The metal-insulator transition for two-dimensional interacting Dirac electrons

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Outline

The metal insulator transition (MIT), existing theories

Study of two model Hamiltonian with MIT at Uc:
1) The Hubbard model on the Honeycomb lattice
2) The Pi-Flux Hubbard model

Numerically exact results and finite size scaling:
Establishing the transition and its
universal critical exponents

Study of criticality in the metallic side (U<Uc):
quasiparticle weight and density structure factor

Hubbard model , any lattice (i.e. even frustrated) one gets a Metal-Insulator transition at half-filling as a function of the Hubbard U/t

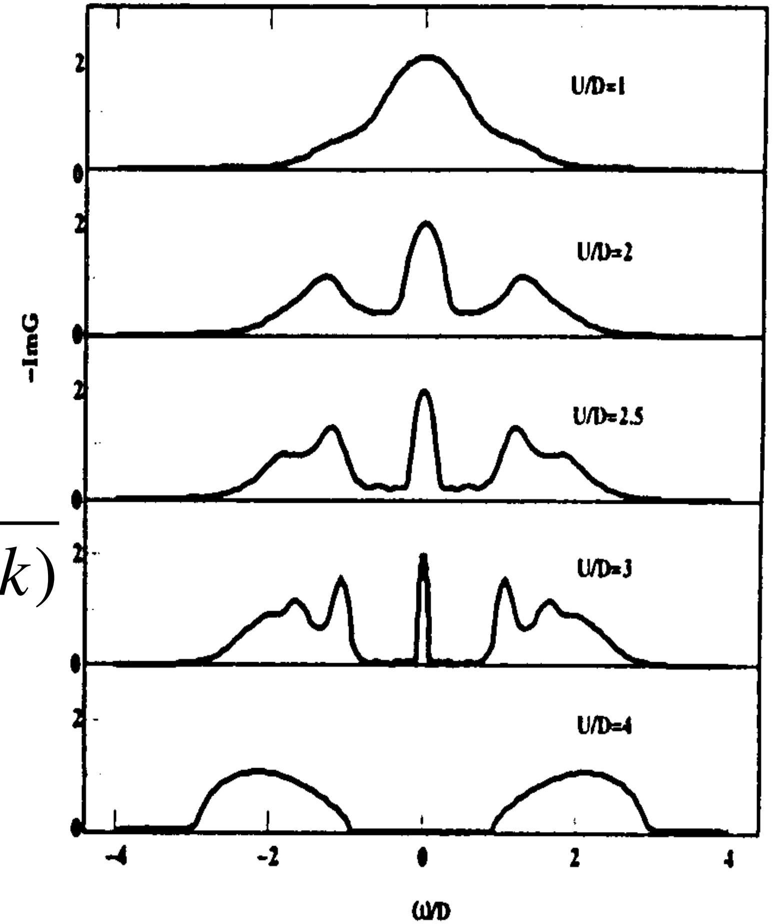
Gutzwiller approximation:
The Brinkman-Rice transition PRB '70

The quasiparticle weight Z renormalizes the Hopping $t \rightarrow Z t$ and there is absence of Kinetic energy at the MIT $Z \rightarrow 0$ as well as Bandwidth, Fermi velocity …

Solving Hubbard model in ∞ dimensions

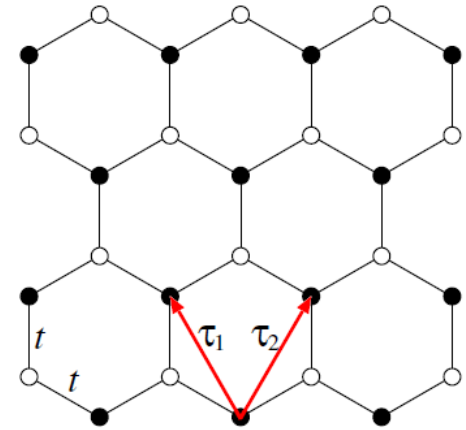
- In ∞-D, spatial fluctuation can be neglected.
  → mean-field solution becomes exact.
- Hubbard model → single-impurity Anderson model in a mean-field bath.
- Solve exactly in the time domain
  → "dynamical" mean-field theory♪

$$G(\omega,k)=\frac{1}{\omega-\varepsilon(k)-\Sigma(\omega)}\approx\frac{Z}{\omega-\varepsilon_{QP}(k)}$$

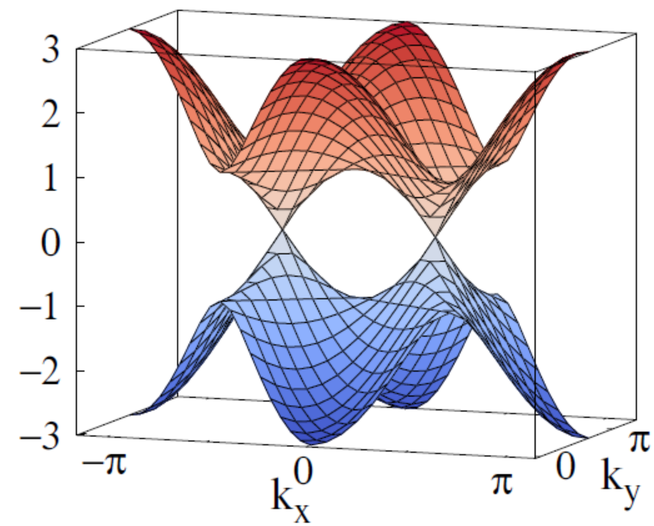


However momentum independent Self energy implies Z~ Bandwith or Z ~Fermi velocity→ 0 at MIT

Hubbard model on honeycomb lattice



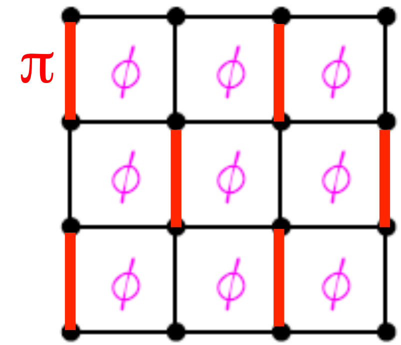
- model for graphene
- massless Dirac fermion
  → semi-metal at U/t=0
- bipartite
  → AF order for large U/t
- not geometrically frustrated
  → negative-sign free in QMC
- smallest coordination number in 2D
  → large quantum fluctuations



Mott transition at $U/t \approx 4$ S.S., E. Tosatti, EPL (1992)

- (peculiar) model for CuO_2

π-flux Hubbard model



$$\mathcal{H} = \sum_{<j,k>,\sigma} \left(c^\dagger_{j\sigma} t_{jk} c_{k\sigma} + c^\dagger_{k\sigma} t^*_{jk} c_{j\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$t_{jk} = t \ e^{i\theta_{jk}} \qquad \phi = \sum\nolimits_{\square} \theta_{jk} = \pi$$

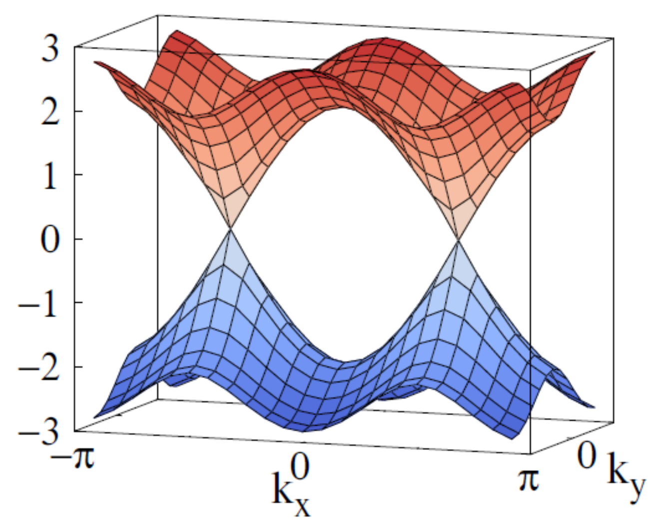
Affleck, Marston, PRB (1998)

Lieb, PRL (1994)

$\phi = \pi$: most stable for half filling even with interaction (U/t)

- time-reversal invariant
- equivalent to staggered π-flux state

- massless Dirac fermion
- bipartite
- not geometrically frustrated
- different non-interacting dispersion than honeycomb lattice



Mott transition at $U/t > 4$

YO, Hatsugai, PRB (2002)

The method in one slide: N sites, projection τ

$\exp(-\tau H)$ → Trotter approx. → Error $O(\Delta\tau^2)$

The discrete Hubbard-Stratonovich transformation (HST, Hirsch '85):

$$\exp[g(n_\uparrow - n_\downarrow)^2] = \frac{1}{2}\sum_{\sigma=\pm 1}\exp[\lambda\sigma(n_\uparrow - n_\downarrow)]$$

$$\cosh(\lambda) = \exp(g/2), \quad \text{with } g = \frac{U\Delta\tau}{2}$$

Sequential updates allows to have N^3 τ algorithm

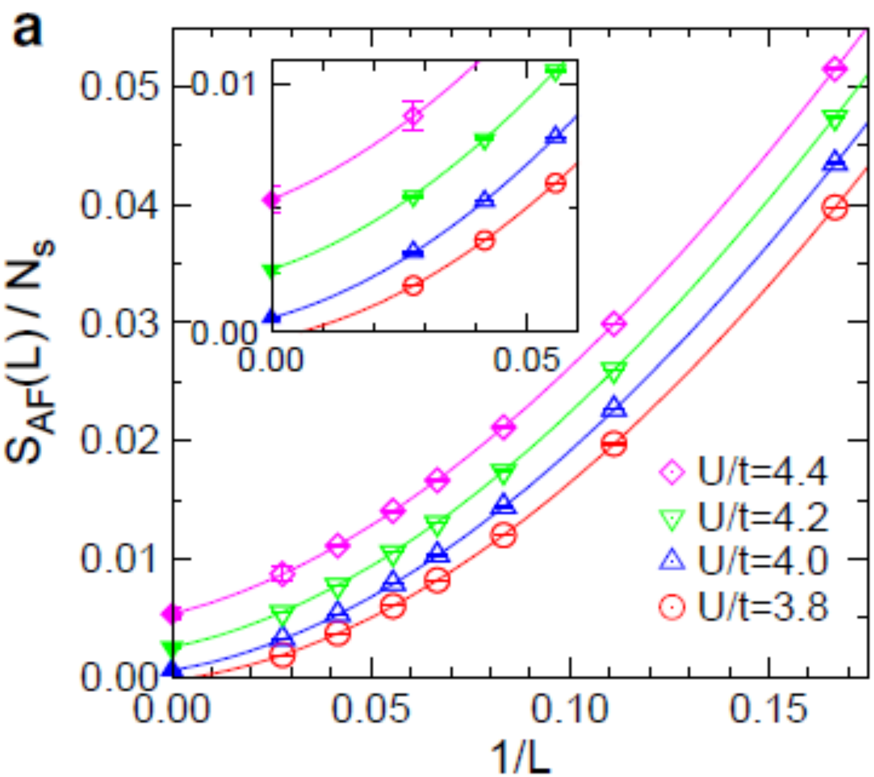
Several Trotter free methods exist now (diagrammatic QMC, continuous time…, but scaling as $(N\,\tau)^3 >> N^3\,\tau$

Thus for ground state standard '85 AFQMC remains convenient

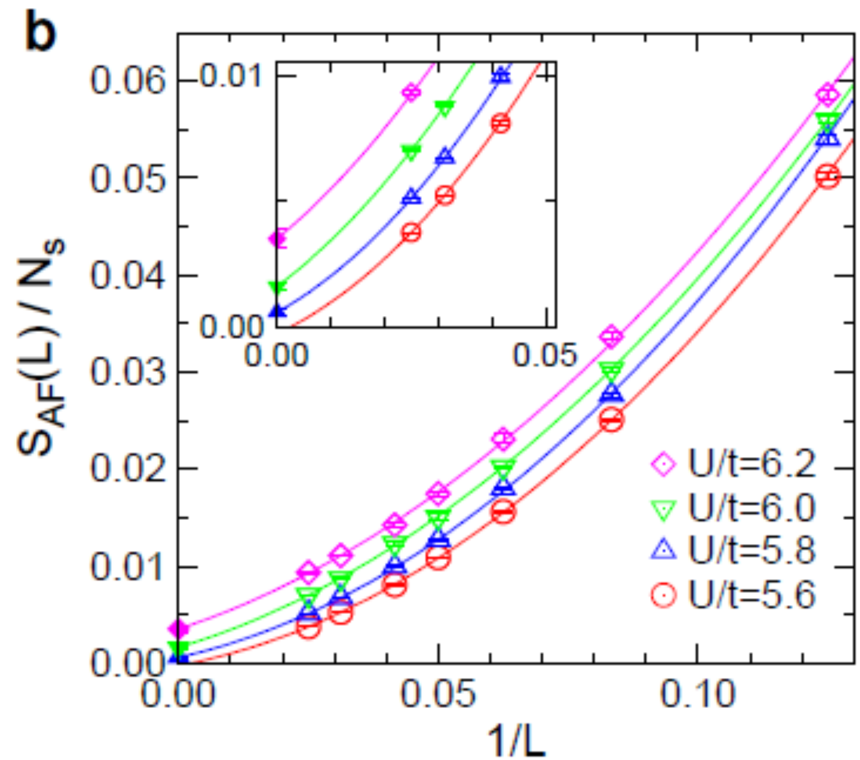
Recent: Trotter Free $N^3\,\tau$ with GFMC by Linearized HST, SS PRB (2011)

N=LxL Extrapolation to $1/L$=0 for various U/t

honeycomb



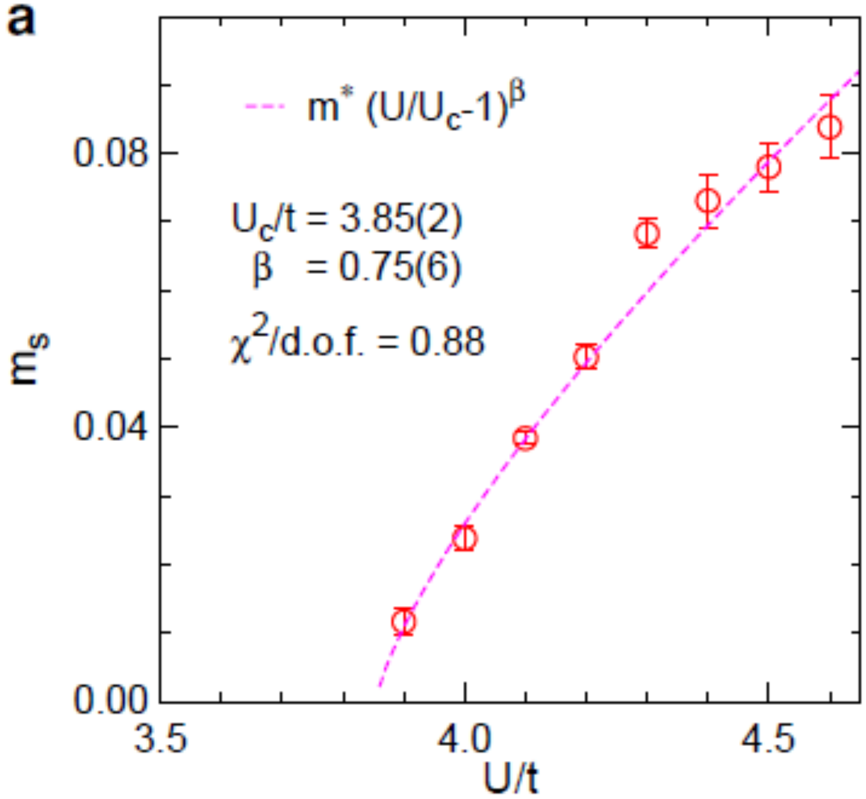
π-flux

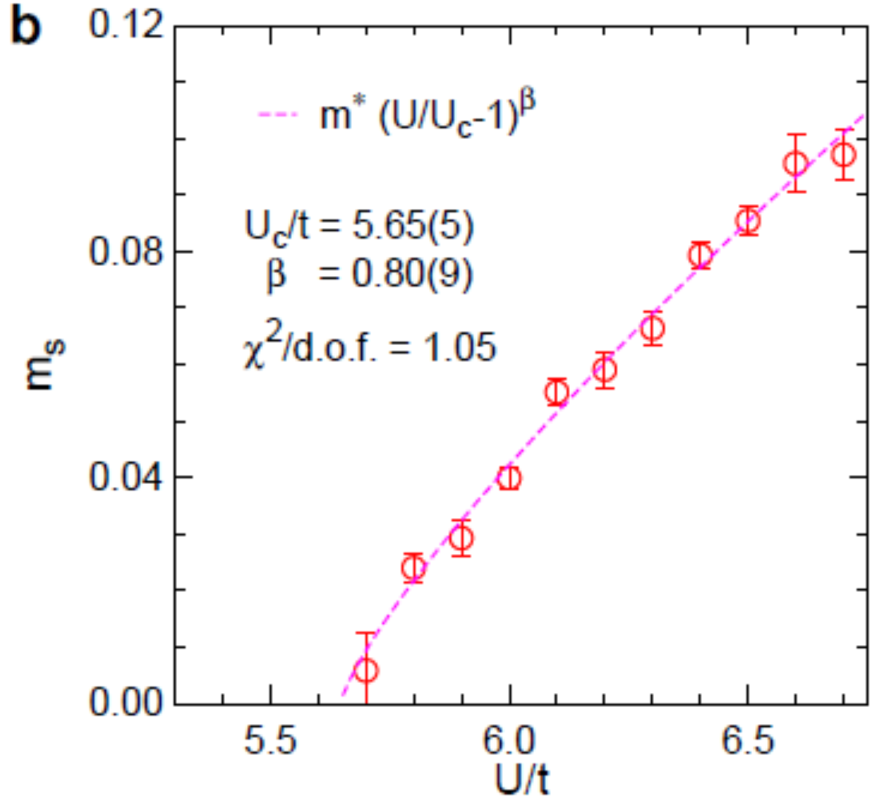


honeycomb

Phase diagram: spin part

π-flux





"spin liquid"

"spin liquid"

Meng *et al.*, Nature (2010)

Chang, Scalettar, PRL (2012)

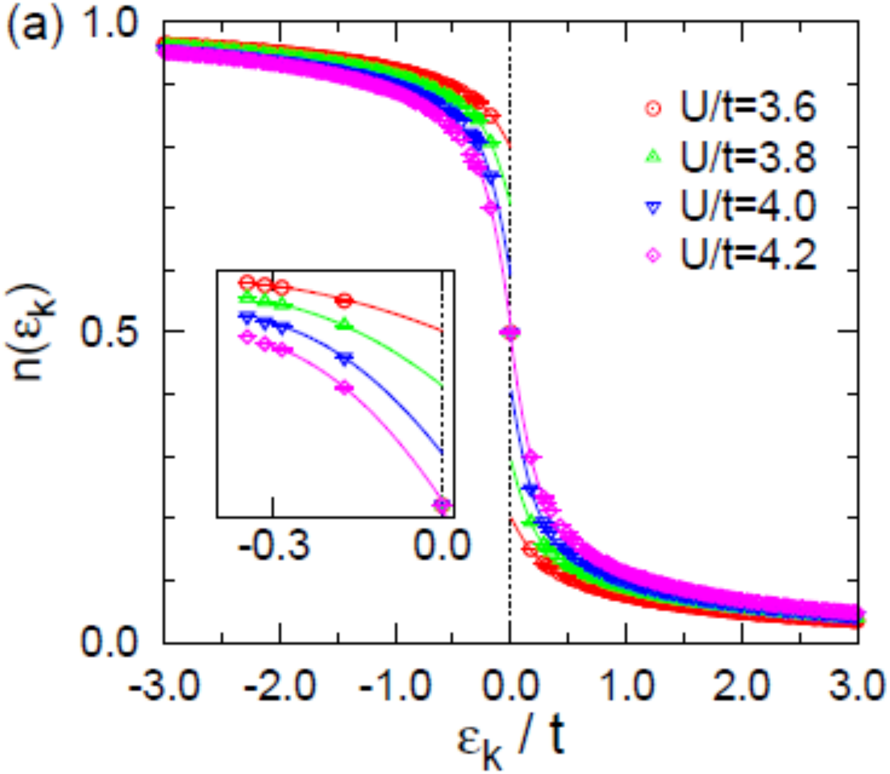
Momentum disribution

honeycomb

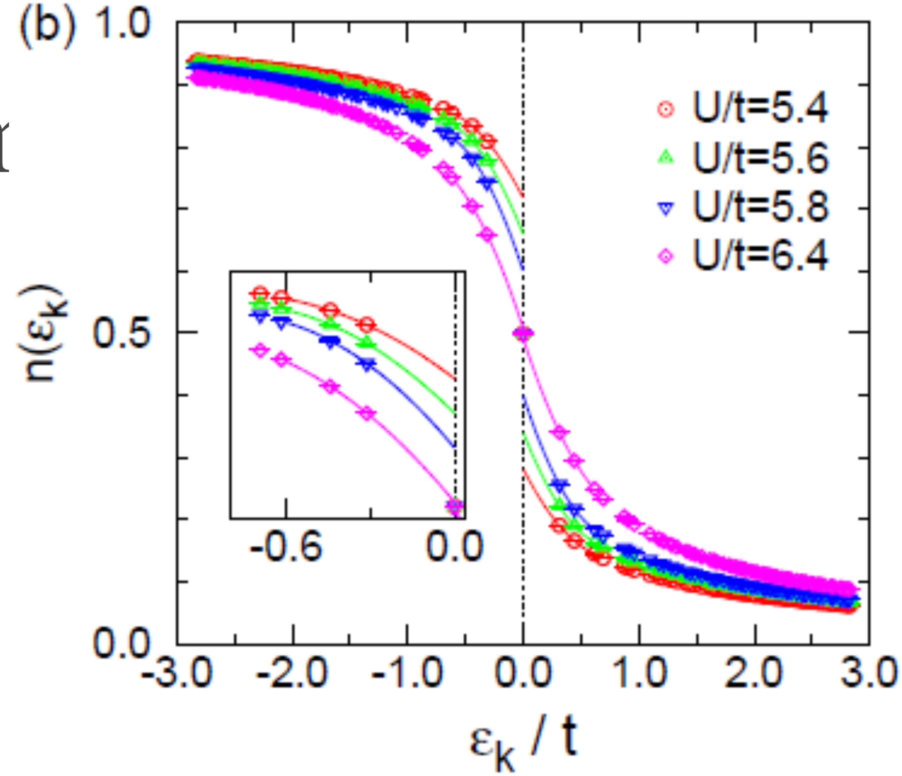
π-flux

L=32

L=40



n

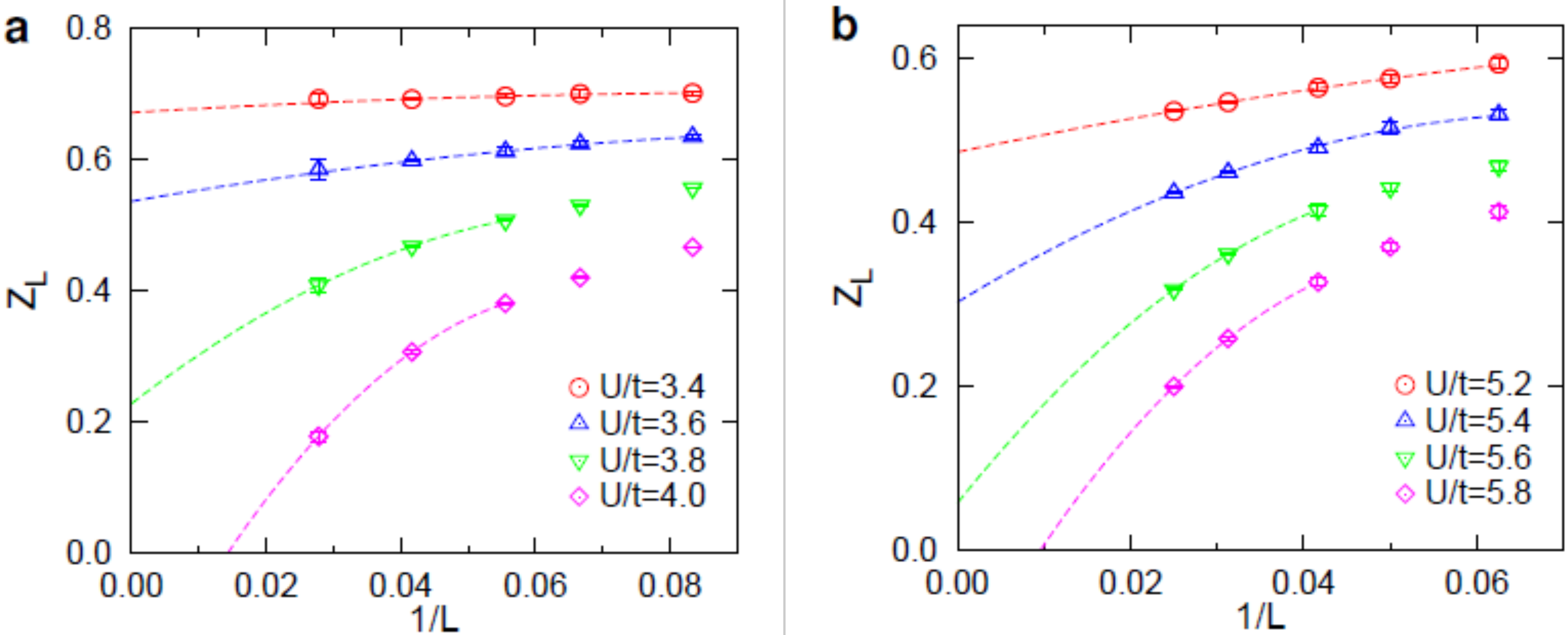


solid curves : least-square fit of 3 data points near Dirac point

$\rightarrow Z_L$

extrapolation of Z_L

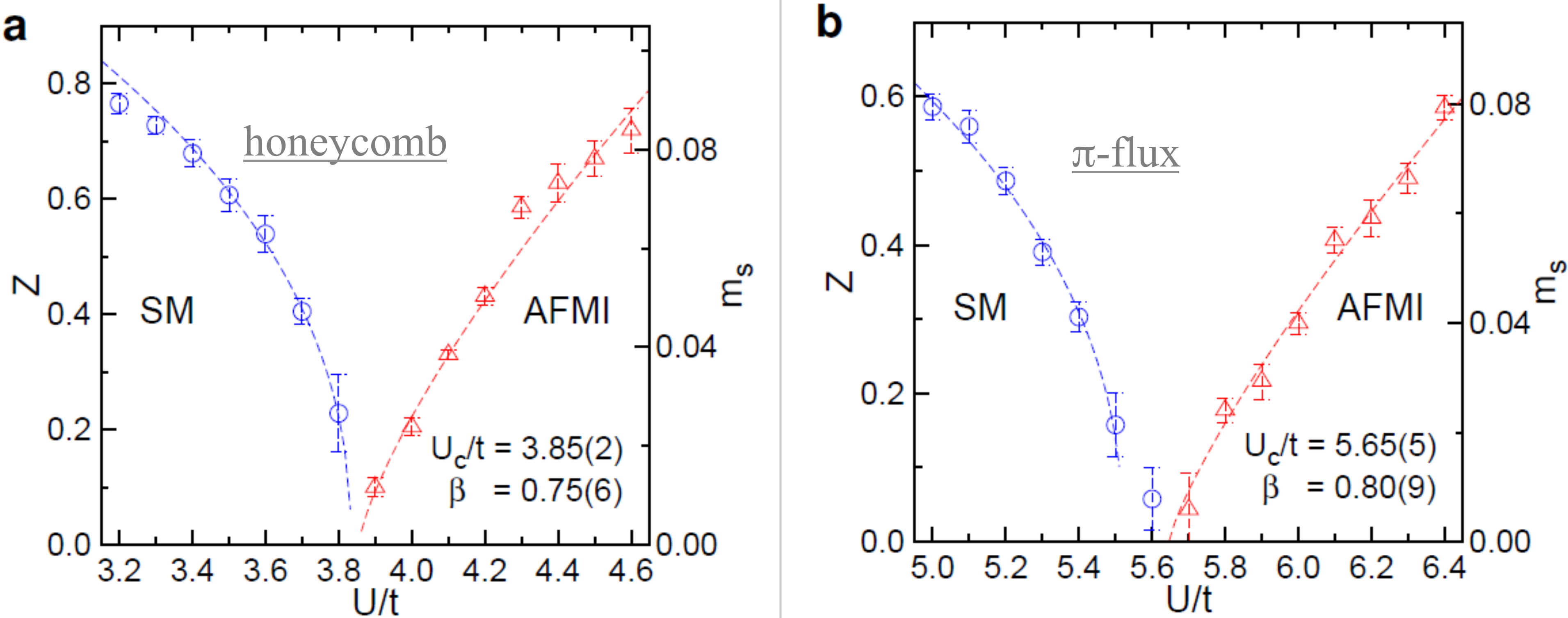
honeycomb π-flux



$$Z = \lim_{L \to \infty} Z_L$$

(clearly power law extr. , does not work for large *U insulator* ➔ *exp.extrapolation*)

The final phase diagram



✓ Direct and continuous transition between SM and AFMI

In agreement with the expected universality of the MIT: the Gross-Neveu model one (Herbut PRL'06)

Purpose of this study

- further check without assuming polynomial functions
- determine the critical exponents with high accuracy for two different lattice models
- universality class in Mott transition ?

Method: finite-size scaling (data collapse)

- ansatz:

$$m_{\mathrm{s}}(u, L) = L^{-\beta/\nu} \left(1 + cL^{-\omega}\right) f_m(uL^{1/\nu})$$

$$u = (U - U_{\mathrm{c}})/U_{\mathrm{c}}$$

Fitting method

– resampling technique: Gauss noise added to raw QMC data

– Bayesian method

Harada, PRE (2011)

critical exponents for AF transition

honeycomb

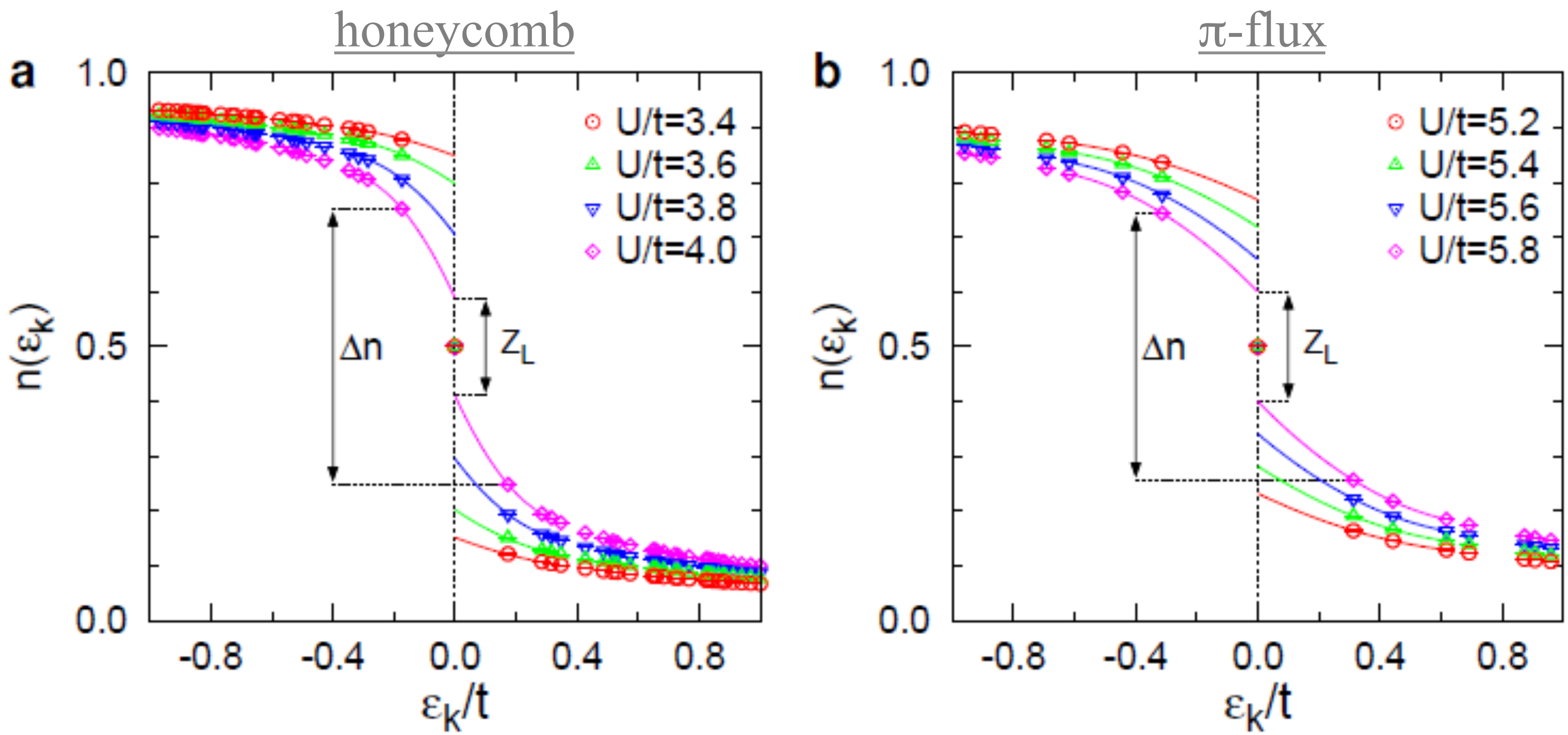
$L_{\min}$	U_c/t	ν	β	ω
6	3.843(8)	1.005(5)	0.74(2)	0.55(4)
9	3.858(9)	1.012(5)	0.74(2)	0.78(5)
12	3.856(10)	1.020(7)	0.75(2)	0.91(5)
15	3.853(10)	1.021(8)	0.75(2)	0.89(6)
18	3.849(10)	1.028(10)	0.76(2)	0.82(12)

π-flux

$L_{\min}$	U_c/t	ν	β	ω
8	5.423(38)	0.998(10)	0.86(5)	0.17(35)
12	5.534(41)	1.007(10)	0.76(5)	0.94(25)
16	5.557(31)	1.008(11)	0.74(3)	1.02(13)
20	5.546(27)	1.021(11)	0.76(3)	0.85(24)
24	5.537(35)	1.050(19)	0.78(4)	0.83(17)

$L_{\min}$: smallest L used in collapse fit

Lmax=36 (honeycomb), Lmax=40 (π-flux)



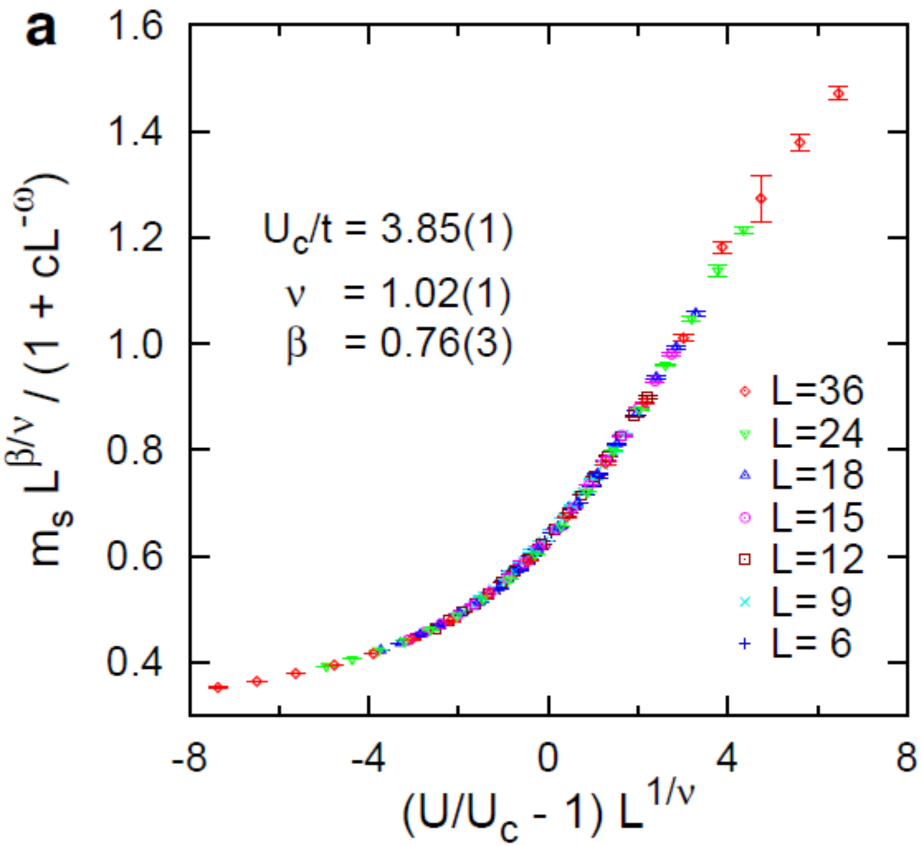
$$\rightarrow \Delta n(u, L) = L^{-\eta_\psi} f_n(uL^{1/\nu})$$

honeycomb lattice		π-flux model	
$L_{\min}$	η_ψ	$L_{\min}$	η_ψ
6	0.17(2)	8	0.19(2)
9	0.18(2)	12	0.21(2)
12	0.19(2)	16	0.22(2)
15	0.20(2)	20	0.23(2)
18	0.20(2)	24	0.24(2)

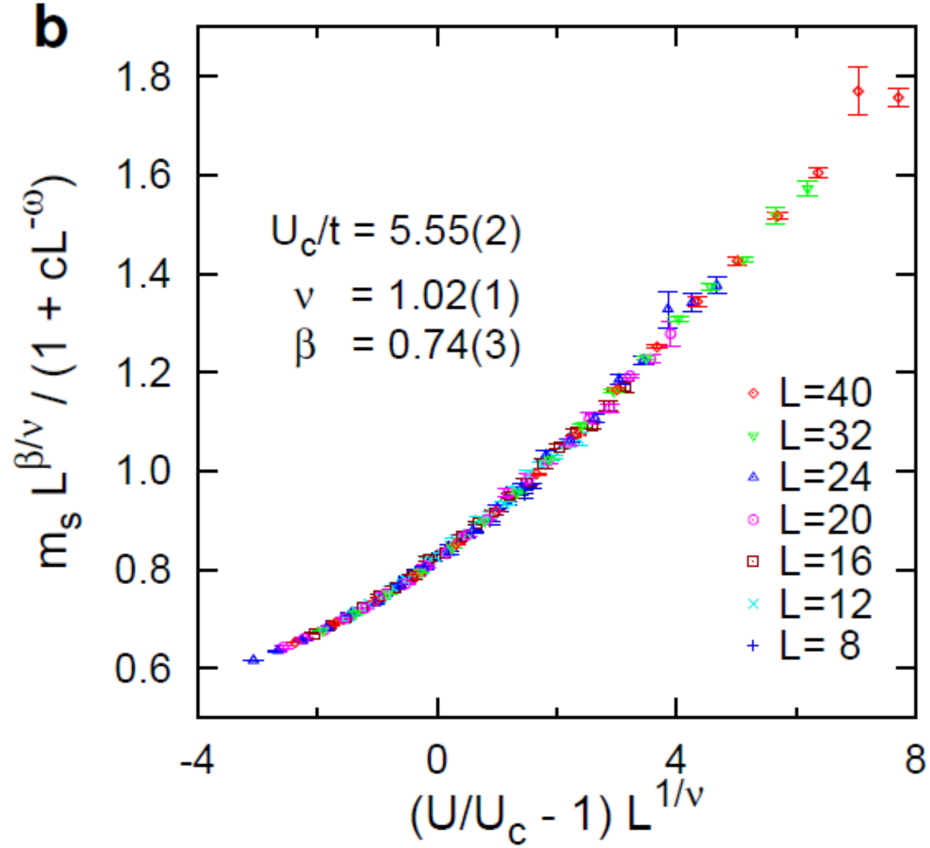
Uc/t & ν : fixed

collapse fits: AF order parameter

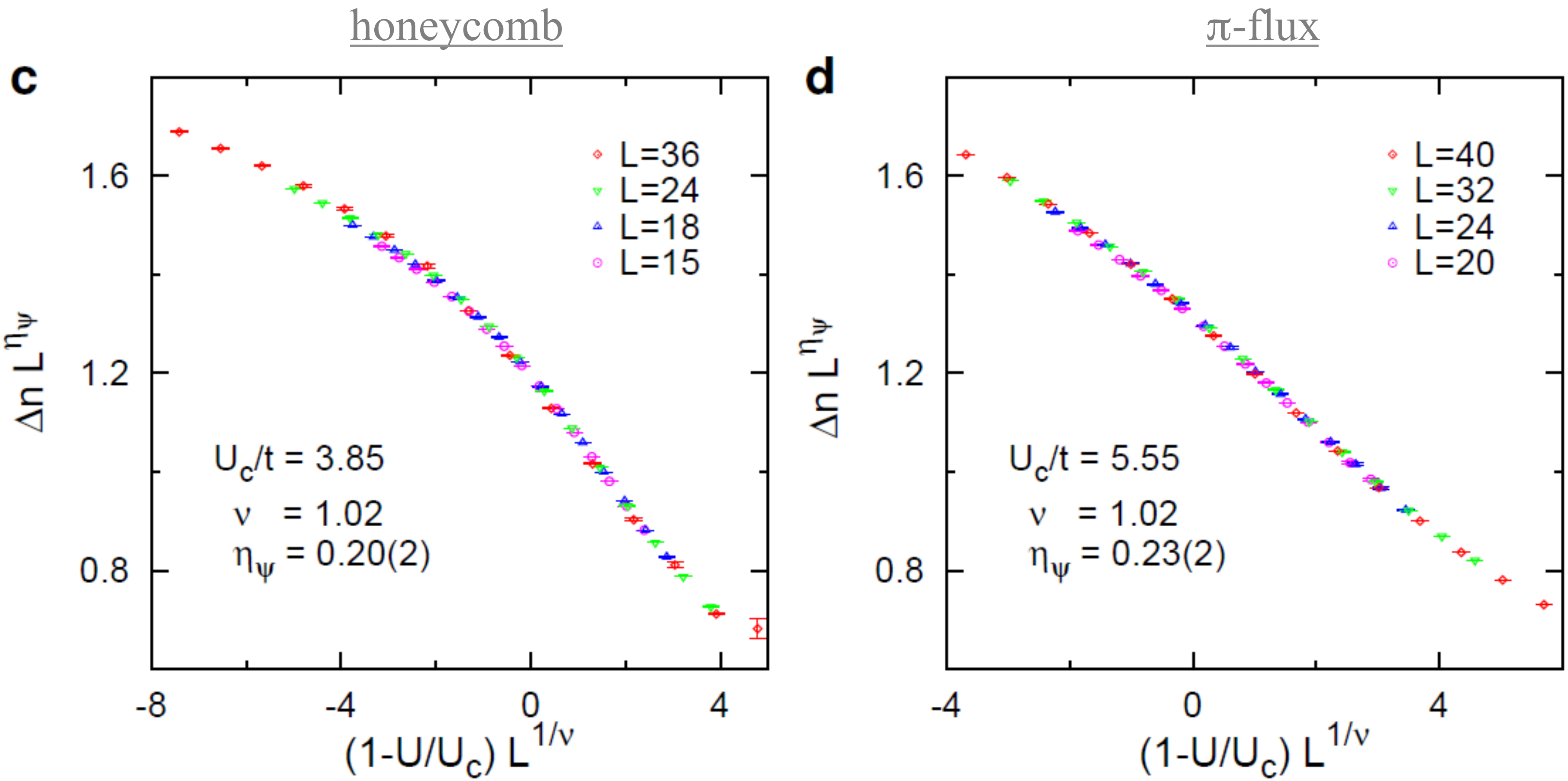
honeycomb



π-flux



collapse fits: Jump in momentum distribution Δn→Z



Fermionic quantum criticality in honeycomb and π-flux Hubbard models

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arXiv: 1411.2502

Fermionic quantum critical point of spinless fermions on a honeycomb lattice

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arXiv: 1407.0029

Fermion-sign-free Majarana-quantum-Monte-Carlo studies of quantum critical phenomena of Dirac fermions in two dimensions

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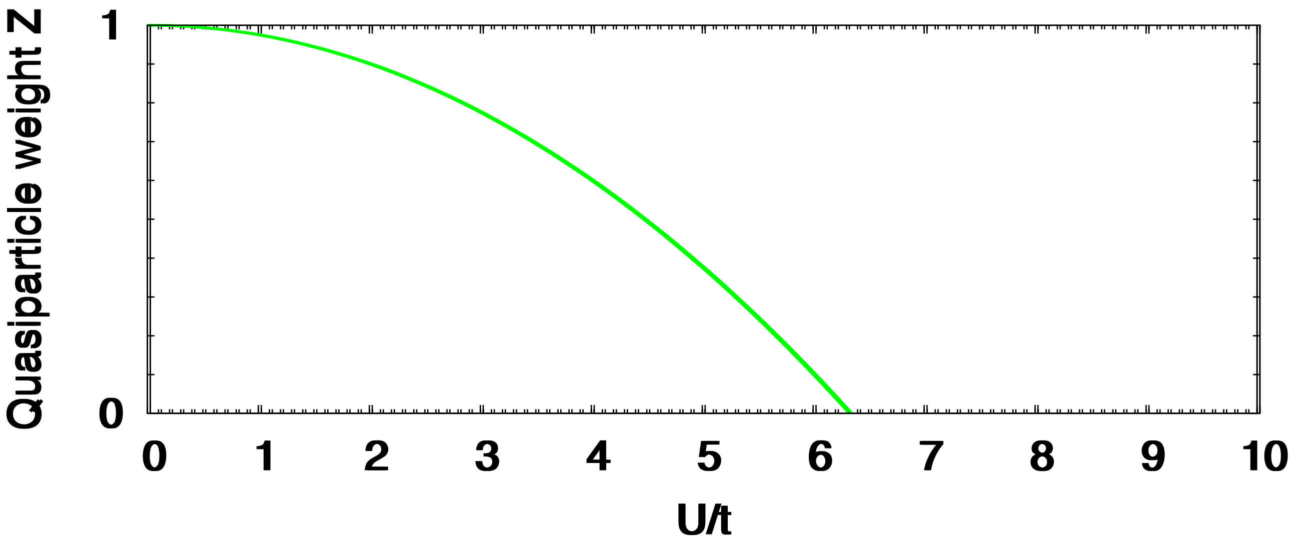
arXiv: 1411.7383

Discussion & Summary

Method	ν	β	η_ψ
Present QMC	1.02(1)	0.75(2)	0.21(2)
4-ε First order	0.882	0.794	0.3
4-ε Second order N=4(8Herbut)	1.083	1.035	0.242
4-ε Second order N=8 (Rosenstein '93.)	1.01	0.995	0.101

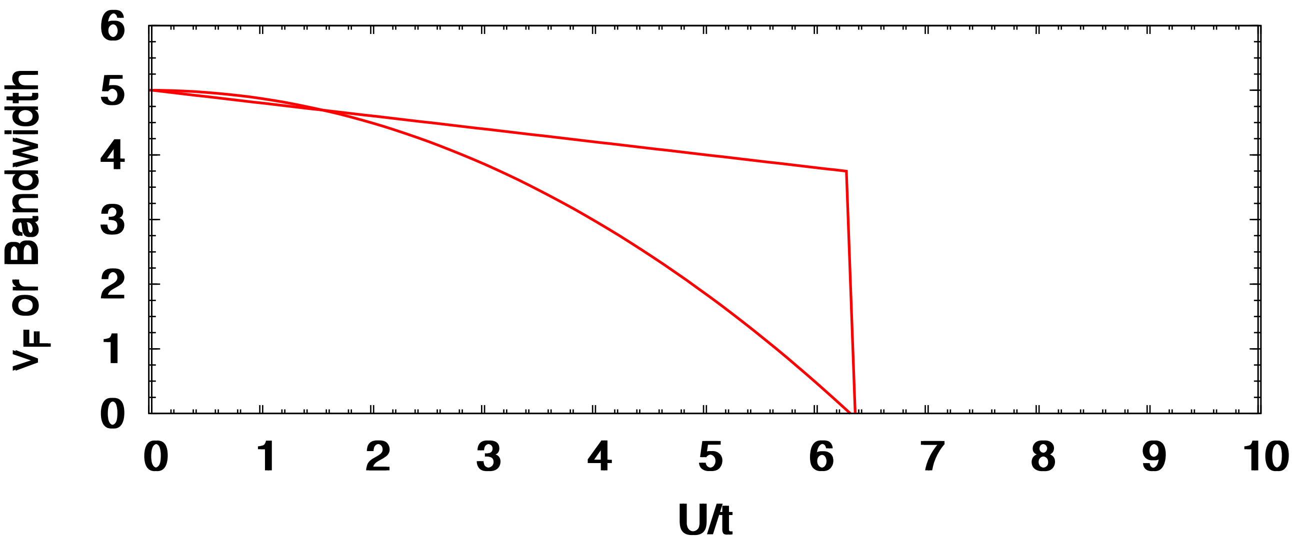
The second order expansion is controversial…
it should be done again, possible errors

Mott transition: the scenario



Brinkman-Rice
Gutzwiller Appr.
DMFT
Infinite dimension

All agree….



This is the truth…

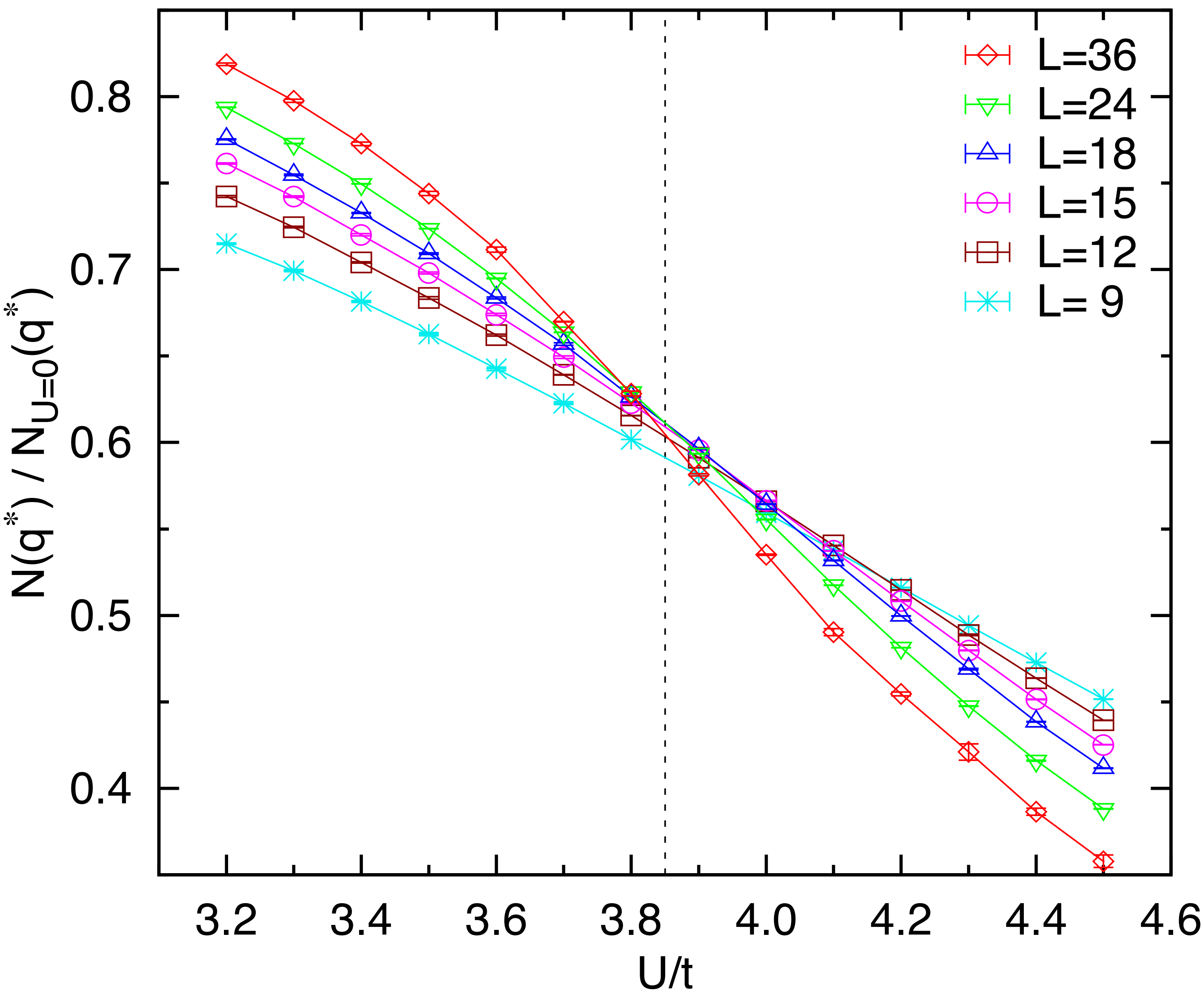
We cannot compute directly the Fermi velocity but we can assume is proportional to the sound velocity→ dynamical charge correlations N(q,ω)

→ We measure $N(q) = \int N(q,\omega) d\omega \quad q \to 0$

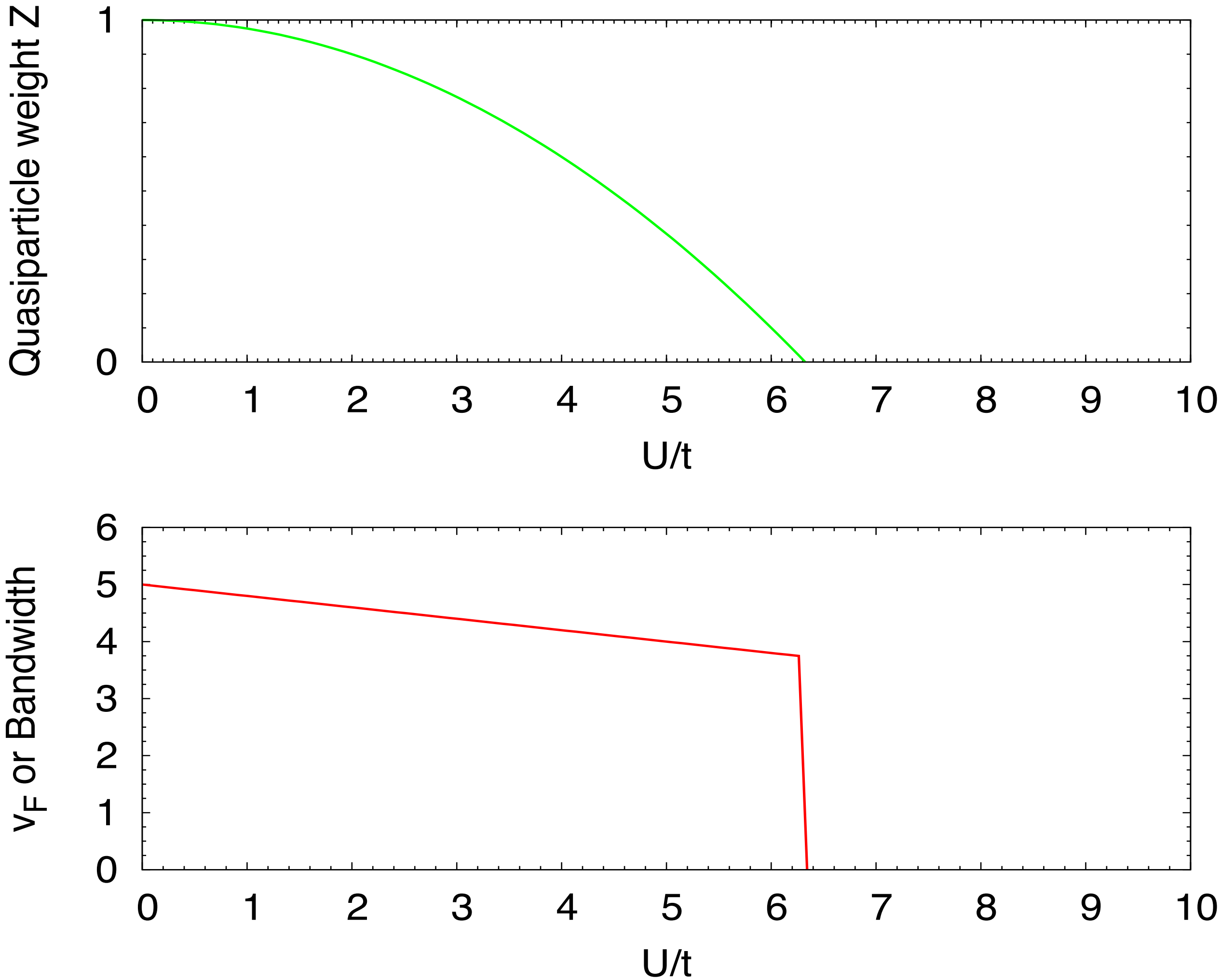
e.g. in 1D N(q) ~K q K~ $v_F dn/d\mu$

In 2D chiral N(q)~K q^2 ln(q) (e.g. U=0, K=..)
We assume: K should also in this case proportional to v_F in the metallic phase

We compute the U=0 ratio of N(q) for the smallest q=q*



Though this may represent an indirect evidence of a qualitative different scenario as compared to mean-field (dynamical or not) theories, it is confirmed mostly by the agreement of the critical behavior of these realistic Hubbard models with the Gross-Neveau behavior, where the Fermi velocity remains unrenormalized at the transition.



This is the truth…

Conclusions

We have obtained an unbiased and accurate description of the universal criticality of the MIT in Dirac fermions

Most importantly we have not found criticality in the Fermi velocity, effective mass, bandwidth, in agreement with the Gross-Neuveu criticality and In contrast with (dynamical) mean field theories: Only $Z \rightarrow 0$ at the transition for $U<Uc$.