Hybrid-Monte-Carlo simulations at the van Hove singularity in monolayer graphene

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Outline

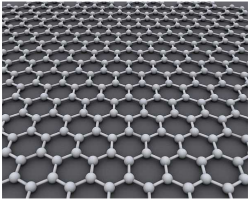
Graphene - Overview

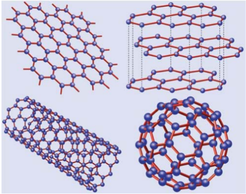
History:

- **1947** - First calculation of the band structure (*Wallace et. al.*)
- **1962** - First experimental realization (*Boehm et. al.*)
- **2004** - Measurement of the electron properties (*Novoselov, Geim*)
- **2010** - Nobel Prize for Novoselov and Geim
- **since at least 2010** - 2D Materials as a independent field of research

Graphene: 2-dimensional hexagonal lattice of Carbon Atoms

Basic building block for Graphite, Fullerene, etc.





http://www.nobelprize.org

Castro Neto, Guinea, Peres, Novoselov, Geim., Rev. Mod. Phys., Vol. 81, No. 1,

Graphene - Overview

Remarkable physical properties:

- Tensile strength: $130 \cdot 10^3 \frac{N}{mm^2}$
  (Structural steel: 310 - 630 $\frac{N}{mm^2}$)
- Thermal conductivity: 5000 $\frac{W}{mK}$
  (Copper: 400 $\frac{W}{mK}$)
- Electrical conductivity: $9.6 \cdot 10^5 \frac{1}{\Omega cm}$
  (Copper: $6.0 \cdot 10^5 \frac{1}{\Omega cm}$)
- Nearly transparent: Absorption $\approx 2.3\%$

Focus on electrons:

3 electrons in sp^2-orbitals build σ-band (responsible for structure)

1 electron in p_z-orbital build π-band (valence band)

π-band electrons are screened by σ-band electrons

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Structure

- Diatomic base:

$$\vec{a} = a \cdot \begin{pmatrix} \sqrt{3} \\ 0 \end{pmatrix} \quad \vec{b} = \frac{a}{2} \cdot \begin{pmatrix} \sqrt{3} \\ 3 \end{pmatrix} \quad \vec{c} = \begin{pmatrix} 0 \\ a \end{pmatrix}$$

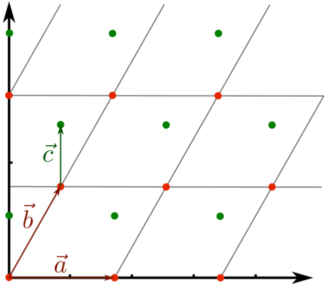
with the lattice constant $a \approx 1.42$ Å

- All lattice points can be described by:

$$\vec{R}_1 = n_1\,\vec{a} + n_2\,\vec{b} \qquad \vec{R}_2 = n_1\,\vec{a} + n_2\,\vec{b} + \vec{c}$$

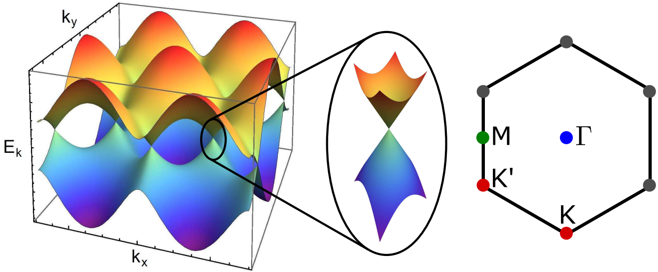
with $n_1,\, n_2 \in \mathbb{Z}$.

- **Two sublattices!**



Tight binding theory of Graphene

$$\mathrm{H}_{TB} = -\kappa \sum_{\langle x,y \rangle, s} \left(\mathrm{a}^{\dagger}_{x,s} \mathrm{a}_{y,s} + h.c. \right)$$



- Linear Dispersion around K-points
- Van Hove Singularity at the M-point

Density of States

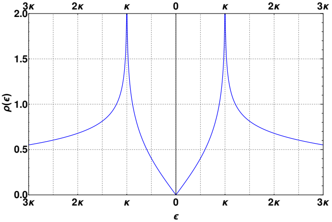
- Important effects are also in the DOS:

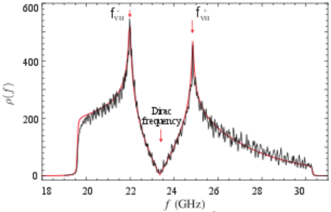
$$\rho(E) = \int_{S(E)} \frac{ds}{(2\pi)^2} \frac{1}{\left|\nabla_{\vec{k}}\epsilon(\vec{k})\right|}$$

- VHS characterized by a divergency in the DOS
- Full tight-binding DOS can be observed in analog experiments with photonic crystals (microwave billiards)
- Logarithmic divergency in finite volumes

$$\rho_{\max} = \frac{3}{\pi\kappa}\left[\ln N_c - 2\ln\pi + 1 + \mathcal{O}(N_c^{-1})\right]$$

- **Neck-disrupting Lifshitz transition**

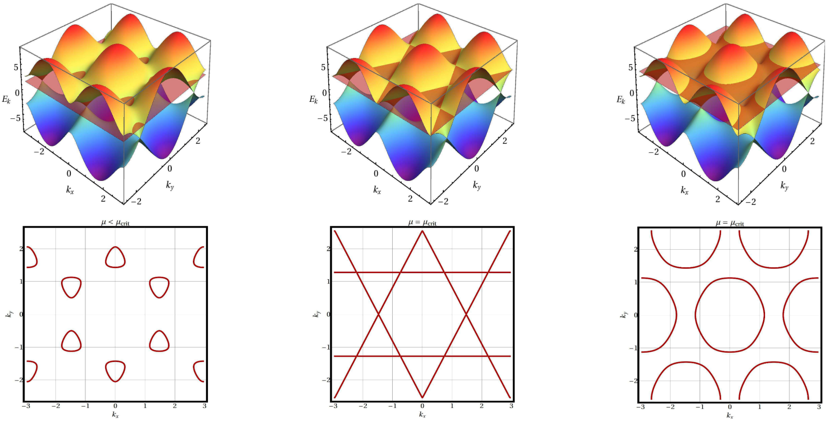




Dietz, Iachello, Miski-Oglu, Pietralla, Richter, v. Smekal, Wambach
Phys. Rev. B 88, 104101 (2013)

Lifshitz Transition

Shifting the Fermi level by a chemical potential μ
$\Rightarrow$ the shape of the fermi "surface" changes



The topology of the fermi "surface" changes when crossing the VHS!

Real Graphene

- Strongly coupled system
  - $\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar v_F} \approx 2.2$
  - non-local exchange effects are not negligible
  - α can be changed experimentally
- Experimental observations:
  - Reshaping of bands $\longrightarrow$ smaller bandwidth
    S. Ulstrup et al.,
    Phys. Rev. B, 94, 081403 (2016).
  - Extended VHS
    J. L. McChesney et. al.,
    PRL 104, 136803 (2010)

Add a long-range potential and a chemical potential to the Hamiltonian:

$$H = -\kappa \sum_{\langle x,y\rangle ,s} (a^\dagger_{x,s} a_{y,s} + \text{h.c.}) + \lambda \sum_{x,y} q_x V_{xy} q_y - \mu \sum_{x,s} a^\dagger_{x,s} a_{x,s}$$

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

Goal:

Use the HMC-Algorithm to study the influence of the long-range interaction on the DOS especially at the VHS.

Hybrid Monte Carlo

- **HMC:** Based on path-integral representation of partition function

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

- Interactions are transmitted by scalar **Hubbard field** ϕ
- Effect of dynamical Fermions encoded in **Fermion matrix** $M(\phi)$

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

- Path-integral approximated by artificial Hamiltonian evolution of ϕ

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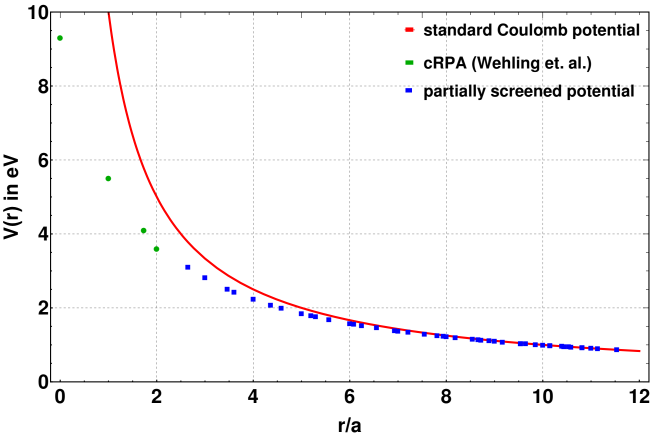
Potential



Sign problem

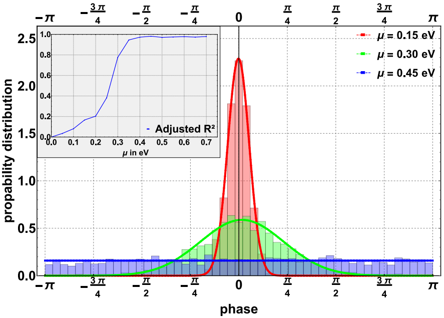
Through a chemical potential in the Hamiltonian the Fermion matrix M respectively $M^\dagger$, turns into

$$M \rightarrow M - \mu \frac{\beta}{N_t} \mathbb{1} = M_\mu$$

$$M^\dagger \rightarrow M^\dagger + \mu \frac{\beta}{N_t} \mathbb{1} \neq M_\mu^\dagger$$

Measure is no longer real and positive definite.

Interpretation as a probability impossible!



Circumvention by introducing a **spin-dependent** chemical potential:

$$\mu = +\mu_s \quad \forall\ s = +1$$

$$\mu = -\mu_s \quad \forall\ s = -1$$

Then the condition is fulfilled and we can write $\det\left[M(\phi)M^\dagger(\phi)\right]$ again.

Observable

- Effects in DOS perserved in Thomas-Fermi-susceptibility

$$\chi(\mu) = A_c \cdot \lim_{\vec{p}\to 0} \lim_{\omega\to 0} \Pi(\omega, \vec{p}, \mu, T) \quad \xrightarrow{T\to 0} \quad \rho(\mu)$$

$$\Pi(\omega, \vec{p}, \mu, T) = -\int_{BZ} \frac{d^2k}{2\pi^2} \sum_{s,s'=\pm 1} \left(1 + \frac{ss'\Phi_{\vec{k}}\Phi_{\vec{k}+\vec{p}}}{|\Phi_{\vec{k}}||\Phi_{\vec{k}+\vec{p}}|}\right)$$

$$\times \frac{f\left(\frac{s'E(\vec{k}+\vec{p})-\mu}{T}\right) - f\left(\frac{sE(\vec{k})-\mu}{T}\right)}{s'E(\vec{k}+\vec{p}) - sE(\vec{k}) - \omega - i\epsilon}$$

- The Thomas-Fermi susceptibility is given by the second derivative of the grand canonical potential

$$\chi(\mu) = -\frac{1}{N_c}\left(\frac{d^2\Phi}{d\mu^2}\right) = \frac{1}{N_c\beta}\left[\frac{1}{Z}\frac{d^2Z}{d\mu^2} - \frac{1}{Z^2}\left(\frac{dZ}{d\mu}\right)^2\right]$$

Observable

- Expectation values of susceptibility in the thermal ensemble:

$$\frac{1}{Z}\frac{d^n Z}{d\mu^n} = \frac{1}{Z}\int D\phi \left[\frac{d^n}{d\mu^n}\mathrm{det}\left(MM^\dagger\right)\right] e^{-S(\phi)}$$

- Using these relations we can write the susceptibility as $\langle\chi\rangle = \langle\chi_{\mathrm{con}}\rangle + \langle\chi_{\mathrm{dis}}\rangle$, with

$$\begin{aligned}\langle\chi_{\mathrm{con}}\rangle =& \frac{-2}{N_c\beta}\left\langle \mathrm{ReTr}\left(M^{-1}\frac{dM}{d\mu}M^{-1}\frac{dM}{d\mu}\right)\right\rangle \\ \langle\chi_{\mathrm{dis}}\rangle =& \frac{4}{N_c\beta}\left\{\left\langle\left[\mathrm{ReTr}\left(M^{-1}\frac{dM}{d\mu}\right)\right]^2\right\rangle \right. \\ & \left. - \left\langle \mathrm{ReTr}\left(M^{-1}\frac{dM}{d\mu}\right)\right\rangle^2\right\}\end{aligned}$$

- The brackets on the right-hand sides are understood as averages over a representative set of field configurations.

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Relevant parameters - An overview

- Temperature T
- Volume N
- Staggered mass m_s
- Discretization of the time axis N_t
- Interaction strength α
- spin-dependent chemical potential μ

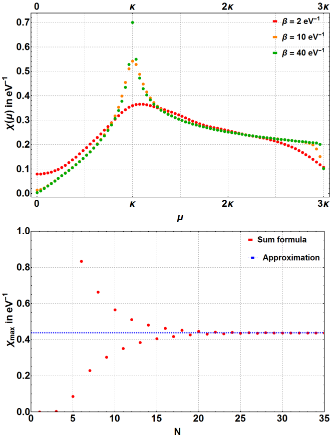
Influence of V and T in non-interacting theory

- **Finite volumina and non-zero temperature**

$$\chi(\mu) = \frac{1}{2TN^2} \sum_{n,m} \left[\text{sech}^2\left(\frac{\mu - E(m,n)}{2T}\right) + \text{sech}^2\left(\frac{\mu + E(m,n)}{2T}\right)\right]$$

- **Behavior at the VHS**

$$\chi_{max} = \frac{3}{\pi^2 \kappa}\left\{ \ln\left(\frac{8\kappa}{\pi T}\right) + \gamma_E + \mathcal{O}(T)\right\}$$



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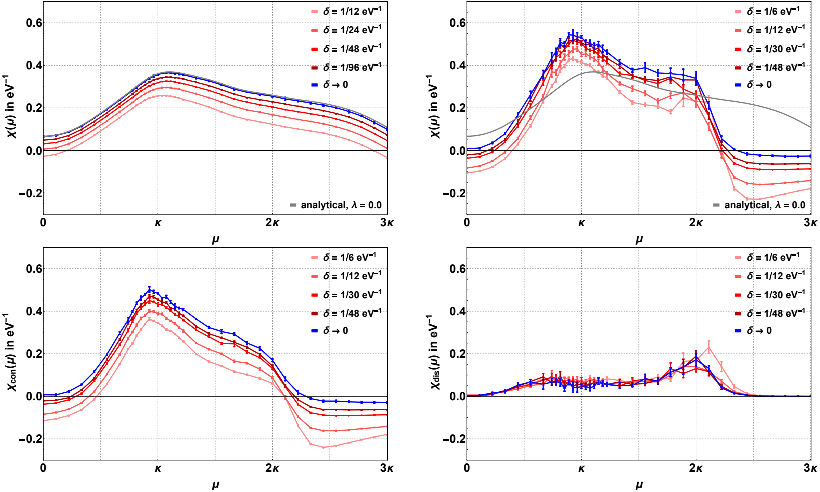
Influence of the time discretization



- discretization generates a constant shift in χ
- χ_{dis} is not affected by the discrete time axis

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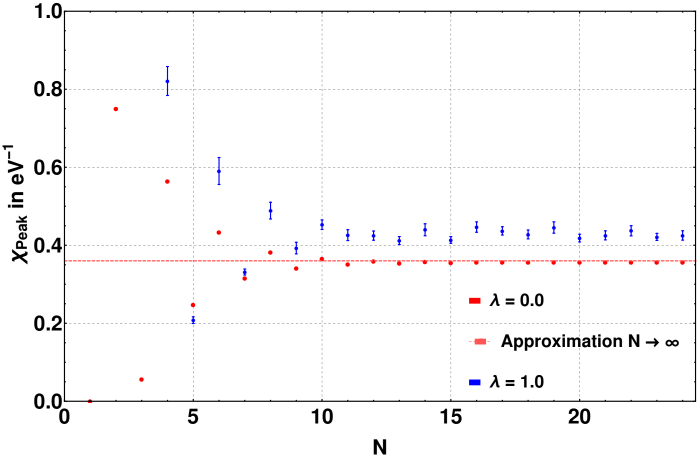
Influence of the volume



Interactions only shift the peak to higher values

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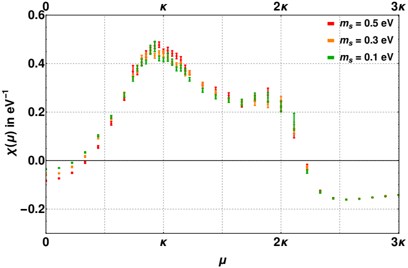
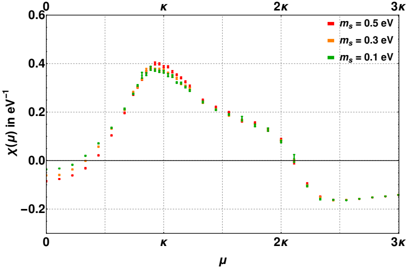
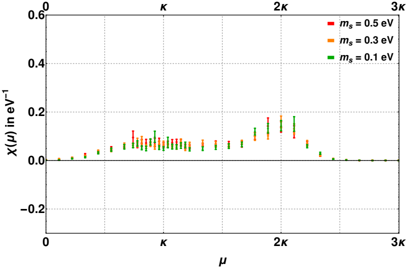
Influence of the staggered mass

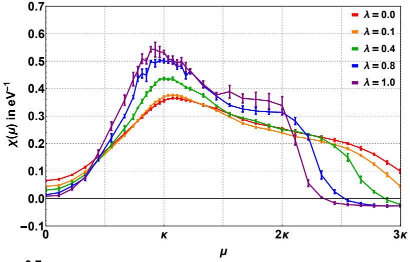


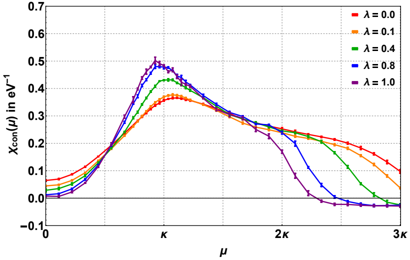


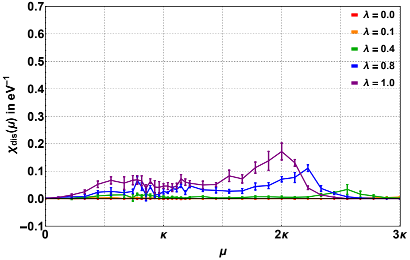


- staggered mass influences χ only at low μ
- χ_{dis} not affected by m_s

Influence of the long-range interaction

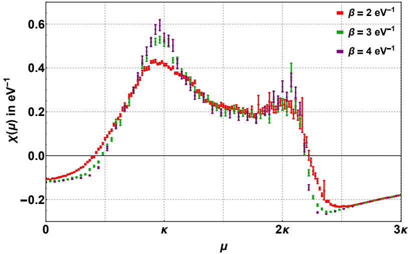


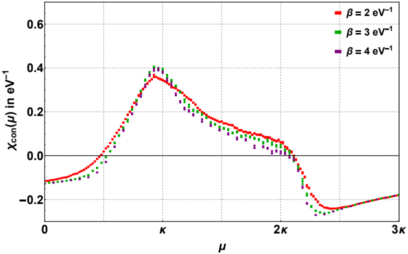


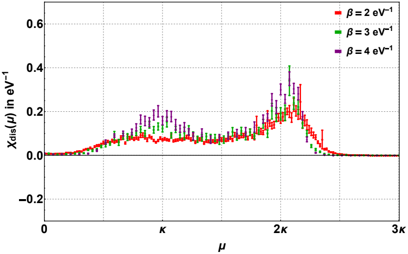


- Simulation agrees qualitativly with the experimental result (bandwidth shrinking)
- Long-range interaction enlarge the VH-peak in finite volumina

Influence ot the Temperature

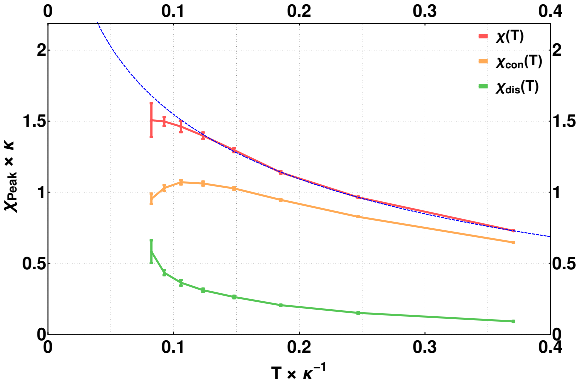






- Lowering temperature enlarge the VH-peak in finite volumina
- Enlargement is mostly driven by χ_{dis} in interacting systems

Influence of the Temperature at the VHS



$$f_1(T) = \frac{3}{\pi^2} \ln\left(\frac{\kappa}{T}\right) + b - c\frac{T}{\kappa}$$

b [eV^{-1}]	0.519(3)
c [eV^{-1}]	0.472(8)

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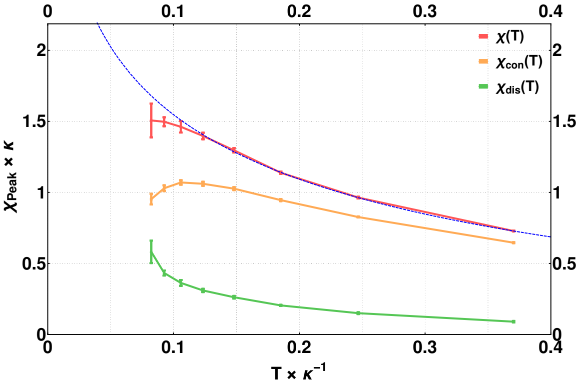

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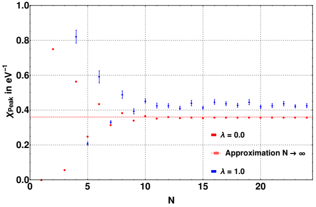
Use volume dependency!



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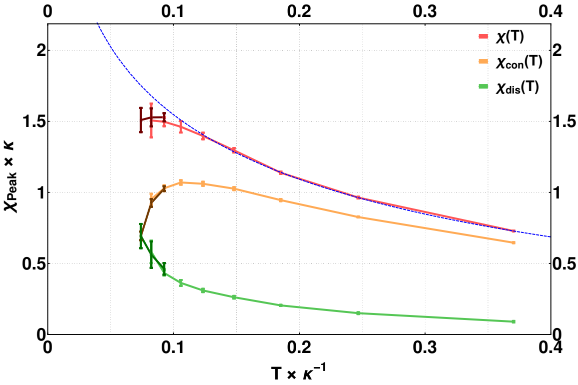

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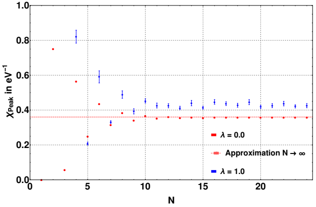

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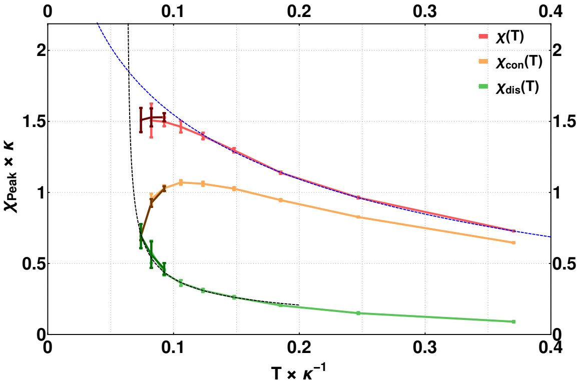

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$$f_2(T) = k\left|\frac{T - T_c}{T_c}\right|^{-\gamma}$$

β_c $[\mathrm{eV}^{-1}]$	6.1(5)
γ	0.52(6)
k $[\mathrm{eV}^{-1}]$	0.12(1)

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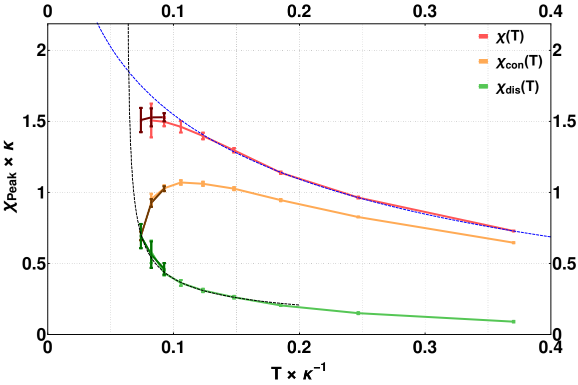
Influence of the Temperature at the VHS



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Evidence for extended van-Hove singularity!

Summary

Graphene

System in which the coupling can be changed experimentally

Method

- Tight-binding description/approximations as a baseline for simulations
- Use spin-dependent chemical potential to avoid the sign problem ("phase quenched theory")
- All influences of the simulation parameters are understood

HMC-simulations agrees with experiments qualitatively

- Bandwith shrinking
- Extended van-Hove singularity

More Information: *MK, Smith, Buividovich, Ulybyshev, von Smekal*, Phys. Rev. B 96, 195408

Outlook

Differences to a pure Hubbard model

Simulations with only on-site interactions

Improved action

Implementation of exponential action (with Maksim Ulybyshev)

Sign problem

Use LLR algorithm to simulate with
real chemical potential (with Kurt Langfeld)

Second peak in χ_{con}

Study and explain the second peak in the
disconnected part of the susceptibilty

Thank you!