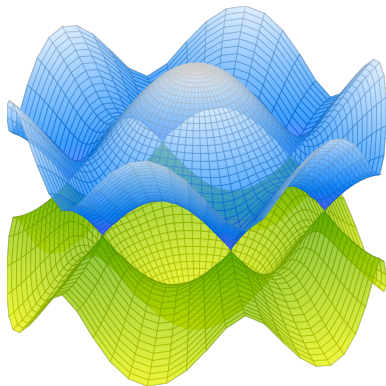


# Dirac Spinors in Graphene: A Good Analogy?

Lars Dehlwes

| IFT-UNESP



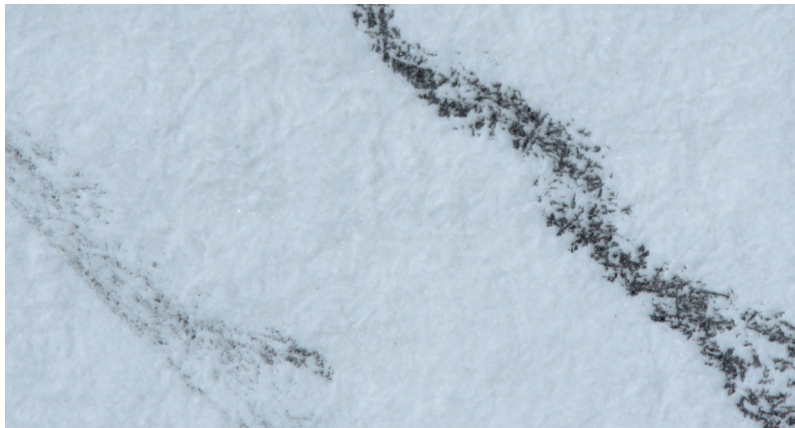


# Graphene?

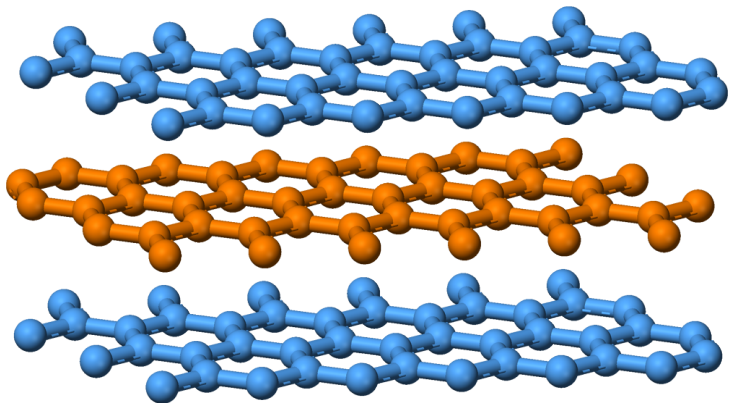
# Graphene?



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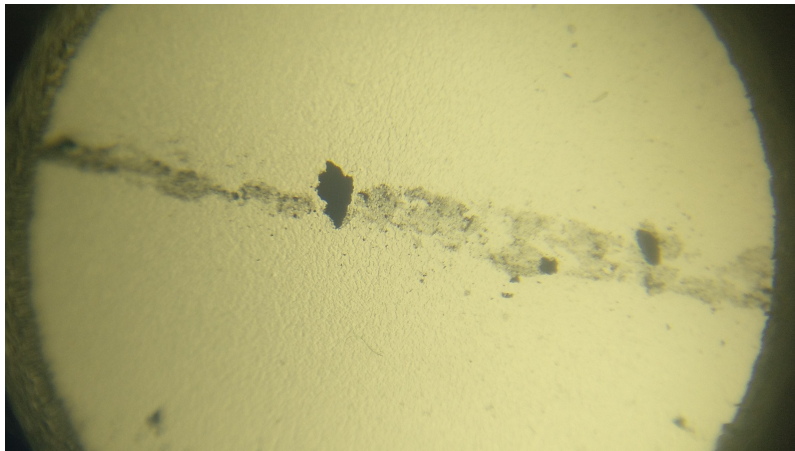


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# Graphene?

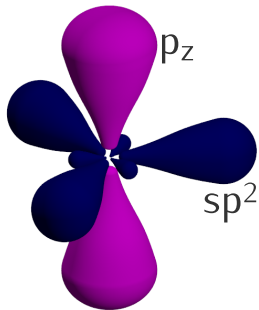
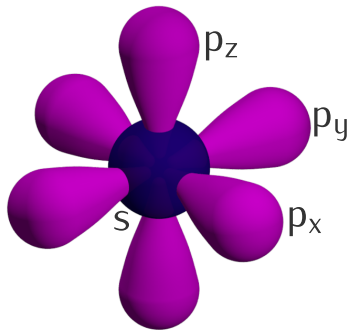


# Graphene?



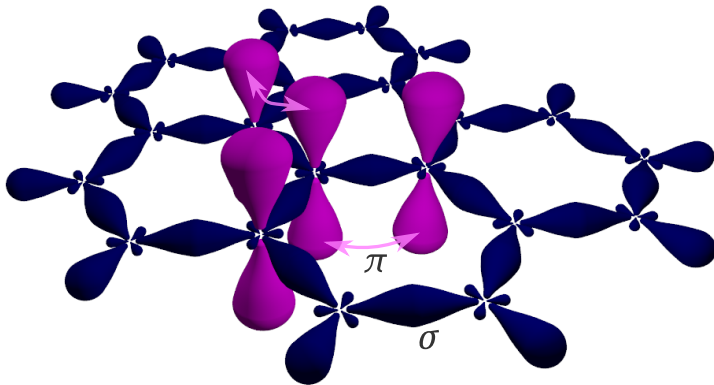


## Why in layers?



2

# Why in layers?



3

# Overview

- 1 Review of Periodic Potentials
- 2 Tight-Binding Approximation
- 3 Relation to Massless Dirac Fermions

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- 1 Review of Periodic Potentials
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- 3 Relation to Massless Dirac Fermions

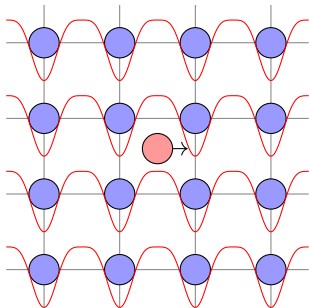
# Review of Periodic Potentials

Revisiting: Non-interacting electrons in a periodic potential  
→ “Bloch” states

- Description:

$$H = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} + V_{\text{periodic}}(\mathbf{r}) \quad (1)$$

- Reduces to single-particle problem



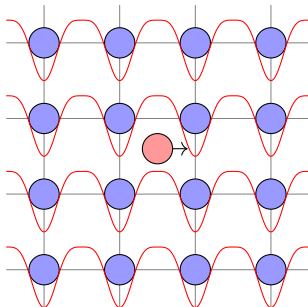
## Review of Periodic Potentials

Properly approaching the problem...

Assume infinite 2D crystal lattice with ions at positions

$$\mathbf{R}_n = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 \quad \mathbf{n} \in \mathbb{Z}^2 \quad (2)$$

- Potential invariant w.r.t. crystal symmetry group; in particular: Translation.
- Thus  $[T_{\mathbf{R}_n}, H] = 0$ , and we can strive for simultaneous eigenstates of all  $T_{\mathbf{R}_n}$  and  $H$ .



# Bloch waves

## Result

Any solution  $\psi(\mathbf{r})$  of

$$H\psi(\mathbf{r}) = E_\psi\psi(\mathbf{r}) \quad \forall \mathbf{n} \in \mathbb{N}^3: T_{\mathbf{R}_n}\psi(\mathbf{r}) = t_{\mathbf{n},\psi}\psi(\mathbf{r}) \quad (3)$$

can be written as

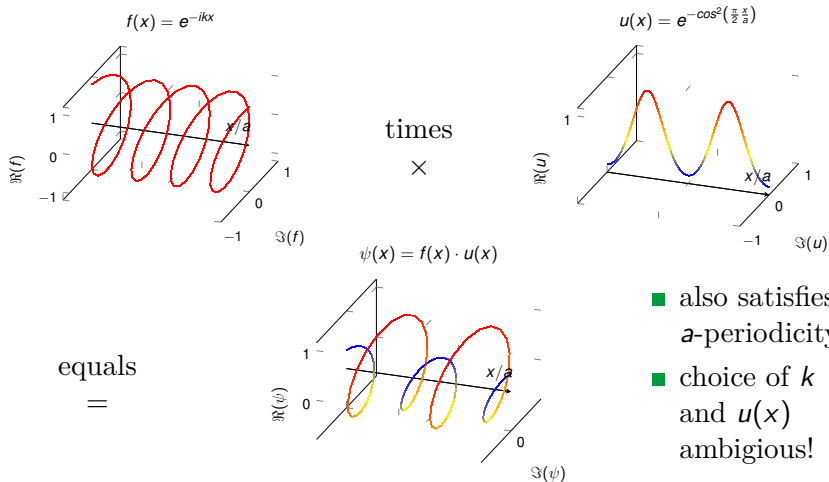
$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u(\mathbf{r}), \quad (4)$$

where  $u(\mathbf{r})$  exhibits the full translational symmetry of the crystal, i.e.

$$\forall \mathbf{n} \in \mathbb{N}^3: T_{\mathbf{R}_n}u(\mathbf{r}) = u(\mathbf{r}) \quad (5)$$

and  $\mathbf{k}$  such that  $e^{i\mathbf{k}_j L_j} = 0, j = 1, 2, 3$ . (periodic boundary conditions)

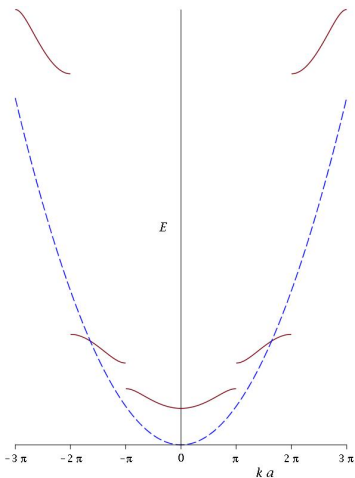
# Ambiguity of of quasi-momentum $k$ : An 1D Example





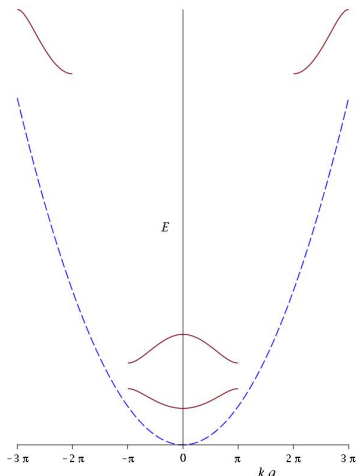
## An one-dimensional visualization

- $H\psi_k = E_k\psi_k$  gives rise to spectrum
- fixing number of revolutions of  $u(x)$  to 0
- obtain a discontinuous, deformed free-particle spectrum



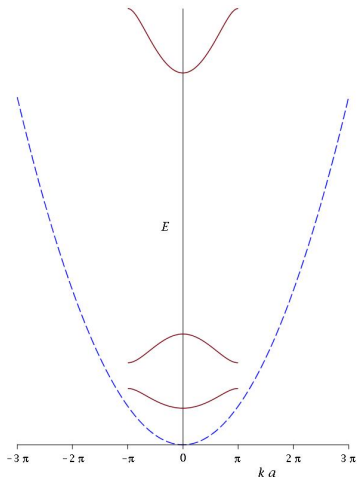
## An one-dimensional visualization

- $H\psi_k = E_k\psi_k$  gives rise to spectrum
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- obtain a discontinuous, deformed free-particle spectrum
- due to the equivalence on reciprocal space, possible to attribute each  $E_k$  to some  $k \in (-\pi/a, \pi/a)$  (first Brillouin zone).



## An one-dimensional visualization

- $H\psi_k = E_k\psi_k$  gives rise to spectrum
- ~~fixing number of revolutions of  $u(x)$  to 0~~
- ~~obtain a discontinuous, deformed free-particle spectrum~~
- due to the equivalence on reciprocal space, possible to attribute each  $E_k$  to some  $k \in (-\pi/a, \pi/a)$  (first Brillouin zone).



⇒ Energy bands

## Reciprocal space and Brillouin zones

- We have seen: Ambiguity in one-dimensional case
- In general, introduce Reciprocal Lattice

$$\text{RL} := \left\{ \mathbf{K} \in \mathbb{R}^2 \mid \forall \mathbf{n} \in \mathbb{Z}^2 : e^{i\mathbf{K} \cdot \mathbf{R}_n} = 1 \right\} \quad (6)$$

- Declare equivalence relation on Reciprocal Space

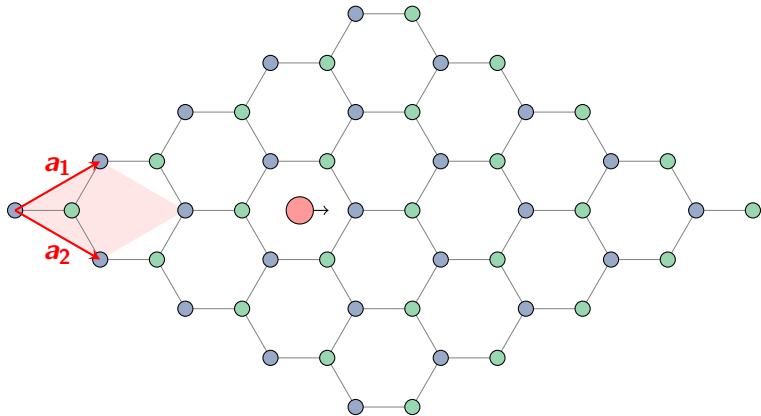
$$\forall \mathbf{k}, \mathbf{k}' \in \mathbb{R}^2 : [\mathbf{k} \sim \mathbf{k}' \iff \exists \mathbf{K} \in \text{RL} : \mathbf{k}' = \mathbf{k} + \mathbf{K}] \quad (7)$$

- We can reduce everything to  $\mathbb{R}^2 / \sim = \mathbb{R}^2 / \text{RL}$
- One possibility: Brillouin zone

$$\text{BZ} := \left\{ \mathbf{k} \in \mathbb{R}^2 \mid \forall \mathbf{K} \in \text{RL} \setminus \{0\} : |\mathbf{k}| \leq |\mathbf{K} - \mathbf{k}| \right\} \quad (8)$$

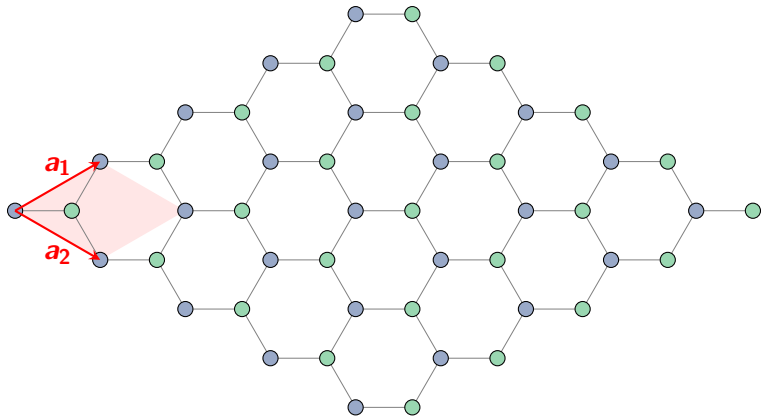
## In the case of Graphene...

Note: The unit cell contains two (identical) carbon atoms.



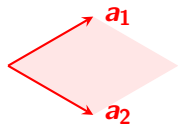
## In the case of Graphene...

Constructing the reciprocal lattice...



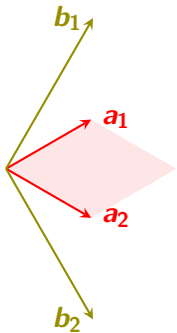
## In the case of Graphene...

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## In the case of Graphene...

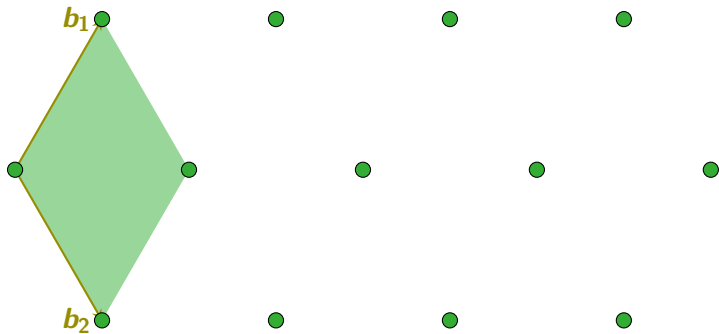
Constructing the reciprocal lattice...





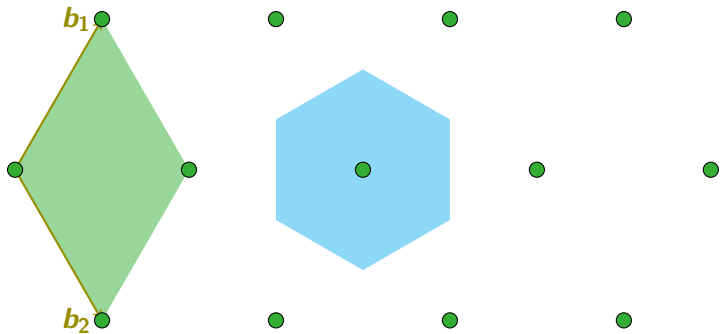
## In the case of Graphene...

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## In the case of Graphene...

Constructing the reciprocal lattice...



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- 1 Review of Periodic Potentials
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## Tight-Binding Ansatz for Graphene

Suppose  $p_z(\mathbf{r})$  represents the  $p_z$ -orbital of a carbon atom, i.e.,

$$H_C(\mathbf{r})p_z(\mathbf{r}) = \underbrace{E_z}_{\text{wlog.} = 0} p_z(\mathbf{r}). \quad (9)$$

The total Hamiltonian is given by

$$H = \frac{\mathbf{p}^2}{2m} + \sum_{\mathbf{n} \in (\mathbb{Z}_1^L)^2} (V_C(\mathbf{r} - \mathbf{r}_A - \mathbf{R}_n) + V_C(\mathbf{r} - \mathbf{r}_B - \mathbf{R}_n)). \quad (10)$$

We make an approximate ansatz

$$\begin{aligned} \Psi_{\mathbf{k}}(\mathbf{r}) = & c_A(\mathbf{k}) \sum_{\mathbf{n} \in (\mathbb{Z}_1^L)^2} e^{i\mathbf{k} \cdot \mathbf{R}_n} p_z(\mathbf{r} - \mathbf{r}_A - \mathbf{R}_n) \\ & + c_B(\mathbf{k}) \sum_{\mathbf{n} \in (\mathbb{Z}_1^L)^2} e^{i\mathbf{k} \cdot \mathbf{R}_n} p_z(\mathbf{r} - \mathbf{r}_B - \mathbf{R}_n). \end{aligned} \quad (11)$$

## Tight-Binding Ansatz for Graphene

We basically restricted ourselves to the subspace spanned by the functions

$$\varphi_{\mathbf{k}}^A(\mathbf{r}) = \frac{1}{L^2} \sum_{\mathbf{n} \in (\mathbb{Z}_1^L)^2} e^{i\mathbf{k} \cdot \mathbf{R}_n} p_z(\mathbf{r} - \mathbf{r}_A - \mathbf{R}_n) \quad (12)$$

and

$$\varphi_{\mathbf{k}}^B(\mathbf{r}) = \frac{1}{L^2} \sum_{\mathbf{n} \in (\mathbb{Z}_1^L)^2} e^{i\mathbf{k} \cdot \mathbf{R}_n} p_z(\mathbf{r} - \mathbf{r}_B - \mathbf{R}_n). \quad (13)$$

Note that  $\langle \varphi_{\mathbf{k}}^\alpha | \varphi_{\mathbf{k}'}^\beta \rangle = 0$  and  $\langle \varphi_{\mathbf{k}}^\alpha | H | \varphi_{\mathbf{k}'}^\beta \rangle = 0$  whenever  $\mathbf{k} \neq \mathbf{k}'$ . The subspaces spanned by  $\{\varphi_{\mathbf{k}}^A, \varphi_{\mathbf{k}}^B\}$  for each  $\mathbf{k}$  are thus orthogonal to each other and the Hamiltonian does not couple these subspaces. Thanks to this fact our ansatz is a good one.

# Tight-Binding Ansatz for Graphene

We then look for the minimum and maximum of the equation

$$\langle E \rangle_{\Psi_{\mathbf{k}}} = \frac{\langle \Psi_{\mathbf{k}} | H | \Psi_{\mathbf{k}} \rangle}{\langle \Psi_{\mathbf{k}} | \Psi_{\mathbf{k}} \rangle}, \quad (14)$$

and the corresponding coefficients  $c_A(\mathbf{k})$  and  $c_B(\mathbf{k})$ . It follows

$$\begin{aligned} \langle E \rangle_{\Psi_{\mathbf{k}}} &= \frac{\begin{pmatrix} c^A(\mathbf{k})^* & c^B(\mathbf{k})^* \end{pmatrix} \begin{pmatrix} \langle \varphi_{\mathbf{k}}^A | H | \varphi_{\mathbf{k}}^A \rangle & \langle \varphi_{\mathbf{k}}^A | H | \varphi_{\mathbf{k}}^B \rangle \\ \langle \varphi_{\mathbf{k}}^B | H | \varphi_{\mathbf{k}}^A \rangle & \langle \varphi_{\mathbf{k}}^B | H | \varphi_{\mathbf{k}}^B \rangle \end{pmatrix} \begin{pmatrix} c^A(\mathbf{k}) \\ c^B(\mathbf{k}) \end{pmatrix}}{\begin{pmatrix} c^A(\mathbf{k})^* & c^B(\mathbf{k})^* \end{pmatrix} \begin{pmatrix} \langle \varphi_{\mathbf{k}}^A | \varphi_{\mathbf{k}}^A \rangle & \langle \varphi_{\mathbf{k}}^A | \varphi_{\mathbf{k}}^B \rangle \\ \langle \varphi_{\mathbf{k}}^B | \varphi_{\mathbf{k}}^A \rangle & \langle \varphi_{\mathbf{k}}^B | \varphi_{\mathbf{k}}^B \rangle \end{pmatrix} \begin{pmatrix} c^A(\mathbf{k}) \\ c^B(\mathbf{k}) \end{pmatrix}} \quad (15) \\ &= \frac{c(\mathbf{k})^\dagger H(\mathbf{k}) c(\mathbf{k})}{c(\mathbf{k})^\dagger S(\mathbf{k}) c(\mathbf{k})} \approx \frac{c(\mathbf{k})^\dagger H(\mathbf{k}) c(\mathbf{k})}{c(\mathbf{k})^\dagger c(\mathbf{k})}. \end{aligned}$$

Simplification: Suppose  $S(\mathbf{k}) = \mathbb{1}_2$ , i.e.  $\langle \varphi_{\mathbf{k}}^A | \varphi_{\mathbf{k}}^B \rangle = 0$ .<sup>4</sup>

## Tight-Binding Ansatz for Graphene

- Now we can use the *min-max-theorem*<sup>5</sup> that states that the minimum and maximum correspond to the eigenvalues of  $H(\mathbf{k})$  and is attained precisely by the eigenvectors.
- ⇒ Found a new eigenvalue problem!
- It remains to calculate  $H(\mathbf{k})$ .
- Tight-binding  $\equiv$  “take only nearest neighbour interactions into account”

$$\langle \varphi_{\mathbf{k}}^A | H | \varphi_{\mathbf{k}}^A \rangle \approx 0 \approx \langle \varphi_{\mathbf{k}}^B | H | \varphi_{\mathbf{k}}^B \rangle \quad (16)$$

$$\langle \varphi_{\mathbf{k}}^A | H | \varphi_{\mathbf{k}}^B \rangle \approx -\gamma_0 \alpha(\mathbf{k}) \approx \overline{\langle \varphi_{\mathbf{k}}^B | H | \varphi_{\mathbf{k}}^A \rangle} \quad (17)$$

where

$$\alpha(\mathbf{k}) = 1 + e^{-i\mathbf{k} \cdot \mathbf{a}_1} + e^{-i\mathbf{k} \cdot \mathbf{a}_2}. \quad (18)$$

## Tight-Binding Ansatz for Graphene

We found

$$H(\mathbf{k}) = \begin{pmatrix} 0 & -\gamma_0 \alpha(\mathbf{k}) \\ -\gamma_0 \alpha(\mathbf{k})^* & 0 \end{pmatrix}, \quad (19)$$

where

$$\alpha(\mathbf{k}) = 1 + e^{-i\mathbf{k}\cdot\mathbf{a}_1} + e^{-i\mathbf{k}\cdot\mathbf{a}_2}. \quad (20)$$

Eigenvalues:

$$\begin{aligned} E_{\pm}(\mathbf{k}) &= \pm \gamma_0 |\alpha(\mathbf{k})| \\ &= \pm \sqrt{3 + 2 \cos(\mathbf{k}\cdot\mathbf{a}_1) + 2 \cos(\mathbf{k}\cdot\mathbf{a}_2) + 2 \cos(\mathbf{k}\cdot(\mathbf{a}_1 - \mathbf{a}_2))} \end{aligned} \quad (21)$$

Note that at

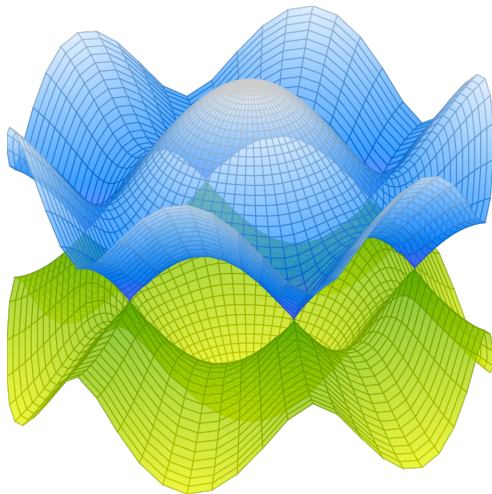
$$\mathbf{K}_{\pm} = \frac{1}{2}(\mathbf{b}_1 + \mathbf{b}_2) \pm \frac{1}{6}(\mathbf{b}_2 - \mathbf{b}_1) \quad (22)$$

we have

$$E_{+}(\mathbf{K}_{\pm}) = E_{-}(\mathbf{K}_{\pm}) = 0. \quad (23)$$

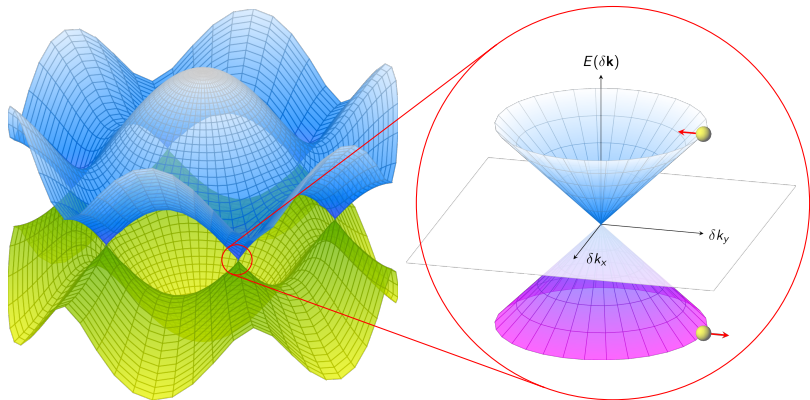


# Band Structure for the $p_z$ -Orbitals in Graphene



$$E_{\pm}(\mathbf{k}) = \pm \sqrt{3 + 2 \cos(\mathbf{k} \cdot \mathbf{a}_1) + 2 \cos(\mathbf{k} \cdot \mathbf{a}_2) + 2 \cos(\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2))} \quad (24)$$

# Band Structure for the $p_z$ -Orbitals in Graphene



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## Dispersion at the Dirac Points

Indeed, for  $\mathbf{k} = \mathbf{K}_{\pm} + \delta\mathbf{k}$ , we have

$$E_{\pm}(\delta\mathbf{k}) \approx \pm \frac{\sqrt{3}\gamma_0 a}{2} |\delta\mathbf{k}| = \pm \hbar v_F |\delta\mathbf{k}|, \quad (25)$$

where we defined the Fermi velocity

$$v_F = \frac{\sqrt{3}\gamma_0 a}{2\hbar} \approx 8.5 \times 10^5 \text{ m s}^{-1} \cong 3\% \times \text{speed of light} \quad (26)$$

that is the electronic group velocity of wave packets.

Next step:

What is the form of the Hamiltonian in the promixity of the points  $\mathbf{K}_{\pm}$ ?

## Dispersion at the Dirac Points

$$H(\mathbf{K}_- + \delta\mathbf{k}) \approx \underbrace{\frac{\sqrt{3}\gamma_0 a}{2}}_{\hbar v_F} \begin{pmatrix} 0 & -\delta\mathbf{k}_y - i\delta\mathbf{k}_x \\ -\delta\mathbf{k}_y + i\delta\mathbf{k}_x & 0 \end{pmatrix} \quad (27)$$

$$H(\mathbf{K}_+ + \delta\mathbf{k}) \approx \underbrace{\frac{\sqrt{3}\gamma_0 a}{2}}_{\hbar v_F} \begin{pmatrix} 0 & \delta\mathbf{k}_y - i\delta\mathbf{k}_x \\ \delta\mathbf{k}_y + i\delta\mathbf{k}_x & 0 \end{pmatrix} \quad (28)$$

## Dispersion at the Dirac Points

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Let us modify our ansatz:

$$\begin{aligned} \Psi_{\mathbf{k}}(\mathbf{r}) = & c_A(\mathbf{k}) \sum_{\mathbf{n} \in (\mathbb{Z}_1^L)^2} e^{i\mathbf{k} \cdot \mathbf{R}_n} p_z(\mathbf{r} - \mathbf{r}_A - \mathbf{R}_n) \\ & + c_B(\mathbf{k}) \sum_{\mathbf{n} \in (\mathbb{Z}_1^L)^2} e^{i\mathbf{k} \cdot \mathbf{R}_n} p_z(\mathbf{r} - \mathbf{r}_B - \mathbf{R}_n). \end{aligned} \quad (29)$$

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## Dispersion at the Dirac Points

$$H(\mathbf{K}_- + \delta\mathbf{k}) \approx \underbrace{\frac{\sqrt{3}\gamma_0 a}{2}}_{\hbar v_F} \begin{pmatrix} 0 & \delta k_x - i\delta k_y \\ \delta k_x + i\delta k_y & 0 \end{pmatrix} \quad (27)$$

$$H(\mathbf{K}_+ + \delta\mathbf{k}) \approx \underbrace{\frac{\sqrt{3}\gamma_0 a}{2}}_{\hbar v_F} \begin{pmatrix} 0 & \delta k_x + i\delta k_y \\ \delta k_x - i\delta k_y & 0 \end{pmatrix} \quad (28)$$

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## Dispersion at the Dirac Points

$$H(\mathbf{K}_- + \delta\mathbf{k}) \approx \underbrace{\frac{\sqrt{3}\gamma_0 a}{2}}_{\hbar v_F} \delta\mathbf{k} \cdot \boldsymbol{\sigma} \quad (27)$$

$$H(\mathbf{K}_+ + \delta\mathbf{k}) \approx \underbrace{\frac{\sqrt{3}\gamma_0 a}{2}}_{\hbar v_F} \delta\mathbf{k} \cdot \boldsymbol{\sigma}^\dagger \quad (28)$$

Let us modify our ansatz:

$$\begin{aligned} \Psi_{\mathbf{k}}(\mathbf{r}) = & c_A(\mathbf{k}) \sum_{\mathbf{n} \in (\mathbb{Z}_L^1)^2} e^{i\mathbf{k} \cdot \mathbf{R}_n} p_z(\mathbf{r} - \mathbf{r}_A - \mathbf{R}_n) \\ & + i c_B(\mathbf{k}) \sum_{\mathbf{n} \in (\mathbb{Z}_L^1)^2} e^{i\mathbf{k} \cdot \mathbf{R}_n} p_z(\mathbf{r} - \mathbf{r}_B - \mathbf{R}_n). \end{aligned} \quad (29)$$

## Weyl Spinors?

$$H(\mathbf{K}_- + \delta\mathbf{k}) \approx \underbrace{\frac{\sqrt{3}\gamma_0 a}{2}}_{\hbar v_F} \delta\mathbf{k} \cdot \boldsymbol{\sigma} \quad (30)$$

$$H(\mathbf{K}_+ + \delta\mathbf{k}) \approx \underbrace{\frac{\sqrt{3}\gamma_0 a}{2}}_{\hbar v_F} \delta\mathbf{k} \cdot \boldsymbol{\sigma}^\dagger \quad (31)$$

It definitively “looks like” the Weyl equation  $\sigma^\mu p_\mu \psi = 0!$

### A word of warning

The states  $\Psi_{\mathbf{k}}$  are not eigenvectors of the momentum operator  $\hat{p}$ ! Even worse,  $\delta\mathbf{k}$  is not even remotely related to the expectation value of  $\hat{p}$  in the state  $\Psi_{\mathbf{K}_\pm + \delta\mathbf{k}}$ !

Anyway, as long as we do not take the analogy too literally, it is a valid comparison between wave phenomena!

## Massless Dirac fermions?

We can build a four-component object:

$$\begin{aligned} |\psi_{\delta\mathbf{k}}\rangle = & c_A^-(\delta\mathbf{k}) |\varphi_{\mathbf{K}_-+\delta\mathbf{k}}^A\rangle - ic_B^-(\delta\mathbf{k}) |\varphi_{\mathbf{K}_-+\delta\mathbf{k}}^B\rangle \\ & + ic_B^+(\delta\mathbf{k}) |\varphi_{\mathbf{K}_++\delta\mathbf{k}}^B\rangle + c_A^+(\delta\mathbf{k}) |\varphi_{\mathbf{K}_++\delta\mathbf{k}}^A\rangle \end{aligned} \quad (32)$$

With respect to the ordered basis

$$\left( |\varphi_{\mathbf{K}_-+\delta\mathbf{k}}^A\rangle, -i |\varphi_{\mathbf{K}_-+\delta\mathbf{k}}^B\rangle, i |\varphi_{\mathbf{K}_++\delta\mathbf{k}}^B\rangle, |\varphi_{\mathbf{K}_++\delta\mathbf{k}}^A\rangle \right), \quad (33)$$

the joint Hamiltonian is given by

$$H(\delta\mathbf{k}) = \hbar v_F \begin{pmatrix} -\delta\mathbf{k} \cdot \boldsymbol{\sigma} & 0 \\ 0 & \delta\mathbf{k} \cdot \boldsymbol{\sigma} \end{pmatrix}. \quad (34)$$

This looks like the massless Fermi-Dirac Hamiltonian in the Weyl representation!

$$H_W^{\text{F.D.}} = \gamma^0 \boldsymbol{\gamma} \cdot \mathbf{p} = \begin{pmatrix} 0 & \mathbb{1}_2 \\ \mathbb{1}_2 & 0 \end{pmatrix} \begin{pmatrix} 0 & \boldsymbol{\sigma} \cdot \mathbf{p} \\ -\boldsymbol{\sigma} \cdot \mathbf{p} & 0 \end{pmatrix} = \begin{pmatrix} -\boldsymbol{\sigma} \cdot \mathbf{p} & 0 \\ 0 & \boldsymbol{\sigma} \cdot \mathbf{p} \end{pmatrix} \quad (35)$$

## Energy eigenstates

Suppose  $\delta \mathbf{k} = |\delta \mathbf{k}| \begin{pmatrix} \cos(\theta) \\ \sin(\theta) \end{pmatrix}$  and denote by  $\xi = \pm 1$  the valley  $\mathbf{K}_\xi$ . The positive ( $s = +1$ ) and negative ( $s = -1$ ) energy eigenstates for the valley  $\mathbf{K}_\xi$  are given by

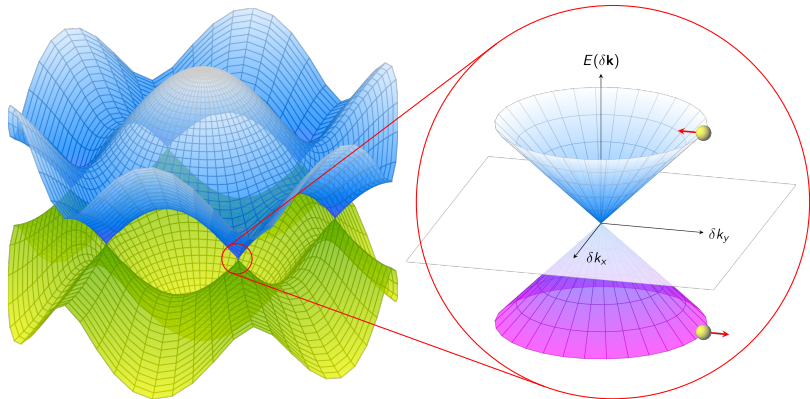
$$\psi_s^\xi = \begin{pmatrix} 1 \\ \xi s e^{i\theta} \end{pmatrix}. \quad (36)$$

Check that:

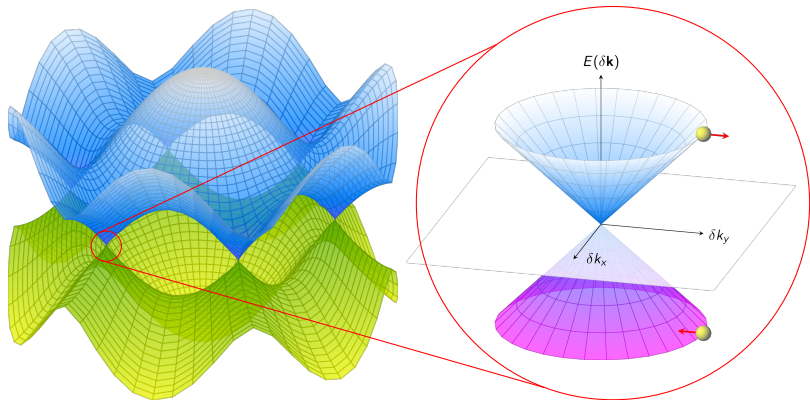
$$H(\mathbf{K}_\xi + \delta \mathbf{k}) \psi_s^\xi = \hbar v_F \xi (\delta \mathbf{k} \cdot \boldsymbol{\sigma}) \psi_s^\xi = s \hbar v_F |\delta \mathbf{k}| \psi_s^\xi \quad (37)$$

$s = +1$  for the “conduction” band and  $s = -1$  for the “valence band”. Note that the pseudohelicity eigenvalue of  $\psi_s^\xi$  is  $\xi s$ . This introduces an artificial distinction of the two valleys  $\mathbf{K}_+$  and  $\mathbf{K}_-$ .

# Pseudohelicity at the Dirac Point $K_-$



# Pseudohelicity at the Dirac Point $K_+$



## Conclusion

Similarities:

Differences:



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- linear dispersion

Differences:

- only in the rest frame!

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## Curiosity

Dirac fermions only exist in  $1 + 3$  dimensions due to the double cover  $SL(2, \mathbb{C}) \rightarrow SO(1, 3)$  of the Lorentz group.

The “massless Dirac fermions” of Graphene appear in a  $1 + 2$  dimensional system, with “z-momentum” always equal to zero.

# Conclusion

Leads to:

- no intravalley backscattering ( $\Rightarrow$  high mobility)
  
- Klein tunneling (we cannot electrostatically confine charge carriers)
  
- half integer quantum hall effect

Thank you for your attention!