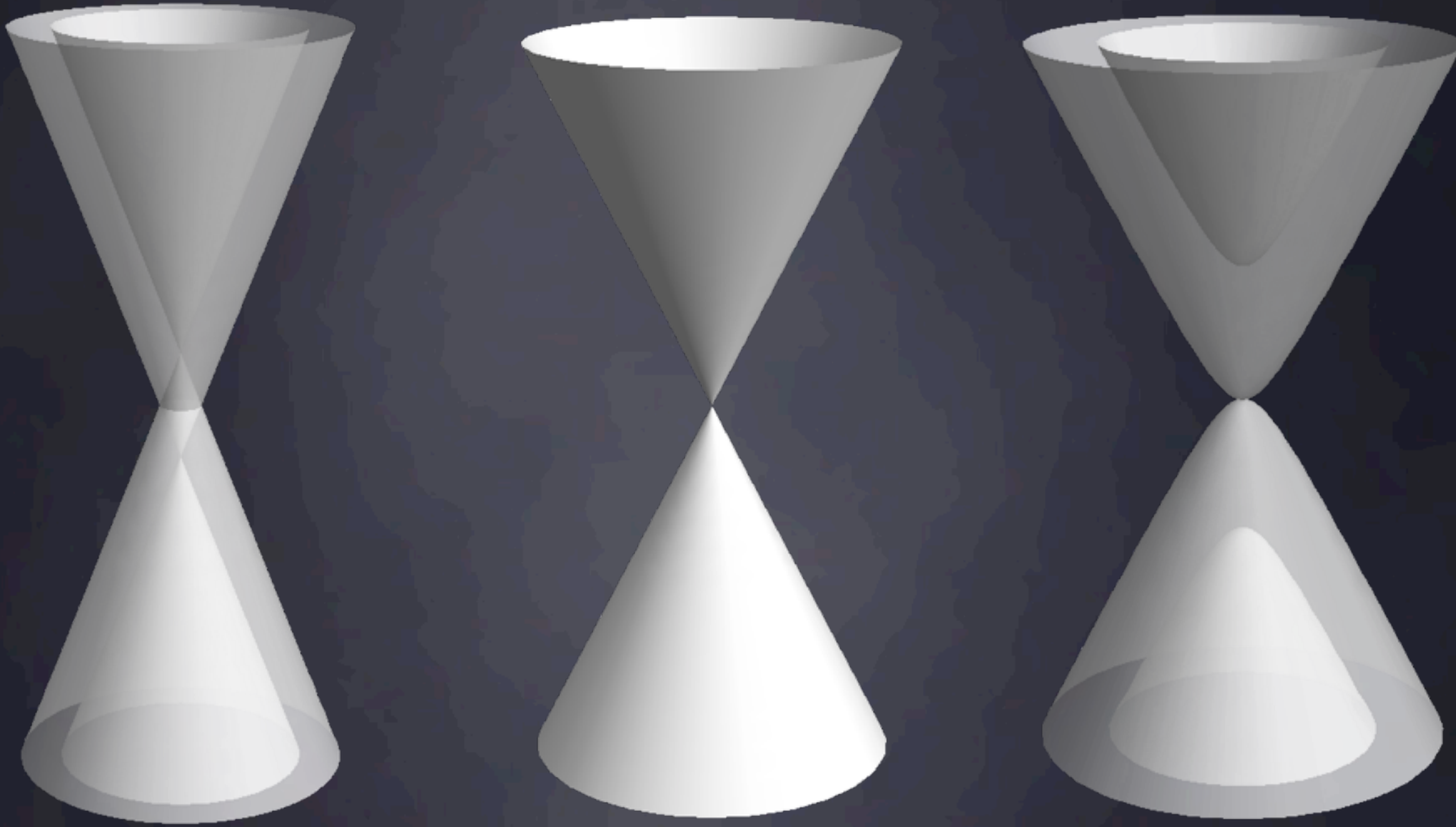
Modeling twisted bilayers

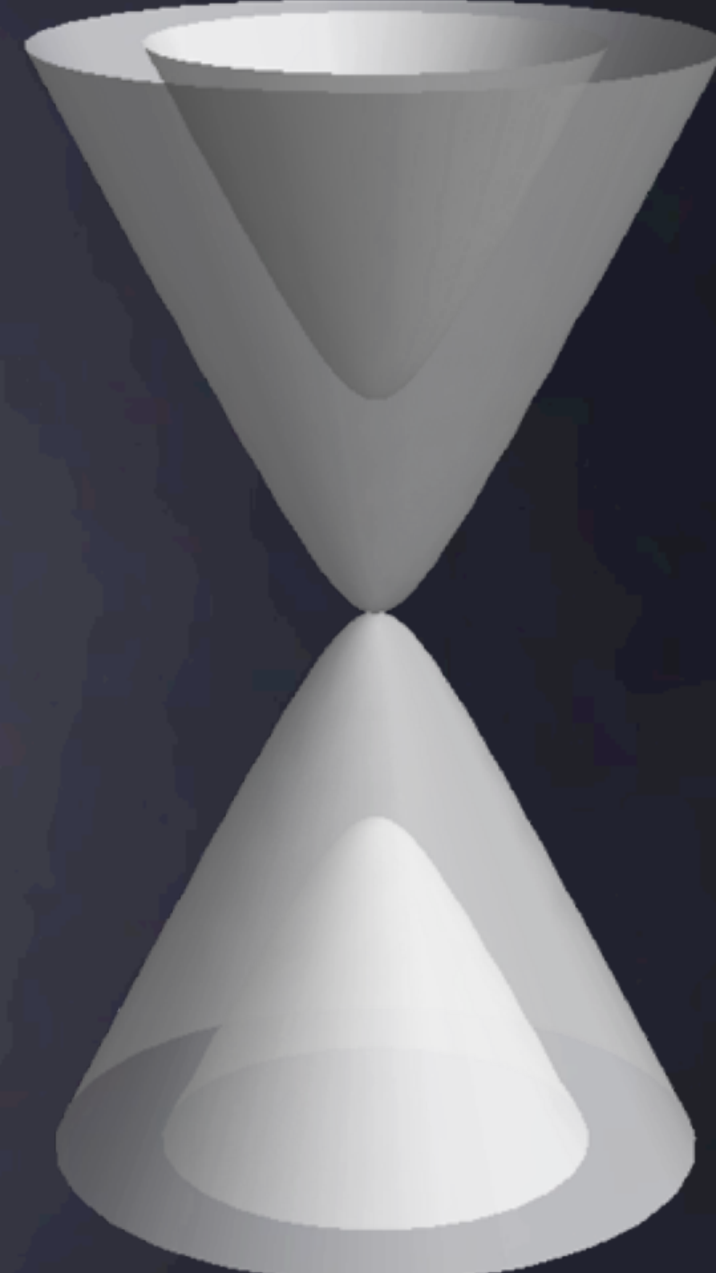
Simple stackings at low energy



AA bilayer Monolayer AB bilayer

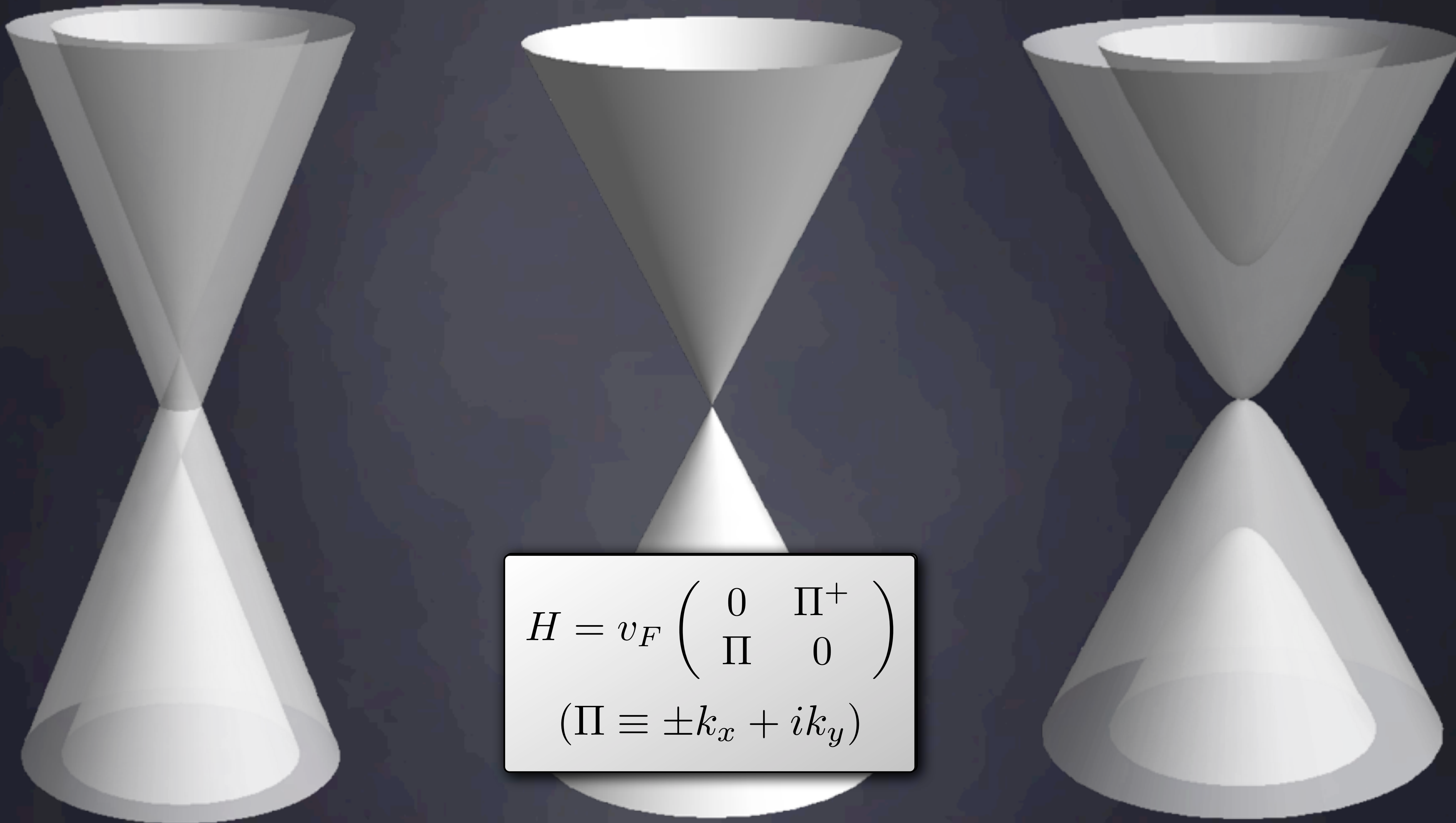
Simple stackings at low energy

$$H = v_F \mathbf{k} \cdot \boldsymbol{\sigma}$$



AA bilayer *Monolayer* *AB bilayer*

Simple stackings at low energy

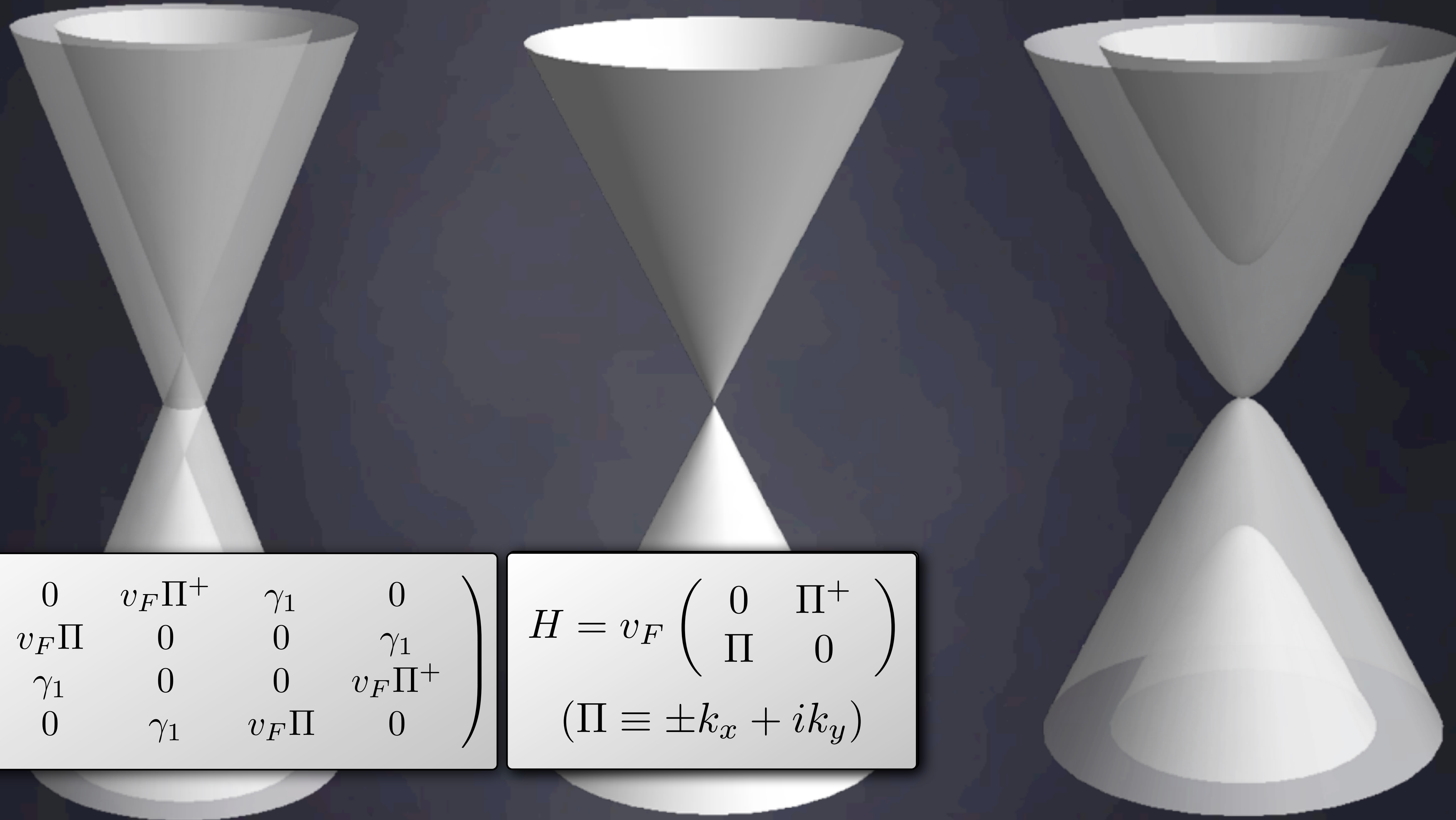


$$H = v_F \begin{pmatrix} 0 & \Pi^+ \\ \Pi & 0 \end{pmatrix}$$

$$(\Pi \equiv \pm k_x + i k_y)$$

AA bilayer Monolayer AB bilayer

Simple stackings at low energy



$$H = \begin{pmatrix} 0 & v_F\Pi^+ & \gamma_1 & 0 \\ v_F\Pi & 0 & 0 & \gamma_1 \\ \gamma_1 & 0 & 0 & v_F\Pi^+ \\ 0 & \gamma_1 & v_F\Pi & 0 \end{pmatrix}$$

$$H = v_F \begin{pmatrix} 0 & \Pi^+ \\ \Pi & 0 \end{pmatrix}$$

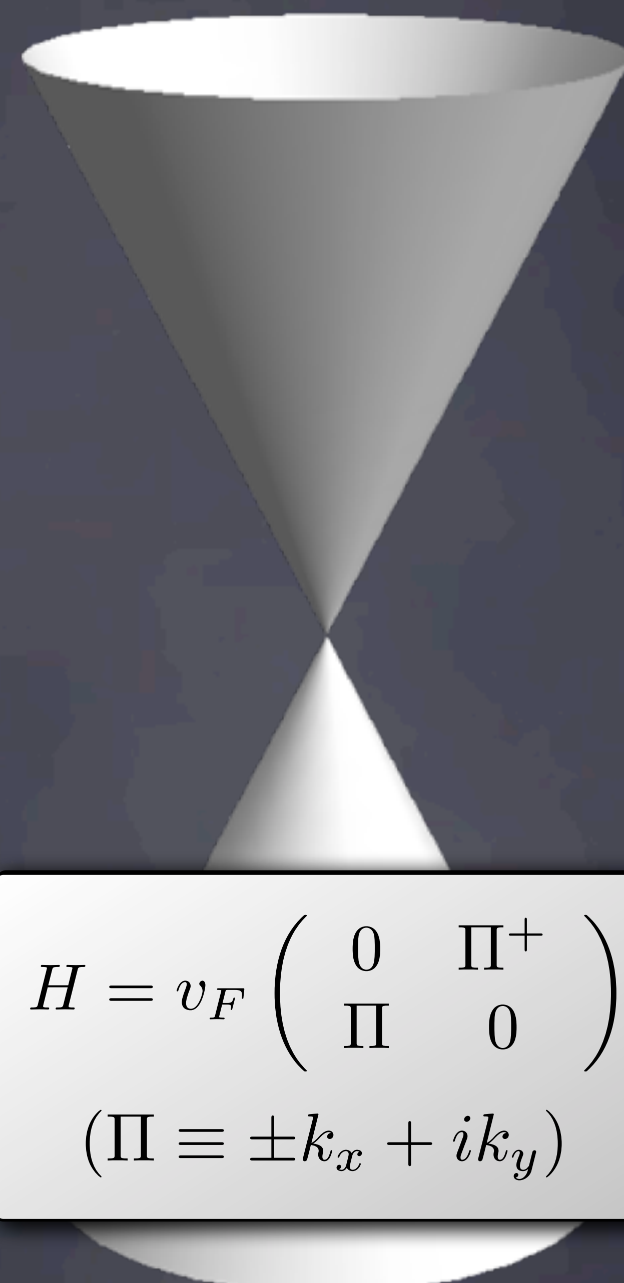
$$(\Pi \equiv \pm k_x + i k_y)$$

AA bilayer **Monolayer** **AB bilayer**

Simple stackings at low energy

$$H = \begin{pmatrix} 0 & v_F\Pi^+ & \gamma_1 & 0 \\ v_F\Pi & 0 & 0 & \gamma_1 \\ \gamma_1 & 0 & 0 & v_F\Pi^+ \\ 0 & \gamma_1 & v_F\Pi & 0 \end{pmatrix}$$

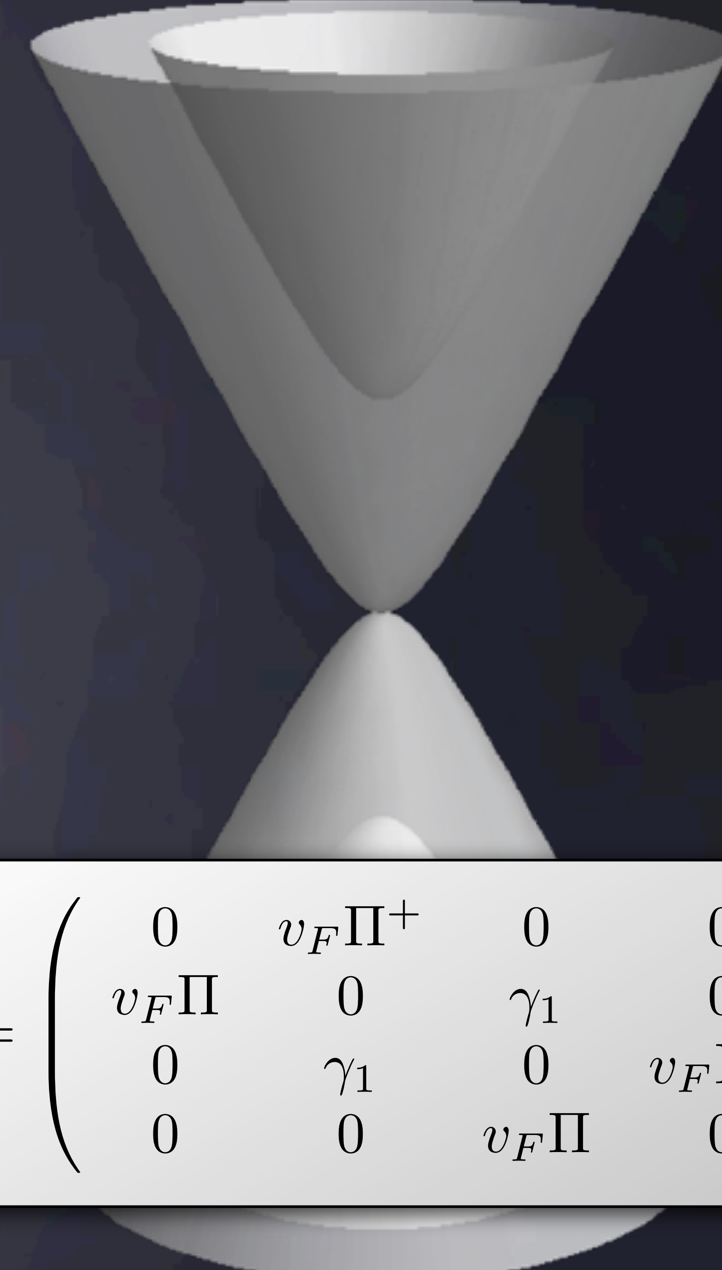
AA bilayer



$$H = v_F \begin{pmatrix} 0 & \Pi^+ \\ \Pi & 0 \end{pmatrix}$$

$$(\Pi \equiv \pm k_x + i k_y)$$

Monolayer



$$H = \begin{pmatrix} 0 & v_F\Pi^+ & 0 & 0 \\ v_F\Pi & 0 & \gamma_1 & 0 \\ 0 & \gamma_1 & 0 & v_F\Pi^+ \\ 0 & 0 & v_F\Pi & 0 \end{pmatrix}$$

AB bilayer

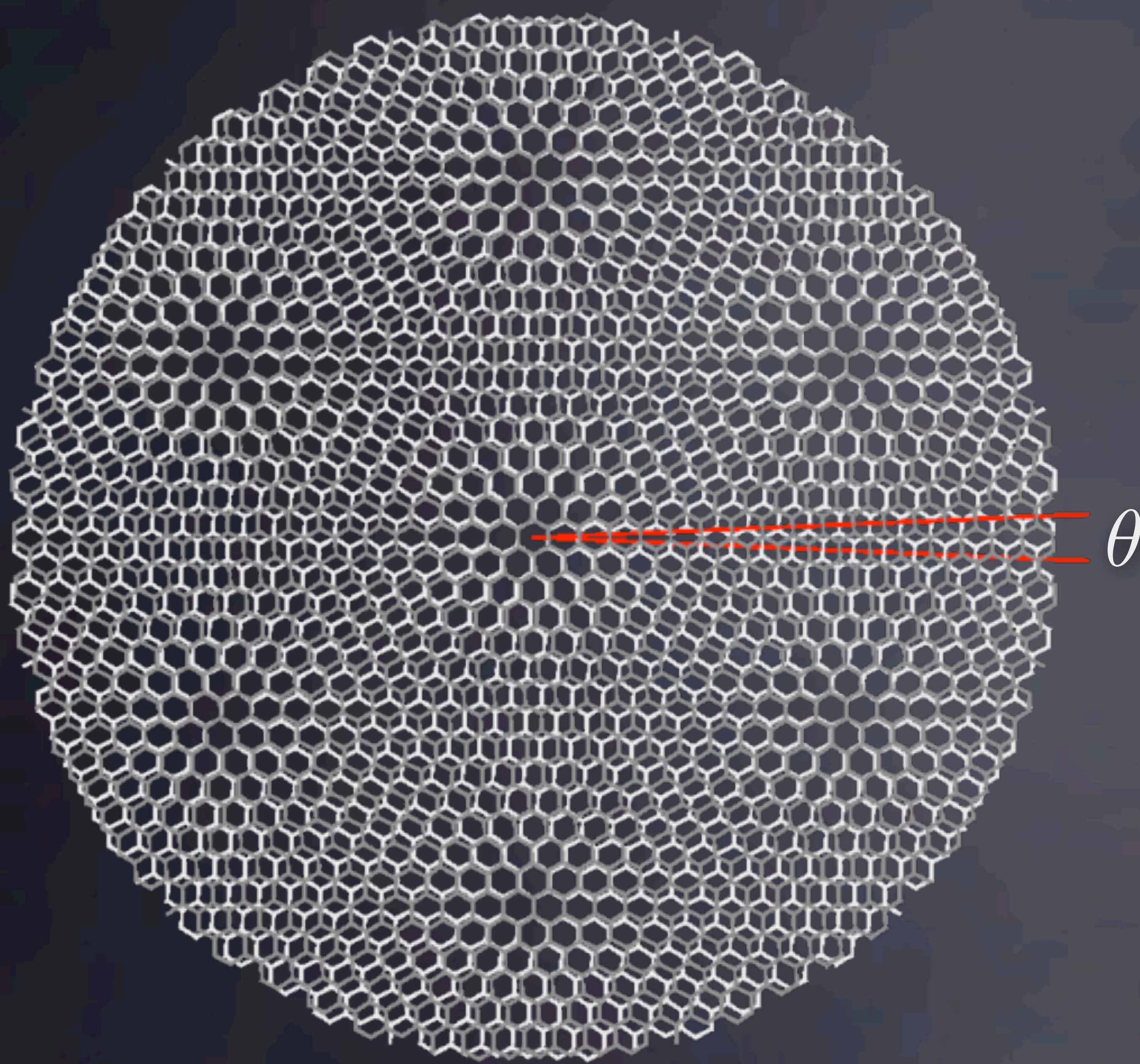
Twisted bilayer

$$L = \frac{a}{2\sin\frac{\theta}{2}}$$

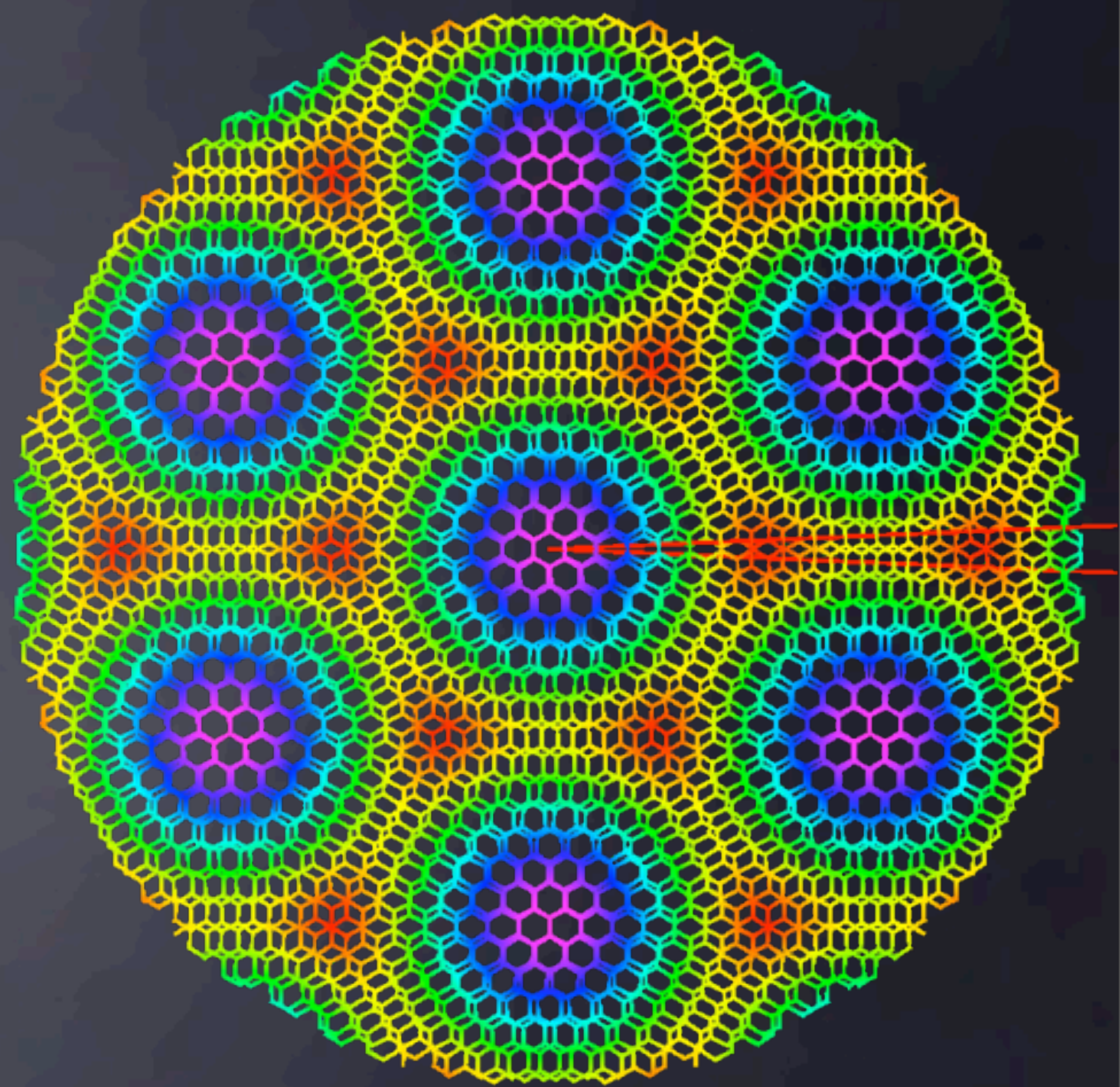
Gray: Top layer
White: Bottom layer

Pink: AA stacking
Red: AB/BA stacking

Twisted bilayer

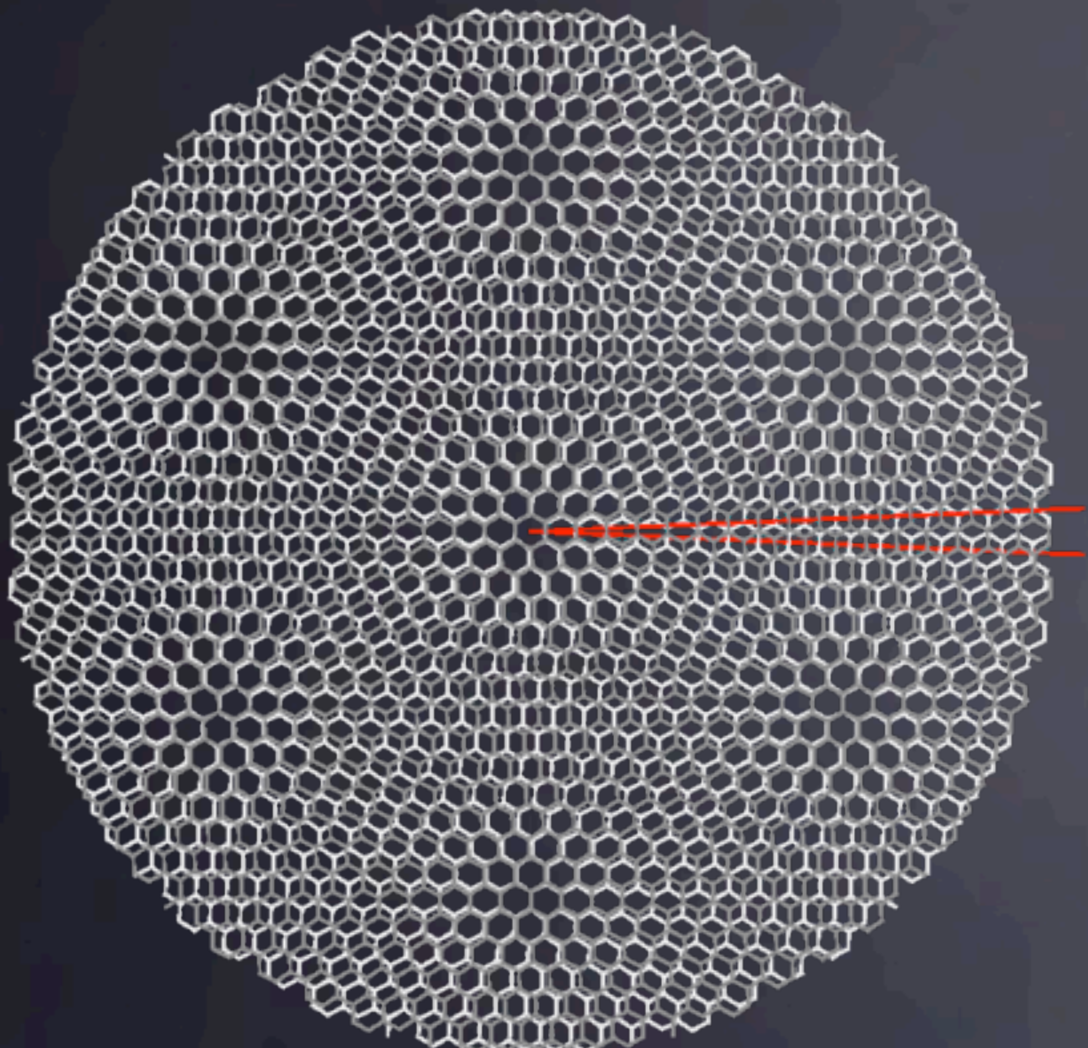


Gray: Top layer
White: Bottom layer



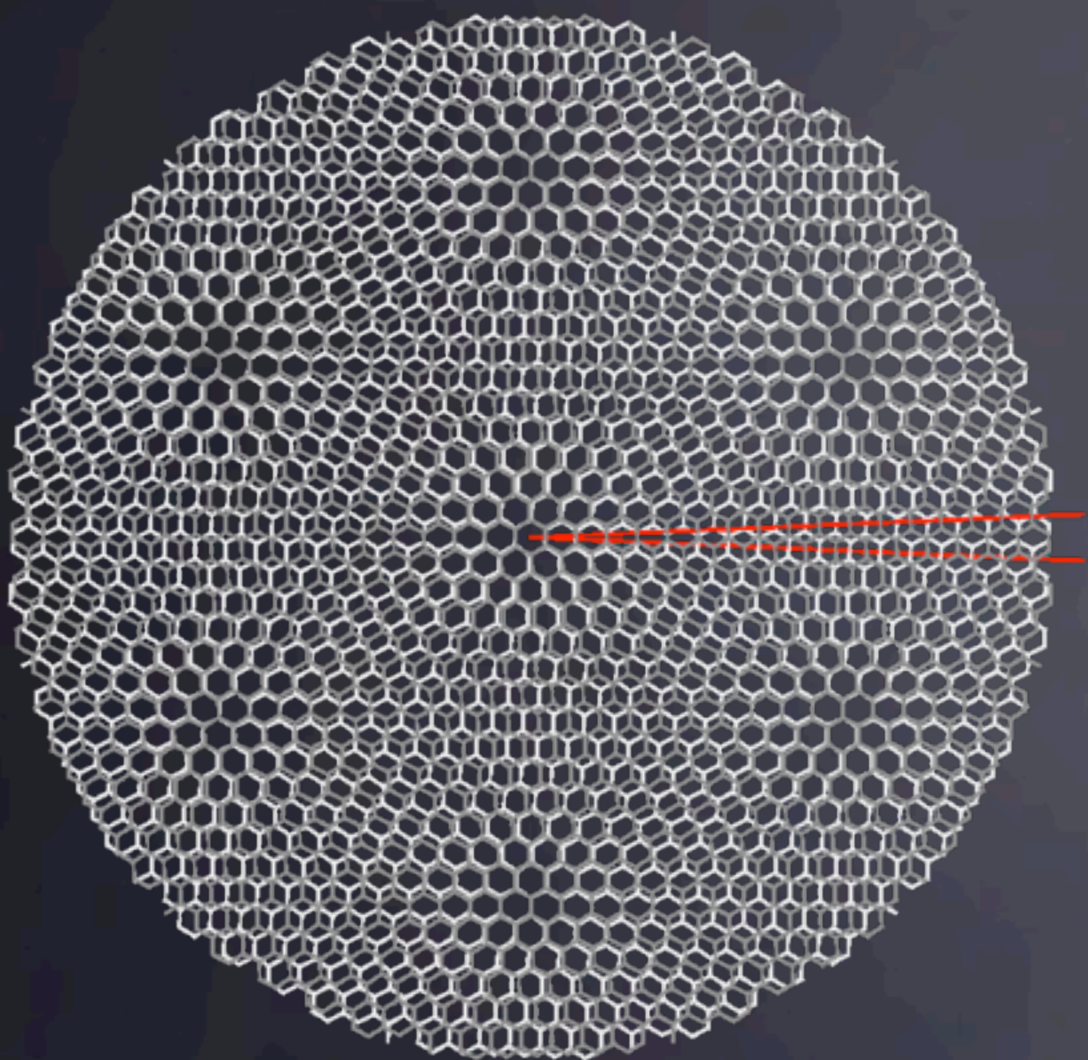
Pink: AA stacking
Red: AB/BA stacking

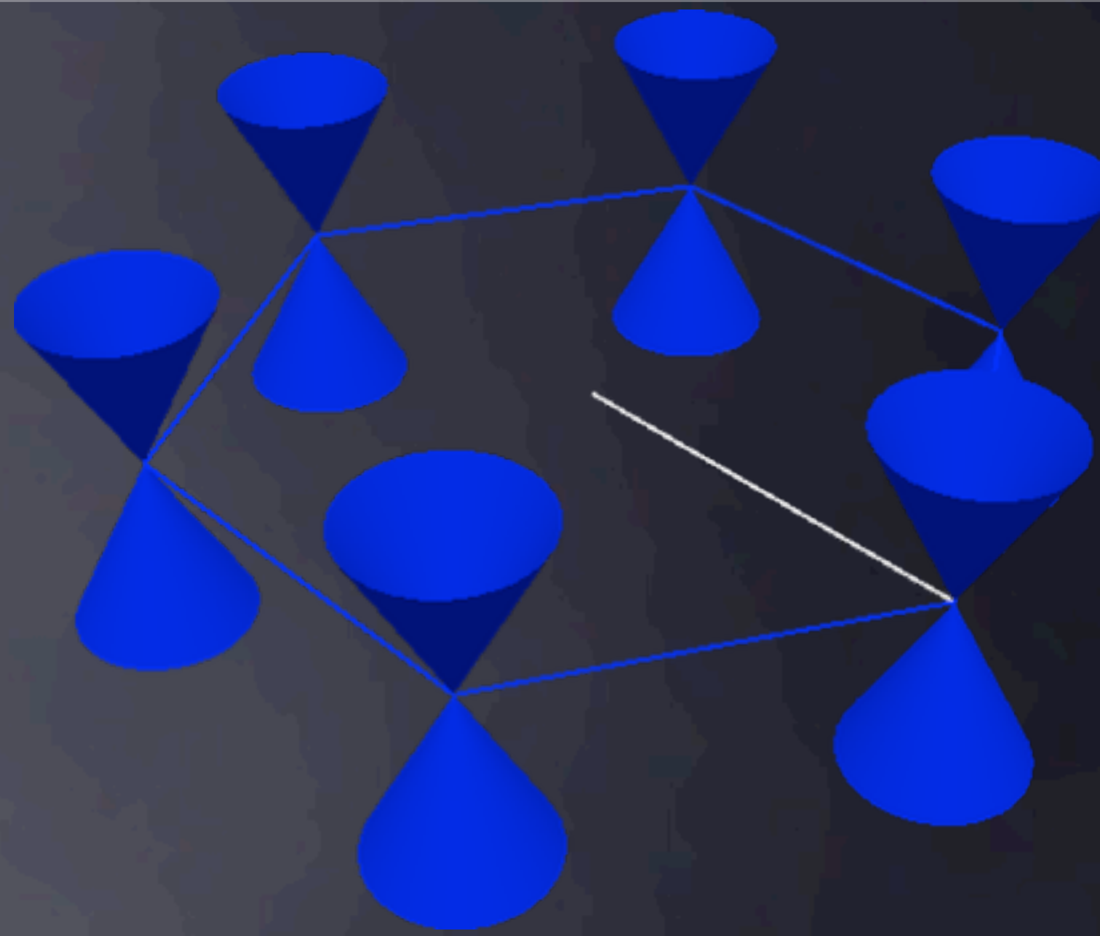
Twisted bilayer at low energy



J. M. B. Lopes dos Santos et al. Phys. Rev. Lett., 99, 256802 (2007)

Twisted bilayer at low energy





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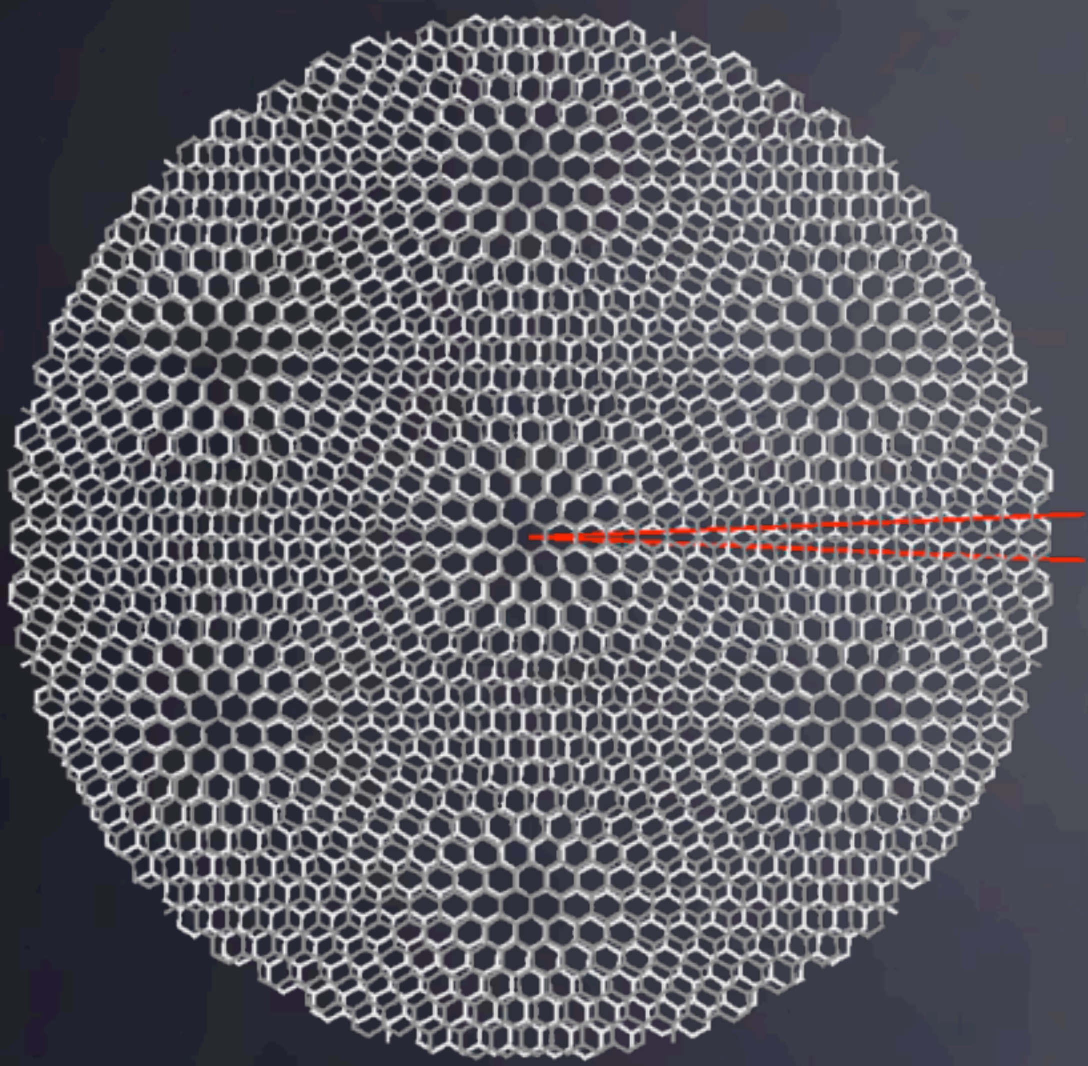
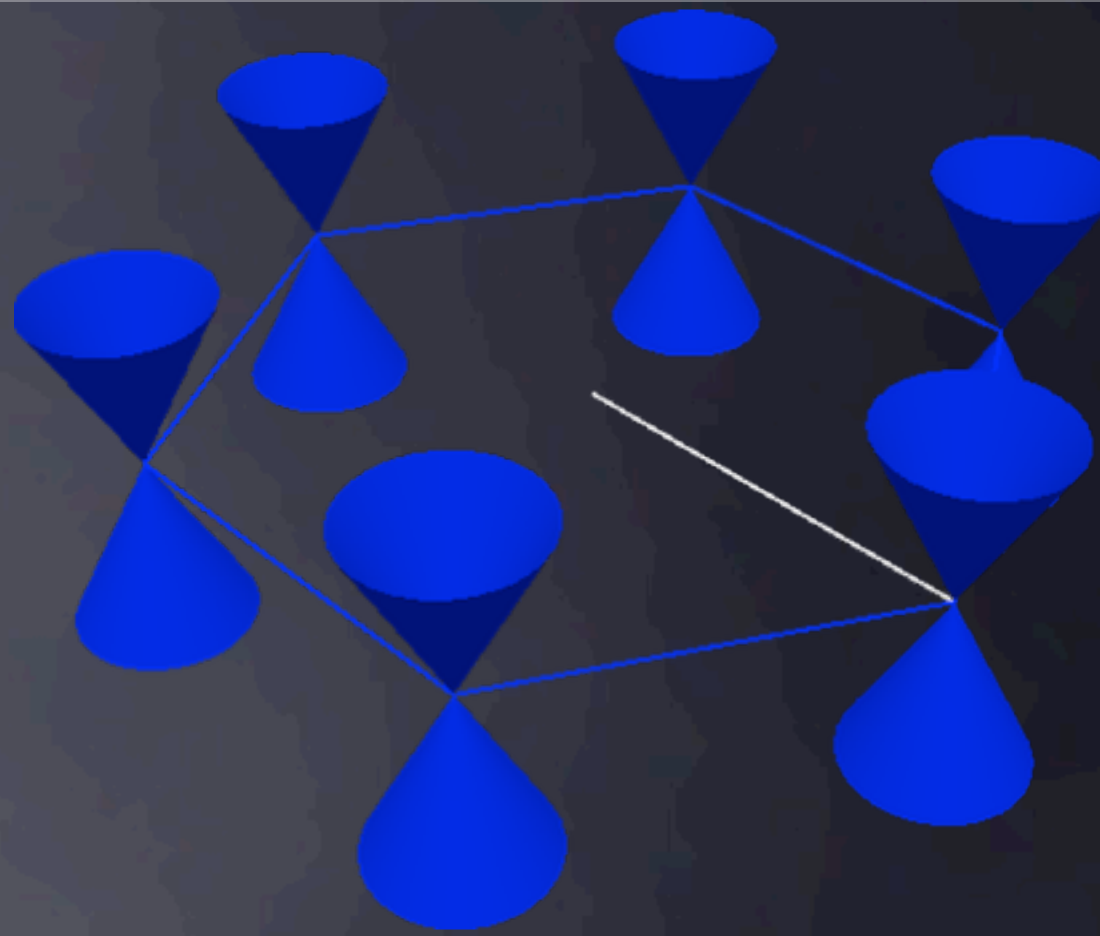
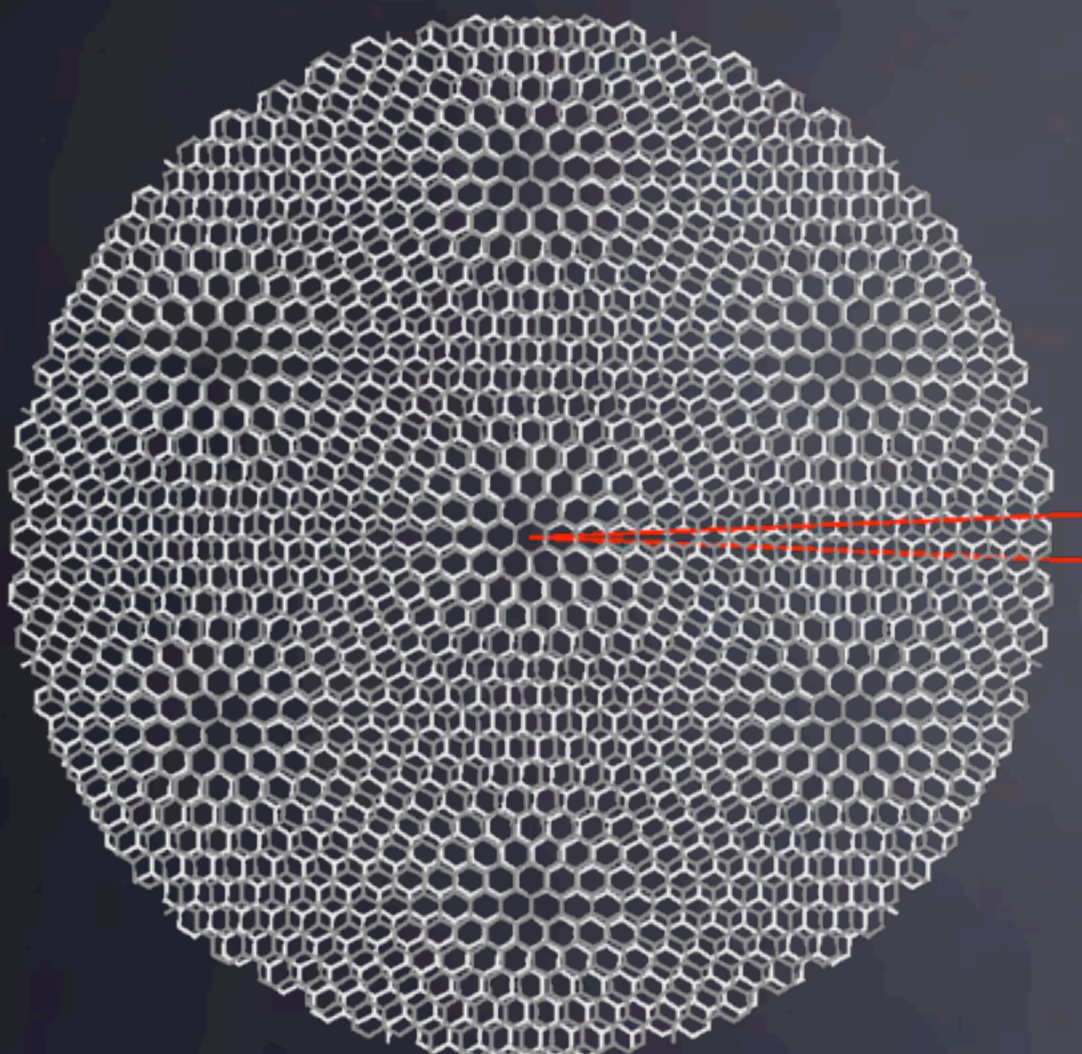


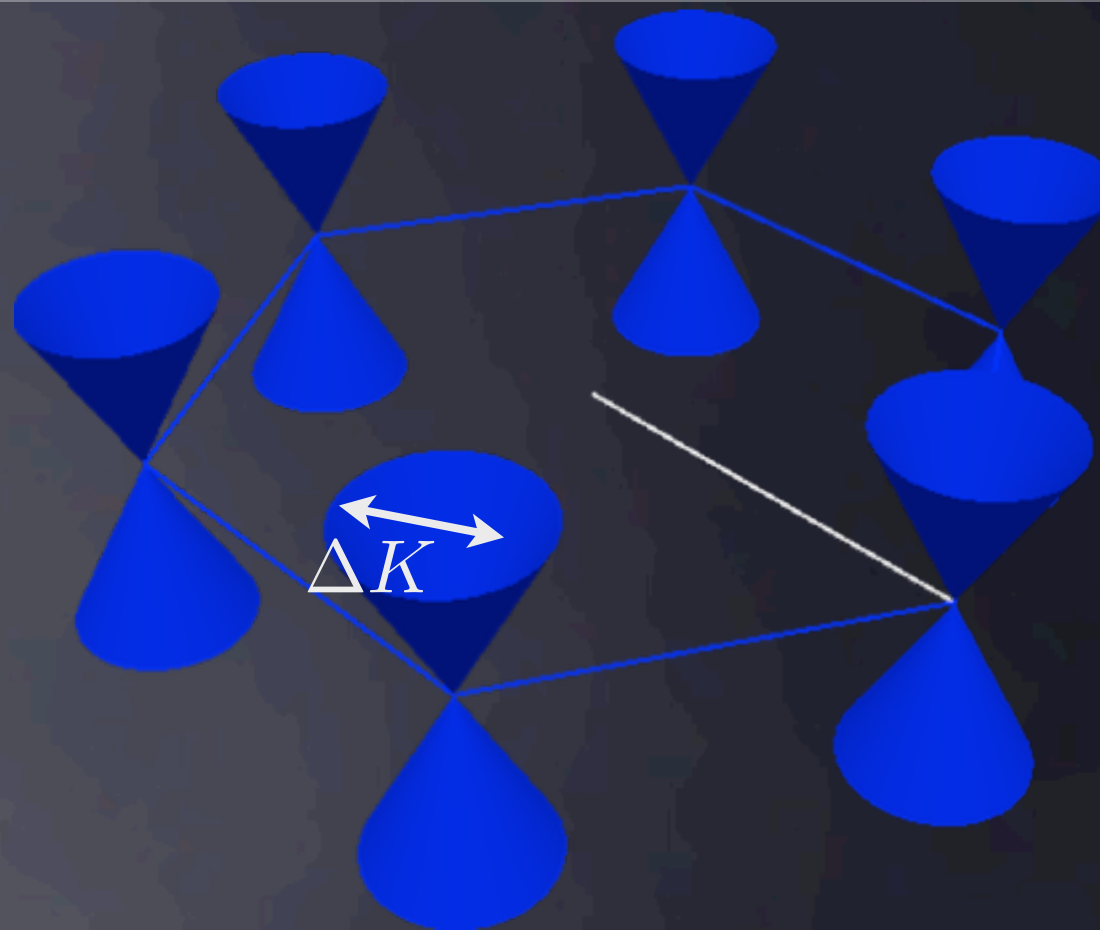


$$H_0 = v_F \begin{pmatrix} 0 & \Pi_+^\dagger & 0 & 0 \\ \Pi_+ & 0 & 0 & 0 \\ 0 & 0 & 0 & \Pi_-^\dagger \\ 0 & 0 & \Pi_- & 0 \end{pmatrix}$$

J. M. B. Lopes dos Santos et al. Phys. Rev. Lett., 99, 256802 (2007)

Twisted bilayer at low energy





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$$\Pi_\pm = -i\partial_x + \partial_y \mp i\frac{\Delta K}{2} \quad ; \quad \Delta K = 2K \sin\frac{\theta}{2}$$

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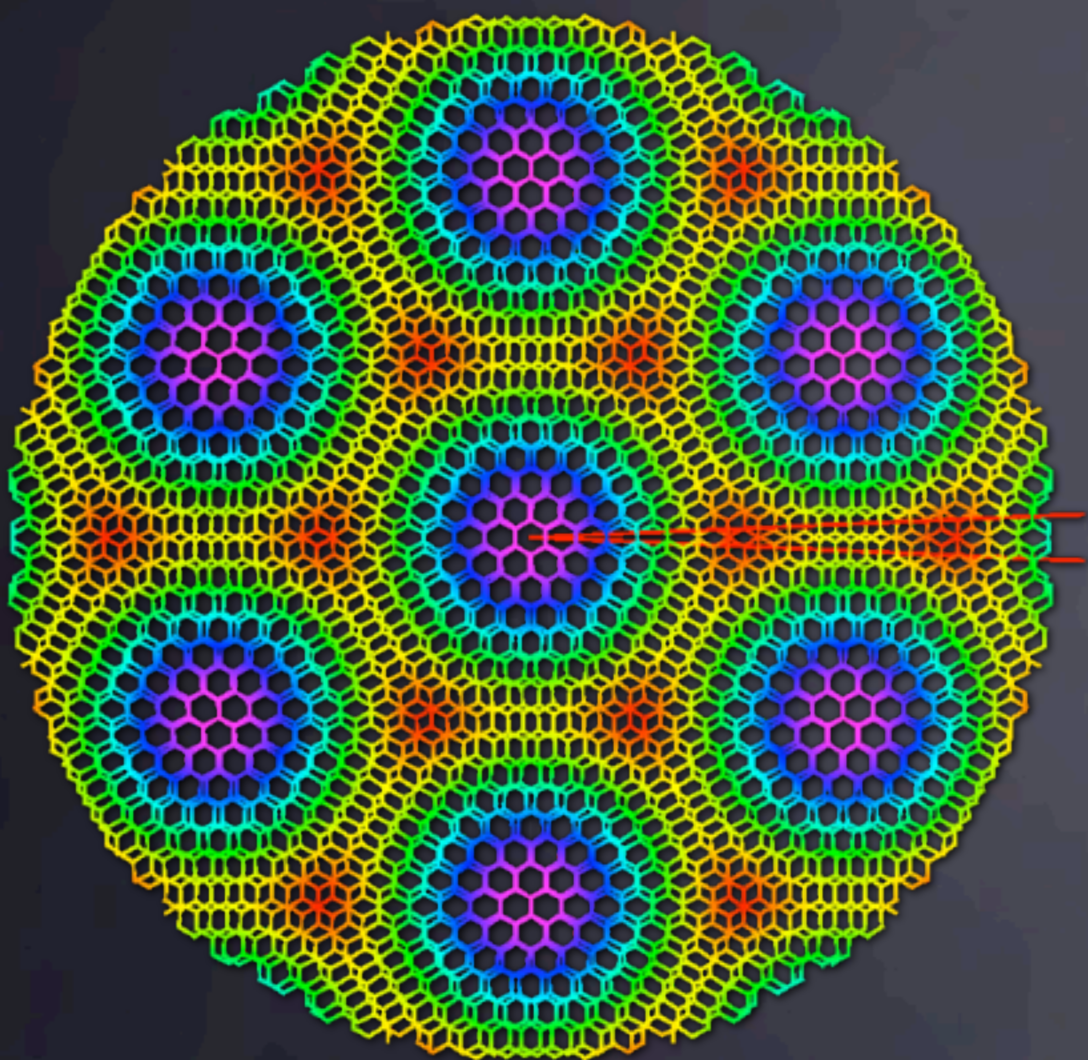
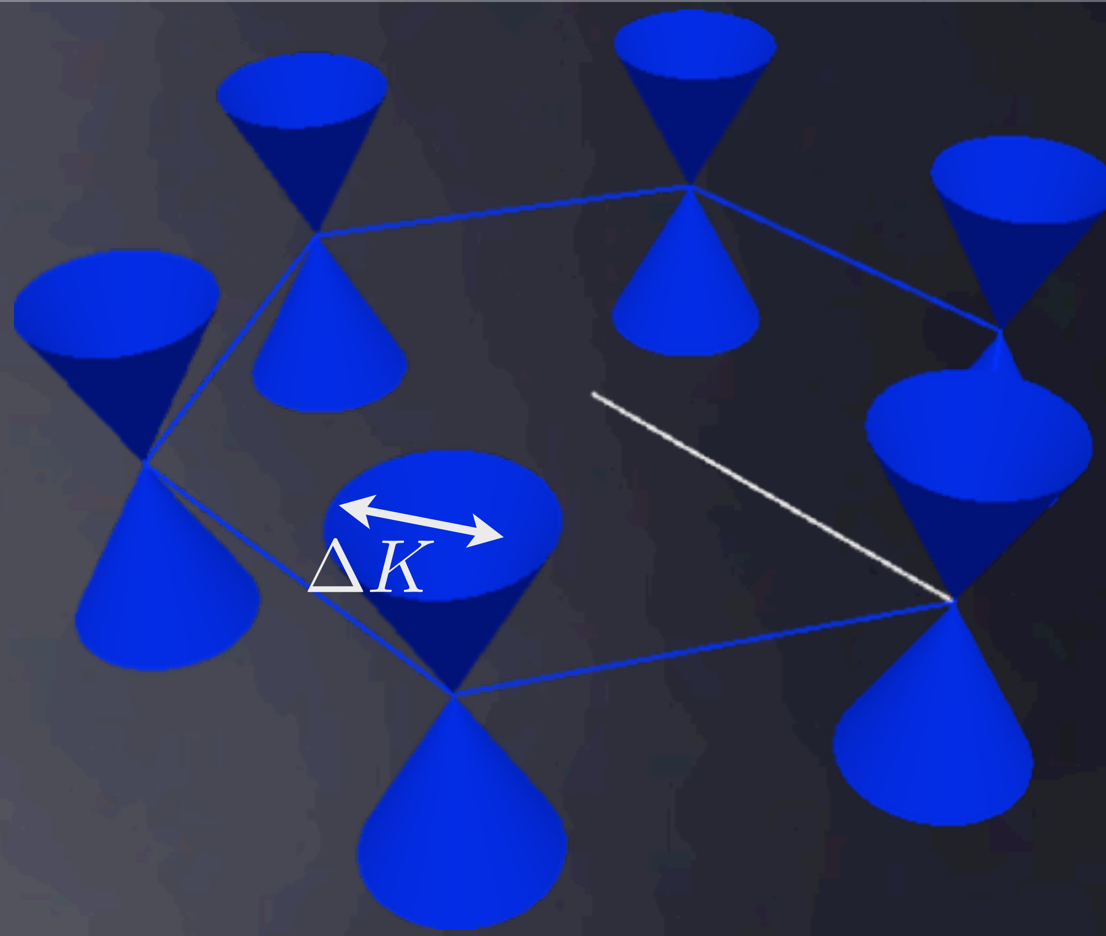
Twisted bilayer at low energy





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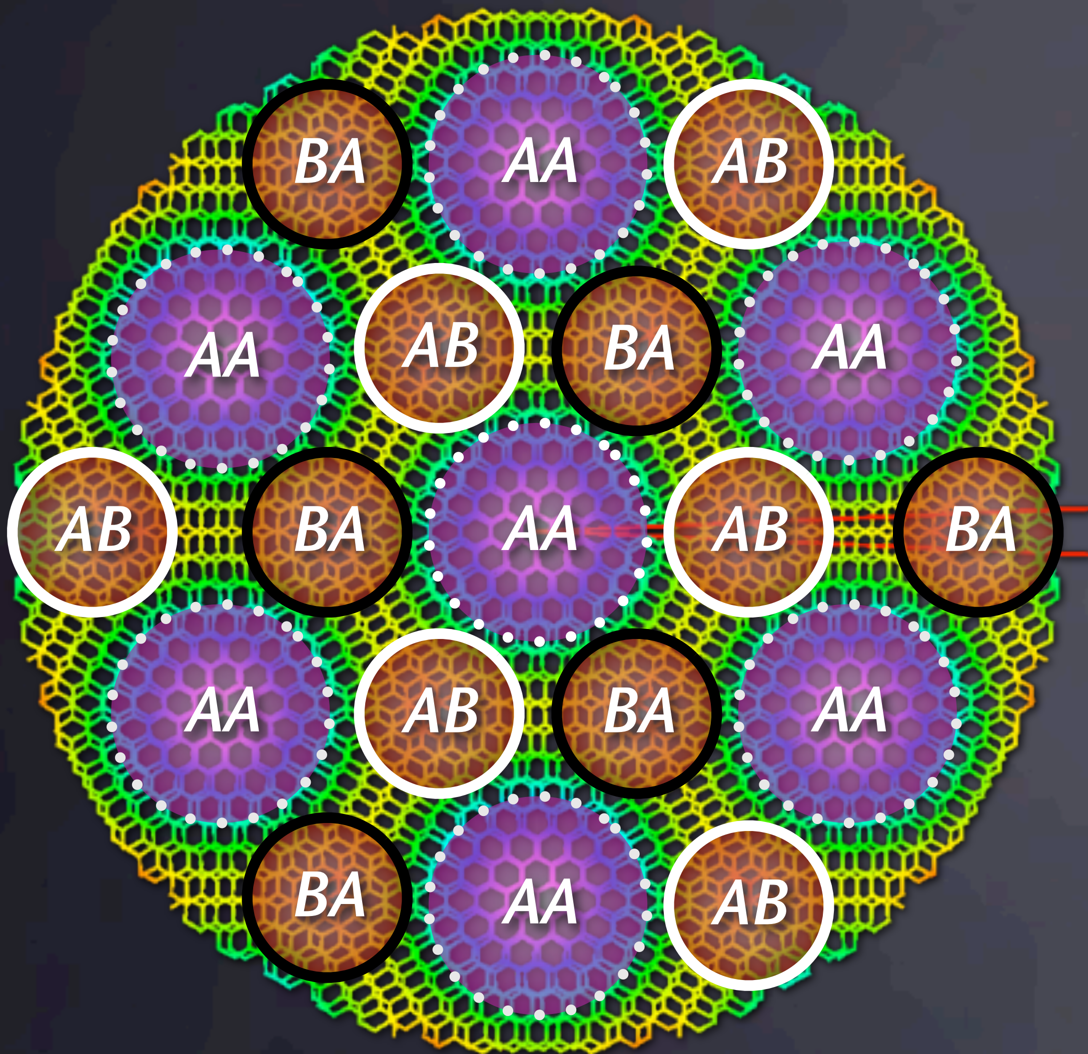
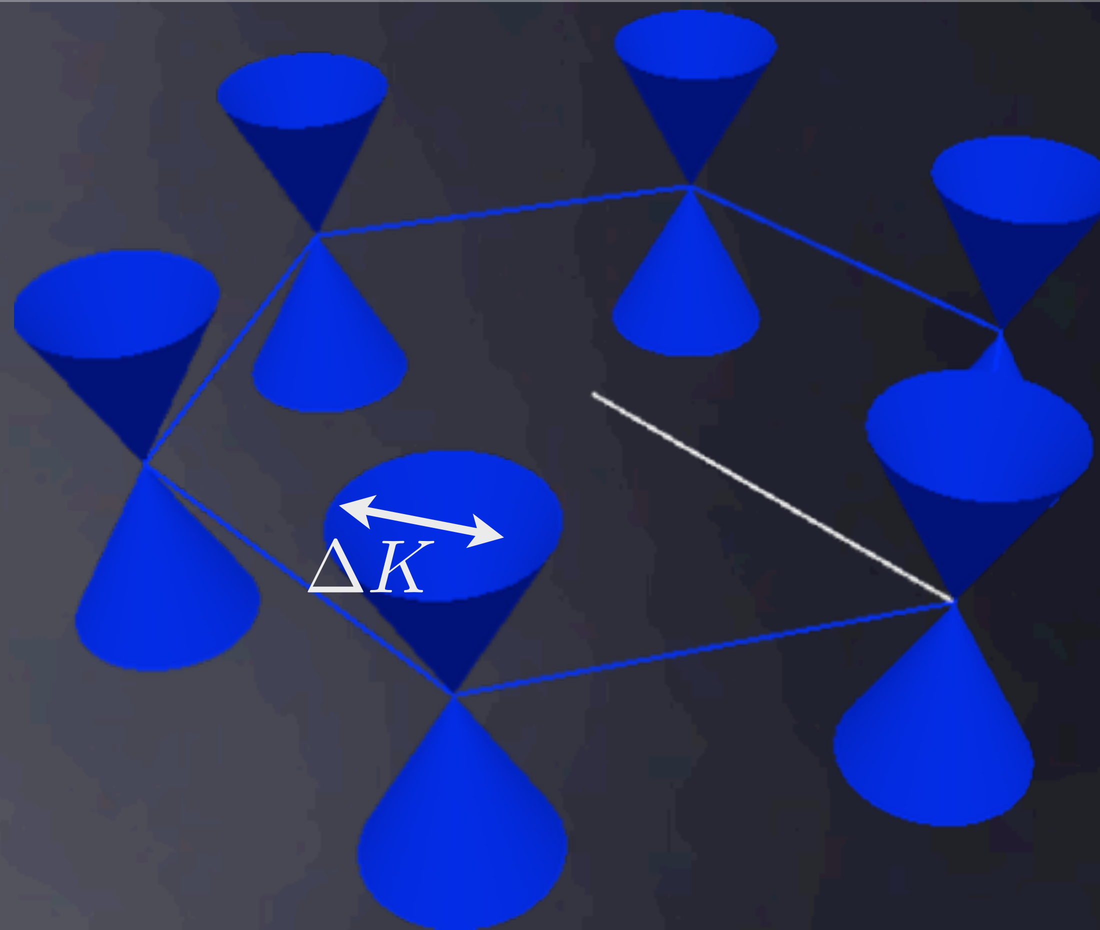
Twisted bilayer at low energy





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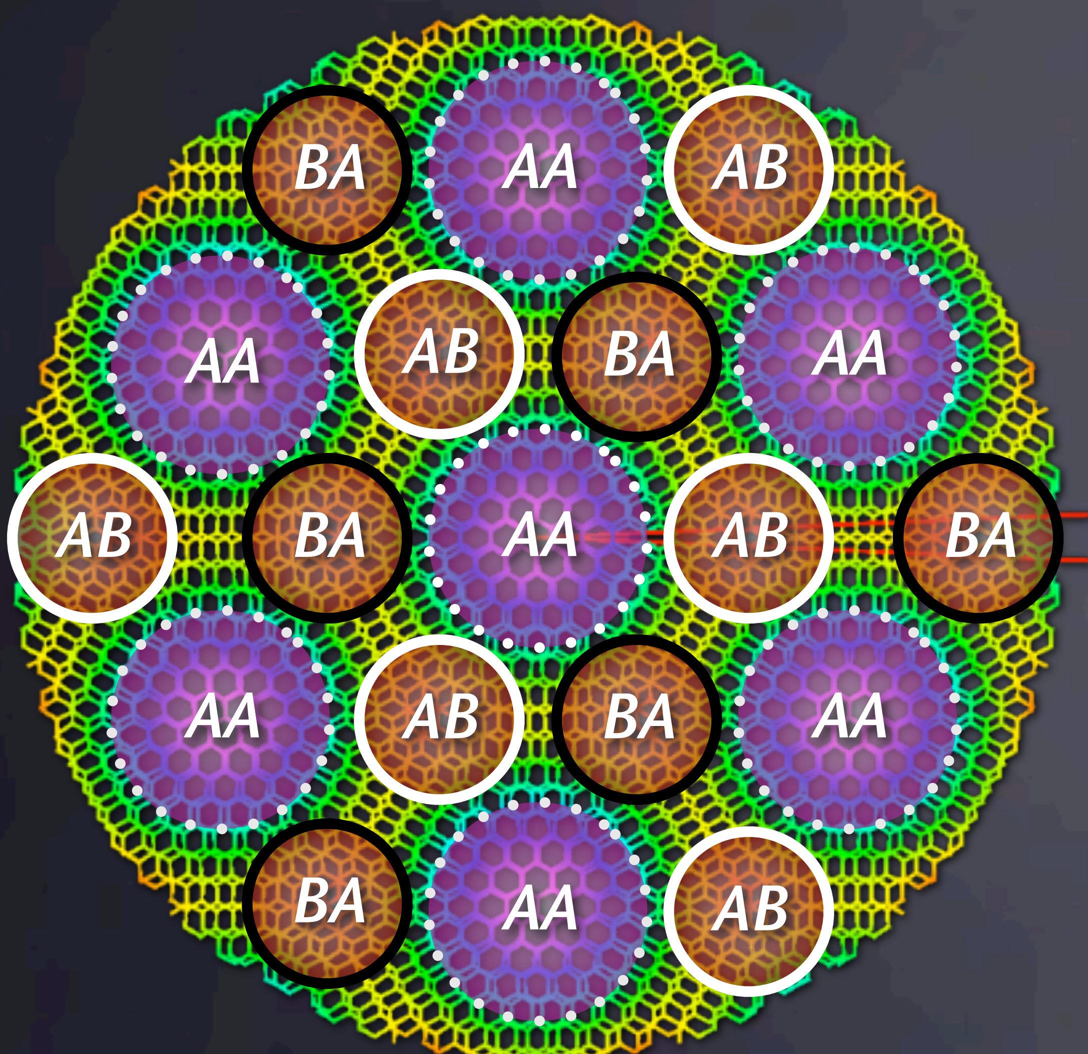
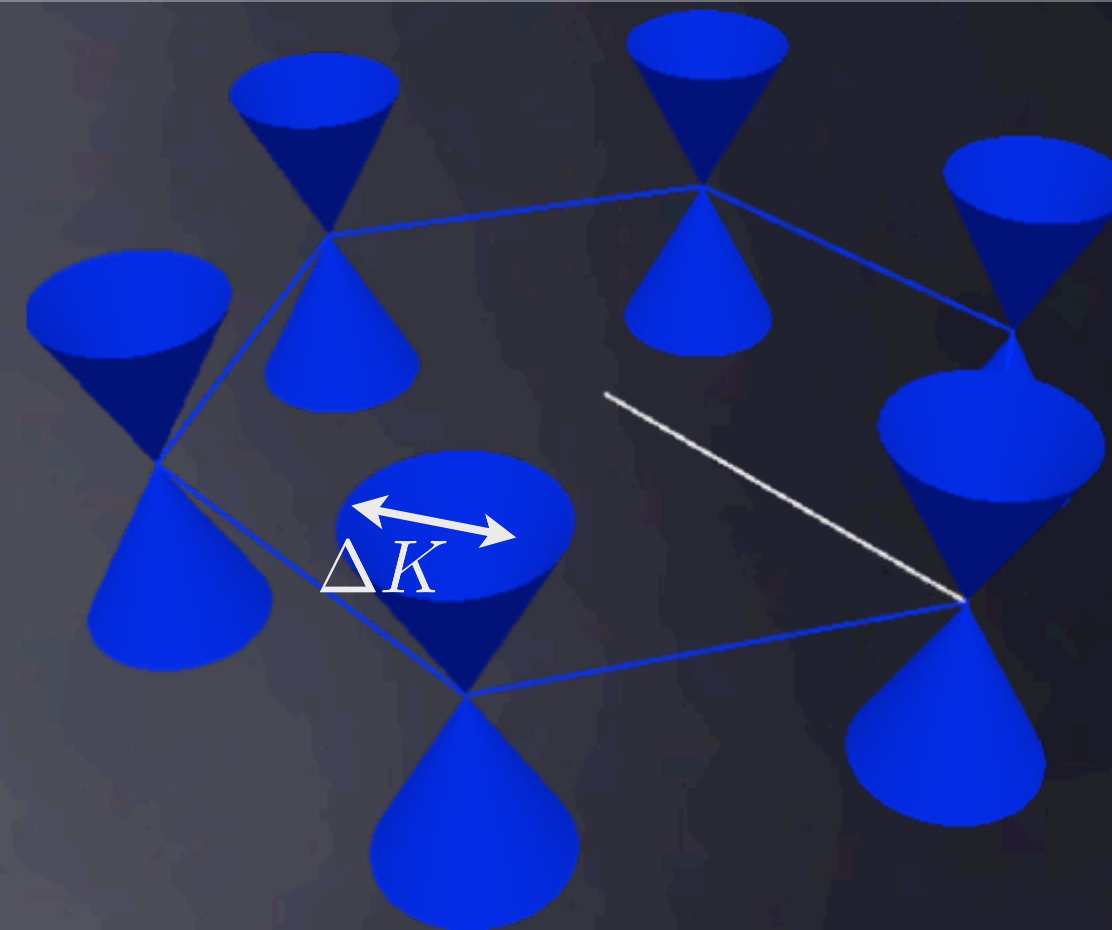
Twisted bilayer at low energy



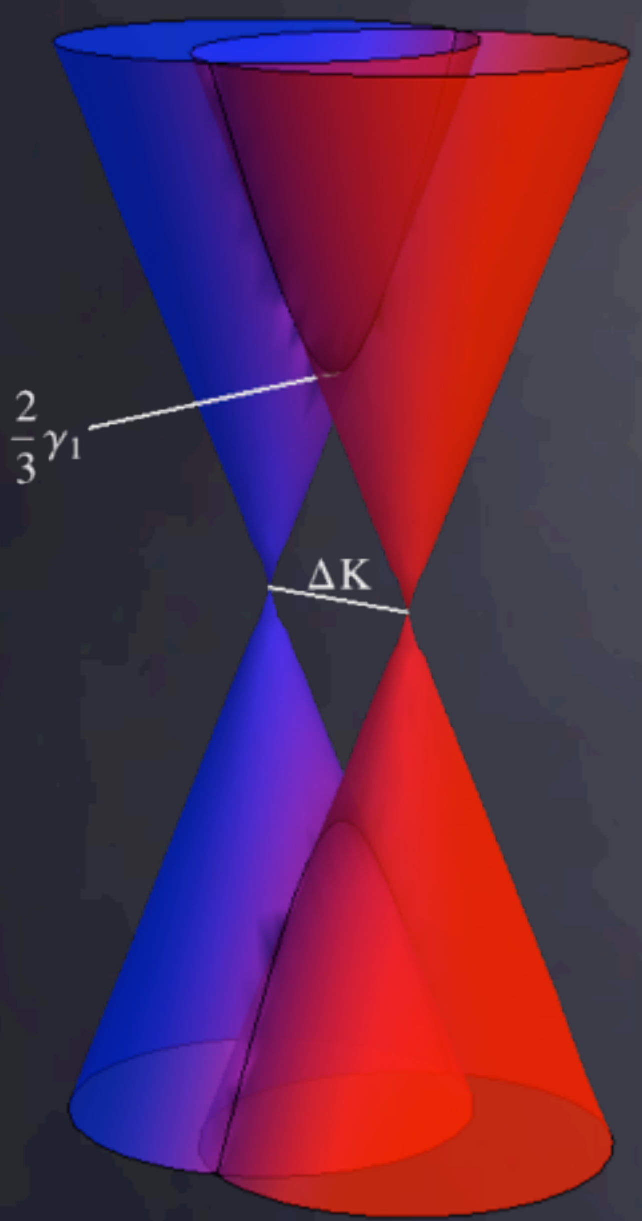


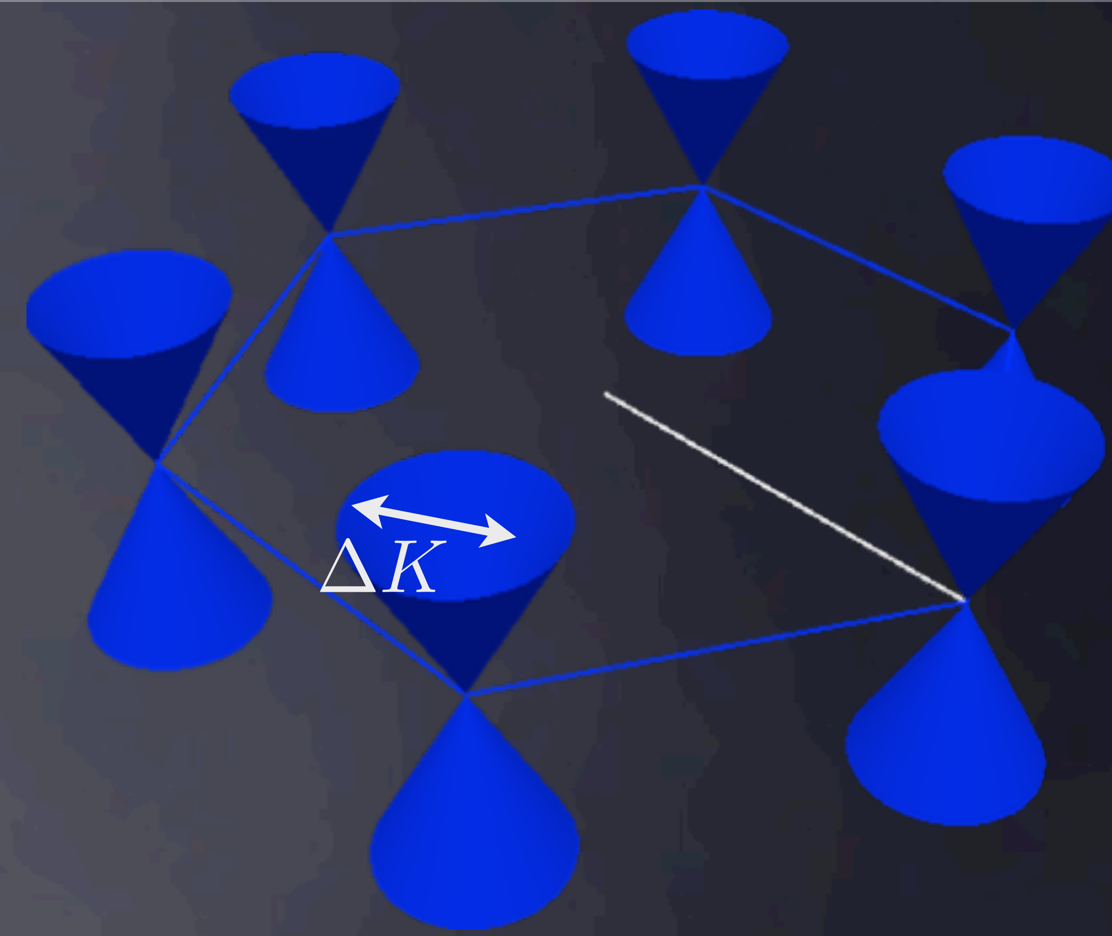
$$H = v_F \begin{pmatrix} 0 & \Pi_+^\dagger & V_{AA}(\mathbf{r}) & V_{AB}(\mathbf{r}) \\ \Pi_+ & 0 & V_{BA}(\mathbf{r}) & V_{AA}(\mathbf{r}) \\ V_{AA}^\star(\mathbf{r}) & V_{BA}^\star(\mathbf{r}) & 0 & \Pi_-^\dagger \\ V_{AB}^\star(\mathbf{r}) & V_{AA}^\star(\mathbf{r}) & \Pi_- & 0 \end{pmatrix}$$

$$V_{ij}(\mathbf{r}) = \frac{\gamma_1}{3v_F}\left(1 + e^{i\mathrm{G}_1\cdot(\mathrm{r}-\mathrm{r}_{ij}^{(0)})} + e^{i\mathrm{G}_2\cdot(\mathrm{r}-\mathrm{r}_{ij}^{(0)})}\right)$$

J. M. B. Lopes dos Santos et al. Phys. Rev. Lett., 99, 256802 (2007)

Twisted bilayer at low energy





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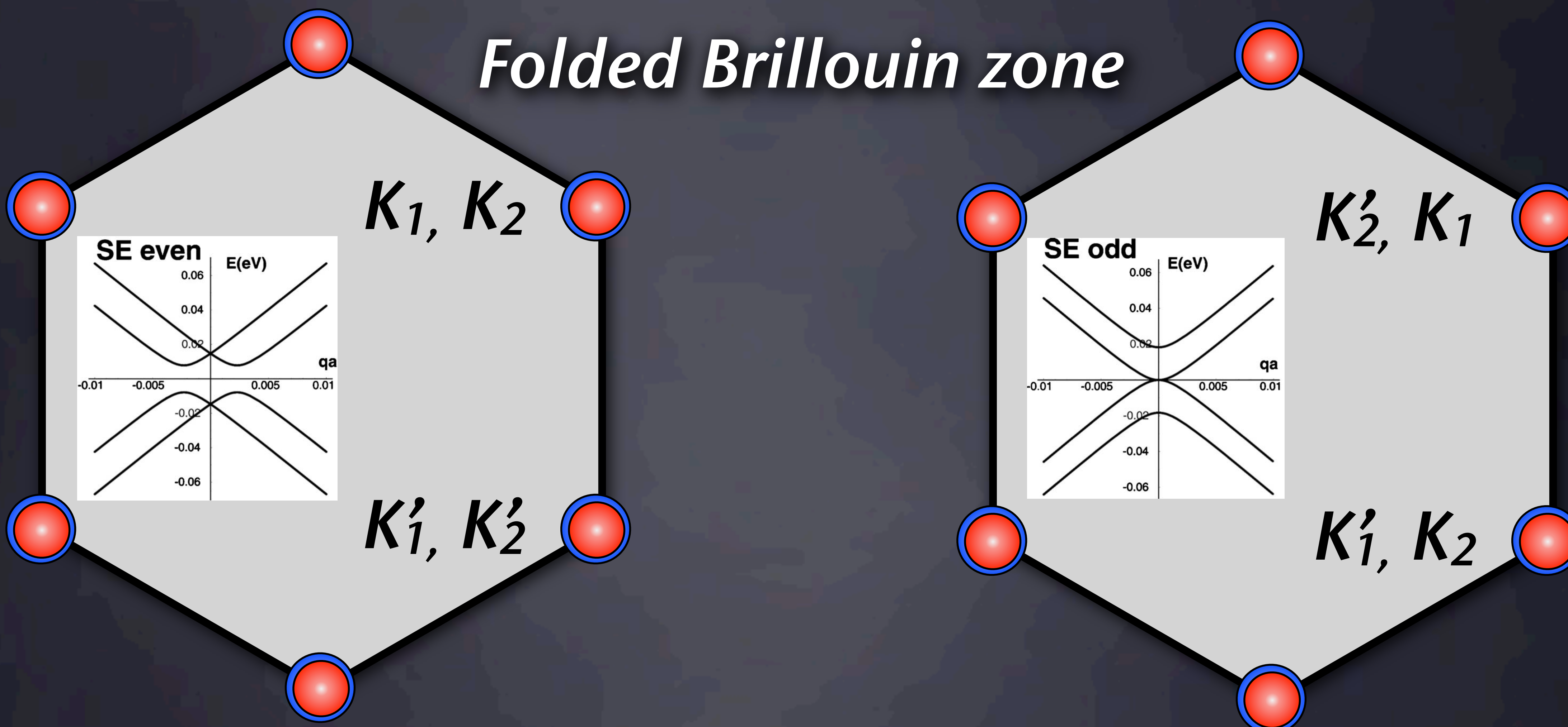
J. M. B. Lopes dos Santos et al. Phys. Rev. Lett., 99, 256802 (2007)

Brillouin zone

- *Two different classes, depending on the microscopic stacking*



SE-even (gapped) *SE-odd (parabolic)*

E. J. Mele. Phys. Rev. B 81, 161405 (2010)
E. J. Mele. arXiv:1112.2620 (2011)

Tunable gaps?? Let's see...

- *Tight-binding model for SE-even and SE-odd lattices*
- *Overlap for two π orbitals separated by* $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$

$$V(\mathbf{r}) = \gamma_0 \frac{x^2+y^2}{|\mathrm{r}|^2} e^{-\lambda(|\mathrm{r}|-a_{cc})} + \gamma_1 \frac{z^2}{|\mathrm{r}|^2} e^{-\lambda(|\mathrm{r}|-d)}$$

- *Range and number of neighbors are unconstrained*

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- *Range and number of neighbors are unconstrained*

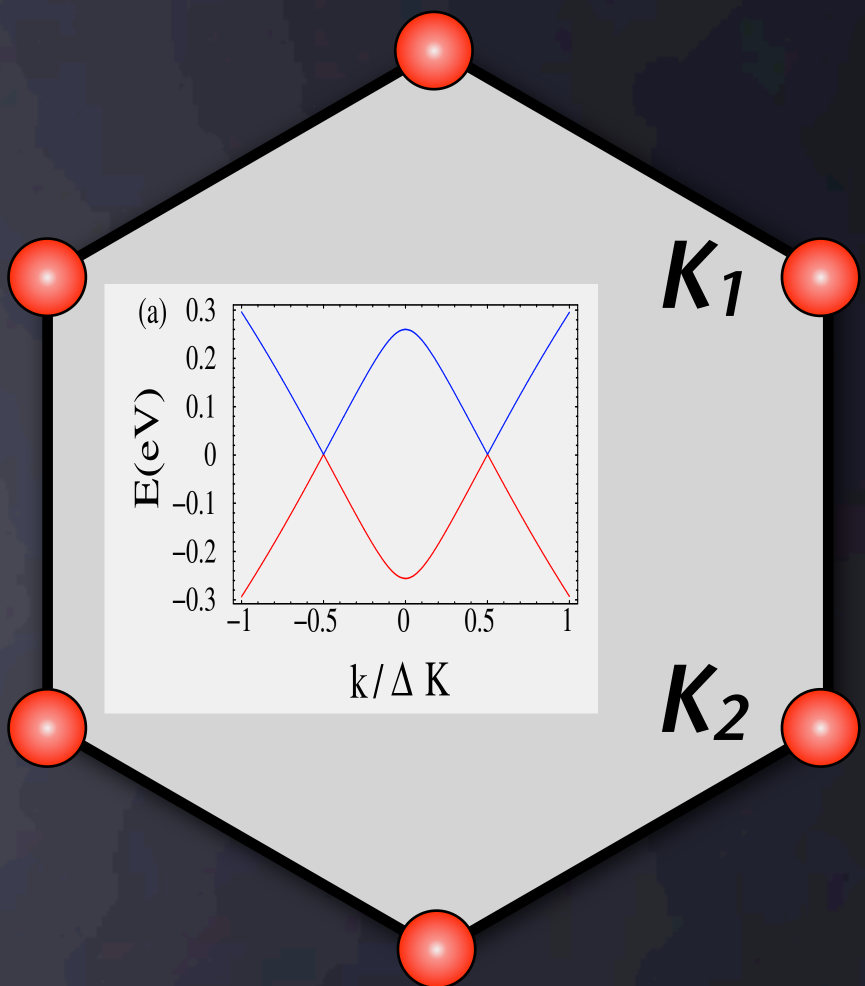
But...
No gaps to be seen, anywhere!

Tunable gaps?? Let's see...

- *Tight-binding model for SE-even and SE-odd lattices*
- *Overlap for two π orbitals separated by* **r=r₁-r₂**

$$V(\mathbf{r}) = \gamma_0 \frac{x^2+y^2}{|\mathbf{r}|^2} e^{-\lambda(|\mathbf{r}|-a_{cc})} + \gamma_1 \frac{z^2}{|\mathbf{r}|^2} e^{-\lambda(|\mathbf{r}|-d)}$$

- *Range and number of neighbors are unconstrained*

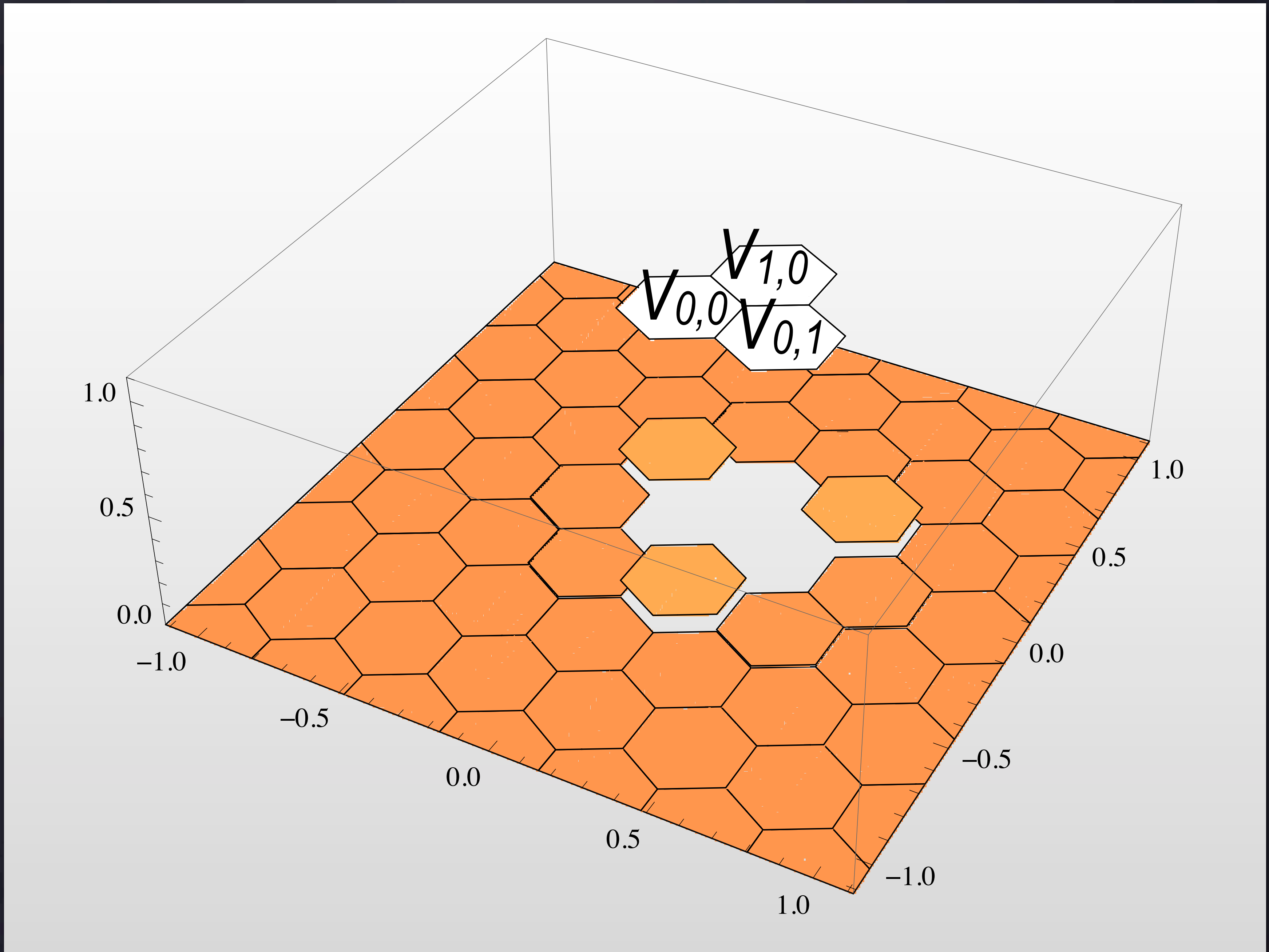


Valley-decoupled!

But...
No gaps to be seen, anywhere!

Tight-binding calculation

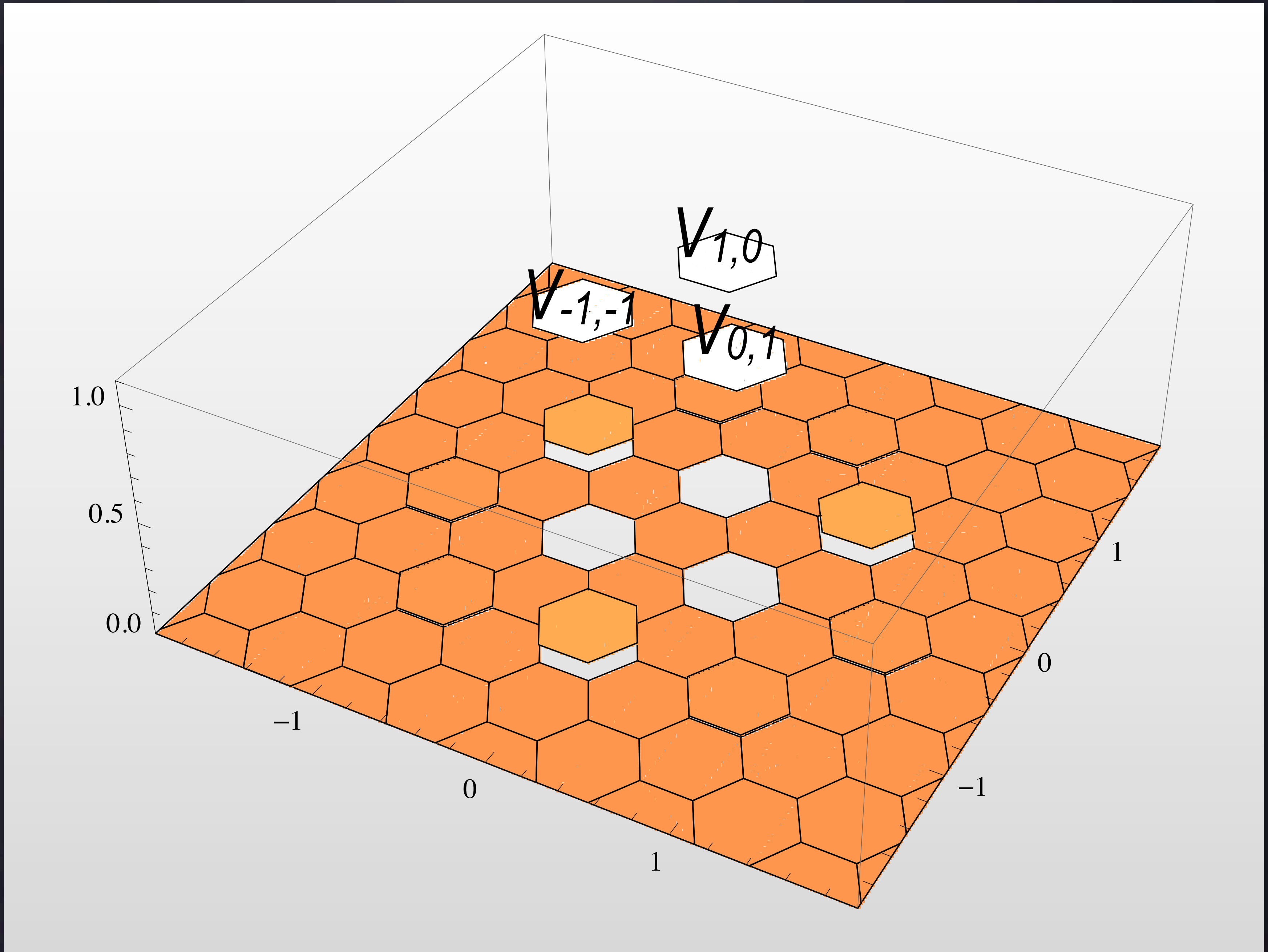
$$V_{nm} \equiv \langle k + nG_1 + mG_2 | V | k \rangle$$



SE-odd

Tight-binding calculation

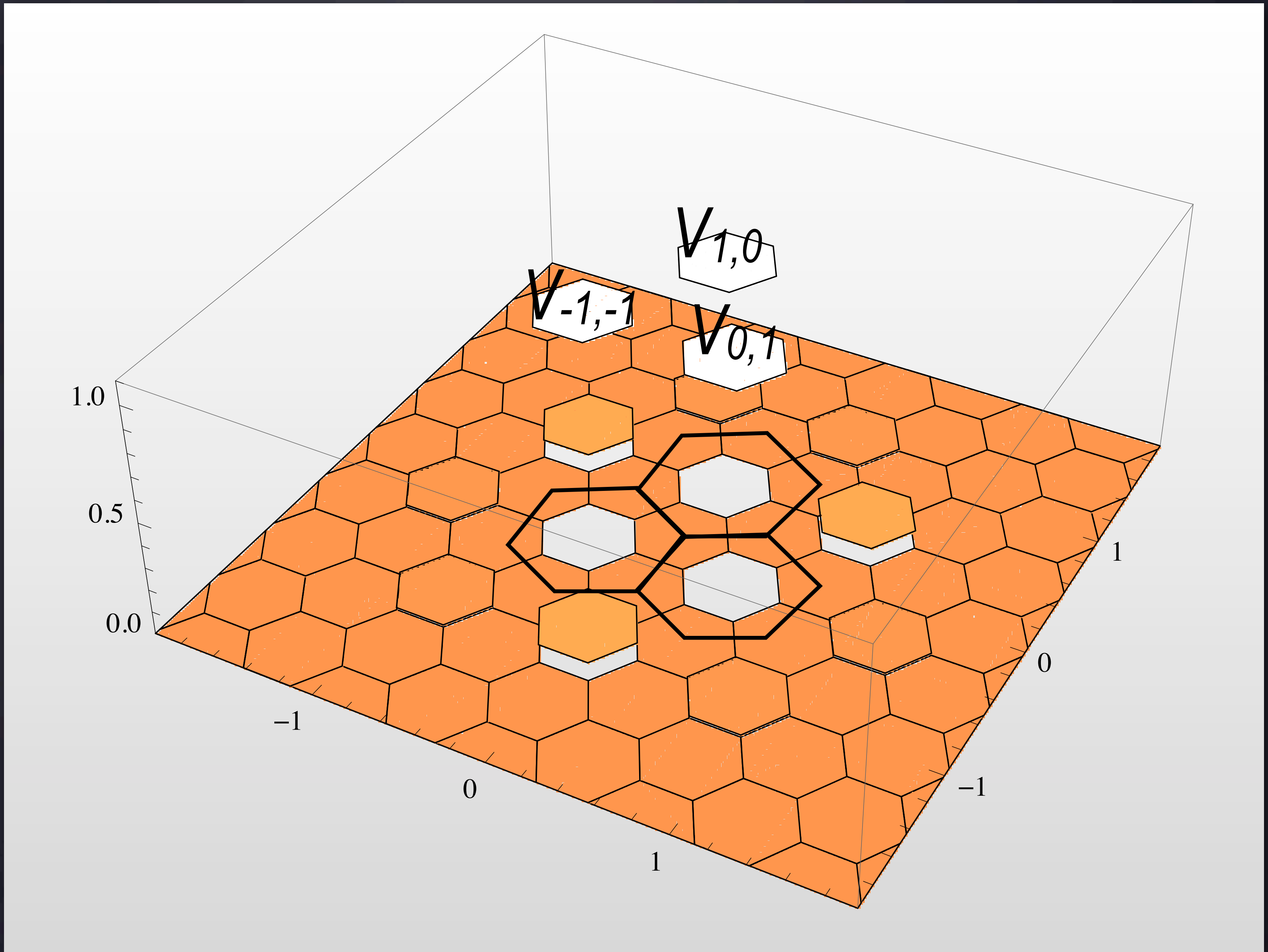
$$V_{nm} \equiv \langle k + nG_1 + mG_2 | V | k \rangle$$



SE-even

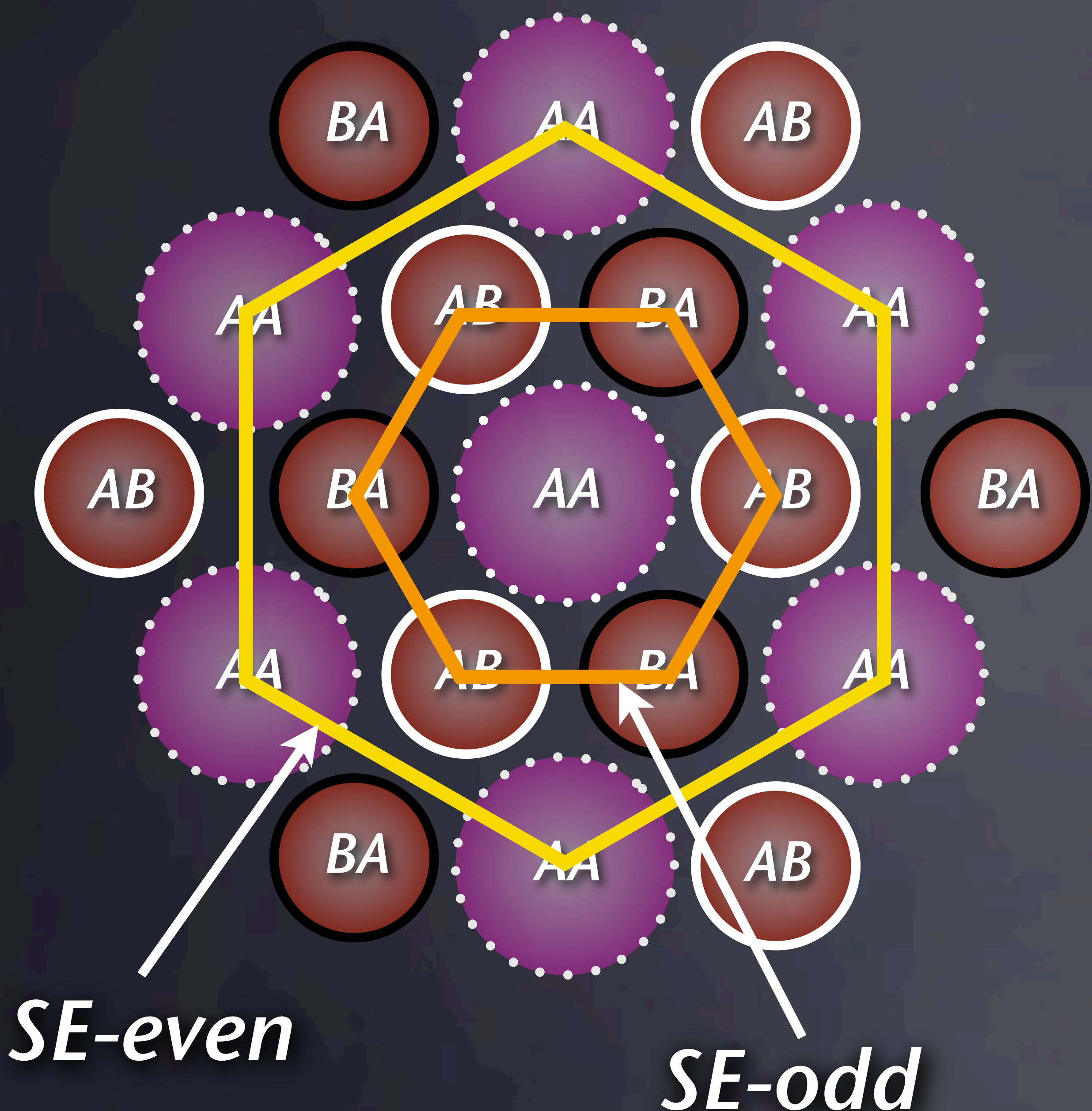
Tight-binding calculation

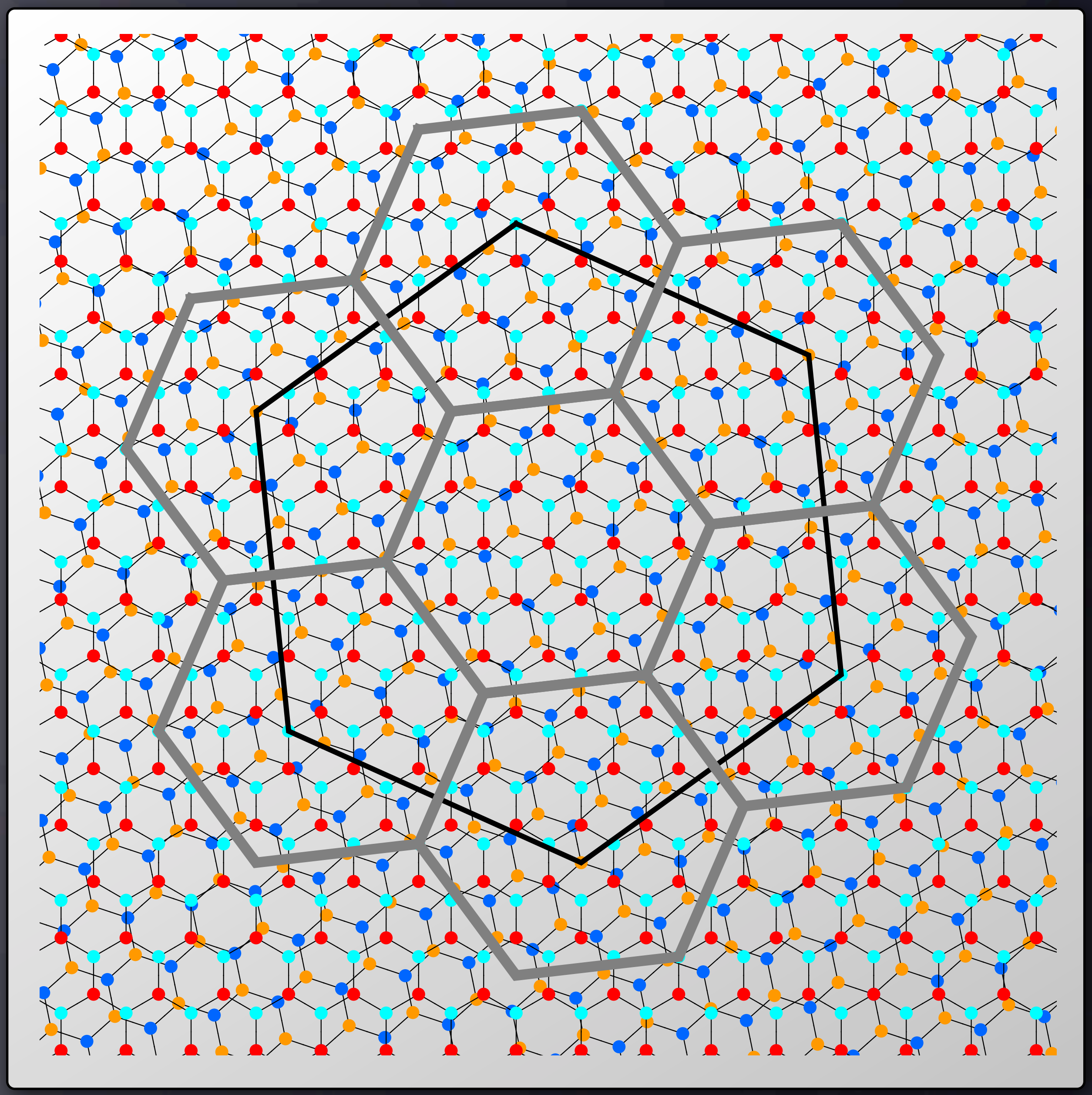
$$V_{nm} \equiv \langle k + nG_1 + mG_2|V|k\rangle$$



SE-even

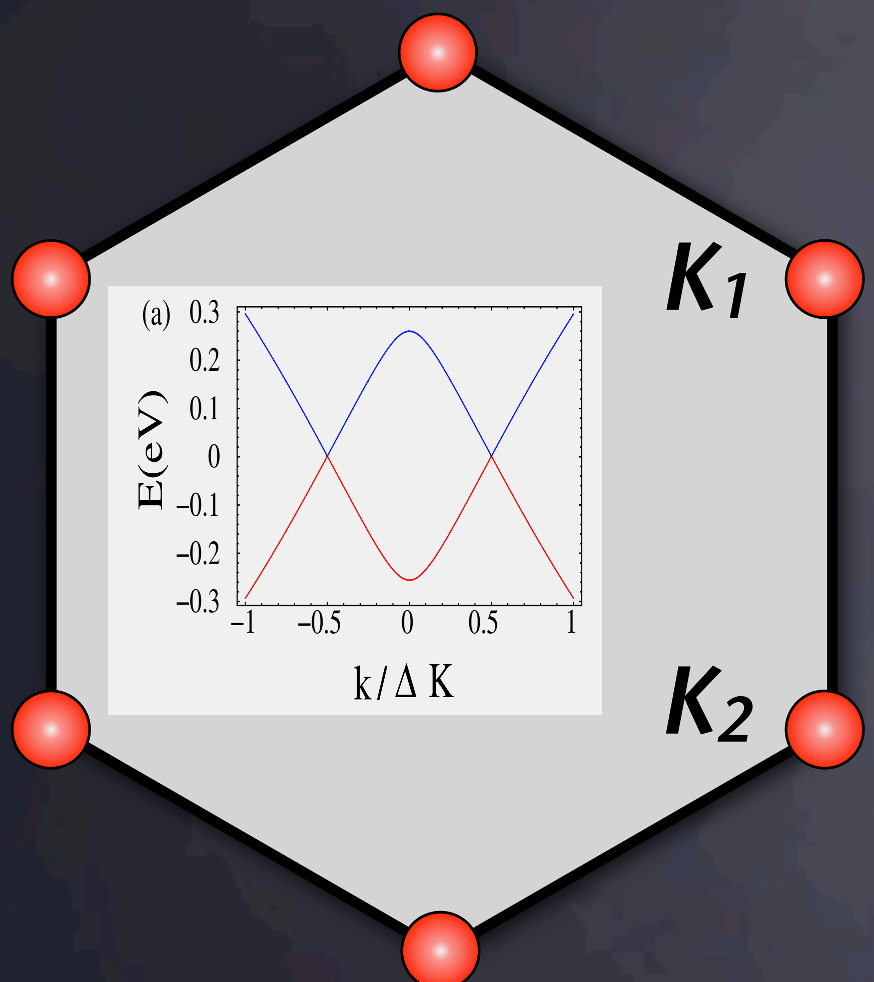
Crystallography versus Moiré





Universality of the continuum limit

- *Both SE-even and SE-odd have the same low angle physics*

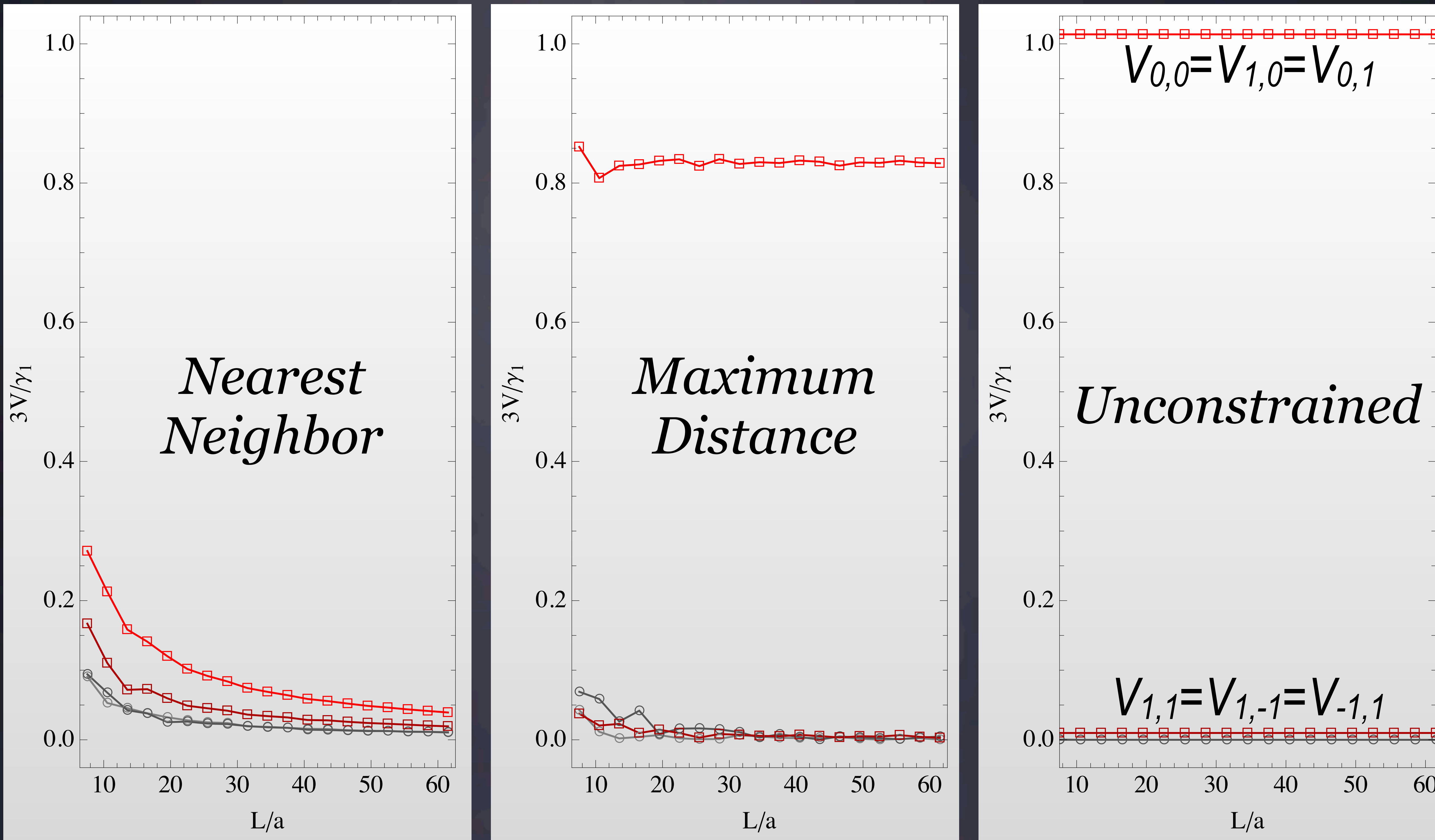


$$H = v_F \begin{pmatrix} 0 & \Pi_+^\dagger & V_{AA}(\mathbf{r}) & V_{AB}(\mathbf{r}) \\ \Pi_+ & 0 & V_{BA}(\mathbf{r}) & V_{AA}(\mathbf{r}) \\ V_{AA}^\star(\mathbf{r}) & V_{BA}^\star(\mathbf{r}) & 0 & \Pi_-^\dagger \\ V_{AB}^\star(\mathbf{r}) & V_{AA}^\star(\mathbf{r}) & \Pi_- & 0 \end{pmatrix}$$

Valley-decoupled

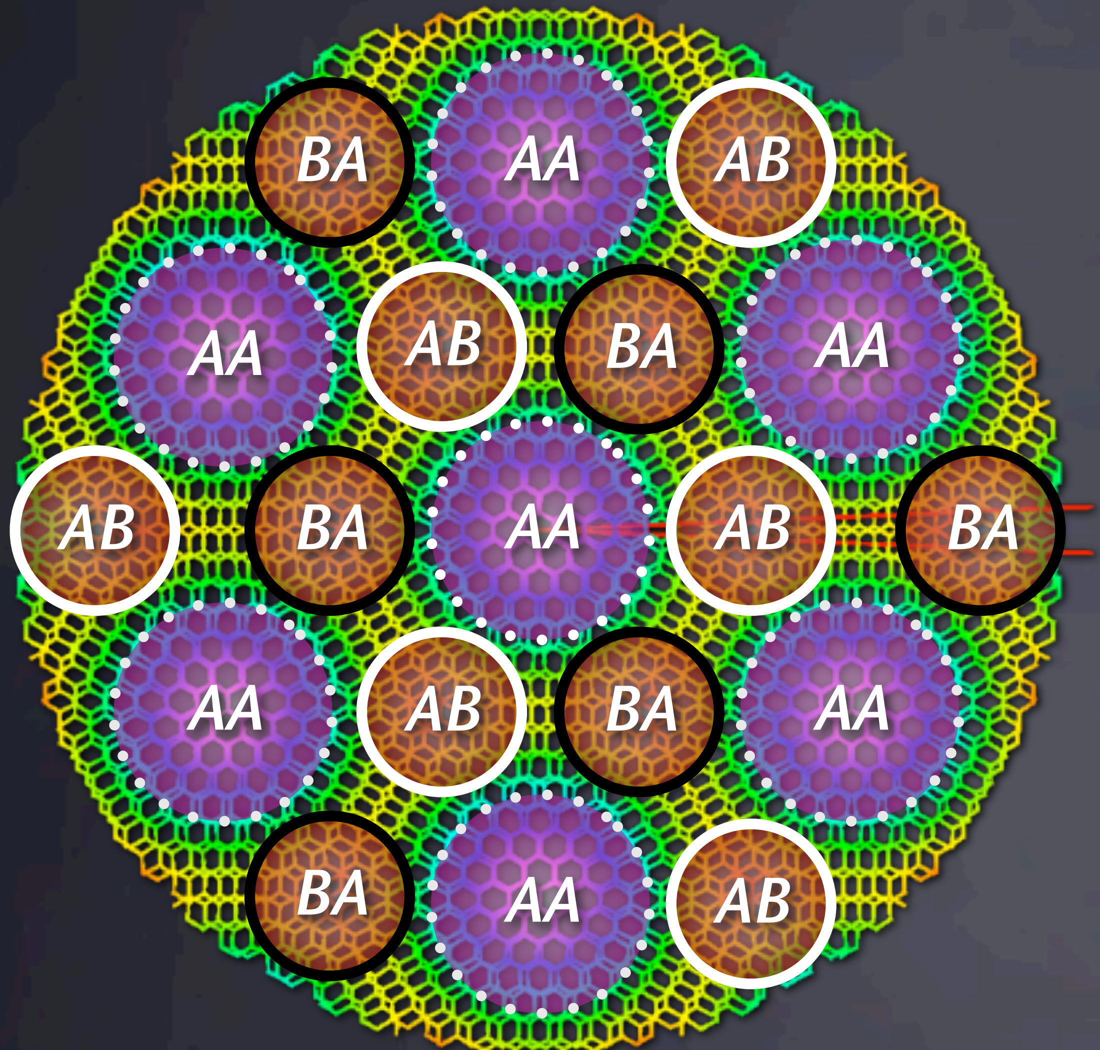
J. M. B. Lopes dos Santos, N. M. R. Peres and A. H. Castro Neto. arXiv:1202.1088

Mele in tight-binding models



Electronic structure

Twisted bilayer at low energy



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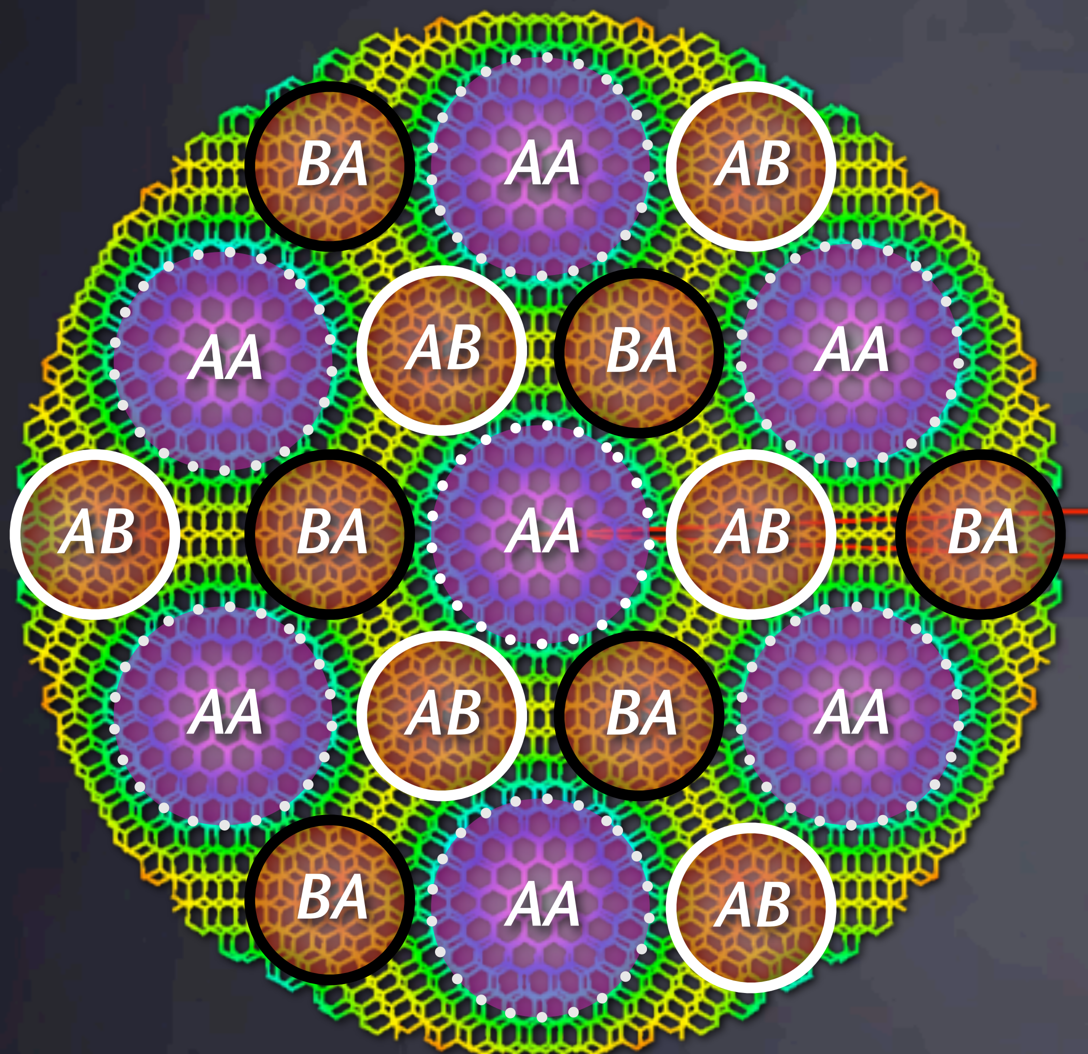
$$\Pi_\pm = -i\partial_x + \partial_y \mp i\frac{\Delta K}{2} \quad ; \quad \Delta K = 2K \sin\frac{\theta}{2}$$

Twisted bilayer at low energy



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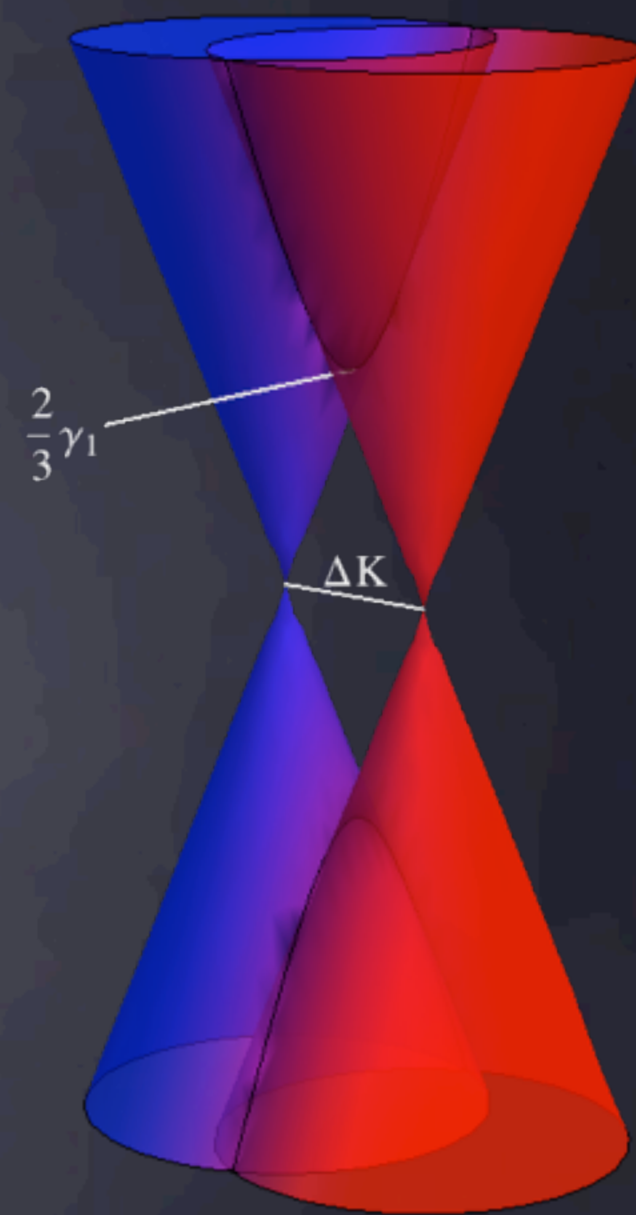
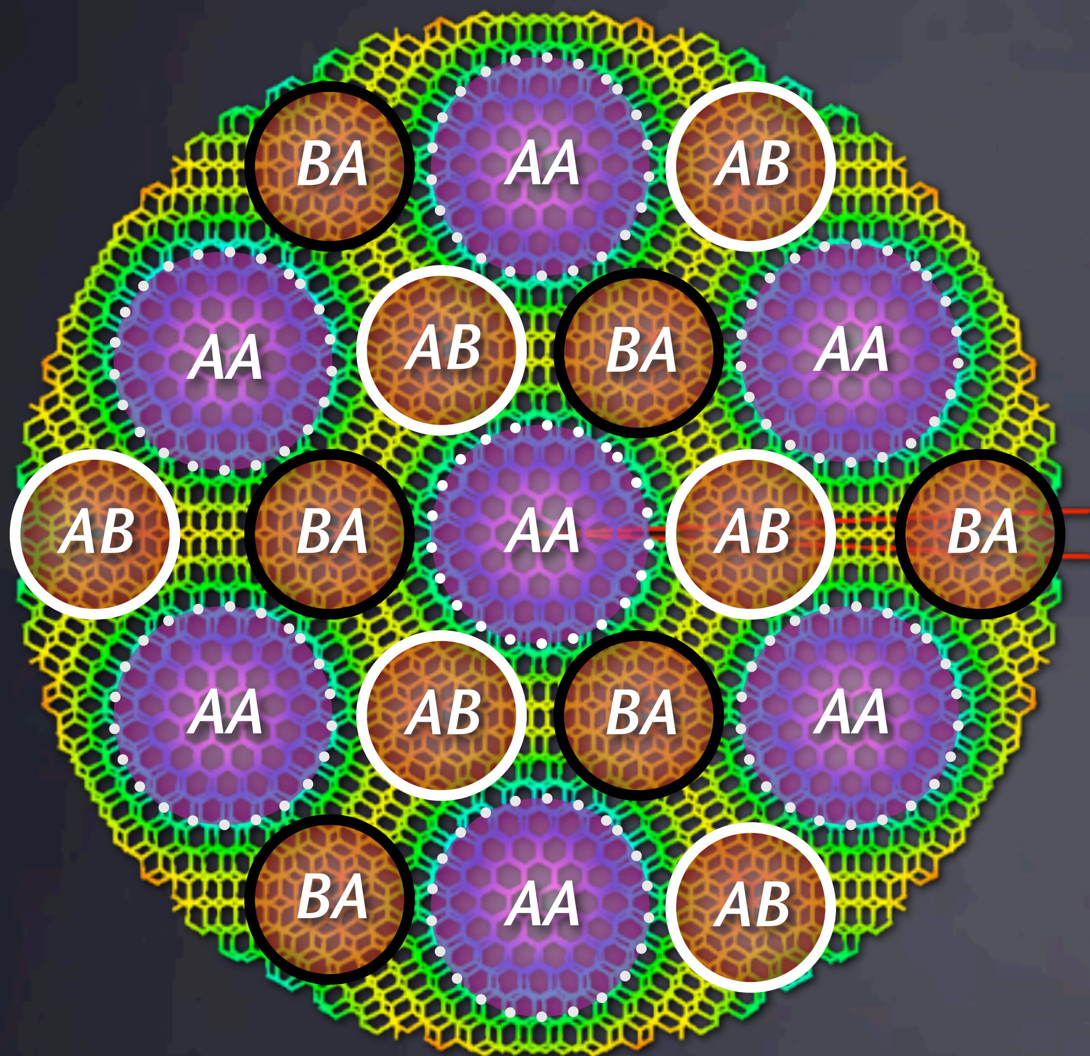


Low energy saddle point

Twisted bilayer at low energy



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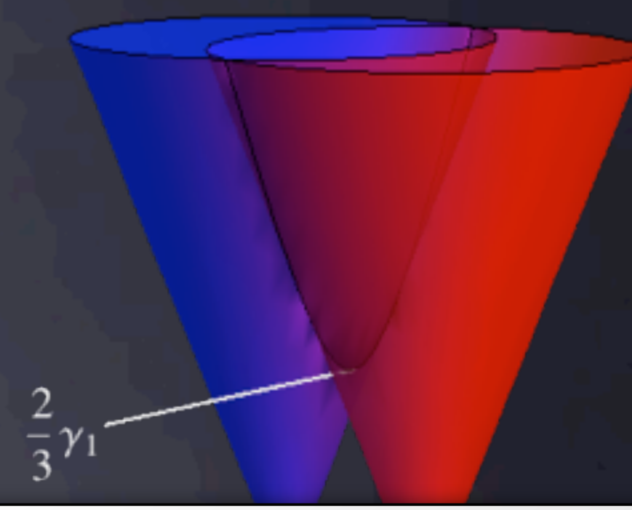
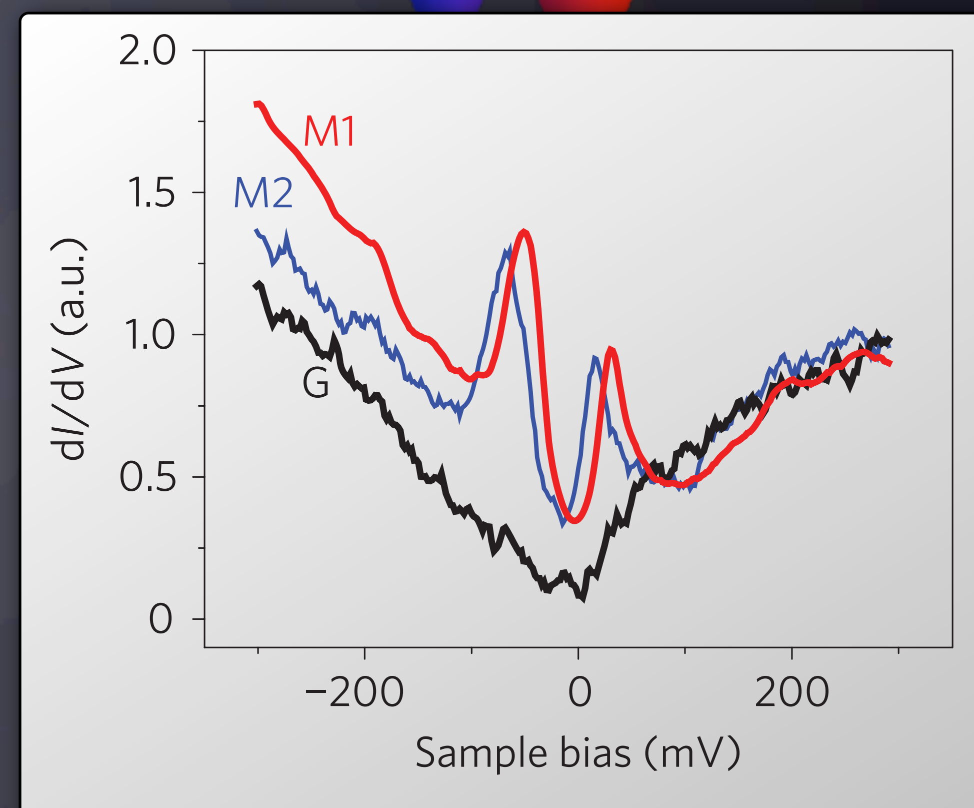
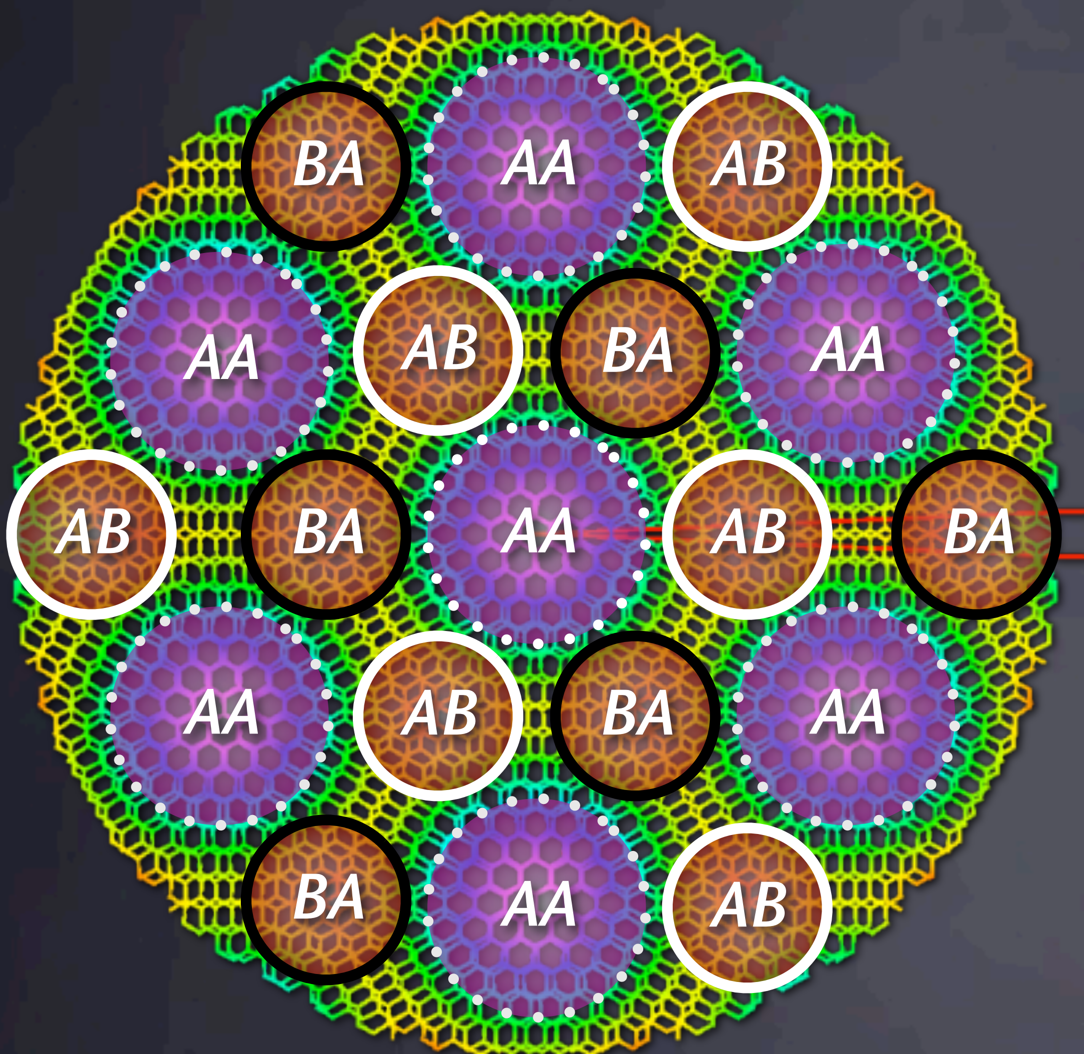




Low energy saddle point

G. Li, A. Luican, et al. Nat Phys, 6(2):109, 2010.

Twisted bilayer at low energy



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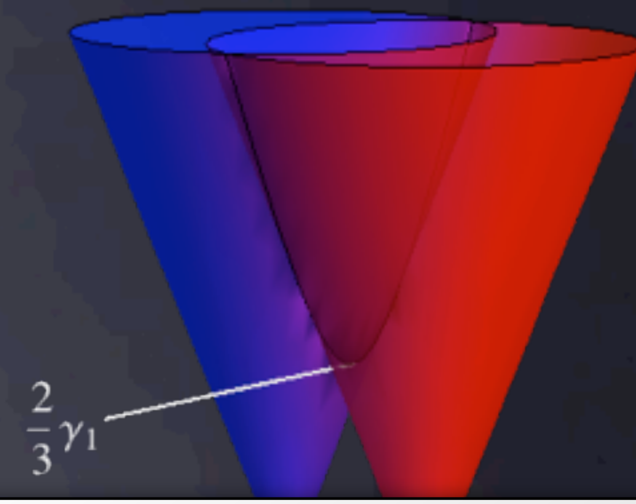
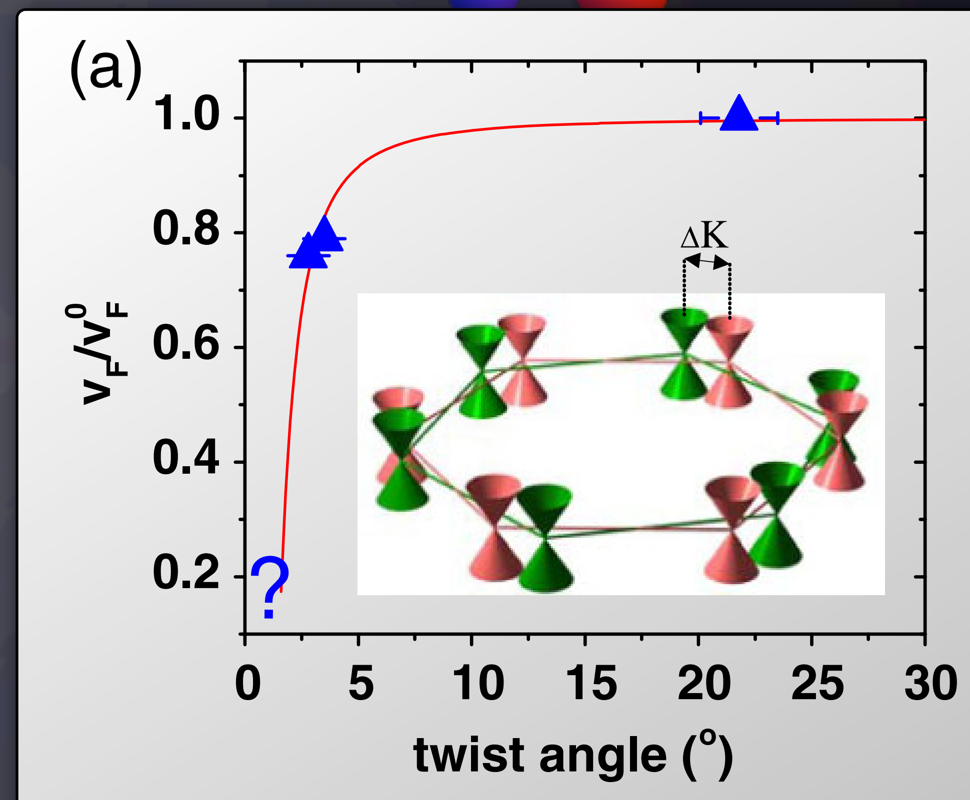
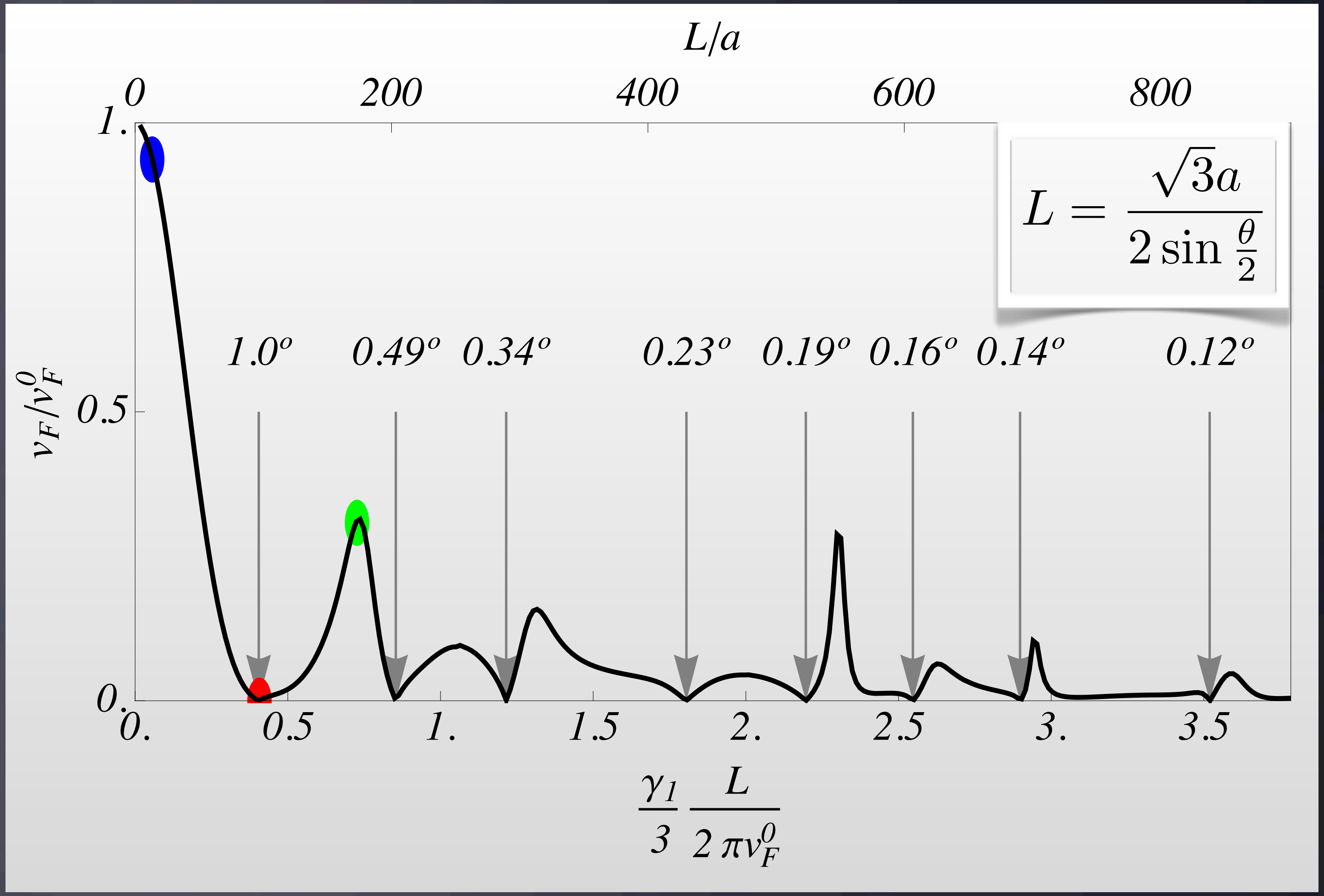




Fermi velocity suppression

J. M. B. Lopes dos Santos et al. Phys. Rev. Lett., 99, 256802 (2007)
A. Luican et al. Phys. Rev. Lett., 106, 126802, (2011)

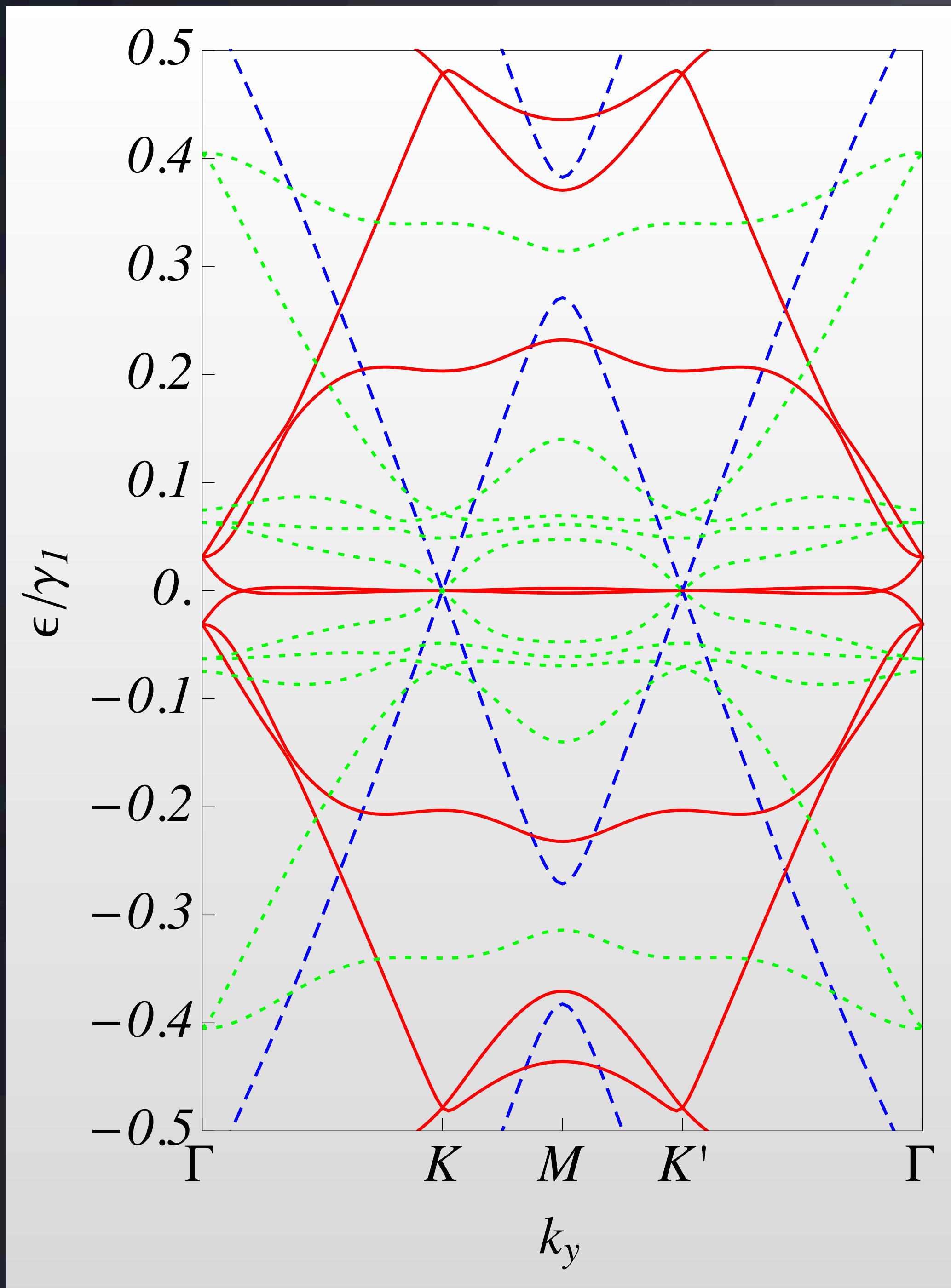
Recurrent zero energy modes

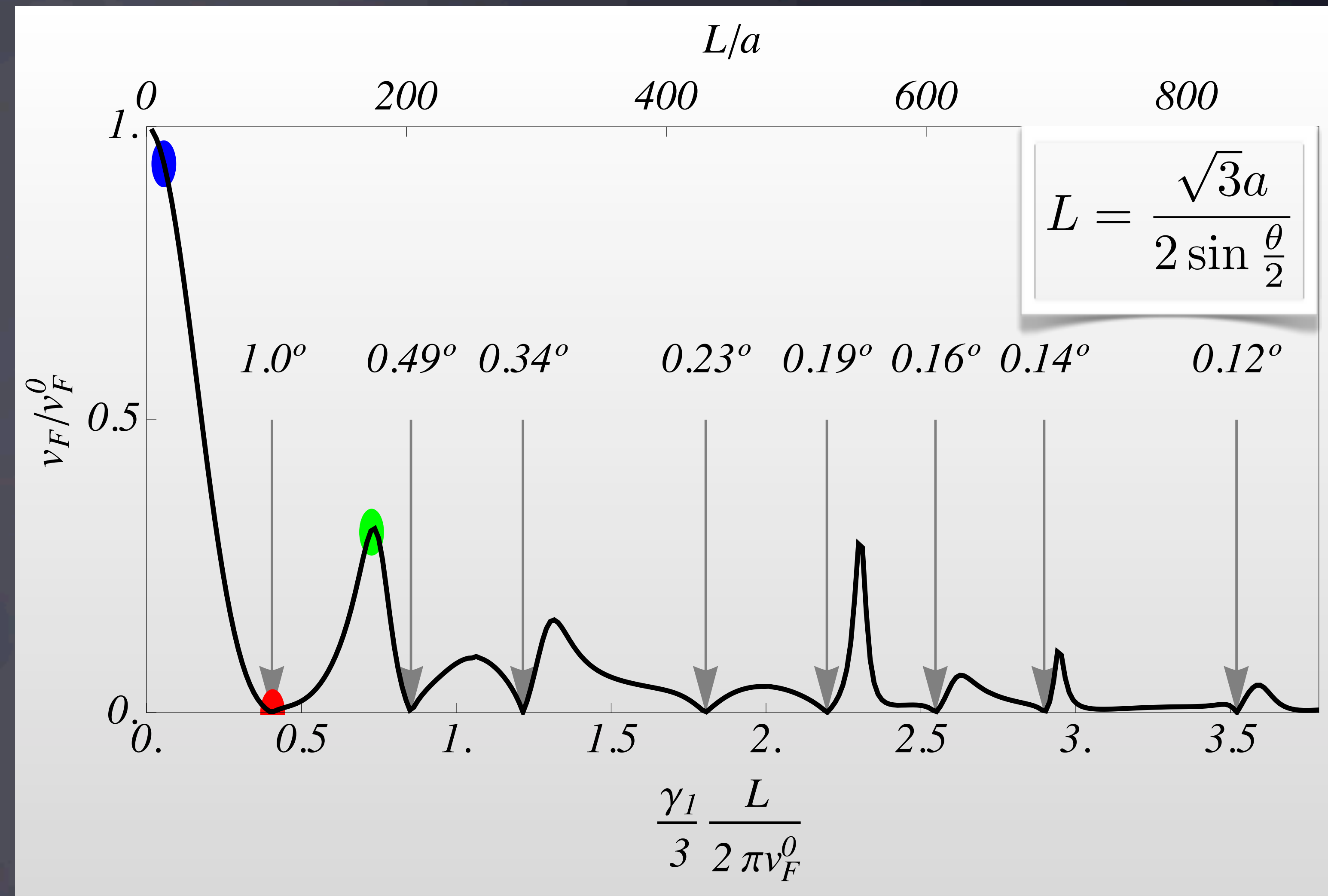


- *Magical angles θ_c^n with vanishing velocity at irregular intervals*

R. Bistritzer and A. MacDonald. PNAS 108, 12233 (2011)

Recurrent zero energy modes

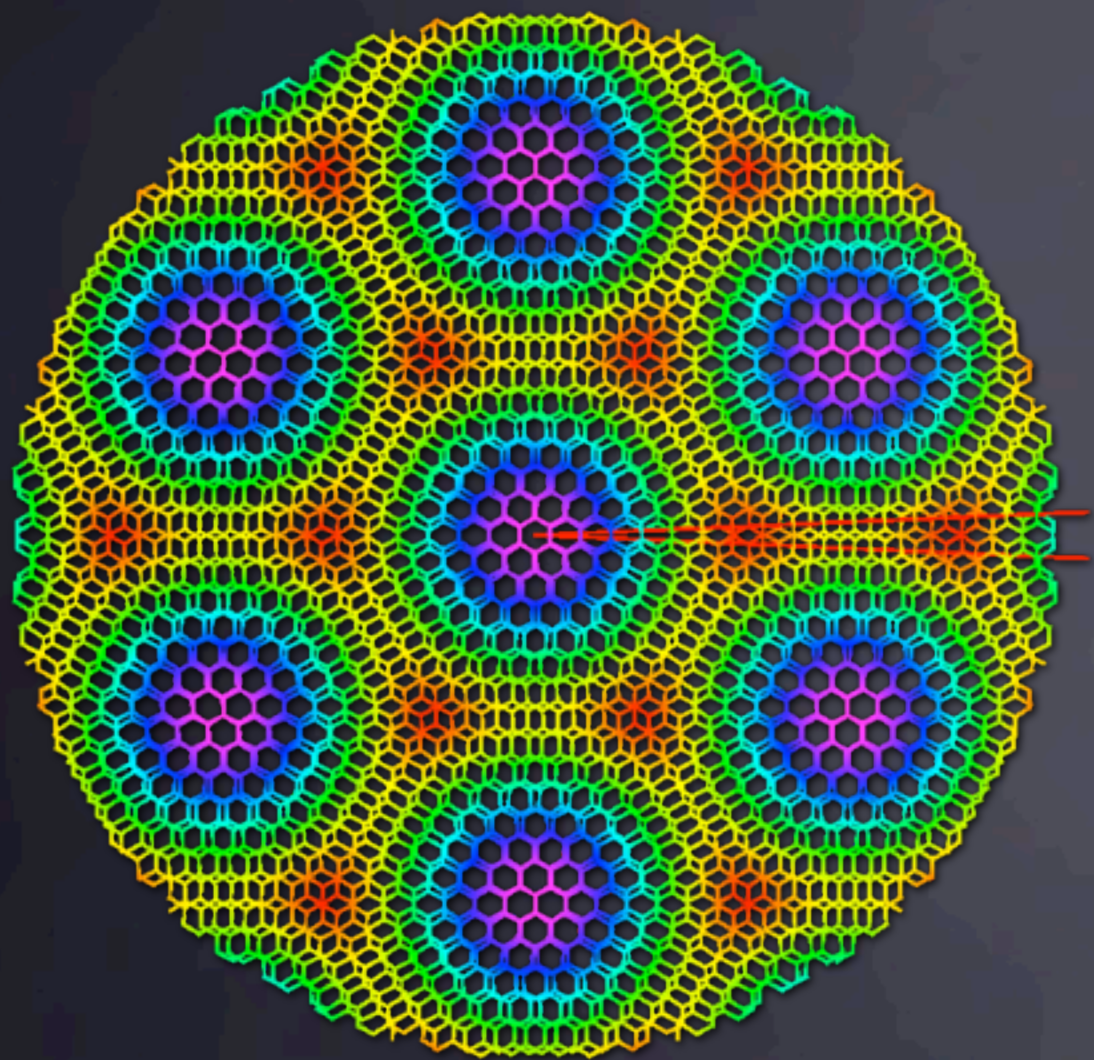


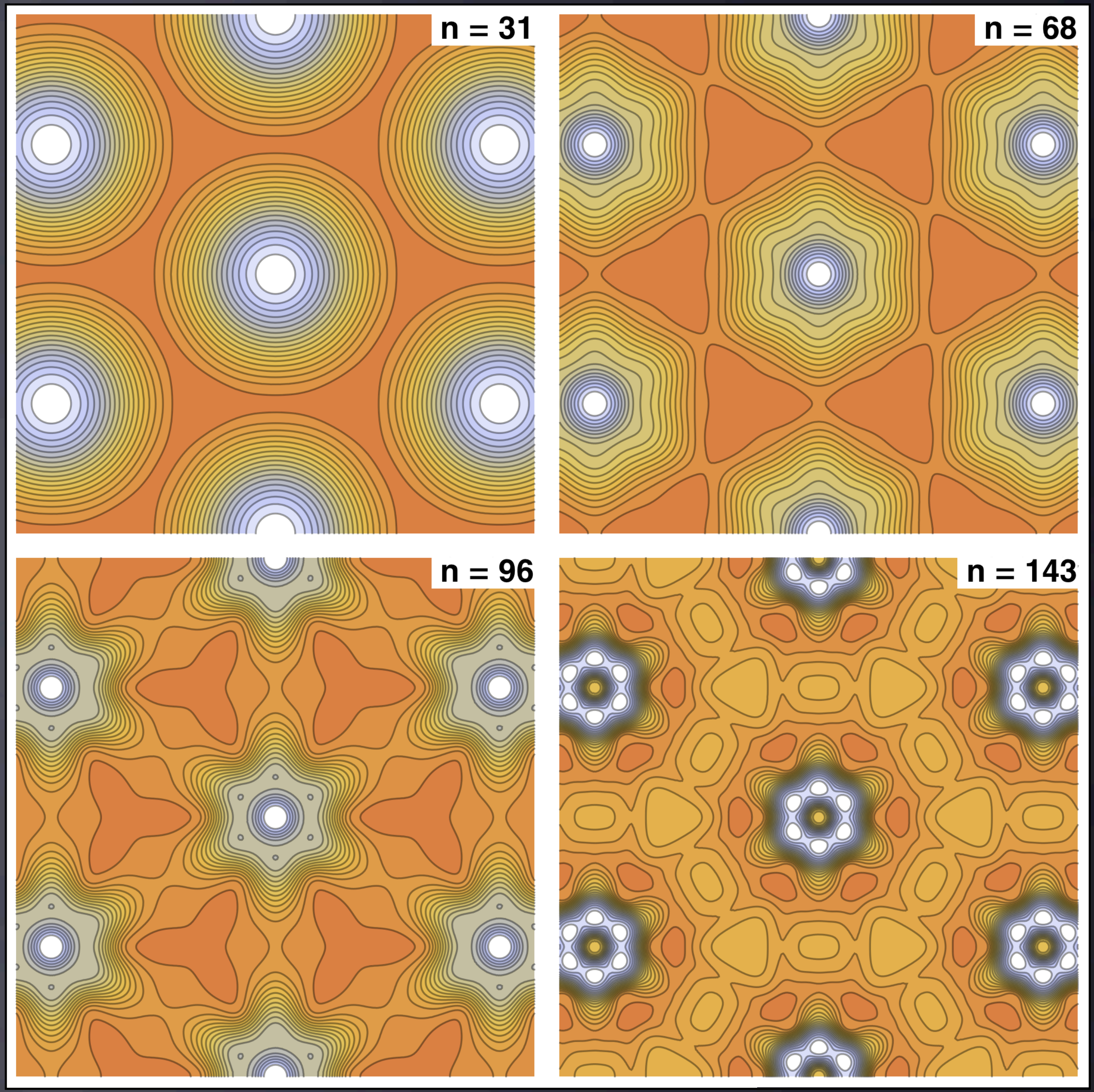


- *Magical angles θ_c^n with vanishing velocity at irregular intervals*
- *Almost flat band at $\theta=\theta_c^n$*

R. Bistritzer and A. MacDonald. PNAS 108, 12233 (2011)

Localized zero energy state





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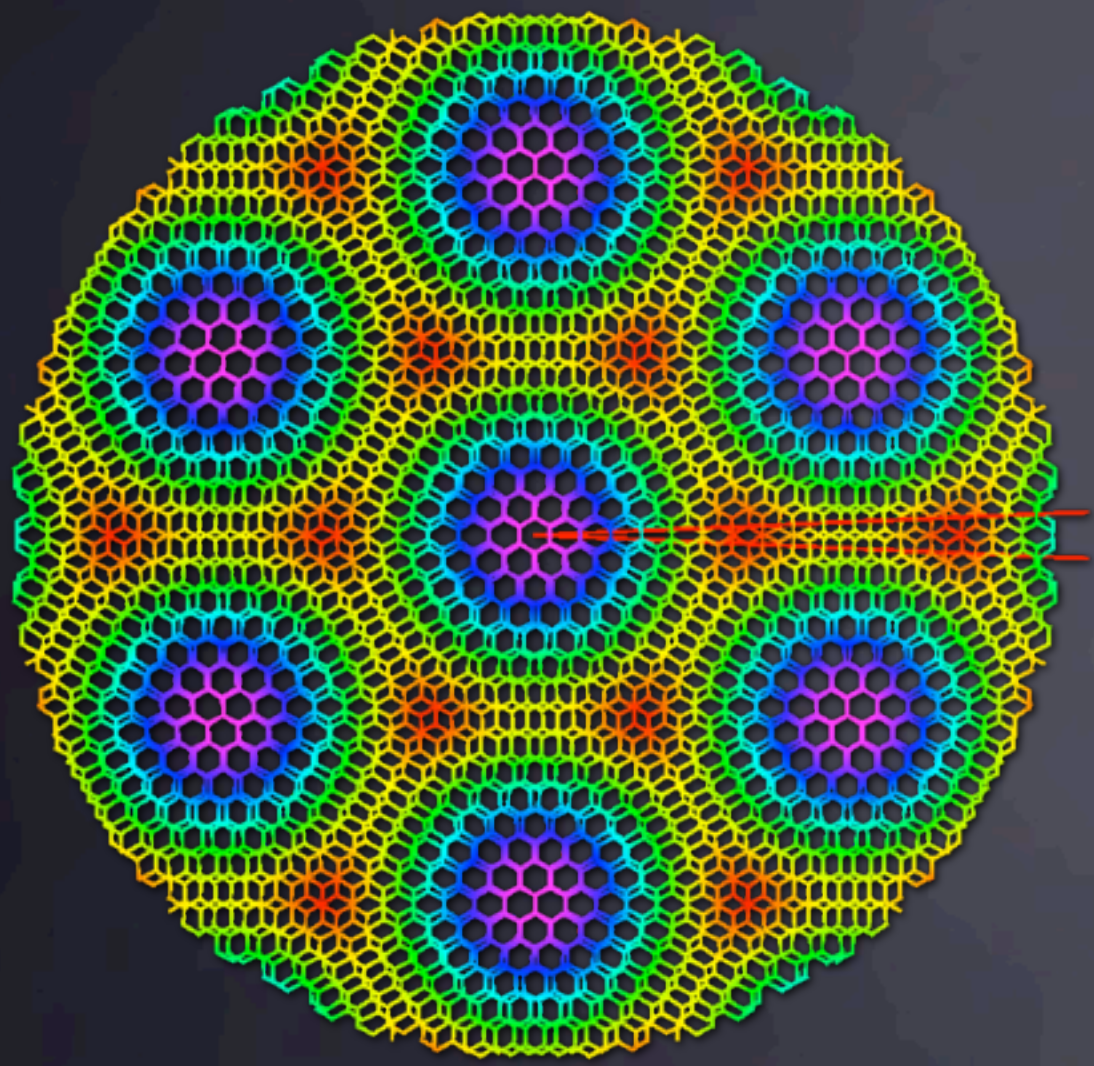

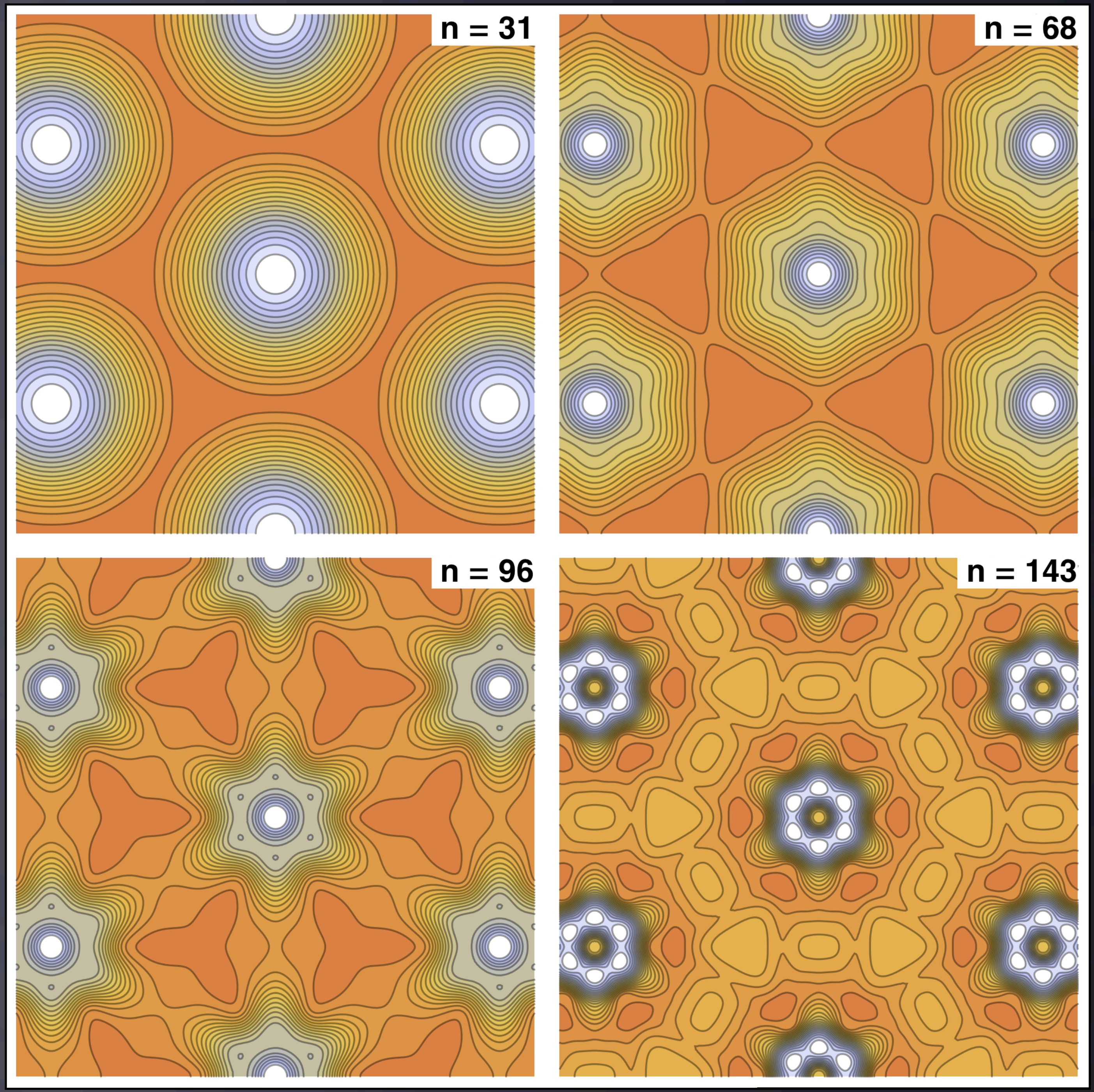

P. San-Jose, J. González and F. Guinea, arxiv:1110.2883

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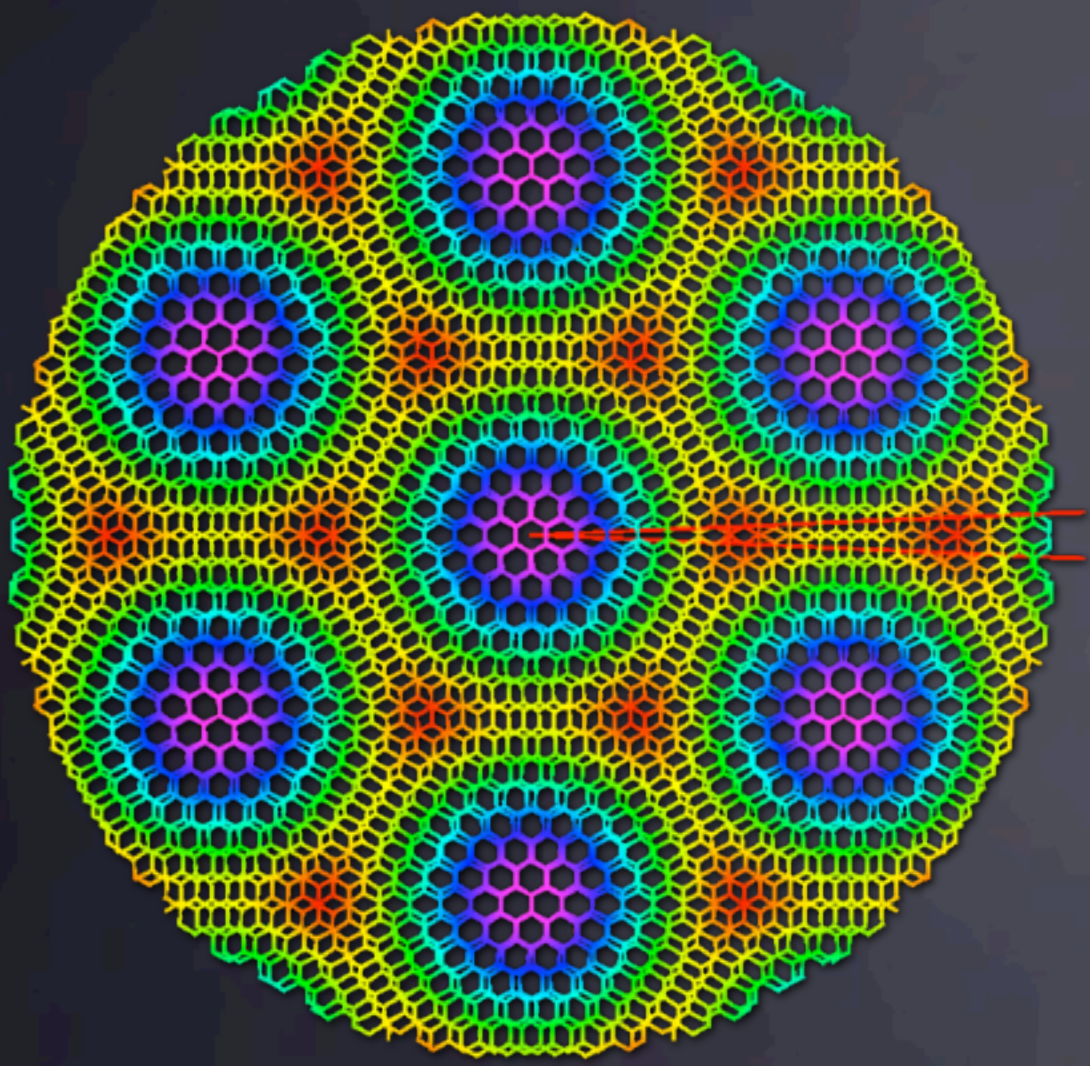

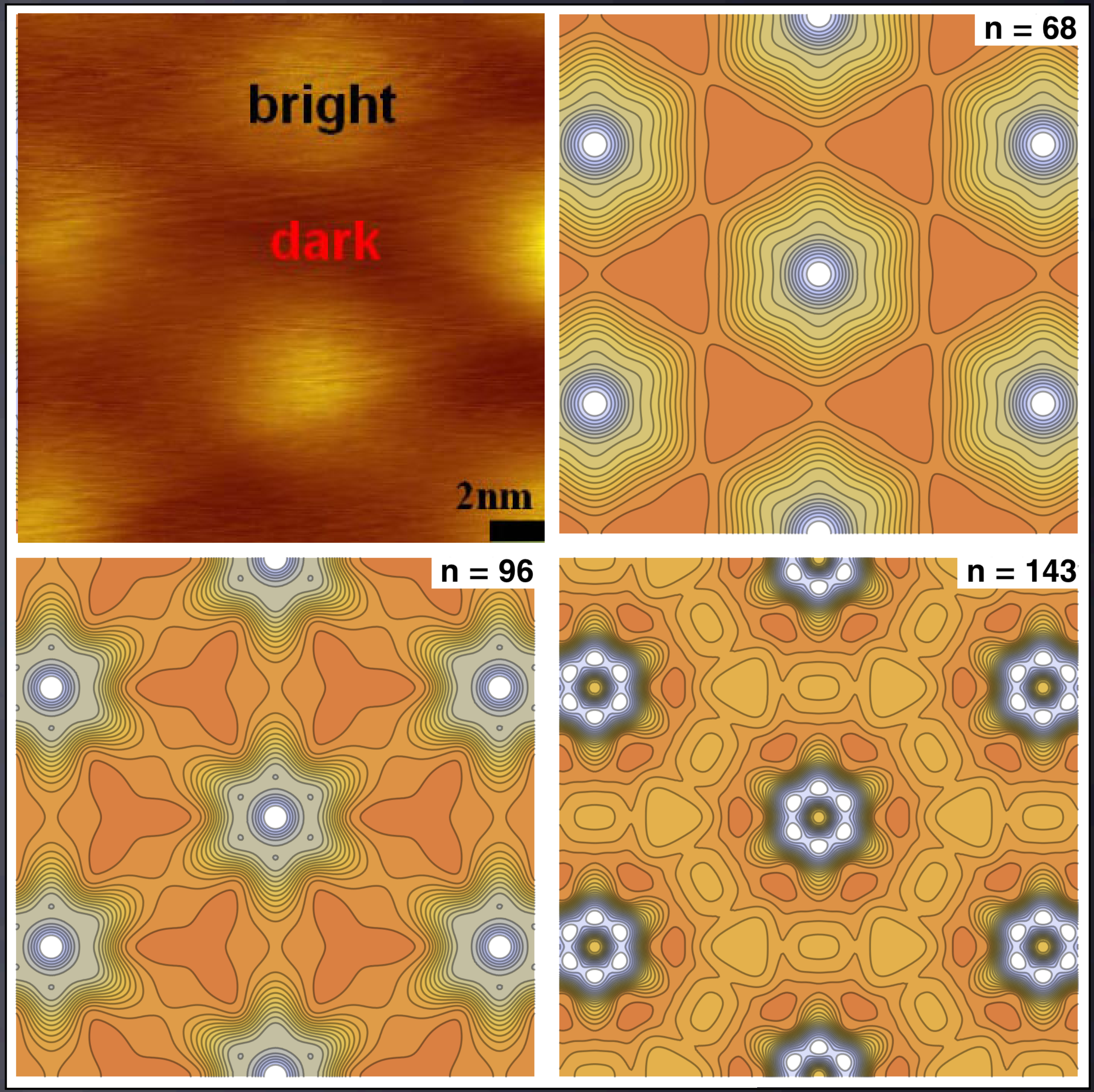

P. San-Jose, J. González and F. Guinea, arxiv:1110.2883
A. Luican, G. Li, A. Reina, J. Kong, R. R. Nair, K. S. Novoselov, A. K. Geim, and E. Y. Andrei. Phys. Rev. Lett., 106 (2011).

Non-Abelian fields

- *Why do zero-energy states arise?*

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$$H = v_F \begin{pmatrix} 0 & \Pi^\dagger & \tilde{V}_{AA}(\mathbf{r}) & \tilde{V}_{AB}(\mathbf{r}) \\ \Pi & 0 & \tilde{V}_{BA}(\mathbf{r}) & \tilde{V}_{AA}(\mathbf{r}) \\ \tilde{V}^\star_{AA}(\mathbf{r}) & \tilde{V}^\star_{BA}(\mathbf{r}) & 0 & \Pi^\dagger \\ \tilde{V}^\star_{AB}(\mathbf{r}) & \tilde{V}^\star_{AA}(\mathbf{r}) & \Pi & 0 \end{pmatrix}$$

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Dirac Hamiltonian

$$H = v_F \vec{\boldsymbol{\sigma}} \cdot \left[\tau_0 \vec{\mathbf{k}} - \hat{\vec{\mathbf{A}}}(\mathbf{r}) \right] + v_F \hat{\Phi}(\mathbf{r})$$

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Non-Abelian gauge field   *Non-Abelian scalar field*

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Non-Abelian gauge field

Non-Abelian scalar field

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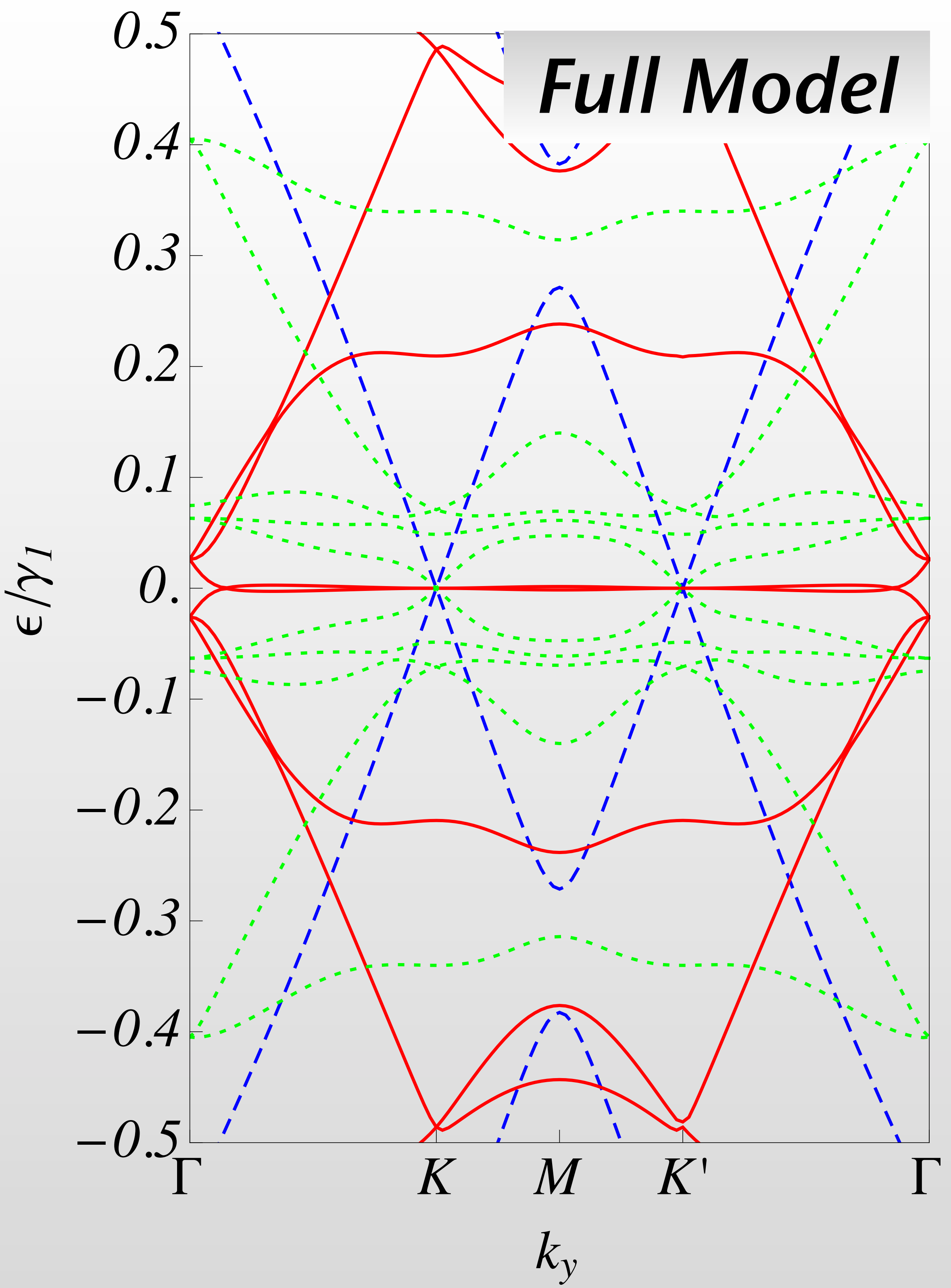
Origin of zero-energy bands



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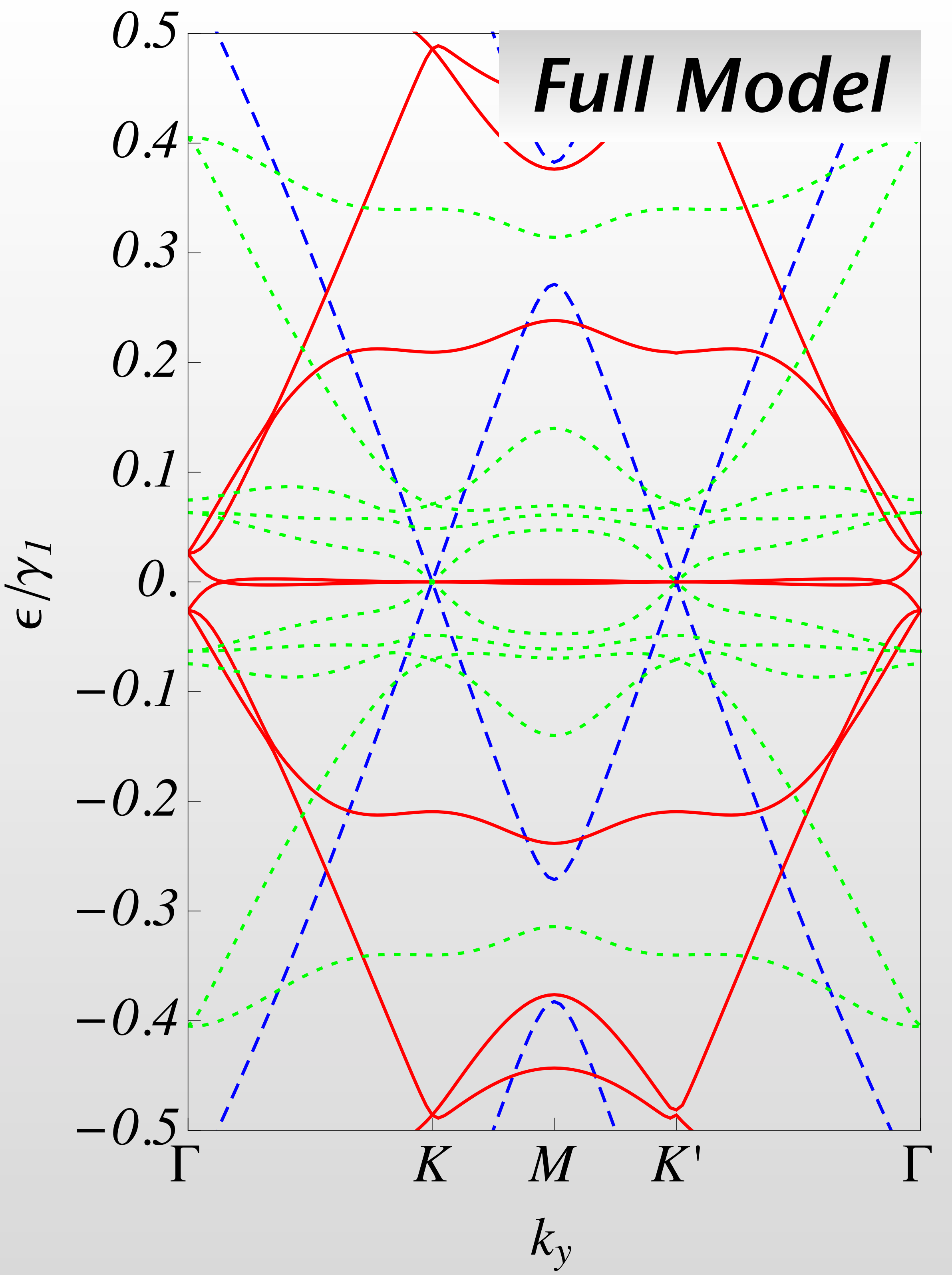

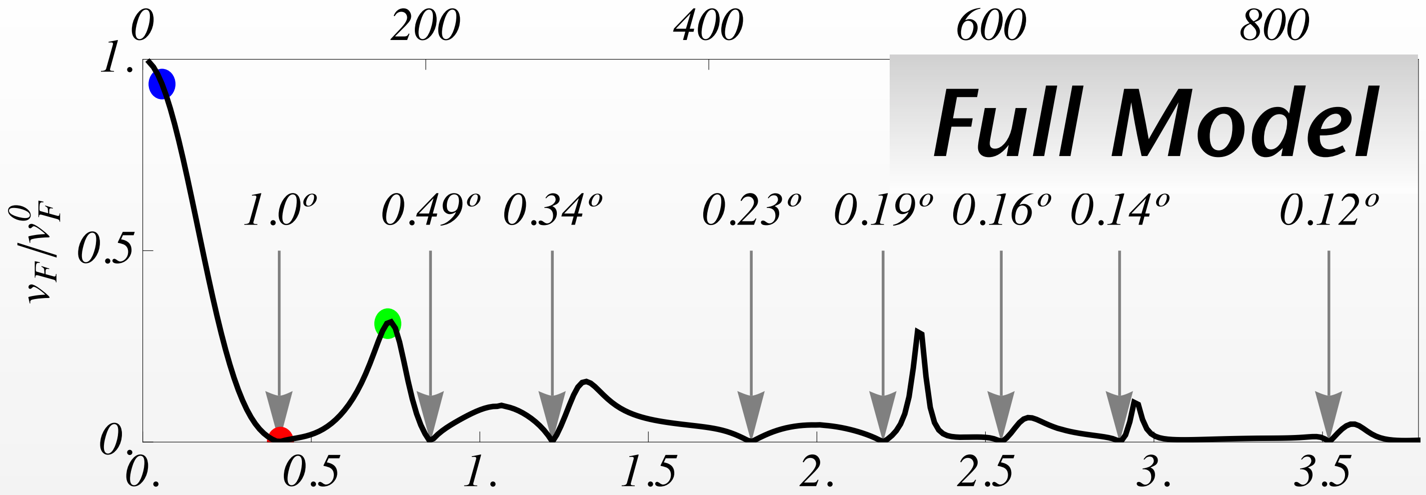

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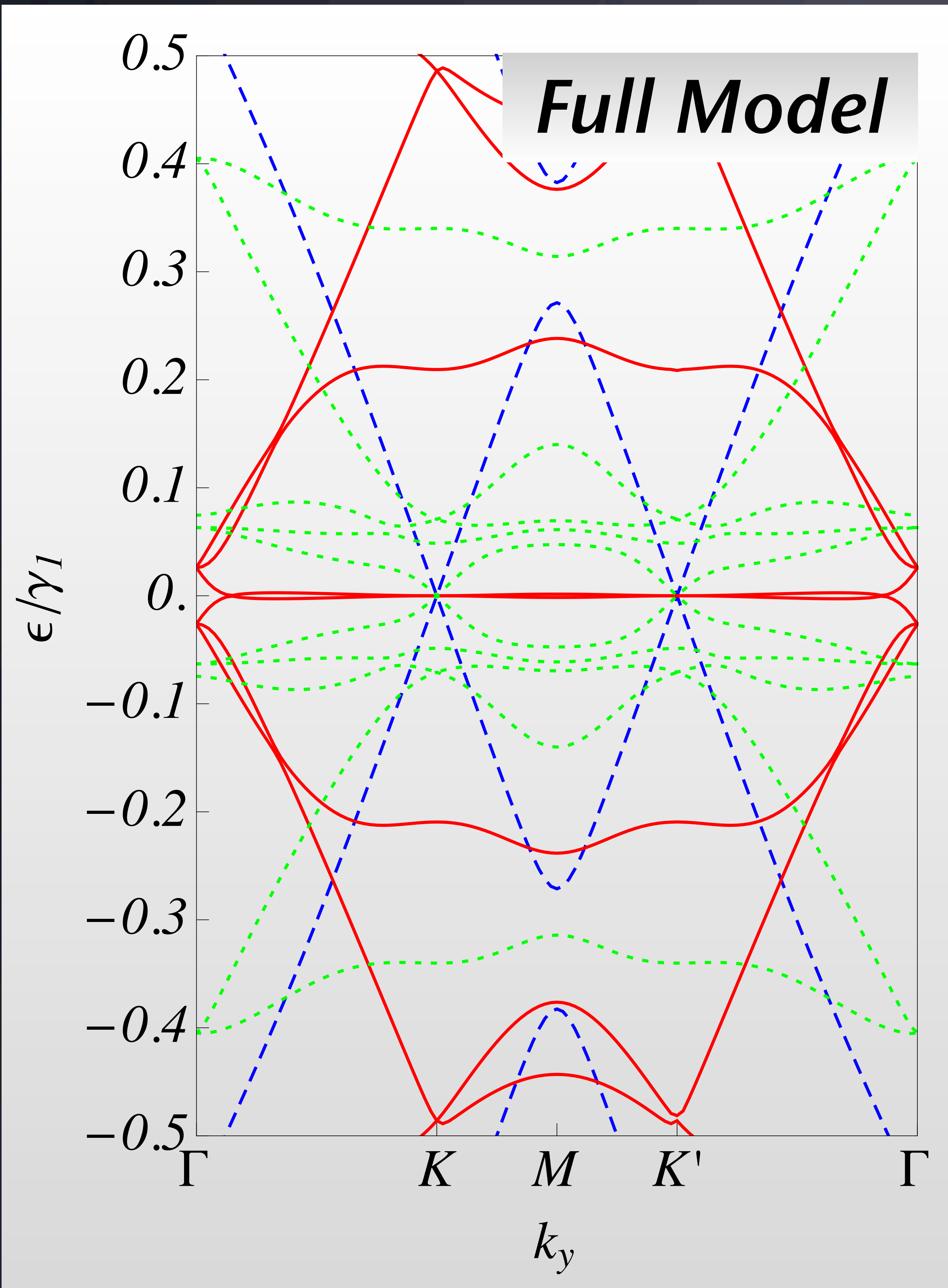

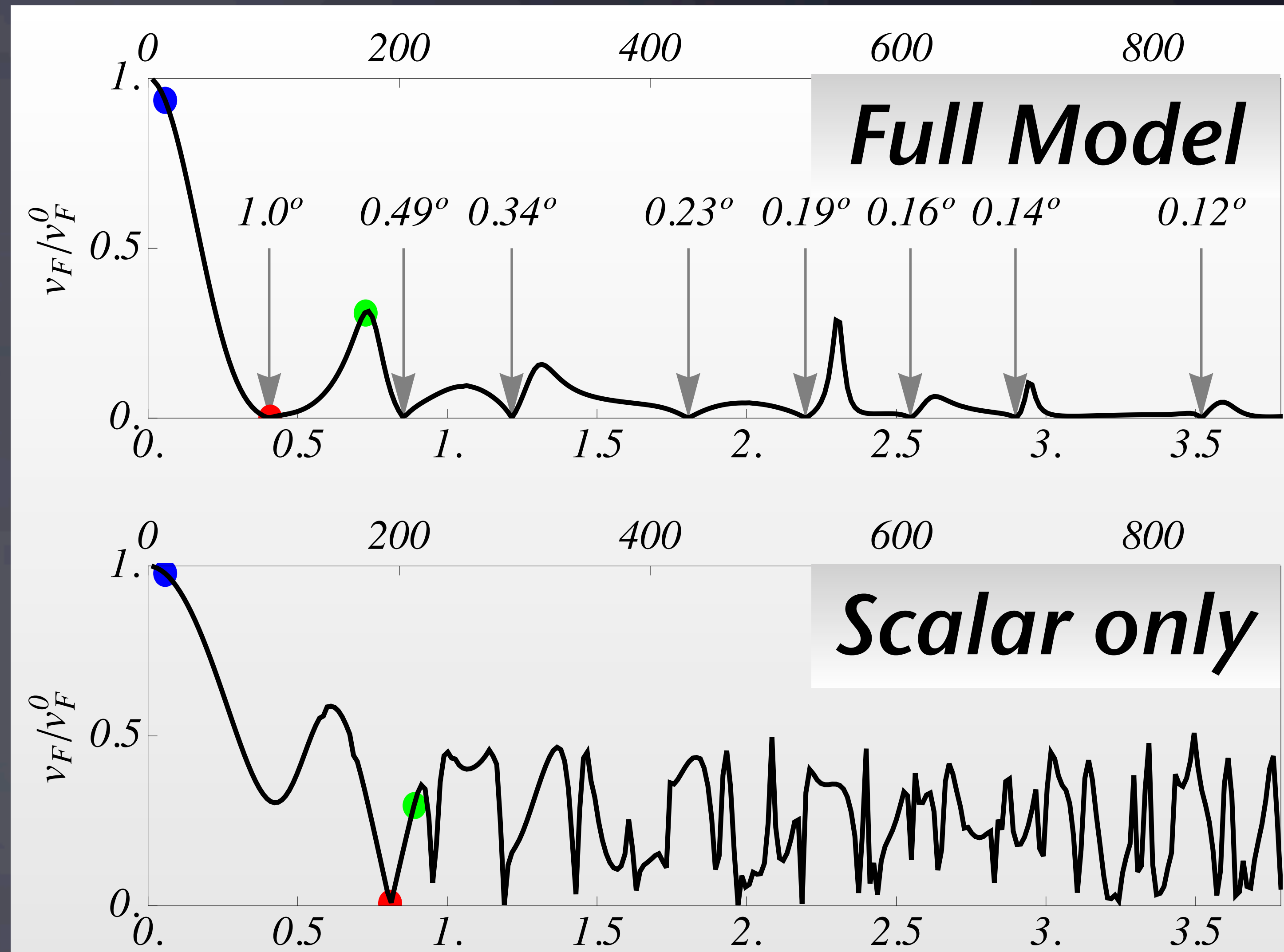

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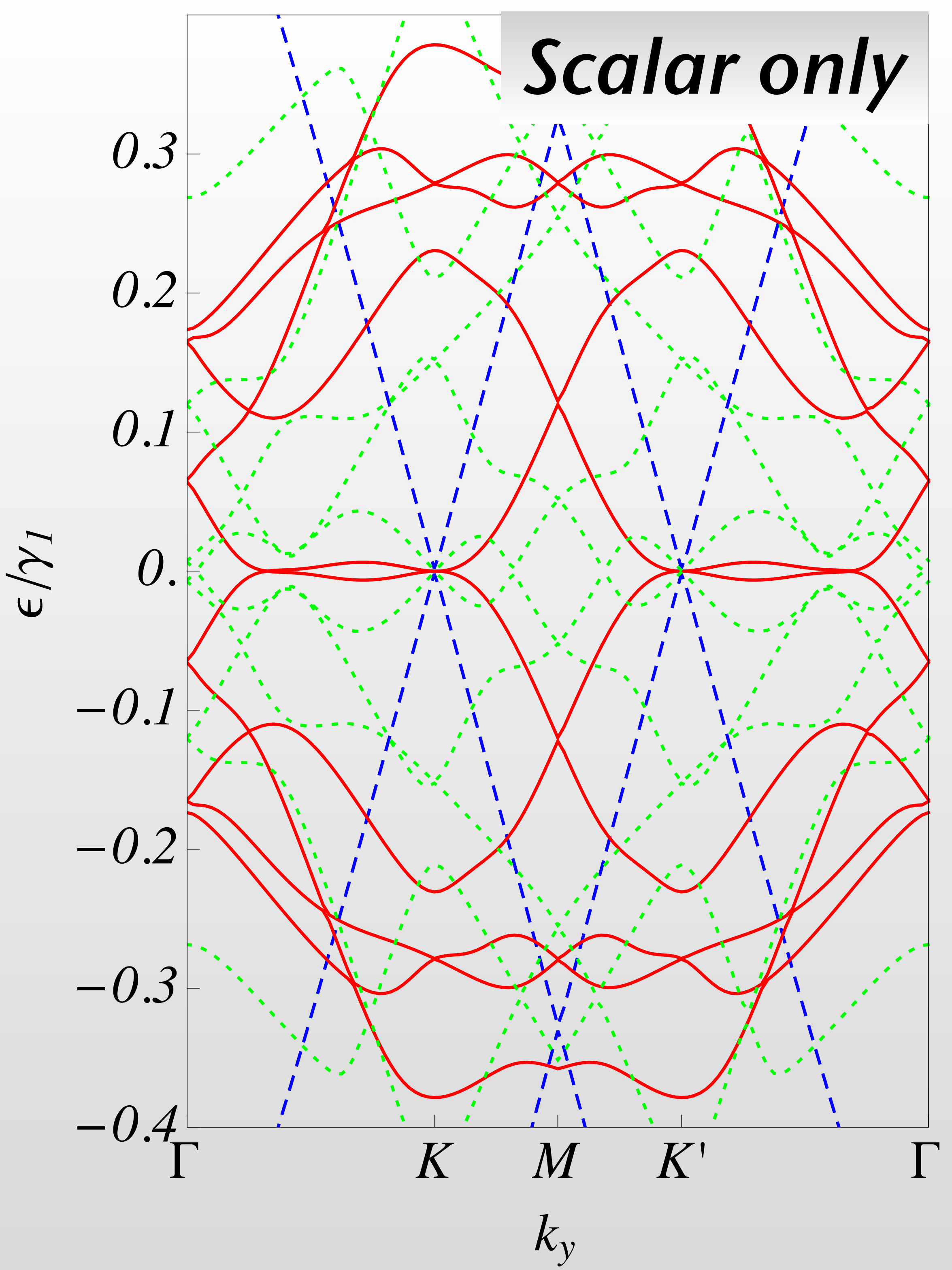

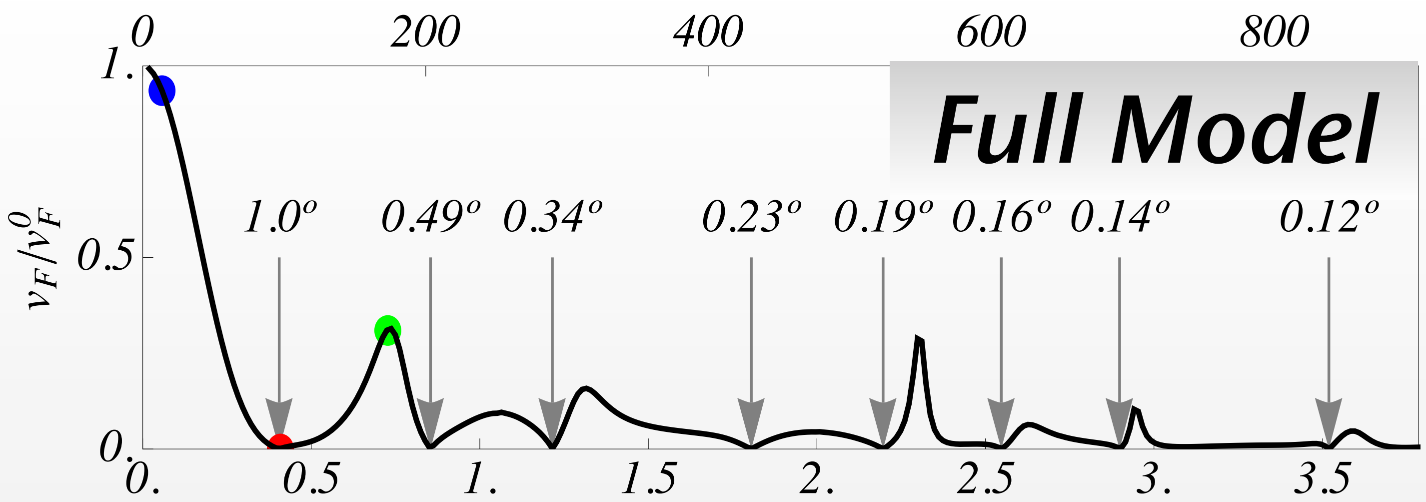

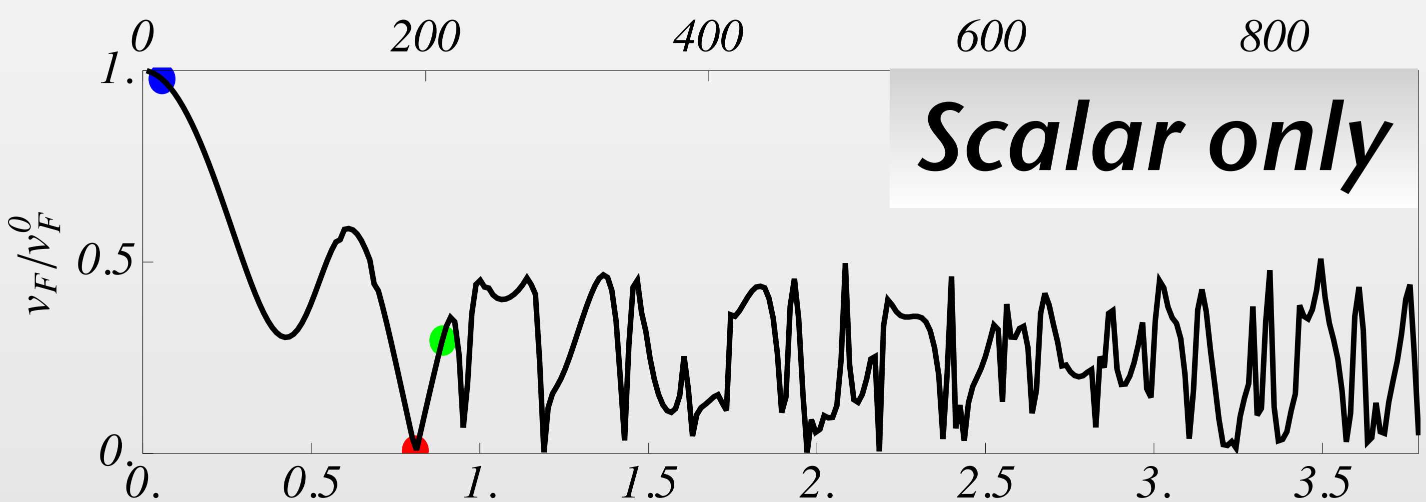

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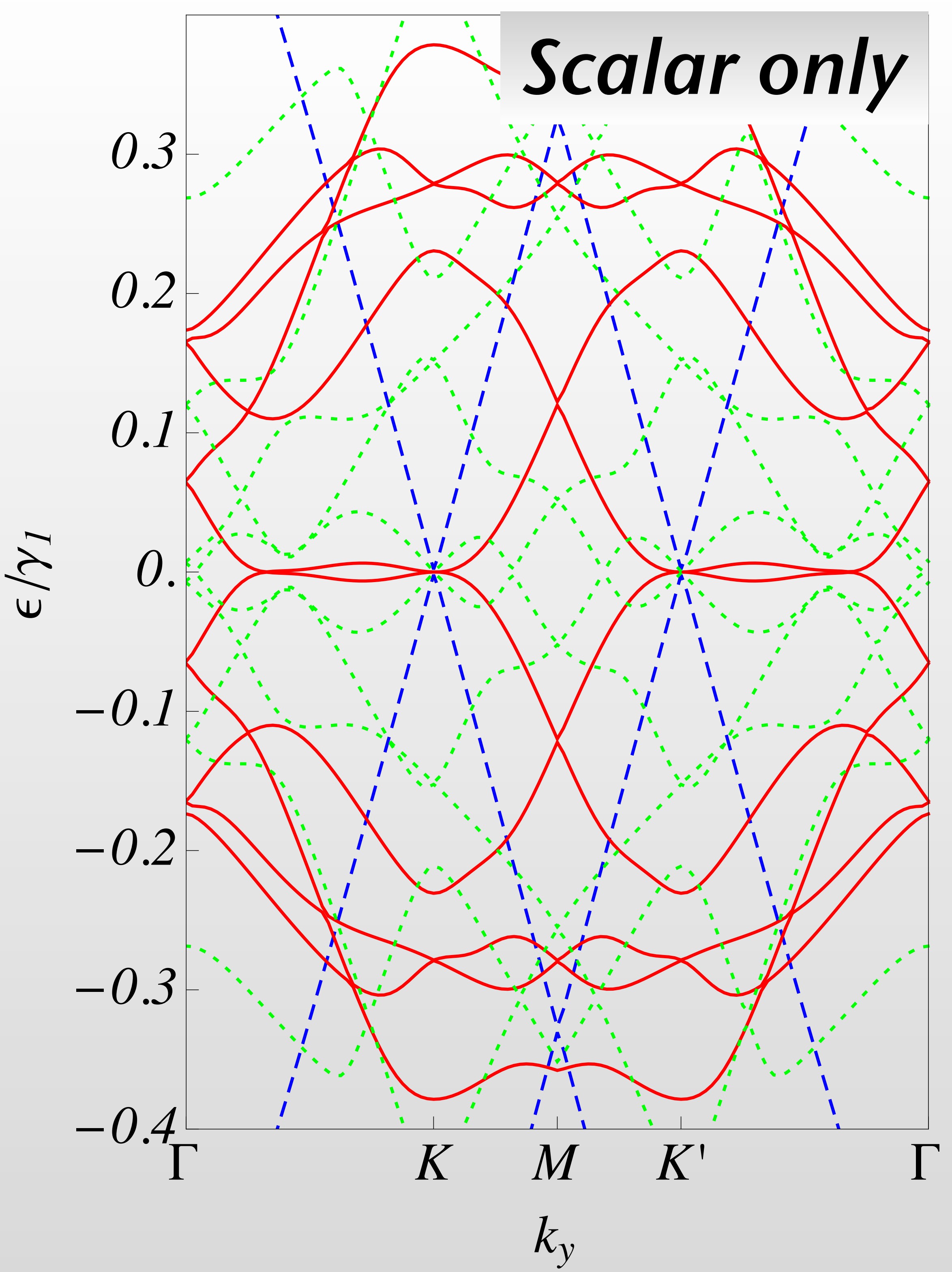

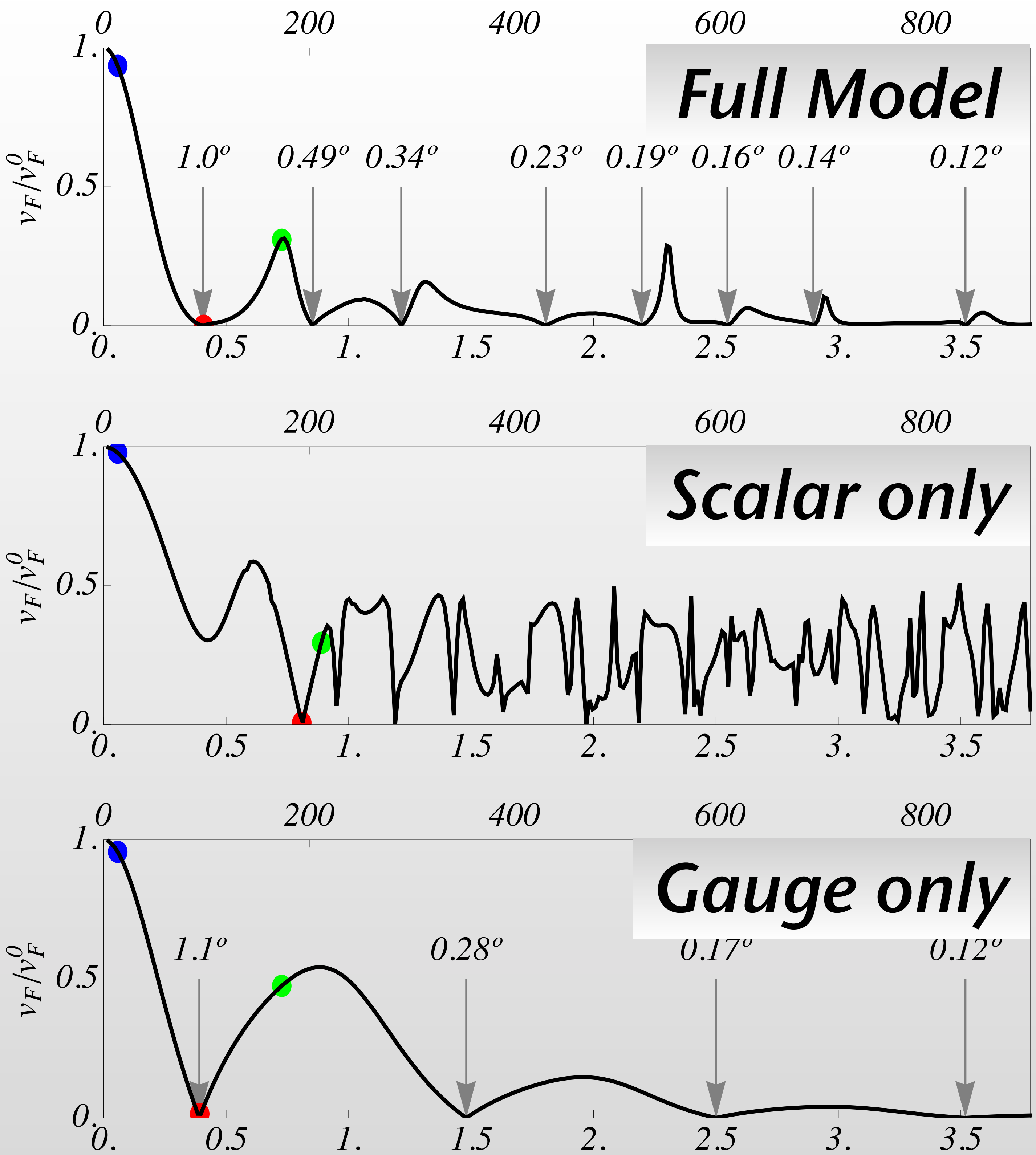

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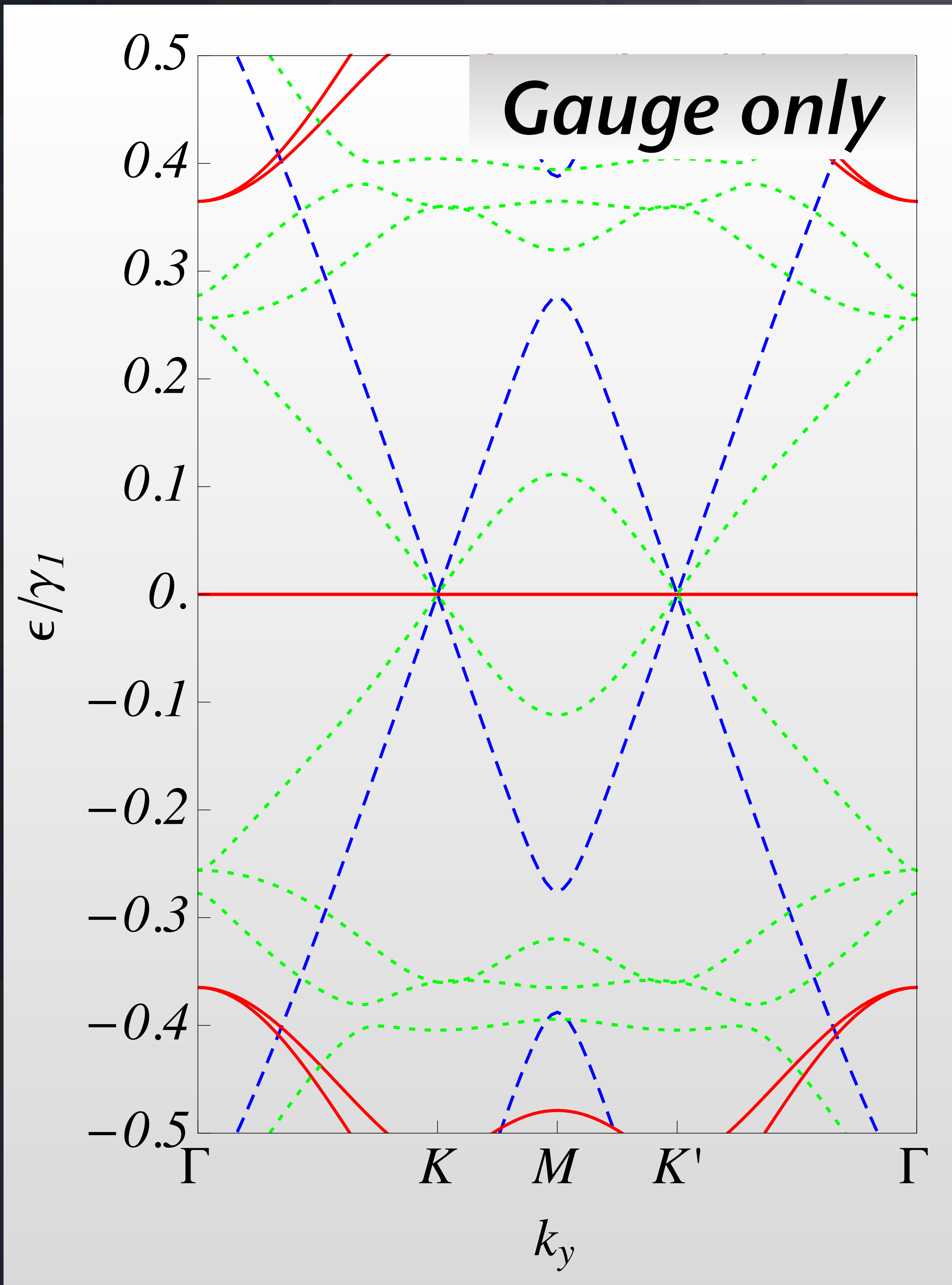
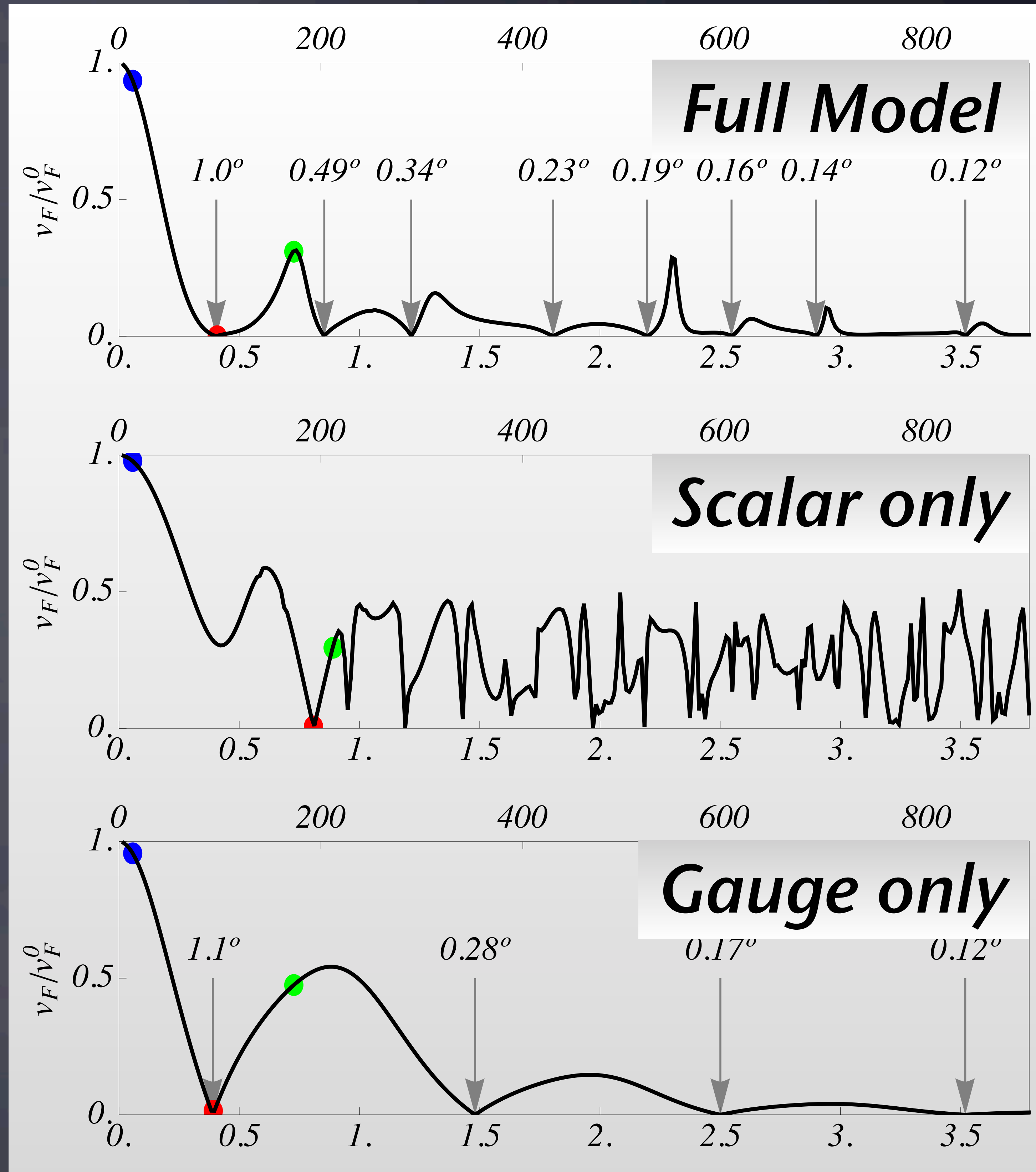
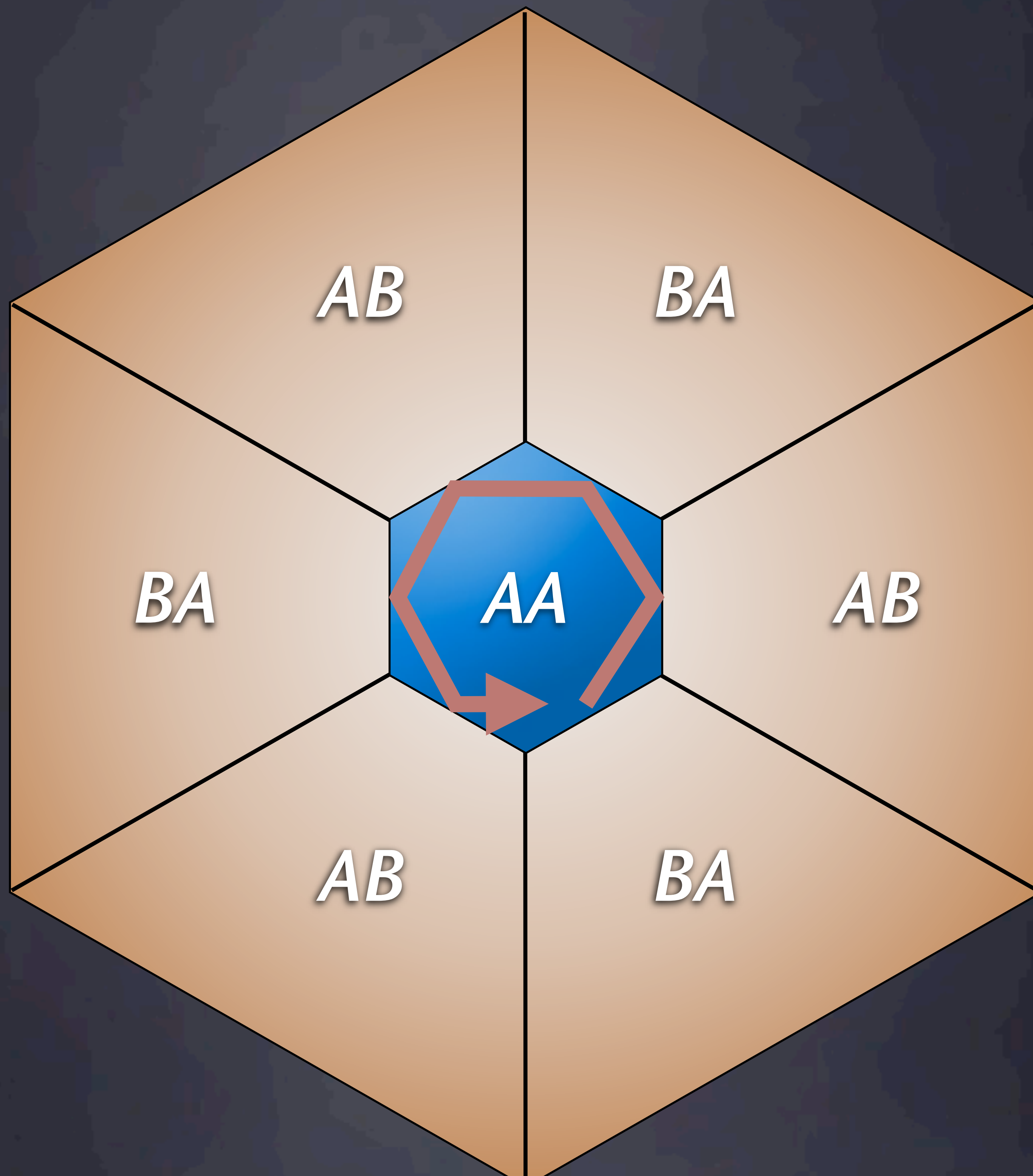




Confinement mechanism?



J. M. B. Lopes dos Santos, N. M. R. Peres and A. H. Castro Neto. arXiv:1202.1088