Graphene as a lattice field theory

Dominik Smith
Lorenz von Smekal
smith@theorie.ikp.physik.tu-darmstadt.de

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Outline

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Part I - Graphene, basics & history

- Introduction
- Tight-binding & low-energy effective theory (“graphene as a field theory”)

Part II - Lattice simulations of graphene

- Derivation of the graphene path-integral
- Hybrid-Monte-Carlo algorithm

Part III - Results

- Semimetal-insulator phase transition (“chiral symmetry-breaking”)
- Neck-disrupting Lifshitz transition
- Conclusions & Outlook

Part I - Graphene, basics & history

Introduction

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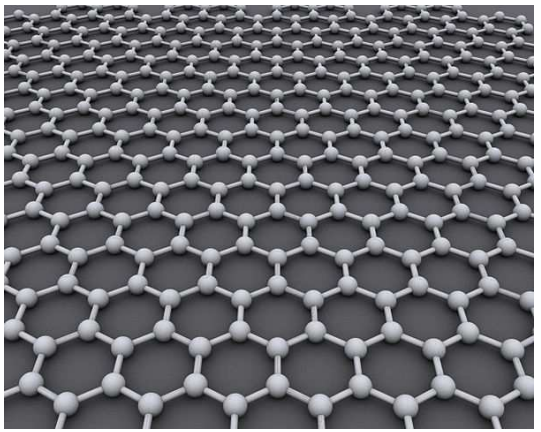
- **Graphene:** Single 2D layer of Carbon atoms arranged on hexagonal lattice.

  Inter-atomic distance: $d \approx 0.142\,\text{nm}$

  Basic building block of graphitic materials.



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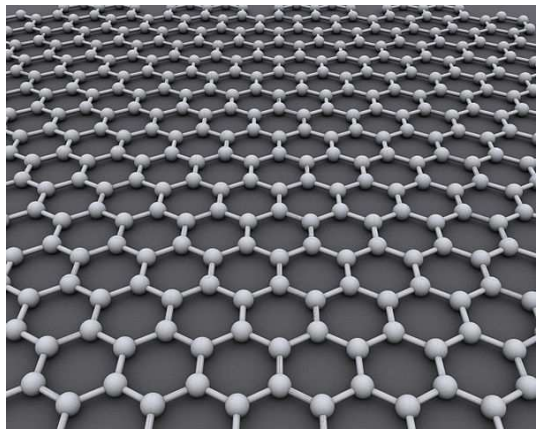
  Basic building block of graphitic materials.

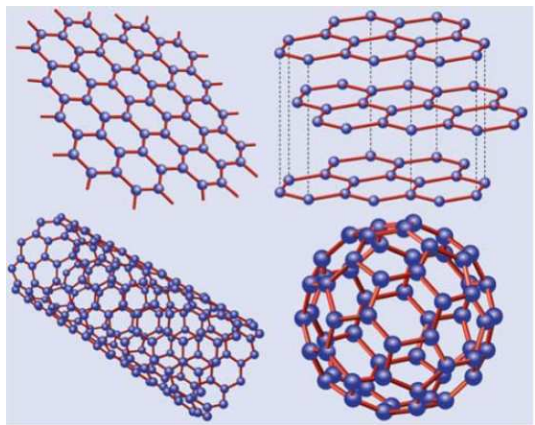
- **Graphite:** Many stacked layers of graphene (e.g. pencil trace: $\approx 3 \cdot 10^6$ layers).

  Inter-layer distance: $d' \approx 0.335\,\text{nm}$

- **Carbon nanotubes:** Rolled-up cylinders of graphene.

- **Fullerenes (C_{60}):** Wrapped graphene (introduction of pentagons produces curvature).





Bottom figure:
A. H. Castro Neto et al.,
Rev. Mod. Phys. 81, 109 (2009).

Introduction

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Novoselov & Geim, 2004: Experimental discovery of free-standing graphene.

Photo: PA

$\longrightarrow$ **Nobel prize for physics 2010**

Reconciliation with theory: Graphene is stabilized by a number of mechanisms (slight crumbling in 3rd dimension, small size ($<$ 1mm), strong atomic bonds,. . .).

Introduction

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Why are people interested in graphene?

Many unusual properties of interest for applications:

- **Density:** $0.77\,\mathrm{mg/m^2}$ (blocks passage of Helium atom).
- **Optical transparency:** Absorbs only 2.3% of visible light intensity.
- **Breaking strength:** $42\,\mathrm{N/m}$ (steel: $\sim 0.3\,\mathrm{N/m}$) - “carries weight of cat”.
- **Thermal conductivity:** At room temperature $10\times$ better than copper.
- **Electrical conductivity:** As good as copper (high electron mobility even in doped devices, carrier density $n \approx 10^{12}\,\mathrm{cm^{-2}}$)

Graphene based devices (processors, solar panels etc.) are imaginable.

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But: Why are high-energy physicists interested in graphene?

Introduction

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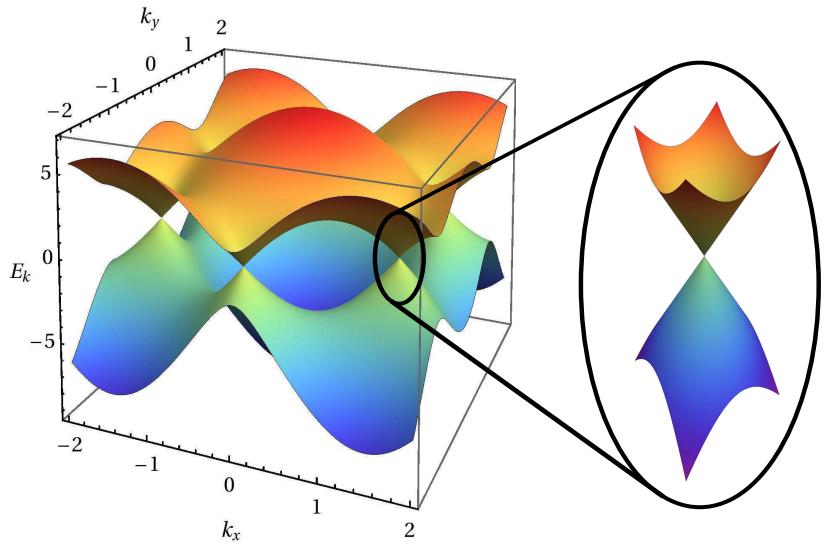
Graphene has linear dispersion relation at low energies:

$$E = \pm\hbar v_F \left|\vec{k}\right| , \quad v_F \approx c/300$$

Low-energy dynamics governed by massless Dirac equation!

Physics of relativistic field theory realized in a condensed matter system!



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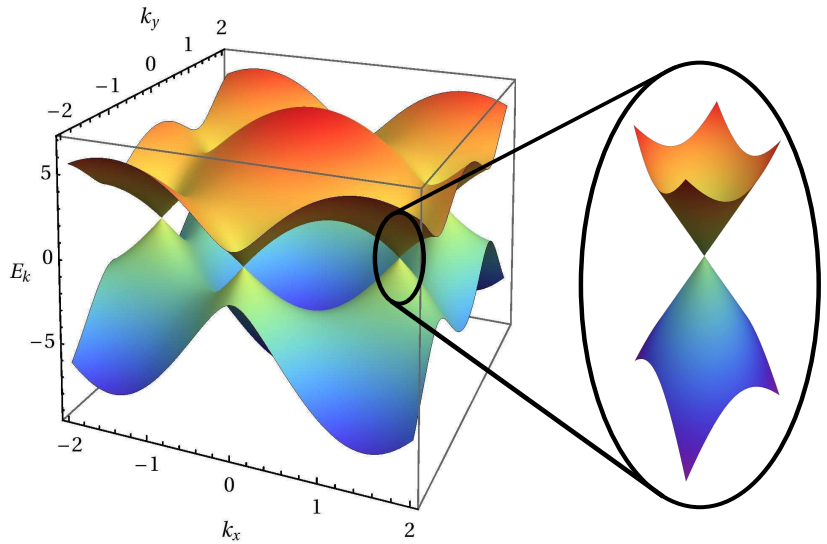

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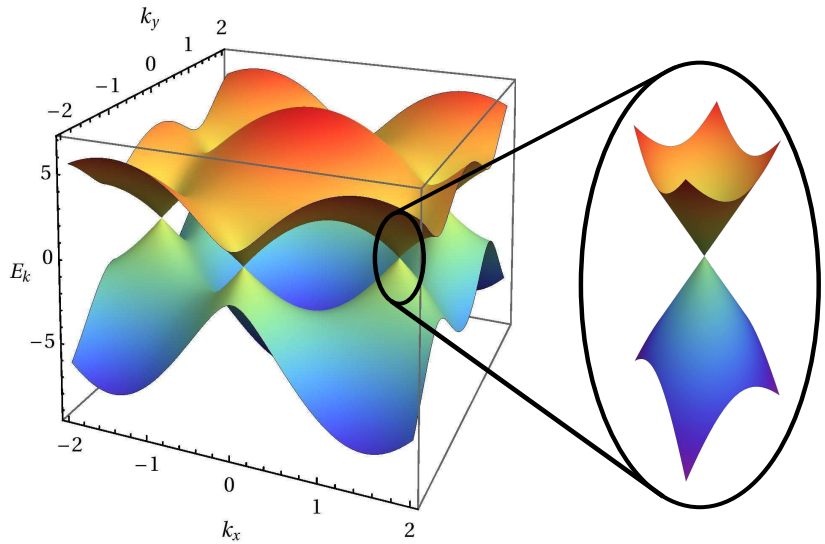

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Moreover: small Fermi-velocity leads to strong EM-interactions. $\alpha_{\text{eff}} = \frac{e^2}{\hbar v_F} \approx 2.2$

Suggests application of non-perturbative methods:

- Dyson-Schwinger equations, renormalization group, **lattice simulations**, . . .

Tight-binding & low-energy effective theory

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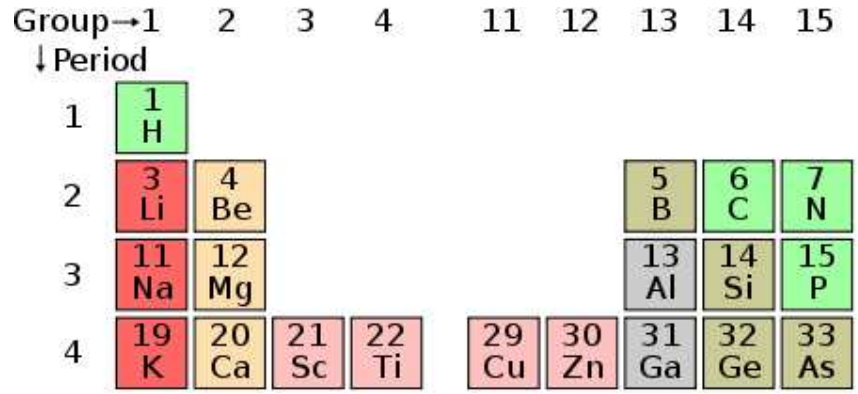

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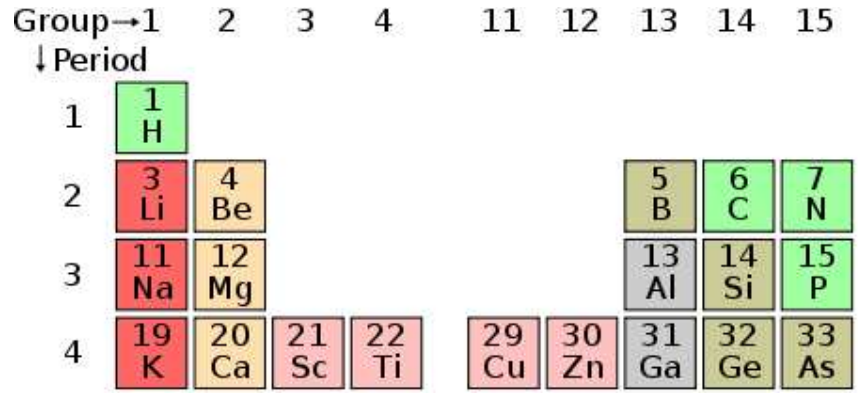

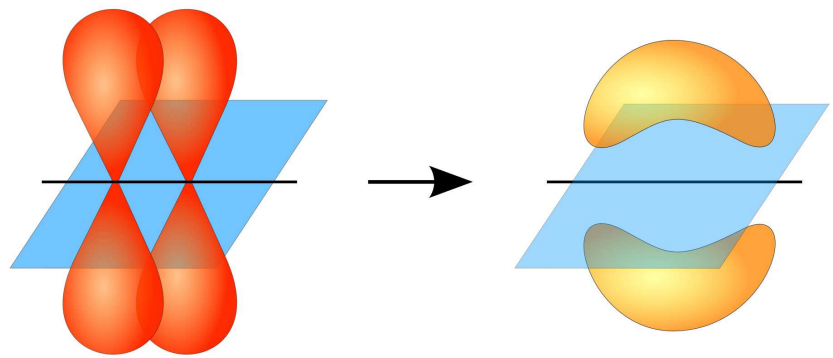

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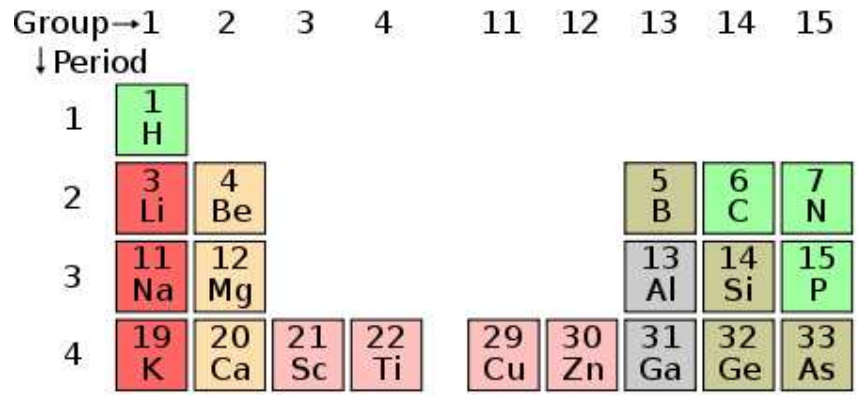
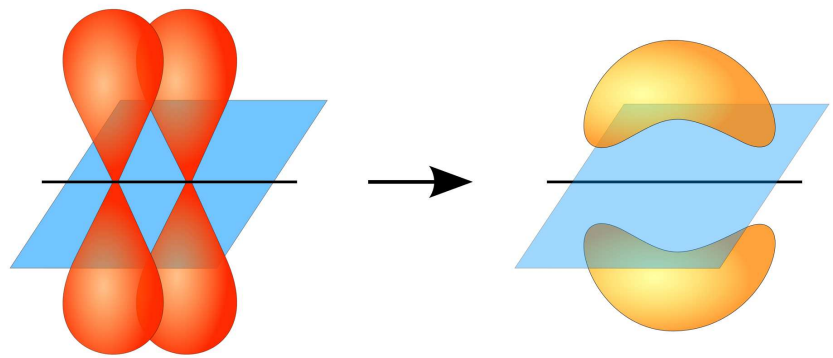
- **Tight-binding model:** "Nearest neighbor hopping" description of valence band.
  $H_{tb} = -\kappa \sum_{\langle x,y \rangle, s} (a^\dagger_{x,s} a_{y,s} + a^\dagger_{y,s} a_{x,s})$
  Neglects higher-hopping ($\sim$ 3%-effect) and two-body interactions.





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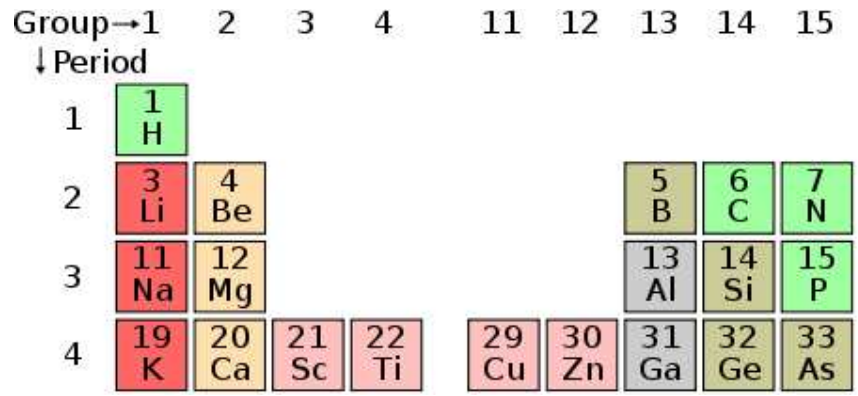

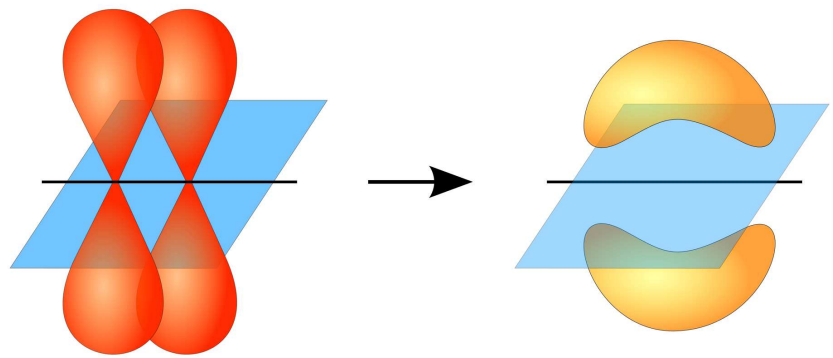

p_z-orbitals form π-bonds!

First goal: Understand properties of non-interacting tight-binding model!

Tight-binding & low-energy effective theory

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Bravais lattice: Given a set of N (not necessarily orthogonal/orthonormal) linear independent vectors $\vec{a}_i \in \mathbb{R}^N$, the set of points which can be reached as

$$\vec{r} = \sum_i n_i \, \vec{a}_i \,, \quad (n_i \in \mathbb{Z})$$

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Consider another vector $\vec{x}$. In general it does **not** hold that: $|\vec{x}| = \sqrt{\sum_i (\vec{x}\vec{a}_i)^2}$

Dual base ("reciprocal lattice") $\{\vec{b}_i \in \mathbb{R}^N \;,\; \vec{a}_i\vec{b}_j = 2\pi\,\delta_{ij}\}$ is required:

$|\vec{x}| = \sqrt{\sum_i (\vec{x}\vec{a}_i)(\vec{x}\vec{b}_i)/2\pi}$ $\quad$ ($(\vec{x}\vec{a}_i)$ are $(\vec{x}\vec{b}_i)$ are **"co-/contravariant"** components)

For $N = 3$: $\quad \vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1(\vec{a}_2 \times \vec{a}_3)} \;, \quad \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1(\vec{a}_2 \times \vec{a}_3)} \;, \quad \vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1(\vec{a}_2 \times \vec{a}_3)}$

Reciprocal lattice spans momentum space ("$\vec{k}$-space")!

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Unit cell: Cell with same volume as parallelepiped spanned by $\vec{a}_i$, which generates entire lattice when repeated.

Brillouin zone: (special) Unit cell in reciprocal lattice.

Tight-binding & low-energy effective theory

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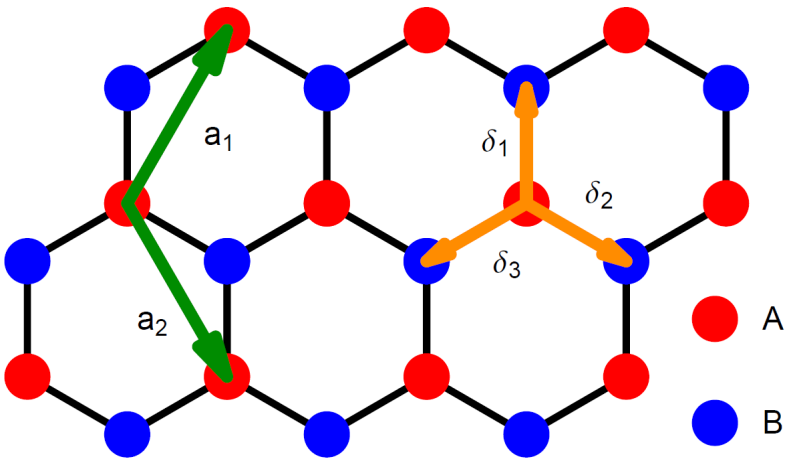
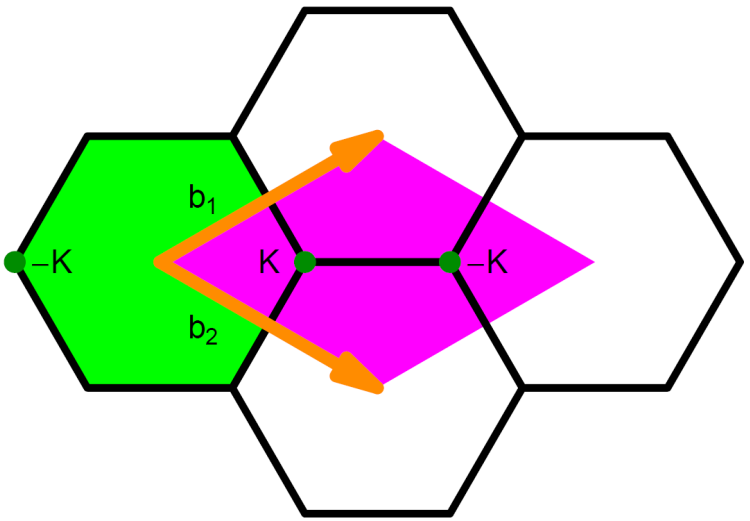
Graphene lattice: Not a Bravais lattice! Consists of two triangular sub-lattices.





Figures:
Gusynin et al.
Int. J. Mod. Phys.
B21: 4611-4658
(2007)

Base vectors: $\vec{a_1} = \sqrt{3}d\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$, $\vec{a_2} = \sqrt{3}d\left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right)$

Dual base: $\vec{b_1} = \frac{2\pi}{\sqrt{3}d}\left(1, \frac{1}{\sqrt{3}}\right)$, $\vec{b_2} = \frac{2\pi}{\sqrt{3}d}\left(1, -\frac{1}{\sqrt{3}}\right)$

($d \approx 0.142$nm “inter-atomic spacing”)

$\vec{\delta_1} = d\,(0, 1)$

$\vec{\delta_2} = d\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$

$\vec{\delta_3} = d\left(-\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$

Two types of lattice sites: **A-sites** **B-sites**

Tight-binding & low-energy effective theory

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Goal: Derive band-structure of non-interacting tight-binding model.

Tight-binding & low-energy effective theory

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Rewrite Hamiltonian in terms of ladder-operators acting on A and B sites:

$$H_{tb} = -\kappa \sum_{\vec{x},\vec{\delta},s} \left(a^{\dagger}_{\vec{x},s} b_{\vec{x}+\vec{\delta},s} + h.c. \right) \ , \quad \vec{\delta_1} = d\,(0,1) \ , \ \vec{\delta_2} = d\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \ , \ \vec{\delta_3} = d\left(-\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$$

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Dispersion relation $E(\vec{k})$ is desired. $\rightarrow$ Transform H to momentum space!

Fourier transformation on the triangular sub-lattices:

$$a^{\dagger}_{\vec{x},s} = \sqrt{S} \int_{\mathrm{BZ}} \frac{d^2k}{(2\pi)^2}\, e^{-i\vec{k}\vec{x}} a^{\dagger}_{s}(\vec{k}) \ , \quad b_{\vec{x}+\vec{\delta},s} = \sqrt{S} \int_{\mathrm{BZ}} \frac{d^2k}{(2\pi)^2}\, e^{i\vec{k}(\vec{x}+\vec{\delta})} b_{s}(\vec{k}) \ , \quad S = 3\sqrt{3}d^2/2$$

Rhombic Brillouin zone (“BZ”) defines ultra-violet cut-off.

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$$= -\kappa \sum_{\vec{\delta},s} \int_{\mathrm{BZ}} \frac{d^2k}{(2\pi)^2} \left[a^\dagger_s(\vec{k}) e^{i\vec{k}\vec{\delta}} b_s(\vec{k}) + h.c. \right] \quad \left(\text{Used} : \sum_{\vec{x}} e^{-i\vec{x}(\vec{k}-\vec{k}')} = \frac{(2\pi)^2}{S} \delta(\vec{k}-\vec{k}') \right)$$

Tight-binding & low-energy effective theory

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Compact notation: $H_{tb} = \sum_{\vec{\delta},s} \int_{\mathrm{BZ}} \frac{d^2k}{(2\pi)^2} \left[a_s^\dagger(\vec{k})\, \phi(\vec{k})\, b_s(\vec{k}) + h.c. \right]$, $\phi(\vec{k}) = -\kappa \sum_{\vec{\delta}_i} e^{i\vec{k}\vec{\delta}_i}$

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Can be re-written in vector/matrix form:

$$H_{tb} = \sum_{\vec{\delta},s} \int_{\mathrm{BZ}} \frac{d^2k}{(2\pi)^2} \left(a_s^\dagger(\vec{k}) , b_s^\dagger(\vec{k}) \right) \begin{pmatrix} 0 & \phi(\vec{k}) \\ \phi(\vec{k})^* & 0 \end{pmatrix} \begin{pmatrix} a_s(\vec{k}) \\ b_s(\vec{k}) \end{pmatrix} , \quad \mathcal{H} = \begin{pmatrix} 0 & \phi(\vec{k}) \\ \phi(\vec{k})^* & 0 \end{pmatrix}$$

Energy levels $E(\vec{k})$ i.e. "dispersion relation" given by eigenvalues of $\mathcal{H}$!

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Diagonalization through similarity transformation is easy:

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$A_s^\dagger(\vec{k}), B_s^\dagger(\vec{k})$ create energy eigenstates.

Dispersion relation given by $E(\vec{k}) = \pm|\phi(\vec{k})|$.

Tight-binding & low-energy effective theory

TECHNISCHE UNIVERSITÄT DARMSTADT

Reminder: $H_{tb} = \sum_{\vec{\delta},s} \int_{\mathrm{BZ}} \frac{d^2k}{(2\pi)^2} \left[a_s^\dagger(\vec{k})\, \phi(\vec{k})\, b_s(\vec{k}) + h.c. \right]$, $\phi(\vec{k}) = -\kappa \sum_{\vec{\delta}_i} e^{i\vec{k}\vec{\delta}_i}$

Writing out $\phi(\vec{k})$ explicitly leads to: $\vec{a_1} = \sqrt{3}d \left(\frac{1}{2}, \frac{\sqrt{3}}{2} \right)$, $\vec{a_2} = \sqrt{3}d \left(\frac{1}{2}, -\frac{\sqrt{3}}{2} \right)$

$$\phi(\vec{k}) = -\kappa\, e^{i\vec{k}(\vec{a}_1 - \vec{a}_2)/3} \left[1 + e^{i\vec{k}\vec{a}_2} + e^{-i\vec{k}\vec{a}_2} \right] = -\kappa \left[\exp\left(ik_y d\right) + \exp\left(-i\frac{k_y d}{2} \right) 2\cos\left(\frac{k_x\sqrt{3}d}{2} \right) \right]$$

Tight-binding & low-energy effective theory

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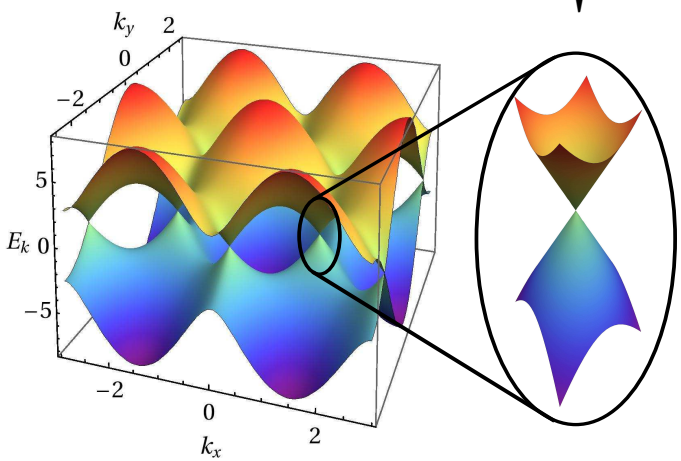
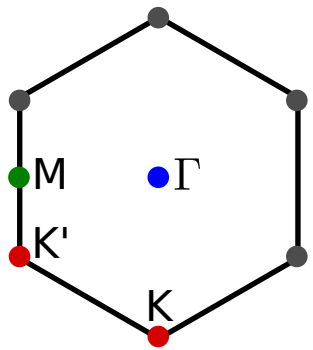
Dispersion relation ("tight-binding bands") given by absolute value of $\phi(\vec{k})$:

$$E(\vec{k}) = \pm|\phi(\vec{k})| = \pm\kappa\sqrt{1 + 4\cos^2\left(\frac{k_x\sqrt{3}d}{2}\right) + 4\cos\left(\frac{k_x\sqrt{3}d}{2}\right)\cos\left(\frac{3k_y d}{2}\right)}$$





Linear around zero points at corners of Brillouin zone!

(Figure by M. Körner)

Tight-binding & low-energy effective theory

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Corners of Brillouin zone ("K-points") are zero-points of $\phi(\vec{k})$!

$$\vec{K}_{1,2} = \pm\frac{2\pi}{\sqrt{3}d}\begin{pmatrix}1/3\\1/\sqrt{3}\end{pmatrix}, \quad \vec{K}_{3,4} = \pm\frac{2\pi}{\sqrt{3}d}\begin{pmatrix}2/3\\0\end{pmatrix}, \quad \vec{K}_{5,6} = \pm\frac{2\pi}{\sqrt{3}d}\begin{pmatrix}1/3\\-1/\sqrt{3}\end{pmatrix}.$$

Only two are inequivalent! Choice: $\vec{K}_+ \equiv \vec{K}_3$, $\vec{K}_- \equiv \vec{K}_4$

Goal: Understand physics close to $\vec{K}_\pm$ (low-energy limit).

Tight-binding & low-energy effective theory

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Goal: Understand physics close to $\vec{K}_\pm$ (low-energy limit).

Taylor expansion:

$$\phi(\vec{K}_\pm + \vec{p}) = -\kappa\left[\exp\left(ip_y d\right) + \exp\left(-i\frac{p_y d}{2}\right)2\cos\left(\frac{(\pm\frac{4\pi}{3\sqrt{3}d} + p_x)\sqrt{3}d}{2}\right)\right] \approx \pm\hbar v_F\left(p_x \mp ip_y\right)$$

Leads to linear ("relativistic massless") dispersion relation at low energies:

$$E(\vec{p}) = |\phi(\vec{K}_\pm + \vec{p})| \approx \hbar v_F\sqrt{p_x^2 + p_y^2} = \hbar v_F|\vec{p}|$$

Hopping parameter: $\kappa \approx 2.8\text{eV}$ $\longrightarrow$ Fermi-velocity: $v_F = \frac{3\kappa d}{2\hbar} \approx c/300$

All electronic excitations move with limiting velocity v_F. Effective "speed of light" is reduced by factor $\sim 1/300$.

Tight-binding & low-energy effective theory

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Tight-binding Hamiltonian in low energy limit: $\left(\phi(\vec{K}_\pm + \vec{p}) \approx \pm\hbar v_F \left(p_x \mp i p_y\right)\right)$

$$H_{tb} = \sum_{\vec{\delta},s} \int_{\mathrm{BZ}} \frac{d^2k}{(2\pi)^2} \left[a_s^\dagger(\vec{k})\, \phi(\vec{k})\, b_s(\vec{k}) + h.c.\right]$$

$$\approx \sum_{\vec{\delta},s} \int_{\mathrm{DC}} \frac{d^2p}{(2\pi)^2} \left[a_s^\dagger(\vec{K}_+ + \vec{p})\, \phi(\vec{K}_+ + \vec{p})\, b_s(\vec{K}_+ + \vec{p}) + a_s^\dagger(\vec{K}_- + \vec{p})\phi(\vec{K}_- + \vec{p})\, b_s(\vec{K}_- + \vec{p}) + h.c.\right]$$

Integration runs over Dirac cones (ultra-violet cutoff preserves number of states).

Tight-binding & low-energy effective theory

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Integration runs over Dirac cones (ultra-violet cutoff preserves number of states).

Low-energy Hamiltonian can be re-written using matrix/spinor notation:

$$H_{tb} \approx \hbar v_F \sum_{\vec{\delta},s} \int_{\mathrm{DC}} \frac{d^2p}{(2\pi)^2} \Psi_s^\dagger(\vec{p})\, \mathcal{H}_0\, \Psi_s(\vec{p}) \equiv H_0$$

$$\Psi_s(\vec{p}) = \begin{pmatrix} a_s^\dagger(\vec{K}_+ + \vec{p}) \\ b_s^\dagger(\vec{K}_+ + \vec{p}) \\ b_s^\dagger(\vec{K}_- + \vec{p}) \\ a_s^\dagger(\vec{K}_- + \vec{p}) \end{pmatrix}, \quad \mathcal{H}_0 = \begin{pmatrix} 0 & p_x - ip_y & 0 & 0 \\ p_x + ip_y & 0 & 0 & 0 \\ 0 & 0 & 0 & -p_x + ip_y \\ 0 & 0 & -p_x - ip_y & 0 \end{pmatrix}$$

Tight-binding & low-energy effective theory

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Using Pauli-matrices $\tau_{1,2}$ we obtain:

$$\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

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$$\equiv \alpha_1 p_x + \alpha_2 p_y$$

Tight-binding & low-energy effective theory

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Dirac algebra is fulfilled! $\{\gamma_\mu, \gamma_\nu\} = 2g^{\mu\nu}$, $g^{\mu\nu} = diag(1, -1, -1, -1)$

Tight-binding & low-energy effective theory

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Tight-binding Hamiltonian at low-energies is Dirac-Hamiltonian in 2+1D:

$$H_0 = \hbar v_F \sum_{\vec{\delta},s} \int_{DC} \frac{d^2p}{(2\pi)^2} \overline{\Psi}_s(\vec{p}) \left[\gamma_1 p_x + \gamma_2 p_y\right] \Psi_s(\vec{p}) , \qquad \overline{\Psi}_s(\vec{p}) = \Psi_s^\dagger(\vec{p})\gamma_0$$

Lagrangian: $\mathcal{L} = i\hbar \sum_s \overline{\Psi}_s(t, \vec{r}) \left[\gamma_0\partial_t + v_F(\gamma_1\partial_x + \gamma_2\partial_y)\right] \Psi_s(t, \vec{r})$

Part II - Lattice simulations of graphene

The graphene path-integral

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Low energy theory of graphene (variant of QED_{2+1}) simulated with staggered fermions:	Drut, Lähde, Phys.Rev.Lett. 102, 026802 (2009)	Drut, Lähde, Phys.Rev. B 79, 165425 (2009)	Drut, Lähde, Phys.Rev. B 79, 241405 (2009)
Thirring model in 2+1 dimensions simulated:	Hands, Strouthos, Phys.Rev. B 78, 165423 (2008)	Armour, Hands, Strouthos, Phys.Rev. B 81, 125105 (2010)	Armour, Hands, Strouthos, Phys.Rev. B 84, 075123 (2011)

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First derivation of path-integral for hexagonal lattice: Brower,Rebbi,Schaich, PoS(Lattice 2011)056

Recently:

- Tight-binding with gauge-links. Buividovich, Polikarpov, Phys. Rev. B 86, 245117 (2012)
- **Tight-binding with instantaneous interactions.** Ulybyshev et al. (ITEP), Phys. Rev. Lett. 111, 056801 (2013); DS, von Smekal, Phys. Rev. B 89, 195429 (2014)

The graphene path-integral

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Goal: Simulate (grand) canonical ensemble of interacting tight-binding theory.

$$Z = \mathrm{Tr}\, e^{-\beta H}\,, \quad \langle O \rangle = \frac{1}{Z}\mathrm{Tr}\left[\widehat{O} e^{-\beta H}\right]\,, \quad H = -\kappa \sum_{\langle x,y\rangle,s} (a^\dagger_{x,s} a_{y,s} + a^\dagger_{y,s} a_{x,s}) + H_{\mathrm{int}}$$

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Usual strategy in field theory:

- Express Z as a path integral (i.e. functional integral).
- Operators are replaced by “coordinates” (field variables) which can be stored in computer memory.
- Generate exemplary field configurations which represent ensemble.
- Measure observables in coordinate representation.

$$\langle O \rangle = \frac{1}{Z} \int \prod_i \mathcal{D}\phi_i \; O(\phi_1, \ldots, \phi_N) \exp\left[-S(\phi_1, \ldots, \phi_N)\right]\,,$$

$$Z = \int \prod_i \mathcal{D}\phi_i \; \exp\left[-S(\phi_1, \ldots, \phi_N)\right]\,.$$

The graphene path-integral

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Crucial differences for graphene:

- No Lorentz-invariance (i.e. Hilbert-space is regular Fock-space of non-relativistic many-body QM) .
- Spacelike lattice-spacing is physical.

Hexagonal geometry is unusual but not problematic.

The graphene path-integral

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Roadmap:

- Express trace in convenient base of Hilbert space: $\mathrm{Tr}\, e^{-\beta H} = \sum_n \langle n| e^{-\beta H} |n\rangle$
- Factorize exponential: $e^{-\beta H} = e^{-\delta H}\, e^{-\delta H} \ldots e^{-\delta H}$, $\quad \delta = \beta / N_t$
- Insert unit operators between factors: $\mathbf{1} = \sum_m |m\rangle\langle m|$
- Leads to: $Z = \lim_{N_t \to \infty} \sum_n \prod_{i=0}^{N_t - 1} \langle n_{i+1}| e^{-\delta H} |n_i\rangle$
- Replace operators by eigenvalues.

The graphene path-integral

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What is proper choice of basis for Fermionic Fock space?

The graphene path-integral

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Consider a **Bosonic** Fock space: $[a_i^\dagger, a_j^\dagger] = [a_i, a_j] = 0\ , \quad [a_i, a_j^\dagger] = \delta_{ij}\ .$

Associate a complex number ϕ_i with each a_i.

Construct **coherent states** as: $|\phi\rangle = e^{\sum_i \phi_i a_i^\dagger} |0\rangle\ , \quad \langle\phi| = \langle 0| e^{\sum_i a_i \phi_i^*}$

(each set ϕ_i defines a different state)

Can be interpreted as “classical” field configurations.

The graphene path-integral

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(each set ϕ_i defines a different state)

Can be interpreted as “classical” field configurations.

Properties:

- Right (left) eigenstates of a_j ($a_j^\dagger$) operators: $a_j|\phi\rangle = \phi_j|\phi\rangle\ , \ \langle\phi|a_j^\dagger = \langle\phi|\phi_j^*$
- Scalar product: $\langle\phi|\chi\rangle = e^{\sum_i \phi_i^* \chi_i}$
- **Closure relation:** $\frac{1}{2\pi i}\int \left[\prod_i d\phi_i^*\, d\phi_i\right]\ e^{-\sum_i \phi_i^* \phi_i}|\phi\rangle\langle\phi| = \mathbf{1}$
- ...

Coherent states are basis of (Bosonic) Fock space!

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Trace can be expressed using coherent states:

$$\mathrm{Tr}\, A = \sum_n \langle n|A|n\rangle = \frac{1}{2\pi i}\int \left[\prod_i d\phi_i^*\, d\phi_i\right] e^{-\sum_i \phi_i^*\phi_i} \sum_n \langle n|\phi\rangle\langle\phi|A|n\rangle$$

$$= \frac{1}{2\pi i}\int \left[\prod_i d\phi_i^*\, d\phi_i\right] e^{-\sum_i \phi_i^*\phi_i} \langle\phi|A|\phi\rangle$$

The graphene path-integral

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Theorem for **normal-ordered** functions of ladder operators:

$$\langle\phi|A(a_i^\dagger, a_i)|\chi\rangle = A(\phi_i^*, \chi_i)\, e^{\sum_i \phi_i^*\chi_i}$$

The graphene path-integral

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Partition function can be expressed with complex numbers ϕ_i, ϕ_i^* (up to non-normal-ordered contributions to $e^{-\delta H}$ which vanish as $\beta/N_t = \delta \to 0$):

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The graphene path-integral

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But: Tight-binding Hamiltonian acts on Fermionic space!

The graphene path-integral

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Goal: Construct coherent states for **Fermionic** Fock space.

$$\{a_i^\dagger, a_j^\dagger\} = \{a_i, a_j\} = 0 \,, \quad \{a_i, a_j^\dagger\} = \delta_{ij} \,.$$

Anti-commutation relations generate technical and conceptual issues!

The graphene path-integral

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Anti-commutation relations generate technical and conceptual issues!

Assume coherent states $|\xi\rangle$,$\langle\xi|$ exist: $\quad |\xi\rangle = e^{\sum_i \xi_i a_i^\dagger}|0\rangle \ , \quad \langle\xi| = \langle 0| \, e^{\sum_i a_i \xi_i^*}$

Should be eigenstates of ladder operators:

$$a_j|\xi\rangle = \xi_j|\xi\rangle \ , \ \langle\xi|a_j^\dagger = \langle\xi|\xi_j^*$$

Anti-commutation relations for $a_i, a_i^\dagger$ imply:

$$a_i a_j|\xi\rangle = -a_j a_i|\xi\rangle \ \rightarrow \ \xi_i\xi_j|\xi\rangle = -\xi_j\xi_i|\xi\rangle \ ,$$
$$\langle\xi|a_i^\dagger a_j^\dagger = \langle\xi|(-a_j^\dagger a_i^\dagger) \ \rightarrow \ \langle\xi|\xi_i^*\xi_j^* = \langle\xi|(-\xi_j^*\xi_i^*)$$

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Anti-commutation relations generate technical and conceptual issues!

Assume coherent states $|\xi\rangle$,$\langle\xi|$ exist: $|\xi\rangle = e^{\sum_i \xi_i a_i^\dagger}|0\rangle$, $\langle\xi| = \langle 0| e^{\sum_i a_i \xi_i^*}$

Should be eigenstates of ladder operators:

$$a_j|\xi\rangle = \xi_j|\xi\rangle \,, \; \langle\xi|a_j^\dagger = \langle\xi|\xi_j^*$$

Anti-commutation relations for $a_i, a_i^\dagger$ imply:

$$a_i a_j|\xi\rangle = -a_j a_i|\xi\rangle \;\rightarrow\; \xi_i\xi_j|\xi\rangle = -\xi_j\xi_i|\xi\rangle \,,$$
$$\langle\xi|a_i^\dagger a_j^\dagger = \langle\xi|(-a_j^\dagger a_i^\dagger) \;\rightarrow\; \langle\xi|\xi_i^*\xi_j^* = \langle\xi|(-\xi_j^*\xi_i^*)$$

Eigenvalues ξ_i, ξ_i^* cannot be regular complex numbers.

The graphene path-integral

TECHNISCHE UNIVERSITÄT DARMSTADT

Construction of Fermionic coherent states requires Grassmann algebra!

Grassmann algebra: Set of generators $\{\xi_\alpha\}$, $\alpha = 1, \ldots, n$ which anticommute.

$$\xi_\alpha \xi_\beta + \xi_\beta \xi_\alpha = 0 \;\rightarrow \xi_\alpha^2 = 0$$

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Grassmann numbers: Linear combinations with complex coefficients of

$$\{1, \xi_1, \xi_2, \ldots, \xi_1 \xi_2 \ldots \xi_n\} \quad \text{(ordering is convention)}$$

The graphene path-integral

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For $n = 2p$, conjugation can be defined (by forming groups of two ξ_i each):

$$(\xi_\alpha)^* = \xi_\alpha^* \,, \quad (\xi_\alpha^*)^* = \xi_\alpha \,, \quad (\lambda \xi_\alpha)^* = \lambda^* \xi_\alpha^* \quad (\lambda \in \mathbb{C})$$

Functions $A(\xi_0^*, \xi_0, \ldots, \xi_n^*, \xi_n)$ can be defined. Due to $\xi_\alpha^2 = 0$, are at most linear in any ξ_i, ξ_i^*, e.g.:

$$A(\xi^*, \xi) = a_0 + a_1 \xi + \overline{a_1} \xi^* + a_{12} \xi^* \xi$$

The graphene path-integral

TECHNISCHE UNIVERSITÄT DARMSTADT

More properties/definitions:

$$A(\xi^*, \xi) = a_0 + a_1\xi + \overline{a_1}\xi^* + a_{12}\xi^*\xi$$

- Derivative: $\frac{\partial}{\partial\xi}(\xi^*\xi) = \frac{\partial}{\partial\xi}(-\xi\xi^*) = -\xi^* \;\rightarrow\; \frac{\partial}{\partial\xi}A(\xi^*, \xi) = a_1 - a_{12}\xi^*$, ...
- Integral: $\int d\xi\, 1 = 0\,, \;\int d\xi\, \xi = 1 \;\rightarrow\; \int d\xi\, A(\xi^*, \xi) = \frac{\partial}{\partial\xi}A(\xi^*, \xi)$, ...
- ...

The graphene path-integral

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- ...

To construct **Fermionic coherent states**:

- Associate a generator ξ_α with each operator a_α and ξ^*_α with each $a^\dagger_\alpha$.
- Require that: $\{\bar{\xi}, \bar{a}\} = 0$, $(\bar{\xi}\bar{a})^\dagger = \bar{a}^\dagger\bar{\xi}^*$ ($\bar{a}$ / $\bar{\xi}$ label any $a, a^\dagger$ / ξ, ξ^*)

Fermionic coherent states $|\xi\rangle$,$\langle\xi|$ are: $|\xi\rangle = e^{\sum_i \xi_i a_i^\dagger}|0\rangle$, $\langle\xi| = \langle 0| e^{\sum_i a_i \xi_i^*}$

Eigenvalue property can easily be verified:

$$a_\alpha|\xi\rangle = a_\alpha e^{\sum_i \xi_i a_i^\dagger}|0\rangle = a_\alpha \prod_i \left(1 + \xi_i a_i^\dagger\right)|0\rangle = \xi_\alpha|\xi\rangle \quad \text{(likewise } \langle\xi|a^\dagger_\alpha = \langle\xi|\xi^*_\alpha\text{)}$$

The graphene path-integral

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Fermionic coherent states differ from Bosonic ones in fundamental ways:

- No classical limit (particle number is not well-defined etc.).
- $|\xi\rangle, \langle\xi|$ are not themselves elements of the Fock space.

However: Closure relation still holds.

$$\int \left[\prod_i d\xi_i^* \, d\xi_i\right] \, e^{-\sum_i \xi_i^* \xi_i} |\xi\rangle \, \langle\xi| = \mathbf{1}$$

The graphene path-integral

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Likewise, for normal-ordered functions $A(a_i^\dagger, a_i)$ of ladder operators:

$$\langle\xi| A(a_i^\dagger, a_i) |\xi'\rangle = A(\xi_i^*, \xi_i')\, e^{\sum_i \xi_i^* \xi_i'}$$

The graphene path-integral

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Due to the relation $\langle\psi_i|\xi\rangle\langle\xi|\psi_j\rangle = -\langle\xi|\psi_j\rangle\langle\psi_i|\xi\rangle$, an additional minus sign appears in the trace:

$$\mathrm{Tr}\, A = \int \left[\prod_\alpha d\xi_\alpha^*\, d\xi_\alpha\right] e^{-\sum_\alpha \xi_\alpha^* \xi_\alpha} \langle -\xi| A |\xi\rangle \ .$$

Fermionic coherent states can be used to derive functional integral of Z.

Break

Outline

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Part I - Graphene, basics & history

- Introduction
- Tight-binding & low-energy effective theory (“graphene as a field theory”)

Part II - Lattice simulations of graphene

- **Derivation of the graphene path-integral**
- Hybrid-Monte-Carlo algorithm

Part III - Results

- Semimetal-insulator phase transition (“chiral symmetry-breaking”)
- Neck-disrupting Lifshitz transition
- Conclusions & Outlook

Reminder

TECHNISCHE UNIVERSITÄT DARMSTADT

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- Theorem for normal-ordered functions: $\langle\phi|A(a_i^\dagger, a_i)|\chi\rangle = A(\phi_i^*, \chi_i)\, e^{\sum_i \phi_i^* \chi_i}$

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Goal: Derive path integral for Z of interacting tight-binding theory.

The graphene path-integral

TECHNISCHE UNIVERSITÄT DARMSTADT

Starting point: Interacting tight-binding Hamiltonian in second-quantized form.

$$H = \sum_{\langle x,y\rangle,s} (-\kappa)(a^\dagger_{x,s} a_{y,s} + a^\dagger_{y,s} a_{x,s}) + \frac{1}{2} \sum_{x,y} q_x V_{xy} q_y \ ,$$

Fermionic anti-commutation relations apply:

$$\{a^\dagger_i, a^\dagger_j\} = \{a_i, a_j\} = 0 \ , \quad \{a^\dagger_i, a_j\} = \delta_{ij} \ .$$

Hopping parameter is $\kappa \approx 2.8\,\mathrm{eV}$ (experimental input).

Charge-operator:

$$q_x = a^\dagger_{x,1} a_{x,1} + a^\dagger_{x,-1} a_{x,-1} - 1$$

Constant is subtracted from q_x for neutrality at half-filling.

Interactions are approximately instantaneous (non-local), since $v_F \approx c/300 \ll c$.

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Freedom to choose any (positive-definite) interaction matrix V!

The graphene path-integral

TECHNISCHE UNIVERSITÄT DARMSTADT

To proceed, a few modifications are required!

First: Introduce "hole" operators $b_x^\dagger, b_x$ for electrons with $s = -1$:

$$a_x = a_{x,1}\ ,\ a_x^\dagger = a_{x,1}^\dagger\ ,\quad b_x^\dagger = a_{x,-1}\ ,\ b_x = a_{x,-1}^\dagger$$ **(not A- and B-sites!)**

Changes form of charge operator and Hamiltonian:

$$q_x = a_x^\dagger a_x - b_x^\dagger b_x\ ,$$

$$H = \sum_{\langle x,y\rangle}(-\kappa)(a_x^\dagger a_y - b_x^\dagger b_y + \mathrm{h.c.}) + \sum_{x,y} q_x V_{xy} q_y .$$

The graphene path-integral

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Next: Flip sign of $b_x^\dagger, b_x$ on one sublattice. Affects non-interacting term:

$$H_{tb} = \sum_{\langle x,y\rangle}(-\kappa)(a_x^\dagger a_y - b_x^\dagger b_y + \mathrm{h.c.}) \longrightarrow \sum_{\langle x,y\rangle}(-\kappa)(a_x^\dagger a_y + b_x^\dagger b_y + \mathrm{h.c.})\ .$$

Changes make absence of Fermion sign-problem obvious (will be discussed).

The graphene path-integral

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Next: Hamiltonian must be brought into **normal ordered** form (required for the replacement of operators by eigenvalues).

$$H = \sum_{\langle x,y\rangle,s} (-\kappa)(a_x^\dagger a_y + b_y^\dagger b_x + \mathrm{h.c.}) + \frac{1}{2}\sum_{x,y} :q_x V_{xy} q_y: + \frac{1}{2}\sum_x V_{xx}(a_x^\dagger a_x + b_x^\dagger b_x)$$

Normal ordering produces additional term!

The graphene path-integral

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Finally: Add "staggered" mass term to break sublattice symmetry explicitly.

$$H \to H + \sum_x m_S(a_x^\dagger a_x + b_x^\dagger b_x) \quad (m_S = \pm m, x \in A, B)$$

(sign of m_s differs on the sub-lattices).

Removes zero-modes from the Hamiltonian! Physics is obtained in the limit $m \to 0$.

Hamiltonian is now in proper form for application of coherent state formalism!

The graphene path-integral

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Fermionic coherent states for $a_x, a_x^\dagger, b_x, b_x^\dagger$:

$$\langle \psi, \eta | = \langle 0 | e^{-\sum_x (a_x \psi_x^* + b_x \eta_x^*)} , \quad |\psi, \eta\rangle = e^{-\sum_x (\psi_x a_x^\dagger + \eta_x b_x^\dagger)} |0\rangle .$$

Introduction of two symbols η, ψ only a matter of notation!

Grand canonical partition function:

$$Z = \mathrm{Tr}\, e^{-\beta H} = \int \left[\prod_x d\psi_x^* \, d\psi_x \, d\eta_x^* \, d\eta_x \right] e^{-\sum_x (\psi_x^* \psi_x + \eta_x^* \eta_x)} \langle -\psi, -\eta | \, e^{-\beta H} \, |\psi, \eta\rangle .$$

For normal ordered functions $F(...)$ it holds that:

$$\langle \psi, \eta | F(a_x^\dagger, a_x, b_x^\dagger, b_x) | \psi', \eta' \rangle = F(\psi_x^*, \psi_x', \eta_x^*, \eta_x') \; e^{\sum_x \psi_x^* \psi_x' + \eta_x^* \eta_x'} .$$

Hamiltonian is normal-ordered but $e^{-\beta H}$ is not.

The graphene path-integral

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Hamiltonian is normal-ordered but $e^{-\beta H}$ is not.

$\longrightarrow$ Factorize exponential and exploit closure relation!

The graphene path-integral

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Exponential is split into N_t separate factors ($\delta = \beta / N_t$):

$$Z = \int \left[\prod_x d\psi_x^* \, d\psi_x \, d\eta_x^* \, d\eta_x \right] \; e^{-\sum_x (\psi_x^* \psi_x + \eta_x^* \eta_x)} \langle -\psi, -\eta | \, e^{-\delta H} \, e^{-\delta H} \ldots e^{-\delta H} \, | \psi, \eta \rangle \; .$$

Unit operators inserted between factors:

$$\mathbf{1} = \int \left[\prod_x d\psi_x^* \, d\psi_x d\eta_x^* \, d\eta_x \right] \; e^{-\sum_x (\psi_x^* \psi_x + \eta_x^* \eta_x)} | \psi, \eta \rangle \, \langle \psi, \eta | \; .$$

Introduce "time-index": $\langle \psi_t, \eta_t | = \langle 0 | e^{-\sum_x (a_x \psi_{x,t}^* + b_x \eta_{x,t}^*)}$, $| \psi_t, \eta_t \rangle = e^{-\sum_x (\psi_{x,t} a_x^\dagger + \eta_{x,t} b_x^\dagger)} | 0 \rangle$

Obtain "functional integral":

$$Z = \int \prod_{t=0}^{N_t - 1} \left[\prod_x d\psi_{x,t}^* \, d\psi_{x,t} \, d\eta_{x,t}^* \, d\eta_{x,t} \right] \; e^{-\sum_x (\psi_{x,t+1}^* \psi_{x,t+1} + \eta_{x,t+1}^* \eta_{x,t+1})} \langle \psi_{t+1}, \eta_{t+1} | e^{-\delta H} | \psi_t, \eta_t \rangle \; .$$

Anti-periodic boundary conditions implied:

$$\psi_{x,N_t} = -\psi_{x,0} \; , \; \eta_{x,N_t} = -\eta_{x,0} \; .$$

The graphene path-integral

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Functional integral:

$$Z = \int \prod_{t=0}^{N_t-1} \left[\prod_x d\psi^*_{x,t}\, d\psi_{x,t}\, d\eta^*_{x,t}\, d\eta_{x,t} \right] \; e^{-\sum_x (\psi^*_{x,t+1}\psi_{x,t+1} + \eta^*_{x,t+1}\eta_{x,t+1})} \langle \psi_{t+1}, \eta_{t+1} | e^{-\delta H} | \psi_t, \eta_t \rangle \; .$$

Last step: Compute "matrix elements" $\langle \psi_{t+1}, \eta_{t+1} | e^{-\delta H} | \psi_t, \eta_t \rangle$

Reminder:

$$H = \sum_{\langle x,y \rangle, s} (-\kappa)(a^\dagger_x a_y + b^\dagger_y b_x + \text{h.c.}) + \frac{1}{2} \sum_{x,y} :q_x V_{xy} q_y:$$

$$+ \frac{1}{2} \sum_x V_{xx}(a^\dagger_x a_x + b^\dagger_x b_x) + \sum_x m_S (a^\dagger_x a_x + b^\dagger_x b_x)$$

For normal ordered functions F it holds:

$$\langle \psi, \eta | F(a^\dagger_x, a_x, b^\dagger_x, b_x) | \psi', \eta' \rangle = F(\psi^*_x, \psi'_x, \eta^*_x, \eta'_x) \; e^{\sum_x \psi^*_x \psi'_x + \eta^*_x \eta'_x}$$

Hamiltonian is in normal order, but $e^{-\delta H}$ is not!

Deviations from normal-ordering generate discretization error $\mathcal{O}(\delta^2)$.

The graphene path-integral

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After computing all matrix elements:

$$\mathrm{Tr}\, e^{-\beta H} = \int \prod_{t=0}^{N_t-1} \left[\prod_x d\psi^*_{x,t}\, d\psi_{x,t}\, d\eta^*_{x,t}\, d\eta_{x,t} \right] \exp\Big\{ -\delta \Big[\frac{1}{2} \sum_{x,y} Q_{x,t+1,t}\, V_{xy}\, Q_{y,t+1,t}$$
$$- \sum_{\langle x,y \rangle} \kappa(\psi^*_{x,t+1}\psi_{y,t} + \psi^*_{y,t+1}\psi_{x,t} + \eta^*_{y,t+1}\eta_{x,t} + \eta^*_{x,t+1}\eta_{y,t}) + \sum_x m_s(\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t})$$
$$+ \frac{1}{2} \sum_x V_{xx}(\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t}) \Big] - \sum_x \left[\psi^*_{x,t+1}(\psi_{x,t+1} - \psi_{x,t}) + \eta^*_{x,t+1}(\eta_{x,t+1} - \eta_{x,t}) \right] \Big\}$$

Shorthand notation introduced for “charge field”:

$$Q_{x,t,t'} = \psi^*_{x,t}\psi_{x,t'} - \eta^*_{x,t}\eta_{x,t'} \ . \quad (q_x = a^\dagger_x a_x - b^\dagger_x b_x)$$

The graphene path-integral

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After computing all matrix elements:

$$\mathrm{Tr}\, e^{-\beta H} = \int \prod_{t=0}^{N_t-1} \left[\prod_x d\psi^*_{x,t}\, d\psi_{x,t}\, d\eta^*_{x,t}\, d\eta_{x,t} \right] \exp\Big\{ -\delta \Big[\frac{1}{2} \sum_{x,y} Q_{x,t+1,t}\, V_{xy}\, Q_{y,t+1,t}$$
$$- \sum_{\langle x,y \rangle} \kappa(\psi^*_{x,t+1}\psi_{y,t} + \psi^*_{y,t+1}\psi_{x,t} + \eta^*_{y,t+1}\eta_{x,t} + \eta^*_{x,t+1}\eta_{y,t}) + \sum_x m_s(\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t})$$
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First goal achieved: Partition function is expressed as functional integral over Grassmann fields.

But how to proceed?

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Functional integral for partition function of interacting tight-binding theory:

$$Z = \int \mathcal{D}\psi\, \mathcal{D}\psi^*\, \mathcal{D}\eta\, \mathcal{D}\eta^*\ \exp\Big(- S_0[\psi, \psi^*, \eta, \eta^*] - \frac{\delta}{2} \sum_{x,y,t} Q_{x,t+1,t}\, V_{x,y}\, Q_{y,t+1,t} \Big)$$

Shorthand notation (will be used frequently): $\mathcal{D}\phi = \big[\prod_{t=0}^{N_t - 1} \prod_x d\phi_{x,t} \big]$

The graphene path-integral

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Grassmann variables are hard to deal with numerically (complicated representation, no positive-definite measure, ...)

Usual strategy:

- "Integrate out" Grassman fields using Gaussian integration:

  $$\int \big[\prod_{m=1}^{n} d\chi_m^*\, d\chi_m \big]\ \exp\Big(- \sum_{i,j=1}^{n} \chi_i^* H_{ij} \chi_j \Big) \propto [\det H]^{\pm 1}$$

  (+1 for Grassmann numbers, -1 for complex numbers)
- "Fermion determinant" is sampled stochastically (using c-numbers).

The graphene path-integral

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  (+1 for Grassmann numbers, -1 for complex numbers)
- "Fermion determinant" is sampled stochastically (using c-numbers).

However: Interacting term contains fourth powers of fields!

The graphene path-integral

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Hubbard-Stratonovich transformation:

$$\exp\left\{-\frac{\delta}{2}\sum_{t=0}^{N_t-1}\sum_{x,y} Q_{x,t+1,t}\,V_{xy}\,Q_{y,t+1,t}\right\} \propto \int \mathcal{D}\phi\, \exp\left\{-\frac{\delta}{2}\sum_{t=0}^{N_t-1}\sum_{x,y}\phi_{x,t}\,V_{xy}^{-1}\,\phi_{y,t} - i\,\delta\sum_{t=0}^{N_t-1}\sum_{x}\phi_{x,t}\,Q_{x,t+1,t}\right\}.$$

Eliminate fourth powers with auxiliary field $\phi \in \mathbb{R}$ (“Hubbard field”). Applied to Z:

$$Z = \int \mathcal{D}\left[\psi,\psi^*,\eta,\eta^*,\phi\right] \exp\left\{-\delta\sum_{t=0}^{N_t-1}\left[\frac{1}{2}\sum_{x,y}\phi_{x,t}\,V_{xy}^{-1}\,\phi_{y,t} + \sum_{x} i\phi_{x,t}\,Q_{x,t+1,t}\right.\right.$$

$$-\sum_{\langle x,y\rangle}\kappa(\psi^*_{x,t+1}\psi_{y,t} + \psi^*_{y,t+1}\psi_{x,t} + \eta^*_{y,t+1}\eta_{x,t} + \eta^*_{x,t+1}\eta_{y,t}) + \sum_{x} m_s(\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t})$$

$$\left.\left.+\frac{1}{2}\sum_{x} V_{xx}(\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t})\right] - \sum_{t=0}^{N_t-1}\sum_{x}\left[\psi^*_{x,t+1}(\psi_{x,t+1} - \psi_{x,t}) + \eta^*_{x,t+1}(\eta_{x,t+1} - \eta_{x,t})\right]\right\}.$$

The graphene path-integral

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$$Z = \int \mathcal{D}[\psi, \psi^*, \eta, \eta^*, \phi] \exp\Big\{ -\delta \sum_{t=0}^{N_t-1} \Big[\frac{1}{2} \sum_{x,y} \phi_{x,t} V_{xy}^{-1} \phi_{y,t} + \sum_x i\phi_{x,t}(\psi^*_{x,t+1}\psi_{x,t} - \eta^*_{x,t+1}\eta_{x,t})$$

$$- \sum_{\langle x,y \rangle} \kappa(\psi^*_{x,t+1}\psi_{y,t} + \psi^*_{y,t+1}\psi_{x,t} + \eta^*_{y,t+1}\eta_{x,t} + \eta^*_{x,t+1}\eta_{y,t}) + \sum_x m_s(\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t})$$

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Introduce Fermion matrix M:

$$M_{(x,t)(y,t')} = \delta_{xy}(\delta_{tt'} - \delta_{t-1,t'}) - \kappa \frac{\beta}{N_t} \sum_{\vec{n}} \delta_{y,x+\vec{n}} \delta_{t-1,t'} + \left(m_s + \frac{V_{xx}}{2} + i\phi_{x,t} \right) \frac{\beta}{N_t} \delta_{xy} \delta_{t-1,t'}$$

Yields:

$$Z = \int \mathcal{D}[\psi, \psi^*, \eta, \eta^*, \phi] \exp\Big\{ -\frac{\delta}{2} \sum_{t=0}^{N_t-1} \sum_{x,y} \phi_{x,t} V_{xy}^{-1} \phi_{y,t}$$

$$- \sum_{t,t'=0}^{N_t-1} \sum_{x,x'} \left[\psi^*_{x,t} M_{(x,t)(x',t')} \psi_{x',t'} + \eta^*_{x,t} M^*_{(x,t)(x',t')} \eta_{x',t'} \right] \Big\}$$

The graphene path-integral

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Carry out Gaussian integration: $\int \left[\prod_{m=1}^{n} d\chi_m^* \, d\chi_m\right] \exp\left(-\sum_{i,j=1}^{n} \chi_i^* H_{ij} \chi_j\right) \propto [\det H]$

$$Z = \int \mathcal{D}\phi \, \det M^*(\phi) \det M(\phi) \exp\left\{-\frac{\delta}{2} \sum_{t=0}^{N_t-1} \sum_{x,y} \phi_{x,t} V_{xy}^{-1} \phi_{y,t}\right\}$$

$$= \int \mathcal{D}\phi \, \det\left[M(\phi) M^\dagger(\phi)\right] \exp\left\{-\frac{\delta}{2} \sum_{t=0}^{N_t-1} \sum_{x,y} \phi_{x,t} V_{xy}^{-1} \phi_{y,t}\right\}$$

Final form is similar to lattice QCD: Dynamical Bosonic "gauge field" with positive definite measure. Effect of Fermions contained in determinant.

The graphene path-integral

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Final form is similar to lattice QCD: Dynamical Bosonic "gauge field" with positive definite measure. Effect of Fermions contained in determinant.

Observations:

- "Gauge field" is non-compact scalar field (rather than $\in SU(3)$).
- Introducing hole-operators $b_x, b_x^\dagger$ flipped sign of $\mathrm{Im}\,(M)$ for $s = -1$. Change of sign of $b_x, b_x^\dagger$ on sub-lattice "symmetrized" kinetic terms. **Sign-problem circumvented!**

The graphene path-integral

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Side remark: Non-compact field ϕ in det(M) amplifies rounding errors (polynomic contribution). **Numerically unstable!**

The graphene path-integral

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Side remark: Non-compact field ϕ in $\det(M)$ amplifies rounding errors (polynomic contribution). **Numerically unstable!**

Better: Transform to **compact Hubbard field** (additive contribution).

Original Fermion matrix:

$$M_{(x,t)(y,t')} = \delta_{xy}(\delta_{tt'} - \delta_{t-1,t'}) - \kappa\frac{\beta}{N_t}\sum_{\vec{n}}\delta_{y,x+\vec{n}}\delta_{t-1,t'} + \left(m_s + \frac{V_{xx}}{2} + i\phi_{x,t}\right)\frac{\beta}{N_t}\delta_{xy}\delta_{t-1,t'}$$

Fermion matrix with compact Hubbard field:

$$M_{(x,t)(y,t')} = \delta_{xy}(\delta_{tt'} - e^{-i\frac{\beta}{N_t}\phi_{x,t}}\delta_{t-1,t'}) - \kappa\frac{\beta}{N_t}\sum_{\vec{n}}\delta_{y,x+\vec{n}}\delta_{t-1,t'} + m_s\frac{\beta}{N_t}\delta_{xy}\delta_{t-1,t'} \ ,$$

(without proof...)

Hybrid-Monte-Carlo

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Status: Partition function expressed as functional integral over Hubbard ("Coulomb") field. Expression for Fermion matrix $M(\phi)$ obtained.

$$Z = \int \mathcal{D}\phi \, \det\left[M(\phi)M^\dagger(\phi)\right] e^{-S(\phi)} \,, \qquad S(\phi) = \frac{\delta}{2} \sum_{t=0}^{N_t-1} \sum_{x,y} \phi_{x,t} V_{xy}^{-1} \phi_{y,t}$$

$$M_{(x,t)(y,t')} = \delta_{xy}(\delta_{tt'} - e^{-i\frac{\beta}{N_t}\phi_{x,t}}\delta_{t-1,t'}) - \kappa\frac{\beta}{N_t}\sum_{\vec{n}} \delta_{y,x+\vec{n}}\delta_{t-1,t'} + m_s\frac{\beta}{N_t}\delta_{xy}\delta_{t-1,t'} \,,$$

Measure is positive definite!

Goal: Construct algorithm to generate configurations of ϕ, such that

$$P(\phi) = \frac{1}{Z}\det\left[M(\phi)M^\dagger(\phi)\right] e^{-S(\phi)} \,, \quad \langle O\rangle = \int \mathcal{D}\phi \, O(\phi)P(\phi) \,.$$

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Well suited task for application of **Hybrid-Monte-Carlo** method!

- Sample Fermion determinant stochastically using Pseudofermion sources.
- Evolve gauge field through phase-space with fictitious dynamical process.

Hybrid-Monte-Carlo

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Gaussian integration for $\chi \in \mathbb{C}$: $\int \left[\prod_{m=1}^{n} d\chi_m^* \, d\chi_m\right] \exp\left(-\sum_{i,j=1}^{n} \chi_i^* H_{ij} \chi_j\right) \propto [\det H]^{-1}$

Fermion determinant expressed with **Pseudofermion sources**:

$$Z = \int \mathcal{D}\phi \, \det\left[\left(M(\phi)M^\dagger(\phi)\right)^{-1}\right]^{-1} \exp\left\{-\frac{\delta}{2}\sum_{t=0}^{N_t-1}\sum_{x,y}\phi_{x,t}\,V_{xy}^{-1}\,\phi_{y,t}\right\}$$

$$= \int \mathcal{D}\phi\,\mathcal{D}\chi\,\mathcal{D}\chi^* \exp\left\{-\frac{\delta}{2}\sum_{t=0}^{N_t-1}\sum_{x,y}\phi_{x,t}\,V_{xy}^{-1}\,\phi_{y,t} - \sum_{t,t'=0}^{N_t-1}\sum_{x,x'}\chi^*_{x,t}(MM^\dagger)^{-1}_{(x,t)(x',t')}\chi_{x',t'}\right\}.$$

Inverse of $MM^\dagger$ introduced.

Hybrid-Monte-Carlo

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Inverse of $MM^\dagger$ introduced.

Introduce momentum field π (conjugate of ϕ):

$$\mathcal{H} = \frac{\delta}{2}\sum_{t=0}^{N_t-1}\sum_{x,y}\phi_{x,t}V_{xy}^{-1}\phi_{y,t} + \sum_{t,t'=0}^{N_t-1}\sum_{x,x'}\chi^*_{x,t}(MM^\dagger)^{-1}_{(x,t)(x',t')}\chi_{x',t'} + \frac{1}{2}\sum_{t=0}^{N_t-1}\sum_{x}\pi^2_{x,t}.$$

Shothand in vector/matrix notation: $\mathcal{H} = \frac{\delta}{2}\phi^T V^{-1}\phi + \chi^\dagger(MM^\dagger)^{-1}\chi + \frac{\pi^T\pi}{2}$

Hybrid-Monte-Carlo

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Summary of algorithm (repeat following steps):

- Update momentum π using Gaussian noise: $P(\pi) \sim e^{-\pi^2/2}$.
- Update χ by generating $\rho \in \mathbb{C}$ with $P(\rho) = e^{-\rho^\dagger \rho}$ and obtaining $\chi = M\rho$.
- Evolve ϕ, π by integrating Hamilton equations: $\left[\frac{d\phi}{d\tau}\right]^T = \frac{\partial \mathcal{H}}{\partial \pi}$, $\left[\frac{d\pi}{d\tau}\right]^T = -\frac{\partial \mathcal{H}}{\partial \phi}$. ("molecular dynamics"). Symplectic integrator is used (introduces error $\Delta\mathcal{H}$)!
- Metropolis check to correct error: Accept new ϕ, π with $P = \min(1, e^{-\Delta\mathcal{H}})$.

Hybrid-Monte-Carlo

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- Metropolis check to correct error: Accept new ϕ, π with $P = \min(1, e^{-\Delta\mathcal{H}})$.

Symplectic integrator (e.g. "Leapfrog"):

- Approximate time-derivatives with differences:
  $\frac{d\phi}{d\tau} \approx \frac{1}{\epsilon}[\phi(\tau+\epsilon) - \phi(\tau)] \equiv \frac{1}{\epsilon}(\phi_{\tau+1} - \phi_\tau)$, $\frac{d\pi}{d\tau} \approx \frac{1}{\epsilon}[\pi(\tau+\epsilon) - \pi(\tau)] \equiv \frac{1}{\epsilon}(\pi_{\tau+1} - \pi_\tau)$.
- Define position steps $V_\phi(\epsilon)$ and momentum steps $V_\pi(\epsilon)$:
  $V_\phi(\epsilon) \;:\; \phi_{\tau+1} = \phi_\tau + \epsilon(\partial\mathcal{H}/\partial\pi)^T$, $V_\pi(\epsilon) \;:\; \pi_{\tau+1} = \pi_\tau - \epsilon(\partial\mathcal{H}/\partial\phi)^T$.
- Leapfrog integration: Iterate $V_\pi(\epsilon/2)V_\phi(\epsilon)V_\pi(\epsilon/2)$ or $V_\phi(\epsilon/2)V_\pi(\epsilon)V_\phi(\epsilon/2)$.
- Error $\Delta\mathcal{H}$ depends on ϵ and length of MD trajectory!

Hybrid-Monte-Carlo

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Last ingredient: Right-hand sides of Hamilton's equations ("Force terms").

$$\left[\frac{d\phi}{d\tau}\right]^T = \frac{\partial \mathcal{H}}{\partial \pi}\,, \quad \left[\frac{d\pi}{d\tau}\right]^T = -\frac{\partial \mathcal{H}}{\partial \phi}\,.$$

Required for Leapfrog steps: $\phi_{\tau+1} = \phi_\tau + \epsilon(\partial\mathcal{H}/\partial\pi)^T\,, \quad \pi_{\tau+1} = \pi_\tau - \epsilon(\partial\mathcal{H}/\partial\phi)^T\,.$

Are obtained from:

$$\mathcal{H} = \frac{\delta}{2}\phi^T V^{-1}\phi + \chi^\dagger (MM^\dagger)^{-1}\chi + \frac{\pi^T\pi}{2}$$

Hybrid-Monte-Carlo

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Are obtained from:

$$\mathcal{H} = \frac{\delta}{2}\phi^T V^{-1}\phi + \chi^\dagger (MM^\dagger)^{-1}\chi + \frac{\pi^T\pi}{2}$$

Useful identities (ρ/ϕ = vectors, A = symmetric matrix which doesn't depend on ρ):

$$\frac{d(\sigma^T\sigma)}{d\rho} = 2\,\sigma^T\frac{d\sigma}{d\rho}\,, \quad \frac{d(\rho^T A\rho)}{d\rho} = 2\,\rho^T A$$

Leads to:

$$\left[\frac{d\phi}{d\tau}\right]^T = \frac{\partial\mathcal{H}}{\partial\pi} = \pi^T\,, \quad \left[\frac{d\pi}{d\tau}\right]^T = -\frac{\partial\mathcal{H}}{\partial\phi} = -\delta\,\phi^T V^{-1} - \frac{\partial}{\partial\phi}\left[\chi^\dagger(MM^\dagger)^{-1}\chi\right] \equiv F_\phi + F_\chi\,.$$

"Gauge/Fermion force". To do: Evaluate F_χ component-wise!

Hybrid-Monte-Carlo

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Useful identities (s is scalar, U and V are matrices which depend on s):

$$\frac{dU^{-1}}{ds} = -U^{-1}\frac{dU}{ds}U^{-1}\,, \quad \frac{d(UV)}{ds} = U\frac{dV}{ds} + \frac{dU}{ds}V$$

Shorthand notations: $\eta = (MM^\dagger)^{-1}\chi\,, \quad \xi = M^{-1}\chi = M^\dagger\eta\,.$

Computation of Fermion force:

$$(F_\chi)_k = -\frac{\partial}{\partial\phi_k}\left[\chi^\dagger(MM^\dagger)^{-1}\chi\right] = -\chi^\dagger\left[\frac{\partial(MM^\dagger)^{-1}}{\partial\phi_k}\right]\chi = \chi^\dagger(MM^\dagger)^{-1}\left[\frac{\partial(MM^\dagger)}{\partial\phi_k}\right](MM^\dagger)^{-1}\chi$$

$$= \chi^\dagger(MM^\dagger)^{-1}\left[\frac{\partial M}{\partial\phi_k}M^\dagger + M\frac{\partial M^\dagger}{\partial\phi_k}\right](MM^\dagger)^{-1}\chi = \eta^\dagger\frac{\partial M}{\partial\phi_k}\xi + \xi^\dagger\frac{\partial M^\dagger}{\partial\phi_k}\eta = 2\,\mathrm{Re}\left[\eta^\dagger\frac{\partial M}{\partial\phi_k}\xi\right]$$

Precise form of F_χ depends on the choice of M!

Non-compact Hubbard field: $(F_\chi)_{(x,t)} = -2\frac{\beta}{N_t}\mathrm{Im}\left[\eta^*_{(x,t)}\xi_{(x,t-1)}\right]$

Compact Hubbard field: $(F_\chi)_{(x,t)} = -2\frac{\beta}{N_t}\mathrm{Im}\left[\eta^*_{(x,t)}e^{-i\frac{\beta}{N_t}\phi_{x,t}}\xi_{(x,t-1)}\right]$

Part III - Results

Semimetal-insulator phase transition

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Of immediate interest for application: **Do interactions generate band-gap?**

Semimetal-insulator phase transition

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Order parameter: Difference of spin-density "chiral condensate" (or charge-density) on triangular sublattices.

$$\Delta_N = n_A - n_B = \frac{1}{N_x N_y}\left\{ \sum_{x\in X_A} (a^\dagger_{x,1} a_{y,1} - a^\dagger_{x,-1} a_{y,-1}) - \sum_{x\in X_B} (a^\dagger_{x,1} a_{y,1} - a^\dagger_{x,-1} a_{y,-1}) \right\}.$$

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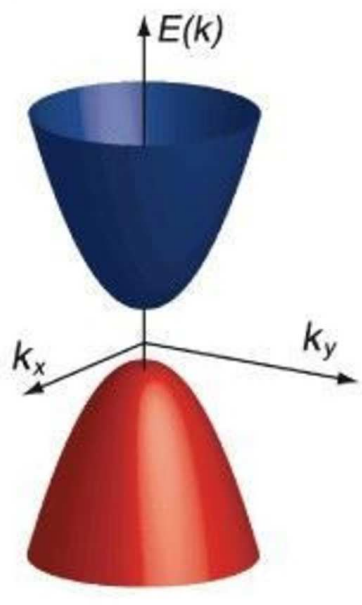
Substrate generates re-scaling of effective coupling constant:
$\alpha_{\text{eff}} \to \alpha_{\text{eff}}/\epsilon \approx 2.2/\epsilon$

Expectation: Gapped phase for $\alpha_{\text{eff}}/\epsilon > \alpha_c$. **Is α_c smaller than upper-bound given by suspended graphene ($\alpha_c < 2.2$)?**

Calculations/simulations with $V(r) = 1/r$ yield $\alpha_c \approx 1.0$. But: Experiments suggest suspended graphene is conductor.

Discrepancy likely due to wrong assumption about $V(r)$.



Semimetal-insulator phase transition

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Interactions are screened by lower orbitals!

Screening by (lower) σ-band electrons calculated in constrained random phase approximation (cRPA):

Wehling et al.
Phys.Rev. Lett. 106, 236805 (2011)

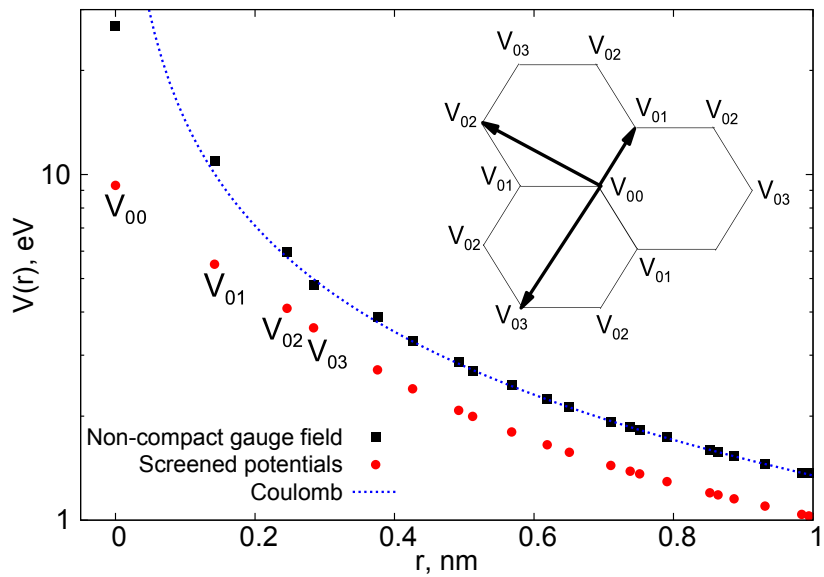
Results for on-site (V_{00}), nearest-neighbor (V_{01}), next-nearest-neighbor (V_{02}) and third-nearest-neighbor (V_{03}) potentials!

Ulybyshev et al.
Phys.Rev. Lett. 111, 056801 (2013)

$$V(r) = \begin{cases} V_{00}, V_{01}, V_{02}, V_{03} & : r \leq 2a \\ e^2/(1.4\,r) & : r > 2a \end{cases},$$

Simulations show: $\alpha_c \approx 3.14\ (\gg 2.2)$ **!**

But: Screening isn't constant at large r.
Might be a problem...



Semimetal-insulator phase transition

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Our follow-up work: Use di-electric screening function at long distances!

$$\epsilon^{-1}(\vec{k}) = \frac{1}{\epsilon_1}\frac{\epsilon_1 + 1 + (\epsilon_1 - 1)e^{-kd}}{\epsilon_1 + 1 - (\epsilon_1 - 1)e^{-kd}}$$

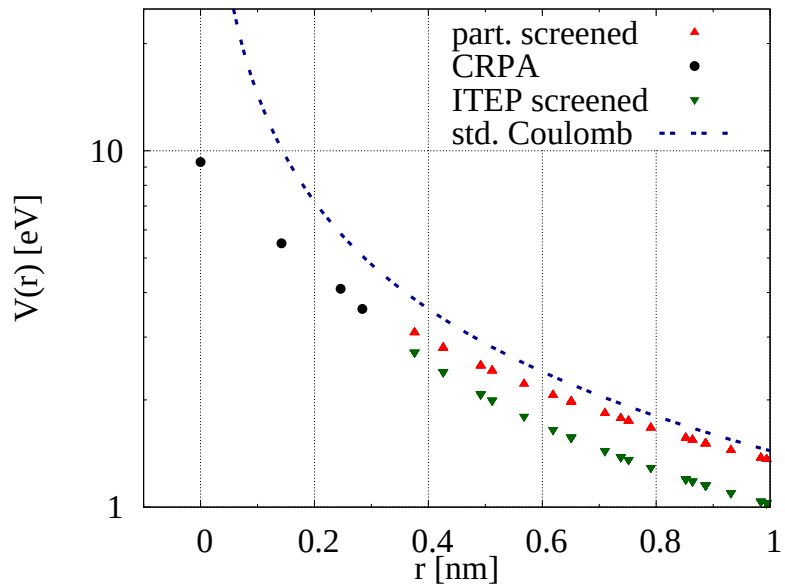
Wehling et al.
Phys.Rev. Lett. 106, 236805 (2011)

($\epsilon_1 = 2.4$ and $d = 2.8\text{Å}$)

Obtain partially screened potential from Fourier back-transform of $\widetilde{V}_0(\vec{k}) = (2\pi e^2)/k$:

$$V(\vec{r}) = \frac{1}{(2\pi)^2}\int_{\mathbb{K}^2} d^2k\, \widetilde{V}_0(\vec{k})\,\epsilon^{-1}(\vec{k})\,e^{-i\vec{k}\vec{r}}$$

$$= e^2 \int_0^\infty dk\, \epsilon^{-1}(\vec{k})\, J_0(kr)\ .$$



Asymptotically approaches unscreened potential.

Results recently published: DS, von Smekal, Phys. Rev. B 89, 195429 (2014)

Semimetal-insulator phase transition

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Order-parameter: Spin-density difference.

$$\Delta_N = n_A - n_B = \frac{1}{L_x L_y}\left\{ \sum_{x\in X_A} (a_x^\dagger a_x + b_x^\dagger b_x) - \sum_{x\in X_B} (a_x^\dagger a_x + b_x^\dagger b_x)\right\}, \quad \langle \Delta_N \rangle = \frac{1}{Z}\mathrm{Tr}\left[\Delta_N e^{-\beta H}\right],$$

Functional integral representation:

$$\langle \Delta_N \rangle = \frac{1}{N_t L_x L_y Z}\int \mathcal{D}[\psi,\psi^*,\eta,\eta^*]\left\{ \sum_{X_A,t} \left(\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t}\right) - \sum_{X_B,t} \left(\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t}\right)\right\} e^{-\beta H}$$

$$= \frac{-1}{\beta L_x L_y Z}\frac{\partial}{\partial m}\int \mathcal{D}[\psi,\psi^*,\eta,\eta^*]\, e^{-\beta H} = \frac{-1}{\beta L_x L_y}\frac{1}{Z}\frac{\partial Z}{\partial m}$$

Reminder:

$$Z = \int \mathcal{D}[\psi,\psi^*,\eta,\eta^*,\phi] \exp\left\{ -\frac{\beta}{N_t}\sum_{t=0}^{N_t-1}\left[\ldots + \sum_x m_s(\psi^*_{x,t+1}\psi_{x,t} + \eta^*_{x,t+1}\eta_{x,t}) + \ldots \right] - \ldots \right\}$$

Analogous to chiral condensate in QCD!

Semimetal-insulator phase transition

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Carry out derivative: $\left(\frac{d}{dx}\det[A] = \det[A]\mathrm{Tr}\left[\frac{dA}{dx}A^{-1}\right]\ ,\ \frac{d(UV)}{ds} = U\frac{dV}{ds} + \frac{dU}{ds}V\right) \quad V \equiv L_x L_y$

$$\langle \Delta_N \rangle = \frac{-1}{\beta V Z}\frac{\partial}{\partial m}\int \mathcal{D}\phi \det\left(MM^\dagger\right) e^{-S[\phi]} = \frac{-2}{\beta V Z}\int \mathcal{D}\phi \det\left(MM^\dagger\right)\mathrm{ReTr}\left[M^{-1}\frac{\partial M}{\partial m}\right] e^{-S[\phi]}$$

$$= \frac{-2}{N_t V}\sum_{t=0}^{N_t-1}\mathrm{Re}\left\langle \sum_{x\in X_A} M^{-1}_{(x,t)(x,t+1)} - \sum_{x\in X_B} M^{-1}_{(x,t)(x,t+1)}\right\rangle .$$

Reminder:

$$M_{(x,t)(y,t')} = \delta_{xy}(\delta_{tt'} - e^{-i\frac{\beta}{N_t}\phi_{x,t}}\delta_{t-1,t'}) - \kappa\frac{\beta}{N_t}\sum_{\vec{n}}\delta_{y,x+\vec{n}}\delta_{t-1,t'} + m_s\frac{\beta}{N_t}\delta_{xy}\delta_{t-1,t'}\ ,$$

Technical remark: Expectation value is of the form $\langle \Delta_N \rangle = \mathrm{Re}\,\langle \mathrm{Tr}\,[A]\rangle$. Trace is computed using **noisy estimators** (random noise vectors ρ_i).

$$\langle \mathrm{Tr}\,[A]\rangle = \frac{1}{N}\sum_i^N \rho_i^\dagger A \rho_i\ , \quad P(\rho) = e^{-\rho^\dagger\rho}$$

Semimetal-insulator phase transition

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Two different setups:

(a) Potential as ITEP (constant screening at large r, cRPA at small r).
Goal: Reproduction and consistency check.

(b) Partially screened Coulomb potential.
Goal: Improved results!

Interaction strength controlled by re-scaling of α_{eff}.

"di-electric constant": $\epsilon \approx 2.2/\alpha_{\text{eff}}, \quad \alpha_{\text{eff}} \to \alpha_{\text{eff}}/\epsilon \qquad (V(r) \to V(r)/\epsilon)$

Parameters:

- $N_x = N_y = 18$
- $\alpha_{eff} \approx 2.0 \ldots 5.0$ ($\epsilon = 0.45 \ldots 1.0$)
- $m = 0.1, 0.2, 0.3, 0.4, 0.5\,\text{eV}$
- $T \approx 5.8 \cdot 10^3\,\text{K}$, (low temperature phase)
- Several hundreds of independent Δ_N measurements.

Semimetal-insulator phase transition

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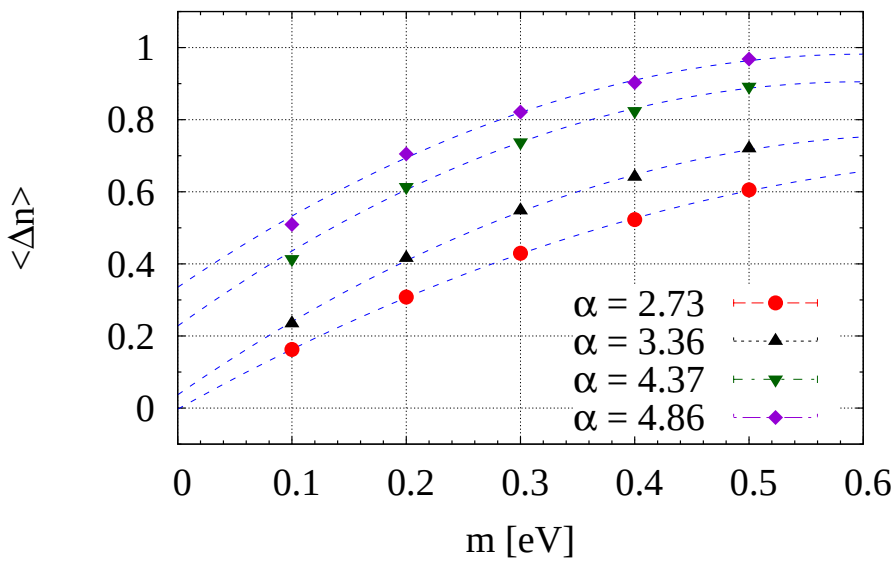
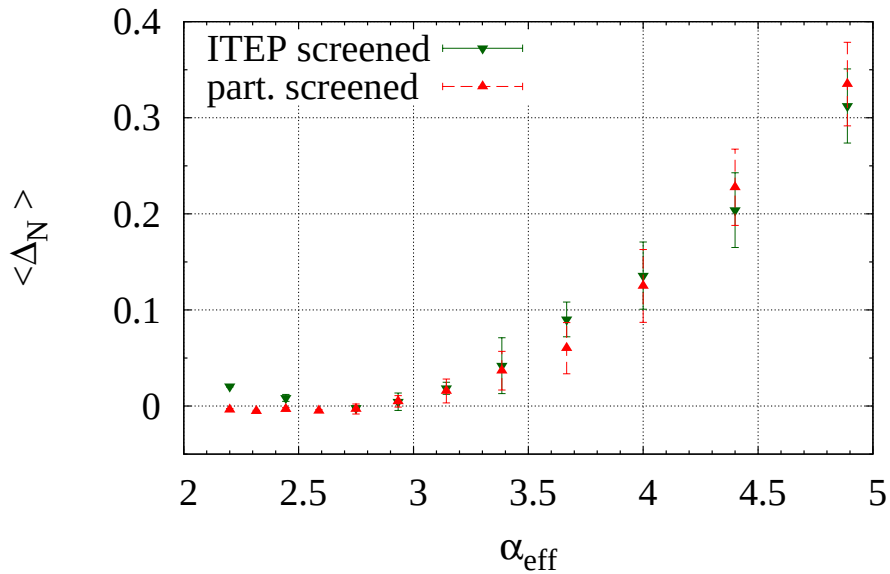
"Chiral limit": $m \to 0$ extrapolation done with $\langle \Delta_N \rangle = a_0 + a_1 m + a_2 m^2$.





Phase transition sets in around $\alpha \approx 3.0 \gg 2.2$.
Far in unphysical regime! **No significant difference between two setups!**

Semimetal-insulator phase transition

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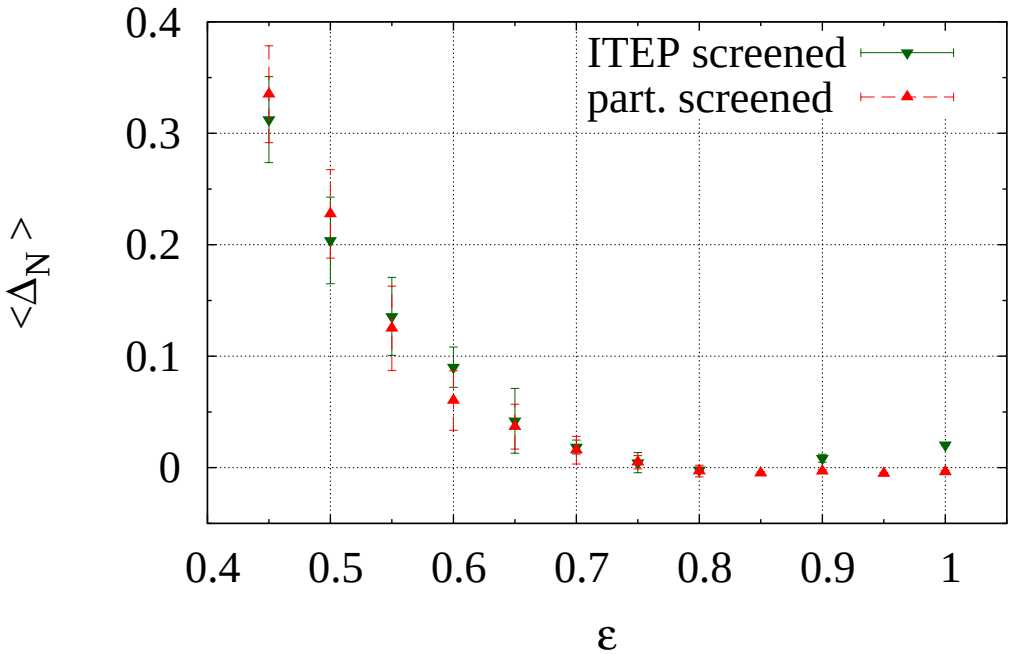
Expressed in terms of di-electric screening $\epsilon \approx 2.2/\alpha_{\text{eff}} = 0.45 \ldots 1.0$:



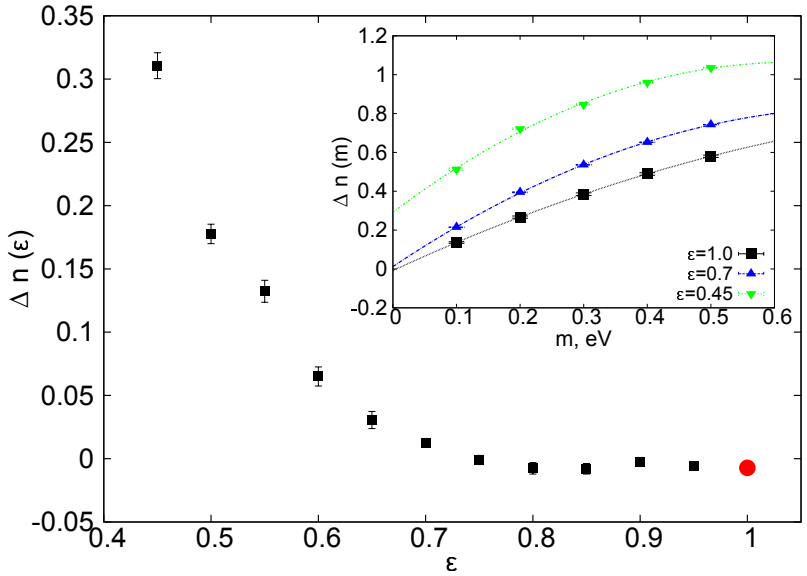


Figure on right: Ulybyshev et al. (ITEP), Phys.Rev. Lett. 111, 056801 (2013).
Clearly consistent!

Results indicate long-range tails don't matter much on $N_x = N_y = 18$.

Semimetal-insulator phase transition

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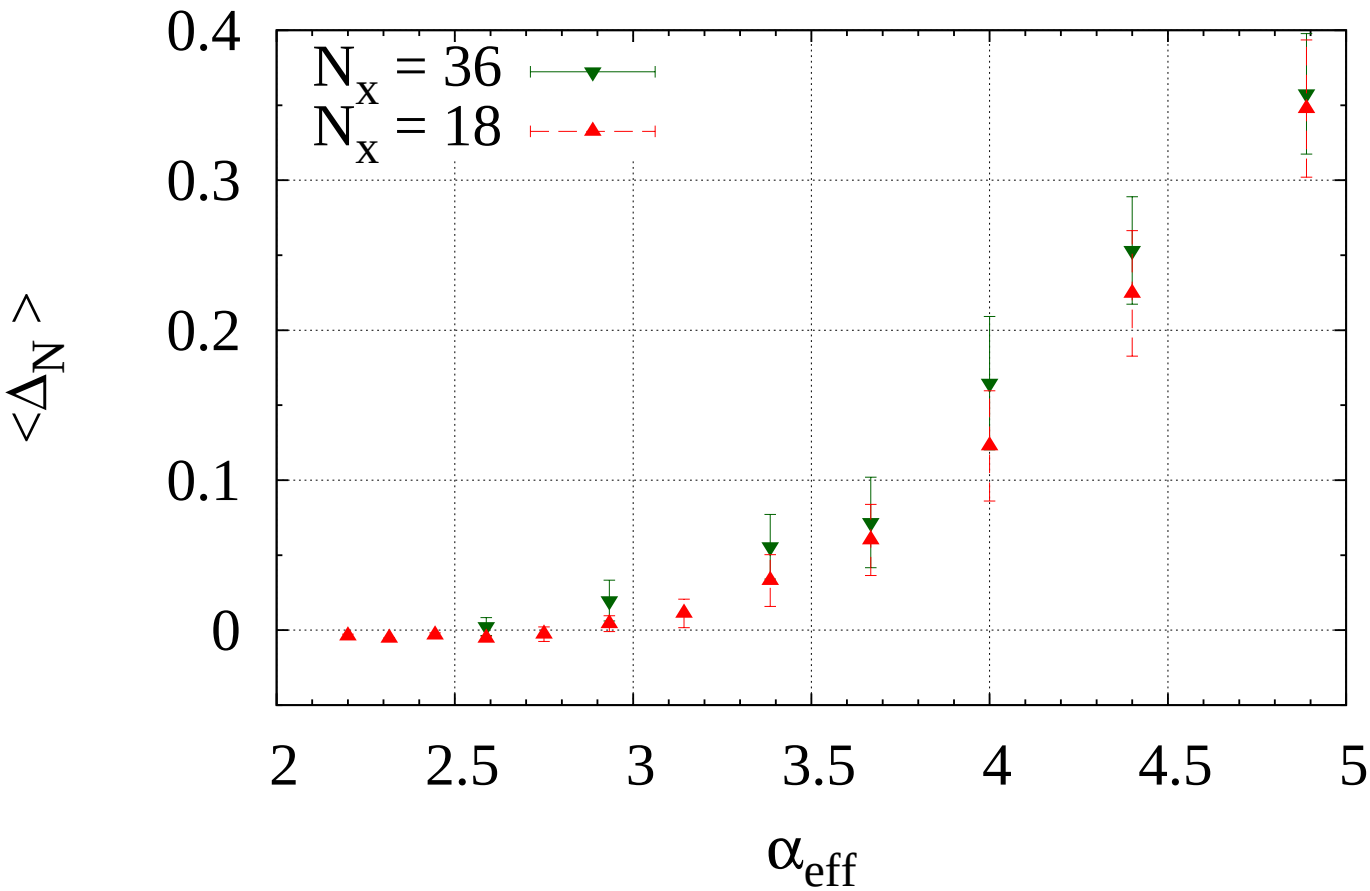
Currently checking volume effects ($N_x, N_y \to 36$). Maybe relevant...



Neck-disrupting Lifshitz transition

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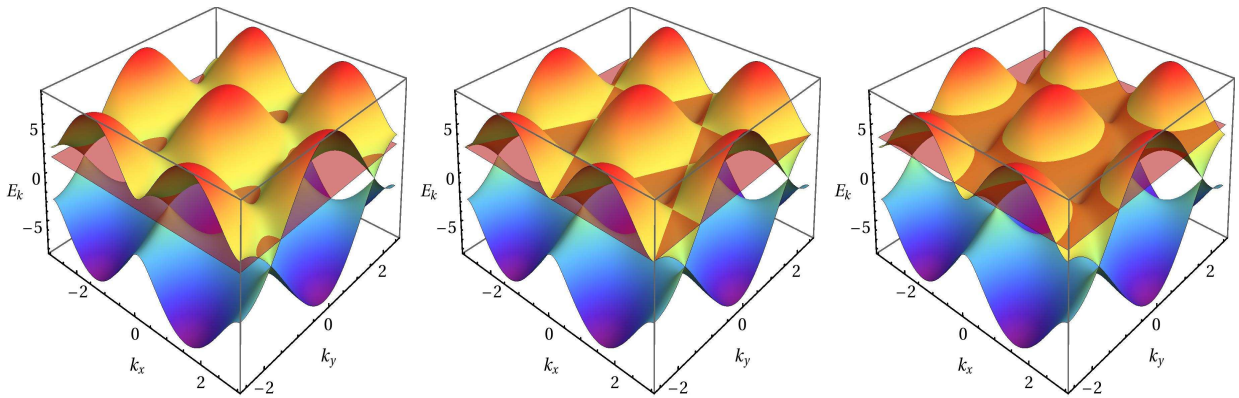
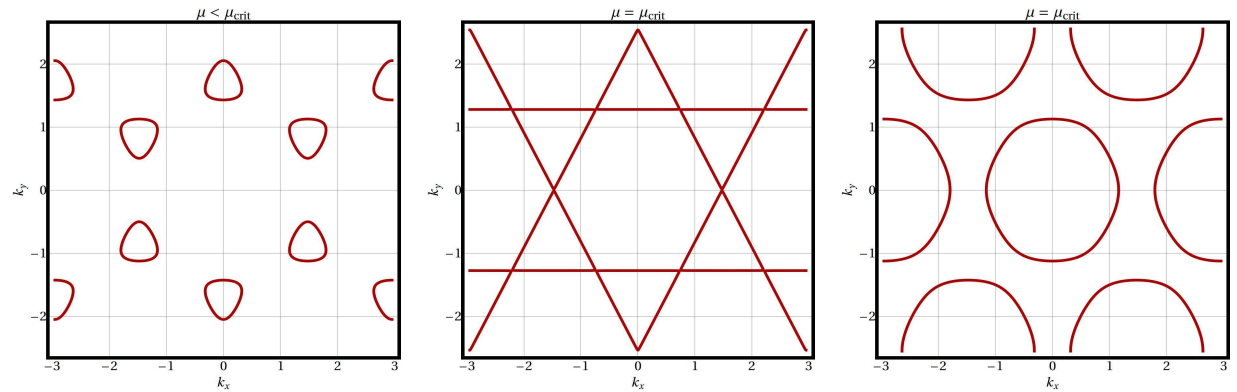
Adding a chemical potential μ shifts the Fermi level in non-interacting theory!
Topology of iso-energy lines changes when crossing saddle-points at $\mu = \mu_c$.





$$\hat{H}_{tb} \rightarrow \hat{H}_{tb} + \mu \sum_{i,s} \hat{n}$$

$$\hat{n} = \hat{a}^{\dagger}_{i,s} \hat{a}_{i,s}$$

Left: $\mu < \mu_c$

Middle: $\mu = \mu_c$

Right: $\mu > \mu_c$

Topological “Neck-disrupting Lifshitz transition” occurs. (Figures by M. Körner)

Neck-disrupting Lifshitz transition

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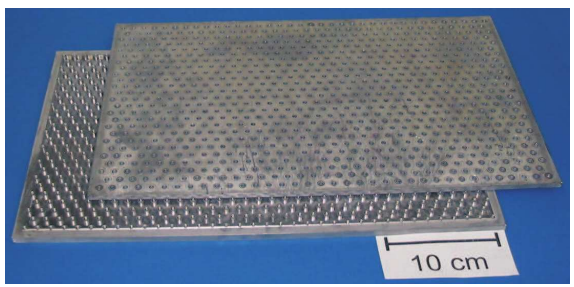
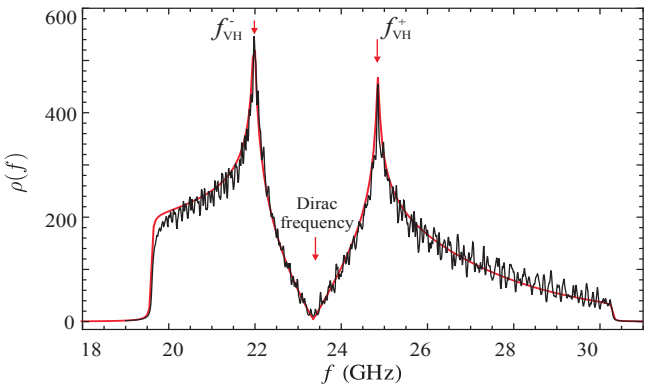
Density of states: $\rho(E) = \int_{BZ} \frac{d\vec{k}}{\left|\nabla_k E(\vec{k})\right|} \delta(E - E(\vec{k}))$

Diverges for $E = \mu_c$ (**"Van-Hove singularity"**). Can be observed e.g. with photonic crystals (microwave billiards):





Dietz et al., Phys. Rev. B 88, 104101 (2013)

Not observed in real graphene (with interactions). Why?

Goal: Study effect of interactions on Lifshitz-transition through simulation.

Neck-disrupting Lifshitz transition

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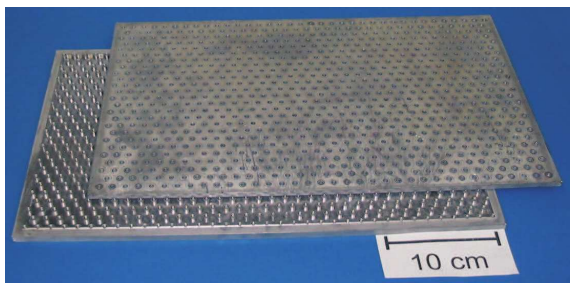

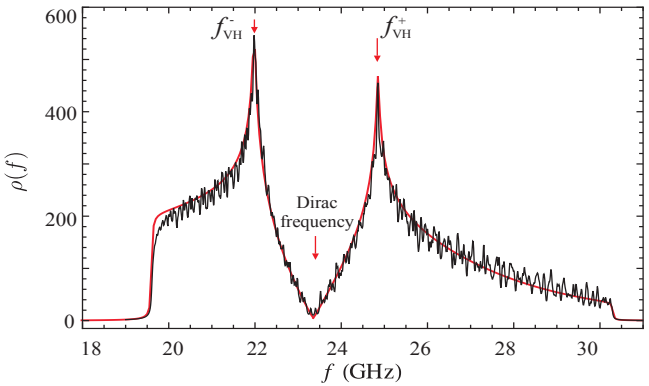

Dietz et al., Phys. Rev. B 88, 104101 (2013)

Not observed in real graphene (with interactions). Why?

Goal: Study effect of interactions on Lifshitz-transition through simulation.

However: Finite μ creates sign-problem. $Z = \int \mathcal{D}\phi \, \det\left[M(\phi)M^\dagger(\phi)\right] e^{-S(\phi)}$

$$M \to M + \mu \frac{\beta}{N_t} \mathbb{1} = M_\mu \,, \qquad M^\dagger \to M^\dagger - \mu \frac{\beta}{N_t} \mathbb{1} \neq M_\mu^\dagger$$

Neck-disrupting Lifshitz transition

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Sign-problem can be circumvented with spin-dependent μ:

$$\hat{H}_{tb} \rightarrow \hat{H}_{tb} + \mu \sum_{i,s} s\, \hat{n}\,, \quad s = \pm 1\,.$$

Leads to: $M \rightarrow M + \mu \frac{\beta}{N_t} \mathbb{1} = M_\mu\,, \quad M^\dagger \rightarrow M^\dagger + \mu \frac{\beta}{N_t} \mathbb{1} = M_\mu^\dagger$ **No sign-problem!**

Neck-disrupting Lifshitz transition

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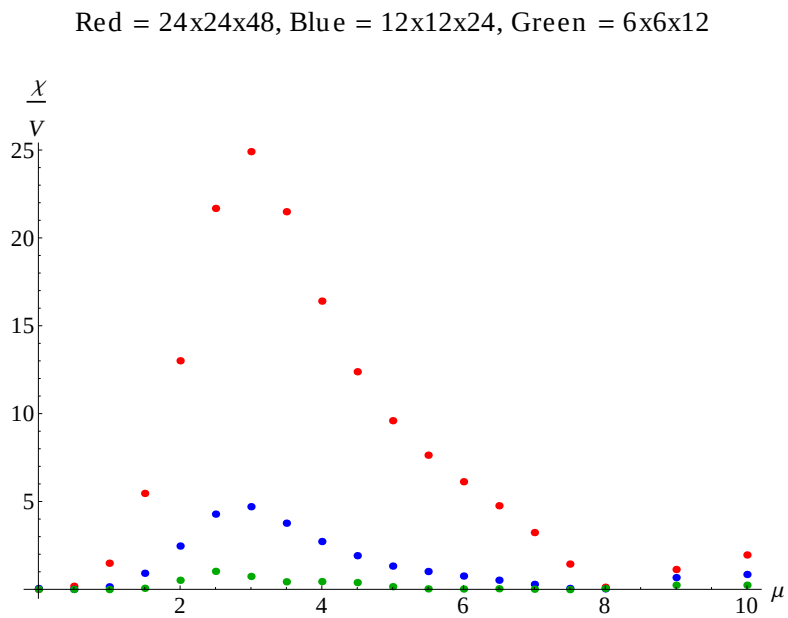
Leads to: $M \rightarrow M + \mu \frac{\beta}{N_t} \mathbb{1} = M_\mu\,, \quad M^\dagger \rightarrow M^\dagger + \mu \frac{\beta}{N_t} \mathbb{1} = M_\mu^\dagger$ **No sign-problem!**

Lifshitz-transition in non-interacting model is blind to sign of spin. Results:

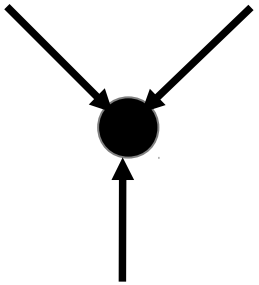
- Number susceptibility: $\chi = -\frac{\beta}{V} \frac{\partial^2}{\partial \mu^2} \log Z$ (related to $\rho(\mu)$)
- $\epsilon = 5000 \rightarrow \alpha_{\mathit{eff}} \approx 0$ (pure tight-binding)
- Peak position correct!
- What happens at finite α_{eff}?

(Figure by M. Körner) **Preliminary!**



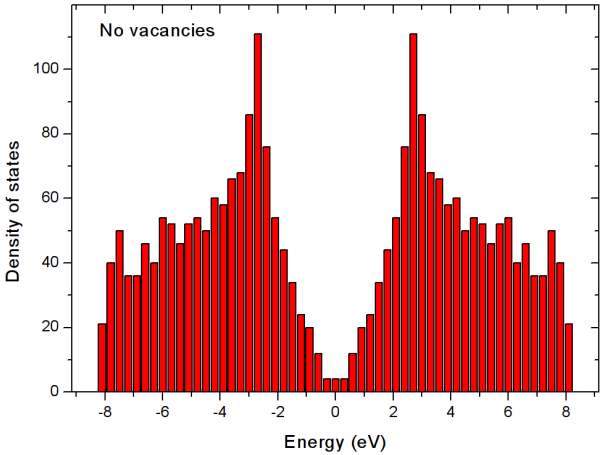
Graphene with vacancies

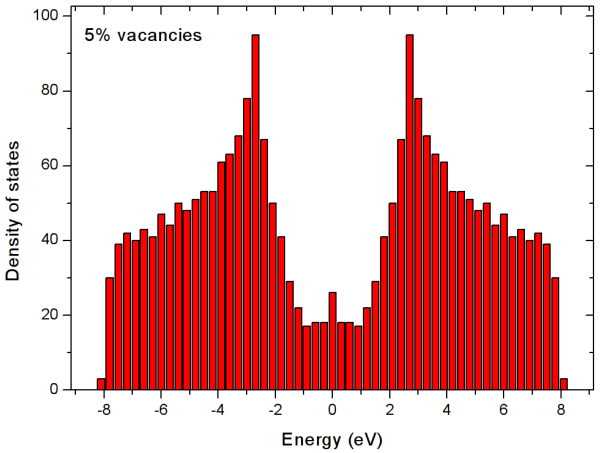
M. V. Ulybyshev (ITEP, Moscow and Regensburg University)



Hoppings are equal to zero for all links connecting vacant site with its neighbors. Charge of the site is also zero.

Approximately corresponds to Hydrogen adatoms.



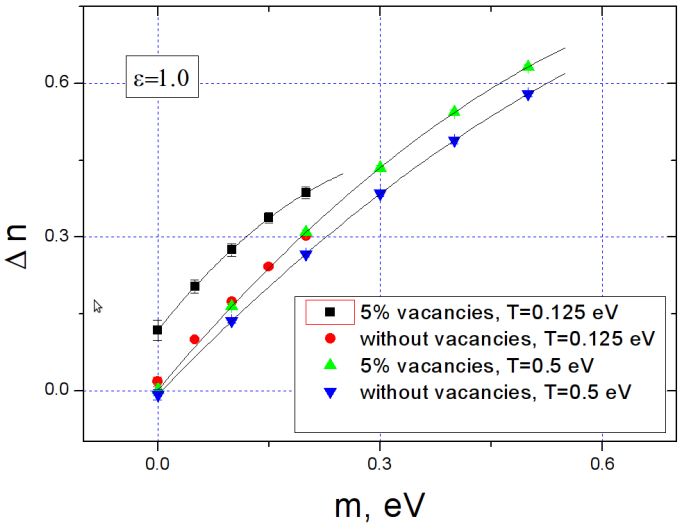


They work very similar to instantons in QFT because near-zero energy states appear in the vicinity of vacant sites. Increasing of the Density of states at Fermi-points will probably lead to instability with respect to formation of some condensate (mean field arguments, analogy to Banks-Casher relation in QCD).

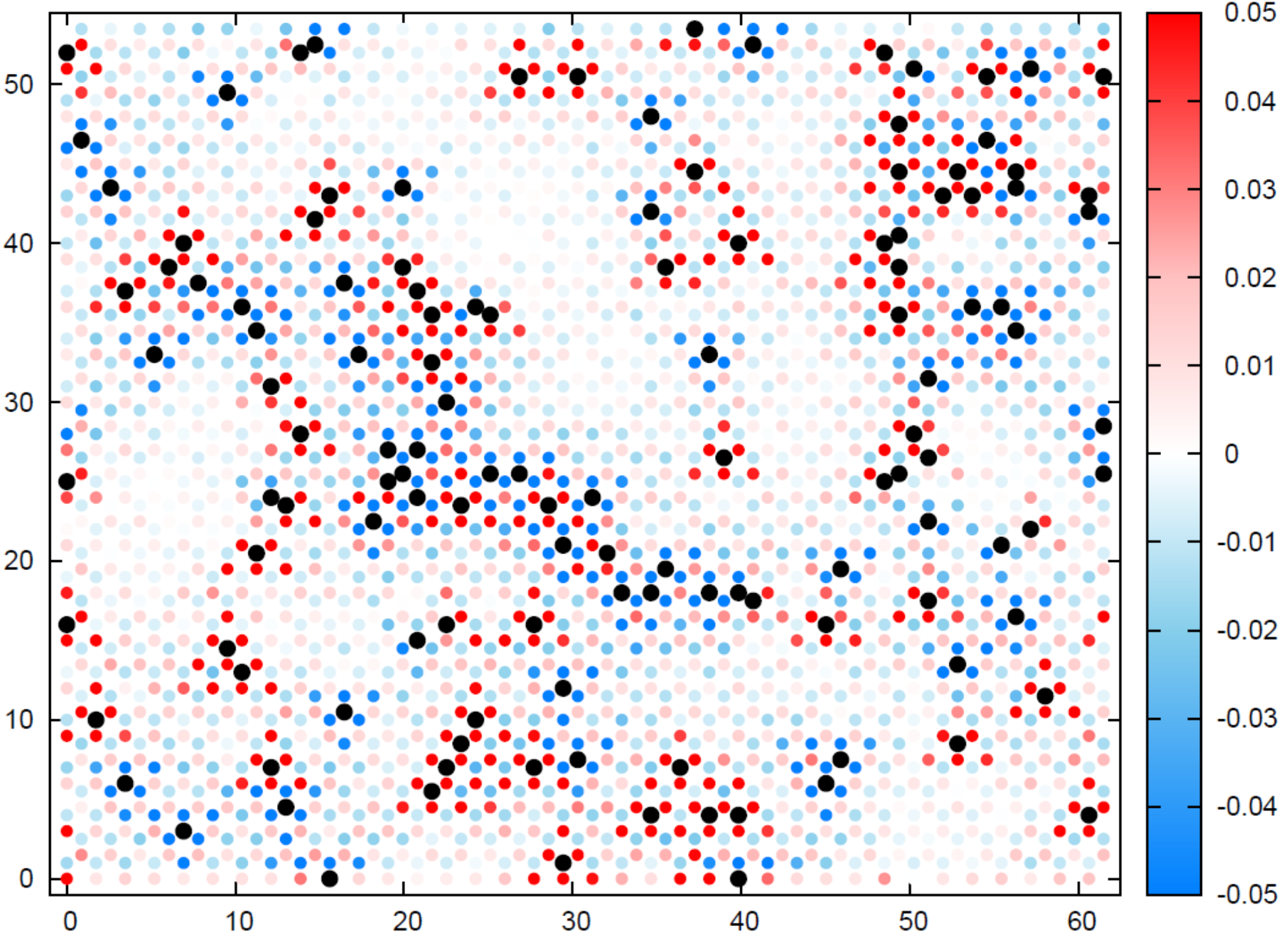
Antiferromagnetic condensate measurements at different temperatures without vacancies and in presence of 5% vacancies (suspended graphene):

Lattice size is 36 x 36 x 80.

Temperature suppresses the effect of vacancies.



Distribution of electron spin



Conclusion

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Past: Investigation of spin-density wave formation concluded (except volume effects).

DS, von Smekal,
Phys. Rev. B 89, 195429 (2014)

Present: Study Neck-disrupting Lifshitz transition.

Future: Additional problems (perhaps external fields, phonons etc.)

Thanks for coming!