

Metal-insulator crossover in the 2d Hubbard model

Evgeny Kozik

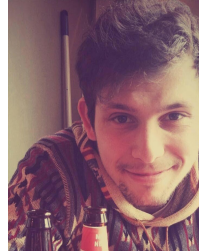


KING'S
College
LONDON

Metal-insulator crossover in the 2d Hubbard model



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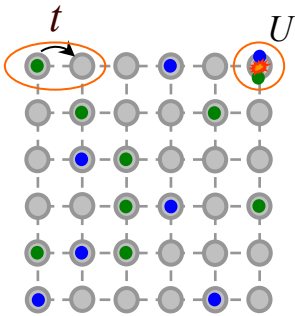
Nikolay Prokof'ev (Umass Amherst)
Boris Svistunov (Umass Amherst)

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SIMONS
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Research Council



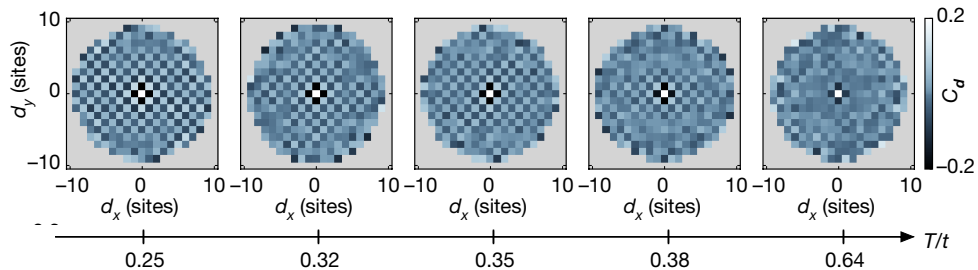
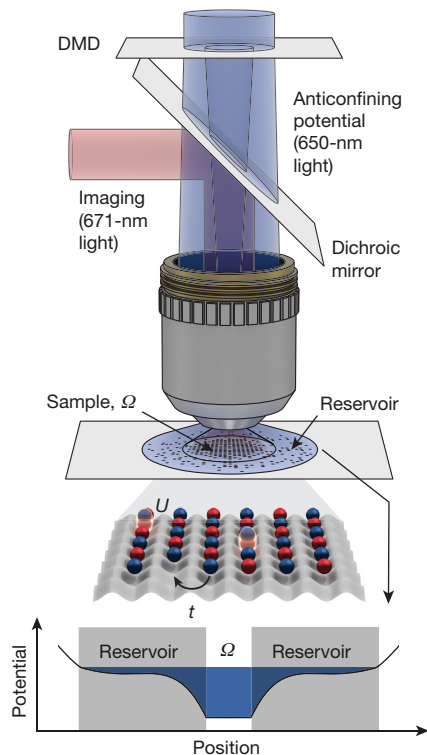
Hubbard model:
$$H = -t \sum_{\langle ij \rangle, \sigma} a_{i\sigma} a_{j\sigma}^\dagger - \mu \sum_{i, \sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

A cold-atom Fermi-Hubbard antiferromagnet

Anton Mazurenko¹, Christie S. Chiu¹, Geoffrey Ji¹, Maxwell F. Parsons¹, Márton Kanász-Nagy¹, Richard Schmidt¹, Fabian Grusdt¹, Eugene Demler¹, Daniel Greif¹ & Markus Greiner¹

¹Department of Physics, Harvard University, Cambridge, Massachusetts, USA.

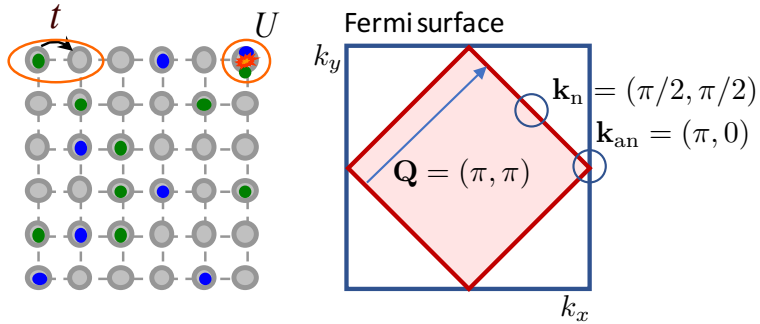
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- **experiments** have reached a regime **with long-range correlations**
- at low enough T to **study the metal vs. insulator physics** - central feature of the Hubbard model

Reliable theoretical predictions are needed

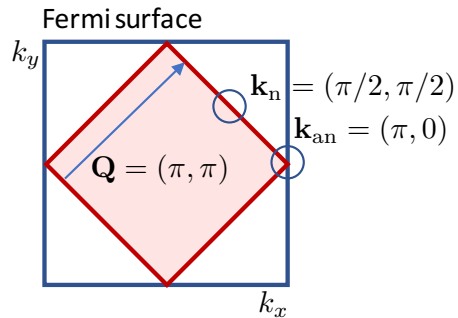
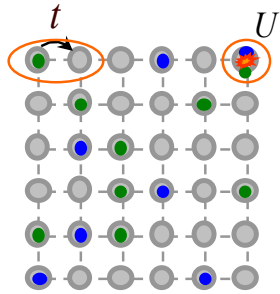
Metal-to-insulator transition in half-filled 2D Hubbard model (square lattice)



Key ingredients:

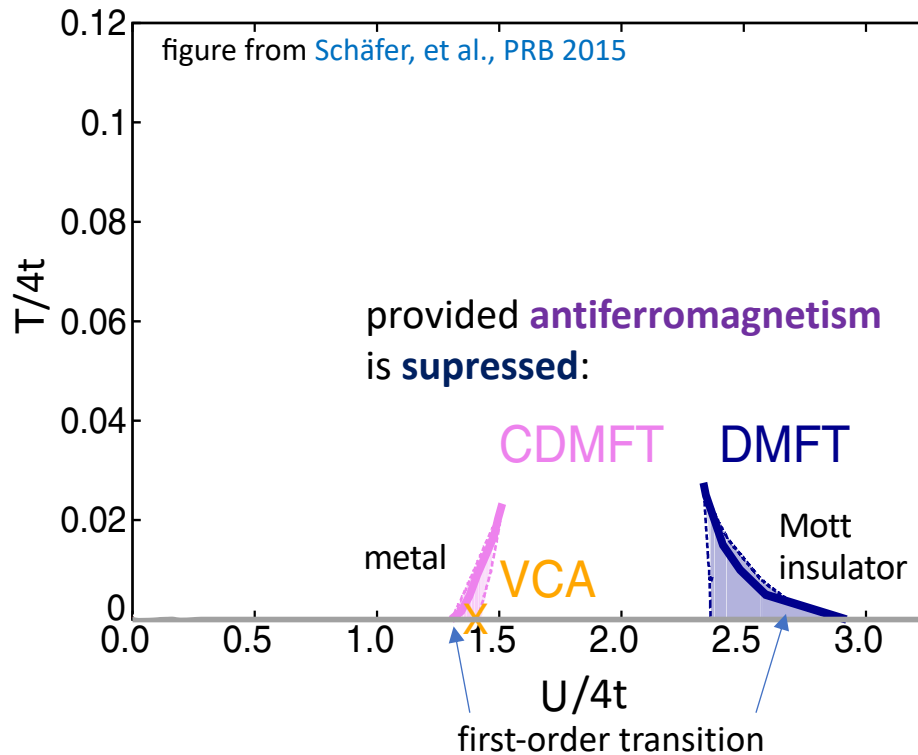
- Fermi surface nesting => tendency towards **AFM ordering (band insulator in the ground state at any $U>0$)**
- Mermin-Wagner => **no long-range order** at $T>0$

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DMFT:

Georges, Kotliar, Krauth, Rozenberg (review) '96

CDMFT/DCA (up 16-site clusters):

Maier, Jarrell, Pruschke, Hettler (review) '05

Park, Haule, Kotliar '08

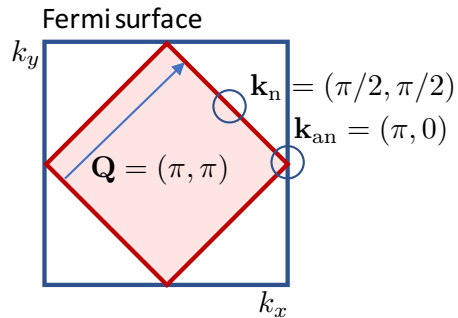
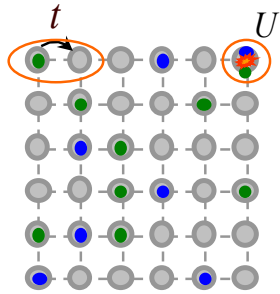
Werner, Gull, Parcollet, Millis '09

Gull, Parcollet, Millis '13

Fratino, Sémon, Charlebois, Sordi, Tremblay '17

Ect, etc...

Meatal-to-insulator crossover in half-filled 2D Hubbard model (square lattice)

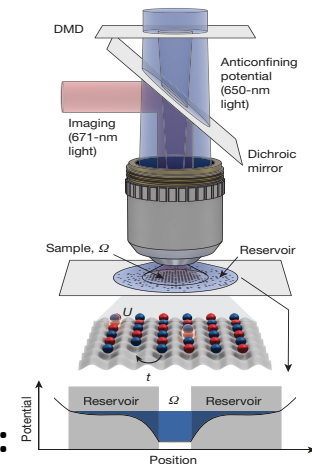
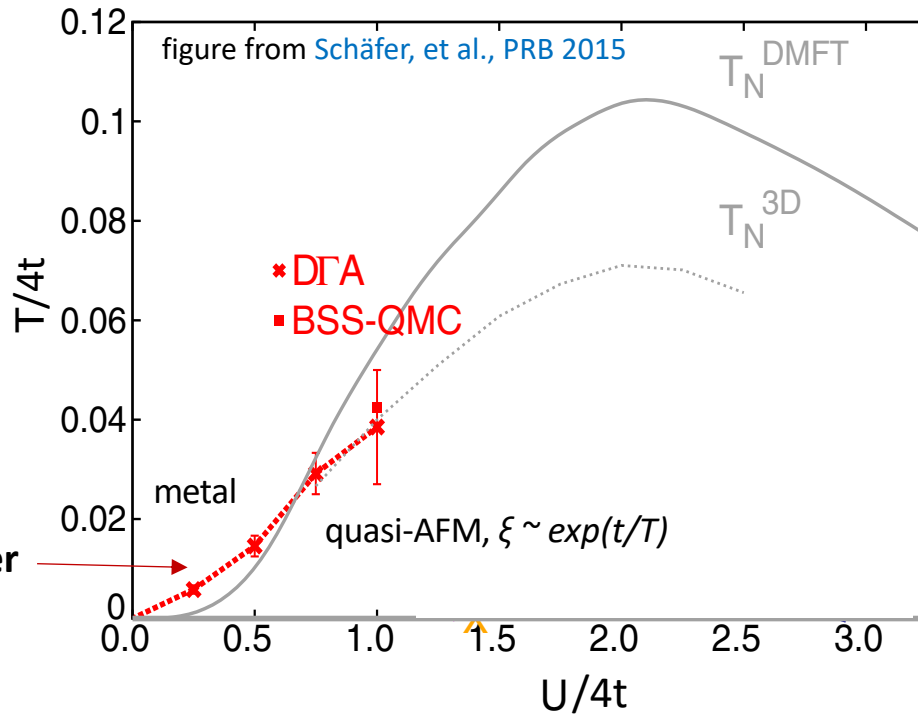


Key ingredients:

- Fermi surface nesting => tendency towards **AFM ordering (band insulator in the ground state at any $U > 0$)**
- Mermin-Wagner => **no long-range order at $T > 0$**

DGA/QMC: Schäfer, Geles, Rost, Rohringer, Arrigoni, Held, Blümer, Aichhorn, Toschi '15

Rohringer, Toschi '16



in current experiments:
pure 2d Hubbard model

Hard problem to solve with controlled accuracy:

- at $T > 0$ long-range AFM correlations with correlation length $\xi \sim \exp(t/T)$ => **quasi-antiferromagnet**
- extrapolation to the **thermodynamic limit** is **extremely challenging**

DiagMC in the thermodynamic limit

observable (correlator) in TD limit
(G, Σ, P, Γ , etc.)

$$A = \sum_{n=0}^{\infty} a_n \xi^n$$

(auxiliary) expansion parameter, coupling

sum of **all** $\sim n!$ diagrams of order n

$\Sigma[G_0] =$

$\propto \xi^2$ $\propto \xi^3$ $\propto \xi^4$ + ...

- Flexibility of diagrammatic space: **bare/bold G**, **bare/screened coupling**, **shifted-action expansions**, etc. etc.
- Stochastic schemes to compute a_n **efficiently** (depends on the diagrammatic space/regime of parameters)
- Powerful **resummation** methods (*standard and developed*) to reconstruct physical observables from divergent series

$$S_\xi = - \sum_{\omega_n, \mathbf{k}, \sigma} c_{\omega_n, \mathbf{k}, \sigma}^\dagger \tilde{G}_0(i\omega_n, \mathbf{k})^{-1} c_{\omega_n, \mathbf{k}, \sigma} + \xi \left[U \int_0^\beta n_{\tau\uparrow} n_{\tau\downarrow} d\tau - \xi^l \sum_{\omega_n, \mathbf{k}, \sigma} \alpha_{\mathbf{k}}(i\omega_n) c_{\omega_n, \mathbf{k}, \sigma}^\dagger c_{\omega_n, \mathbf{k}, \sigma} \right]$$

$\tilde{G}_0(i\omega_n, \mathbf{k}) = \frac{1}{G_0(i\omega_n, \mathbf{k})^{-1} - \alpha_{\mathbf{k}}(i\omega_n)}$

can be anything expansion parameter (eventually set $\xi = 1$) arbitrary field

bare-series expansion (Taylor series): $A(\mathbf{x}_1, \mathbf{x}_2, \dots) = \sum_{n=0}^{\infty} a_n(\mathbf{x}_1, \mathbf{x}_2, \dots) \xi^n$

Determinantal Diagrammatic Monte Carlo for connected diagrams (CDet)

Rossi 2016

In the spirit of: Rubtsov, Savkin, Lichtenstein 2005
Burovski, Prokof'ev, Svistunov, Troyer 2006

$$a_n(\mathbf{k}, \omega) = \underbrace{\sum_{\mathbf{r}_1 \dots \mathbf{r}_n} \int d\tau_1 \dots d\tau_n}_{\text{sampled by Monte Carlo}} \left[\underbrace{\text{all possible } (n!)^2 \text{ diagrams}}_{\substack{\text{summed in } O(n^3) \text{ steps} \\ \text{by determinant} \times \text{determinant}}} - \underbrace{\text{all disconnected diagrams for } \{\mathbf{r}_n, \tau_n\}}_{\substack{\text{summed in } O(3^n) \text{ steps} \\ \text{(fast subset convolution: } O(n^2 2^n) \text{)}}} \right]$$

typically less than cost $O(n^3 2^n)$ of computing sub-determinants
 (tree algorithm for principle minors: $O(2^n)$)

Šimkovic, PhD Thesis 2018

Self-energy for the Hubbard model

bare-series expansion (Taylor series): $\Sigma(\mathbf{k}, \omega) = \sum_{n=1}^{\infty} a_n(\mathbf{k}, \omega) \xi^n$

Determinantal Diagrammatic Monte Carlo for the self-energy (Σ DDMC)

In the spirit of: [Rubtsov, Savkin, Lichtenstein 2005](#)
[Burovski, Prokof'ev, Svistunov, Troyer 2006](#)
[Rossi 2016](#)

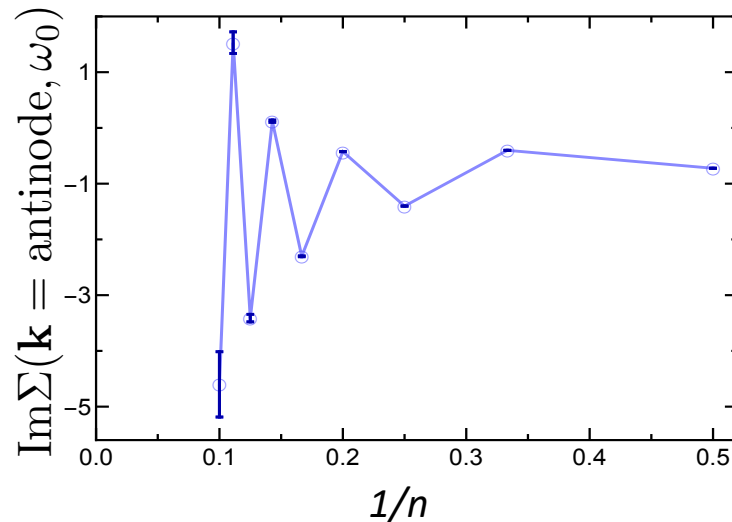
[Šimkovic, EK 2017](#) (similar algorithm: [Moutenet, Wu, Ferrero 2017](#))

$$a_n(\mathbf{k}, \omega) = \underbrace{\sum_{\mathbf{r}_1 \dots \mathbf{r}_n} \int d\tau_1 \dots d\tau_n}_{\text{sampled by Monte Carlo}} \left[\underbrace{\text{all possible } (n!)^2 \text{ diagrams}}_{\substack{\text{summed in } O(n^3) \text{ steps} \\ \text{by determinant} \times \text{determinant}}} - \underbrace{\left[\begin{array}{l} \text{all disconnected diagrams} \\ \text{for } \{\mathbf{r}_n, \tau_n\} \end{array} \right]}_{\text{summed in } O(n^2 3^n) \text{ steps}} - \underbrace{\left[\begin{array}{l} \text{all reducible diagrams} \\ \text{for } \{\mathbf{r}_n, \tau_n\} \end{array} \right]}_{\substack{\text{(fast subset convolution: } O(n^4 2^n) \text{)} \\ \text{typically less than cost } O(n^5 2^n) \\ \text{of computing sub-determinants} \\ \text{(tree algorithm for principle minors } O(n^2 2^n) \text{)}}} \right]$$

2D Hubbard model $T=0.2t$, $U=7t$, $n=0.935(1)$:
(strongly-correlated regime)

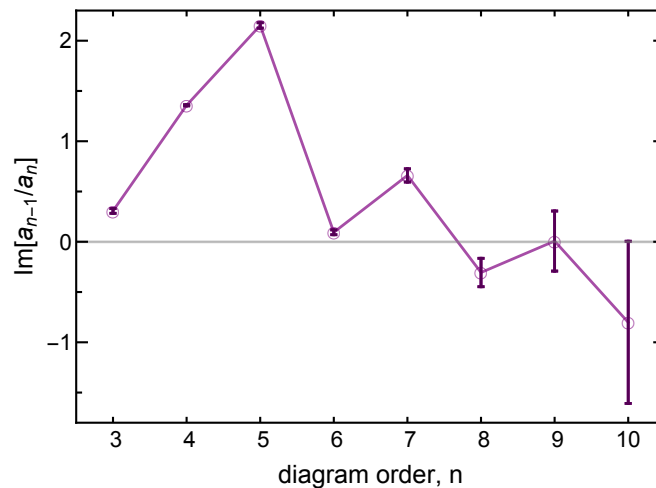
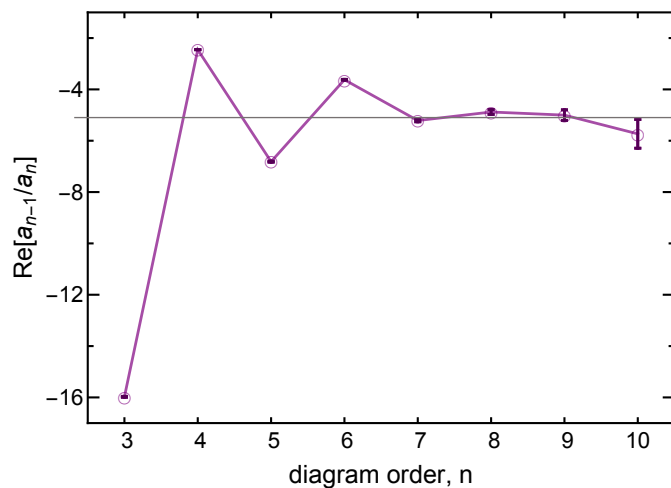
numerically exact partial sums
up to diagram order n

$$\Sigma^{(n)}(\mathbf{k}, \omega) = \sum_{m=1}^n a_m(\mathbf{k}, \omega) \xi^m$$



Reconstruct self-energy from its divergent series:

1. Find location of first singularity from ratio test

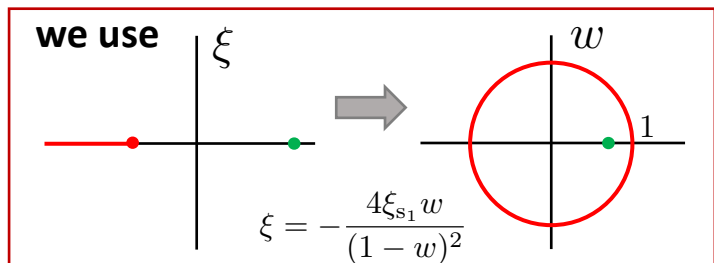


1st singularity at

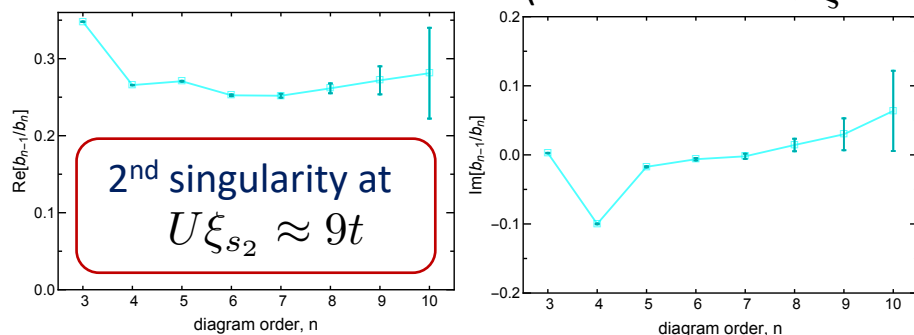
$$U\xi_{s_1} \approx -5t$$

likely corresponds to
phase transition

2. Remove the singularity by conformal map



ratio test for transformed series: (interested in $U\xi = 7t$)



$$\Sigma = \sum_n a_n \xi(w)^n = \sum_n b_n w^n$$

extrapolation to infinite order:

Integral approximant (IA) technique: $\Sigma(w) \approx g(w)$, the solution of

$$Q_M(x)g'(x) + P_L(x)g(x) + R_N(x) = 0$$

and has the same Taylor series up to maximal diagram order

Q_M, P_L, R_N - polynomials of orders M, L, N : $M+L+N+2 = \text{maximal diagram order}$

Hunter, Baker 1979

special cases:

$$Q_M(x) \equiv 0 : \quad g(x) = -\frac{R_N(x)}{P_L(x)} \quad (\text{Padé approximant})$$

$$R_N(x) \equiv 0 : \quad \frac{d \ln[g(x)]}{dx} = -\frac{P_L(x)}{Q_M(x)} \quad (\text{D-log-Padé approximant})$$

general structure of $g(x)$:

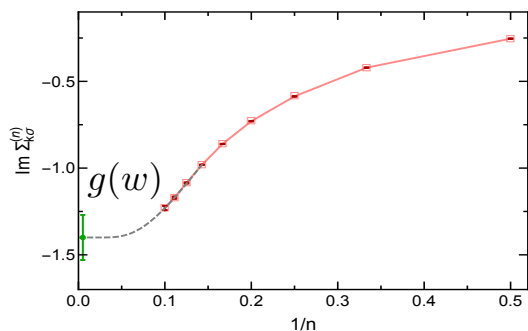
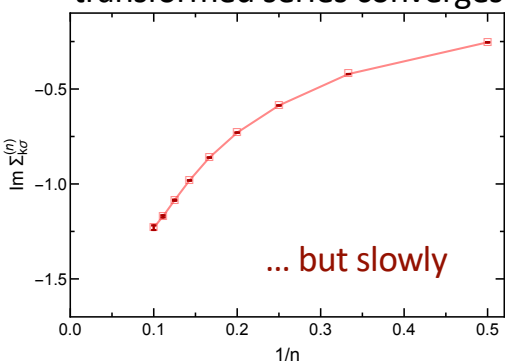
- singularities are zeros of $Q_M(x)$

- close to a singularity x_s , $g(x) = \phi_1(x)(1 - x/x_s)^{-\nu} + \phi_2(x)$

regular

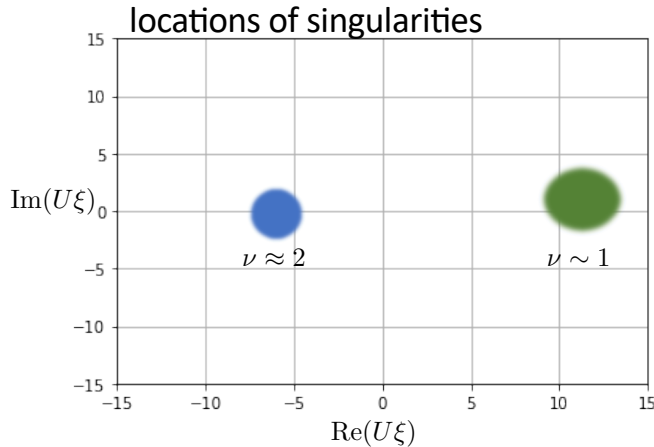
(typical for a phase transition)

transformed series converges:



final result

3. Apply the IA approach to the original series $\Sigma = \sum a_n \xi^n$: $\Sigma(\xi) \approx g(x)$ (no conformal map: automatic way of resumming the series)



$$Q_M(x)g'(x) + P_L(x)g(x) + R_N(x) = 0$$

$g(x)$ has the same Taylor series as $\Sigma(\xi)$ up to maximal diagram order

- singularities are zeros of $Q_M(x)$
- close to a singularity x_s , $g(x) = \phi_1(x)(1 - x/x_s)^{-\nu} + \phi_2(x)$

$\phi_1(x)$

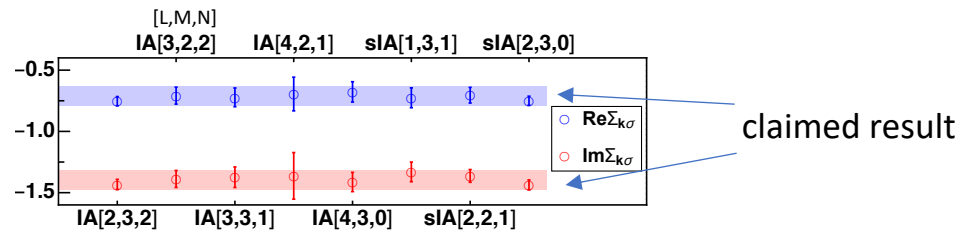
$(1 - x/x_s)^{-\nu}$

$\phi_2(x)$

regular

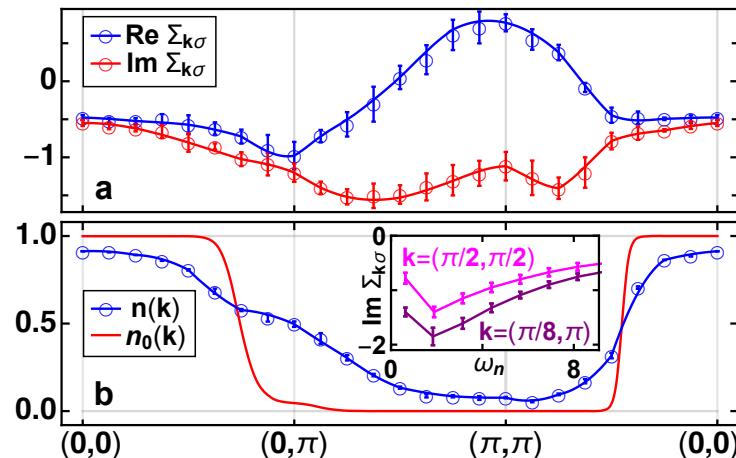
(typical for a phase transition)

controlling the accuracy:

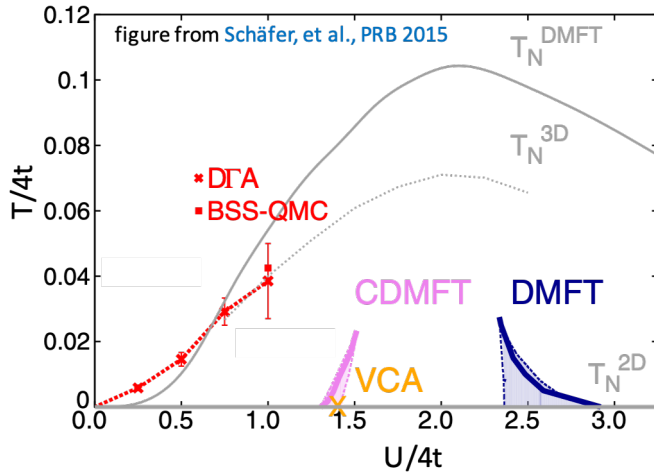


Repeating the reconstruction procedure
for different momentum points:

$T=0.2t$, $U=7t$, $n=0.935(1)$:
(strongly-correlated regime,
best any approach can currently do)



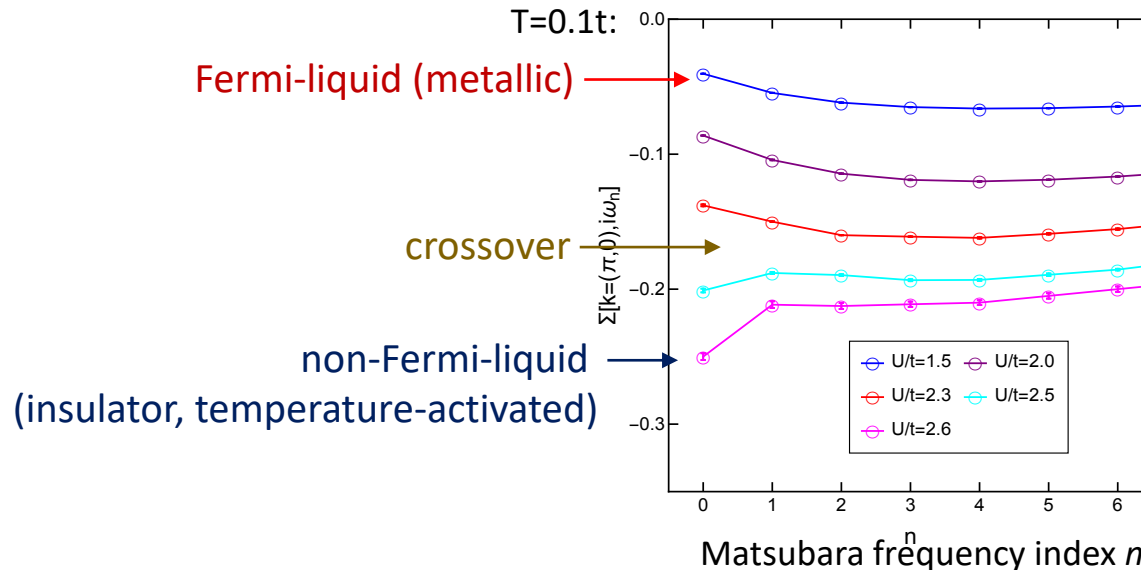
Metal-to-insulator crossover in half-filled 2D Hubbard model (square lattice)



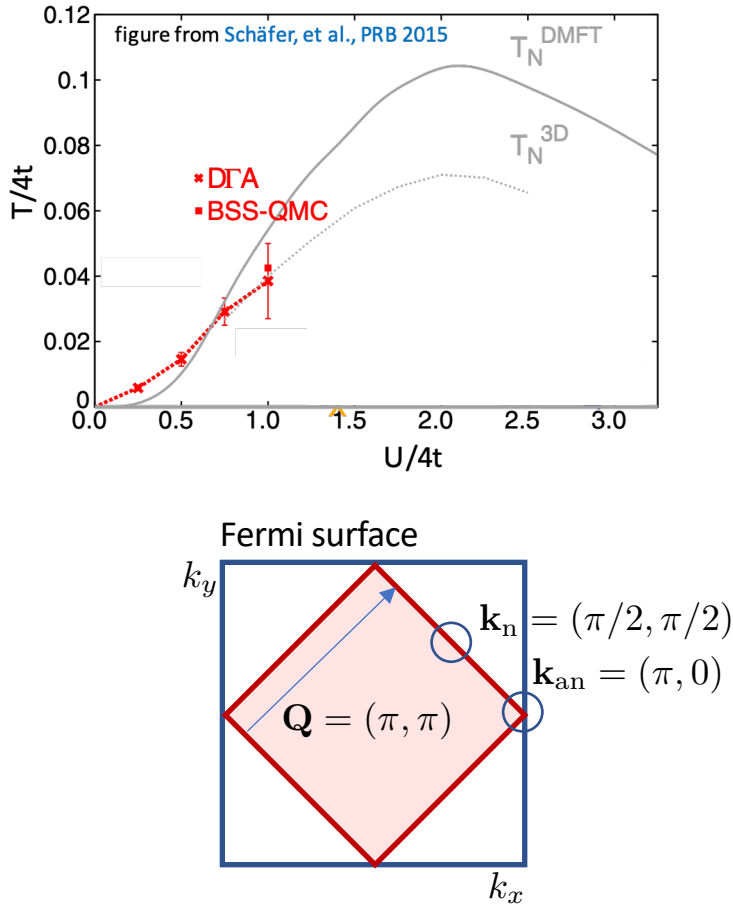
Determinantal Diagrammatic Monte Carlo for the self-energy (Σ DDMC):

- immediately in the thermodynamic limit (no finite-size errors by construction)
- arbitrary momentum resolution
- diagram orders up to 12 with <10% error bars
-> **controlled results in the regime of interest**

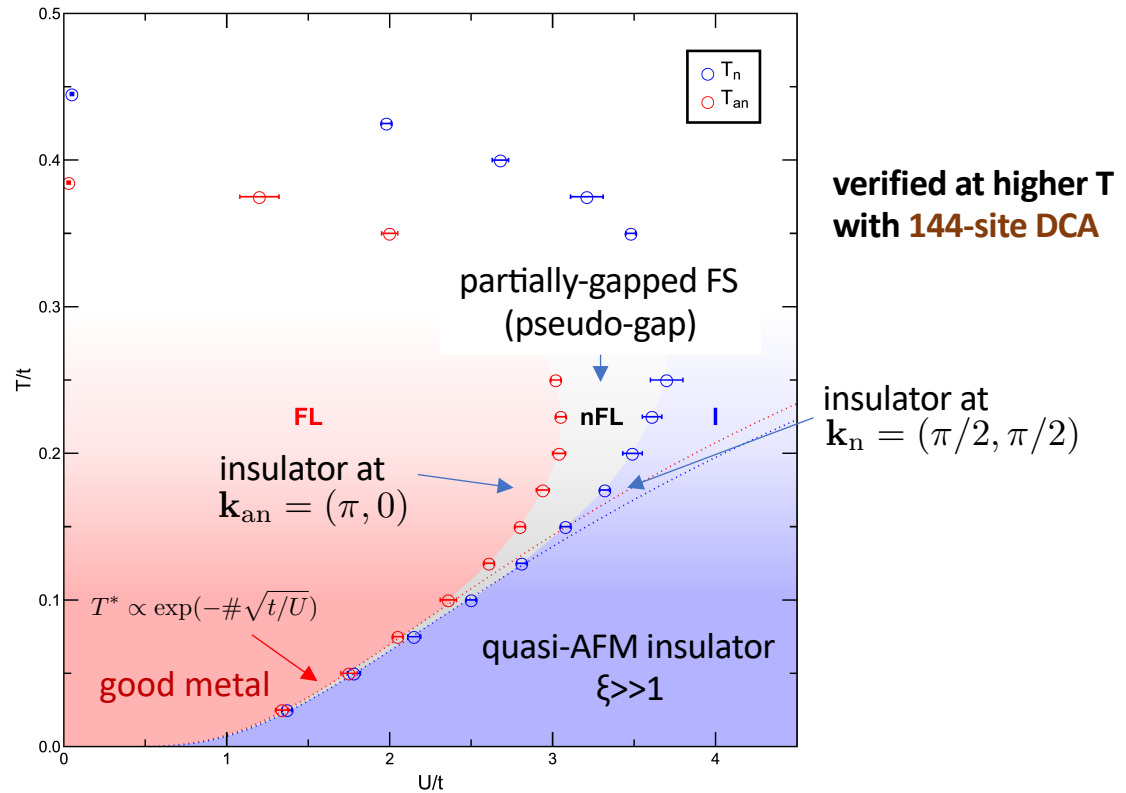
Identifying quasiparticle properties from self-energy



Metal-to-insulator crossover in half-filled 2D Hubbard model (square lattice)

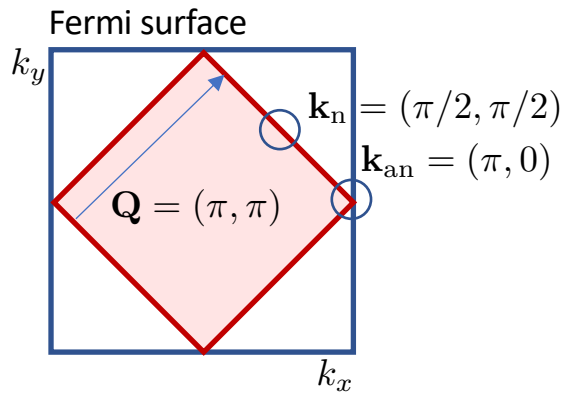


controlled result in the thermodynamic limit:



- extended crossover from Fermi-liquid to quasi-AFM insulator, most interesting regime: $2.5t < U < 4t$
- at $U < 2.5t$: mean-field physics, crossover happens at BCS Néel temperature $T_* = a \exp(b/\sqrt{U})$
- at $U > 4t$: low-T physics is not different from that of the Heisenberg model

Metal-to-insulator crossover in half-filled 2D Hubbard model (square lattice)

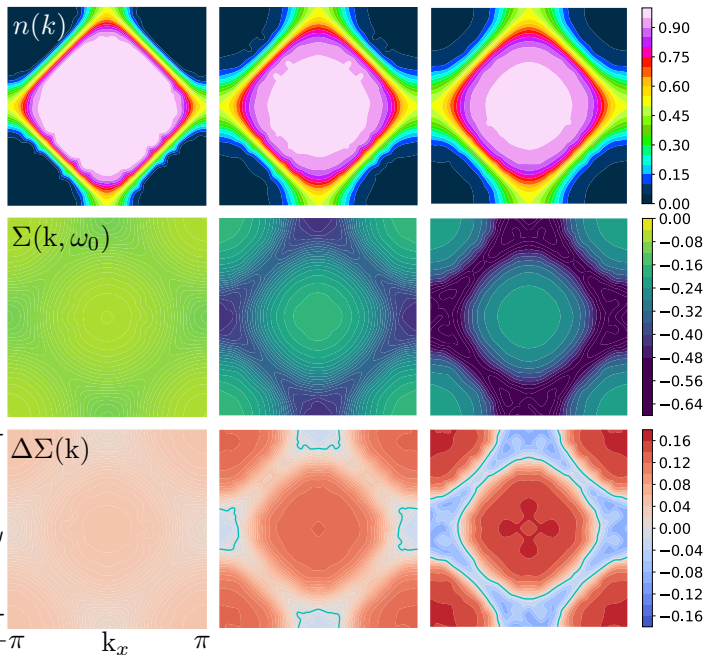


Crossover signatures
in momentum distribution

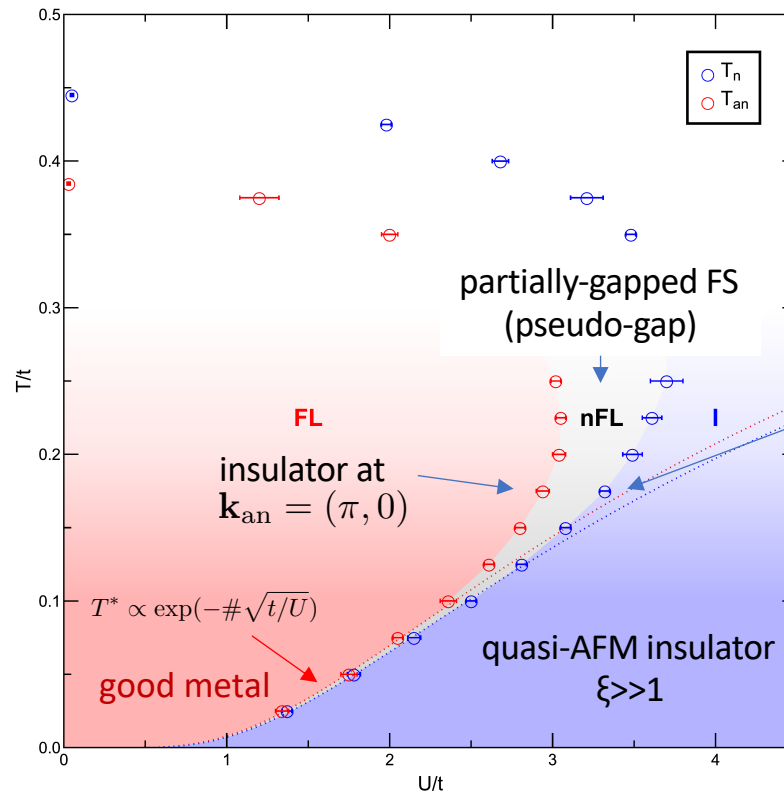
$U=2.0$

$U=3.4$

$U=3.8$



controlled result in the thermodynamic limit:



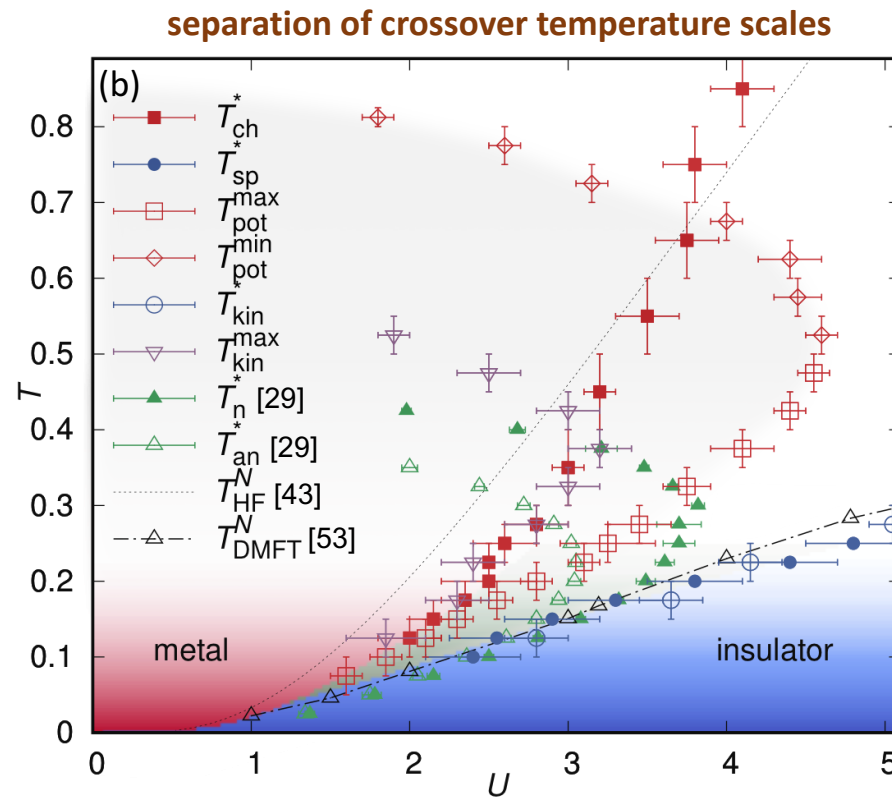
verified at higher T
with **144-site DCA**

insulator at
 $\mathbf{k}_n = (\pi/2, \pi/2)$

difference between self-energies
at the two lowest Matsubara frequencies
(our criterion for **metal** vs. **insulator**)

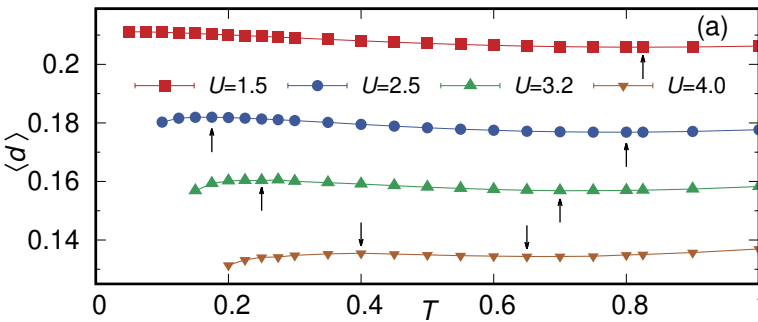
Crossover diagram for charge and spin correlations:
controlled results in the thermodynamic limit
(using CDet + resummations)

Can be measured in cold-atom experiments

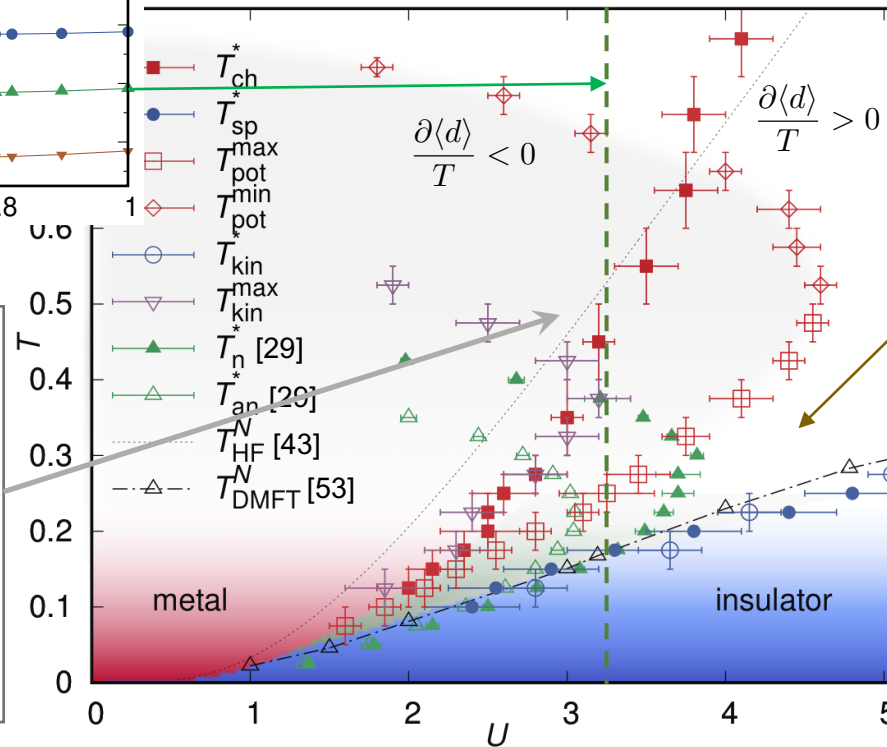


Crossover signatures in charge and spin correlations: Can be measured in cold-atom experiments

double occupancy



crossover diagram



(“Maxwell”) relation to entropy:

$$\frac{\partial \langle d \rangle}{\partial T} = - \frac{\partial s}{\partial U}$$

adiabatic cooling by raising U :

$$\frac{\partial s}{\partial U} > 0$$

local magnetic moment
 $\langle s_z^2 \rangle = (1 - 2\langle d \rangle)/4$

develops

earlier work:

Werner, Parcollet, Georges, Hassan 2005

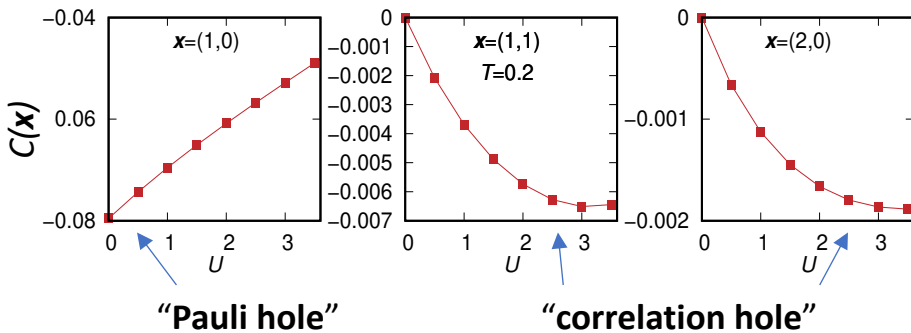
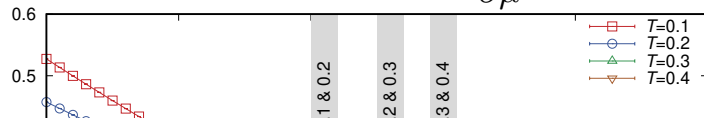
Same qualitative behavior in 3D above Néel temperature

(EK, Burovski, Scarola, Troyer 2013)

Kim, Šimkovic, EK 2019

Crossover signatures in charge and spin correlations: Can be measured in cold-atom experiments

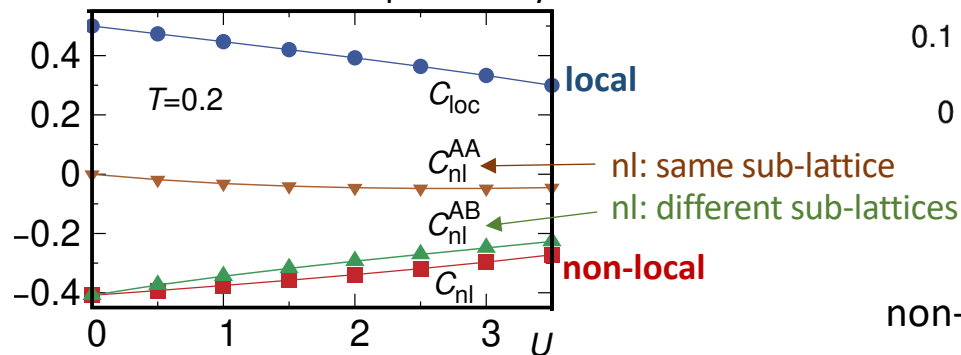
compressibility $\kappa = \frac{\partial n}{\partial \mu}$



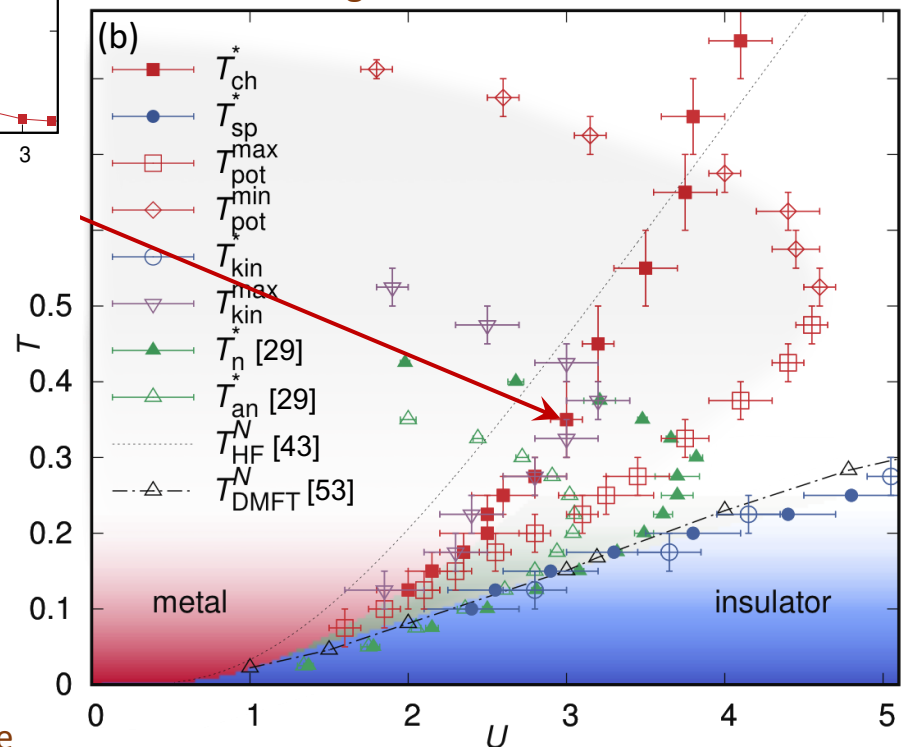
density correlations: $C(\mathbf{x}) = \langle \delta n(0) \delta n(\mathbf{x}) \rangle$

compressibility: $\kappa = \beta \sum_{\mathbf{x}} C(\mathbf{x})$

contributions to compressibility:

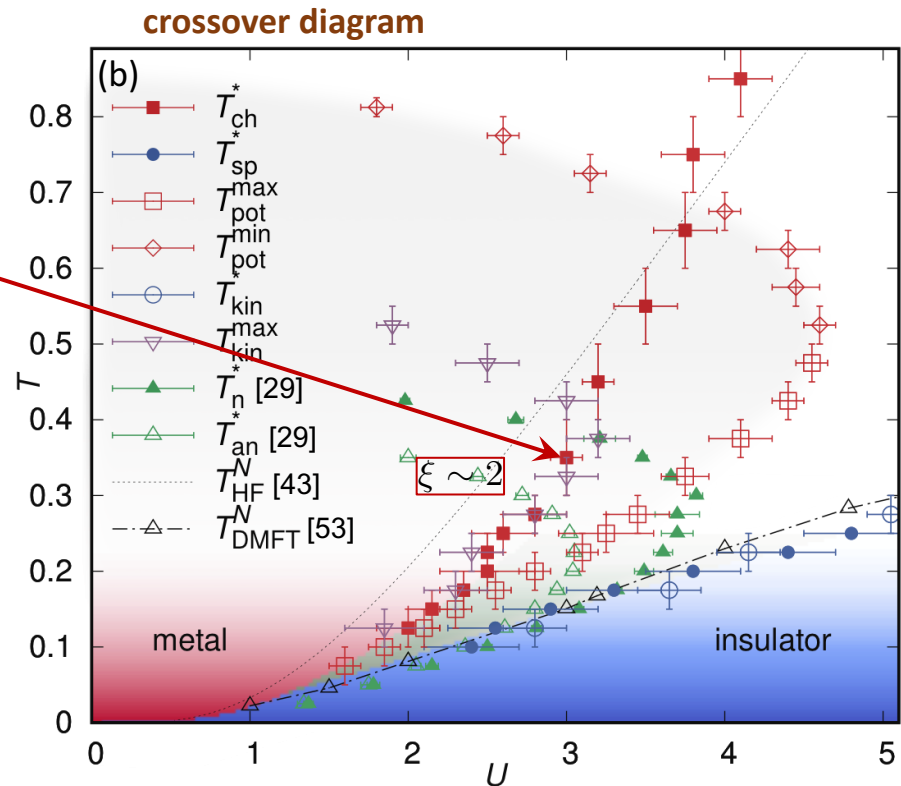
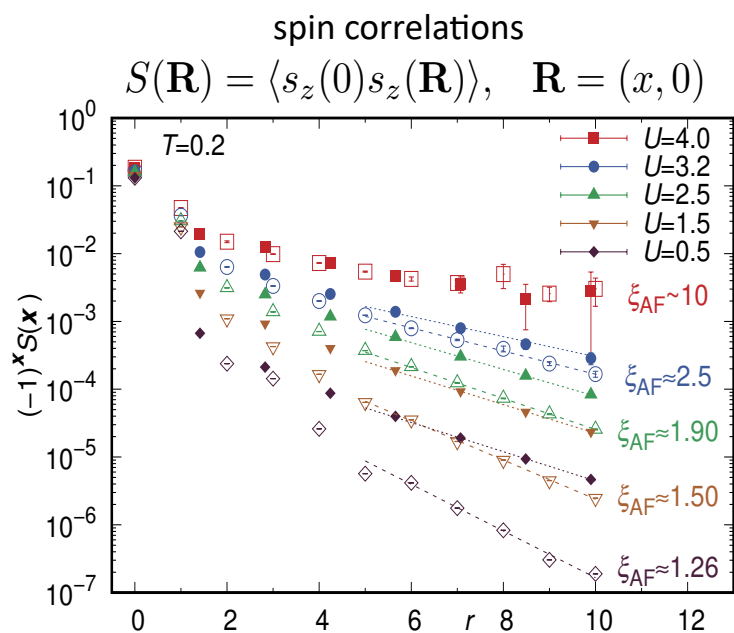
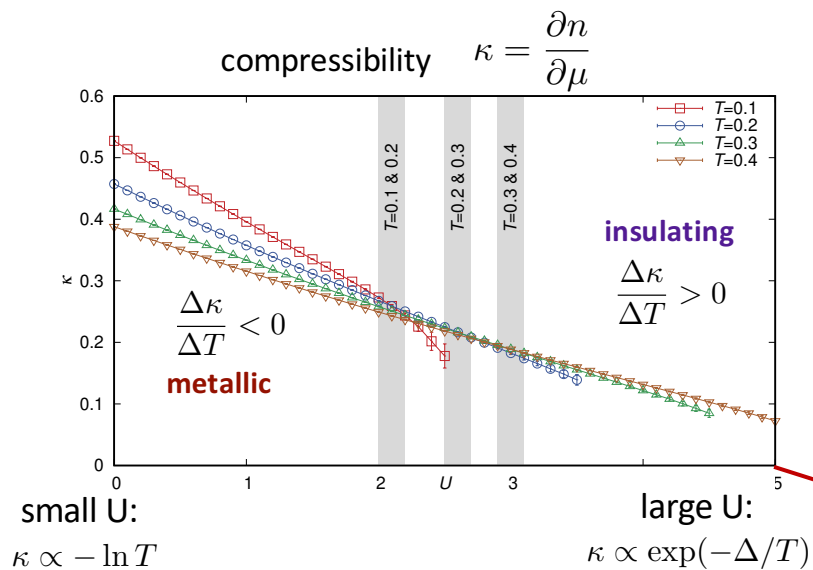


crossover diagram



non-local density correlations are crucial for the crossover

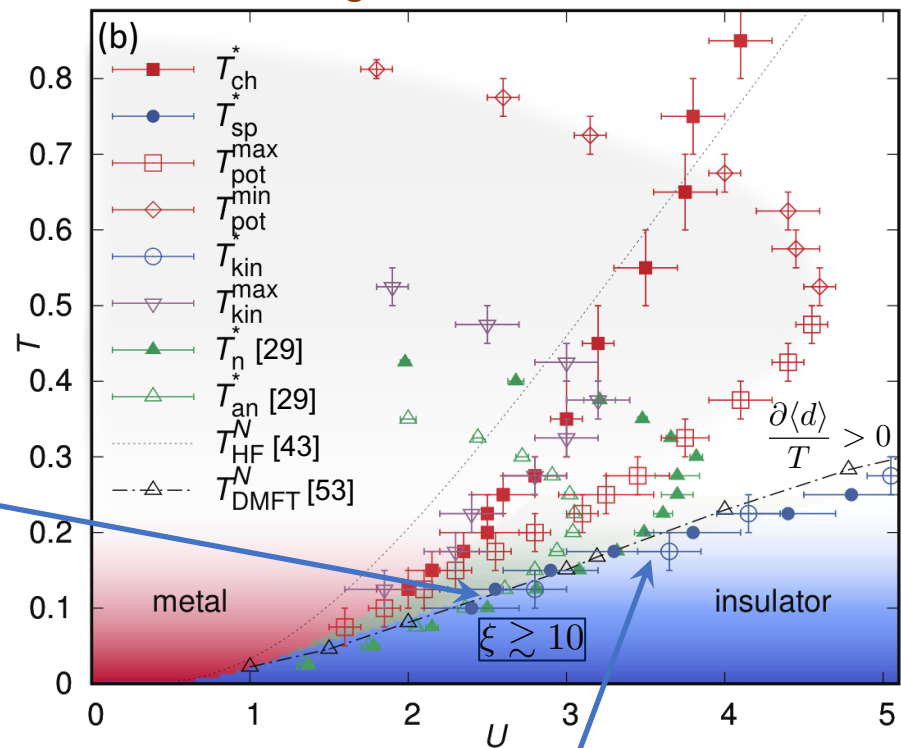
Crossover signatures in charge and spin correlations: Can be measured in cold-atom experiments



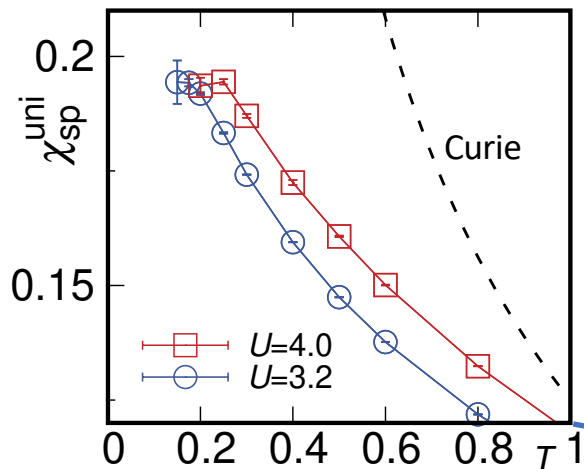
Relatively short-ranged magnetic correlations
at the charge crossover in the correlated regime ($U \sim 3t$)

Crossover signatures in charge and spin correlations: Can be measured in cold-atom experiments

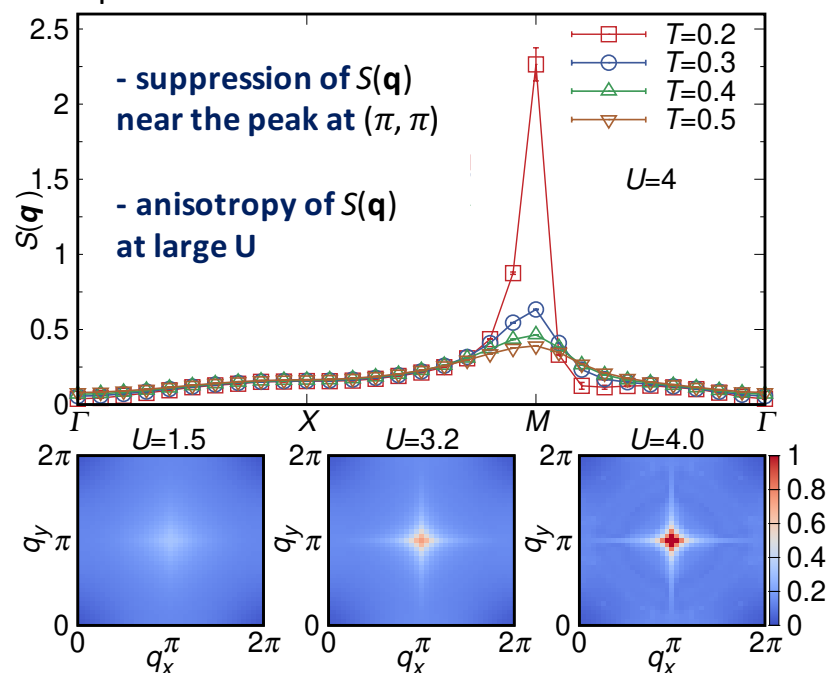
crossover diagram



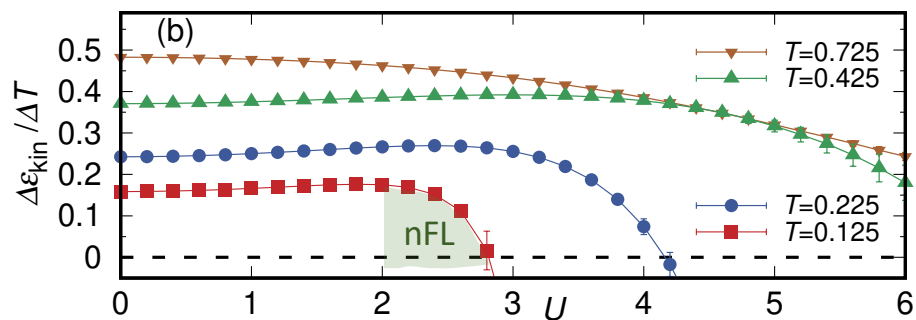
maximum of uniform spin susceptibility:



Spin structure factor:



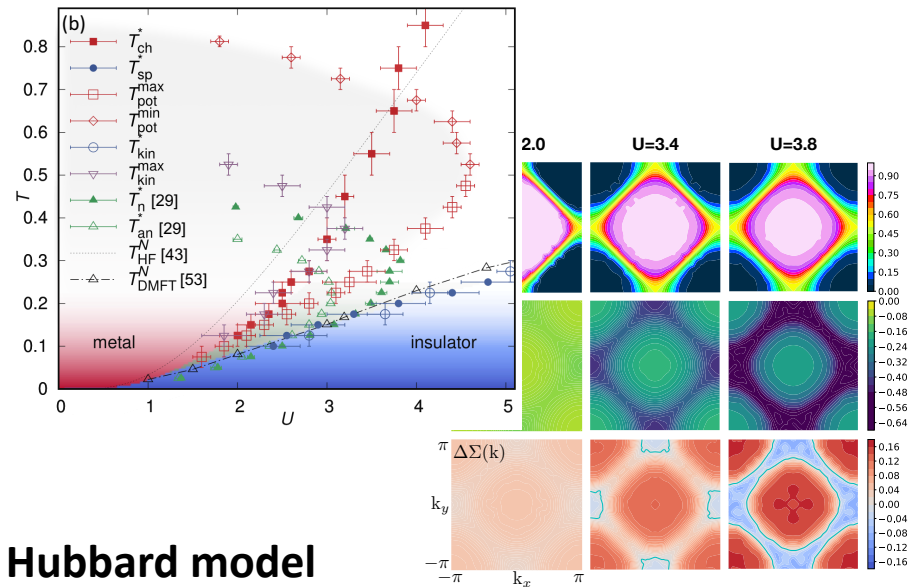
change of sign in $\partial \varepsilon_{kin} / \partial T$ at insulator boundary:



consistent with "Slater" insulator

Conclusions

- Determinantal Diagrammatic Monte Carlo for the self-energy (Σ DDMC) + **resummations** works well in the strongly correlated regime (e.g. $U=7t$, $T=0.2$, 6% doping).
- **Controlled** description of the **metal to insulator crossover** in 2D Hubbard model
- Extended nature of the crossover with a transitional **non-Fermi-liquid regime**
- Signatures in **charge and spin correlations** with controlled accuracy in an **experimentally accessible regime**
- Pronounced **separation of crossover scales**
- Entropy and equations of state of the doped Hubbard model



Šimkovic, LeBlanc, Kim, Deng, Prokof'ev, Svistunov, EK, arXiv:1812.11503
Kim, Šimkovic, EK, arXiv:1905.13337