Ground state construction of Bilayer Graphene

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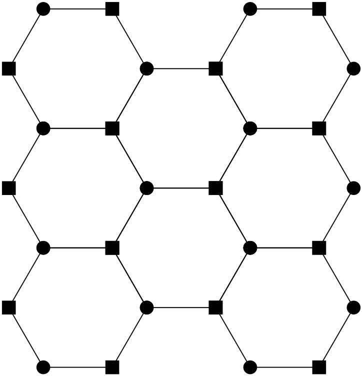
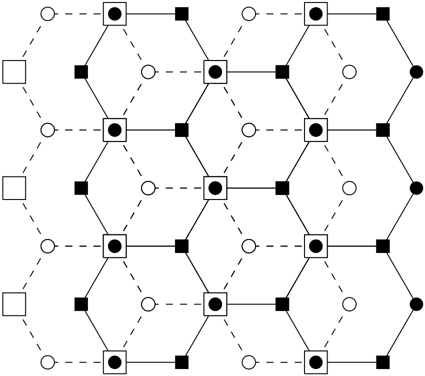
Monolayer graphene

- 2D crystal of carbon atoms on a honeycomb lattice.



Bilayer graphene

- 2 graphene layers in AB stacking.



Hamiltonian

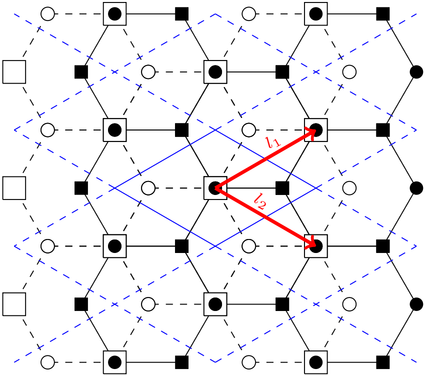
- Model for the electrons.
- Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 + U\mathcal{V}$$

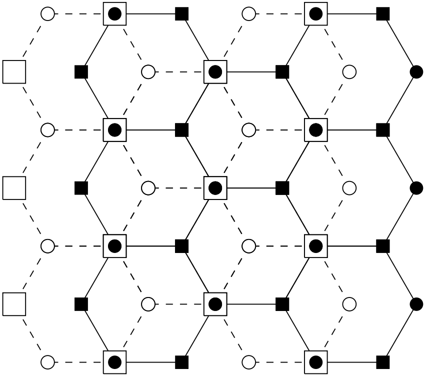
- $\mathcal{H}_0$: kinetic term: hoppings (tight-binding approximation).
- $U\mathcal{V}$: interaction: weak, short-range (screened Coulomb).

Lattice structure

- Rhombic lattice $\Lambda \equiv \mathbb{Z}^2$, 4 atoms per site.



Hoppings



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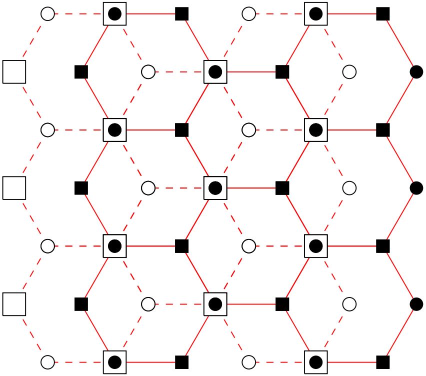

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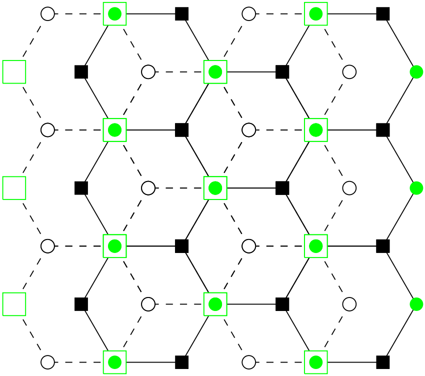

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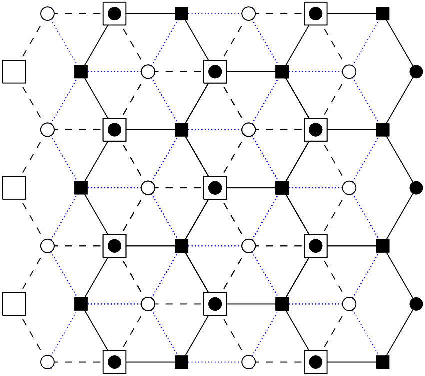

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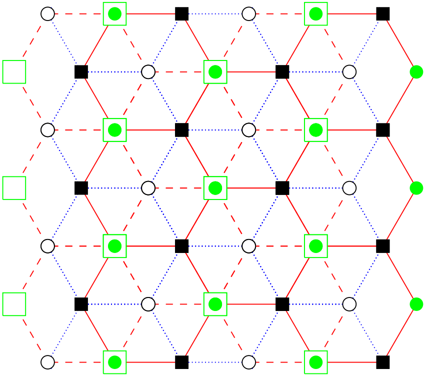


Non-interacting Hamiltonian

$$\mathcal{H}_0 := -\gamma_0 \sum_{\substack{x\in\Lambda\\ j=1,2,3}} \left(a_x^\dagger b_{x+\delta_j} + b_{x+\delta_j}^\dagger a_x + \tilde{b}_x^\dagger \tilde{a}_{x-\delta_j} + \tilde{a}_{x-\delta_j}^\dagger \tilde{b}_x \right)$$

$$-\gamma_1 \sum_{x\in\Lambda} \left(a_x^\dagger \tilde{b}_x + \tilde{b}_x^\dagger a_x \right)$$

$$-\gamma_3 \sum_{\substack{x\in\Lambda\\ j=1,2,3}} \left(\tilde{a}_{x-\delta_1}^\dagger b_{x-\delta_1-\delta_j} + b_{x-\delta_1-\delta_j}^\dagger \tilde{a}_{x-\delta_1} \right)$$

Non-interacting Hamiltonian

- Hopping strengths:

$$\gamma_0 = 1, \quad \gamma_1 = \epsilon, \quad \gamma_3 = 0.33 \times \epsilon$$

- Experimental value $\epsilon \approx 0.1$, here, $\epsilon \ll 1$.

Interaction

$$\mathcal{V} = \sum_{x,y} v(|x-y|) \left(n_x - \frac{1}{2}\right) \left(n_y - \frac{1}{2}\right)$$

- $\sum_{x,y}$: sum over pairs of atoms
- $n_x \equiv \alpha_x^\dagger \alpha_x$
- $v(|x-y|) \leqslant e^{-c|x-y|}$, $c > 0$
- $-\frac{1}{2}$: *half-filling.*

Theorem

$\exists U_0, \epsilon_0 > 0$, independent, such that, for $\epsilon < \epsilon_0$, $|U| < U_0$,

- the free energy

$$f := -\frac{1}{|\Lambda|\beta} \log \mathrm{Tr}(e^{-\beta\mathcal{H}})$$

  is analytic in U, uniformly in β and $|\Lambda|$,

- the two-point Schwinger function: for $\alpha, \alpha' \in \{a, b, \tilde{a}, \tilde{b}\}$,

$$s(x-y) := \frac{\mathrm{Tr}(e^{-\beta\mathcal{H}}\alpha'_x\alpha^\dagger_y)}{\mathrm{Tr}(e^{-\beta\mathcal{H}})}$$

  is analytic in U, uniformly in β and $|\Lambda|$.

Free model

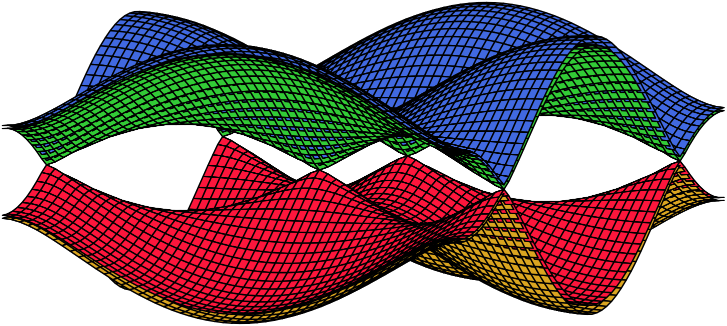
$$\mathcal{H}_0 = \sum_{k \in \hat{\Lambda}} \begin{pmatrix} \hat{a}_k^\dagger \\ \hat{\tilde{b}}_k^\dagger \\ \hat{\tilde{a}}_k^\dagger \\ \hat{b}_k^\dagger \end{pmatrix}^T \hat{H}_0(k) \begin{pmatrix} \hat{a}_k \\ \hat{\tilde{b}}_k \\ \hat{\tilde{a}}_k \\ \hat{b}_k \end{pmatrix}$$

$$\hat{H}_0(k) := - \begin{pmatrix} 0 & \gamma_1 & 0 & \gamma_0\Omega^*(k) \\ \gamma_1 & 0 & \gamma_0\Omega(k) & 0 \\ 0 & \gamma_0\Omega^*(k) & 0 & \gamma_3\Omega(k)e^{3ik_x} \\ \gamma_0\Omega(k) & 0 & \gamma_3\Omega(k)e^{-3ik_x} & \end{pmatrix}$$

$$\Omega(k) := 1 + 2e^{-\frac{3}{2}ik_x} \cos(\tfrac{\sqrt{3}}{2}k_y)$$

Free model

- Eigenvalues of $\hat{H}_0(k)$:



Perturbation theory

- Trotter formula:

$$\frac{\mathrm{Tr}(e^{-\beta(\mathcal{H}_0+U\mathcal{V})})}{\mathrm{Tr}(e^{-\beta\mathcal{H}_0})} = \left\langle \mathbb{T}\exp\left(-U\int_0^\beta dt\ \mathcal{V}(t)\right)\right\rangle_0$$

- "Imaginary time":

$$\mathcal{V}(t) := e^{t\mathcal{H}_0}\mathcal{V}e^{-t\mathcal{H}_0}$$

- "Non-interacting Gibbs measure":

$$\langle A\rangle_0 := \frac{\mathrm{Tr}(e^{-\beta\mathcal{H}_0}A)}{\mathrm{Tr}(e^{-\beta\mathcal{H}_0})}$$

Perturbation theory

- Matsubara frequency: for $\alpha \in \{a, b, \tilde{a}, \tilde{b}\}$,

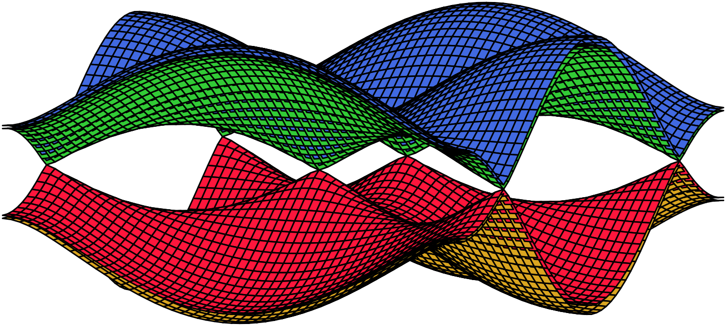
$$\hat{\alpha}_{k_0,k} := \int dt \; e^{ik_0 t} e^{t\mathcal{H}_0} \hat{\alpha}_k e^{-t\mathcal{H}_0}.$$

- Non-interacting Gibbs measure: "Gaussian", and singular: for $\alpha, \alpha' \in \{a, b, \tilde{a}, \tilde{b}\}$,

$$\hat{s}^{(0)}_{\alpha',\alpha}(k_0, k) := \left\langle \hat{\alpha}'_{k_0,k} \hat{\alpha}^{\dagger}_{k_0,k} \right\rangle_0 = (-ik_0 \mathbb{1} + \hat{H}_0(k))^{-1}_{\alpha',\alpha}$$

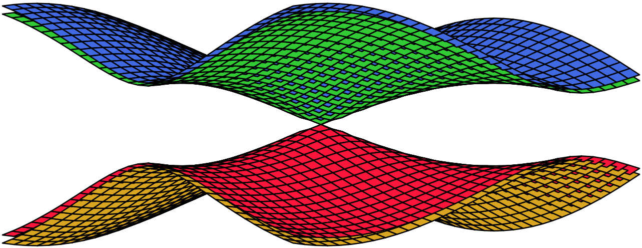
Scaling

- Eigenvalues of $\hat{H}_0(k)$:



Scaling

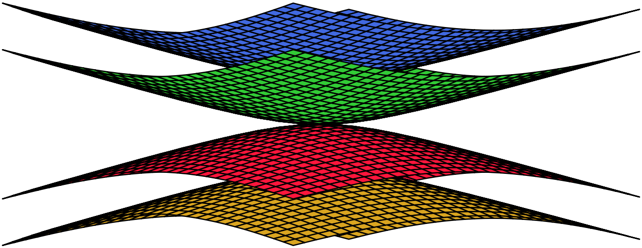
- First regime: $|k| \gg \epsilon$:



$$\hat{s}^{(0)}(k_0, k) \sim (|k_0| + |k|)^{-1}$$

Scaling

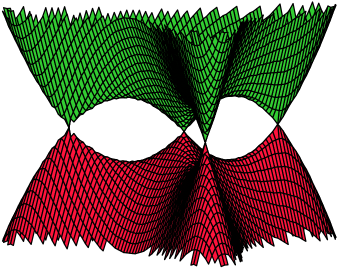
- Second regime: $\epsilon^2 \ll |k| \ll \epsilon$:



$$\hat{s}^{(0)}(k_0, k) \sim \left(|k_0| + \frac{|k|^2}{\epsilon} \right)^{-1}$$

Scaling

- Third regime: $|k| \ll \epsilon^2$:



$$\hat{s}^{(0)}(k_0, k) \sim (|k_0| + \epsilon |k|)^{-1}$$

Renormalization group

- Scale decomposition: scale $h \leqslant 0$:

$$\hat{s}^{(0)}(k_0, k) \sim 2^{-h}$$

- Scale by scale integration:

$$\langle A \rangle_0 = \left\langle \cdots \left\langle \langle A \rangle_{0,0} \right\rangle_{0,-1} \cdots \right\rangle_{0,h} \cdots$$

- Effective potential: $\mathcal{V}_h(t)$:

$$\left\langle \mathbb{T} \exp\left(-U \int dt \ \mathcal{V}_h(t) \right) \right\rangle_{0,h} \text{``} = \text{''} \ \mathbb{T} \exp\left(-U \int dt \ \mathcal{V}_{h-1}(t) \right)$$

Renormalization group flow