Quantum phase transitions on the hexagonal lattice

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II. Lattice simulations of graphene
III. Phase diagram of extended Hubbard model
IV. Conformal phase transition in graphene
V. Lifshitz-transition at finite spin-density
VI. Graphene with lattice defects
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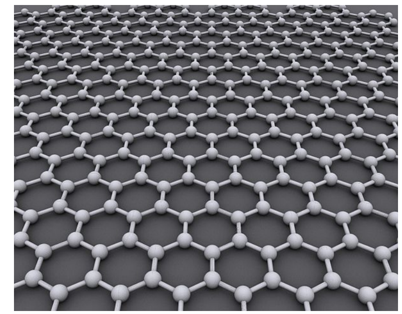
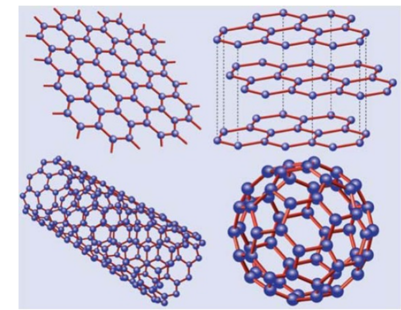
Introduction

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

  Building block of graphitic materials.
  (nano tubes, fullerenes etc.)





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

- **Landau & Peierls, 1935:** 2D crystals are thermodynamically unstable (transverse displacements).

- **Novoselov & Geim, 2004:** Experimental discovery of suspended graphene.

  → **Nobel prize for physics 2010**

(picture removed)

Photo: AP

- **Reconciliation with theory:** Stablized by slight crumbling in 3rd dimension, strong atomic bonds, ...

Why is graphene interesting? Many unusual properties!

- **Area density:** 0.77 mg/m² (single layer blocks Helium atom)
- **Breaking strength:** 42 N/m („carries weight of cat“, nearly 15 times than steel film of equal mass)

→ **Promising material for super strong structures.**

(picture removed) www.head.com

(picture removed) www.spacelift.co

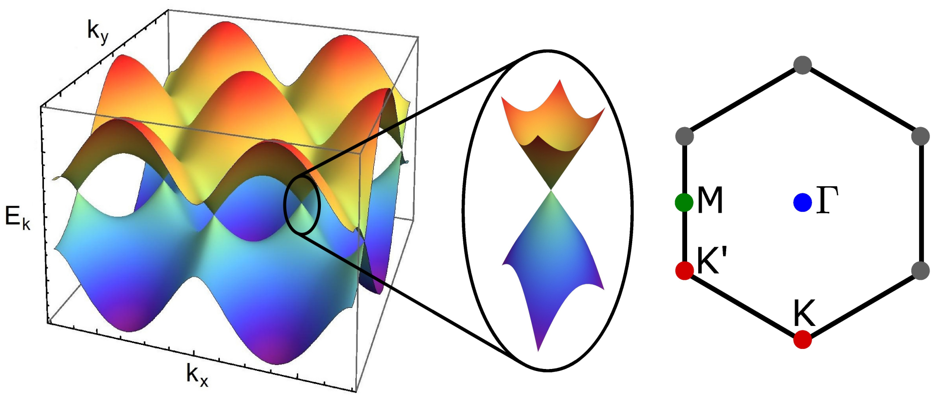
- **Optical conductivity:** Single sheet absorbs 2.3% of visible light.
- **Thermal conductivity:** At room temperature 10x better than copper.
- **Electric conductivity:** As good as copper. High carrier mobility even in doped devices!

→ **Next generation electronic devices!**
(Gigaherz processors, solar panels...)

Why are particle physicists interested?

Linear dispersion around corners of first Brillouin zone:

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



Dirac equation for low-energy dynamics!

⟶ **Relativistic physics in condensed matter system!**

- Klein tunneling, Zitterbewegung, anomalous quantum Hall effect, Atiyah-Singer index theorem, ...

Moreover: Strong electromagnetic interactions!

$$\alpha_{\text{eff}} = \frac{e^2}{\hbar v_F} \approx 2.2$$

- Quantum phase transitions, chiral symmetry breaking, ...

Use non-perturbative techniques: DSEs, FRG, lattice simulations!

Early days: Simulate low-energy effective theories.

- "Reduced" QED_4 (Fermions in 2D, gauge fields in 3D).
- Thirring model in 2+1D.

Drut, Lähde, Phys.Rev.Lett. 102, 026802, (2009)

Hands, Strouthos, Phys.Rev. B 78, 165423 (2008)

Seminal work in 2011: **Path integral for interacting tight-binding theory!**

Brower, Rebbi, Schaich, PoS (Lattice 2011) 056

State of the art 2019: Hybrid-Monte-Carlo simulations of graphene with realistic inter-electron potential.

- Lattice action with exact "chiral" symmetry ($\approx$ "Overlap", non-local).
- Non-iterative Schur complement solver (for dense matrices).
- Molecular-dynamics trajectories with exact Fermion forces.
- Highly-parallelized codes (GPUs, multi-core CPUs).
- Lattice size 24x24x128 on modern hardware.

Buividovich, Smith, Ulybyshev, von Smekal
Phys. Rev. B 98, 235129 (2018)

Buividovich, Smith, Ulybyshev, von Smekal
ArXiv: 1812.06435

Lattice simulations of graphene

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Starting point: Interacting tight-binding Hamiltonian on hexagonal lattice.

$$H = \sum_{\langle x,y\rangle,s} (-\kappa)(\hat{a}^\dagger_{x,s}\hat{a}_{y,s} + \hat{a}^\dagger_{y,s}\hat{a}_{x,s}) + \frac{1}{2}\sum_{x,y} \hat{q}_x V_{xy} \hat{q}_y$$

V positive definite!

Spin directions: $s = \pm 1$

Anti-commutators: $\{\hat{a}^\dagger_i, \hat{a}^\dagger_j\} = 0,\ \{\hat{a}^\dagger_i, \hat{a}_j\} = \delta_{ij}$

Hopping energy: $\kappa \approx 2.8\,\mathrm{eV}$

Charge operator: $\hat{q}_x = \hat{a}^\dagger_{x,1}\hat{a}_{x,1} + \hat{a}^\dagger_{x,-1}\hat{a}_{x,-1} - 1$

Goal: Simulate grand-canonical ensemble.

$$\mathcal{Z} = \mathrm{Tr}\ e^{-\beta\hat{H}},\ \langle O\rangle = \frac{1}{\mathcal{Z}}\mathrm{Tr}\left[\widehat{O}e^{-\beta\hat{H}}\right]$$

Usual strategy (field theory):

- Express Z as functional integral (replace operators by fields).
- Generate field configurations.
- Measure observables in field representation.

Differences for graphene:

- Fock space of non-relativistic QM.
- Spacelike lattice-spacing is physical.

Hexagonal geometry unusual but not problematic.

Two triangular sublattices!

First step: Symmetric Suzuki-Trotter decomposition.

$$\mathcal{Z} = \mathrm{Tr}\left(e^{-\beta\hat{\mathcal{H}}}\right) = \mathrm{Tr}\left(e^{-\delta_\tau\hat{\mathcal{H}}_0} e^{-\delta_\tau\hat{\mathcal{H}}_{\mathrm{int}}} e^{-\delta_\tau\hat{\mathcal{H}}_0}\dots\right) + O(\delta_\tau^2)\ , \qquad \delta_\tau = \beta/N_\tau$$

Fierz-transformation: Ensures ergocity of HMC without mass terms.

$$V_{xx}\hat{\rho}_x^2 = \eta V_{xx}\hat{\rho}_x^2 - (1-\eta)V_{xx}\hat{\sigma}_x^2 + 2V_{xx}(1-\eta)\,\hat{\sigma}_x, \quad (\hat{\sigma}_x\text{= spin density})$$

Hubbard-Stratonovich: Replaces four-fermion terms with bilinears.

$$e^{-\frac{\delta_\tau}{2}\sum\limits_{x,y}\widetilde{V}_{xy}\hat{\rho}_x\hat{\rho}_y} \cong \int D\phi\, e^{-\frac{1}{2\delta_\tau}\sum\limits_{x,y}\phi_x\widetilde{V}_{xy}^{-1}\phi_y}\, e^{i\sum\limits_x\phi_x\hat{\rho}_x} \qquad (\widetilde{V}_{xx} = \eta V_{xx})$$

$$e^{\frac{\delta_\tau}{2}(1-\eta)\sum\limits_x V_{xx}\hat{\sigma}_x^2} \cong \int D\chi\, e^{-\frac{1}{2\delta_\tau}\sum\limits_x\frac{\chi_x^2}{(1-\eta)V_{xx}}}\, e^{\sum\limits_x\chi_x\hat{\sigma}_x}$$

→ **Complex bosonic auxiliary field!** $\Phi_{x,t} = \chi_{x,t} + i\phi_{x,t}$

Last step: Integrate out fermionic operators.

$$\mathrm{Tr}\left(e^{-\hat{A}_1}e^{-\hat{A}_2}\dots e^{-\hat{A}_n}\right) = \det\begin{pmatrix} 1 & -e^{-A_1} & 0 & \dots \\ 0 & 1 & -e^{-A_2} & \dots \\ \vdots & & \ddots & \\ e^{-A_n} & 0 & \dots & 1 \end{pmatrix}$$

Left: Bilinears

$$\hat{A}_k = (A_k)_{xy}\hat{a}^\dagger_x\hat{a}_y$$

Right: Matrices

$$A_k = (A_k)_{xy}$$

Final result: $\mathcal{Z} = \int D\Phi\,|\det M(\Phi)|^2 e^{-S_\eta(\Phi)}$

$$M(\Phi) = \begin{pmatrix} 1 & -e^{-\delta_\tau h} & 0 & 0 & 0 & \dots \\ 0 & 1 & -e^{i\Phi_1} & 0 & 0 & \dots \\ 0 & 0 & 1 & -e^{-\delta_\tau h} & 0 & \dots \\ 0 & 0 & 0 & 1 & -e^{i\Phi_2} & \dots \\ \vdots & & & & \ddots & \\ e^{i\Phi_{N_\tau}} & 0 & 0 & & \dots & 1 \end{pmatrix}$$

$$S_\eta(\Phi) = \frac{1}{2\delta_\tau}\sum_{x,y,t}\phi_{x,t}\widetilde{V}^{-1}_{xy}\phi_{y,t} + \sum_{x,t}\frac{(\chi_{x,t} - (1-\eta)\delta_\tau V_{xx})^2}{2(1-\eta)\delta_\tau V_{xx}}$$

$$e^{i\Phi_t} \equiv \mathrm{diag}\left(e^{\chi_{x,t}+i\phi_{x,t}}\right)$$

($|\cdot|^2$ from two spin components)

h: tight-binding matrix

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$$\mathcal{Z} = \int D\Phi \, |\det M(\Phi)|^2 e^{-S_\eta(\Phi)} \qquad S_\eta(\Phi) = \frac{1}{2\delta_\tau} \sum_{x,y,t} \phi_{x,t} \widetilde{V}^{-1}_{xy} \phi_{y,t} + \sum_{x,t} \frac{(\chi_{x,t} - (1-\eta)\delta_\tau V_{xx})^2}{2(1-\eta)\delta_\tau V_{xx}}$$

Features:

- Measure is positive-definite. **No sign problem!**
- η interpolates between real and imaginary fields.
- $0 \ll \eta \ll 1$: domain walls with $\det M = 0$ cirumvented. **Ergodicity!**
- „Chiral“ symmetry! (combination of spin and sublattice)
- M is dense. Invert with Schur solver!

Buividovich, Smith, Ulybyshev, von Smekal Phys. Rev. B 98, 235129 (2018)

Hybrid Monte-Carlo:

- Evolve fields in computer time with fictitious Hamiltonian process.
- Numerical integrator introduces stepsize error. Correct with Metropolis accept/reject step.

→ **Exact algorithm!**

Results I: Phase diagram of extended Hubbard model

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- **Real graphene:** Strongly coupled due to small Fermi velocity.

$$\alpha_{\text{eff}} = \frac{e^2}{\hbar v_F} \approx 2.2$$ → **Could be Mott insulator!**

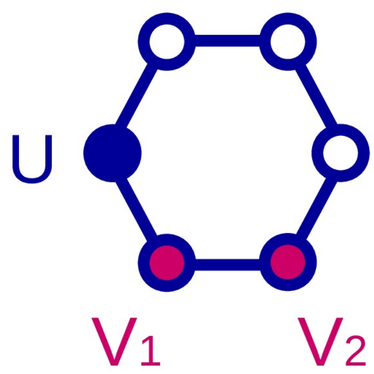
- **Experiments and HMC:** Suspended graphene is conductor.
(interactions screened by σ-band electrons)

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

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

- **However:** Interaction parameters can be modified!
(B-fields, substrates, strain, adatoms, other hexagonal materials, . . .)

- **(Extended) Hubbard model:** On-site (U), nearest neighbor (V_1), next-nearest neighbor (V_2) interactions only.



$$H = \sum_{\langle x,y \rangle, s} (-\kappa)(\hat{a}^\dagger_{x,s}\hat{a}_{y,s} + \hat{a}^\dagger_{y,s}\hat{a}_{x,s}) + \frac{1}{2}\sum_{x,y} \hat{q}_x V_{xy} \hat{q}_y$$

→ **Study competition of ordered phases!**

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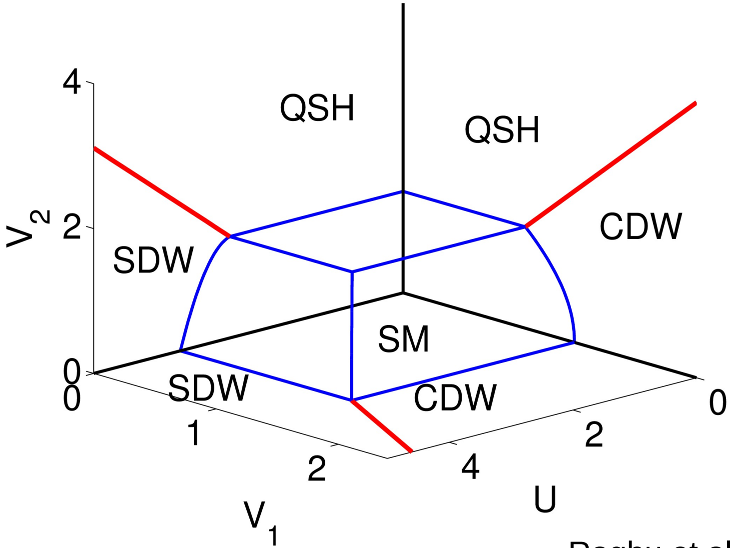
Semi-analytic methods: Renormalization group, random phase approximation, variational Hamiltonian approach, ...

Qualitative phase diagram but large uncertainties (orders / locations of transitions, ...)

→ **Do ab-initio simulations!**



Raghu et al., PRL 100, 156401 (2008)

On-site potential (U) only: Well-studied with „BSS“ Quantum-Monte-Carlo.

Blankenbecler, Scalapino, Sugar Phys. Rev. D 24, 2278 (1981)

- Insulating spin-density-wave (SDW) phase for $U \gtrsim 3.8\kappa$.
- 2nd order phase-transition.
- Universality class of 3D N=2 chiral Gross-Neveu model.
- ...

Assaad and Herbut, Phys. Rev. X. 3, 031010 (2013)

BSS QMC: Faster than HMC for pure on-site Hubbard model.

→ **Method of choice for contact interactions!**

However: Additional auxiliary field for each interaction term.
(cost quickly grows with off-site potentials)

HMC: Single complex auxiliary field!

→ **Method of choice for non-diagonal interaction matrices!**

In 2017/18: Hybrid-Monte-Carlo study of extended Hubbard model with on-site (U) and nearest neighbor potential (V).

- Unbiased study of spin-density-wave (SDW) and charge-density-wave (CDW) order parameters.
- Phase diagram in U-V plane in region V<U/3 (restriction of positive-definite interaction).

Buividovich, Smith, Ulybyshev, von Smekal Phys. Rev. B 98, 235129 (2018)

Results I: Phase diagram of extended Hubbard model

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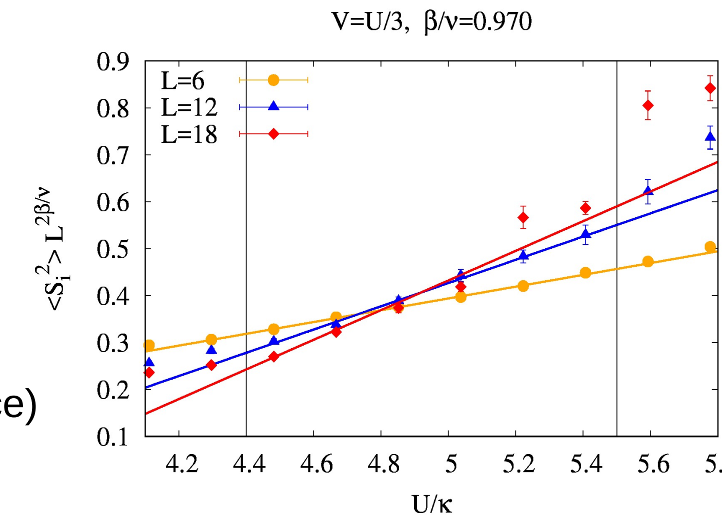
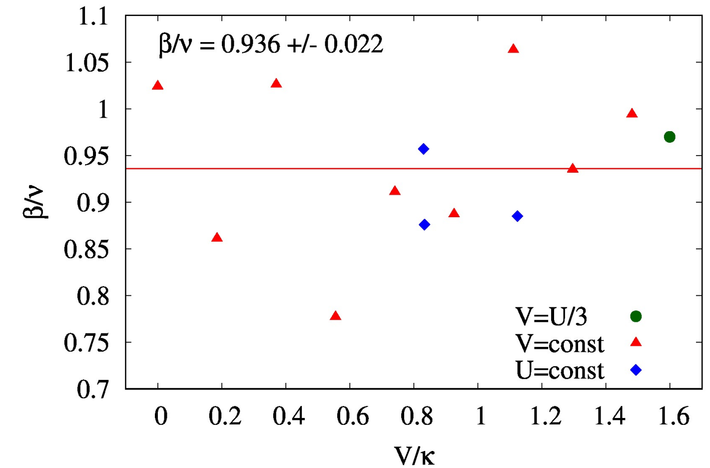
Order parameters:

$$\langle S^2 \rangle = \sum_{SL} \left\langle \frac{1}{L^4} \left(\sum_{x \in SL} \hat{S}_x \right)^2 \right\rangle$$

$$\langle q^2 \rangle = \sum_{SL} \left\langle \frac{1}{L^4} \left(\sum_{x \in SL} \hat{q}_x \right)^2 \right\rangle$$

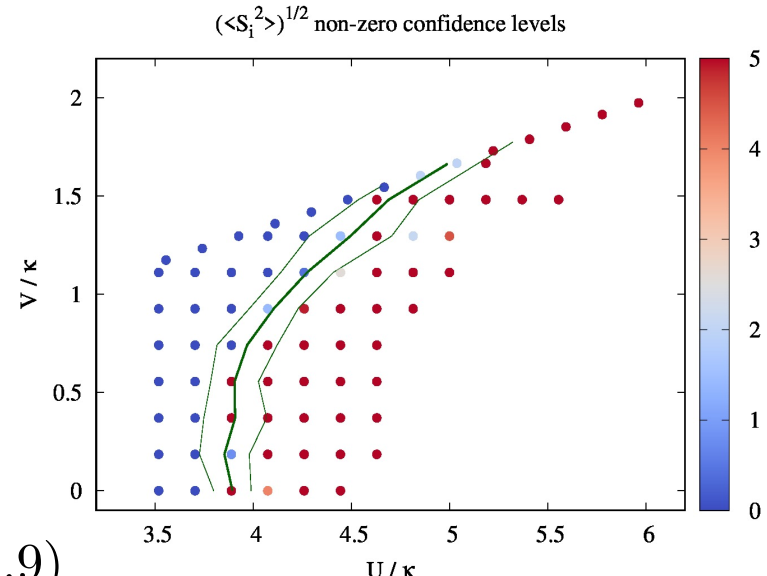
(squared spin/charge per sublattice)





Analysis:

- Extrapolate to infinite volume.
  Use confidence level of non-zero signal!
- Finite-size scaling for U=const. / V=const. lines.
  Use optimal intersection and critical exponents.



Conclusions:

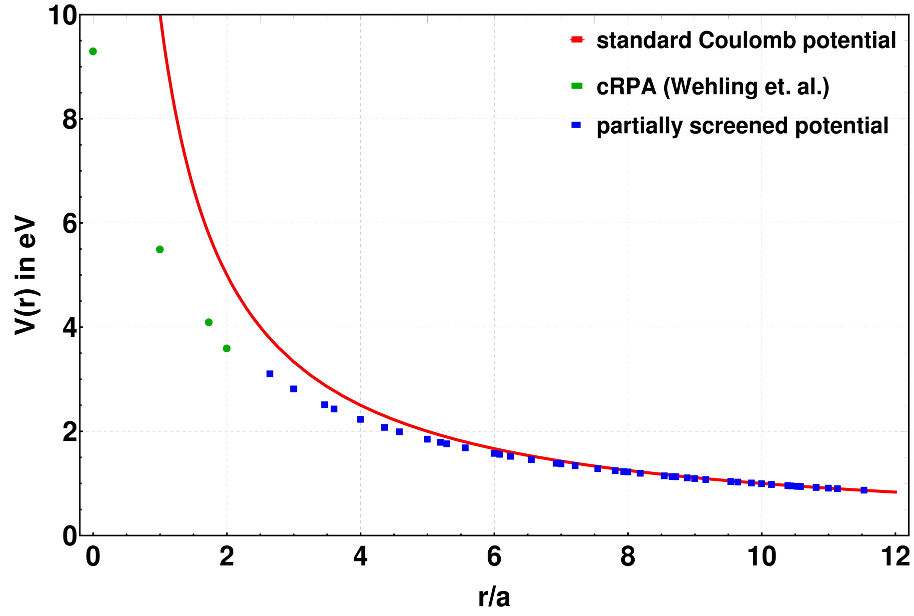
- Extended region with SDW order. **No CDW!**
- 2nd order boundary stretches up to U=3V line.
- Chiral Gross-Neveu class confirmed! $(\beta/\nu \approx 0.9)$

Results II: Conformal phase transition in graphene

- **Graphene:** Long-range potential!
- **Wehling et al.:** cRPA calculation of screened short-range potential. Thin-film model for long-range part.

Wehling, Şaşıoğlu, Friedrich, Lichtenstein, Katsnelson, Blügel
Phys. Rev. Lett. 106, 236805 (2011)

→ **„Partially screened" Coulomb potential!**



But does it matter? Perhaps...

- **Renormalization group:** Coulomb tail is marginally irrelevant.

Herbut, Juričić, Vafek
Phys. Rev. B 80, 075432 (2009)

Juričić, Herbut, Semenoff
Phys. Rev. B 80, 081405 (2009)

- **Strong-coupling expansion:** On-site potential drives transition. (critical properties = Hubbard model)

G. W. Semenoff,
Physica Scripta 2012 , 014016.

But short-range potential is strongly screened...

Dyson-Schwinger: „Reduced“ QED_4 exhibits **conformal phase transition!**

Gamayun, Gorbar, Gusynin, Phys. Rev. B 81, 075429 (2010)

Reduced QED_4: Low-energy effective field theory of graphene.

- Electron fields in 2D plane. Gauge fields in 3D bulk.
- Strongly coupled due to small Fermi velocity.
- Describes long-range physics. Insensitive to short-range physics.

CPT: Phase transition „of infinite order“.

$$M(\lambda) \sim \exp\left(\frac{-c}{\sqrt{\lambda - \lambda_c}}\right)$$

- Observables exhibit exponential „Miransky“ scaling.
- Formal limit $\beta, \nu \to \infty, \delta = 1$ of 2nd order transition.
- In 2D: Kosterlitz-Thouless transition.
- „Conformal window“ in QCD, „Walking technicolor“, ...

2nd order: $M \sim |\lambda - \lambda_c|^\beta, \quad \xi \sim |\lambda - \lambda_c|^{-\nu}, \quad M_{\lambda=\lambda_c} \sim H^{1/\delta}$

But which applies to graphene?

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In 2018: **Hybrid-Monte-Carlo study of competing order in graphene.**

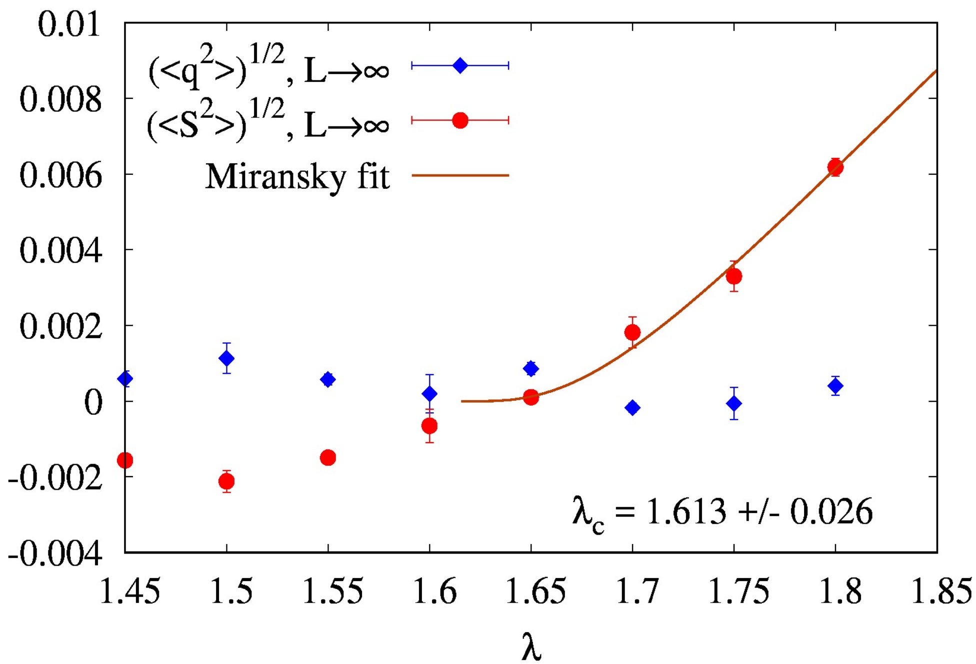
Buividovich, Smith, Ulybyshev, von Smekal
ArXiv: 1812.06435

Study order parameters:

$$\langle S^2 \rangle = \sum_{SL} \left\langle \frac{1}{L^4} \left(\sum_{x \in SL} \hat{S}_x \right)^2 \right\rangle$$

$$\langle q^2 \rangle = \sum_{SL} \left\langle \frac{1}{L^4} \left(\sum_{x \in SL} \hat{q}_x \right)^2 \right\rangle$$

Rescale potential: $V_{xy} \to \lambda V_{xy}$



First conclusions:

- Potential must be scaled up by $\lambda \approx 1.6$ for phase transition.
- SDW favored over CDW order.
- Fit to Miransky function works but doesn‘t mean much. (powerlaw just as good)

$$M(\lambda) \sim \exp\left(\frac{-c}{\sqrt{\lambda - \lambda_c}} \right)$$

→ **Study critical properties!**

Results II: Conformal phase transition in graphene

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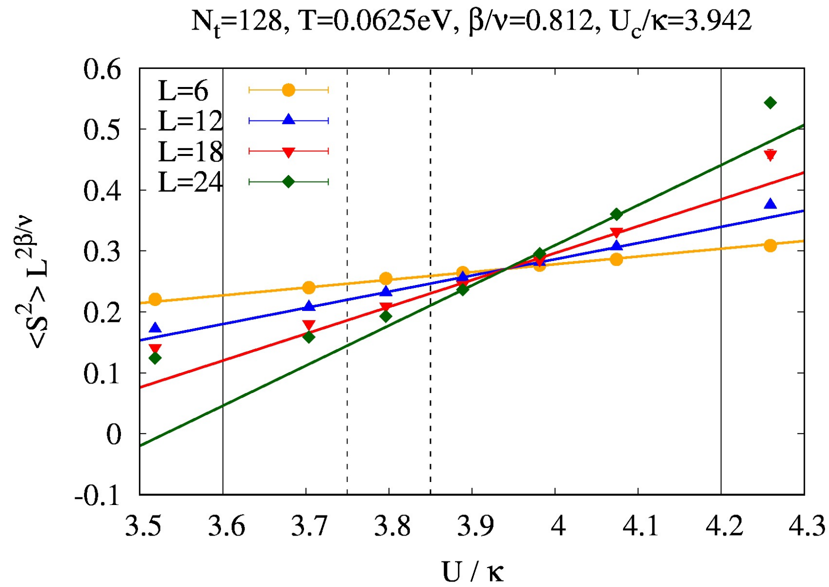
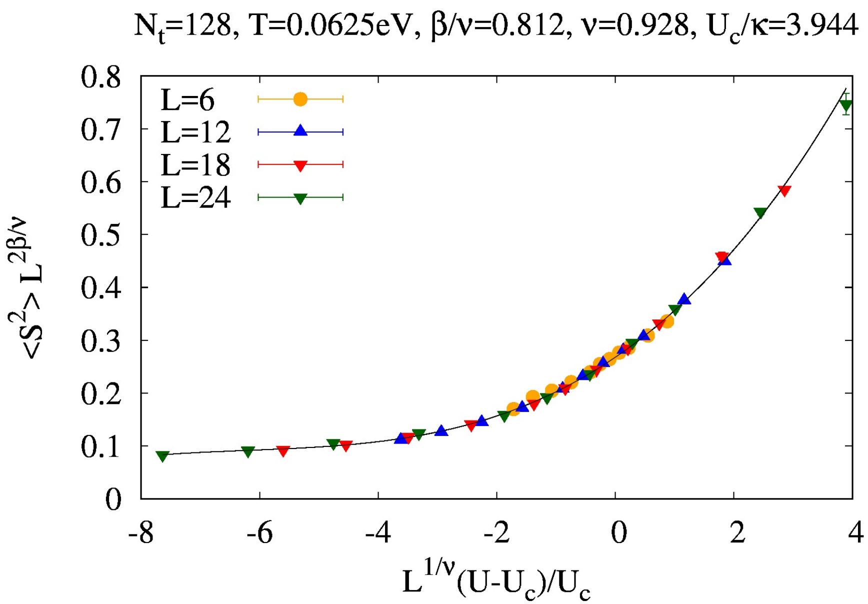
On-site potential, benchmark (new BSS-study):

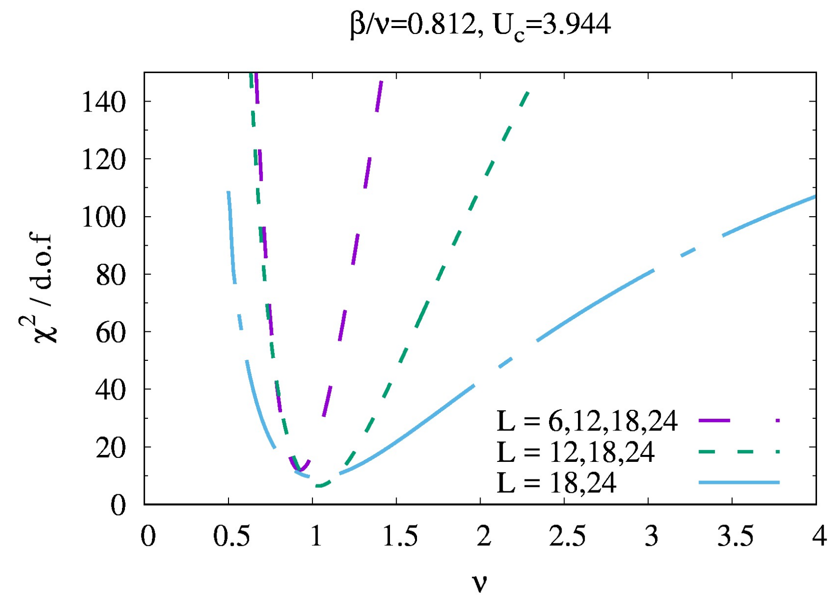
- $U_c \approx 3.9$ and $\beta/\nu \approx 0.8$ (finite-size scaling).
- $\nu \approx 0.9$ from optimized collapse.
- χ^2 of collapse very sensitive.

Exponents tighly constrained!

- Difference to old results: Finite-size effects.



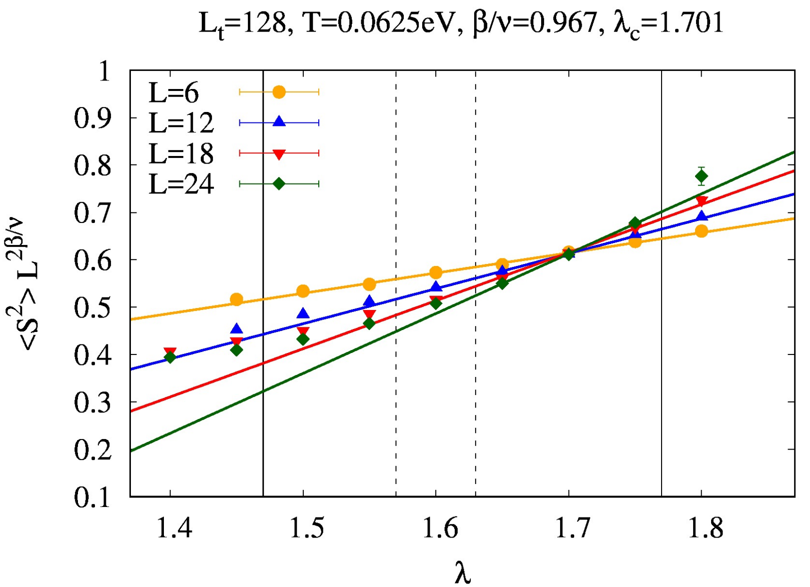




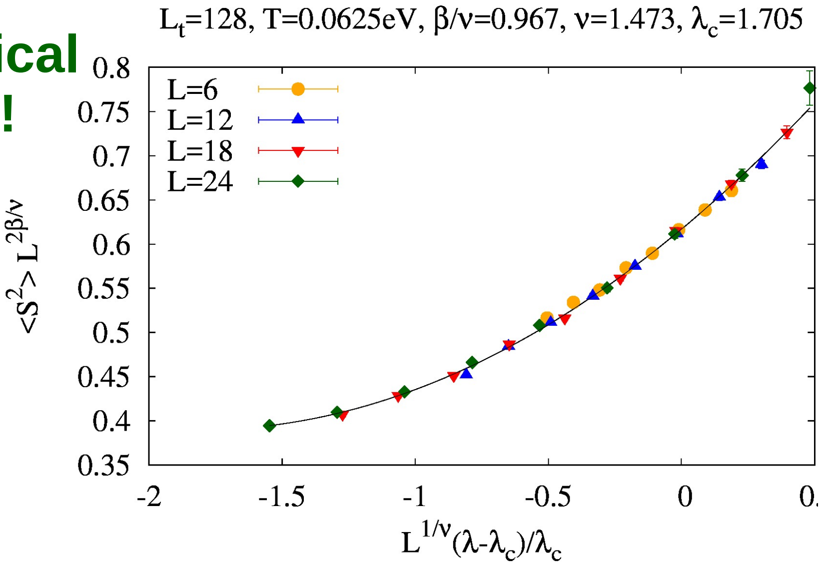
Results II: Conformal phase transition in graphene

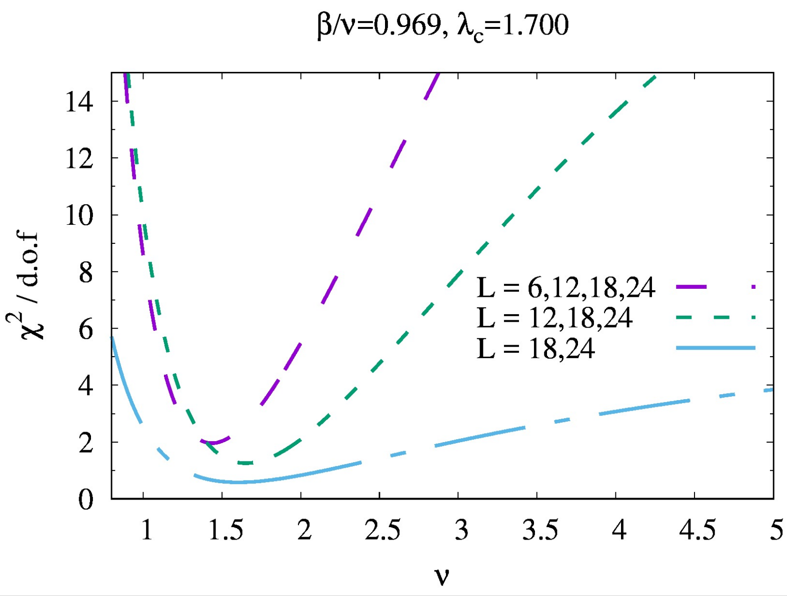
Graphene:

- $\beta/\nu \approx 1.0$ but not tightly constrained. (FSS intersections possible for $0.95 \ldots 1.0$)
- $\lambda_c \approx 1.7$ but can move in range $1.6 \ldots 1.7$.
- $\nu \gtrsim 1.5$ but very weakly constrained on large lattices! (drift towards larger values)
- **Hubbard model exponents fail entirely!**



Very non-typical for 2nd order!





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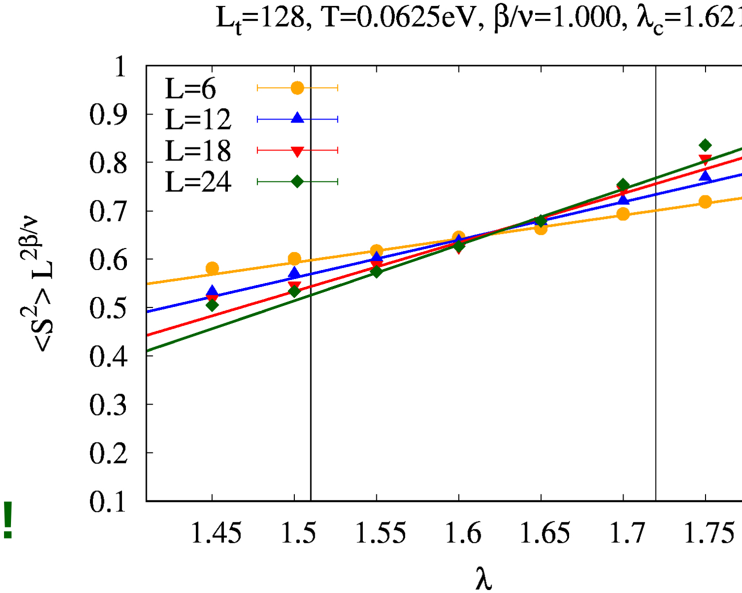
QED2+1, reduced QED4, many-flavor QCD:

- CPT sensitive to infrared cutoff, receives powerlaw corrections.

  (Braun, Fischer, Gies, Goecke, Williams, Gusynin, Reenders, Liu, Li, Cheng)

  → **Mimics 2nd order in finite volume!**

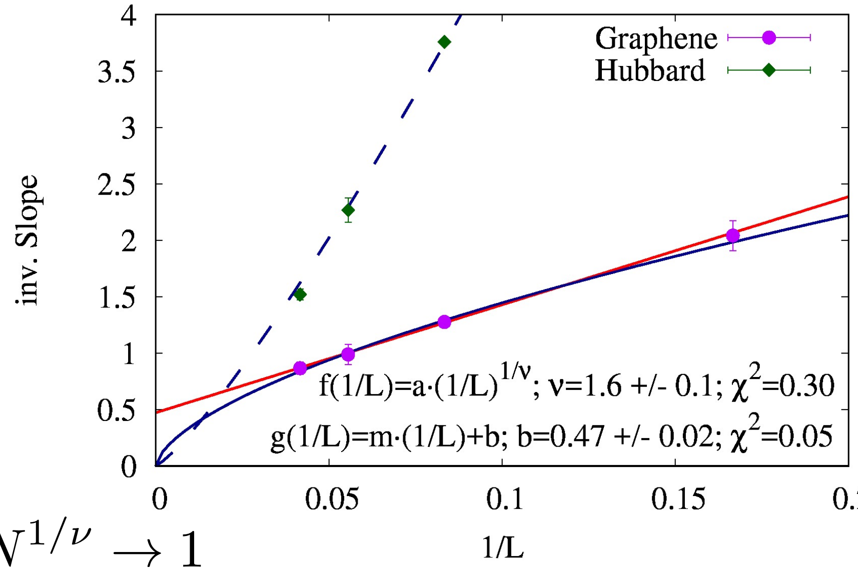


Proposition: (Gusynin et al, 2010) **Hyperscaling relation on finite lattices!**

$\beta, \nu \to \infty$ in infinite volume!

In 2+1D: $\frac{\beta}{\nu} = \frac{d}{\delta + 1} = 1$

- Good FSS intersection! Inverse slopes extrapolate to finite value! **Collapse without rescaling coupling!** $\nu \to \infty\ ,\ N^{1/\nu} \to 1$



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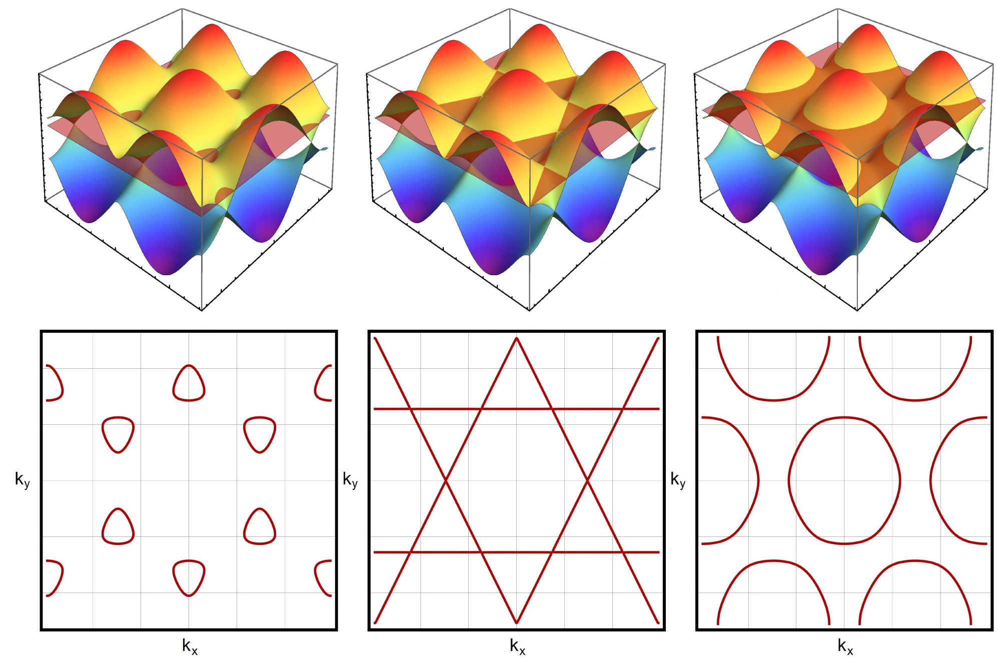
Graphene bands:

- Topology of Fermi „surface“ changes when Fermi level crosses saddle points (charge doping).

„Neck-disrupting Lifshitz- transition“

- Density of states diverges! („Van-Hove singularity“)



(Phys. Rev. B 96,195408)

Electron interactions should produce ordered phase! → **Chubukov et al.: Nature Physics 8, 158163 (2012)** Chiral superconductivity in doped graphene.

(maybe: twisted bilayer)

Monte-Carlo simulation:

$$\mathcal{Z}(\mu) = \int D\Phi \; \det M(\mu,\Phi)\widetilde{M}(\mu,\Phi)e^{-S_\eta(\Phi)}$$

$$M(\mu,\Phi) = M(0,\Phi) - \mu\frac{\beta}{N_t}\mathbf{I}\,, \quad \widetilde{M}(\mu,\Phi) = M^\dagger(0,\Phi) + \mu\frac{\beta}{N_t}\mathbf{I}$$

Sign problem!

2017: HMC study of graphene at finite spin density.

Körner, Smith, Buividovich, Ulybyshev, von Smekal
Phys. Rev. B 96, 195408 (2017)

$$M(\mu_s, \Phi) = M(0, \Phi) - \mu_s \frac{\beta}{N_t}\mathbf{I} \;, \quad \widetilde{M}(\mu_s, \Phi) = M^\dagger(0, \Phi) - \mu_s \frac{\beta}{N_t}\mathbf{I}$$

No sign problem!

(In-plane B-field. Fermi-level shifted in opposite directions for spin orientations)

VHS at finite T (no interactions):

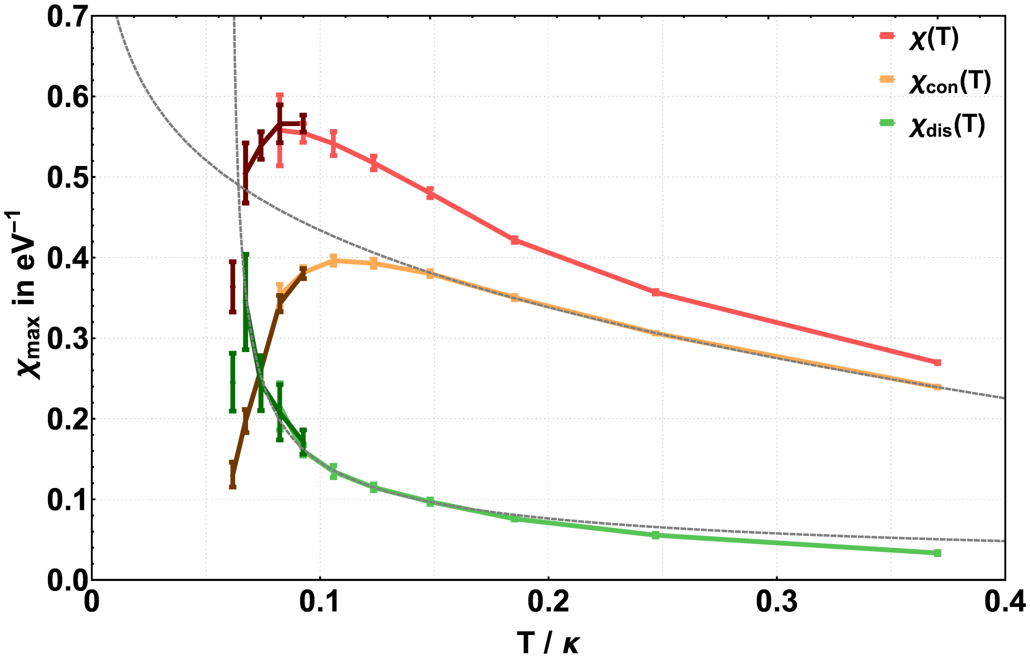
- Log-divergence of **connected part** of particle-hole susceptibility for $T \to 0$.

$$\chi_{\text{con.}} \sim -\ln\left(\pi T/\kappa\right) + \mathcal{O}(T)$$

With interactions:

- Powerlaw-divergence of **disconnected part** at finite T_c .

$$\chi_{\text{dis.}} \sim |T - T_c|^\gamma \;, \quad \gamma \approx 1/2$$



To do: Cooper pair condensates!

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2017: Inter-electron interactions and the RKKY potential between H adatoms in graphene

Buividovich, Smith, Ulybyshev, von Smekal
Phys. Rev. B 96, 165411 (2017)

Hydrogen adatoms:

- Can be modelled as vacant lattice sites (hoppings to site set zero)

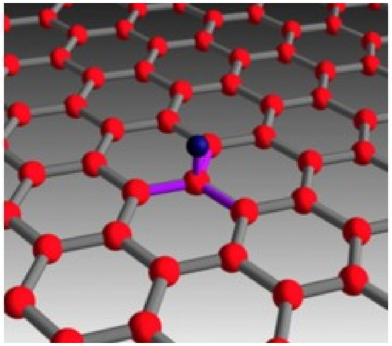
Adatom at z: $$H = -\sum_{\langle x,y\rangle,s} \kappa(x,y)(\hat{a}^\dagger_{x,s}\hat{a}_{y,s} + \hat{a}^\dagger_{y,s}\hat{a}_{x,s}) \;, \quad \kappa(x,z) = 0 \;\forall\; x$$

"Instantons"

- Interact via fermionic Casimir / Van-der-Waals force:
  Free energy of electrons is modified! („Ruderman-Kittel-Kasuya-Yosida“)
- RKKY interaction affected by inter-electron interactions!

Our HMC study:

- Interaction of H-adatom pairs.
- Stability of H-adatom superlattices.



Picture:
Jyioti Katoch
Synthetic Metals, Vol. 210, Part A, 68-79 (2015)

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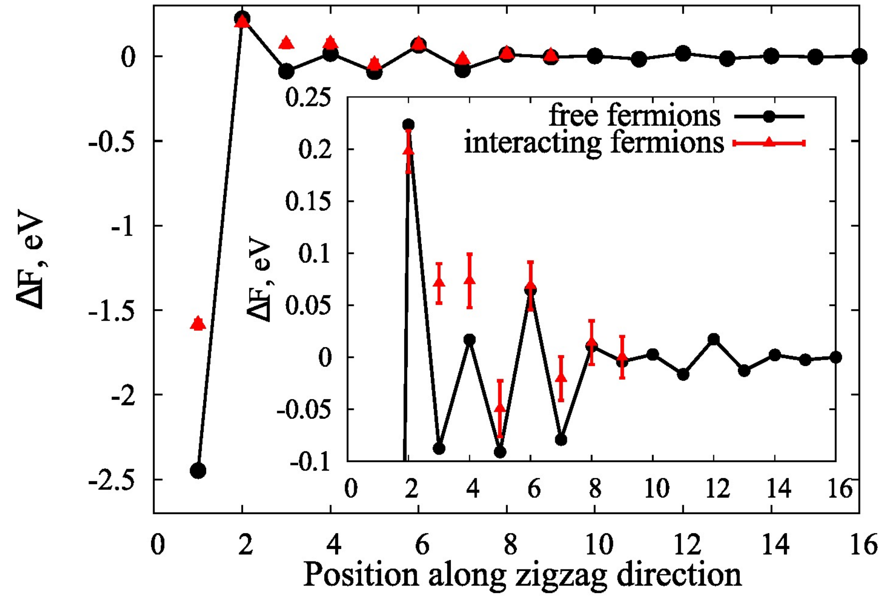
Pairwise interaction:

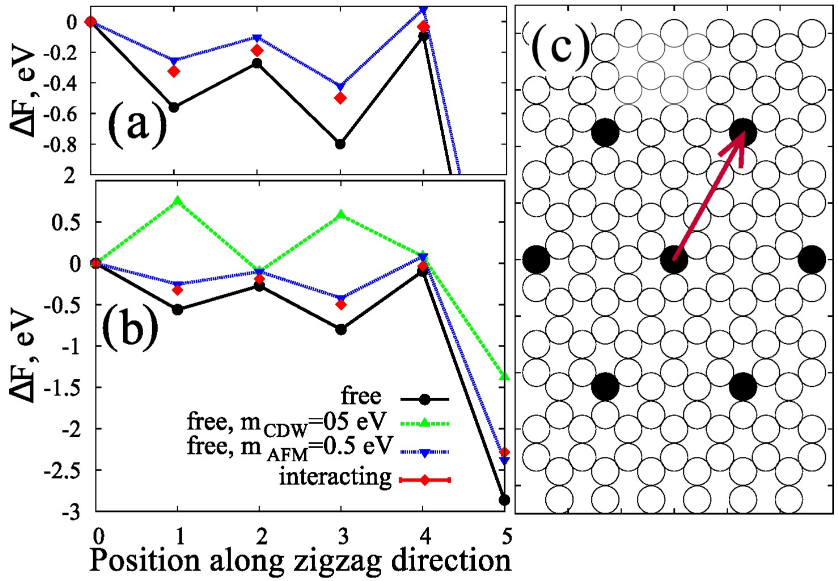
- Alternating sign on different sublattices. Order-of-magnitude enhancement at some distances.
- With interactions: Local minimum at 3-bond distance disappears! (suppression of dimer formation)

Superlattices (example):

- System with 5.56% coverage on one sublattice shown!
- SDW (AFM) has only weak effect. Stabilized by CDW!

Also: Dynamic stability of different superlattices considered! (not shown here)





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Ongoing:

- Hubbard model at finite charge density using generalized density of states method (Körner, Langfeld, von Smekal).

Future:

- Attractive (U < 0) Hubbard model has no sign problem at finite charge density!
- $\widehat{=}$ discretized **Nambu-Jona-Lasinio** model:

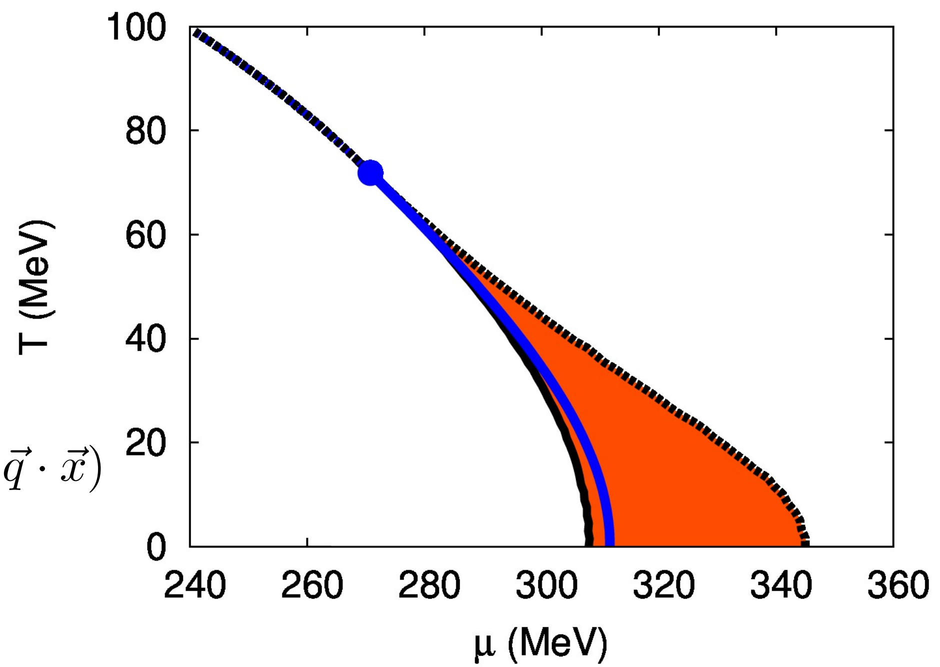
$$\mathcal{L}_{\mathrm{NJL}} = \bar{\psi}(i\gamma^\mu\partial_\mu - m)\psi + G_S\left((\bar{\psi}\psi)^2 + (\bar{\psi}i\gamma^5\vec{\tau}\psi)^2\right)$$

- NJL in 3+1D (D. Nickel): Inhomogeneous "chiral density wave" in mean field.

$$\langle\bar{\psi}\psi\rangle = -\frac{\Delta}{2G_S}\cos(\vec{q}\cdot\vec{x}) \ , \ \langle\bar{\psi}i\gamma^5\vec{\tau}\psi\rangle = -\frac{\Delta}{2G_S}\sin(\vec{q}\cdot\vec{x})$$

($\widehat{=}$ "spin spiral" in Hubbard model)

Verified in 2+1D. Test beyond mean field!



Buballa, Carignano, Prog. Part. Nucl. Phys. 81, 39–96 (2015)

Literature:

1) *Monte-Carlo simulation of the tight-binding model of graphene with partially screened Coulomb interactions*, Smith, von Smekal, Phys. Rev. B 89, 195429 (2014)

2) *Interelectron interactions and the RKKY potential between H adatoms in graphene*, Buividovich, Smith, Ulybyshev, von Smekal, Phys. Rev. B 96, 165411 (2017)

3) *Hybrid Monte Carlo study of monolayer graphene with partially screened Coulomb interactions at finite spin density*, Körner, Smith, Buividovich, Ulybyshev, von Smekal, Phys. Rev. B 96, 195408 (2017)

4) *Hybrid Monte Carlo study of competing order in the extended fermionic Hubbard model on the hexagonal lattice*, Buividovich, Smith, Ulybyshev, von Smekal, Phys. Rev. B 98, 235129 (2018)

5) *Numerical evidence of conformal phase transition in graphene with long-range interactions*, Buividovich, Smith, Ulybyshev, von Smekal, arXiv:1812.06435

Thanks for coming!