Quantum Monte Carlo calculation of the Fermi velocity renormalization in graphene: a test of convergence for perturbative series

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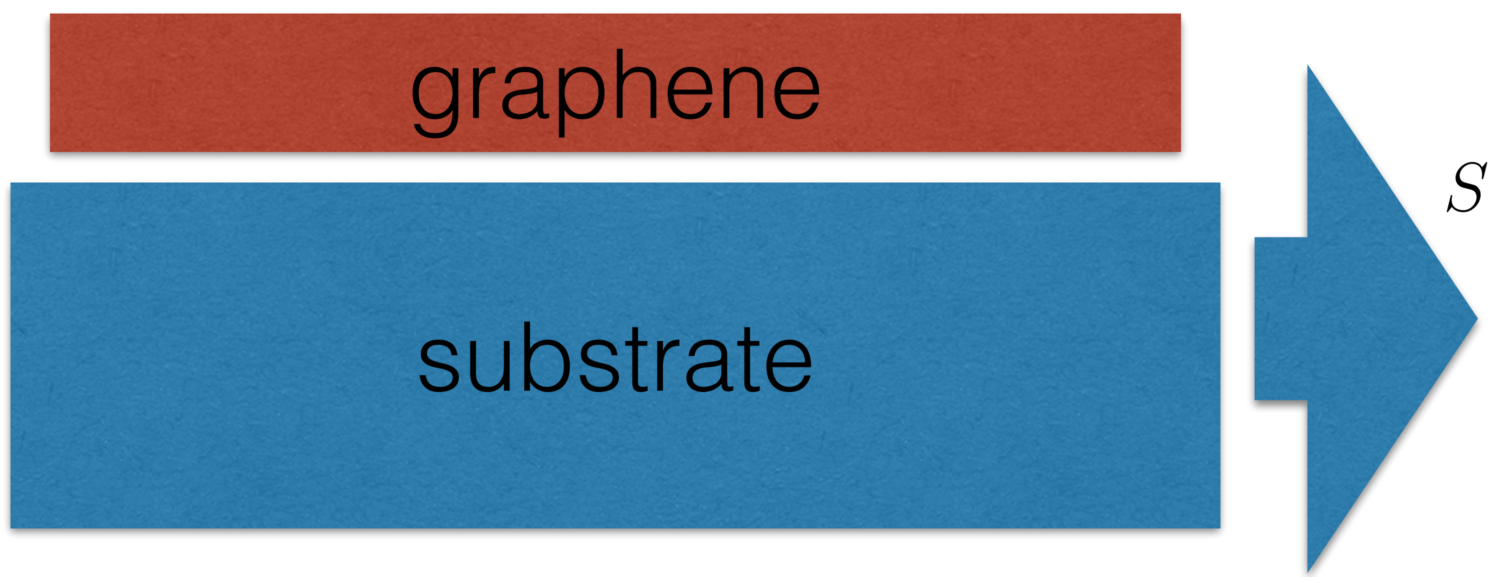
Motivation: strongly correlated QED in graphene



$$S = \int dt d^2x (i\bar{\psi}_a \gamma^0 \partial_0 \psi_a + i v_F \bar{\psi}_a \gamma^i \partial_i \psi_a - e\bar{\psi}_a \gamma^0 \psi_a A_0) + \frac{1}{2} \int dt d^3x (\partial_i A_0)^2$$

Fermi velocity v_F is ~ 1/300 of the speed of light, hence fine structure constant $\alpha \approx 2$.

Thus free-standing graphene is an ideal playground to test the properties of perturbative series in strongly correlated QFT

Following Dyson's argument on the properties of the perturbative series of QED, we have asymptotic series:

Normal QED: we can go up to 137 orders in perturbative series and achieve spectacular precision of at least 12 digits (anomalous magnetic dipole moment of electron)

Graphene effective low energy theory: possible divergence already in the first orders of perturbative expansion

Renormalization of the Fermi velocity (2+1D QED)

$$\boxed{v_F(k) = v_{F,0}(1 + C \ln \Lambda/k)}$$

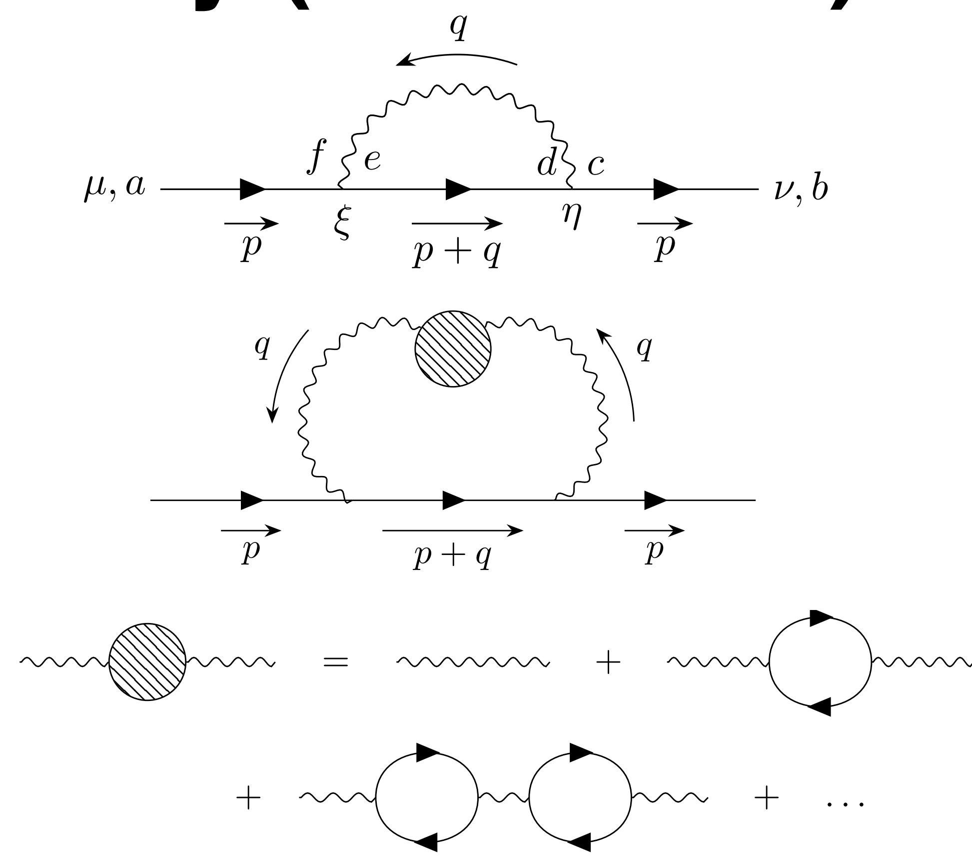
$C = \dfrac{\alpha}{4}$ - one-loop self-energy correction

Random Phase Approximation (RPA): $C = \dfrac{4}{\pi^2 N_f}\left(F_1(\lambda) - F_0(\lambda)\right)$

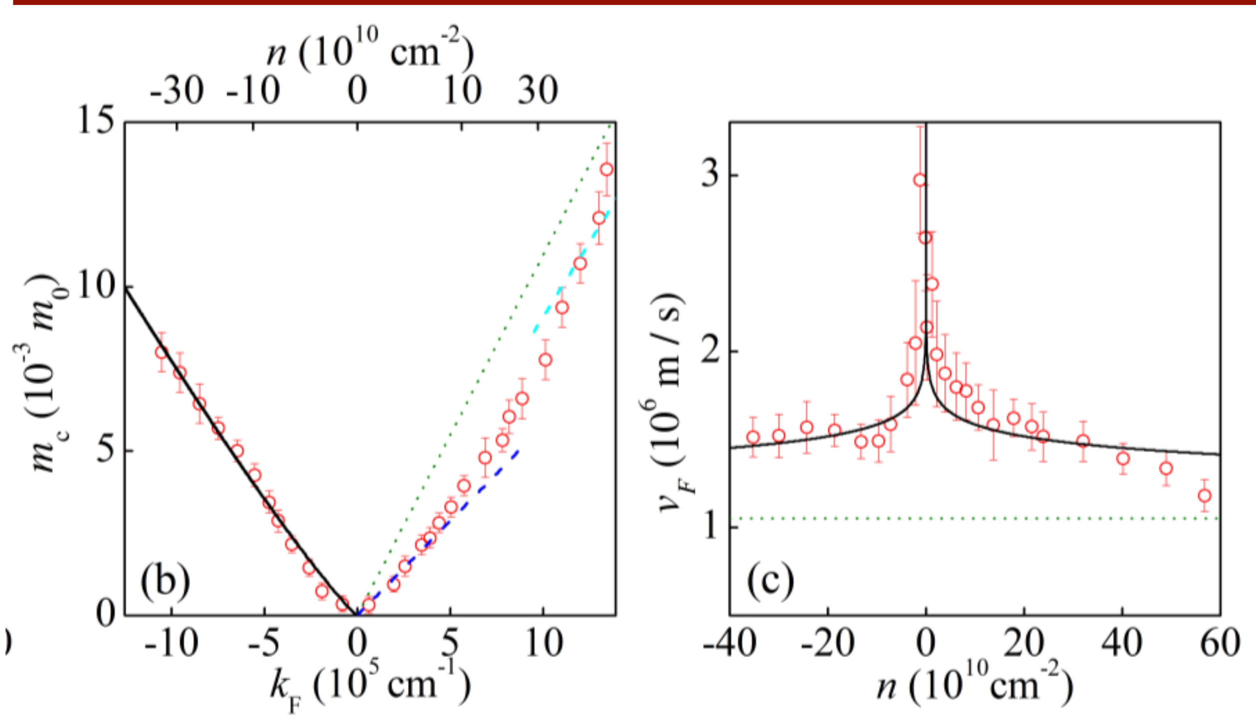
$$F_1(\lambda) = \begin{cases} -(\sqrt{1-\lambda^2}/\lambda)\arccos\lambda - 1 + \pi/(2\lambda) & \lambda < 1 \\ -(\sqrt{\lambda^2-1}/\lambda)\log\left(\lambda + \sqrt{\lambda^2-1}\right) - 1 + \pi/(2\lambda) & \lambda > 1 \end{cases}$$

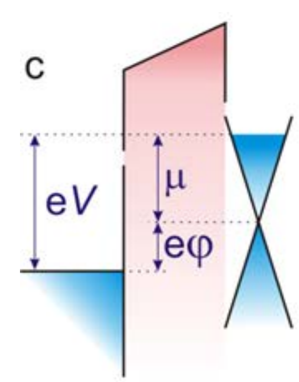
$$F_0(\lambda) = \begin{cases} -((2-\lambda^2)/(\lambda\sqrt{1-\lambda^2}))\arccos\lambda - 2 + \pi/\lambda & \lambda < 1 \\ -((\lambda^2-2)/(\lambda\sqrt{\lambda^2-1}))\log\left(\lambda + \sqrt{\lambda^2-1}\right) - 2 + \pi/\lambda & \lambda > 1 \end{cases}$$

$\lambda \equiv e^2 N_f/(16 v_F) \qquad N_f = 2$



Infrared effect, thus large lattices are crucial for its detection. For this reason we perform auxiliary field QMC simulations on 102x102 lattice with long-range Coulomb interaction.





Experiments

Suspended graphene: Elias et al, Nature Physics 7, 701 (2011)

Graphene encapsulated in hBN: Proceedings of he National Academy of Sciences 110, 3282 (2013)

Important: measurements were maid at finite chemical potential (possible additional screening of Coulomb interaction due to the increased density of charge carriers).

Another possible sources of corrections: charge puddles, strain, lattice defects, curvature, etc.

QMC as an intermediate stage in the study of the convergence of asymptotic series

Questions: Do we really have logarithm in experiment? How close can we get to the experimental value of the coefficient C using asymptotic perturbative series?

Experiment

?

Perturbative series for low energy effective theory (2+1D QED) or for interacting tight-binding Hamiltonian (Lattice Perturbation theory)

QMC

$$\hat{H} = -\kappa \sum_{\sigma,\langle x,y\rangle} (\hat{a}^{\dagger}_{\sigma,x}\hat{a}_{\sigma,y} + \mathrm{h.c}) + \frac{1}{2}\sum_{x,y} V_{x,y}\hat{q}_x\hat{q}_y$$

Verification of the interacting tight-binding Hamiltonian

Check the convergence of perturbative series

We can separate higher-order perturbative corrections from other effects (lattice-scale physics, etc)

Hybrid Monte Carlo simulations on large lattices: Gaussian representation of the fermionic determinant

$$e^{\delta_\tau \sum_{x,y} V_{x,y} \hat{q}_x \hat{q}_y} \cong \int \mathcal{D}\phi e^{-\frac{1}{2\delta_\tau} \sum_{x,y} \phi_x V^{-1}_{x,y} \phi_y} e^{i \sum_x \phi_x \hat{q}_x}$$

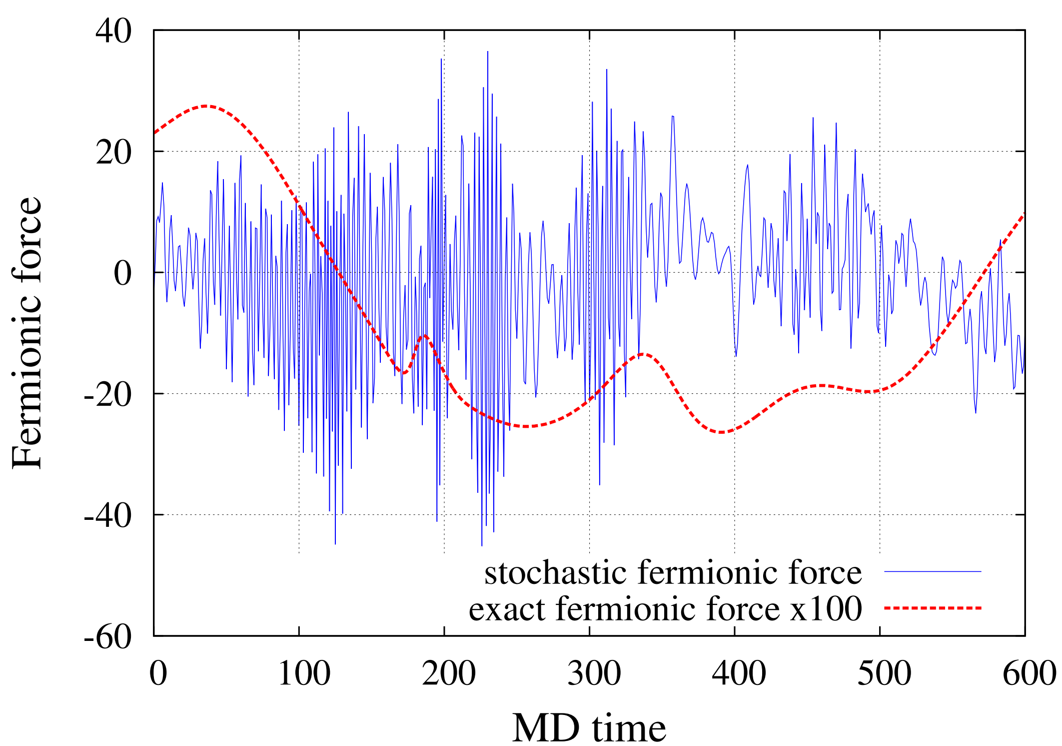
- HS field coupled to charge (long-range interaction)

$$Z = \int \mathcal{D}\phi \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{-S[\bar{\psi},\psi,\phi]}$$

$$S = \int_0^\beta d\tau \left[-\sum_{x,a} \bar{\psi}_{x,a} \partial_\tau \psi_{x,a} + \sum_{x,a;y,a} \bar{\psi}_{x,a} (H_0)_{x,a;y,b} \psi_{y,b} + i \sum_{x,a,b} \phi_x \bar{\psi}_{x,a} \sigma^z_{a,b} \psi_{x,b} - \frac{1}{2} \sum_{x,y} \phi_x V^{-1}_{x,y} \phi_y \right]$$

Fermionic fields are integrated out: $\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\phi \det M[\phi]^2 \mathcal{O} e^{-S_B[\phi]}$

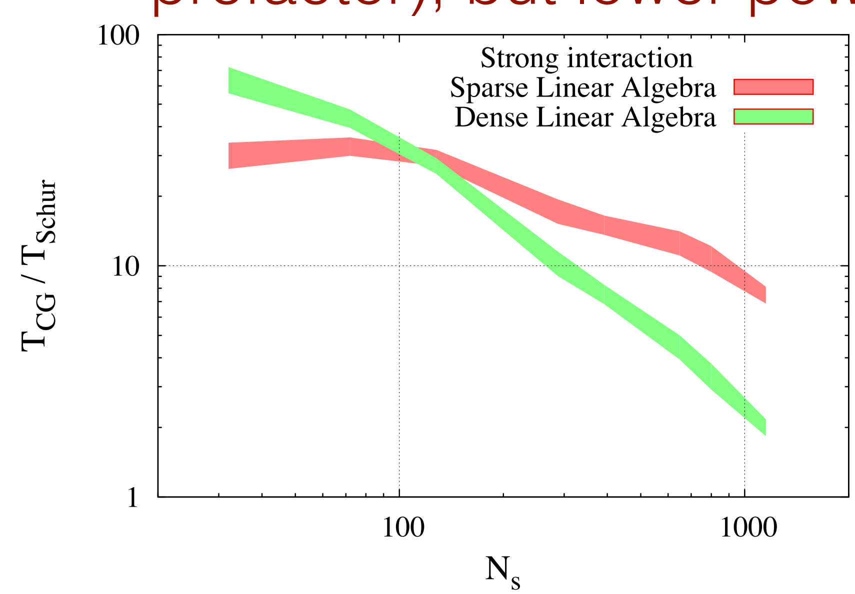
Standard BSS-QMC: direct calculation of the changes of fermionic determinant during updates. Leads to scaling law N^3L.



HMC: Gaussian representation of fermionic determinant

$$\det M[\phi]^2 \propto \int \mathcal{D}\{\eta, \eta^\dagger\} e^{-\eta^\dagger \left(M[\phi] M^\dagger[\phi]\right)^{-1} \eta}$$

Worse statistical fluctuations (thus larger prefactor), but lower power in the scaling:



$$\mathcal{S}_{real} = 1.47$$

$$T \sim (NL)^{\mathcal{S}_{real}}$$

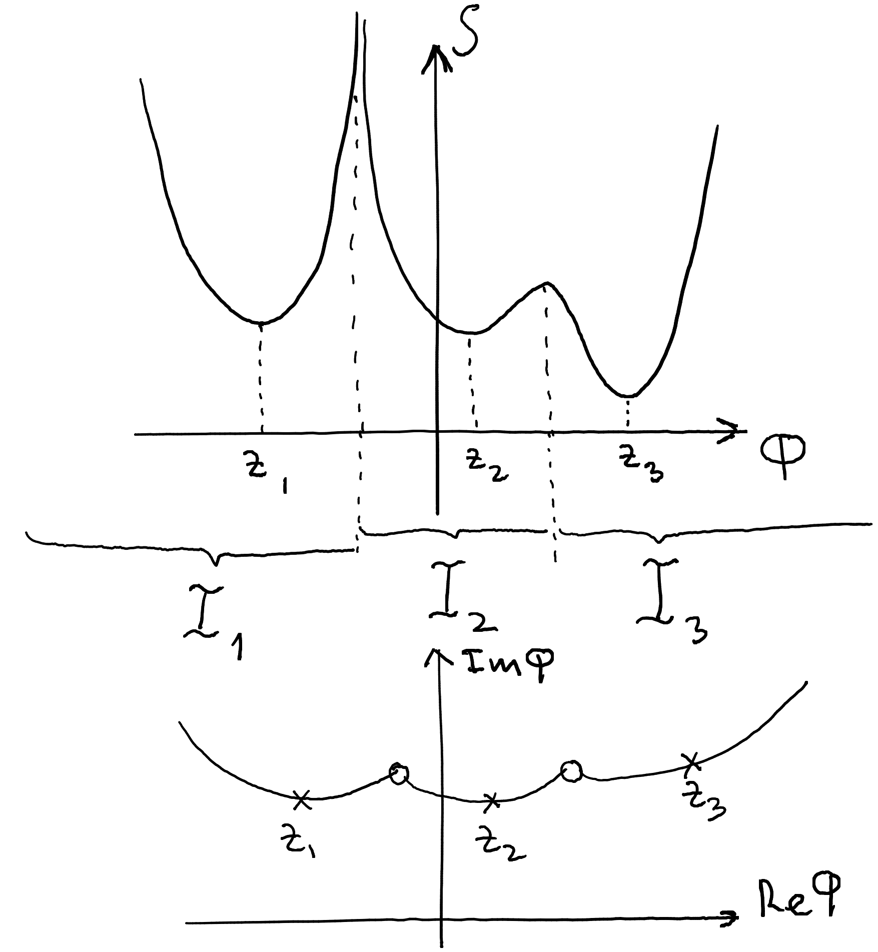
arXiv: 1812.06435
arXiv: 1803.05478

Hybrid Monte Carlo simulations on large lattices: Why better scaling? (1)

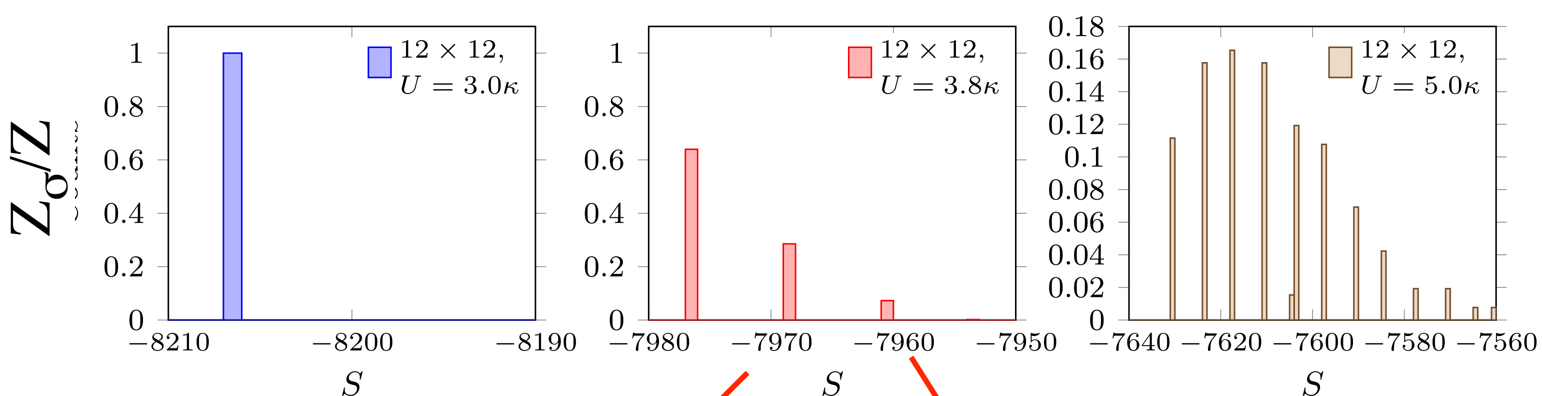
Can be understood in terms of Lefschetz thimbles

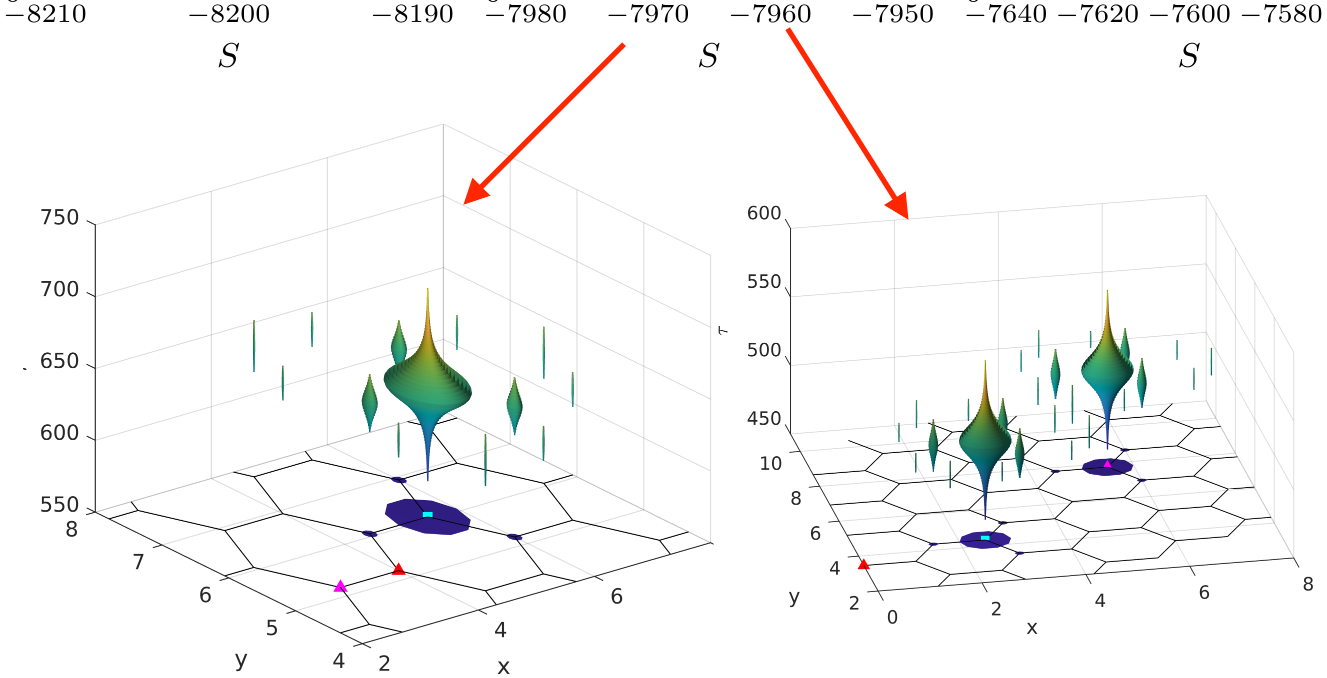
$$\mathcal{Z} = \int_{\mathbb{R}^N} \mathcal{D}\Phi \, e^{-S[\Phi]} = \sum_{\sigma} k_\sigma \mathcal{Z}_\sigma$$

$$\mathcal{Z}_\sigma = \int_{\mathcal{I}_\sigma} \mathcal{D}\Phi \, e^{-S[\Phi]} \qquad \left.\frac{\partial S}{\partial \Phi}\right|_{\Phi = z_\sigma} = 0$$

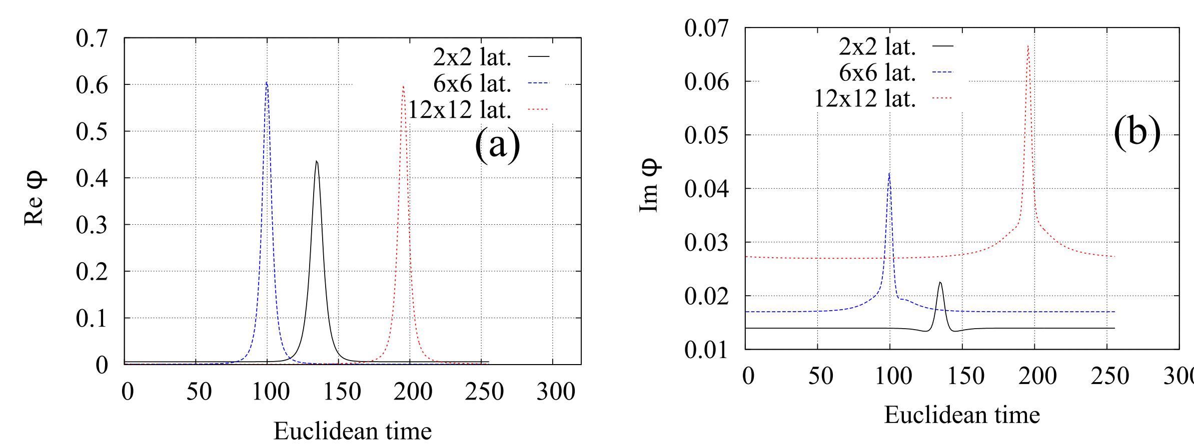


Saddle points at half-filling are multi-instanton solutions: collections of localized instantons





Instantons are shifted into complex space away of half-filling

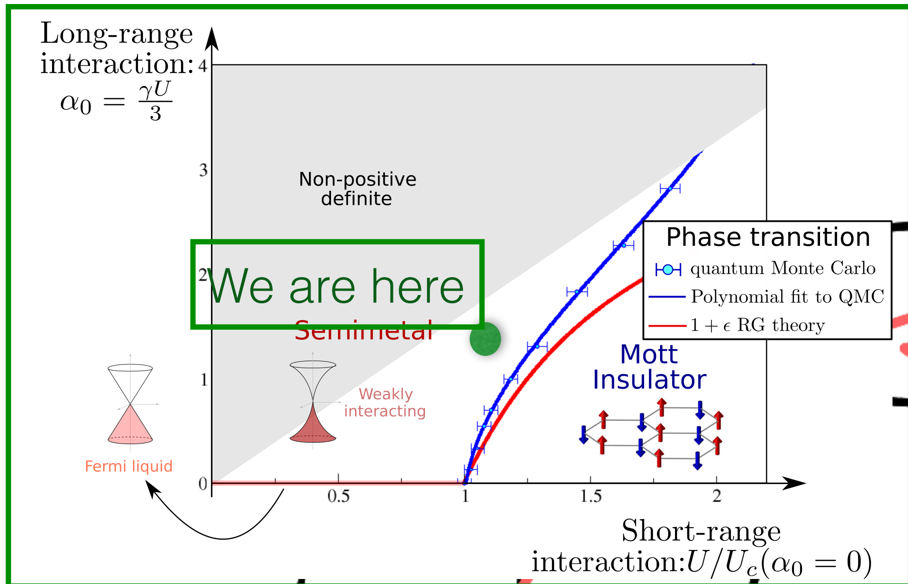


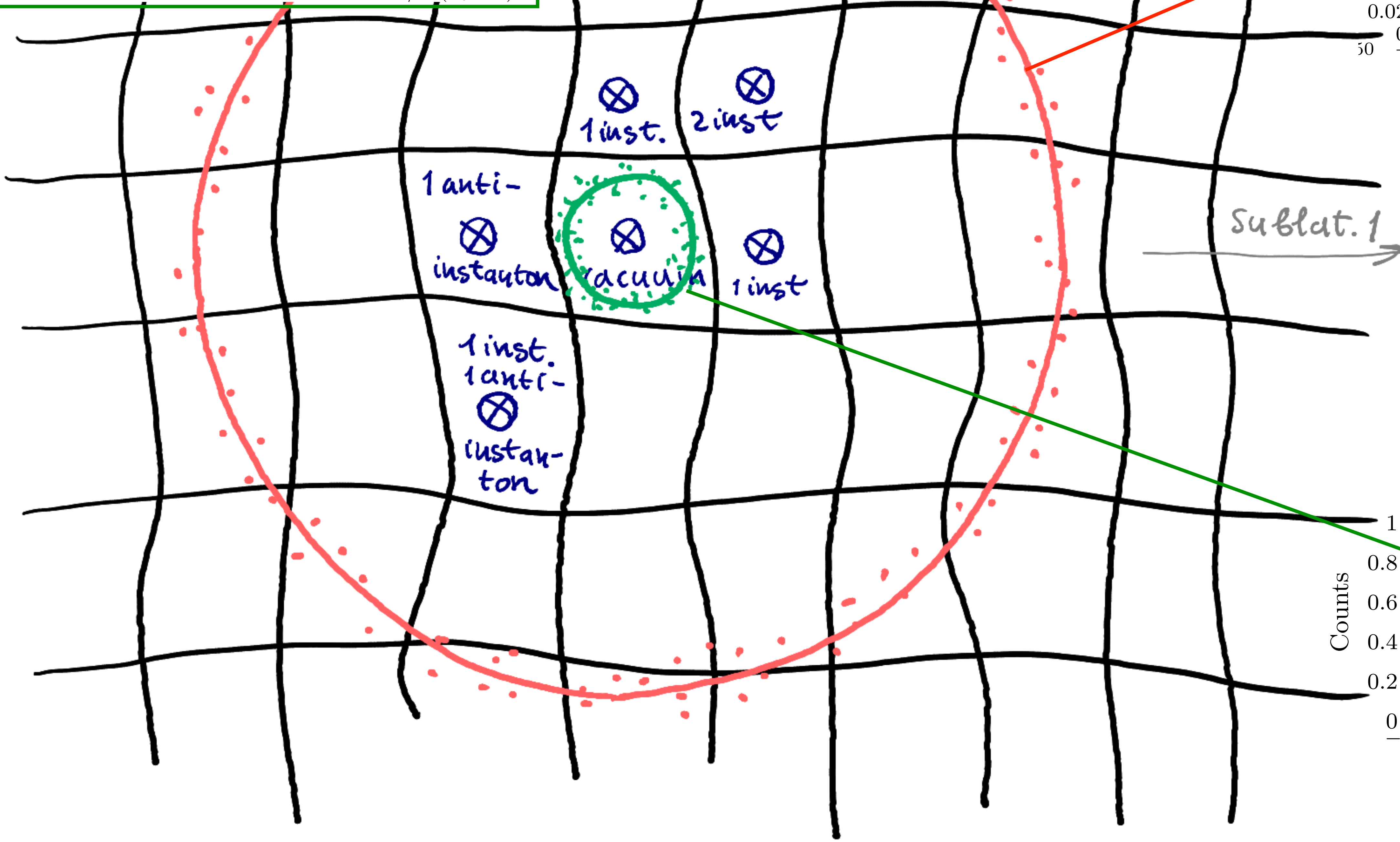
PRD 101, 014508 (2020)

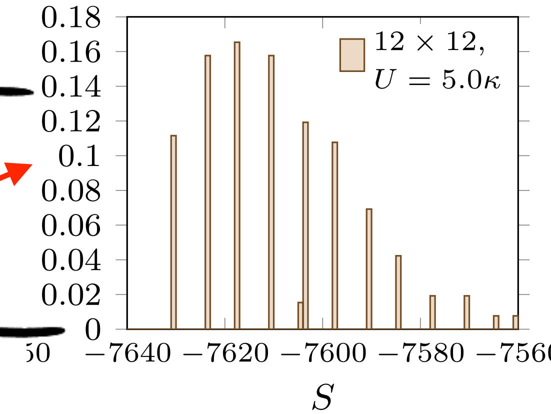
Hybrid Monte Carlo simulations: Why better scaling? (2)

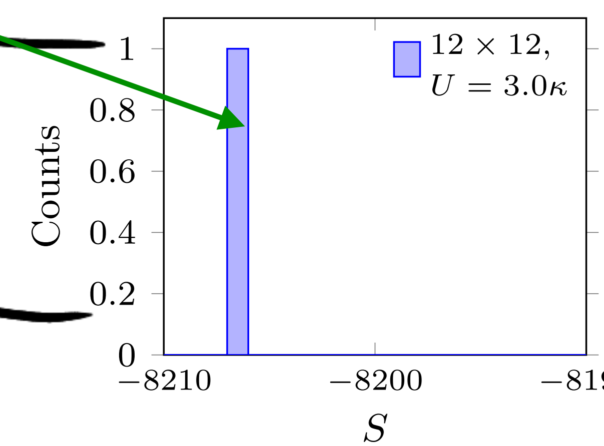
$$\det M[\phi]^2 \propto \int \mathcal{D}\left\{\eta,\eta^\dagger\right\} e^{-\eta^\dagger\left(M[\phi]M^\dagger[\phi]\right)^{-1}\eta}$$

Works well if M doesn't have zero modes



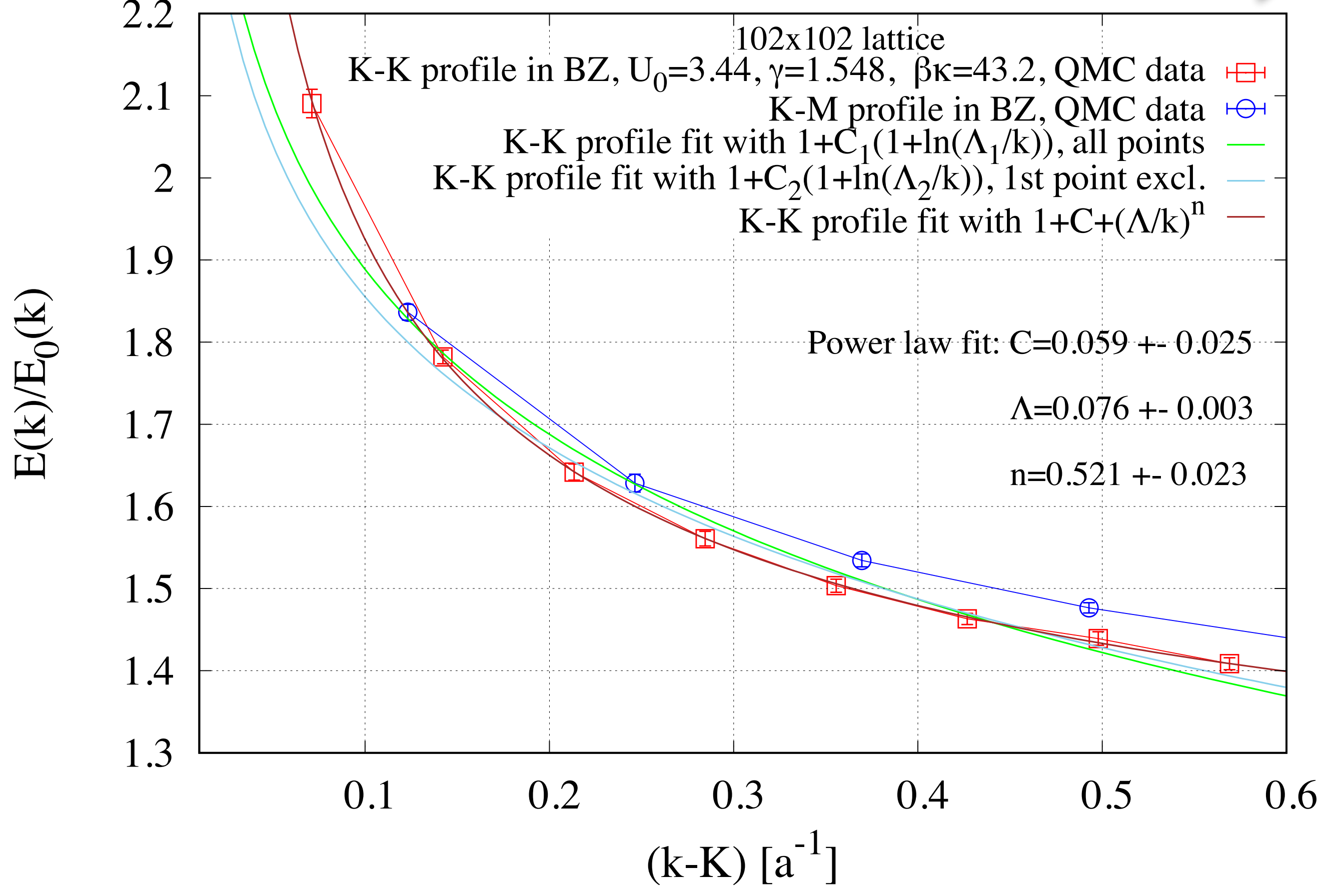


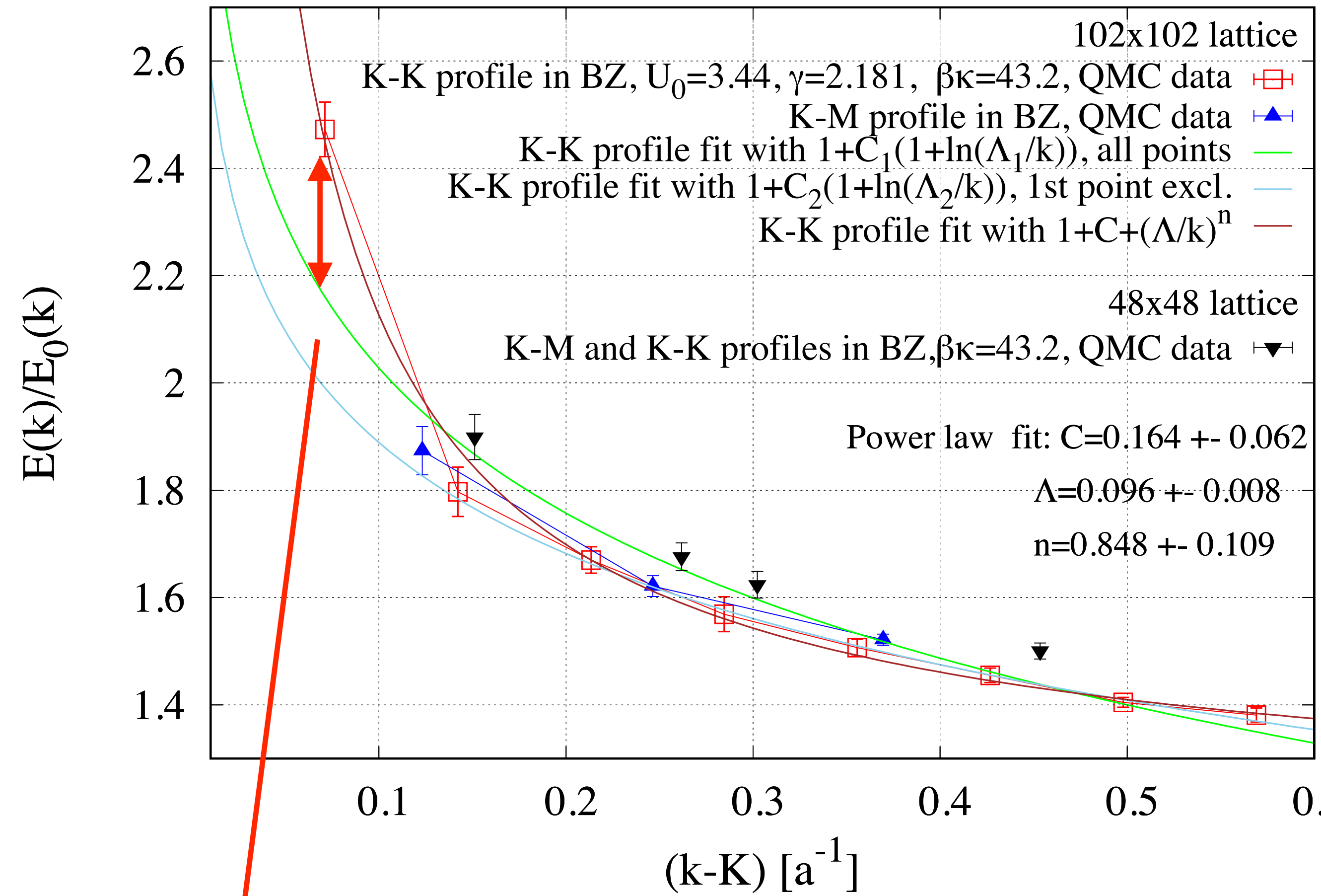


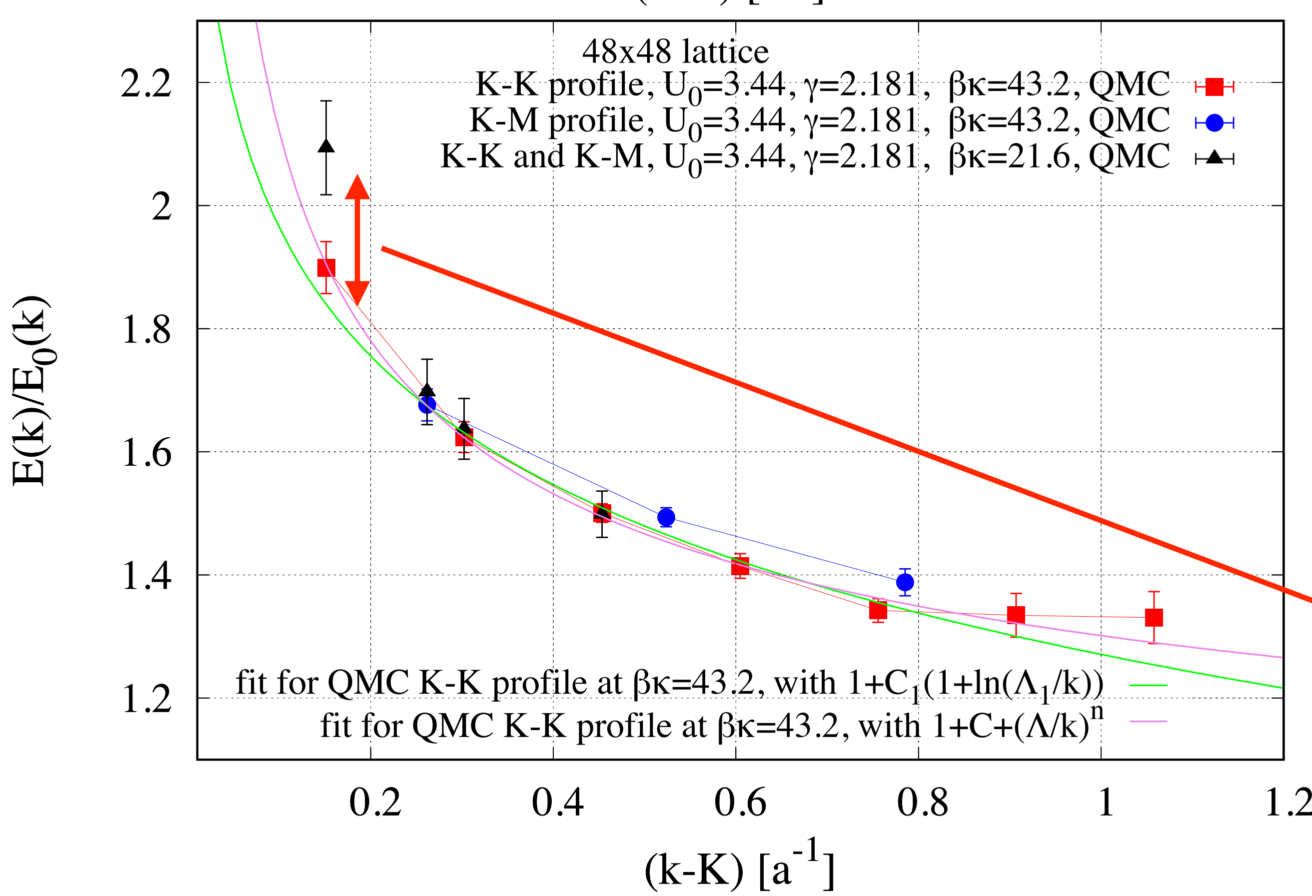


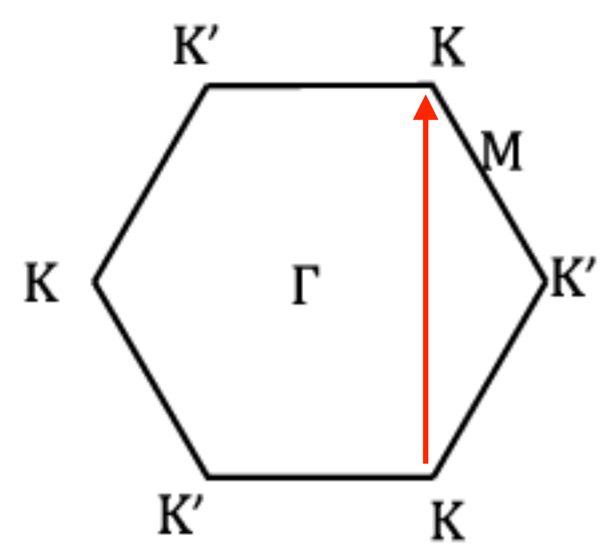
QMC data on 102x102 lattices

$$v_F(k) = v_{F,0}(1 + C \ln \Lambda/k) \Rightarrow E(k) = E_0(k)[1 + C(1 + \ln \Lambda/k)]$$





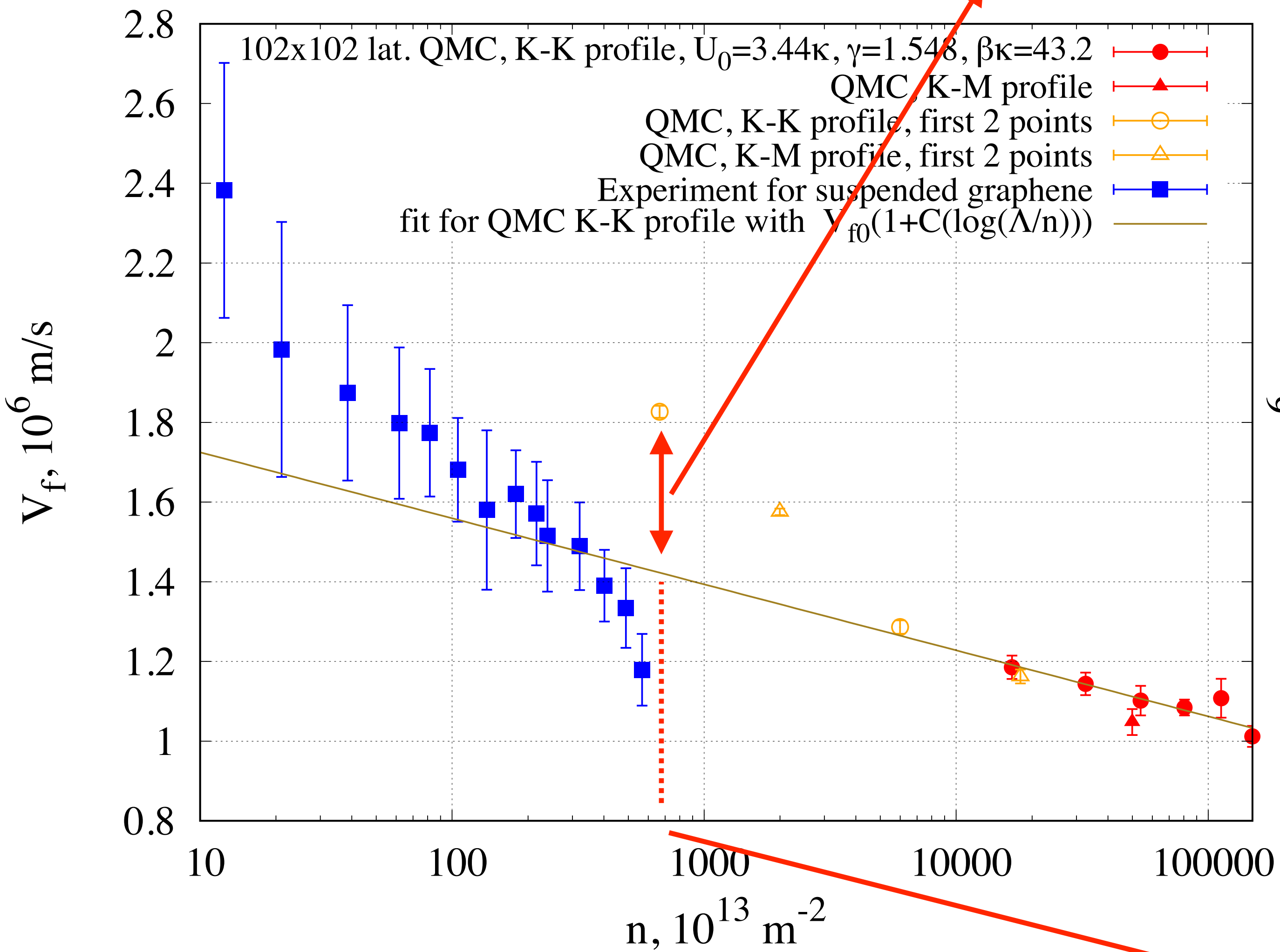


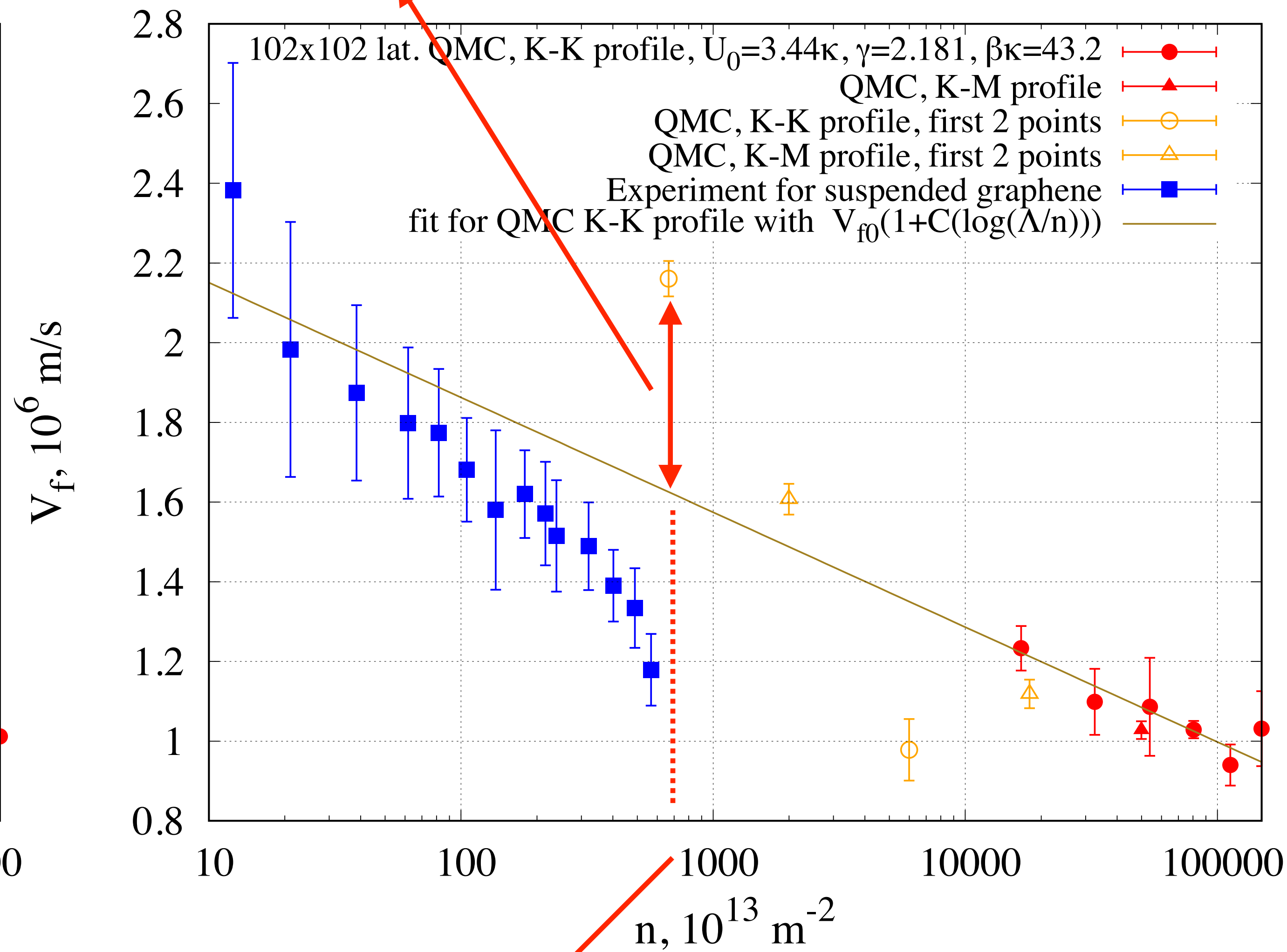


Temperature corrections at low (k-K), of the opposite sign comparing to perturbative predictions

Comparison with experiment

Temperature corrections are still important in QMC data





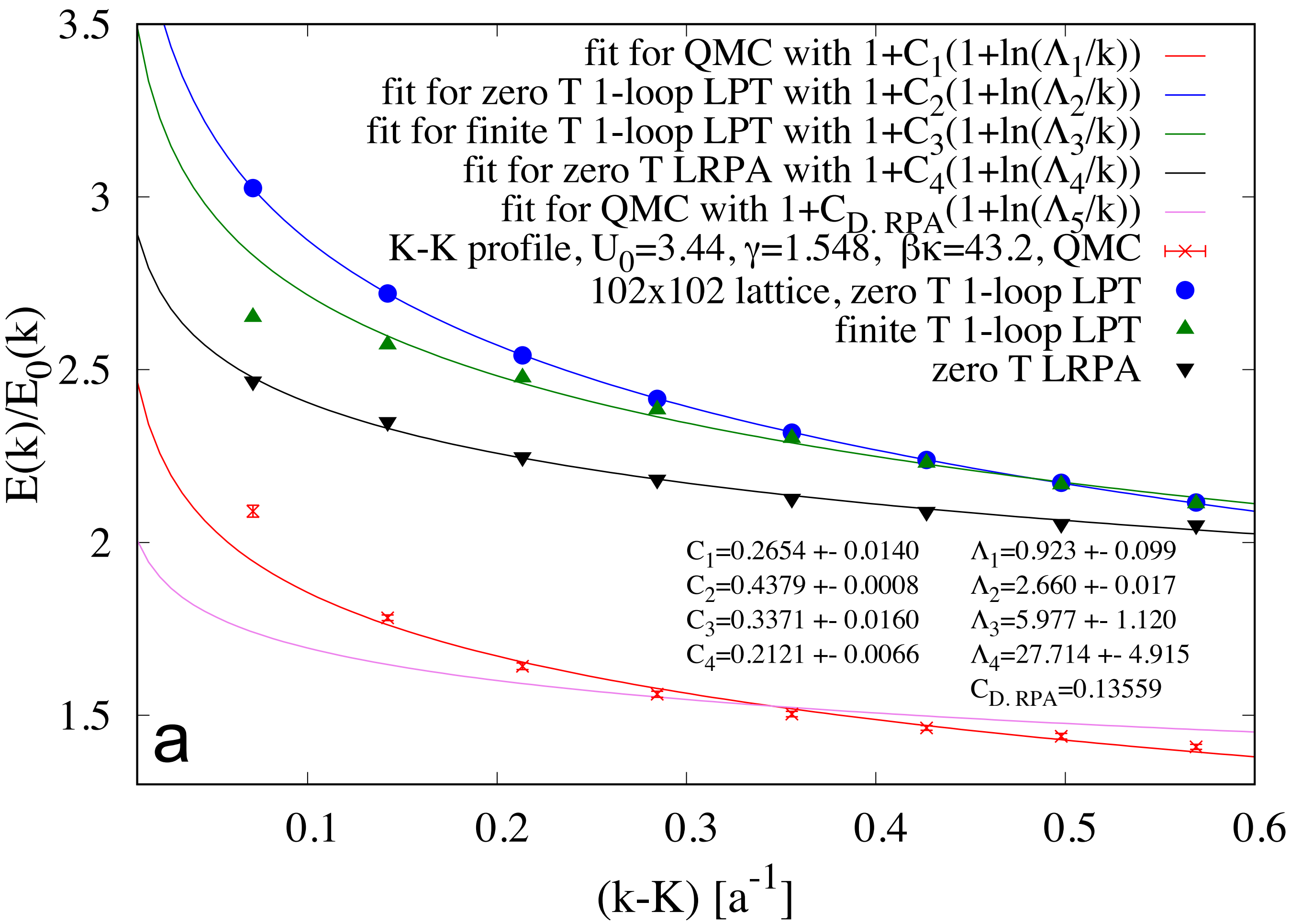
$$v_F\left(\frac{k_1+k_2}{2}\right) = \frac{E(k_1)-E(k_2)}{k_1-k_2}$$

2 times lower temperature: QMC and experimental data meet here.

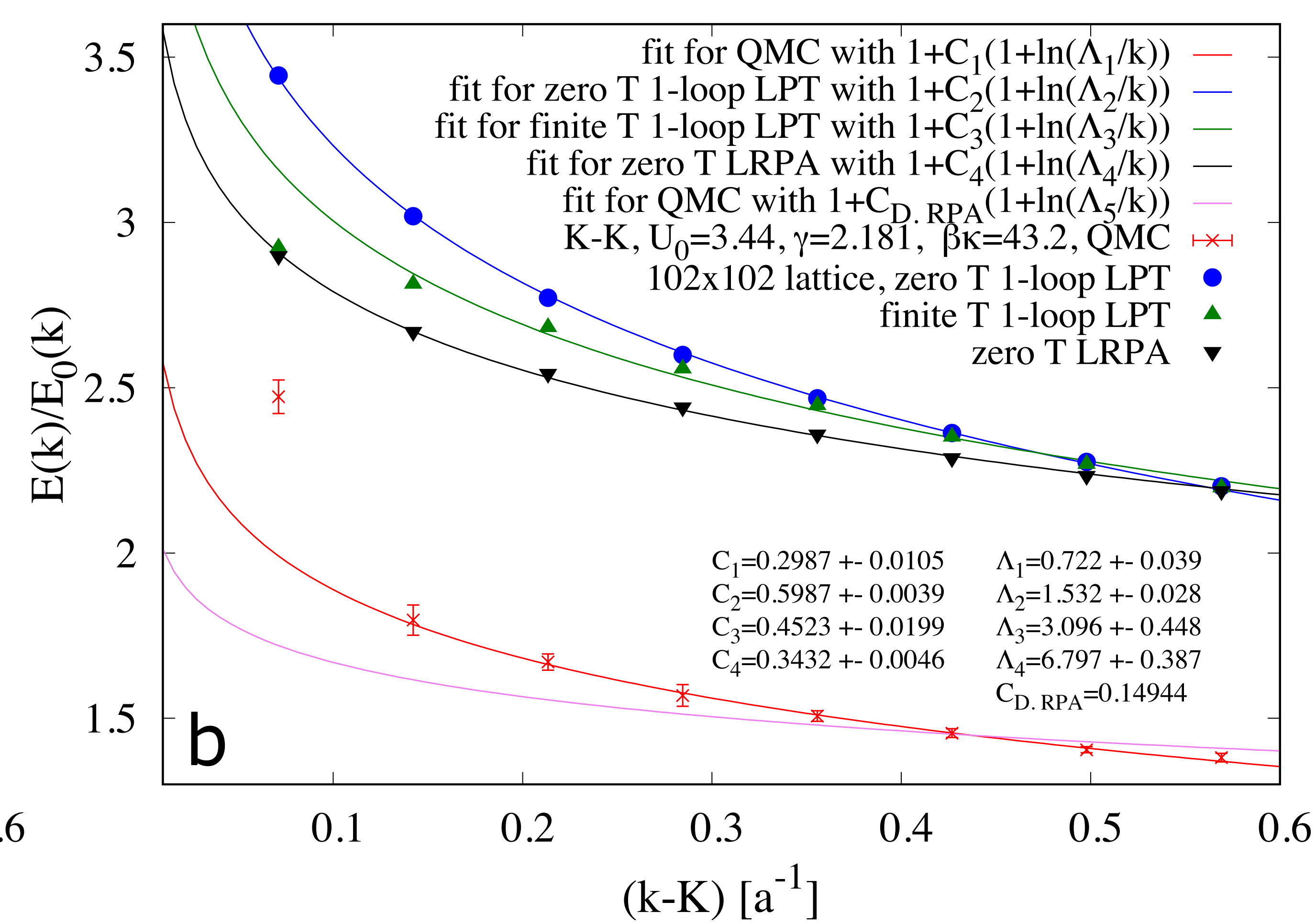
2 times larger lattice: large overlap between experiment and QMC data.

Suggestion for experiment: 1) better precision; 2) temperature effects at low density as qualitative proof of higher-order corrections beyond one-loop approximation

Comparison with perturbative results



Smaller Coulomb tail



Larger Coulomb tail

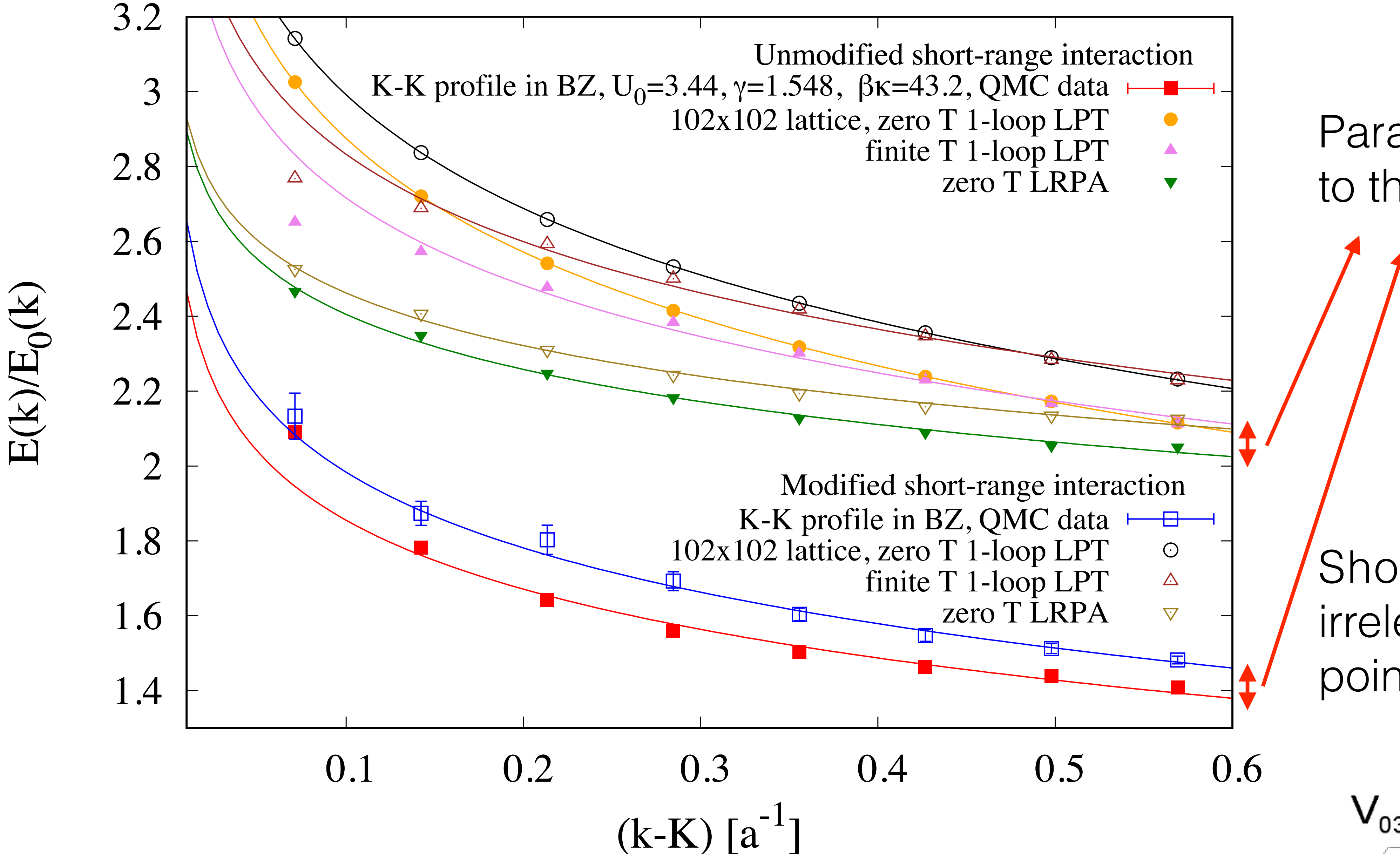
$$V_{x,y} = \gamma U_0 / (2|\vec{R}_{x,y}|)$$

$$V_{x,x} = U_0$$

Still large discrepancies even between lattice RPA and QMC data: higher order corrections are important.

Note: Cutoff is not a free parameter in lattice PT

Role of short-range (irrelevant) couplings



Parallel shift is equivalent to the change of cutoff.

Short-range couplings: irrelevant at infrared fixed point.

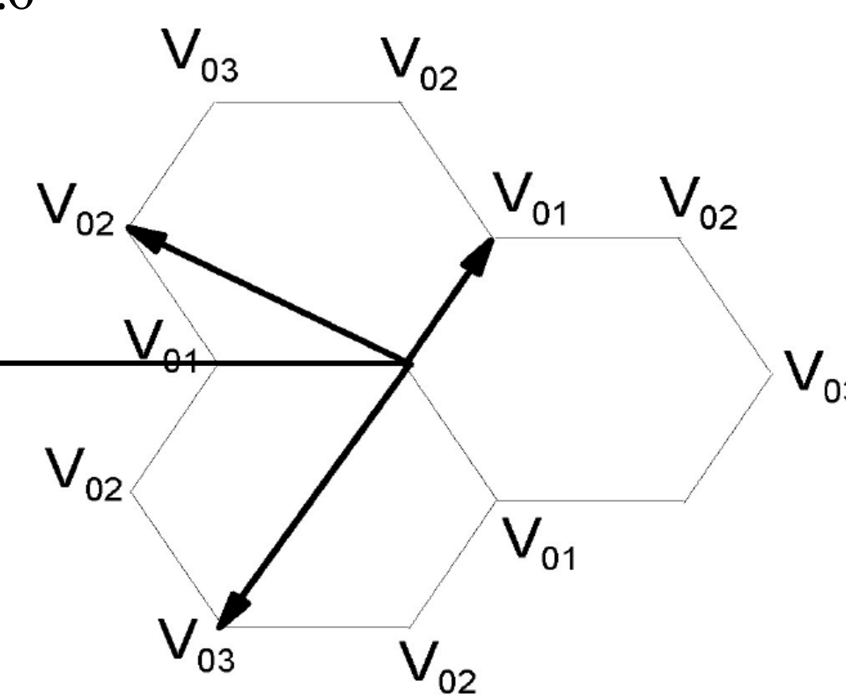
Non-universal (in RG sense) quantities, like cutoff are still dependent on irrelevant interactions

Coulomb tail

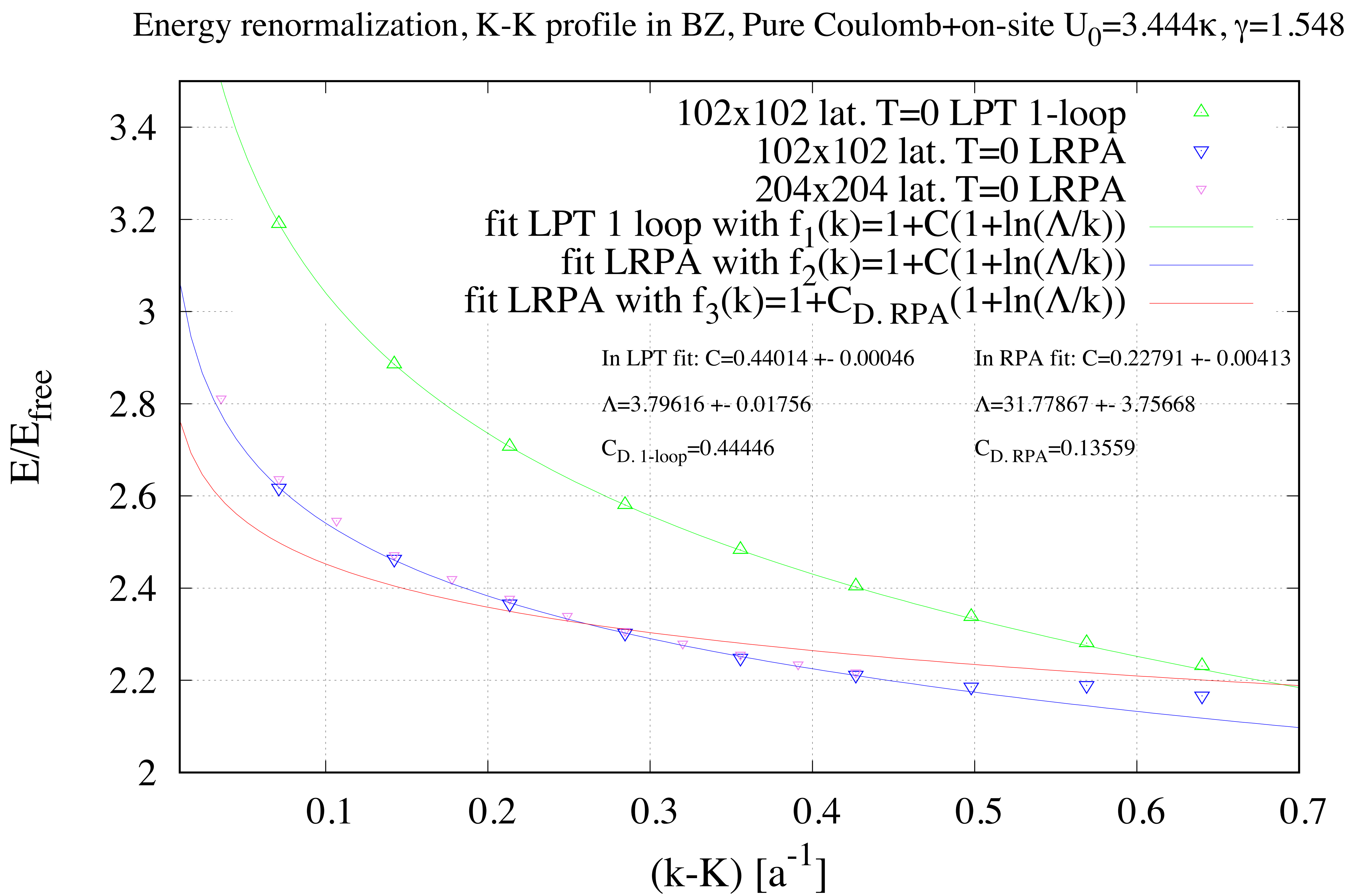
$$V_{x,y} = \gamma U_0/(2|\vec{R}_{x,y}|)$$

$$V_{x,x} = U_0$$

«Marginally irrelevant»: gives main asymptotic for the Fermi velocity renormalization



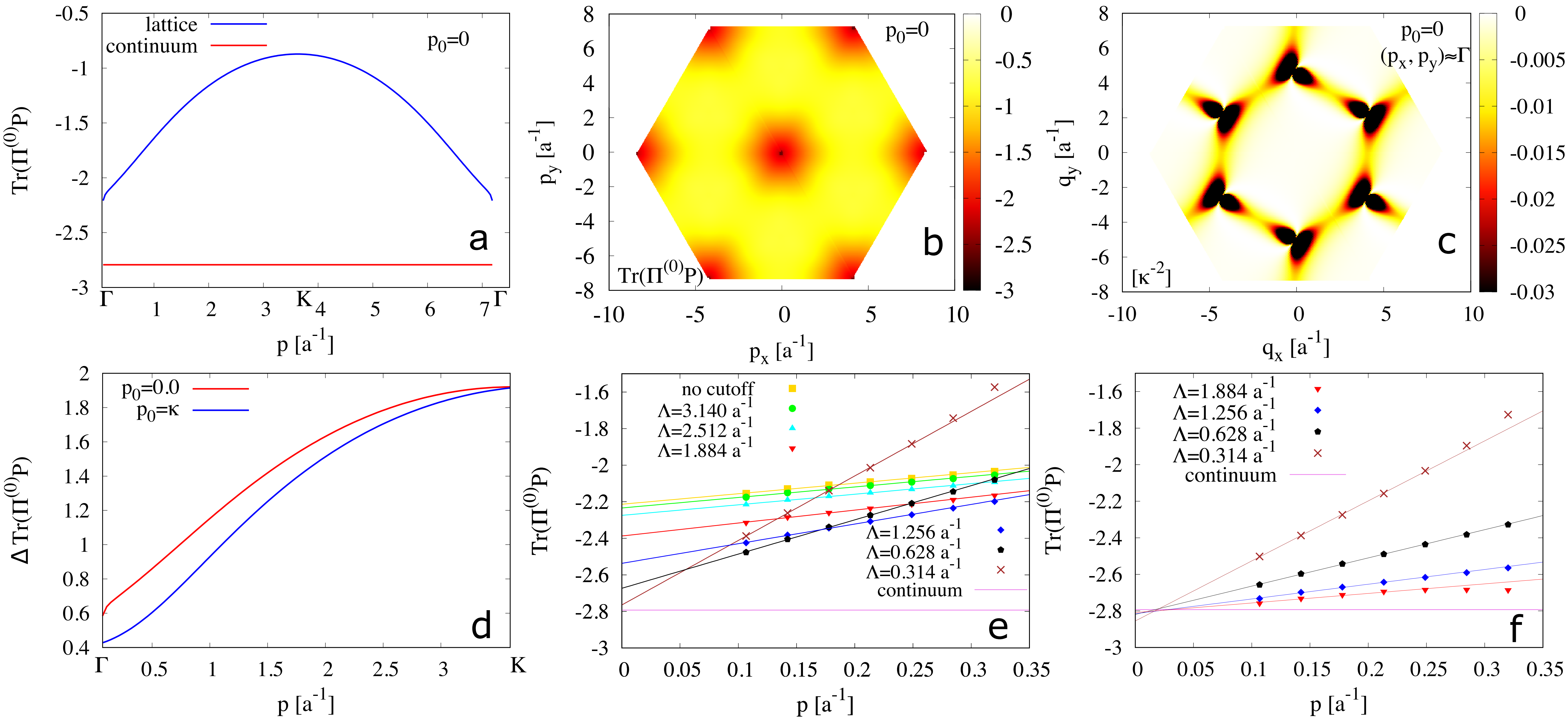
Comparison of lattice and continuum PT

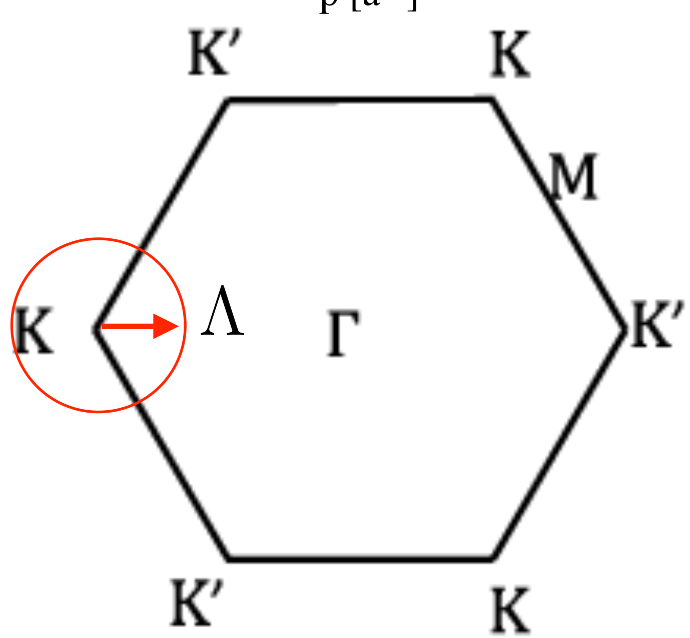


Very good agreement at one-loop level, but quite large difference in RPA coefficient.

This is puzzling, since we are deeply within the infrared regime where both bare Coulomb propagator and dispersion relation of electrons are the same as in 2+1D QED within <1% error.

Polarization on the lattice and in continuum



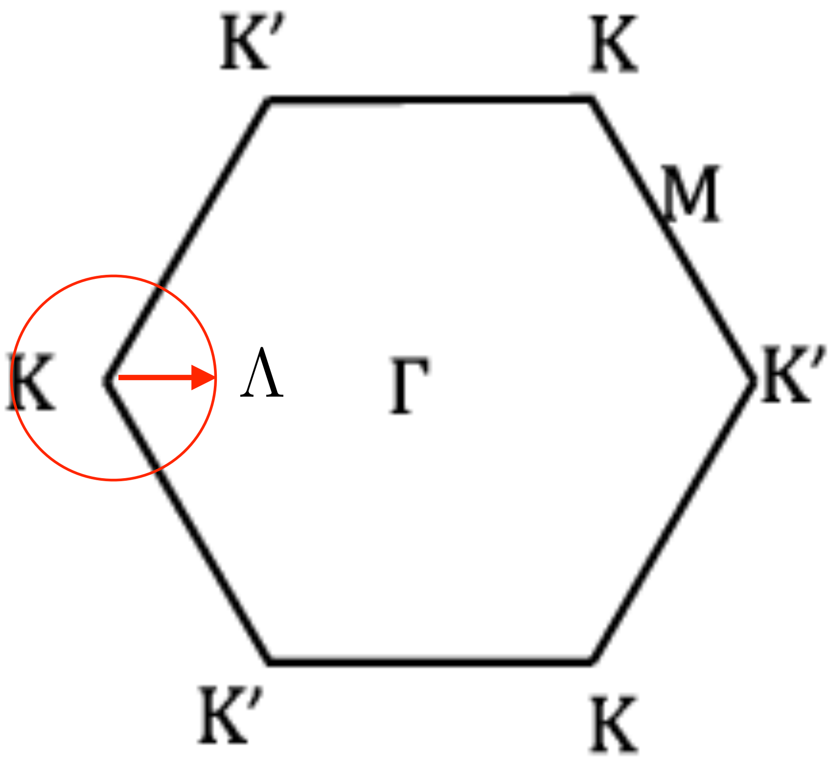


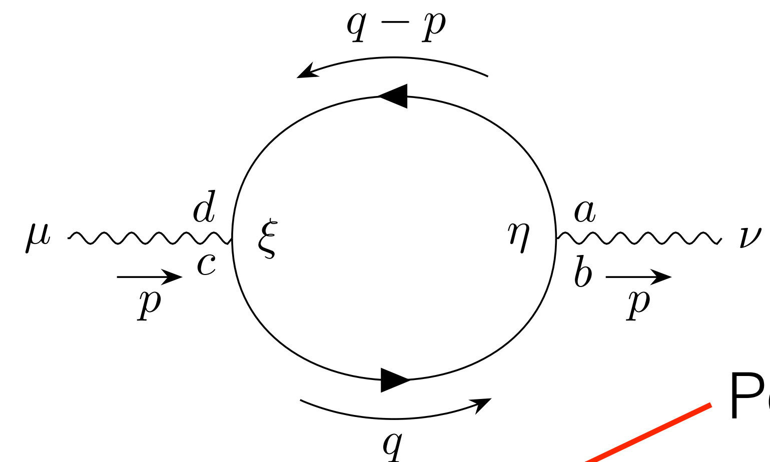
Shift at the origin: inter-valley scattering

Linear asymptotic at the origin: finite cutoff effect (We expand cutoff keeping the linear approximation to the electronic dispersion)

Inter-valley scattering and finite cutoff should be added in 2+1D QED for quantitative description of QMC or experimental data

Cutoff effects in polarization and self-energy in 2+1D QED



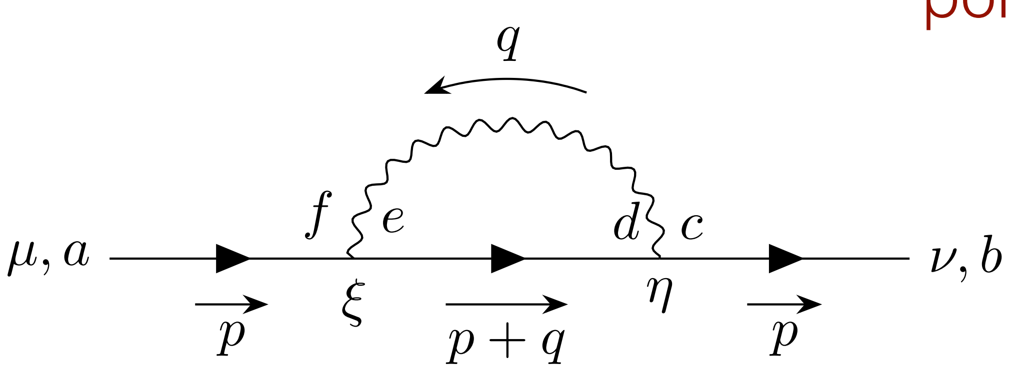


Polarization is finite

$$P_\Lambda^{(0)}(p_0,\vec{p}) = P^{(0)}(p_0,\vec{p}) + \delta P_\Lambda^{(0)}(p_0,\vec{p})$$

$$\delta P_\Lambda^{(0)}(p_0,\vec{p}) = -\frac{7}{16\pi}\frac{\vec{p}^2}{\Lambda} + O\left(\Lambda^{-2}\right)$$

Exactly the same corrections we observed numerically in polarization in LPT



$\delta\Sigma$

$$\Sigma^{(1)}(k_0,\vec{k}) = v_F\gamma_i k_i \frac{\alpha_g}{4}\log\left(\frac{\Lambda}{k}\right) + O(\vec{k}^2/\Lambda^2)$$

Much smaller corrections in one-loop self-energy, also consistent with numerical LPT

Summary

1) With certain QMC algorithms, and in some cases, we can reach sample size/scale really observed in experiment without need for further extrapolations.

2) We were able to directly observe the logarithmic dependence of the Fermi velocity on momentum for the first time in QMC simulations.

3) Comparison with experiment confirms the interacting tight-binding Hamiltonian with cRPA potentials of electron-electron interactions as a quantitatively precise model of the electronic properties of graphene, even in strongly-correlated regime.

4) The standard 2+1D QED can not be really used besides the qualitative prediction of the main asymptotic, since the inter-valley scattering and cutoff effects play important role starting from RPA level. Following this comparison, the most straightforward course of action is to replace continuum perturbation theory with lattice perturbation theory in the study of asymptotic properties of perturbative series in graphene.

5) Besides lattice-scale physics, higher-order corrections are important in quantitative behavior of the Fermi velocity too. The most pronounced effects are: 1) the opposite sign of the temperature corrections in QMC in comparison to perturbative data; 2) large discrepancy in the cutoff when we compare QMC results with LPT.