Tight-binding theory of graphene with partially screened Coulomb interactions

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Outline

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- Introduction / Details of HMC simulation
- Semimetal-Insulator phase transition
- Neck-disrupting Lifshitz transition
- Summary & Outlook

Introduction

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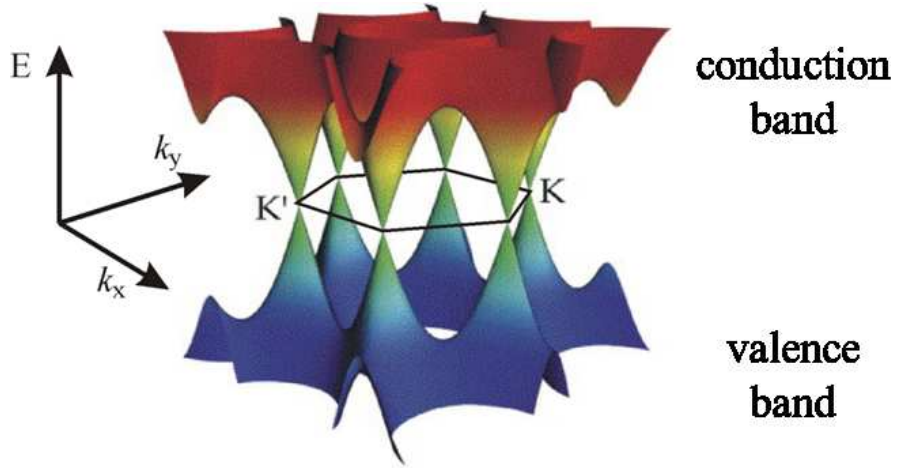
Many properties of graphene are well understood in limit of vanishing two-body interactions.

$$H_{\mathrm{TB}} = \sum_{\langle x,y\rangle,s} (-\kappa)(a^\dagger_{x,s} a_{y,s} + a^\dagger_{y,s} a_{x,s}) \quad , \{a_\mu, a_\nu\} = \{a^\dagger_\mu, a^\dagger_\nu\} = 0 \quad , \{a^\dagger_\mu, a_\nu\} = \delta_{\mu\nu}$$

- Well described by tight-binding theory.
- Conical dispersion at low energies.
- Low energy effective Dirac theory.
- Van Hove singularity at saddle points.
- Semi-metallic behavior (no band gap).
- ...



Include EM interaction: $H = H_{\mathrm{TB}} + H_{\mathrm{INT}}$.

Since $v_F \approx c/300$, $\rightarrow \alpha_{\mathrm{eff}} = e^2/(\hbar v_F) \approx 2.2$

Strongly coupled (difficult, no perturbation theory etc.). Phenomenology much less clear!

Introduction

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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)

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)

Hybrid Monte-Carlo simulation of interacting tight-binding theory

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Tight-binding theory with non-local interactions ($v_F \approx c/300 \ll c$) :

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

Add "staggered" mass to break sublattice ("chiral") symmetry explicitly:

$$H \to H + \sum_x m_S (a^\dagger_{x,1} a_{y,1} - a^\dagger_{x,-1} a_{y,-1}) \quad (m_S = \pm m, x \in A, B)$$

Express partition function with **Fermionic coherent states**: $|\xi\rangle = e^{-\sum_\alpha \xi_\alpha a^\dagger_\alpha}|0\rangle$

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

Timelike lattice-spacing is $\delta = \beta/N_t$, leading error is $\mathcal{O}(\delta^2)$.

Express interaction term with **Hubbard-Stratonovic field**:

$$\exp\left\{-\tfrac{\delta}{2}\sum_{x,y} q_x V_{xy} q_y\right\} \propto \int \left[\prod_x \phi_x\right] \exp\left\{-\tfrac{\delta}{2}\sum_{x,y} \phi_x V^{-1}_{xy} \phi_y - i\,\delta \sum_x \phi_x q_x\right\}$$

Hybrid Monte-Carlo simulation of interacting tight-binding theory

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After integrating out Fermionic fields:

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

Fermion matrix:

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

Components of HMC simulation (force terms etc.) and observables (derivatives of Z) can easily be derived.

Features:

- Non-compact scalar "gauge field" ϕ.
- Potential V_{xy} can be chosen at will (positive definite).
- No sign problem (for $\mu = 0$).
- ...

Semimetal-insulator phase transition

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

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

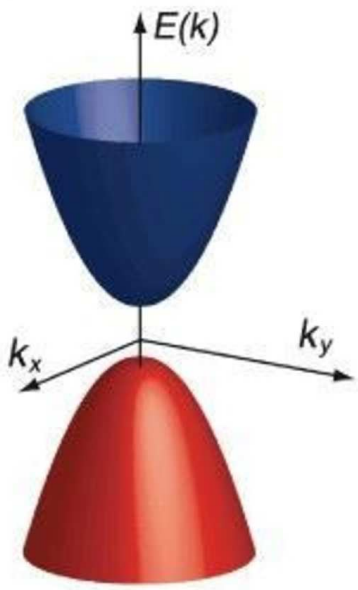
$$\Delta_N = n_A - n_B = \frac{1}{N_x N_y}\Big\{ \sum_{x\in X_A} (a^\dagger_{x,1} a_{y,1} - a^\dagger_{x,-1} a_{y,-1}) - \sum_{x\in X_B} (a^\dagger_{x,1} a_{y,1} - a^\dagger_{x,-1} a_{y,-1}) \Big\}.$$

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)

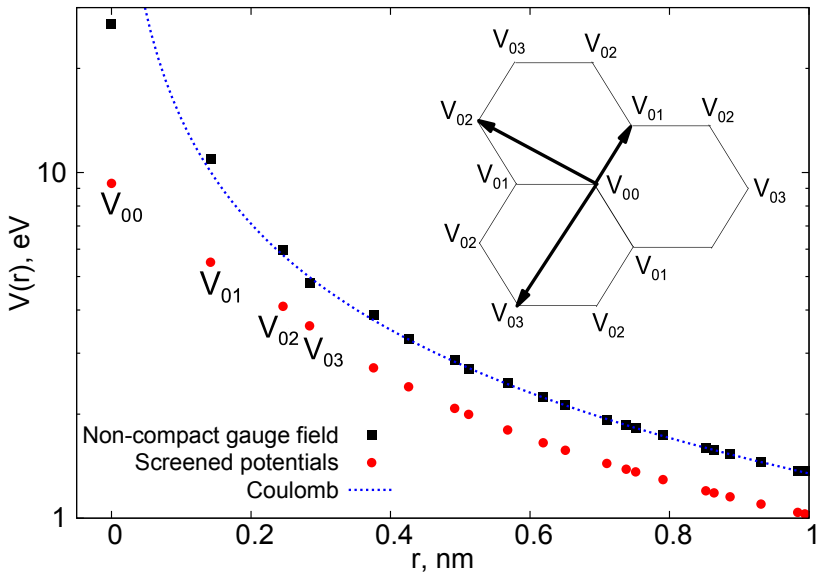
Results for on-site (V_{00}), nearest-neighbor (V_{01}), next-nearest-neighbor (V_{02}) and third-nearest-neighbor (V_{03}) potentials!

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...



Partially screened Coulomb potential

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

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

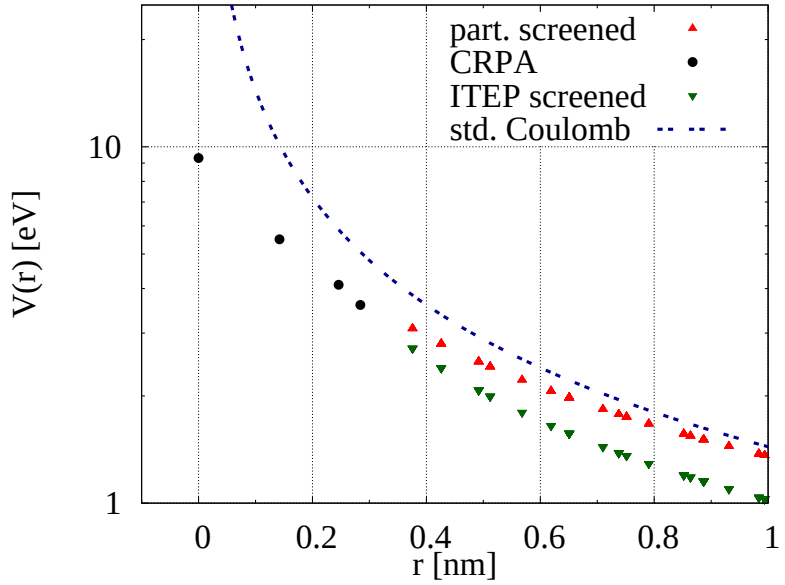
Wehling et al.
Phys.Rev. Lett. 106, 236805 (2011)

($\epsilon_1 = 2.4$ and $d = 2.8$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)

Results (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:

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

Results (semimetal-insulator phase transition)

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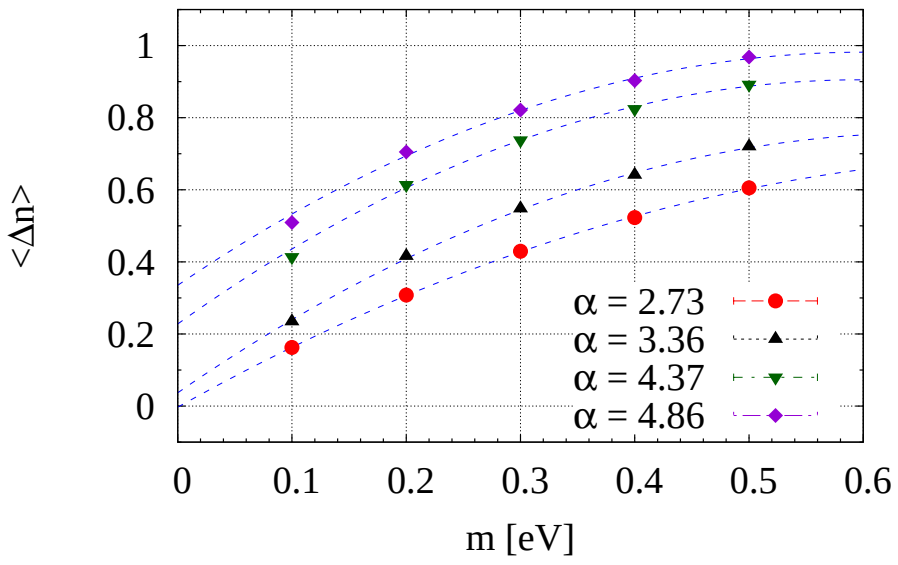
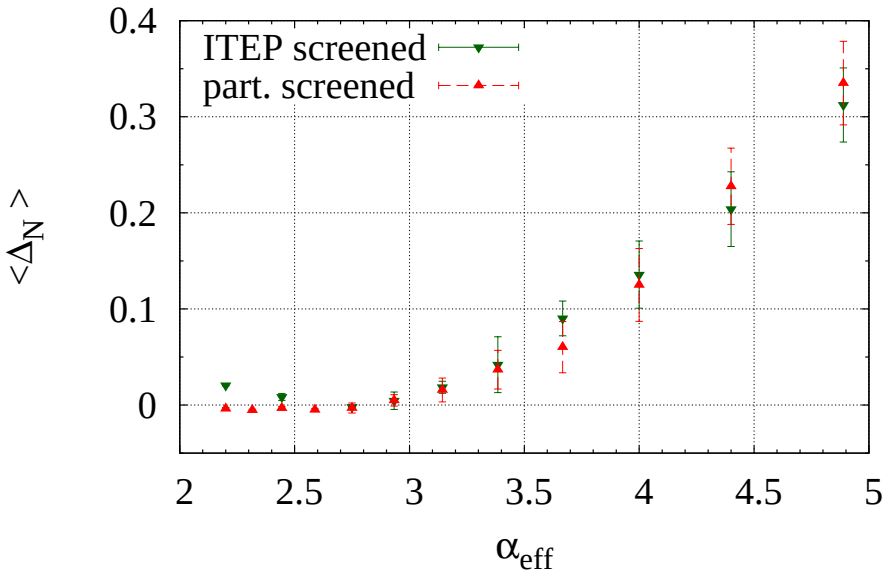
"Chiral limit": $m \to 0$ extrapolation done with $\langle \Delta_N \rangle = a_0 + a_1 m + a_2 m^2$.





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

Results (semimetal-insulator phase transition)

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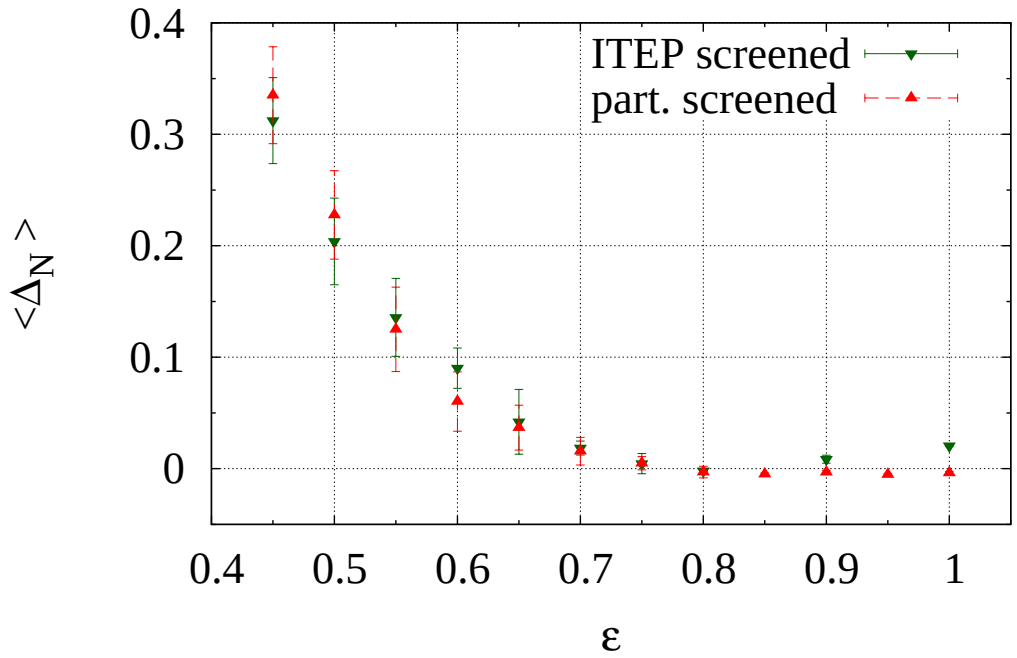
Expressed in terms of di-electric screening $\epsilon \approx 2.2/\alpha_{\text{eff}} = 0.45 \ldots 1.0$:



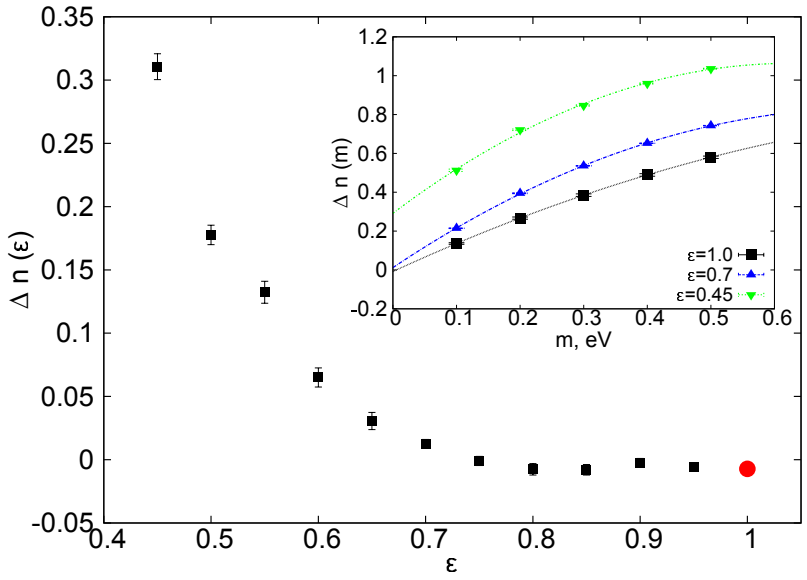


Figure on right: Ulybyshev et al. (ITEP), Phys.Rev. Lett. 111, 056801 (2013).
Clearly consistent!

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

Results (semimetal-insulator phase transition)

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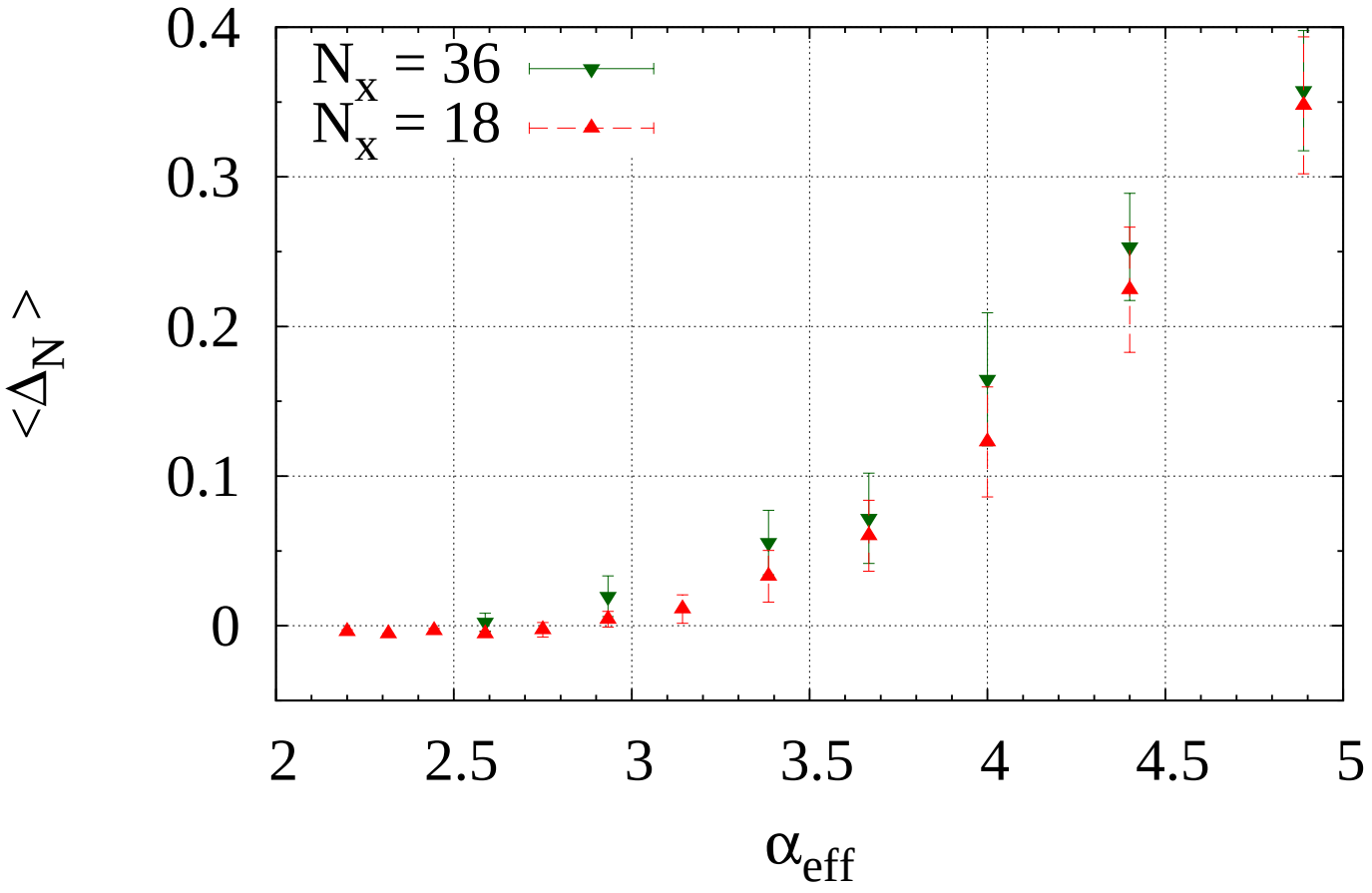
Currently checking volume effects ($N_x, N_y \to 36$). Maybe relevant...



Neck-disrupting Lifshitz transition

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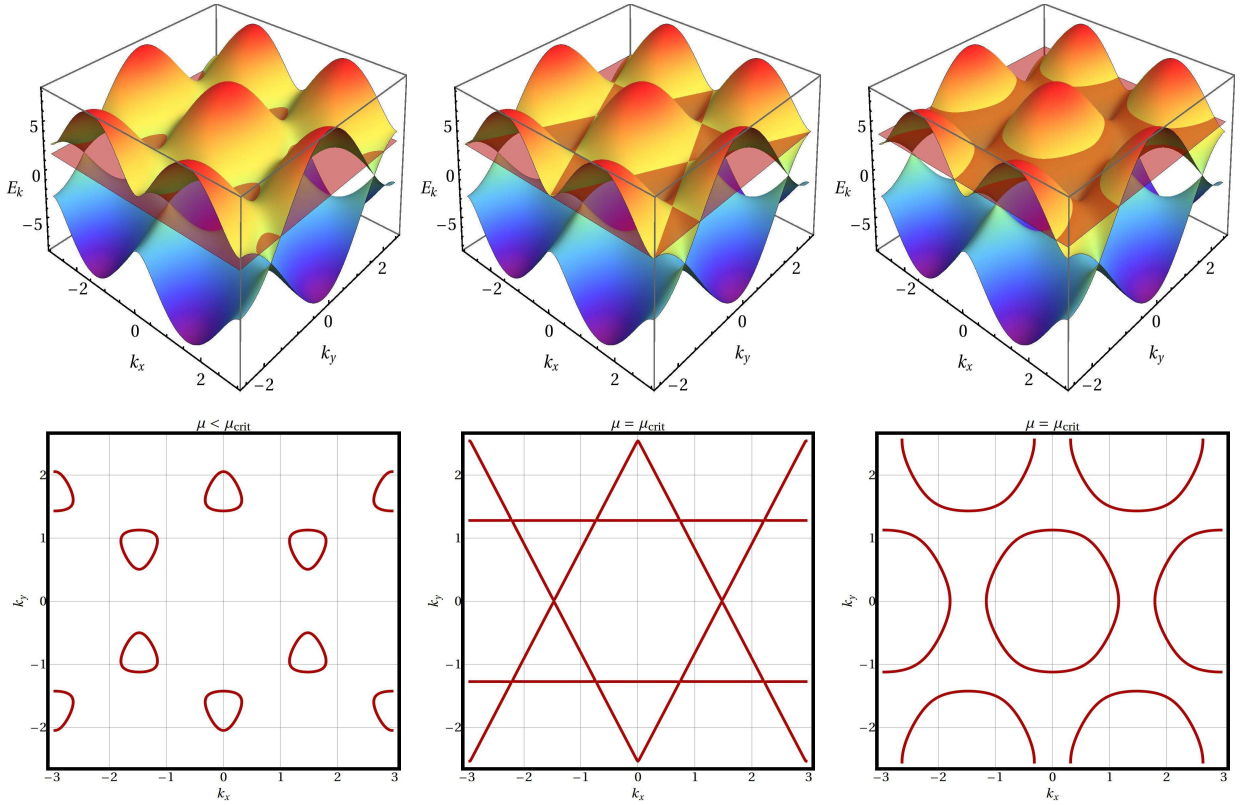
Adding a chemical potential μ shifts the Fermi level in non-interacting theory!
Topology of iso-energy lines changes when crossing saddle-points at $\mu = \mu_c$.



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

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

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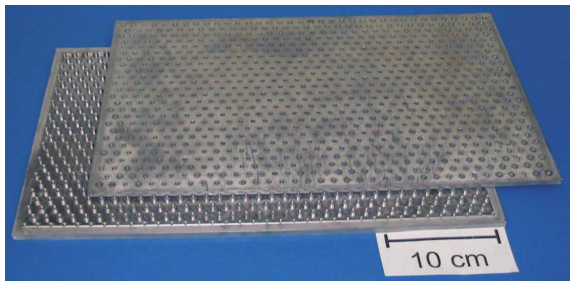
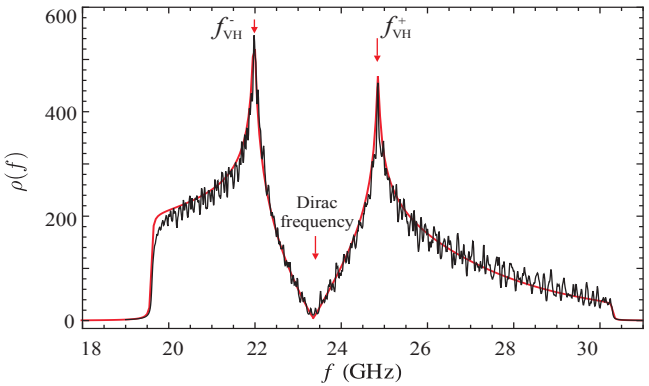
Density of states: $\rho(E) = \int_{BZ} \frac{d\vec{k}}{\left|\nabla_k E(\vec{k})\right|} \delta(E - E(\vec{k}))$

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.

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:

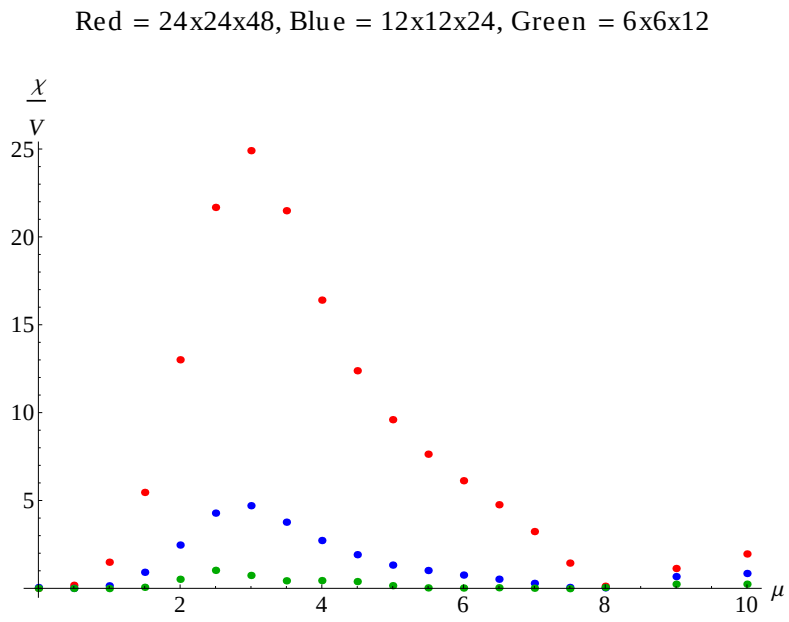
$$\hat{H}_{tb} \to \hat{H}_{tb} + \mu \sum_{i,s} s\, \hat{n}\,, \quad s = \pm 1\,.$$

Leads to: $M \to M + \mu \frac{\beta}{N_t} \mathbb{1} = M_\mu\,, \quad M^\dagger \to M^\dagger + \mu \frac{\beta}{N_t} \mathbb{1} = M_\mu^\dagger$ **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 $\rho(\mu)$)
- $\epsilon = 5000 \to \alpha_{eff} \approx 0$ (pure tight-binding)
- Peak position correct!
- What happens at finite α_{eff}?

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



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!