

Numerical methods for strongly correlated systems

Thereza Paiva



SCHOOL ON RECENT ADVANCES IN STRONGLY CORRELATED QUANTUM MATERIALS

October 5-9, 2026 ICTP-SAIFR

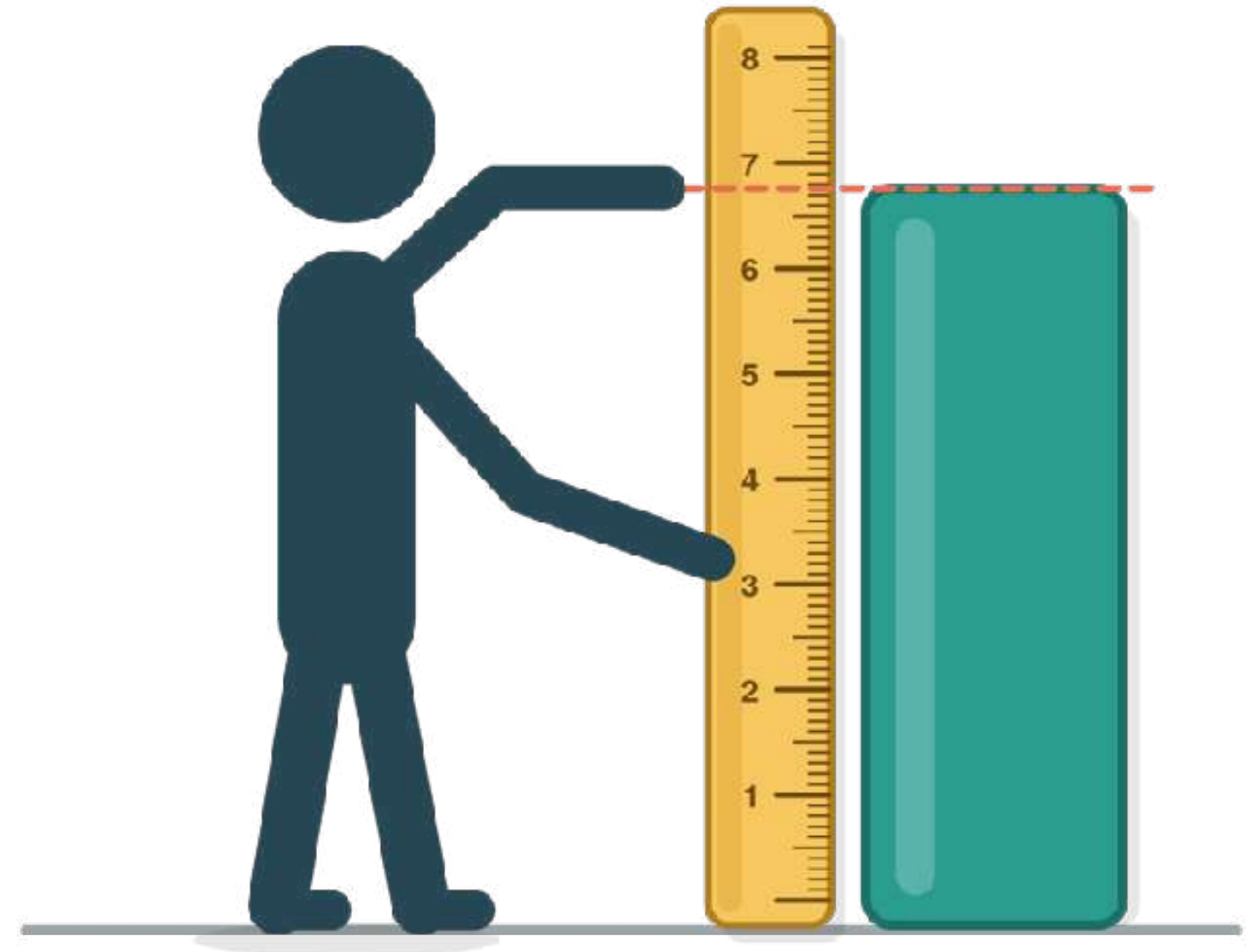
Summary

- 1 – Classical Monte Carlo**
- 2 – Quantum Monte Carlo**
- 3 – Measurements in QMC – I**
- 4 – Measurements in QMC – II**
- 5 – The Sign problem**

Summary

- 1 – Classical Monte Carlo
- 2 – Quantum Monte Carlo
- 3 – **Measurements in QMC – I**
- 4 – Measurements in QMC – II
- 5 – The Sign problem

Measurements in QMC I



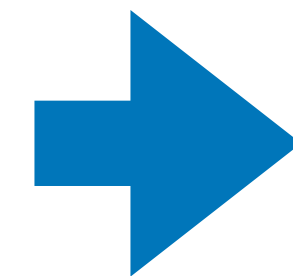
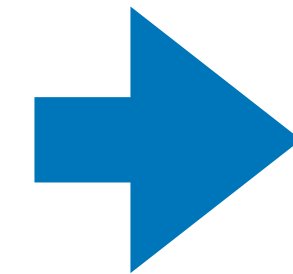
Measurements in QMC

Green's function

Wick's theorems

Charge correlation function

Spin correlation functions



Comparing with
experiments

Quantum gas microscope

Last class

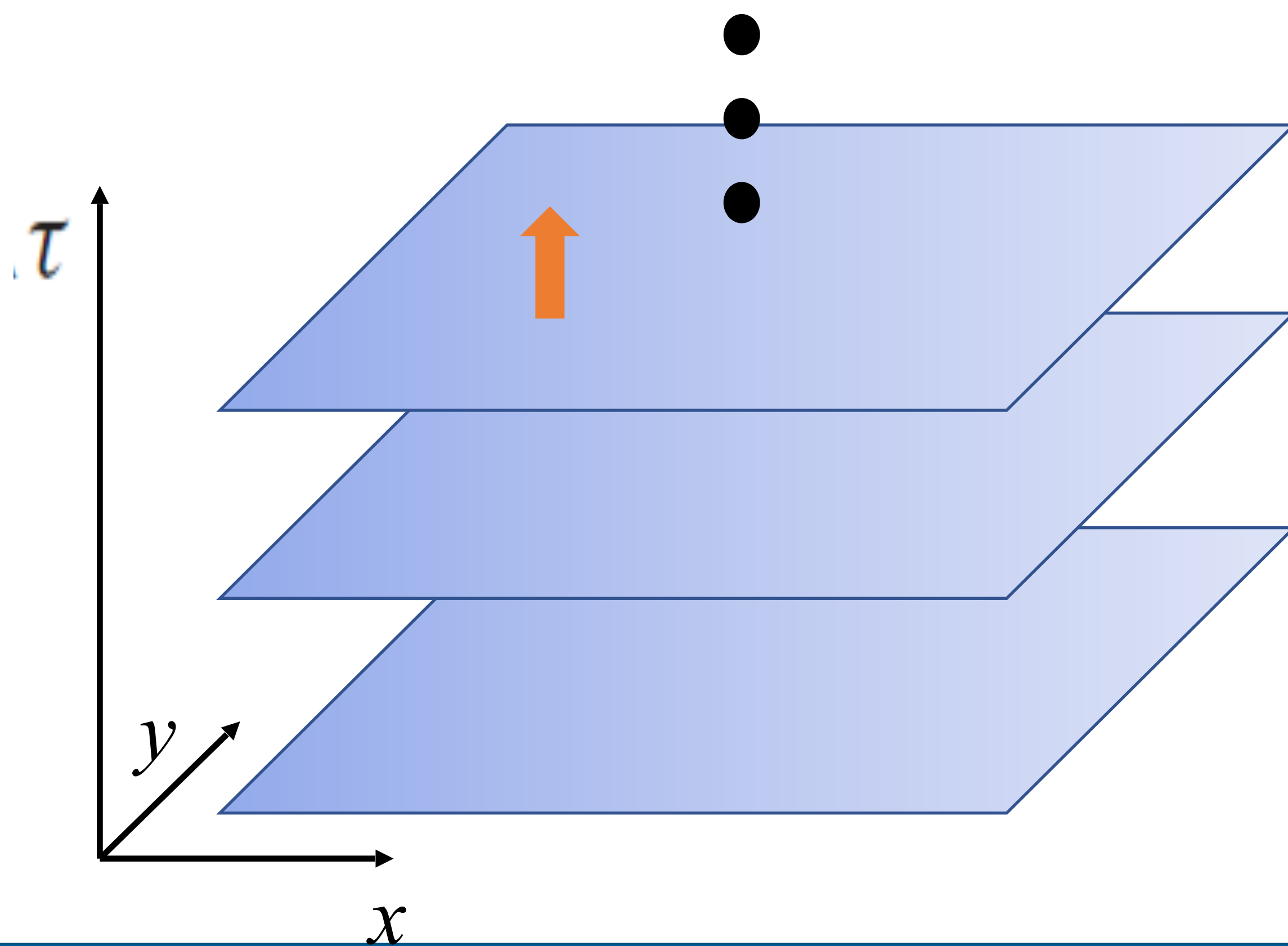
$$\mathcal{Z} = \left(\frac{1}{2}\right)^{L^d M} \text{Tr}_{\{s\}} \prod_{\sigma} \det [\mathbf{1} + \mathbf{B}_M^{\sigma} \mathbf{B}_{M-1}^{\sigma} \cdots \mathbf{B}_1^{\sigma}]$$

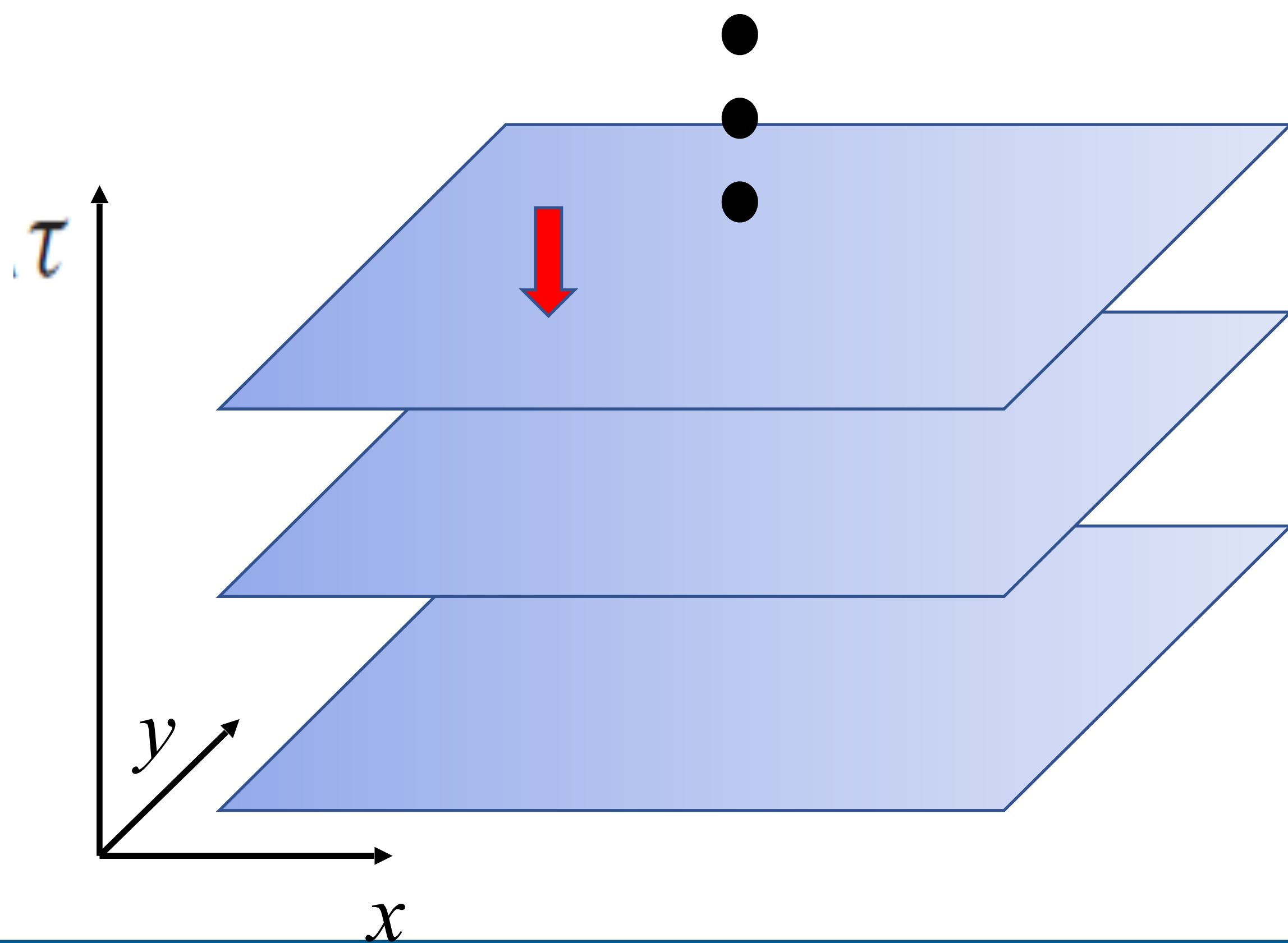
$$\left\{ \begin{array}{l} \mathbf{B}_{\ell}^{\sigma} \equiv e^{-\Delta\tau \mathbf{K}} e^{-\Delta\tau V^{\sigma}(\ell)} \\ O^{\sigma}(\{s\}) \equiv 1 + \mathbf{B}_M^{\sigma} \mathbf{B}_{M-1}^{\sigma} \cdots \mathbf{B}_1^{\sigma} \end{array} \right.$$

$$\left\{ \begin{array}{l} \mathbf{B}_\ell^\sigma \equiv e^{-\Delta\tau \mathbf{K}} e^{-\Delta\tau V^\sigma(\ell)} \\ \mathbf{O}^\sigma(\{s\}) \equiv 1 + \mathbf{B}_M^\sigma \mathbf{B}_{M-1}^\sigma \cdots \mathbf{B}_1^\sigma \end{array} \right.$$

$$\begin{aligned} \mathcal{Z} &= \left(\frac{1}{2}\right)^{L^d M} \mathbf{Tr}_{\{s\}} \det \mathbf{O}^\uparrow(\{s\}) \cdot \det \mathbf{O}^\downarrow(\{s\}) = \\ &= \mathbf{Tr}_{\{s\}} \rho(\{s\}), \end{aligned}$$

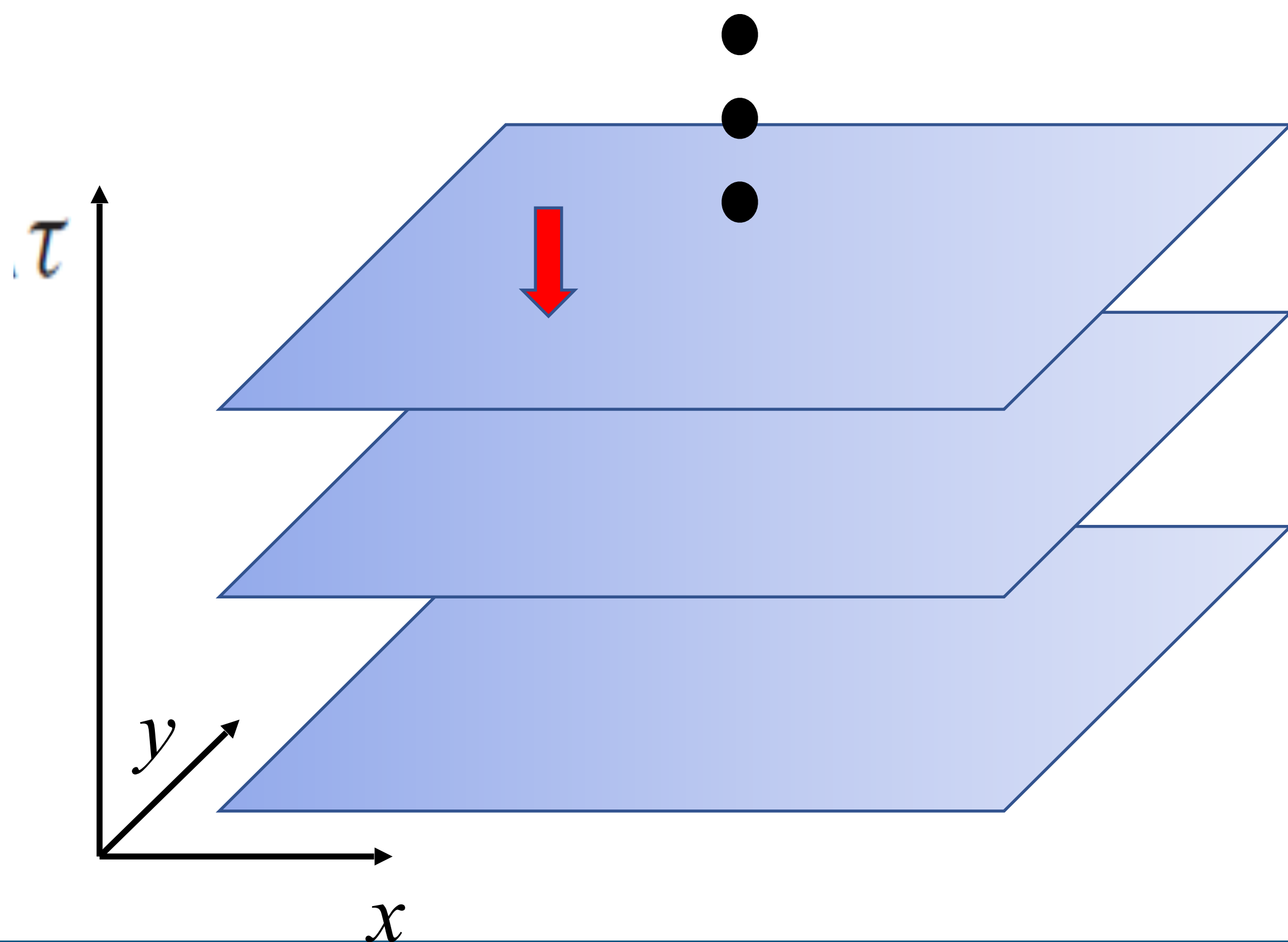
$\rho \rightarrow$ Effective density matrix





$$\mathcal{R}^\sigma = \frac{\det[\mathbb{1} + \mathbf{B}^\sigma(\beta, \beta - \Delta\tau) \dots \mathbf{B}'^\sigma(l+1, l) \dots \mathbf{B}^\sigma(\Delta\tau, 0)]}{\det[\mathbb{1} + \mathbf{B}^\sigma(\beta, \beta - \Delta\tau) \dots \mathbf{B}^\sigma(\Delta\tau, 0)]}$$

$$\mathbf{B}^\sigma(l+1, l) \xrightarrow{x_{i,l} \rightarrow -x_{i,l}} \mathbf{B}'^\sigma(l+1, l)$$



$$\mathcal{R}^\sigma = \frac{\det[\mathbb{1} + \mathbf{B}^\sigma(\beta, \beta - \Delta\tau) \dots \mathbf{B}'^\sigma(l+1, l) \dots \mathbf{B}^\sigma(\Delta\tau, 0)]}{\det[\mathbb{1} + \mathbf{B}^\sigma(\beta, \beta - \Delta\tau) \dots \mathbf{B}^\sigma(\Delta\tau, 0)]}$$

$$\mathbf{B}^\sigma(l+1, l) \xrightarrow{x_{i,l} \rightarrow -x_{i,l}} \mathbf{B}'^\sigma(l+1, l)$$

$$r = \mathcal{R}^\uparrow \mathcal{R}^\downarrow \quad \text{Metropolis}$$

$$r = \frac{\mathcal{R}^\uparrow \mathcal{R}^\downarrow}{1 + \mathcal{R}^\uparrow \mathcal{R}^\downarrow} \quad \text{Heat-bath}$$

Equal time correlations

Operators A and B

$$\langle AB \rangle = \frac{1}{\mathcal{Z}} \text{Tr}_{\{s\}} \mathcal{T} r \left[AB \prod_{\ell\sigma} e^{-\Delta\tau K} e^{-\Delta\tau V^\sigma(\ell)} \right]$$

For a given configuration s of the Hubbard–Stratonovich field

$$\langle AB \rangle_{\{s\}} \equiv \frac{1}{\rho(\{s\})} \mathcal{T} r \left[AB \prod_{\ell\sigma} e^{-\Delta\tau K} e^{-\Delta\tau V^\sigma(\ell)} \right]$$

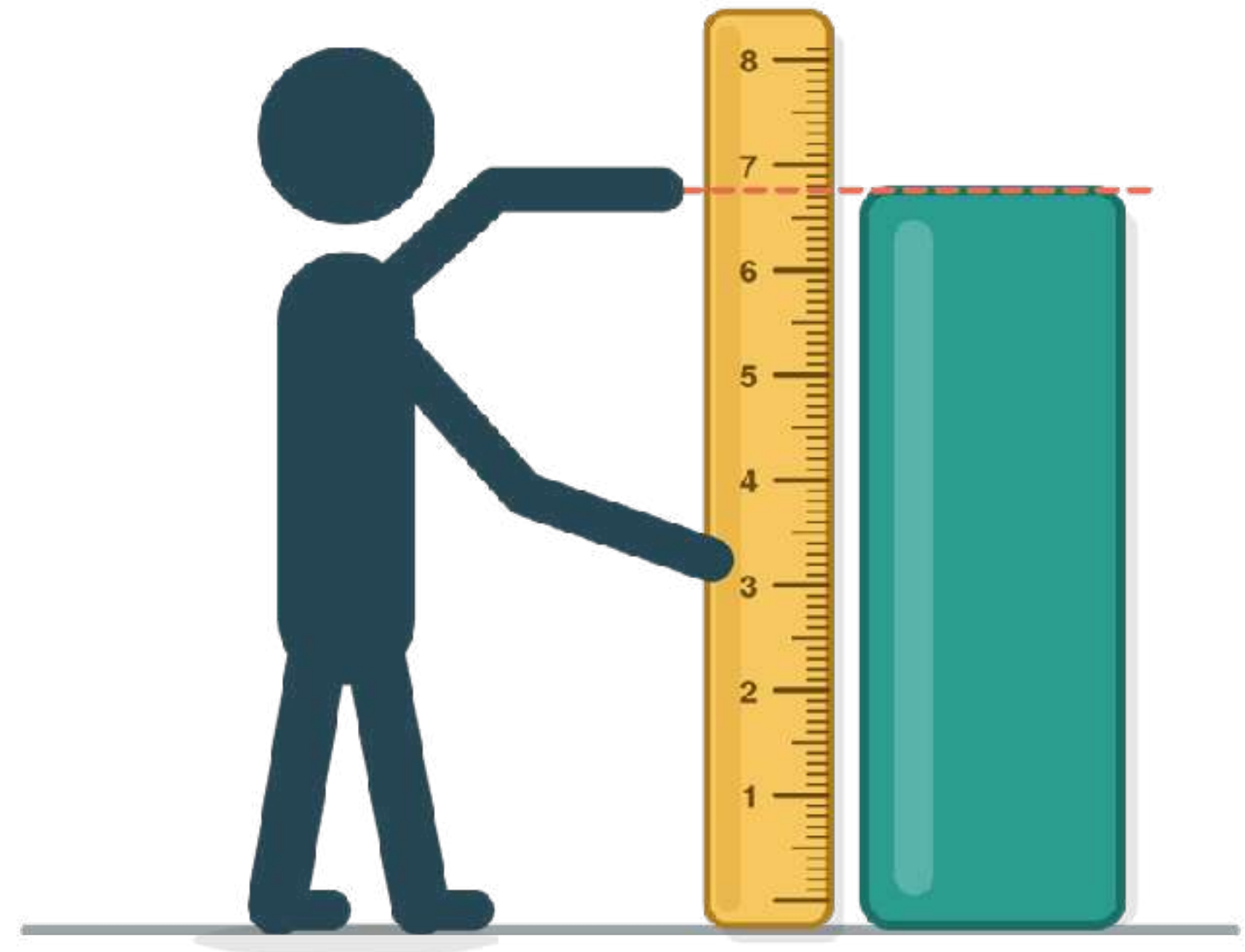
The correlation function becomes

$$\langle AB \rangle = \frac{1}{\mathcal{Z}} \text{Tr}_{\{s\}} \langle AB \rangle_{\{s\}} \rho(\{s\})$$

$$\langle AB \rangle = \frac{1}{\mathcal{Z}_{\{s\}}} \mathbf{Tr}_{\{s\}} \langle AB \rangle_{\{s\}} \rho(\{s\})$$

The average value of an operator is obtained by sampling the corresponding Green's function over the HS configuration weighted by $\rho(\{s\})$

Green's function



Equal time single-particle Green's function

Single-particle Green's function

$$\langle c_i c_j^\dagger \rangle_{\{s\}} = \frac{1}{\mathcal{Z}} \text{Tr} e^{-\beta \mathcal{H}} c_i c_j^\dagger,$$

Omitting spin
indices

Let us define

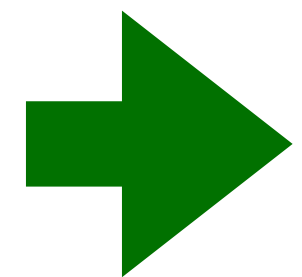
$$D_\ell = e^{-\Delta\tau \sum_{i,j} c_i^\dagger K_{ij} c_j} e^{-\Delta\tau \sum_i c_i^\dagger V_i(\ell) c_i}$$

Then

$$\langle c_i c_j^\dagger \rangle_{\{s\}} = \frac{\text{Tr} D_M \cdots D_1 c_i c_j^\dagger}{\text{Tr} D_M \cdots D_1}.$$

Diagonal representation

$$c_i = \sum_{\alpha} \langle i | \alpha \rangle c_{\alpha} \quad c_i^{\dagger} = \sum_{\alpha} \langle \alpha | i \rangle c_{\alpha}^{\dagger}.$$



$$\langle c_i c_j^{\dagger} \rangle_{\{s\}} = \sum_{\alpha', \alpha''} \langle i | \alpha' \rangle \langle \alpha'' | j \rangle \frac{\text{Tr } c_{\alpha'} c_{\alpha''}^{\dagger} D_M \cdots D_1}{\text{Tr } D_M \cdots D_1}.$$

Taking the trace on the diagonal representation

$$\begin{aligned} \langle c_i c_j^{\dagger} \rangle_{\{s\}} &= \sum_{\alpha'} |\alpha'\rangle \langle i | \frac{1}{1 + e^{-\Delta\tau\epsilon'_{\alpha}}} | j \rangle \langle \alpha' | = \\ &= \left[\frac{1}{1 + B_M \cdots B_1} \right]_{ij} = [g]_{ij}. \end{aligned}$$

**Nonzero contribution only
when $\alpha = \alpha'$**

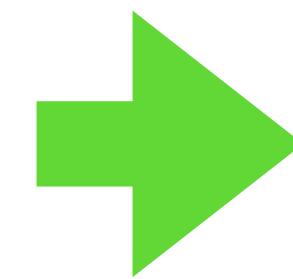
Single-particle Green's function

$$g^\sigma(\ell) \equiv [1 + B_{\ell-1} B_{\ell-2} \dots B_1 B_M \dots B_\ell]^{-1}$$

On a given time-slice ℓ

The average of $g(\ell)$ over all HS fields should be independent of ℓ

$$\langle c_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma}^\dagger \rangle_{\{s\}} = \left[(1 + B_M^\sigma B_{M-1}^\sigma \dots B_1^\sigma)^{-1} \right]_{\mathbf{ij}}$$



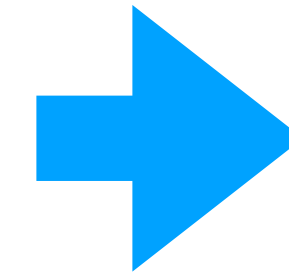
Central quantity in
DQMC calculations

Two particle Green's function

$$\langle c_{i_1}^\dagger c_{i_2} c_{i_3}^\dagger c_{i_4} \rangle_{\{s\}} \quad \rightarrow \quad ?$$

Wick's Theorem

Direct application of all commutation and anticommutation relations is lengthy



Wick's Theorem

Operator identity

Procedure to calculate matrix elements

Creation and destruction operators paired

Destruction operators moved to the right

Contractions and normal ordering

Four two-operator contractions

$$\langle c_{i\sigma} c_{j\sigma}^\dagger \rangle = g_{ij}^\sigma$$

Definition: Annihilator on the left

$$\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle = \delta_{ij} - g_{ji}^\sigma$$

Anticommutation relations

$$\langle c c \rangle = \langle c^\dagger c^\dagger \rangle = 0$$

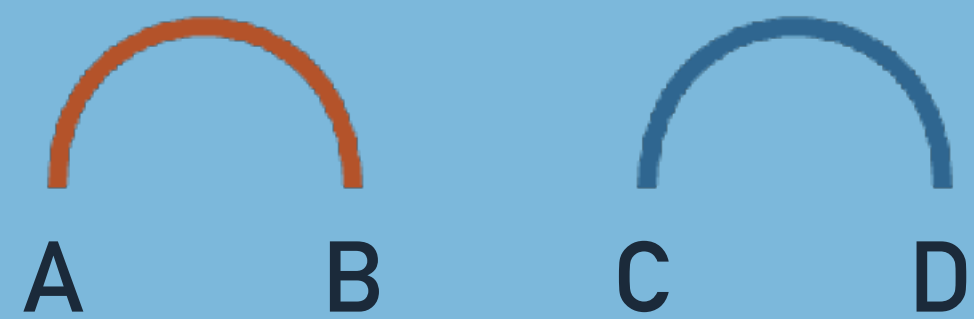
Particle number is conserved

$$\langle c_{i\uparrow}^\dagger c_{j\downarrow} \rangle = 0$$

Oposite spins: S_z is conserved (in the absence of B fields)

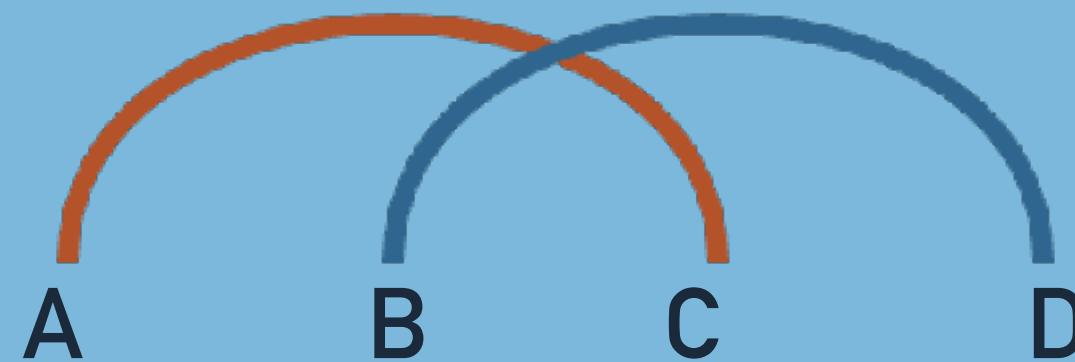
The rule: sum over all pairings

$$\langle ABCD \rangle = \langle AB \rangle \langle CD \rangle - \langle AC \rangle \langle BD \rangle + \langle AD \rangle \langle BC \rangle$$



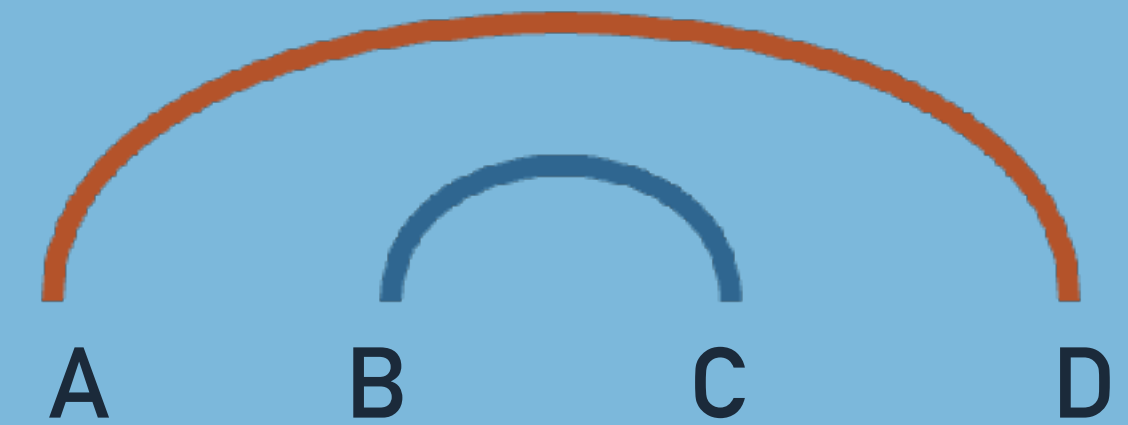
$$+ \langle AB \rangle \langle CD \rangle$$

0 crossings $\rightarrow$ sign +



$$- \langle AC \rangle \langle BD \rangle$$

1 crossings $\rightarrow$ sign -



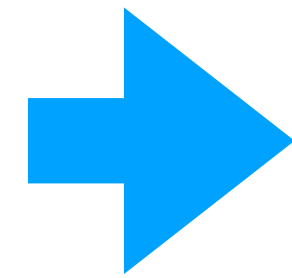
$$+ \langle AD \rangle \langle BC \rangle$$

0 crossings $\rightarrow$ sign +

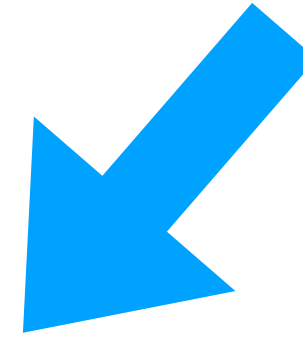
- Within each pair, keep the original order of the operators (A before B, etc.).
- Sign = $(-1)^{(\text{number of crossings})}$, i.e. the parity of the permutation.

Two particle Green's function

$$\langle c_{i_1}^\dagger c_{i_2} c_{i_3}^\dagger c_{i_4} \rangle_{\{s\}}$$



Use Wick's theorem to write in terms of single-particle Green's function



$$\begin{aligned} \langle c_{i_1}^\dagger c_{i_2} c_{i_3}^\dagger c_{i_4} \rangle_{\{s\}} &= \langle c_{i_1}^\dagger c_{i_2} \rangle_{\{s\}} \langle c_{i_3}^\dagger c_{i_4} \rangle_{\{s\}} + \\ &+ \langle c_{i_1}^\dagger c_{i_4} \rangle_{\{s\}} \langle c_{i_2} c_{i_3}^\dagger \rangle_{\{s\}}, \end{aligned}$$

All average values of interest can be written in terms of single-particle Green's functions

Unequal time single-particle Green's function

Operator a in the Heisenberg picture

$$a(\ell) \equiv a(\tau) = e^{\tau \mathcal{H}} a e^{-\tau \mathcal{H}}$$

$$\tau = \ell \Delta\tau$$

Initial time: $\Delta\tau$

Unequal time single-particle Green's function $\ell_1 > \ell_2$

Omitting spin indices

$$G_{ij}(\ell_1; \ell_2) \equiv \langle c_i(\ell_1) c_j^\dagger(\ell_2) \rangle_{\{s\}} = \frac{1}{\mathcal{Z}} \text{Tr} e^{-\beta \mathcal{H}} e^{\ell_1 \Delta \tau \mathcal{H}} c_i e^{-\ell_1 \Delta \tau \mathcal{H}} e^{\ell_2 \Delta \tau \mathcal{H}} c_j^\dagger e^{-\ell_2 \Delta \tau \mathcal{H}}.$$

Using the D matrices again

$$G_{ij}(\ell_1; \ell_2) = \frac{1}{\mathcal{Z}} \text{Tr} D_{\ell_2} \cdots D_1 D_M \cdots D_{\ell+1} D_\ell \cdots D_{\ell_2+1} [D_{\ell_1} \cdots D_{\ell_2+1}]^{-1} c_i [D_{\ell_1} \cdots D_{\ell_2+1}] c_j^\dagger,$$

Diagonal representation

$$D_{\ell_1} \cdots D_{\ell_2+1} = e^{\sum_\alpha |\alpha\rangle \varepsilon_\alpha \langle \alpha|} \quad c_\gamma e^{-\varepsilon_\alpha c_\alpha^\dagger c_\alpha} = \begin{cases} e^{-\varepsilon_\gamma} c_\gamma & \text{if } \alpha = \gamma, \\ e^{-\varepsilon_\alpha c_\alpha^\dagger c_\alpha} c_\gamma & \text{if } \alpha \neq \gamma, \end{cases}$$

$$\sum_{\gamma} \langle i | \gamma \rangle [D_{\ell_1} \cdots D_{\ell_2+1}]^{-1} c_{\gamma} [D_{\ell_1} \cdots D_{\ell_2+1}] = \sum_{\gamma} \langle i | \gamma \rangle e^{-\varepsilon_{\gamma}(1-n_{\gamma})} c_{\gamma}.$$

$$1 - n_{\alpha} = 1, 0 \quad \rightarrow \quad e^{-\varepsilon_{\gamma}(1-n_{\gamma})} = \langle \gamma | B_{\ell_1} \cdots B_{\ell_2+1} | \gamma \rangle;$$

Then $[D_{\ell_1} \cdots D_{\ell_2+1}]^{-1} c_i [D_{\ell_1} \cdots D_{\ell_2+1}] = \sum_k \langle i | B_{\ell_1} \cdots B_{\ell_2+1} | k \rangle c_k;$

$$G_{ij}(\ell_1; \ell_2) \equiv \langle c_i(\ell_1) c_j^{\dagger}(\ell_2) \rangle_{\{s\}} = [B_{\ell_1} B_{\ell_1-1} \cdots B_{\ell_2+1} g(\ell_2 + 1)]_{ij}$$

$$\ell_1 > \ell_2$$

$$G_{ij}(\ell_1; \ell_2) \equiv \langle c_i(\ell_1) c_j^\dagger(\ell_2) \rangle_{\{s\}} = [B_{\ell_1} B_{\ell_1-1} \dots B_{\ell_2+1} g(\ell_2 + 1)]_{ij}$$

$$\tilde{G}_{ij}(\ell_1; \ell_2) \equiv \langle c_i^\dagger(\ell_1) c_j(\ell_2) \rangle_{\{s\}} = \left[[1 - g(\ell_2 + 1)] (B_{\ell_1} B_{\ell_1-1} \dots B_{\ell_2+1})^{-1} \right]_{ij}$$

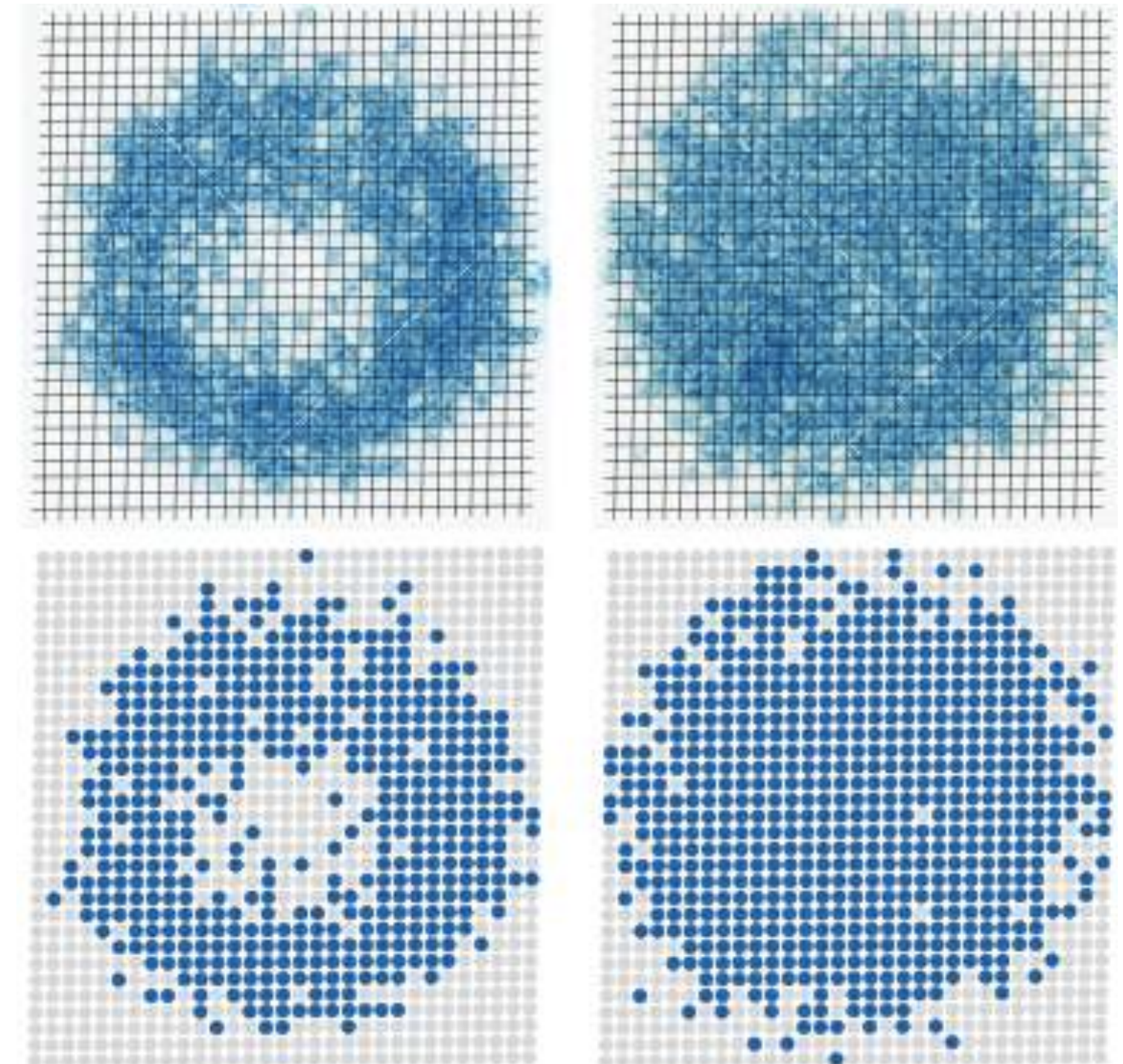
Green's functions

$$\tilde{g}_{ij}^{\sigma} \equiv [1 - g]_{ij} \quad \tilde{G}_{ij}^{\sigma} \equiv [1 - G]_{ij}$$

$$g^{\sigma}(\ell) \equiv \langle c_{i\sigma} c_{j\sigma}^{\dagger} \rangle_{\{s\}} = \left[(1 + B_M^{\sigma} B_{M-1}^{\sigma} \dots B_1^{\sigma})^{-1} \right]_{ij}$$

$$G_{ij}^{\sigma}(\ell_1; \ell_2) \equiv \langle c_{i\sigma}(\ell_1) c_{j\sigma}^{\dagger}(\ell_2) \rangle_{\{s\}} = [B_{\ell_1}^{\sigma} B_{\ell_1-1}^{\sigma} \dots B_{\ell_2+1}^{\sigma} g^{\sigma}(\ell_2 + 1)]_{ij}$$

Charge correlation functions



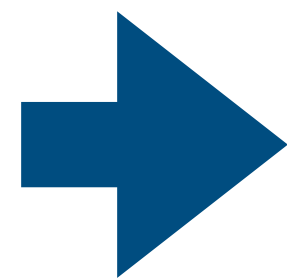
Density

$$\begin{aligned} n &= \frac{1}{MN_s} \sum_{\mathbf{i}, \ell} \sum_{\sigma} \langle c_{\mathbf{i}\sigma}^{\dagger}(\ell) c_{\mathbf{i}\sigma}(\ell) \rangle = \\ &= \frac{1}{MN_s} \sum_{\mathbf{i}, \ell} \sum_{\sigma} \langle\langle 1 - g_{\mathbf{i}\mathbf{i}}^{\sigma}(\ell) \rangle\rangle, \end{aligned}$$

With

$$\langle\langle g_{\mathbf{i}\mathbf{j}}^{\sigma}(\ell) \rangle\rangle \simeq \frac{1}{N_a} \sum_{\zeta=1}^{N_a} g_{\mathbf{i}\mathbf{j}}^{\sigma}(\ell).$$

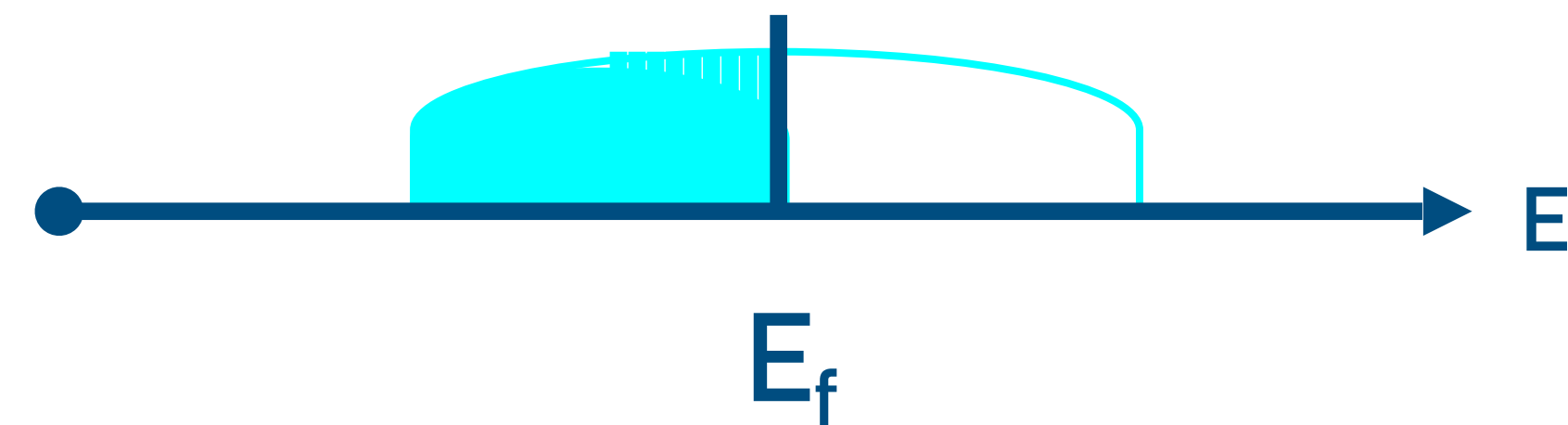
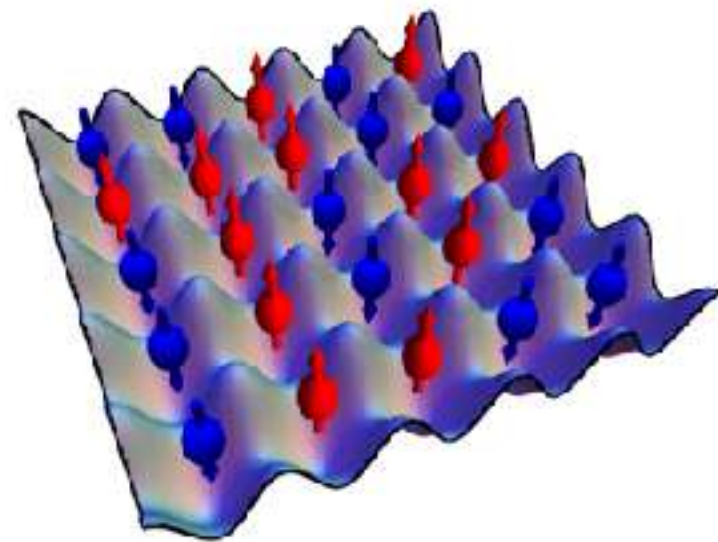
$\langle\langle \dots \rangle\rangle$



Average over N_a HS fields

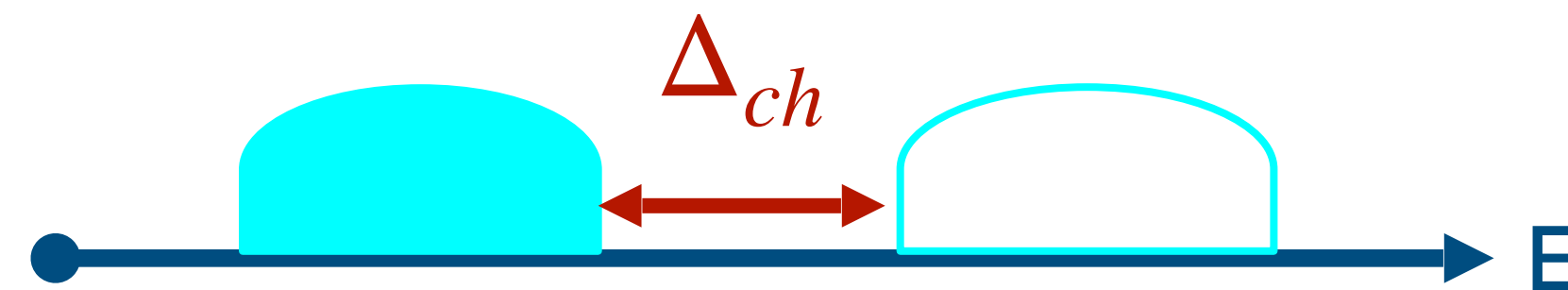
Mott transition

One
fermion
per site



$$U = 0$$

Metal



$$U \neq 0$$

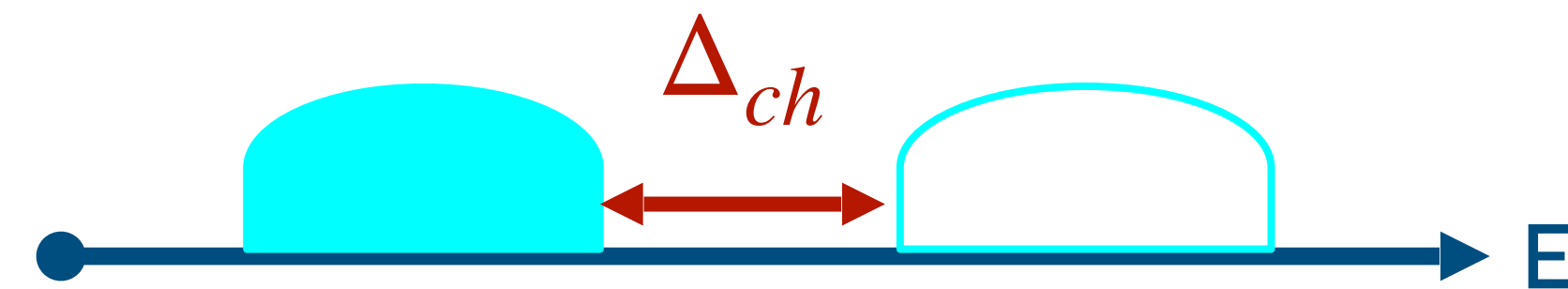
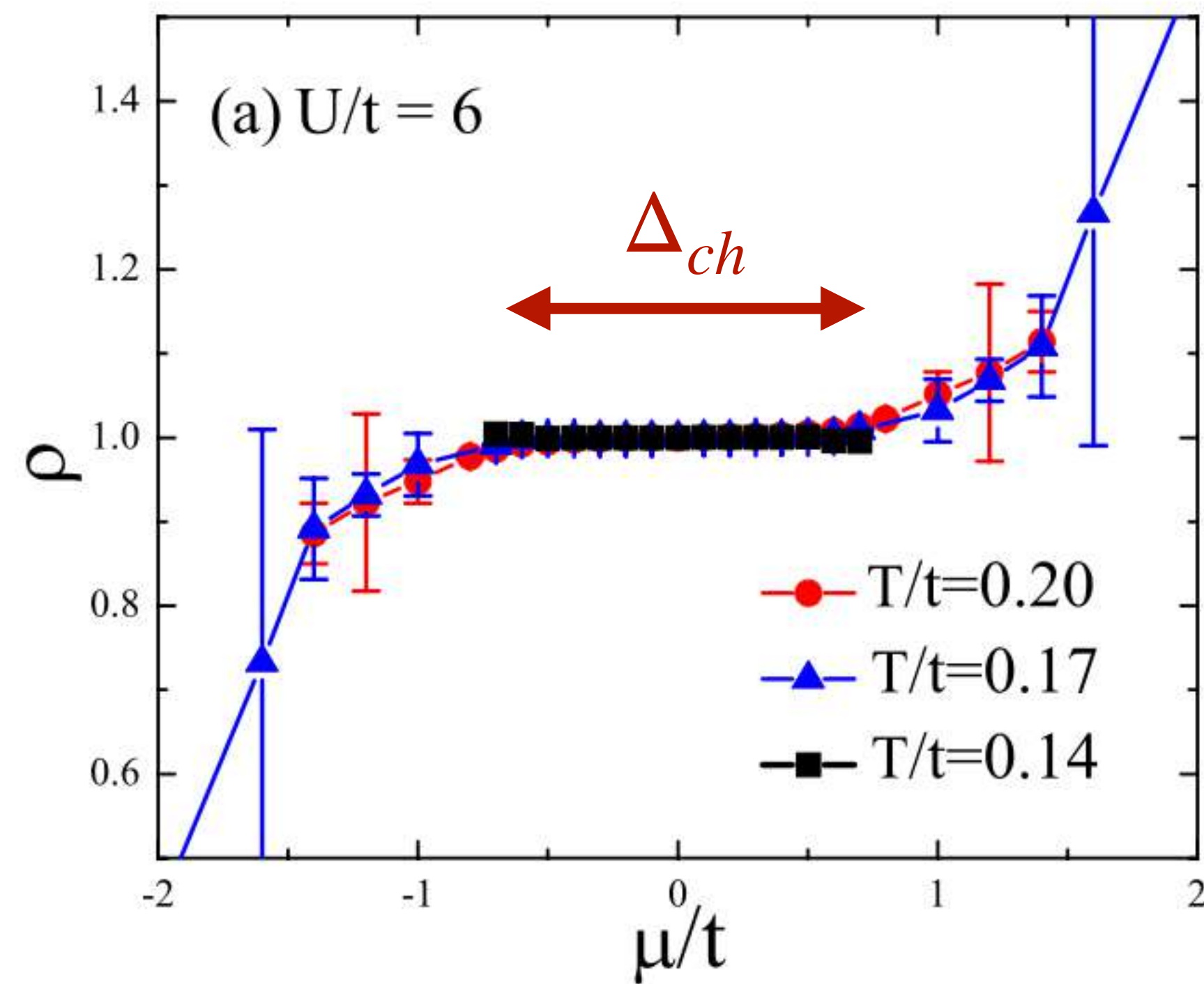
Insulator

Compressibility



$$\kappa = \frac{1}{n^2} \frac{\partial n}{\partial \mu}$$

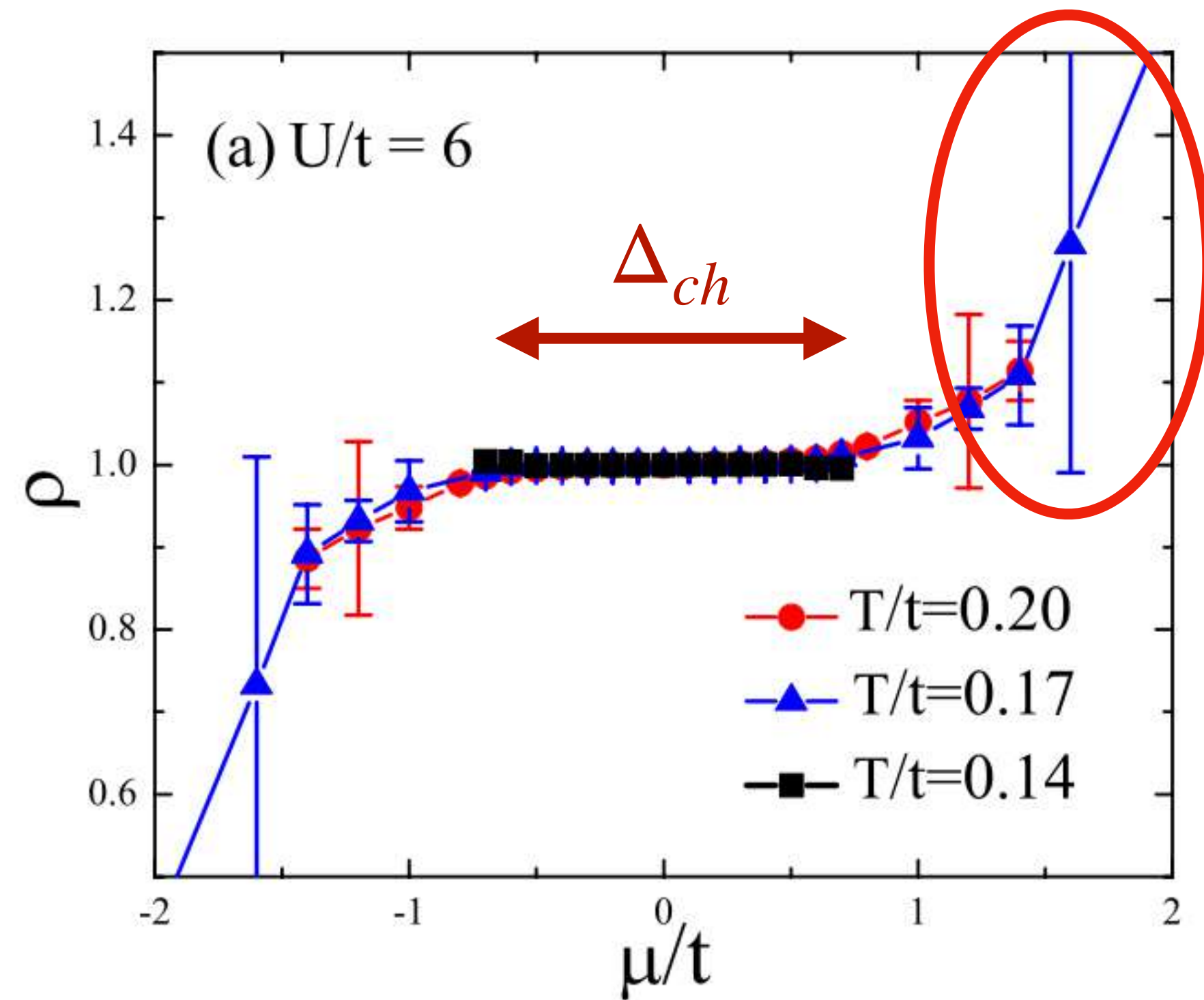
Mott gap



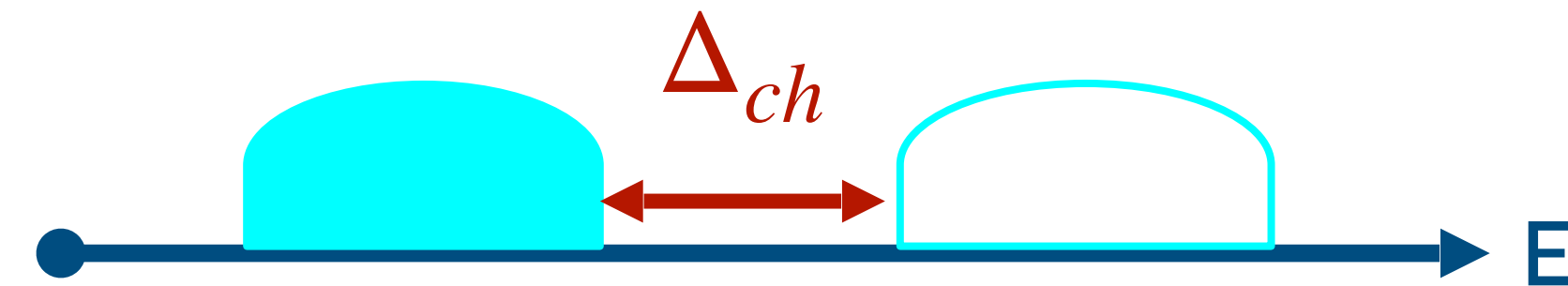
$$\kappa = \frac{1}{n^2} \frac{\partial n}{\partial \mu}.$$

PRL 2010, Paiva et al

Mott gap



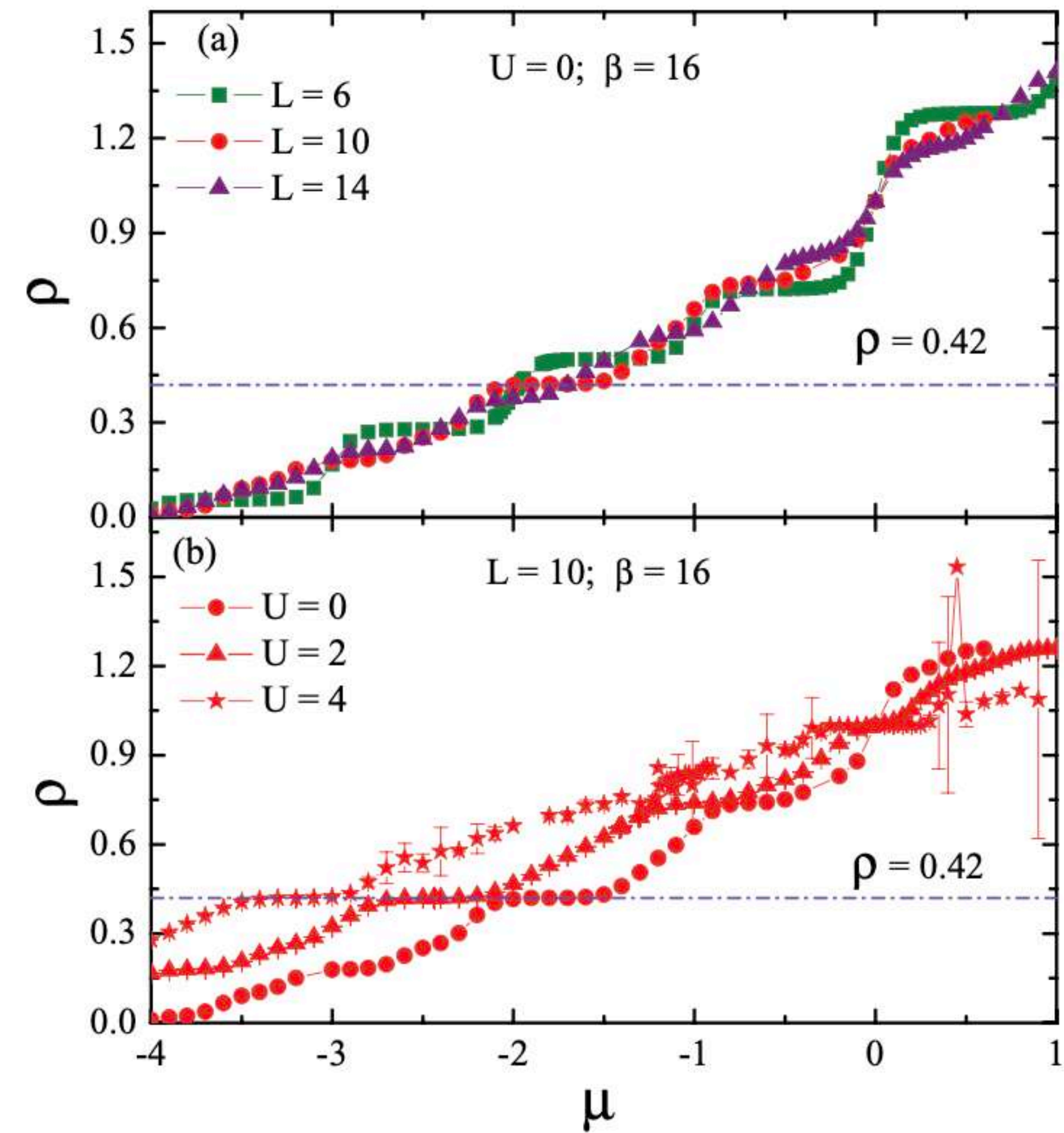
Large error bars: sign problem



$$\kappa = \frac{1}{n^2} \frac{\partial n}{\partial \mu}.$$

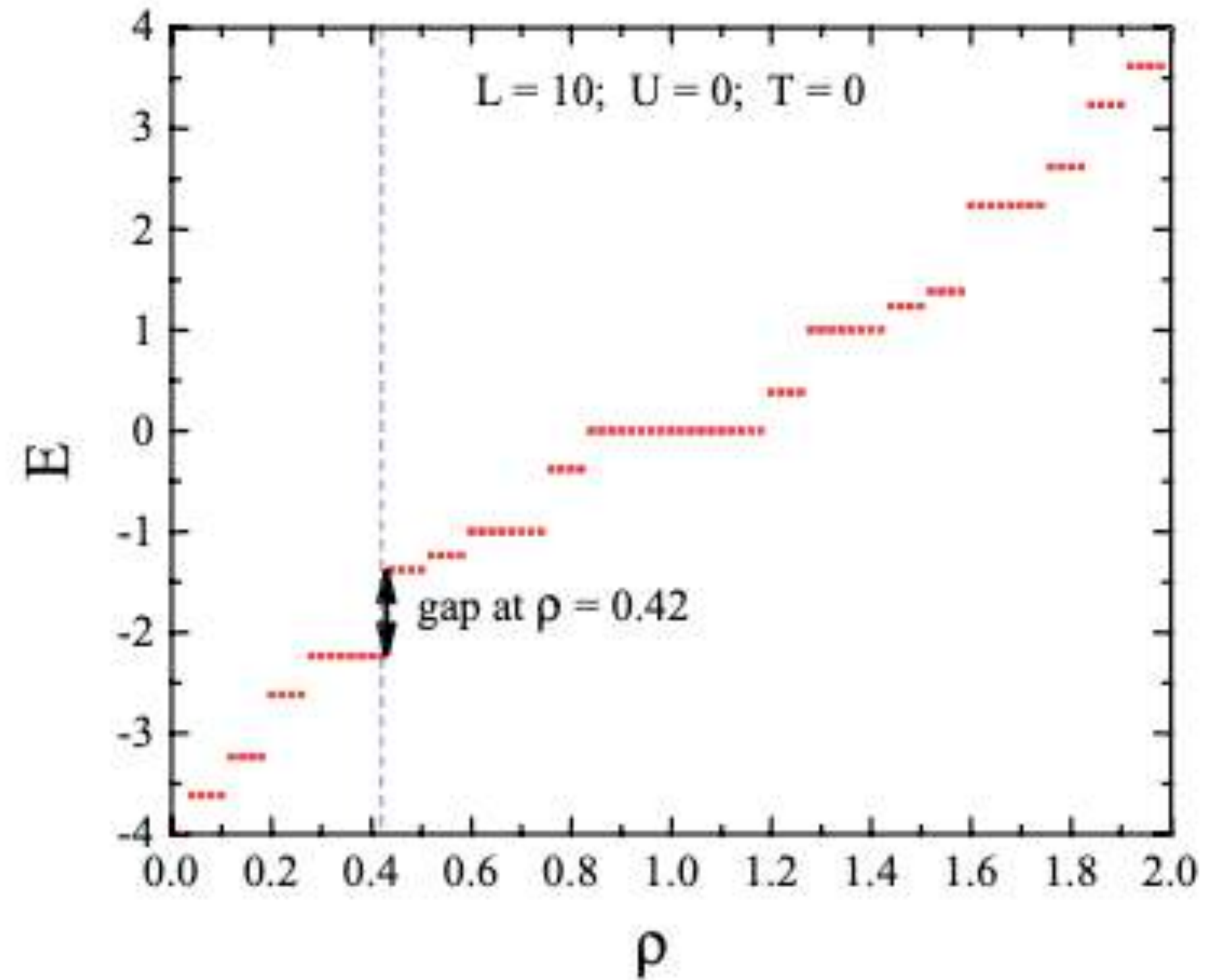
PRL 2010, Paiva et al

Size effects

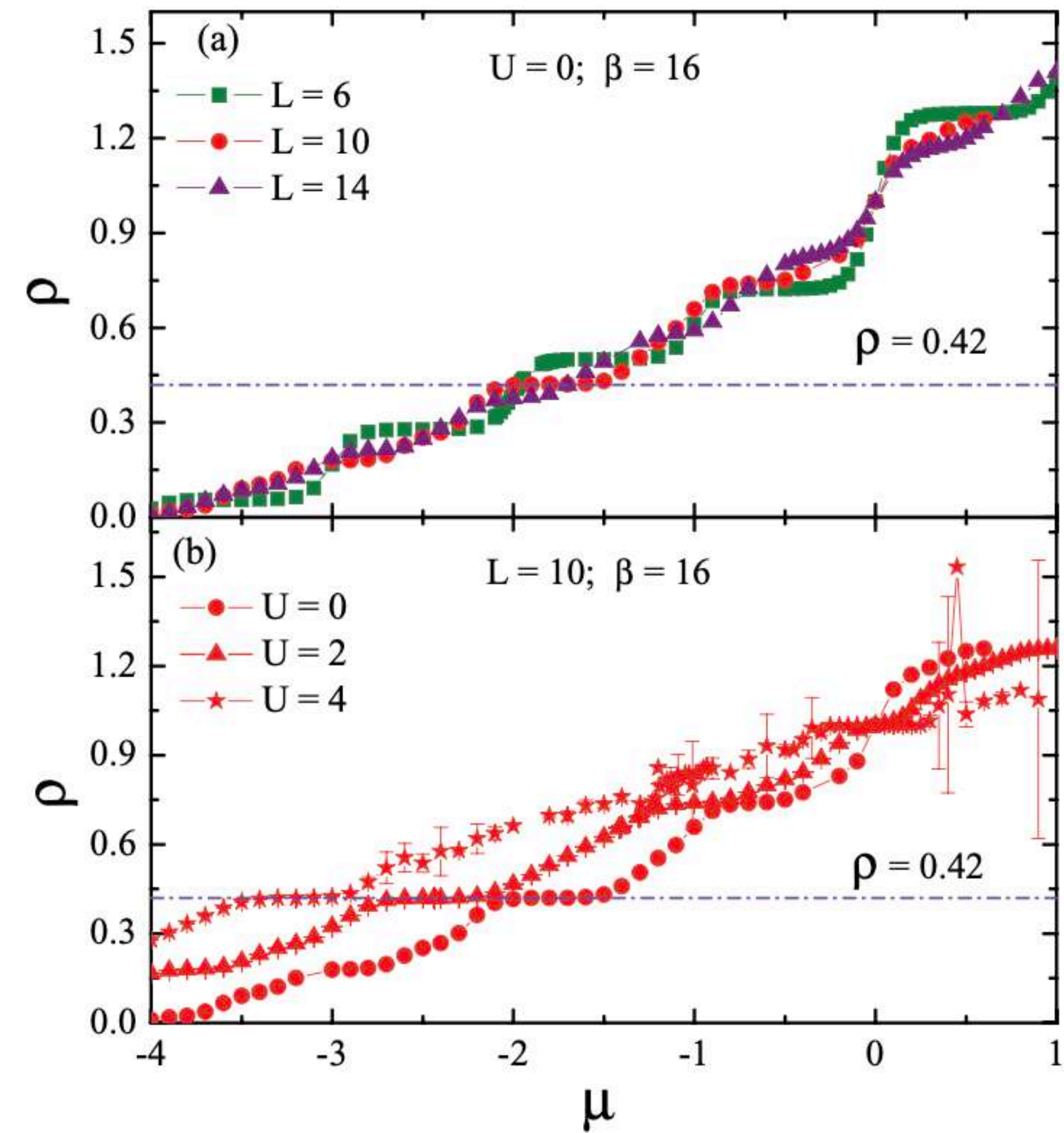


PRB 2012, Mondaini et al

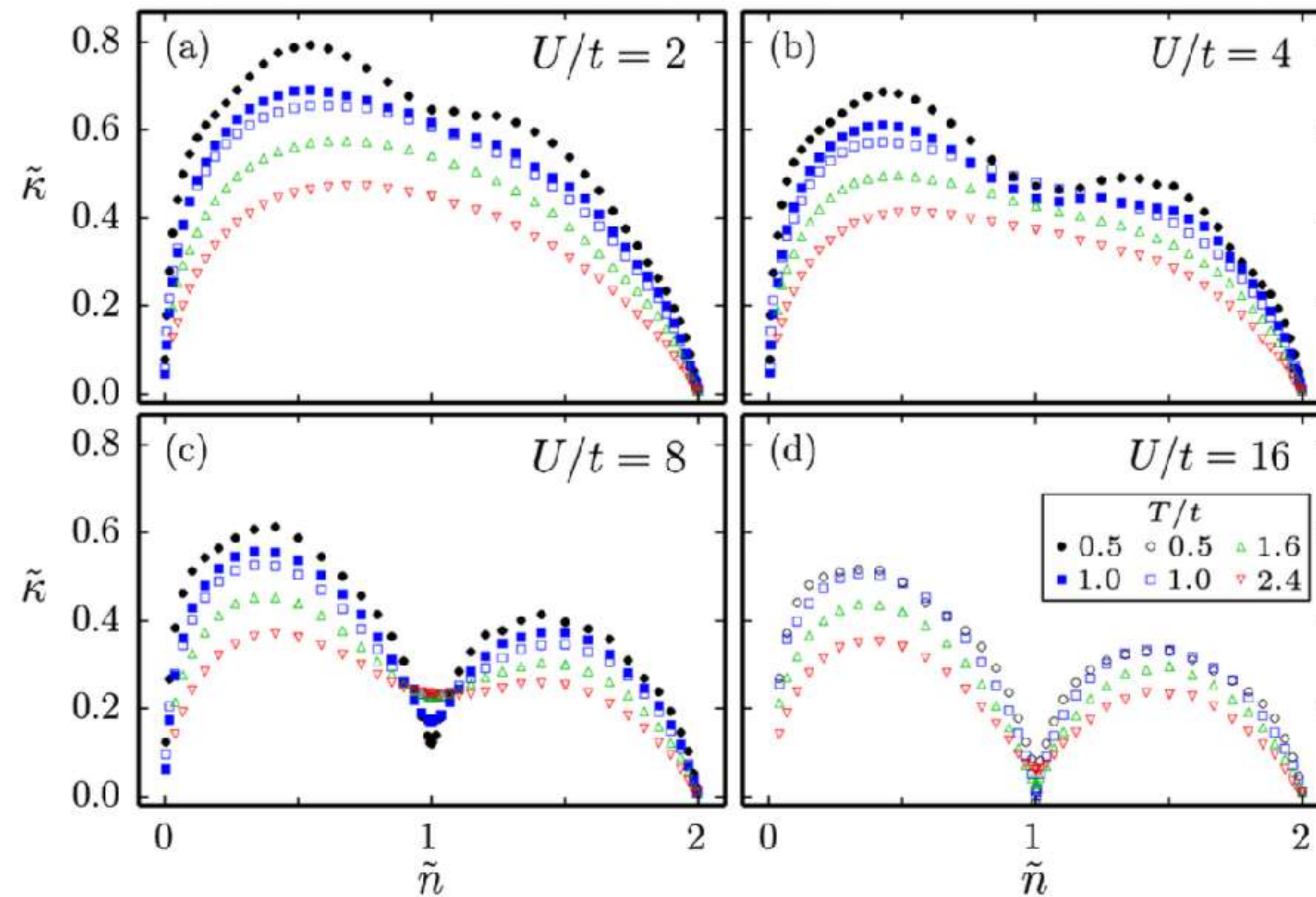
Size effects



PRB 2012, Mondaini et al



Compressibility



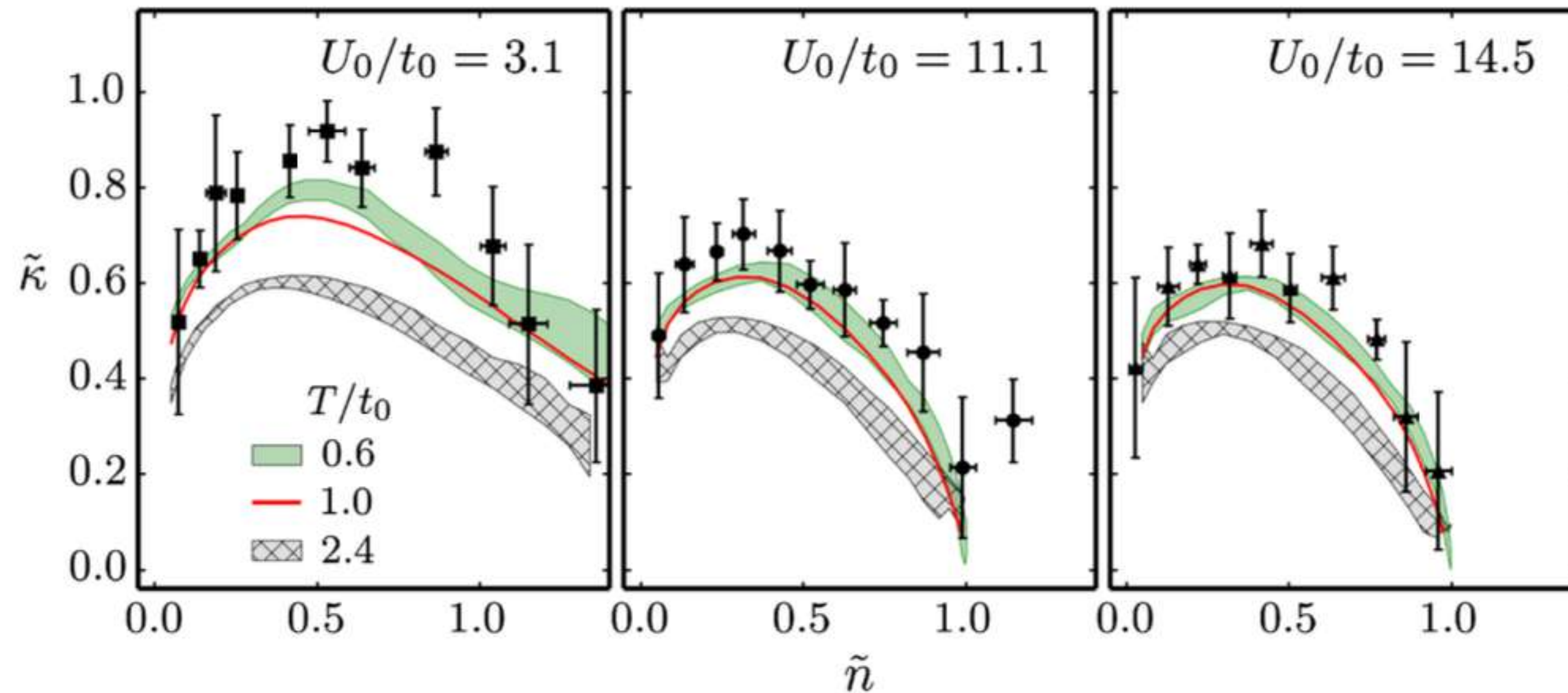
$$\tilde{\kappa} \equiv \frac{(t/a^3)\kappa}{[(2\pi^2/E_r)/a^3]\kappa_0} = \frac{(3\pi^2)^{2/3}}{2} \frac{\partial \tilde{n}^{2/3}}{\partial (\mu/t)},$$

$$\tilde{n} = a^3 n,$$

PRL 2015, Duarte et al

Compressibility

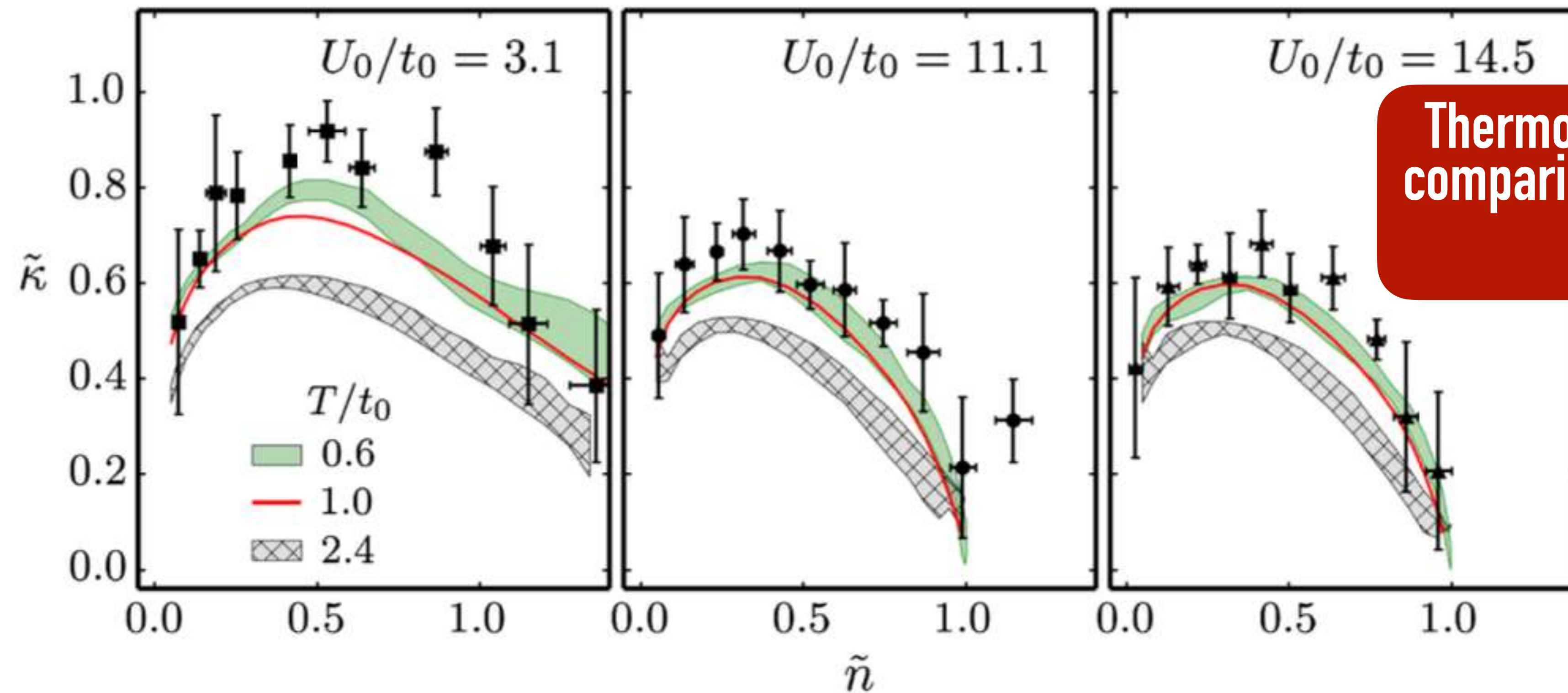
Direct comparison with
optical lattices experiments



PRL 2015, Duarte et al

Compressibility

Direct comparison with
optical lattices experiments

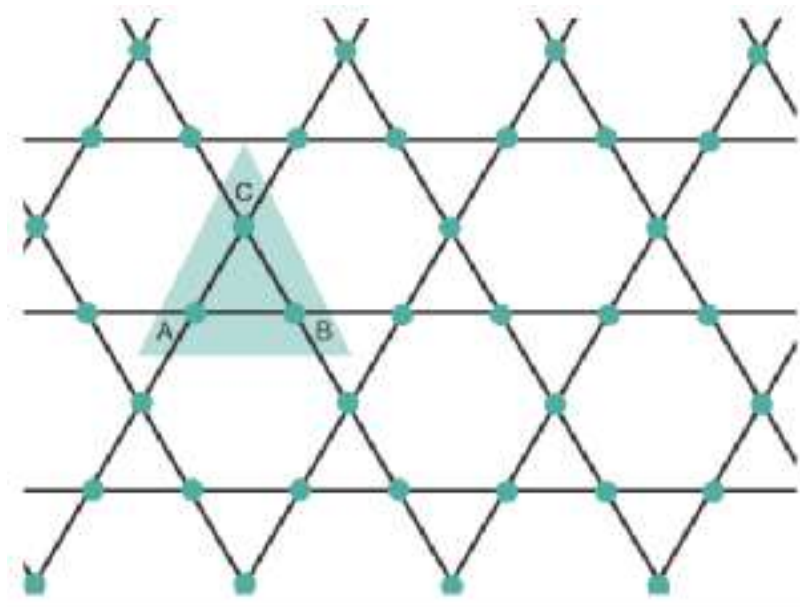


Thermometry from direct
comparison with numerical
data

PRL 2015, Duarte et al

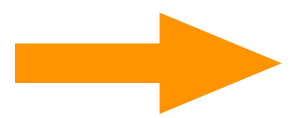
Compressibility

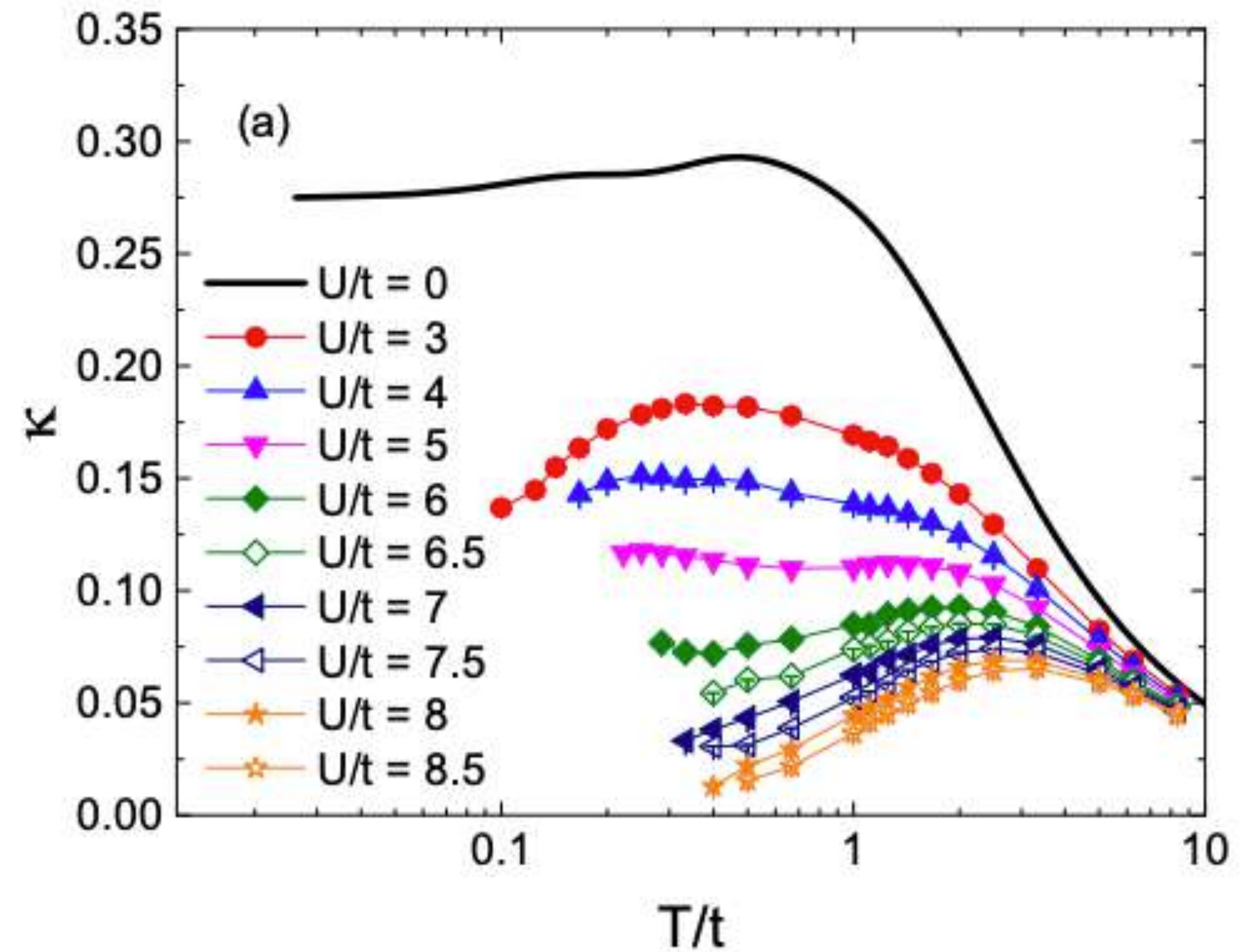
Kagome lattice



$$\kappa = \frac{1}{n^2} \frac{\partial n}{\partial \mu}$$

$$\kappa \propto e^{(-\Delta_c/k_B T)}$$

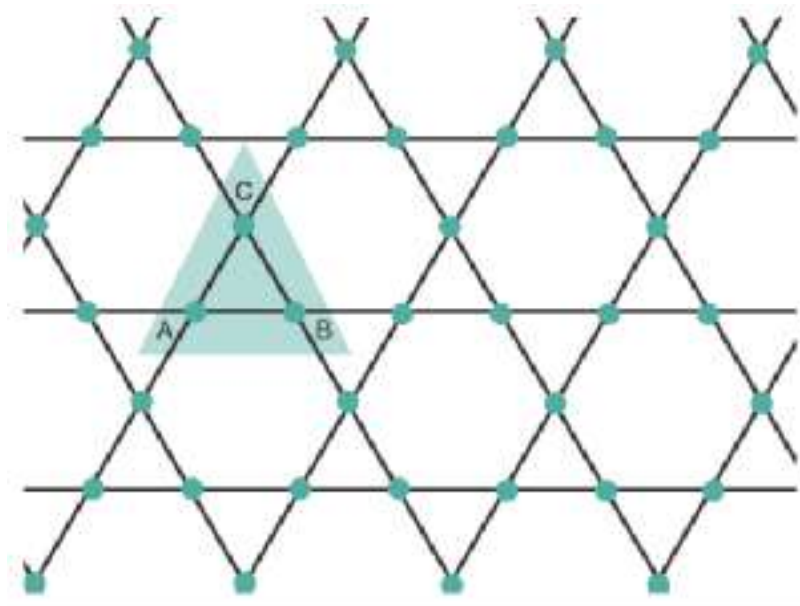
Δ_c  Charge gap



PRB 2013, Medeiros-Silva et al

Compressibility

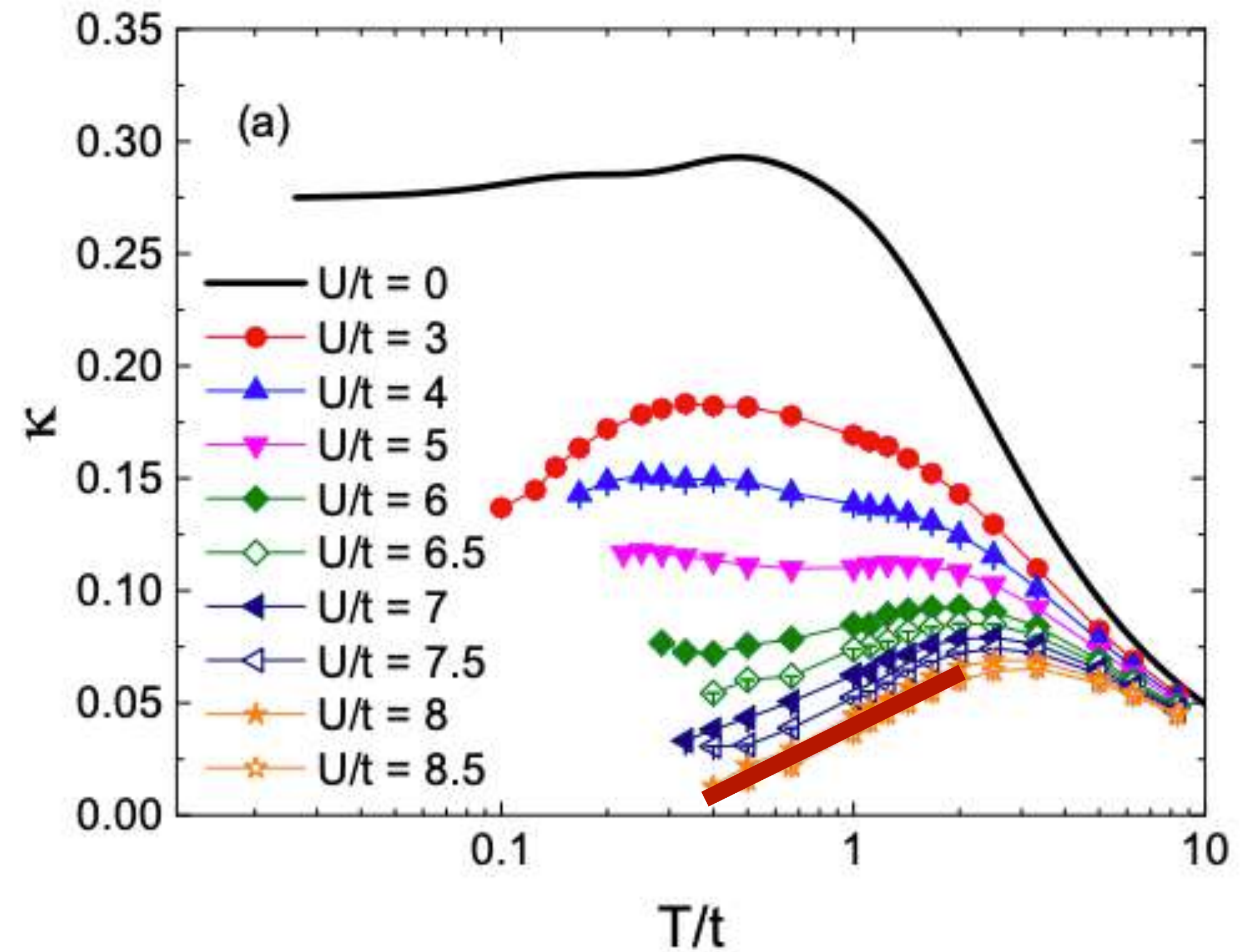
Kagome lattice



$$\kappa = \frac{1}{n^2} \frac{\partial n}{\partial \mu}$$

$$\kappa \propto e^{(-\Delta_c/k_B T)}$$

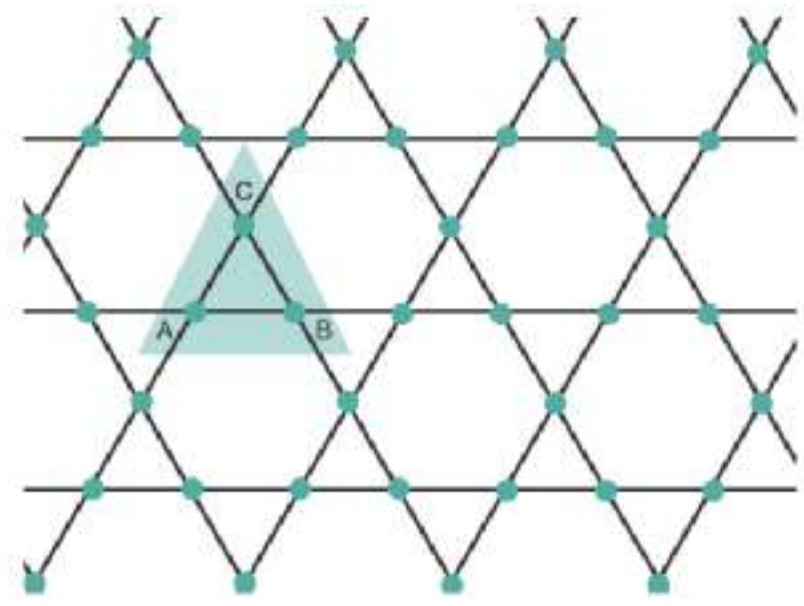
Δ_c  Charge gap



PRB 2013, Medeiros-Silva et al

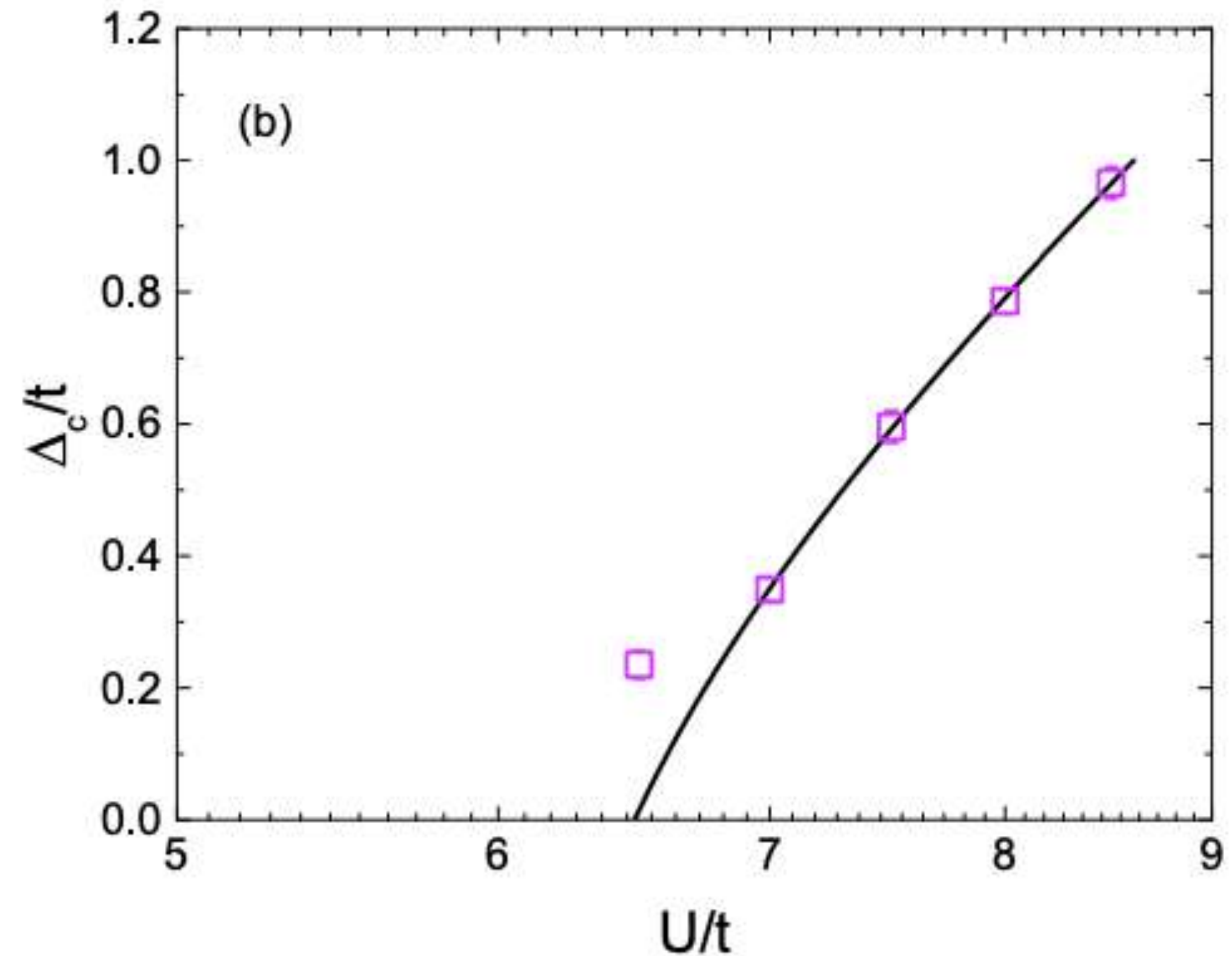
Compressibility

Kagome lattice



$$\kappa \propto e^{(-\Delta_c/k_B T)}$$

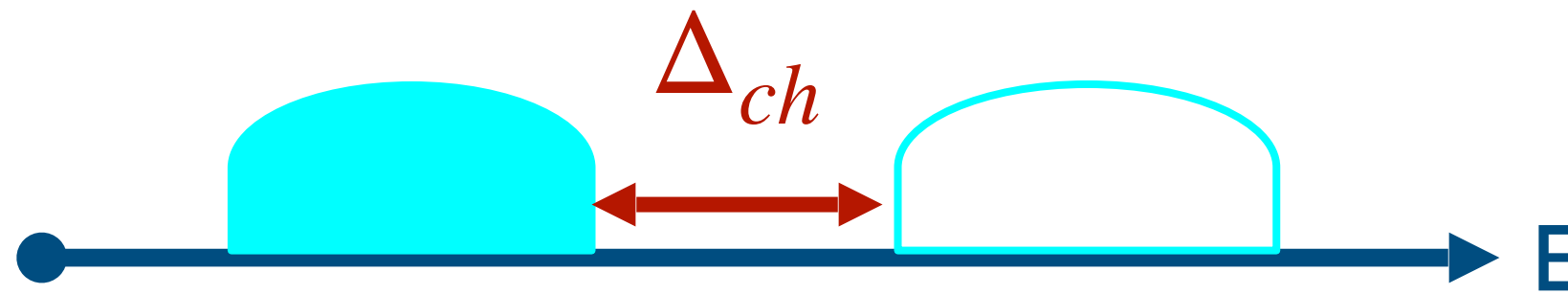
Δ_c  Charge gap



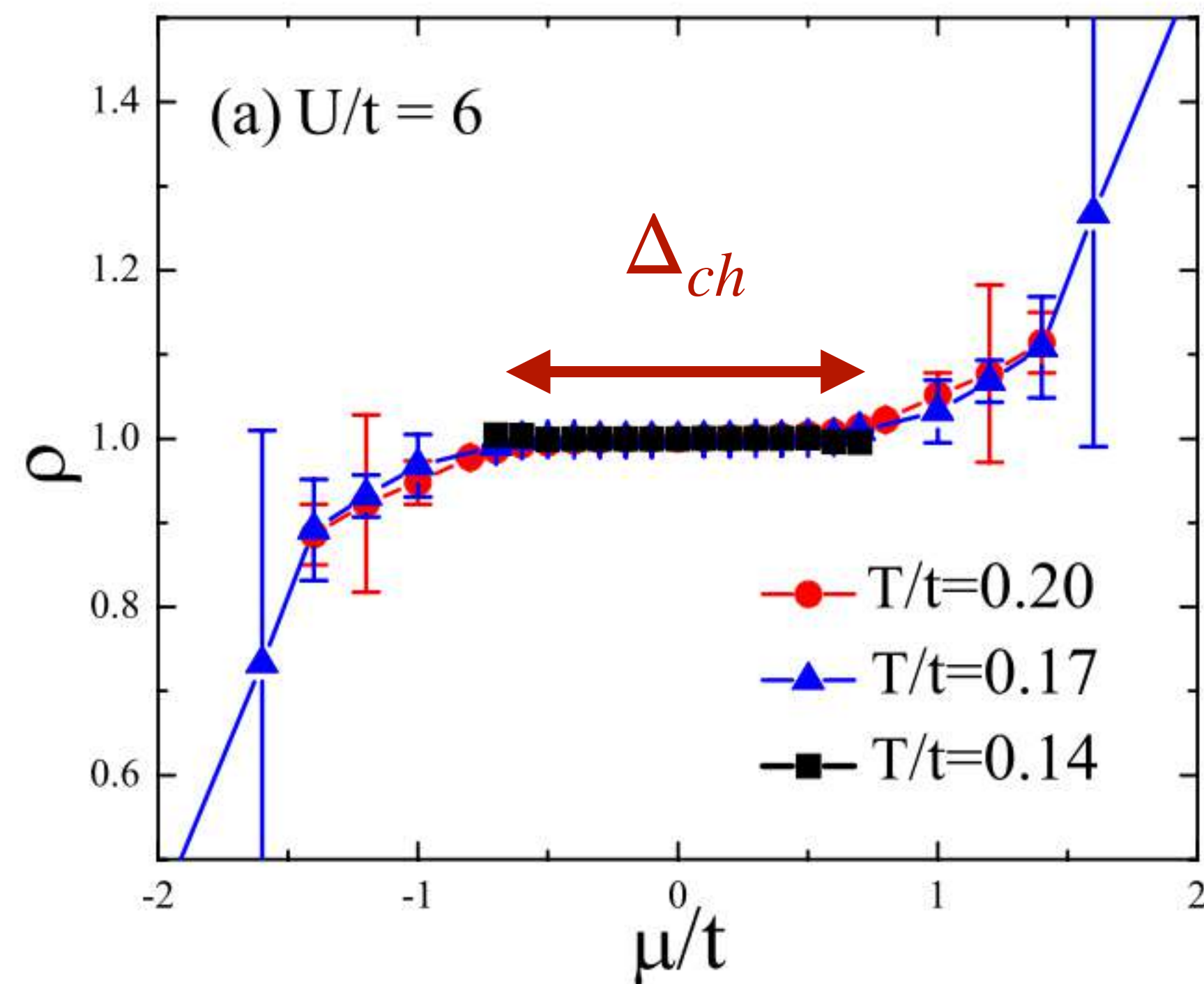
$$U_c/t = 6.5 \pm 0.1$$

PRB 2013, Medeiros-Silva et al

Charge gap

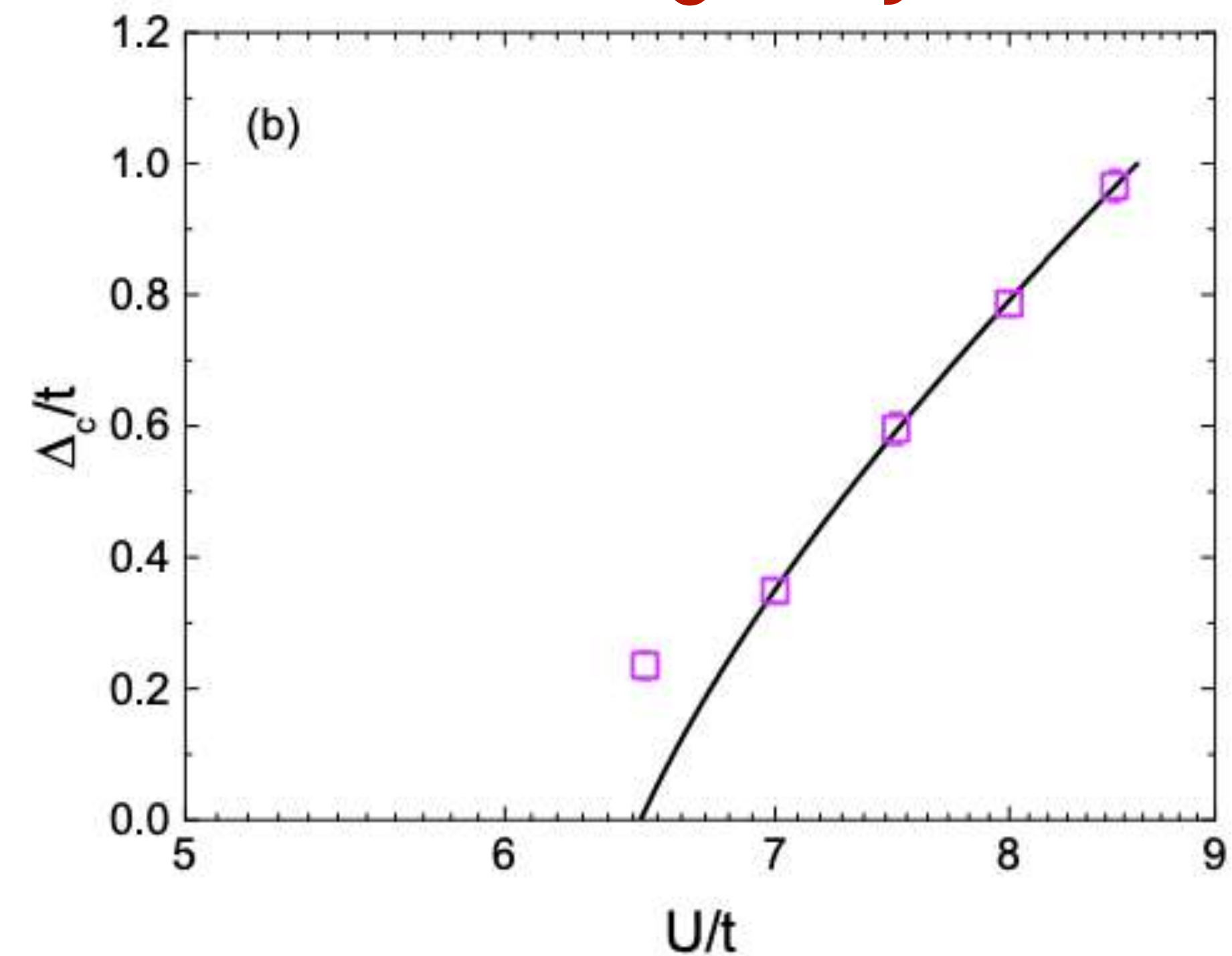


All densities



PRL 2010, Paiva et al

Half-filling only



PRB 2013, Medeiros-Silva et al

Double occupation

$$\langle D \rangle = \langle n_{i\uparrow} n_{i\downarrow} \rangle = \langle c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \rangle$$

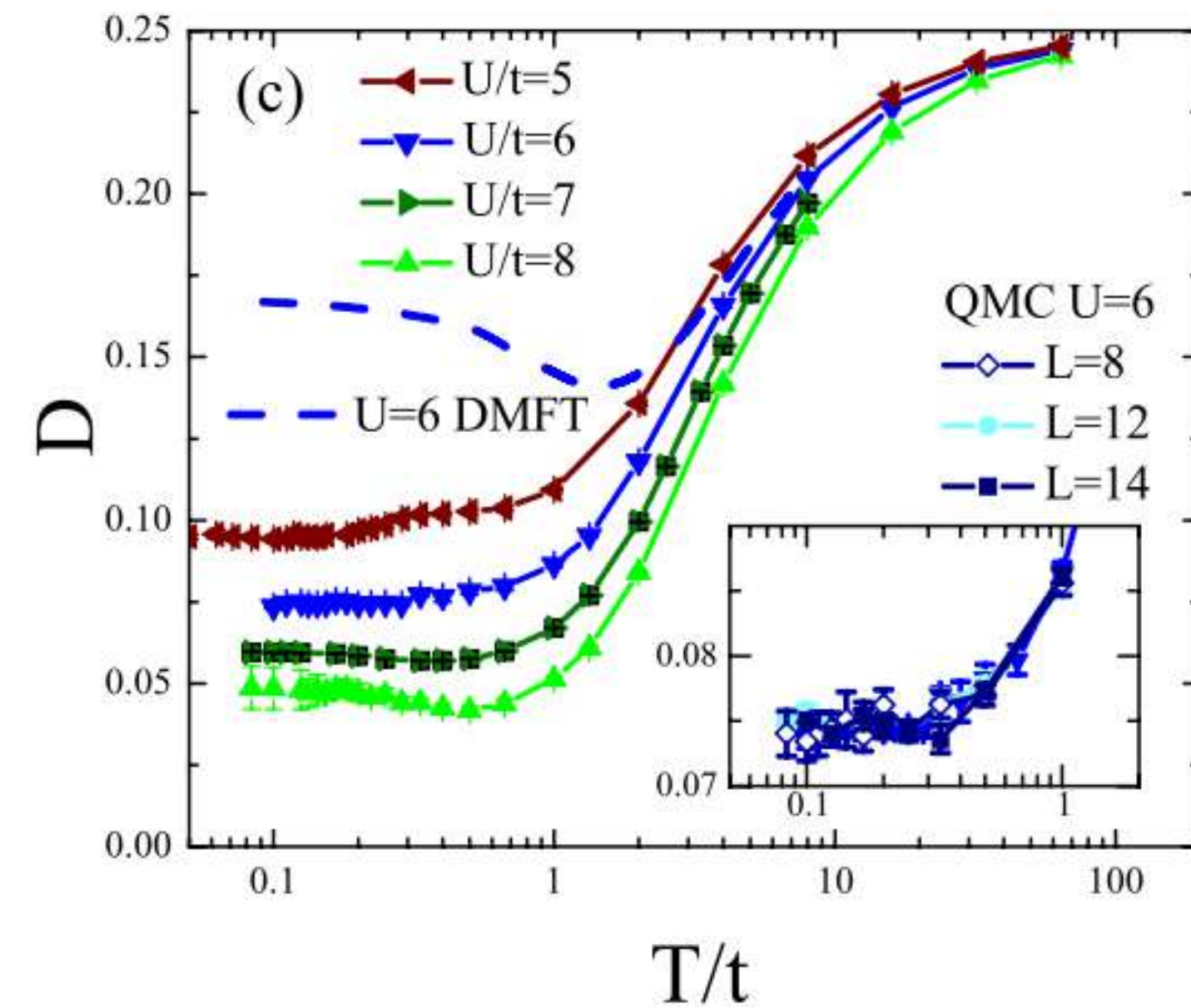
Wick's theorem



$$= \langle c_{i\uparrow}^\dagger c_{i\uparrow} \rangle \langle c_{i\downarrow}^\dagger c_{i\downarrow} \rangle$$

$$\langle D \rangle = \frac{1}{MN_s} \sum_{\mathbf{i}, \ell} \langle \langle 1 - g_{\mathbf{i}\mathbf{i}}^\uparrow(\ell) \rangle \rangle \langle \langle 1 - g_{\mathbf{i}\mathbf{i}}^\downarrow(\ell) \rangle \rangle$$

Double occupation



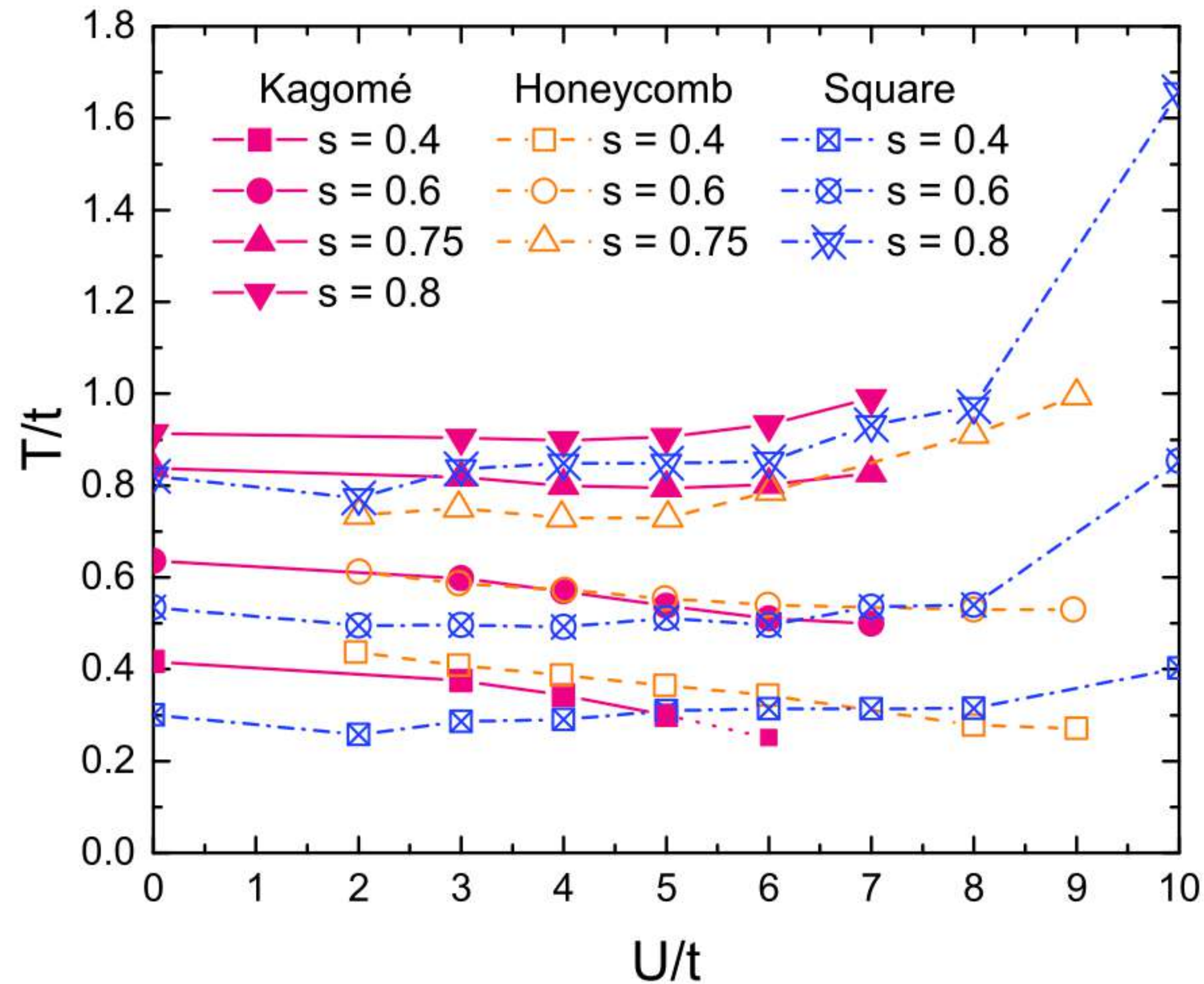
PRL 2010, Paiva et al

Maxwell relation

$$\frac{\partial S}{\partial U} = - \frac{\partial D}{\partial T}$$

Adiabatical cooling

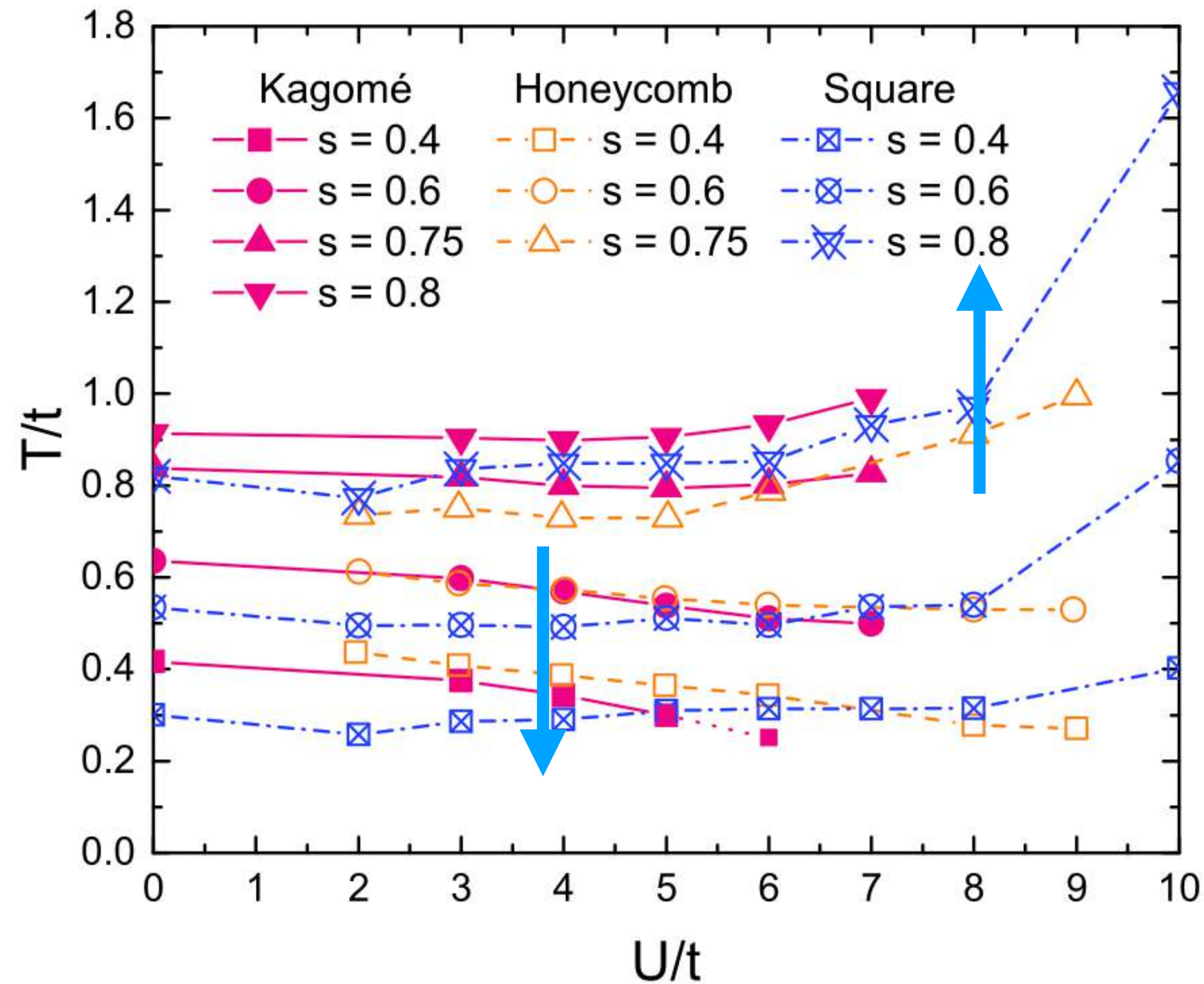
Adiabatic cooling



Important for cold
atom experiments

PRB 2023,
Medeiros-Silva et al

Adiabatic cooling



Important for cold
atom experiments

PRB 2023,
Medeiros-Silva et al

Charge correlations

$$\langle n_{\mathbf{i}} n_{\mathbf{j}} \rangle = \sum_{\sigma, \sigma'} \left[\langle \langle \tilde{g}_{\mathbf{i}\mathbf{i}}^{\sigma} \tilde{g}_{\mathbf{j}\mathbf{j}}^{\sigma'} \rangle \rangle + \delta_{\sigma\sigma'} \langle \langle \tilde{g}_{\mathbf{j}\mathbf{i}}^{\sigma} g_{\mathbf{i}\mathbf{j}}^{\sigma} \rangle \rangle \right]$$

Charge Structure factor

$$\mathcal{C}(\mathbf{q}) = \frac{1}{N_s} \sum_{\mathbf{ij}} e^{i\mathbf{q} \cdot (\mathbf{i} - \mathbf{j})} \langle n_{\mathbf{i}} n_{\mathbf{j}} \rangle$$

Charge correlations

$$\langle n_{\mathbf{i}} n_{\mathbf{j}} \rangle = \sum_{\sigma, \sigma'} \left[\langle \langle \tilde{g}_{\mathbf{ii}}^{\sigma} \tilde{g}_{\mathbf{jj}}^{\sigma'} \rangle \rangle + \delta_{\sigma\sigma'} \langle \langle \tilde{g}_{\mathbf{ji}}^{\sigma} g_{\mathbf{ij}}^{\sigma} \rangle \rangle \right]$$

Charge Structure factor

$$\mathcal{C}(\mathbf{q}) = \frac{1}{N_s} \sum_{\mathbf{ij}} e^{i\mathbf{q} \cdot (\mathbf{i} - \mathbf{j})} \langle n_{\mathbf{i}} n_{\mathbf{j}} \rangle$$

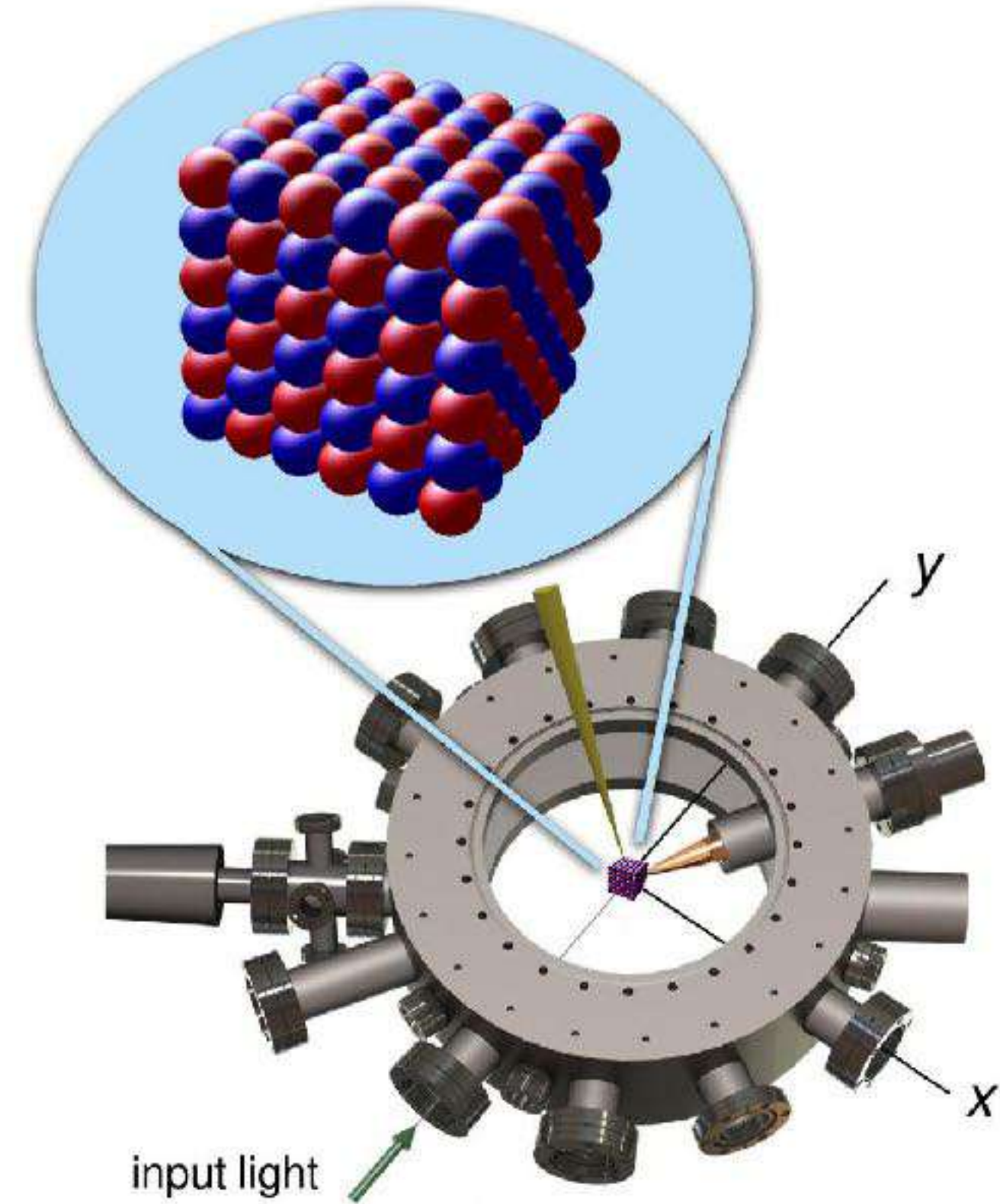
Charge susceptibility

$$\mathcal{N}(\mathbf{q}) = \frac{1}{N_s} \sum_{\mathbf{ij}} e^{i\mathbf{q} \cdot (\mathbf{i} - \mathbf{j})} \int_0^{\beta} d\tau \langle n_{\mathbf{i}}(\tau) n_{\mathbf{j}} \rangle,$$

Unequal time correlations

$$\begin{aligned} \langle n_{\mathbf{i}}(\ell_1) n_{\mathbf{j}}(\ell_2) \rangle = \sum_{\sigma, \sigma'} & \left[\langle \langle \tilde{g}_{\mathbf{ii}}^{\sigma}(\ell_1) \tilde{g}_{\mathbf{jj}}^{\sigma'}(\ell_2) \rangle \rangle + \right. \\ & \left. + \delta_{\sigma\sigma'} \langle \langle \tilde{G}_{\mathbf{ji}}^{\sigma}(\ell_1; \ell_2) G_{\mathbf{ij}}^{\sigma}(\ell_1; \ell_2) \rangle \rangle \right]; \end{aligned}$$

Spin correlation functions



Magnetic correlations

Components of the magnetization operator

$$m_{\mathbf{i}}^x \equiv c_{\mathbf{i}\uparrow}^\dagger c_{\mathbf{i}\downarrow} + c_{\mathbf{i}\downarrow}^\dagger c_{\mathbf{i}\uparrow},$$

$$m_{\mathbf{i}}^y \equiv -i \left(c_{\mathbf{i}\uparrow}^\dagger c_{\mathbf{i}\downarrow} - c_{\mathbf{i}\downarrow}^\dagger c_{\mathbf{i}\uparrow} \right)$$

$$m_{\mathbf{i}}^z \equiv n_{\mathbf{i}\uparrow} - n_{\mathbf{i}\downarrow}$$

Magnetic correlations

Components of the magnetization operator

$$S_i^x = c_{i\downarrow}^\dagger c_{i\uparrow} + c_{i\uparrow}^\dagger c_{i\downarrow}$$

$$S_i^y = -ic_{i\downarrow}^\dagger c_{i\uparrow} + ic_{i\uparrow}^\dagger c_{i\downarrow}$$

$$S_i^z = n_{i,\uparrow} - n_{i,\downarrow}$$

Wick's theorem

$$\langle S_i^z S_j^z \rangle = \langle \langle \tilde{g}_{ii}^\uparrow \tilde{g}_{jj}^\uparrow + \tilde{g}_{ij}^\uparrow g_{ij}^\uparrow - \tilde{g}_{ii}^\uparrow \tilde{g}_{jj}^\downarrow - \tilde{g}_{ii}^\downarrow \tilde{g}_{jj}^\uparrow + \tilde{g}_{ii}^\downarrow \tilde{g}_{jj}^\downarrow + \tilde{g}_{ij}^\downarrow g_{ij}^\downarrow \rangle \rangle,$$

Magnetic correlations

Components of the magnetization operator

$$S_i^x = c_{i\downarrow}^\dagger c_{i\uparrow} + c_{i\uparrow}^\dagger c_{i\downarrow}$$

$$S_i^y = -i c_{i\downarrow}^\dagger c_{i\uparrow} + i c_{i\uparrow}^\dagger c_{i\downarrow}$$

$$S_i^z = n_{i,\uparrow} - n_{i,\downarrow}$$

Wick's theorem

$$\langle S_i^z S_j^z \rangle = \langle \langle \tilde{g}_{ii}^\uparrow \tilde{g}_{jj}^\uparrow + \tilde{g}_{ij}^\uparrow g_{ij}^\uparrow - \tilde{g}_{ii}^\uparrow \tilde{g}_{jj}^\downarrow - \tilde{g}_{ii}^\downarrow \tilde{g}_{jj}^\uparrow + \tilde{g}_{ii}^\downarrow \tilde{g}_{jj}^\downarrow + \tilde{g}_{ij}^\downarrow g_{ij}^\downarrow \rangle \rangle,$$

$$\langle S_i^x S_j^x \rangle = \langle \langle \tilde{g}_{ij}^\uparrow g_{ij}^\downarrow + \tilde{g}_{ij}^\downarrow g_{ij}^\uparrow \rangle \rangle$$

Magnetic correlations

Components of the magnetization operator

$$S_i^x = c_{i\downarrow}^\dagger c_{i\uparrow} + c_{i\uparrow}^\dagger c_{i\downarrow}$$

$$S_i^y = -ic_{i\downarrow}^\dagger c_{i\uparrow} + ic_{i\uparrow}^\dagger c_{i\downarrow}$$

$$S_i^z = n_{i,\uparrow} - n_{i,\downarrow}$$

Local moment

$$\langle m_i^2 \rangle = \langle (m_i^x)^2 + (m_i^y)^2 + (m_i^z)^2 \rangle$$

$$\langle (m_i^z)^2 \rangle = \langle S_i^z S_i^z \rangle$$

Wick's theorem

$$\langle S_i^z S_j^z \rangle = \langle \langle \tilde{g}_{ii}^\uparrow \tilde{g}_{jj}^\uparrow + \tilde{g}_{ij}^\uparrow g_{ij}^\uparrow - \tilde{g}_{ii}^\uparrow \tilde{g}_{jj}^\downarrow - \tilde{g}_{ii}^\downarrow \tilde{g}_{jj}^\uparrow + \tilde{g}_{ii}^\downarrow \tilde{g}_{jj}^\downarrow + \tilde{g}_{ij}^\downarrow g_{ij}^\downarrow \rangle \rangle,$$

$$\langle S_i^x S_j^x \rangle = \langle \langle \tilde{g}_{ij}^\uparrow g_{ij}^\downarrow + \tilde{g}_{ij}^\downarrow g_{ij}^\uparrow \rangle \rangle$$

Magnetic structure factor

$$S(\mathbf{q}) = \frac{1}{N_s} \sum_{\mathbf{ij}} e^{i\mathbf{q} \cdot (\mathbf{i} - \mathbf{j})} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$$

Unequal time Magnetic correlations

Susceptibility

$$\chi(\mathbf{q}) = \frac{1}{N_s} \sum_{\mathbf{ij}} e^{i\mathbf{q} \cdot (\mathbf{i} - \mathbf{j})} \int_0^\beta d\tau \langle \mathbf{S}_{\mathbf{i}}(\tau) \cdot \mathbf{S}_{\mathbf{j}} \rangle$$

$$\begin{aligned} \langle S_{\mathbf{i}}^z(\ell_1) S_{\mathbf{j}}^z(\ell_2) \rangle &= \sum_{\sigma, \sigma'} \left[(2\delta_{\sigma\sigma'} - 1) \langle \langle \tilde{g}_{\mathbf{ii}}^\sigma(\ell_1) \tilde{g}_{\mathbf{jj}}^{\sigma'}(\ell_2) \rangle \rangle \right. \\ &\quad \left. + \delta_{\sigma\sigma'} \langle \langle \tilde{G}_{\mathbf{ij}}^\sigma(\ell_1; \ell_2) G_{\mathbf{ij}}^\sigma(\ell_1; \ell_2) \rangle \rangle \right]. \end{aligned}$$

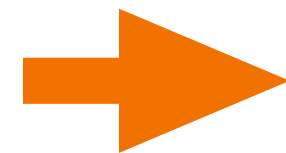
Mermin-Wagner Theorem

$$d \leq 2$$

2d systems

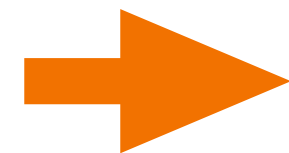
components of the order parameter $\rightarrow n$

$$d > n$$



$$T_c \neq 0$$

$$d < n$$

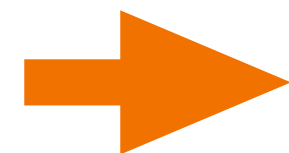


$$T_c = 0$$

SU(2)

half-filling, spin balanced $\mu = 0$ and $h = 0$

$$d = n$$



$$T_{KT} \neq 0$$

$$\left\{ \begin{array}{ll} -U & \mu \neq 0 \rightarrow n \neq 1 \\ +U & h \neq 0 \rightarrow P \neq 1 \end{array} \right.$$

Superfluid

anisotropic AF

Antiferromagnetism

3D → $T_{Neel} \neq 0$

2D → $T_{Neel} = 0$

Early results

Square lattice

PHYSICAL REVIEW B

VOLUME 31, NUMBER 7

1 APRIL 1985

Two-dimensional Hubbard model: Numerical simulation study

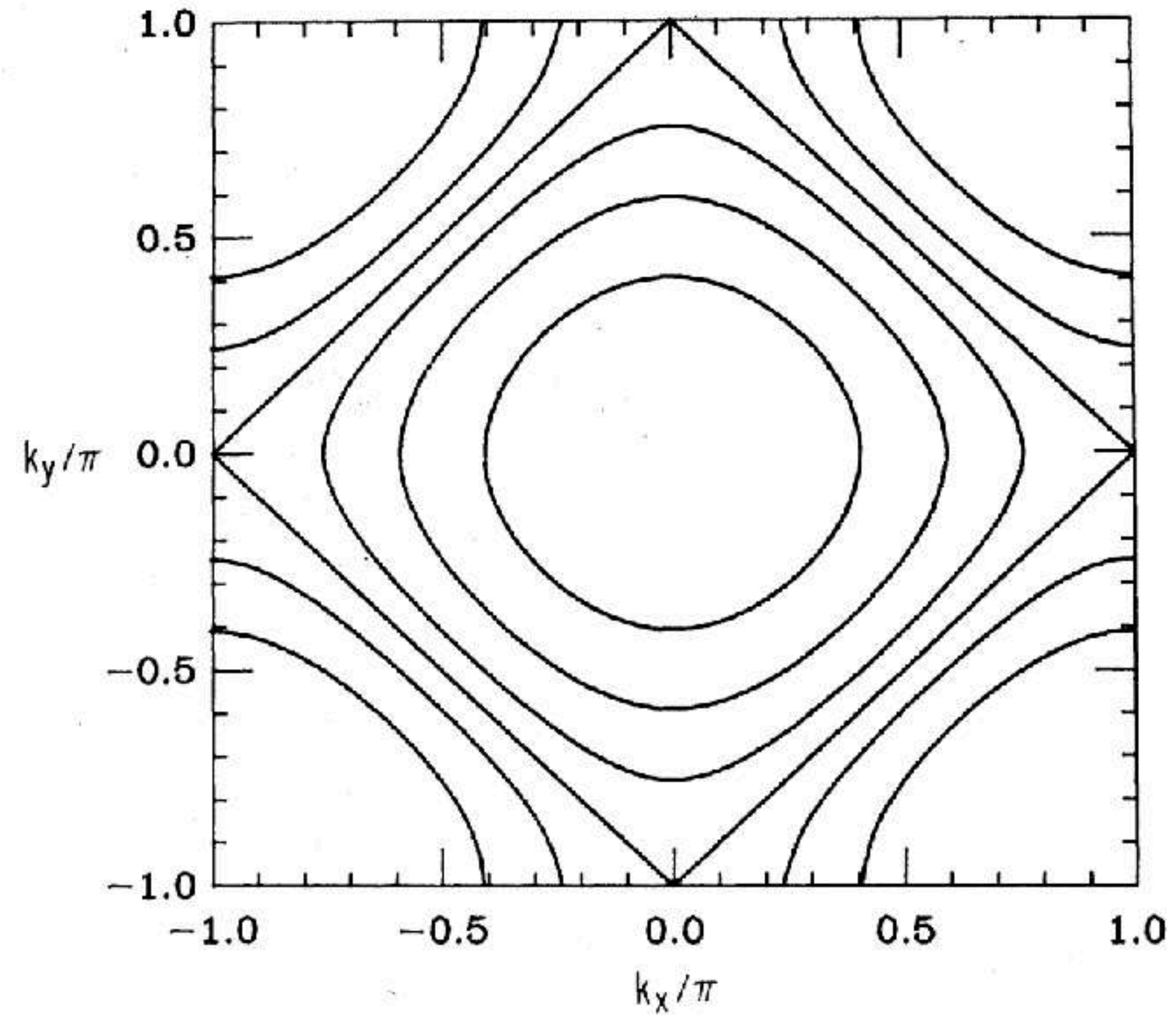
J. E. Hirsch

Department of Physics, University of California, San Diego, La Jolla, California 92093

(Received 1 October 1984)

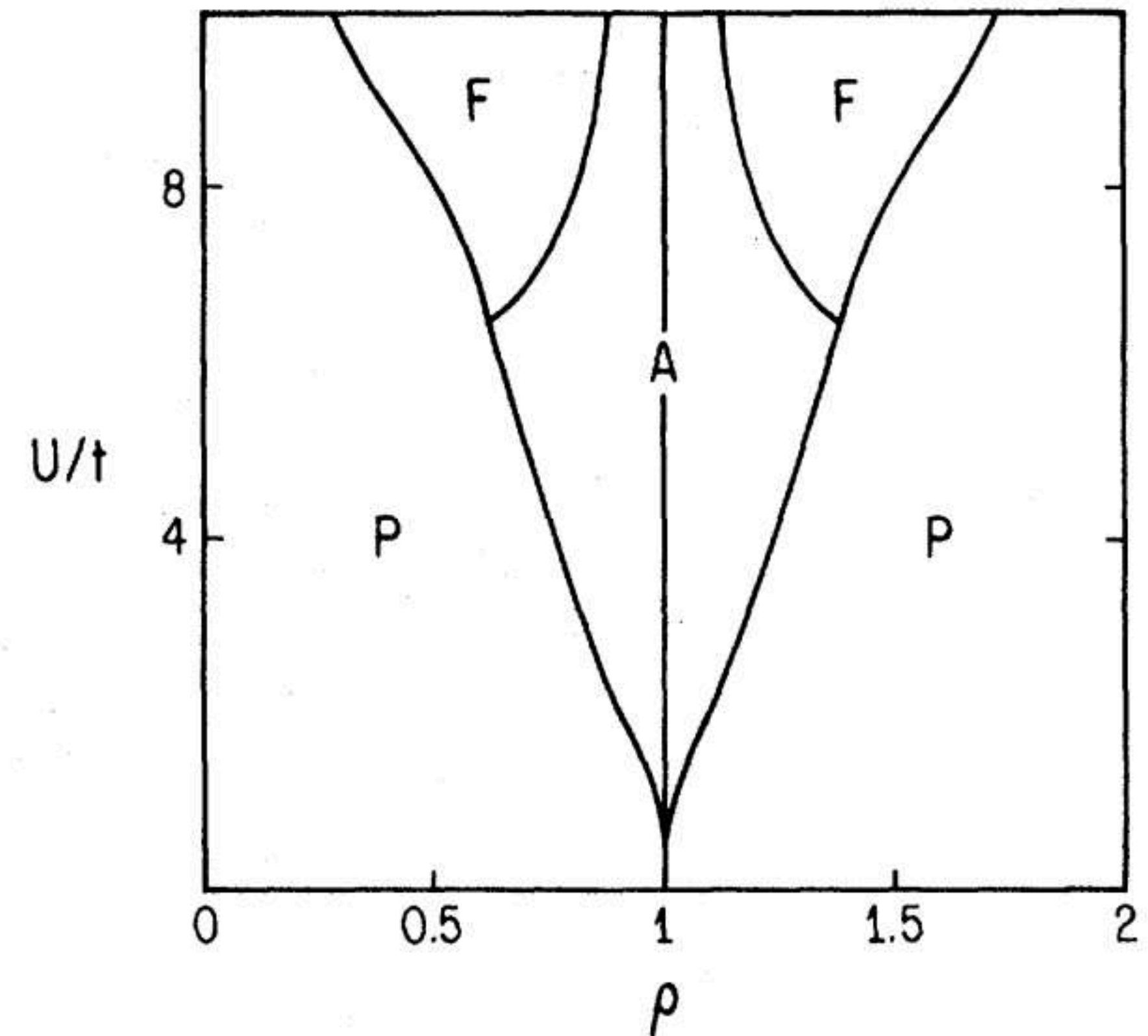
We have studied the two-dimensional Hubbard model on a square lattice with nearest-neighbor hopping. We first discuss the properties of the model within the mean-field approximation: Because of the form of the band structure, some peculiar features are found. We then discuss the simulation algorithm used and compare simulation results with exact results for 6-site chains to test the reliability of the approach. We present results for thermodynamic properties and correlation functions for lattices up to 8×8 in spatial size. The system is found to be an antiferromagnetic insulator for all values of the coupling constant at zero temperature in the half-filled-band case, but the long-range order is much smaller than predicted by mean-field theory. We perform a finite-size-scaling analysis to determine the character of the transition at zero coupling. For non-half-filled-band cases, our results suggest that the system is always paramagnetic, in contradiction with Hartree-Fock predictions. The system does not show tendency to ferromagnetism nor triplet superconductivity in the parameter range studied. We also discuss some properties of the attractive Hubbard model in the half-filled-band case.

Nesting of the Fermi surface



PRB 1985, Hirsch

Hartree-Fock phase diagram



Local moment for the square lattice System sizes, temperature, U

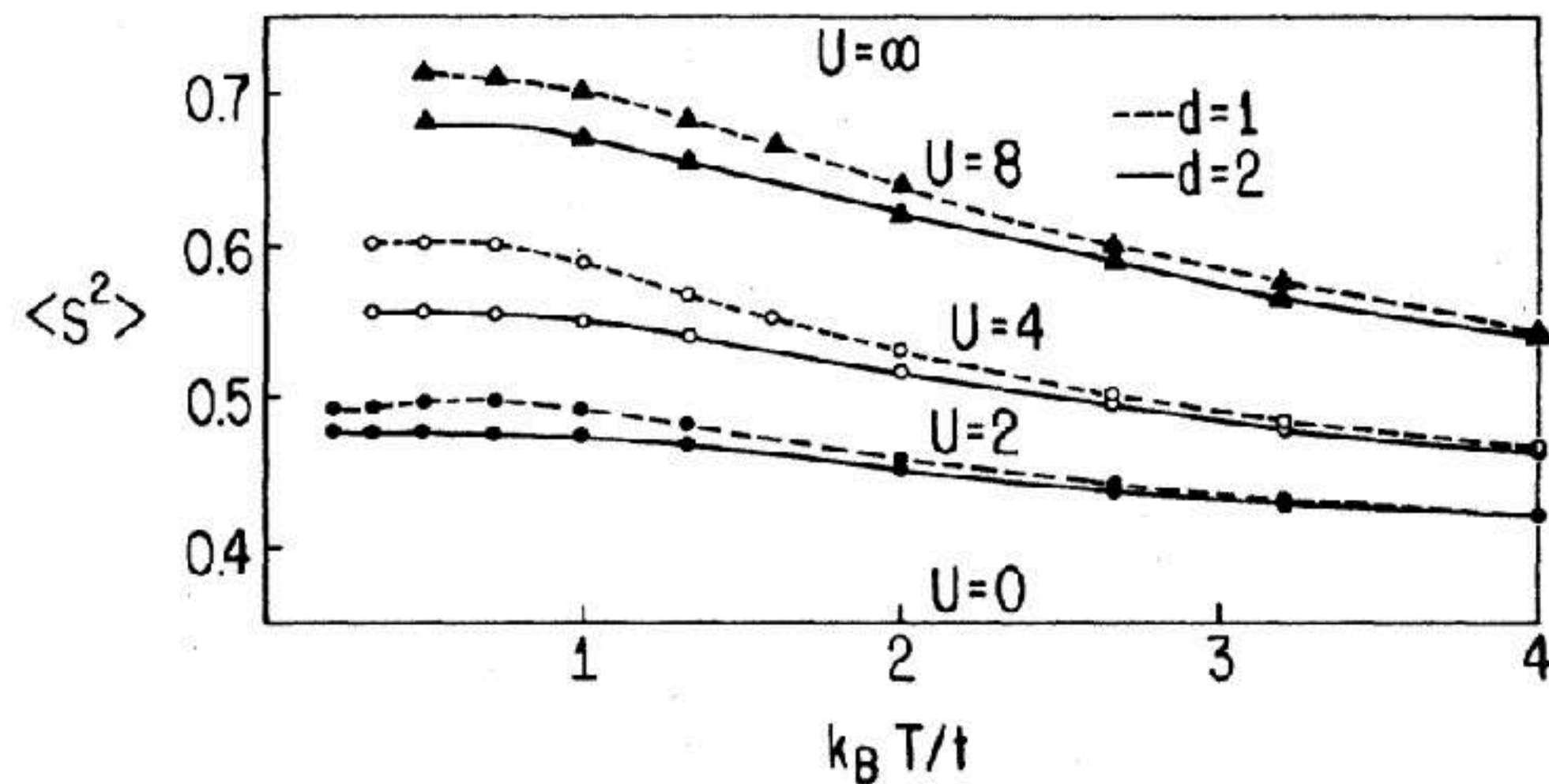
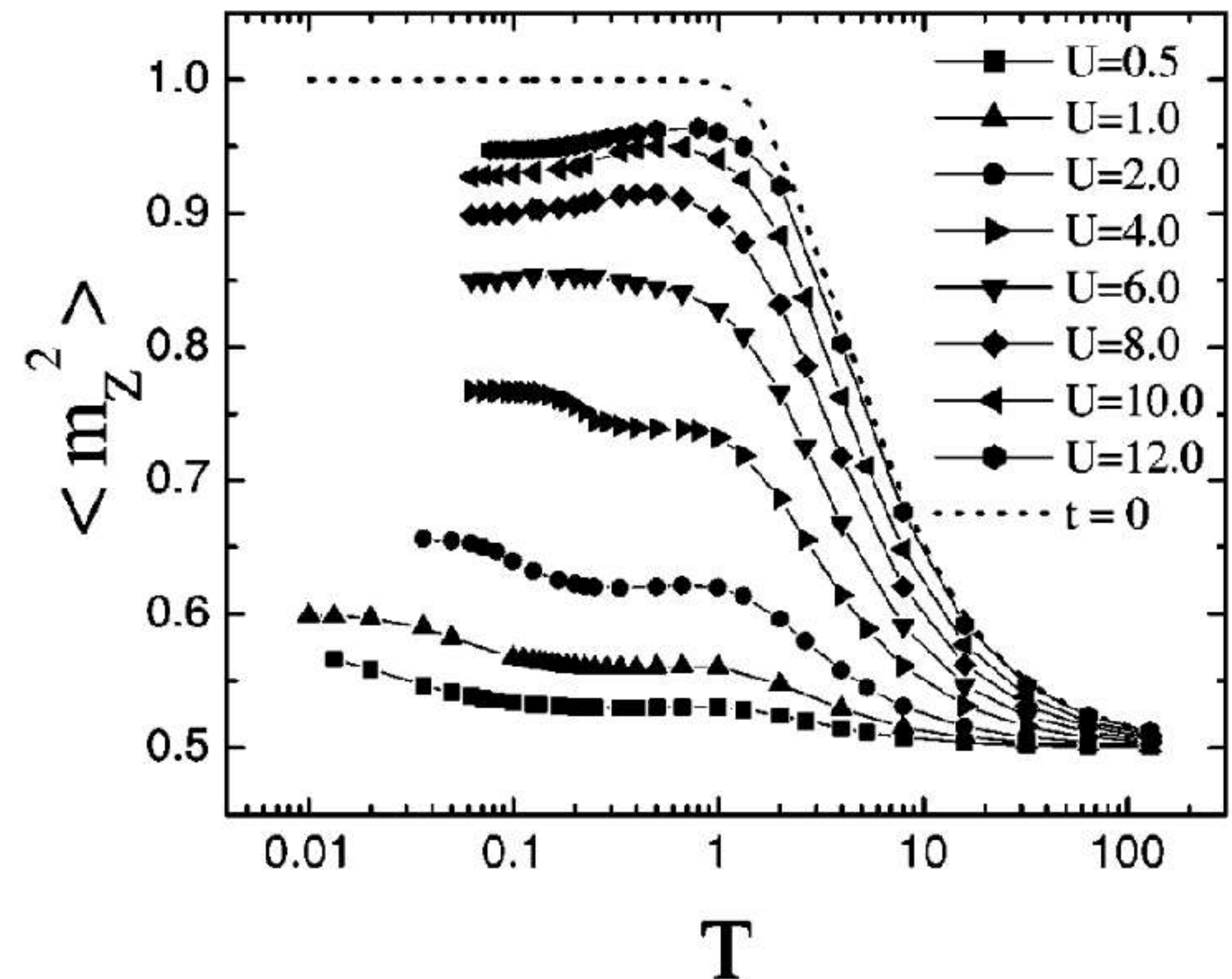


FIG. 6. Local magnetic moment versus temperature on a 6×6 two-dimensional lattice and a 6-site one-dimensional lattice.

PRB 1985, Hirsch



PRB 2001, Paiva et al

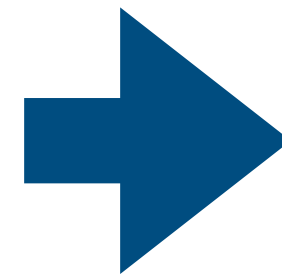
Lower T , larger system sizes, larger U s

Better computers

Lower T, larger system sizes, larger Us

Better computers

Reducing low T instabilities

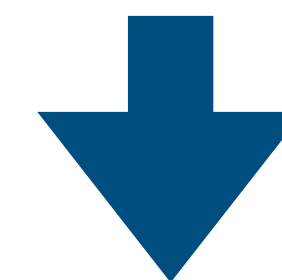


Green's function iterated

$\ell \sim 10$

$\beta > 4$ Green's function iterated at every slice

Ill conditioned matrices

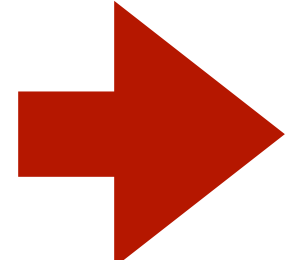


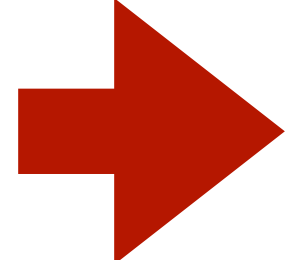
Matrix decomposition stabilization

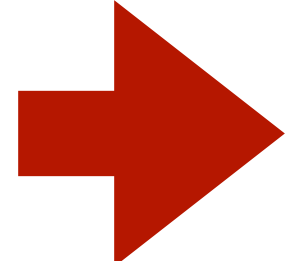
Matrix decomposition stabilization

Graham–Schmidt orthogonalization

$$\tilde{A}_1^\sigma(\ell) = U_1^\sigma D_1^\sigma R_1^\sigma$$

U_1^σ  Well conditioned orthogonal matrix

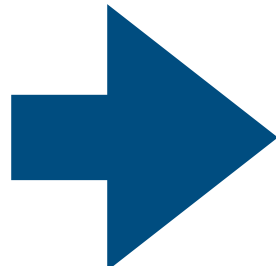
D_1^σ  Diagonal matrix

R_1^σ  Well conditioned right triangular matrix

Lower T , larger system sizes, larger U_s

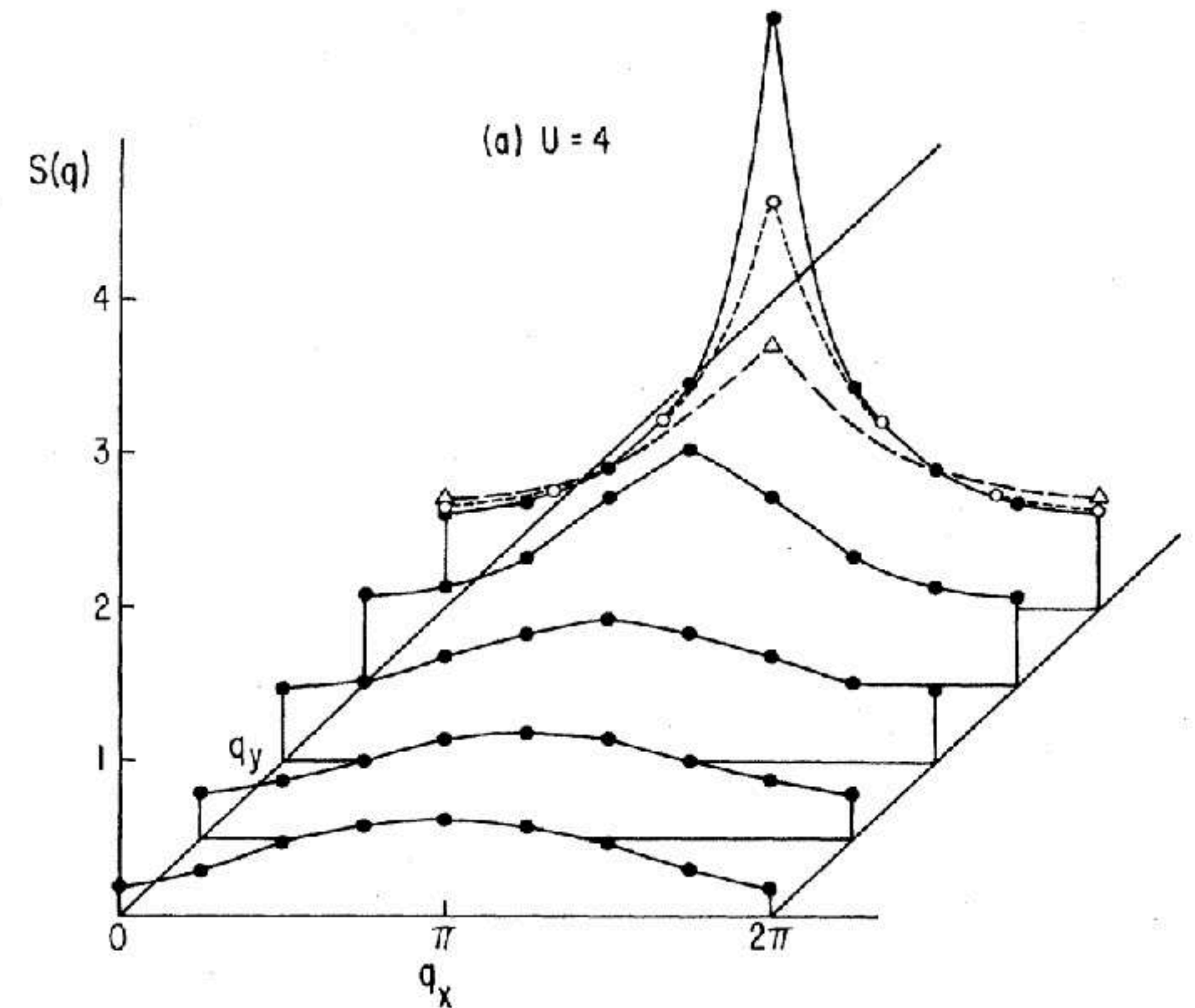
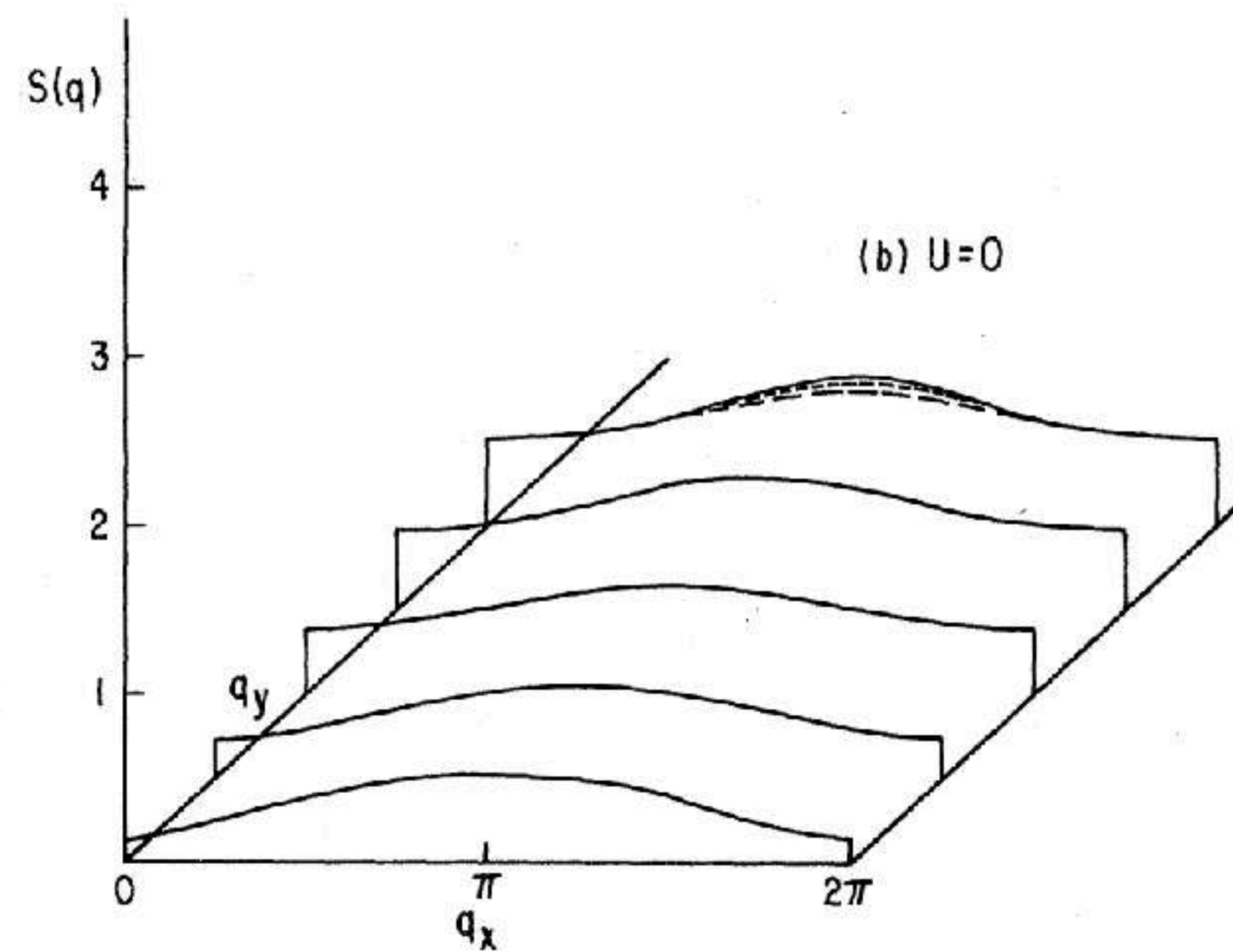
Better computers

Reducing low T instabilities

Reaching larger U_s at low T  Global moves

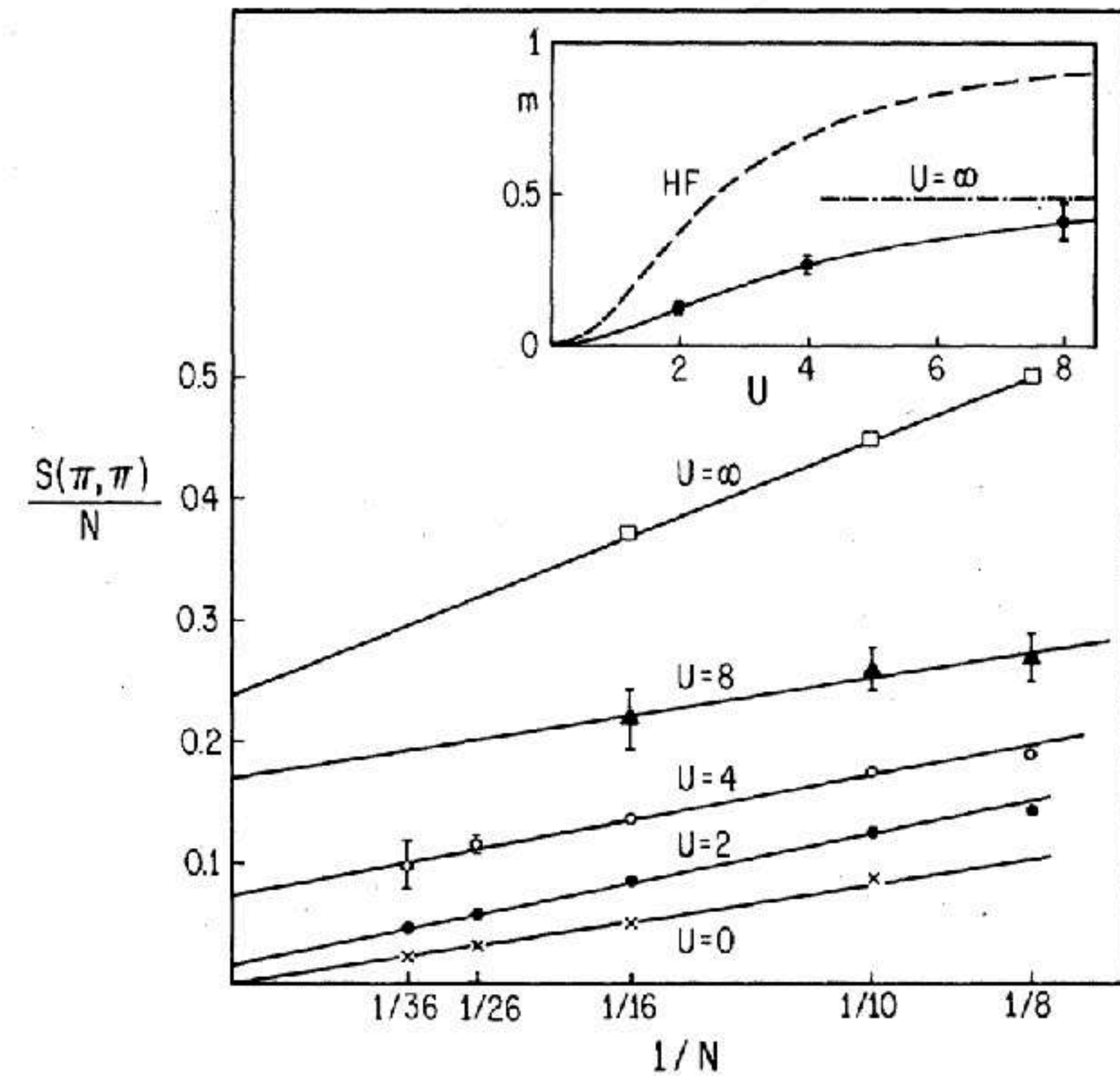
Magnetic structure factor

$$S(\mathbf{q}) = \frac{1}{N_s} \sum_{\mathbf{ij}} e^{i\mathbf{q} \cdot (\mathbf{i} - \mathbf{j})} \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$$

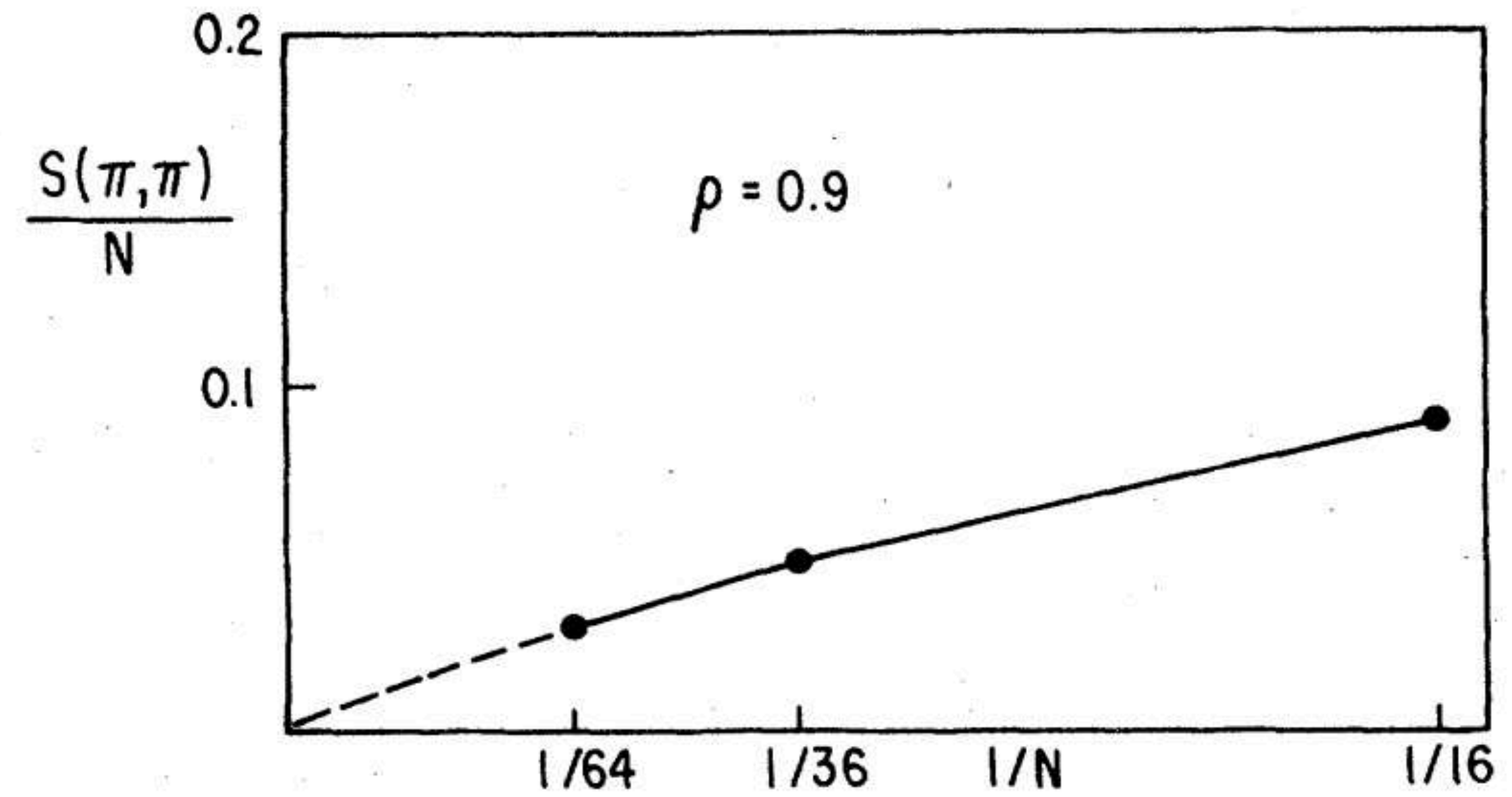


PRB 1985, Hirsch

$n=1$

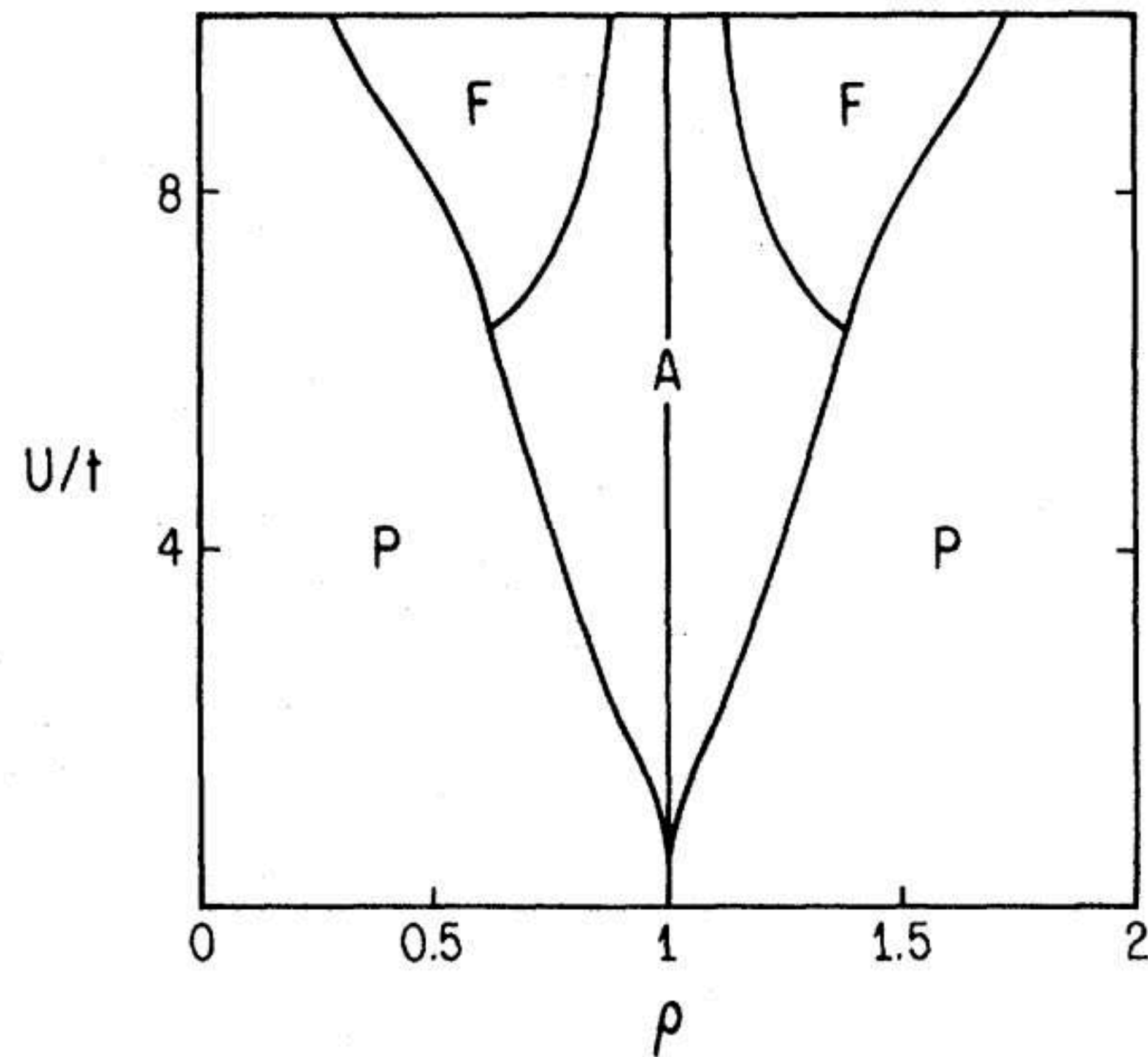


$n=0.9$

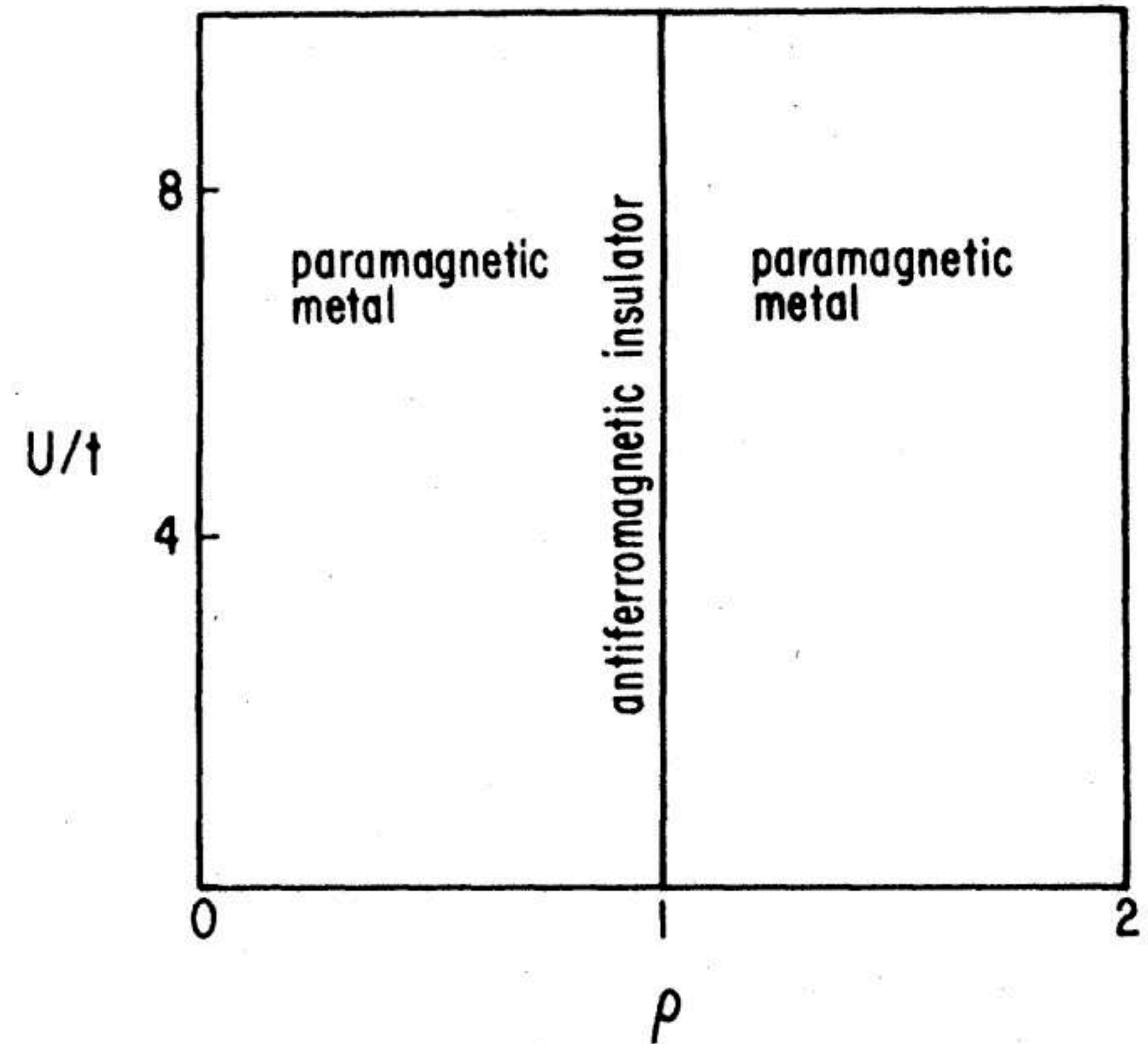


PRB 1985, Hirsch

PRB 1985, Hirsch



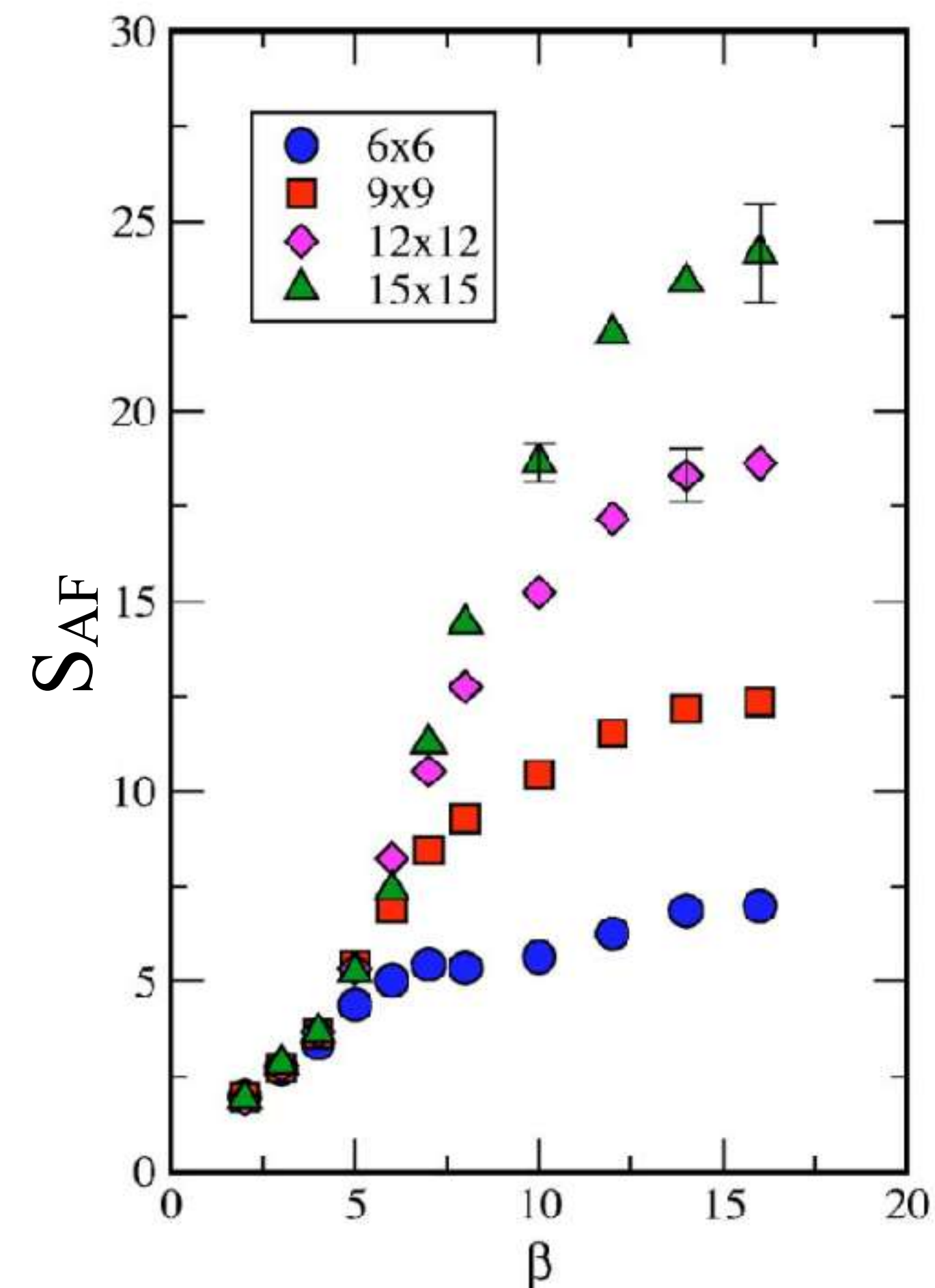
Hartree-Fock phase diagram



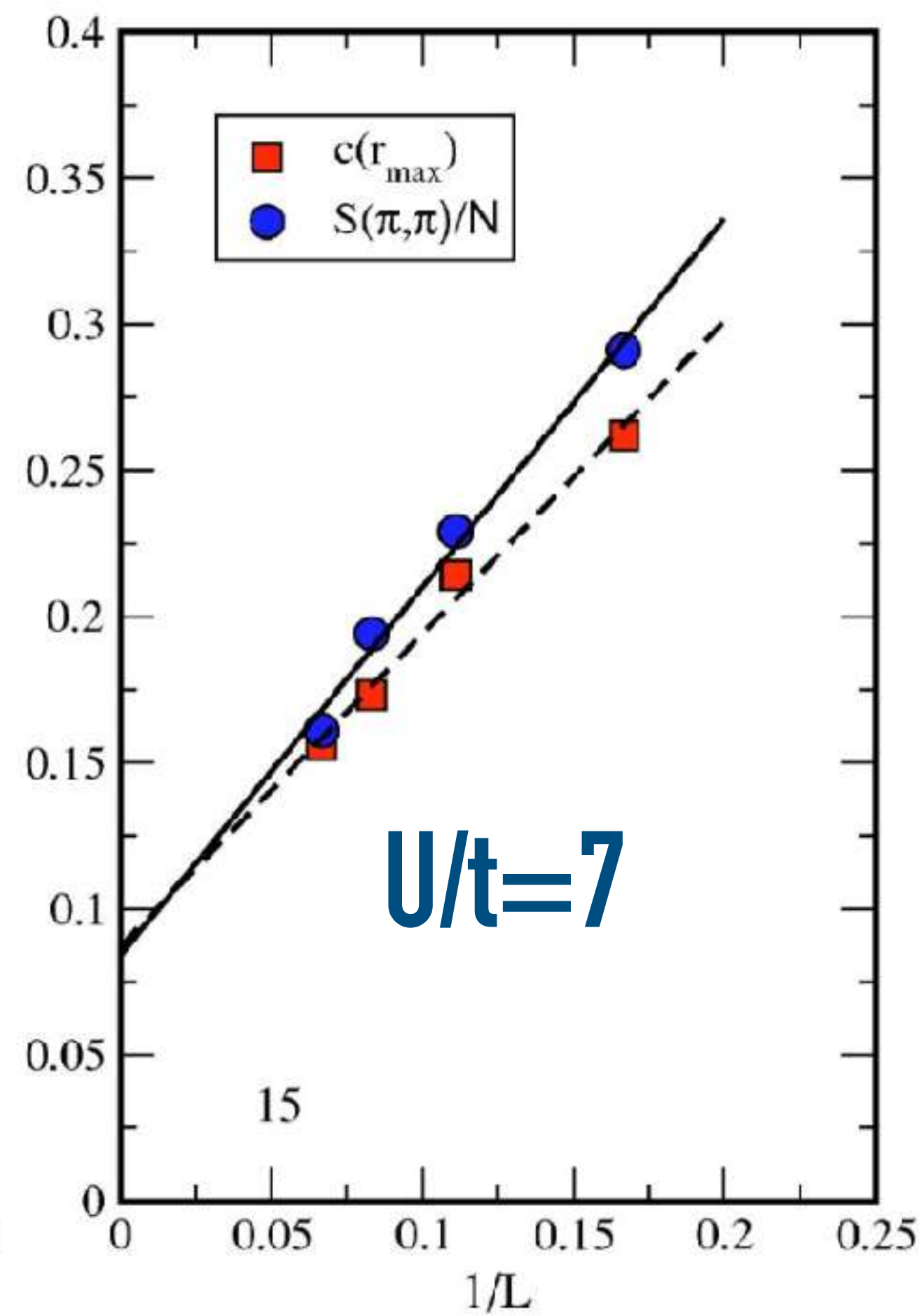
Conjectured QMC phase diagram

Honeycomb lattice

Looking for long-range-order



PRB 2005, Paiva et al

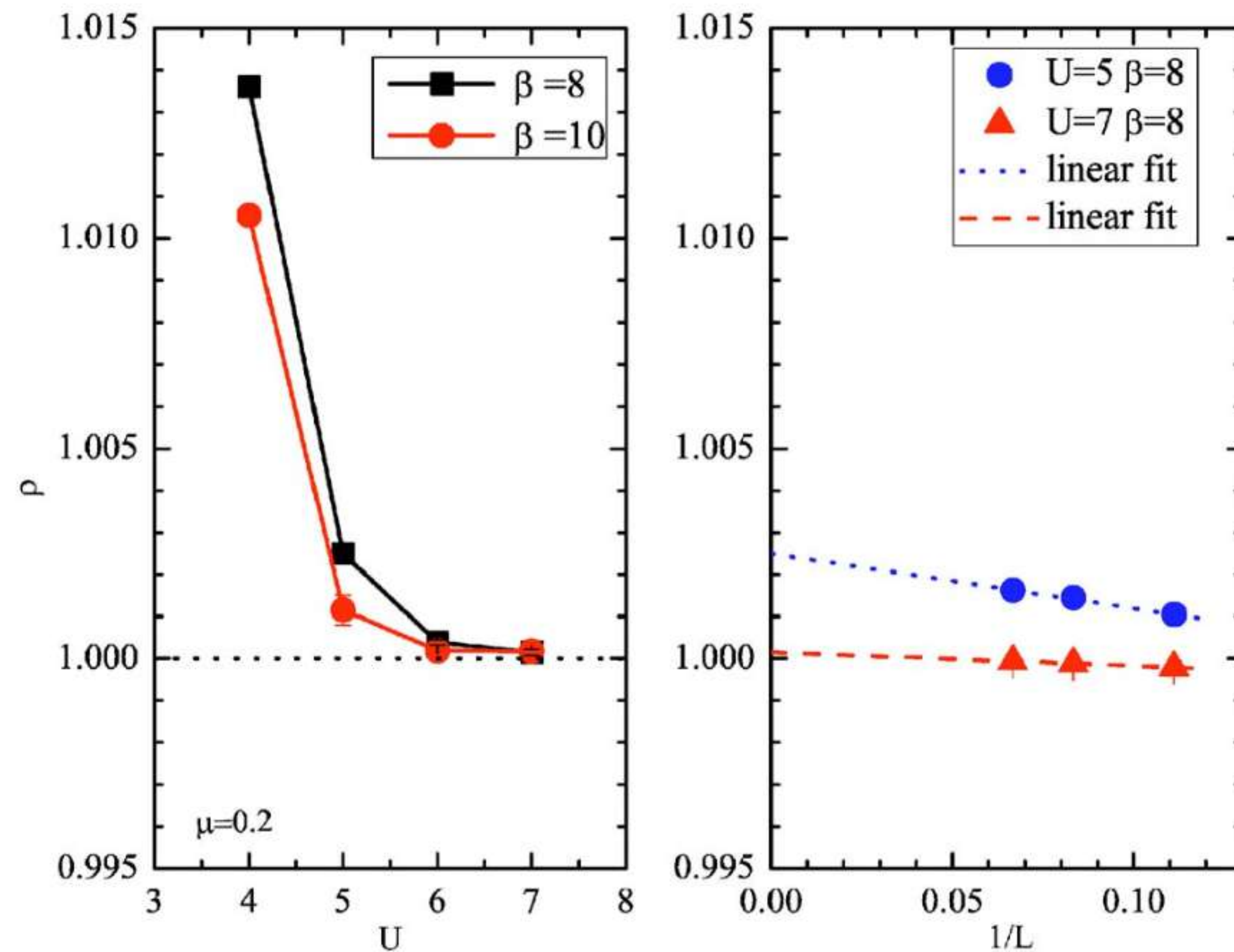


$$S(\mathbf{q}) = \frac{1}{N_s} \sum_{\mathbf{ij}} e^{i\mathbf{q} \cdot (\mathbf{i} - \mathbf{j})} \langle \mathbf{S}_{\mathbf{i}} \cdot \mathbf{S}_{\mathbf{j}} \rangle$$

$$\frac{1}{N} S(\mathbf{q}) = \frac{M^2}{3} + \frac{a}{L},$$

$M \neq 0 \rightarrow \text{LRO}$

Density



PRB 2005, Paiva et al

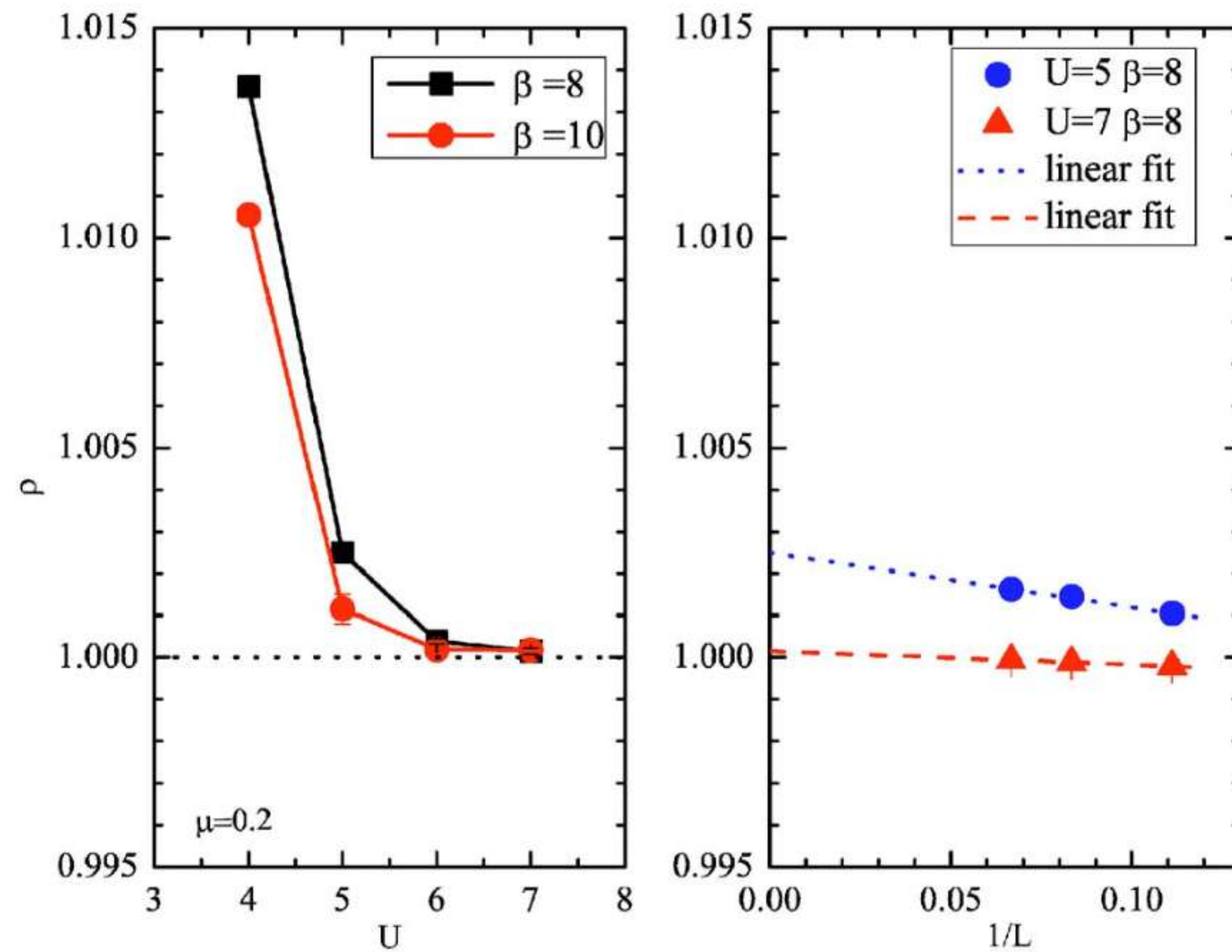
Honeycomb lattice

Used to determine Mott transition

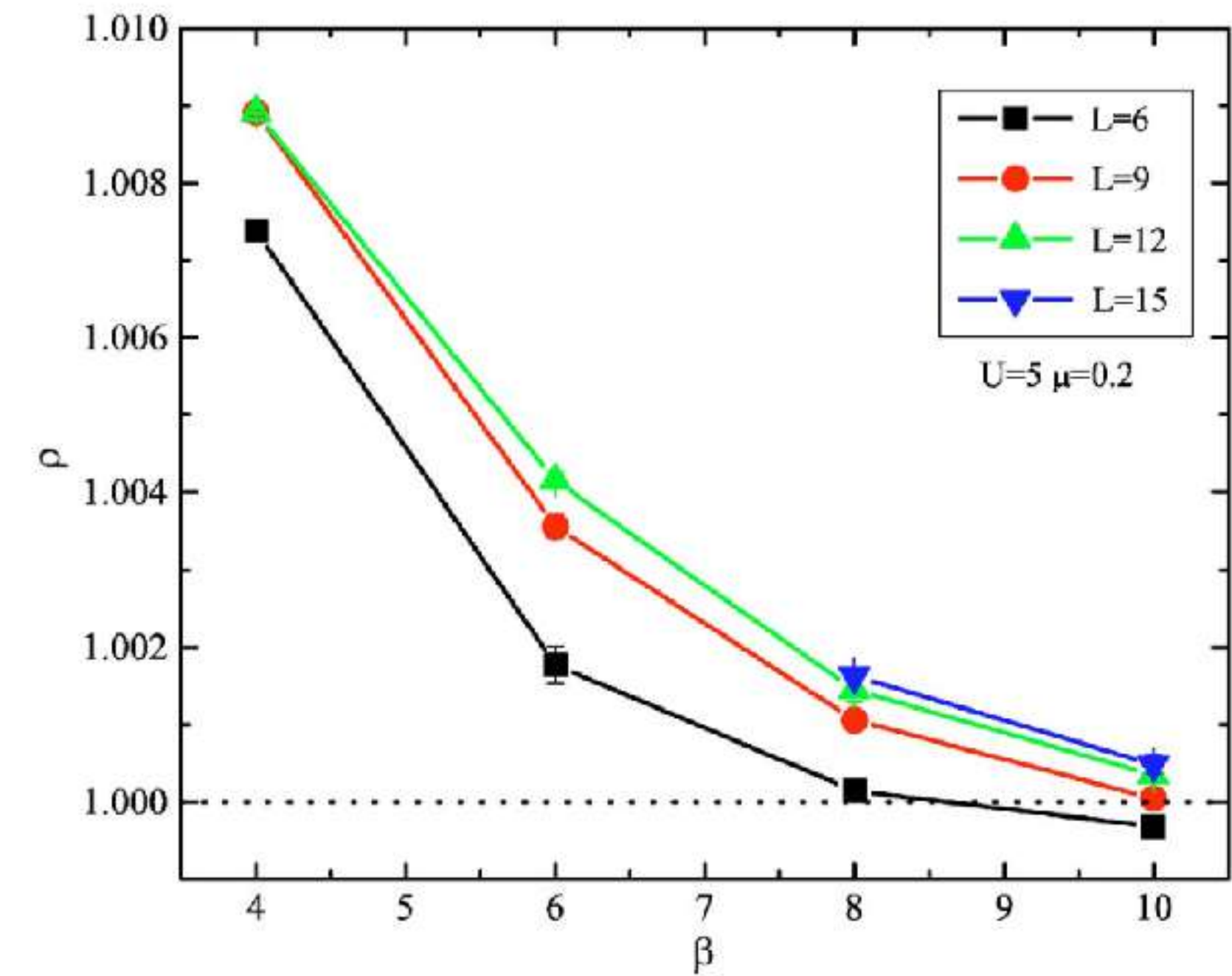
U , size, temperature

$$U_c/t \simeq 3.8$$

Density



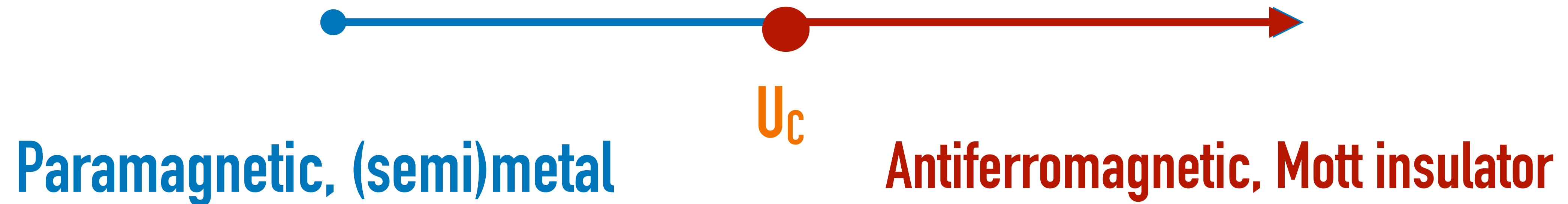
Honeycomb lattice



PRB 2005, Paiva et al

Numerical data to determine a Quantum Phase Transition

Hubbard model on a Honeycomb lattice



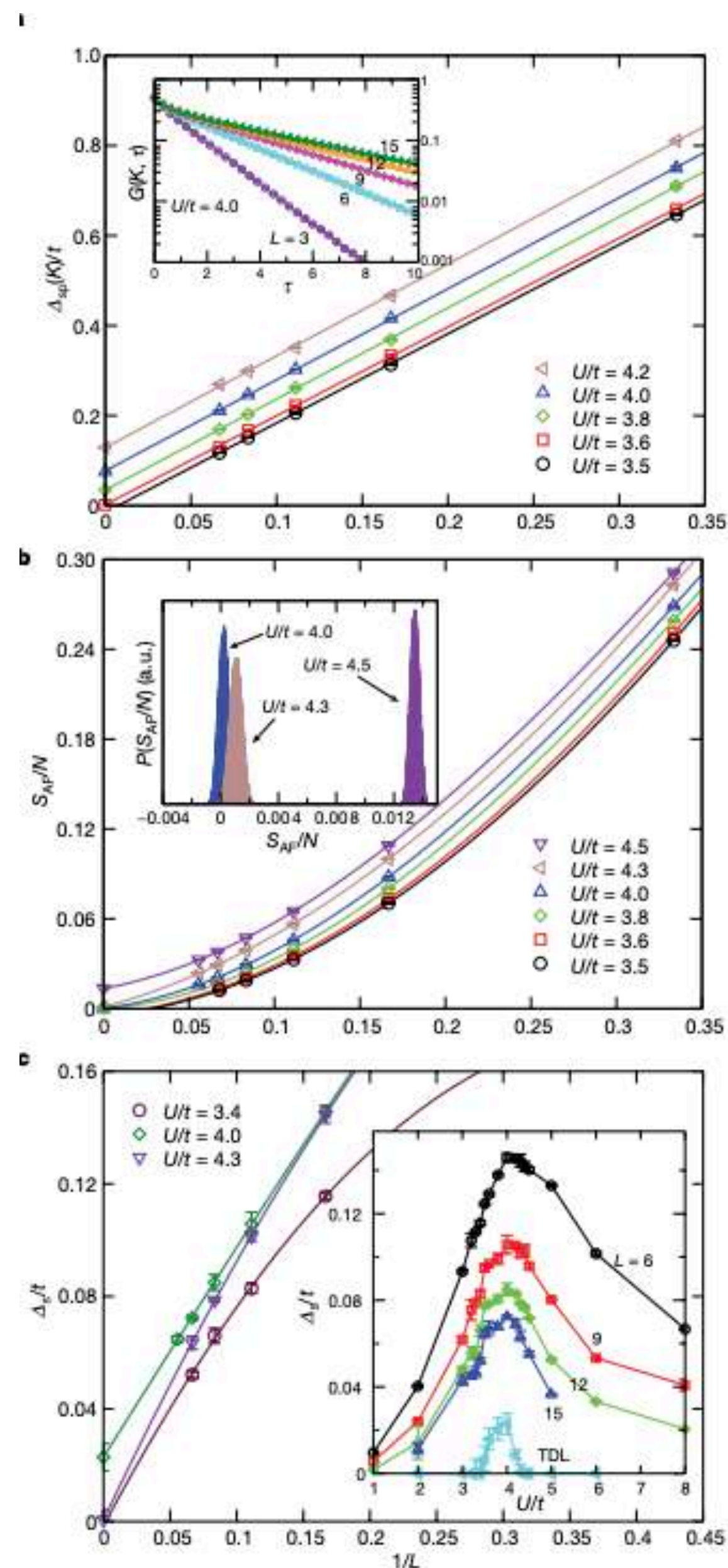
Size effects

ARTICLES

Quantum spin liquid emerging in two-dimensional correlated Dirac fermions

Z. Y. Meng¹, T. C. Lang², S. Wessel¹, F. F. Assaad² & A. Muramatsu¹

Figure 2 | Finite-size extrapolations of the excitation gaps and the antiferromagnetic structure factor. **a**, The single-particle gap at the Dirac point, $\Delta_{sp}(K)$, shown here for different values of U/t , is linear in $1/L$. $\Delta_{sp}(K)$ is obtained by fitting the tail of the Green's function, $G(K, \tau)$ (inset), to the form $e^{-\tau\Delta_{sp}(K)}$. **b**, Antiferromagnetic structure factor, S_{AF} , for various values of U/t , fitted using third-order polynomials in $1/L$. Antiferromagnetic order appears for $U/t > 4.3$, as seen in the histogram $P(S_{AF}/N)$ from a Monte Carlo bootstrapping analysis (inset). a.u., arbitrary units. **c**, Spin gap, Δ_s , for different values of U/t , fitted using second-order polynomials in $1/L$. Inset, Δ_s for $L = 6, 9, 12$ and 15 , and the extrapolated values (TDL), as functions of U/t . Error bars, s.e.m.

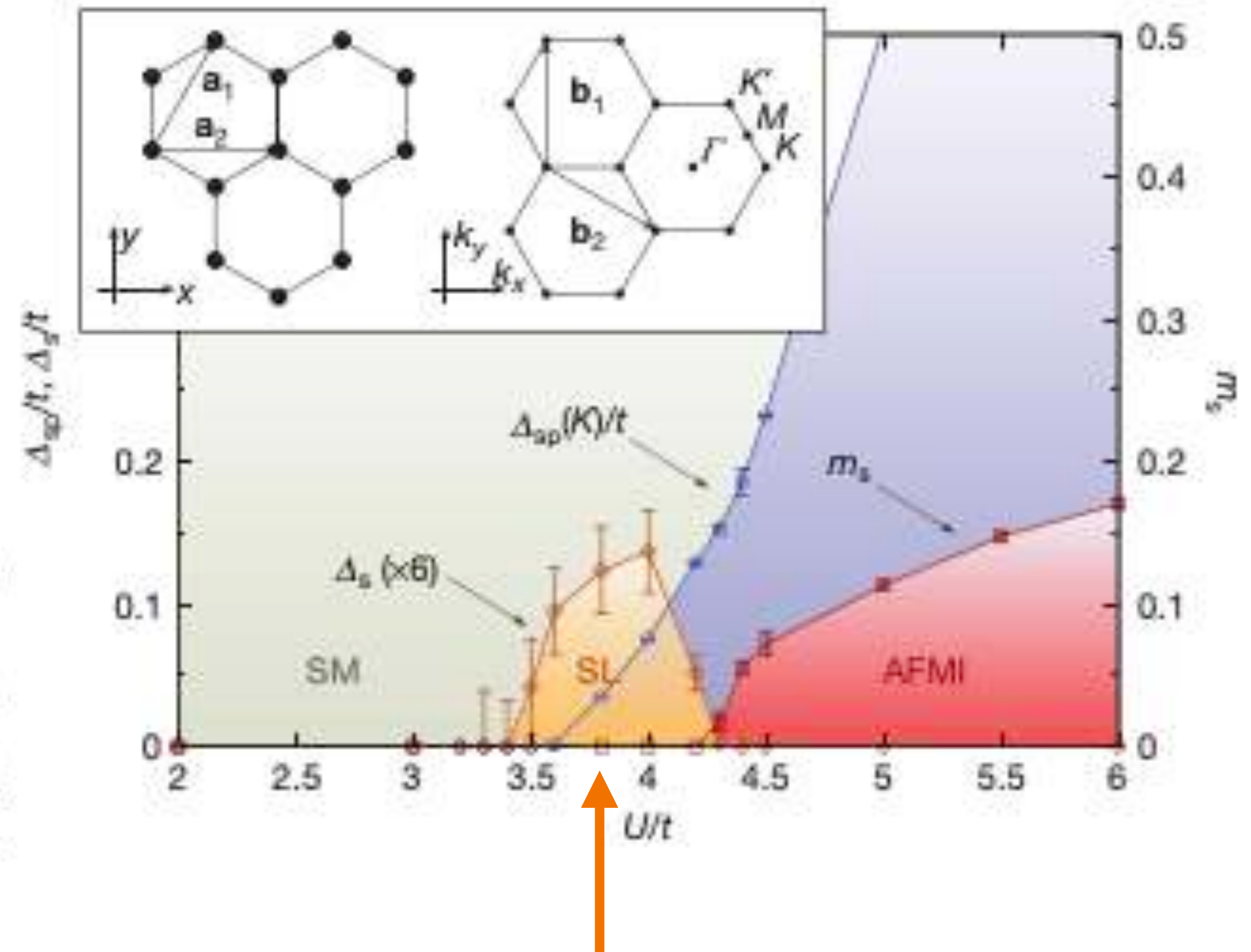


ARTICLES

Quantum spin liquid emerging in two-dimensional correlated Dirac fermions

Z. Y. Meng¹, T. C. Lang², S. Wessel¹, F. F. Assaad² & A. Muramatsu¹

Figure 1 | Phase diagram for the Hubbard model on the honeycomb lattice at half-filling. The semimetal (SM) and the antiferromagnetic Mott insulator (AFMI) are separated by a gapped spin-liquid (SL) phase in an intermediate-coupling regime. $\Delta_{sp}(K)$ denotes the single-particle gap and Δ_s denotes the spin gap; m_s denotes the staggered magnetization, whose saturation value is 1/2. Error bars, s.e.m. Inset, the honeycomb lattice with primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, and the reciprocal lattice with primitive vectors $\mathbf{b}_1$ and $\mathbf{b}_2$. Open and filled sites respectively indicate two different sublattices. The Dirac points K and K' and the M and Γ points are marked.



Spin liquid phase

Absence of a Spin Liquid Phase in the Hubbard Model on the Honeycomb Lattice

Sandro Sorella^{1,2,3}, Yuichi Otsuka³ & Seiji Yunoki^{3,4,5}

Scientific Reports 2, 992 (2012)

Up to 2592 sites

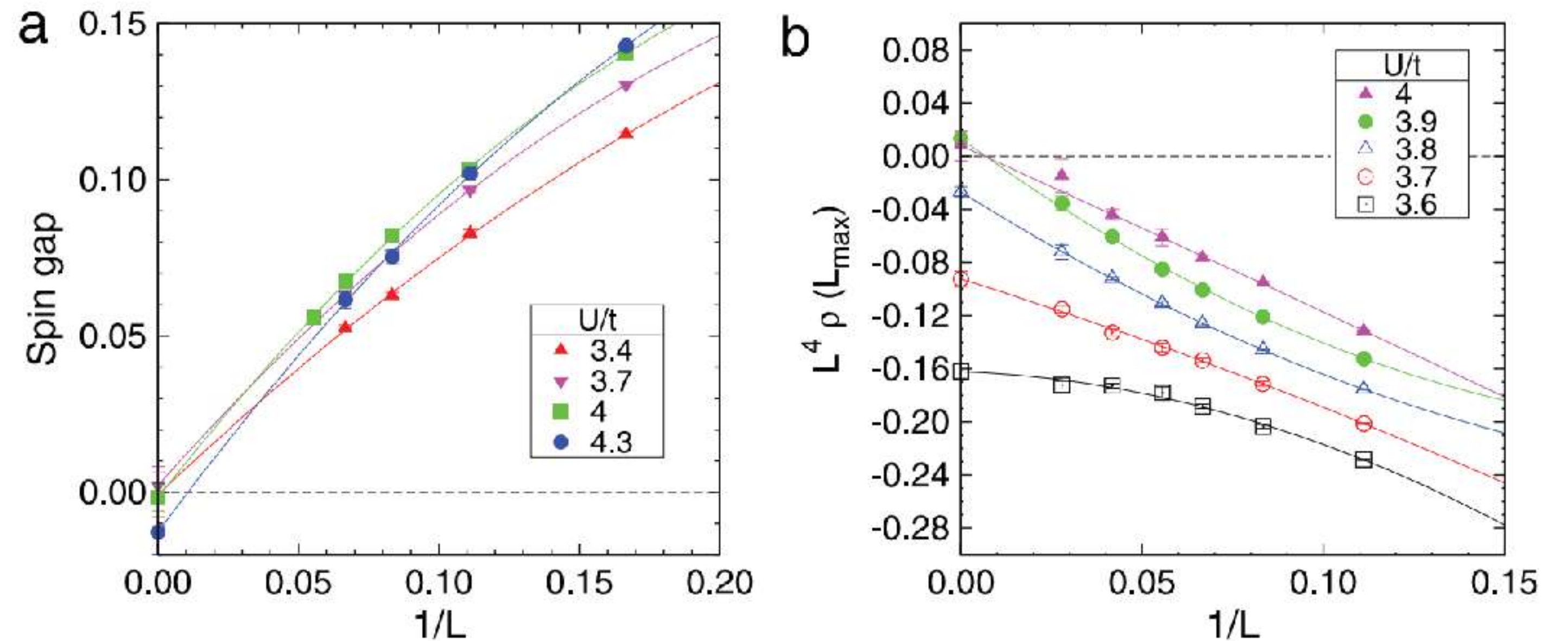


Figure 4 | Finite size scaling of spin gap and charge-charge correlation functions for the Hubbard model on the honeycomb lattice at half-filling. (a) Spin gap $\Delta_s = E(S = 1) - E(S = 0)$ for various U/t , where $E(S)$ is the lowest energy for a given spin S . Solid curves are fits of data by quadratic polynomials in $1/L$. The extrapolated values are also indicated at $1/L = 0$. Error bars of the extrapolated values are computed with the resampling technique. In the semi-metallic region, the spin gap scales to zero with increasing the resolution in momentum space, namely as $1/L$. In the antiferromagnetic region, the spin gap should instead vanish as $1/L^2$. This explains why for $U/t = 4.3$ the gap extrapolates to negative values, as we are well inside the antiferromagnetic phase (see Fig. 3). In any case, a sizable spin gap is not found for any value of U/t . (b) Charge-charge correlation function $\rho(\mathbf{R}) = \langle n_{r,A} n_{r+\mathbf{R},A} \rangle - \langle n_{r,A} \rangle \langle n_{r+\mathbf{R},A} \rangle$ at the maximum distance $|\mathbf{R}| = L_{\max}$ for several values of U/t . In the semi-metallic phase, $\rho(R) \sim 1/R^4$ and $L^4 \rho(L_{\max})$ should converge to a finite value for $L \rightarrow \infty$. Instead, when a charge gap opens, the charge-charge correlations should decay exponentially and $L^4 \rho(L_{\max})$ converges to zero in this limit. Indeed, a quadratic extrapolation to $L \rightarrow \infty$ of this quantity, which is clearly appropriate in the semi-metallic phase, appears to vanish in the interval between $U/t = 3.8$ and $U/t = 3.9$, in remarkable agreement with the critical value $U_c = 3.869 \pm 0.013$ estimated for the antiferromagnetic transition (see Fig. 3). Obviously, a polynomial fit is not consistent in the insulating region and this explains why the extrapolated value to $1/L = 0$ seems slightly positive in this case. For the spin gap and the charge-charge correlation functions, the Trotter $\Delta\tau$ error is negligible, and all data shown here refers to $\Delta\tau t = 0.14$ and 0.1 , respectively.

Comparing with experiments

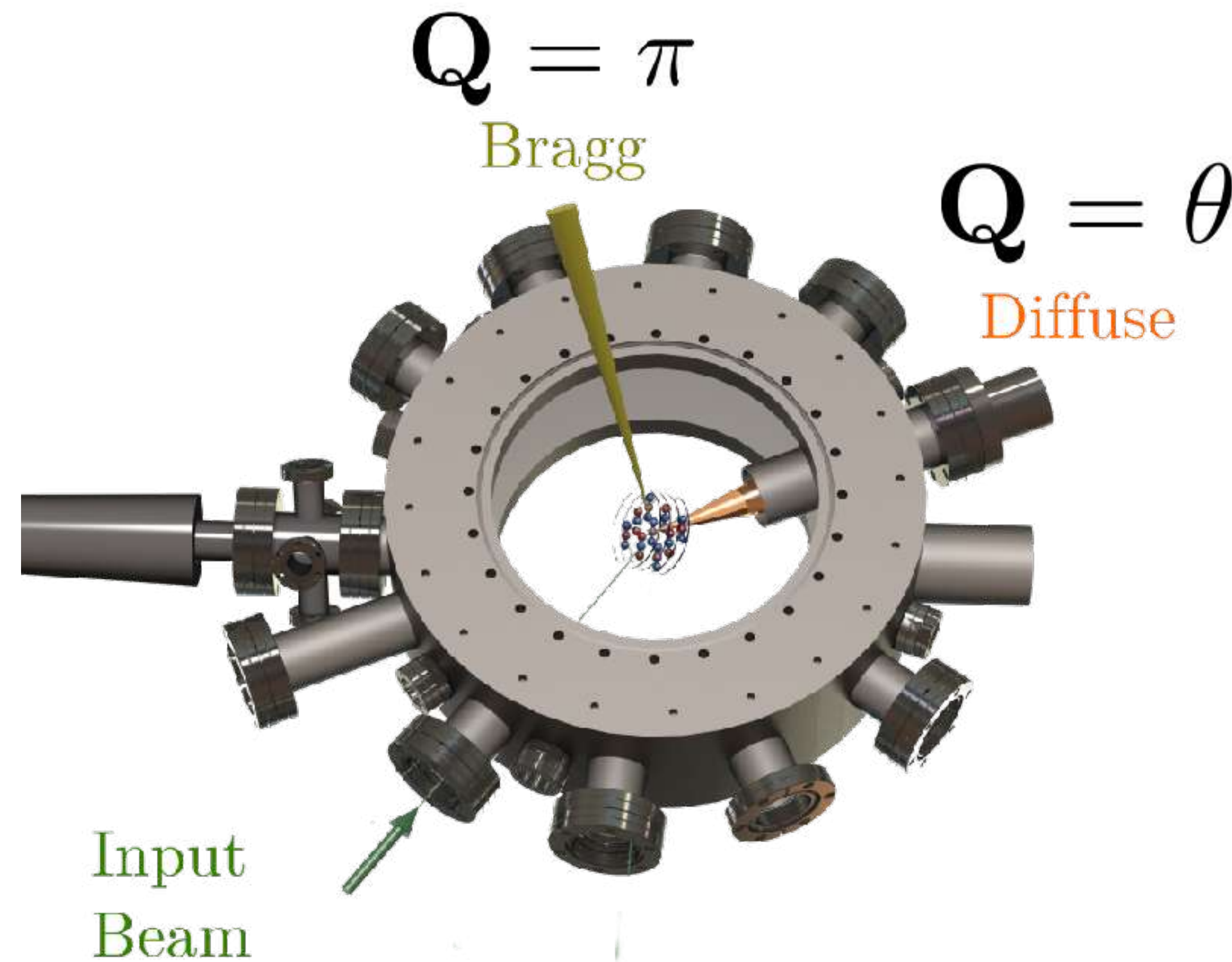
Observation of antiferromagnetic correlations in the Hubbard model with ultracold atoms

Nature 2015

Russell A. Hart^{1*}, Pedro M. Duarte^{1*}, Tsung-Lin Yang¹, Xinxing Liu¹, Thereza Paiva², Ehsan Khatami³, Richard T. Scalettar⁴, Nandini Trivedi⁵, David A. Huse⁶ & Randall G. Hulet¹

Bragg scattering

40K

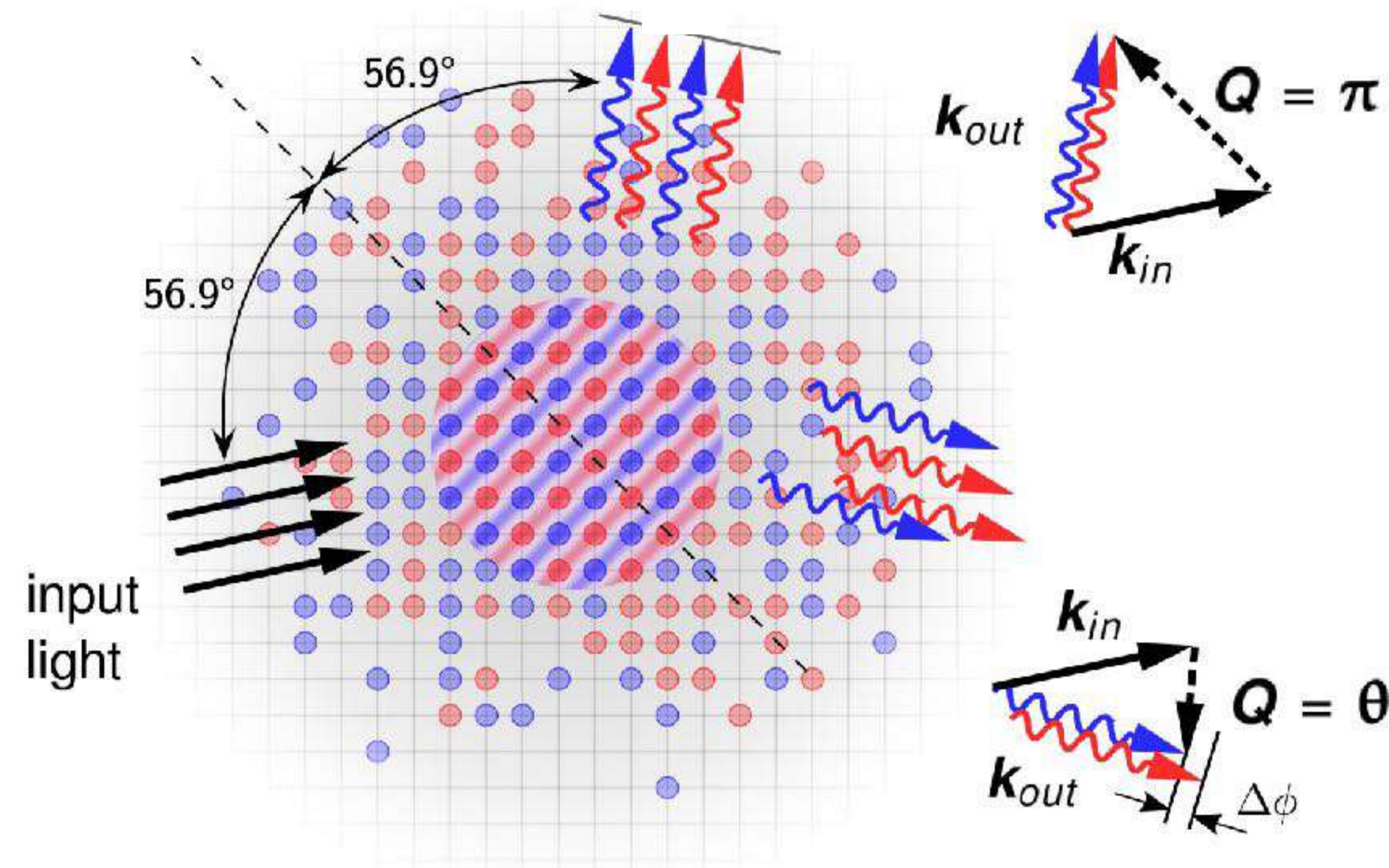


Magnetic structure factor

$$S_Q = \frac{1}{N} \sum_{i,j} e^{iQ \cdot (R_i - R_j)} \langle S_i^z S_j^z \rangle$$

Constructive interference

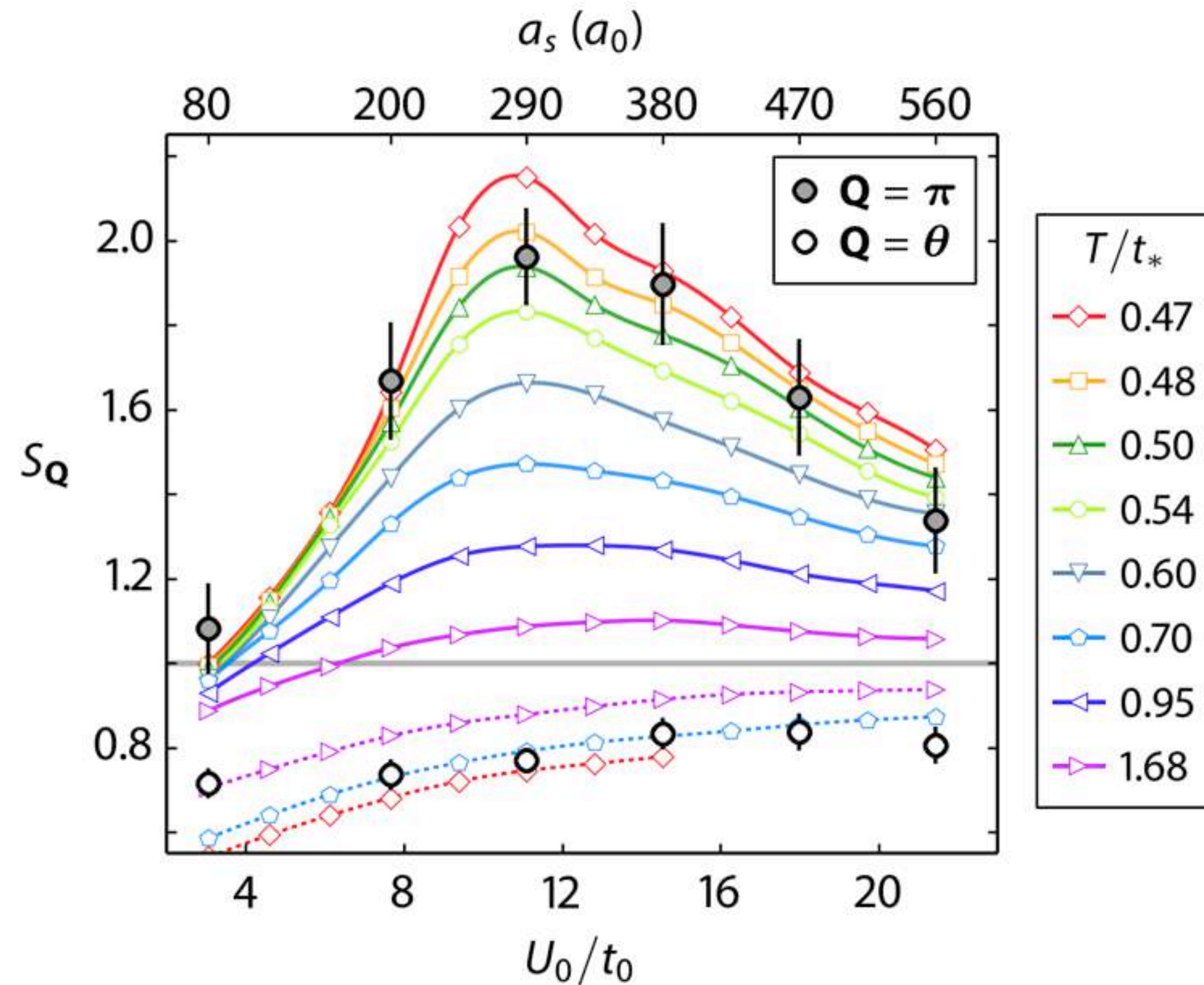
$$\pi = \frac{2\pi}{a}(-0.5, -0.5, +0.5)$$



Destructive interference

$$\theta = \frac{2\pi}{a}(+0.396, -0.105, -0.041)$$

Comparing theory and experiment



Thermometry with support from theory

$U_0/t_0 = 11.1$ $\longrightarrow$ Sweet spot for AF

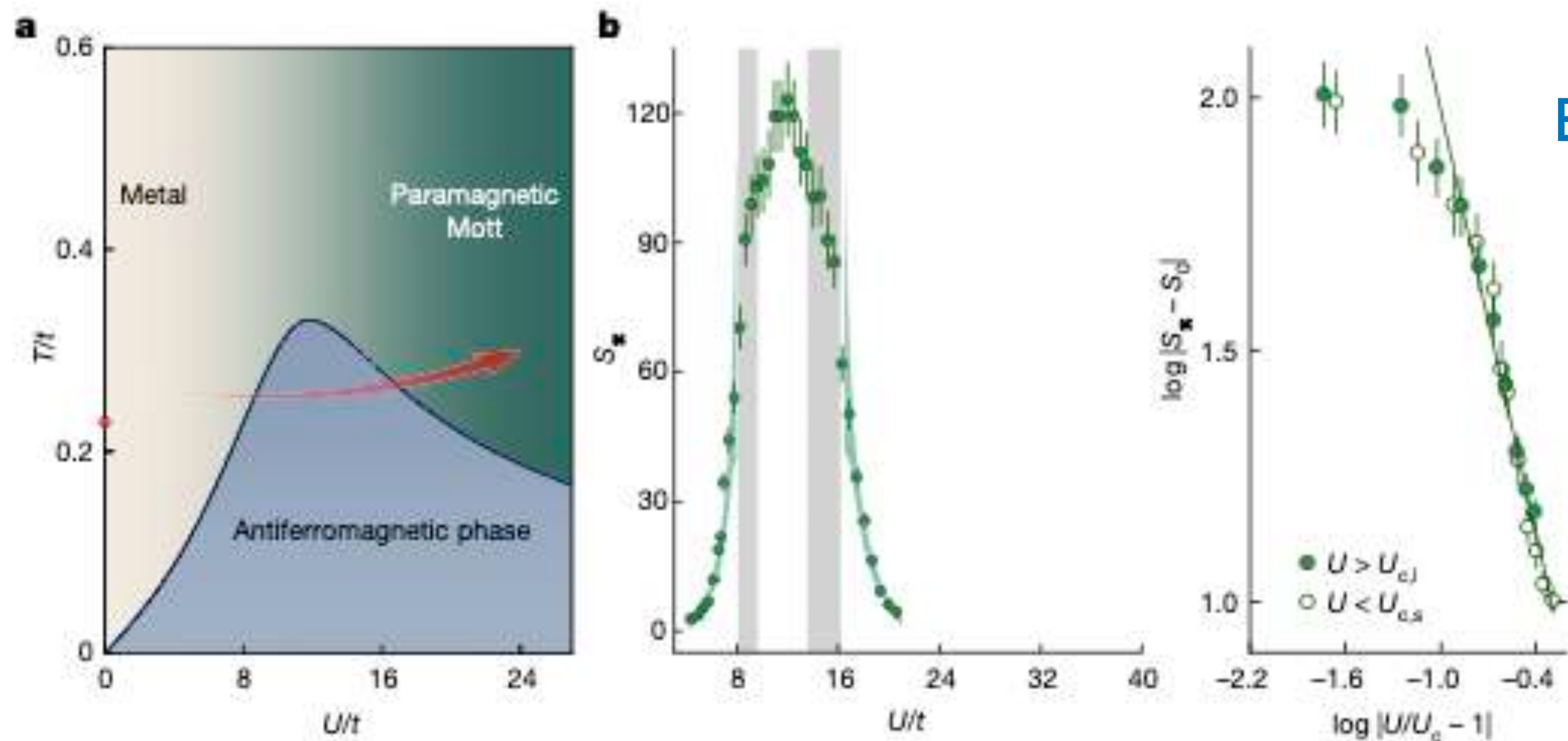
$$T/T_{Neel} = 1.42 \pm 0.16$$

$$T = 32 \pm 4K$$

Antiferromagnetic phase transition in a 3D fermionic Hubbard model

Hou-Ji Shao^{1,2,4}, Yu-Xuan Wang^{1,2,4}, De-Zhi Zhu^{1,2}, Yan-Song Zhu^{1,2}, Hao-Nan Sun^{1,2}, Si-Yuan Chen^{1,2}, Chi Zhang^{1,2}, Zhi-Jie Fan^{1,2,3}, Youjin Deng^{1,2,3}, Xing-Can Yao^{1,2,3}, Yu-Ao Chen^{1,2,3} & Jian-Wei Pan^{1,2,3}

Nature 2024



Bragg scattering

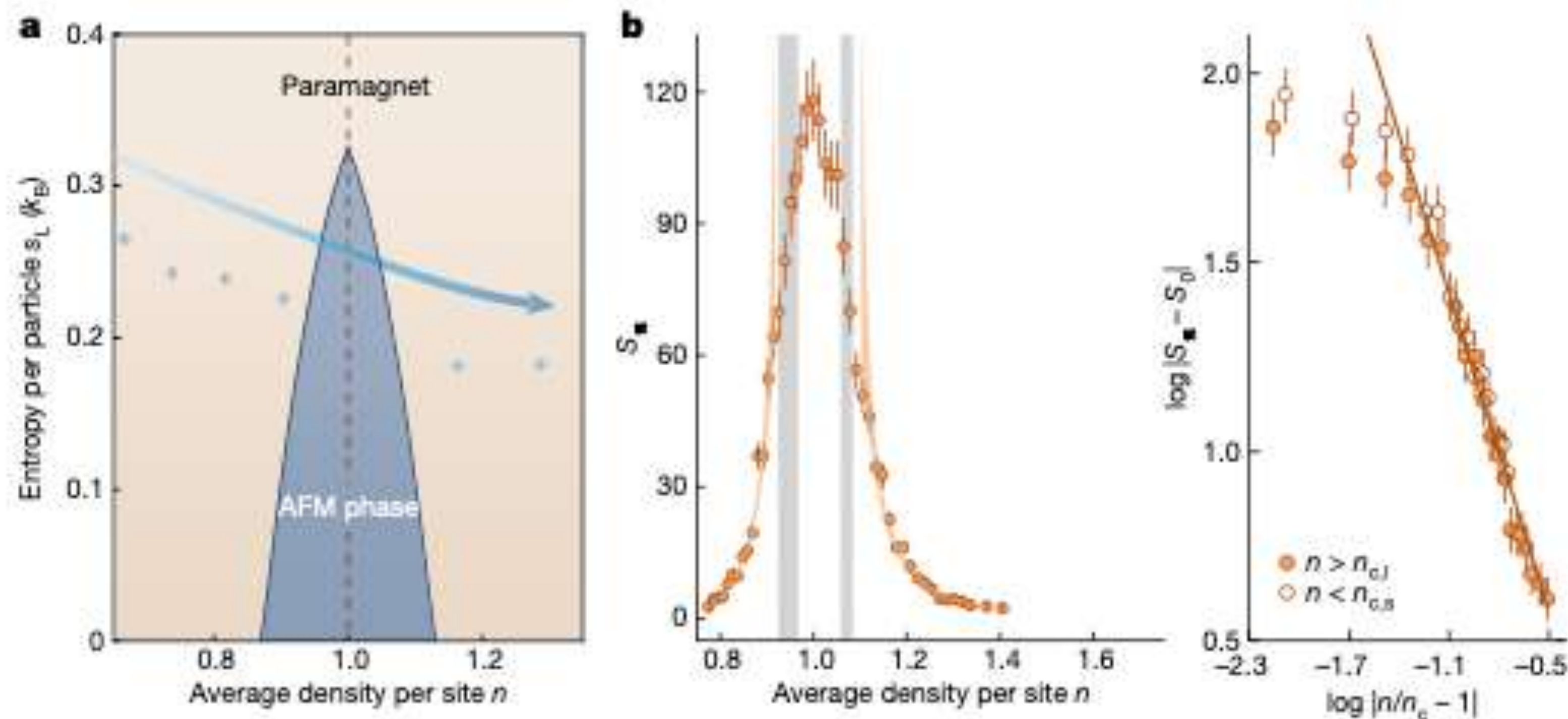
$T/t=0.229(2)$

$S/N=0.216(2) \text{ k}_B$

Antiferromagnetic phase transition in a 3D fermionic Hubbard model

Nature 2024

Hou-Ji Shao^{1,2,4}, Yu-Xuan Wang^{1,2,4}, De-Zhi Zhu^{1,2}, Yan-Song Zhu^{1,2}, Hao-Nan Sun^{1,2},
Si-Yuan Chen^{1,2}, Chi Zhang^{1,2}, Zhi-Jie Fan^{1,2,3}, Youjin Deng^{1,2,3}, Xing-Can Yao^{1,2,3},
Yu-Ao Chen^{1,2,3} & Jian-Wei Pan^{1,2,3}



Bragg scattering

$U/t=11.75$

$T/t=0.229(2)$

Not as easy as it seems...

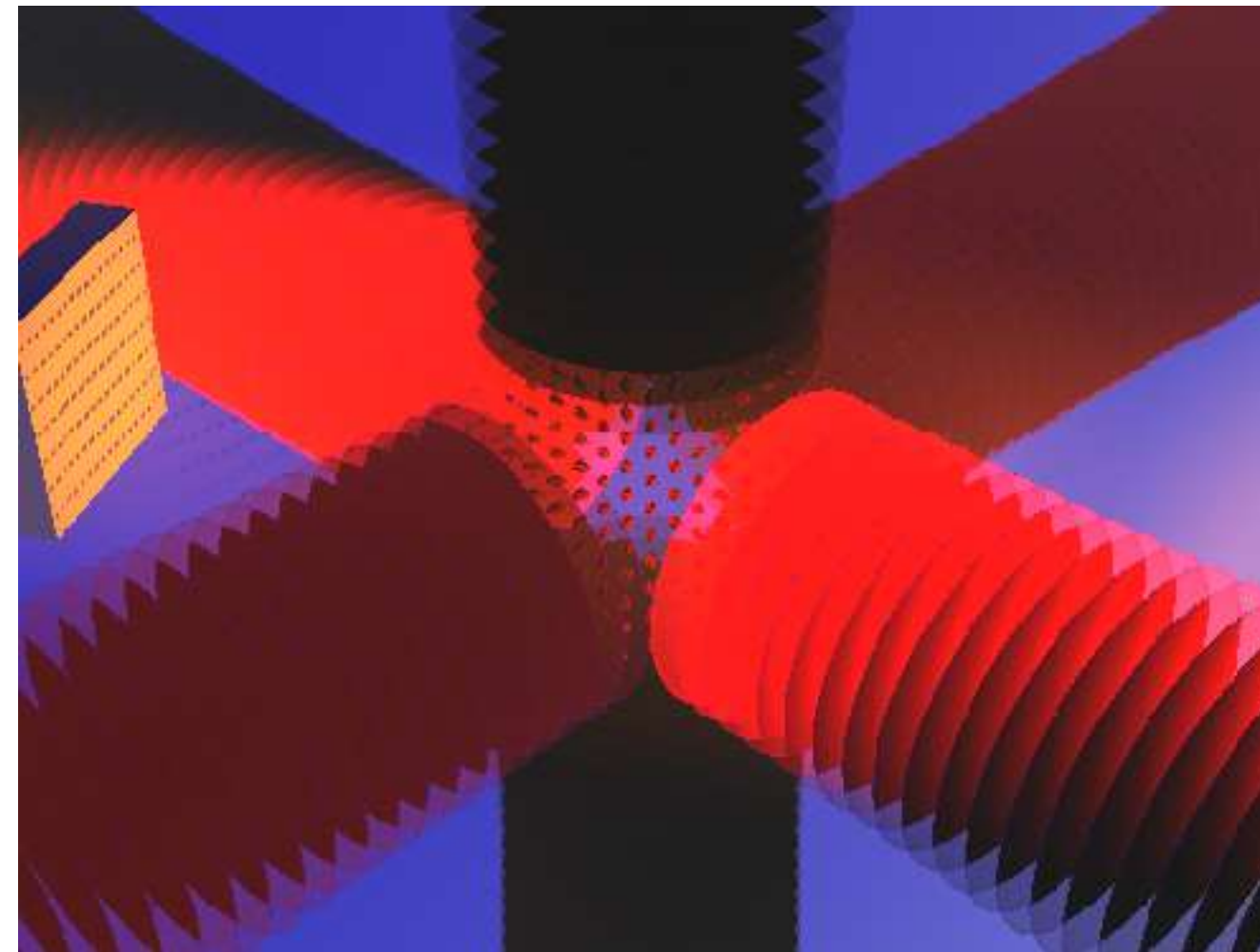
BULK MEASUREMENTS

Fermions in optical lattices

Trap

Optic or
magnetic

Parabolic
compensated



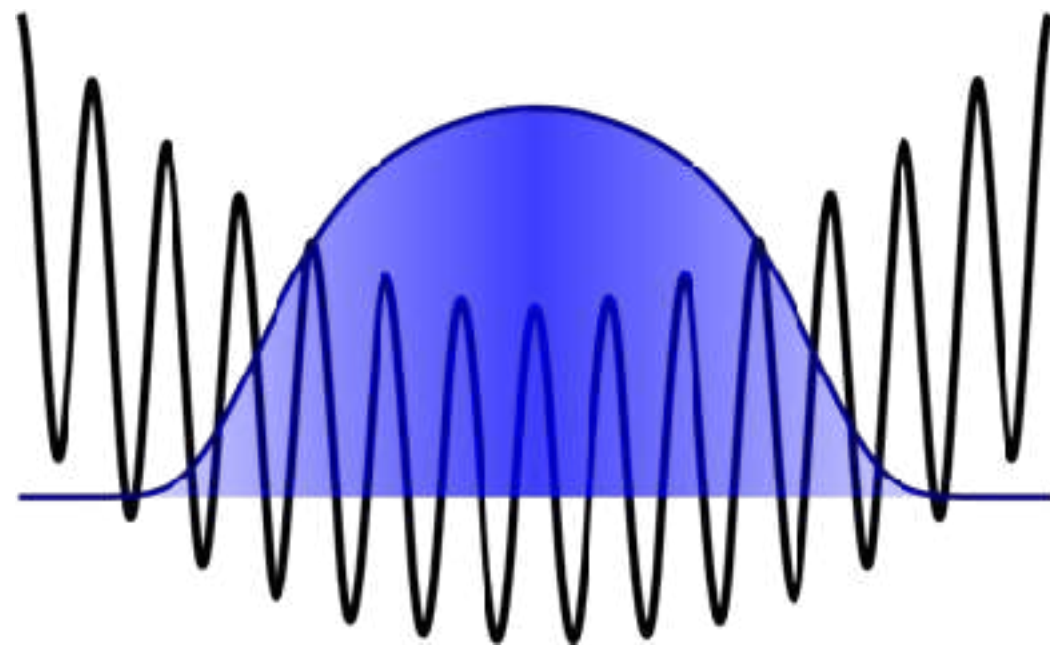
Periodic
potential

Counter
propagating lasers

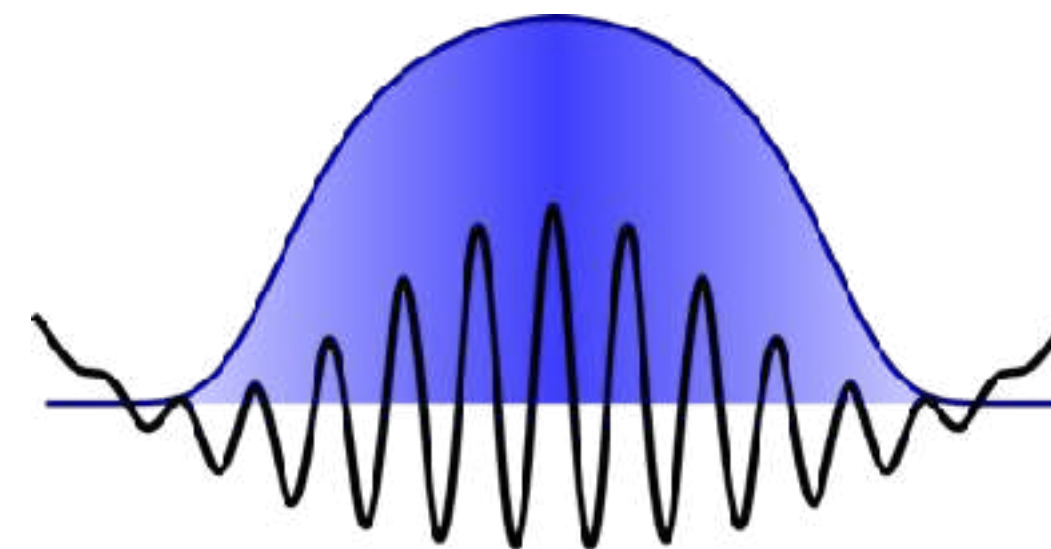
$$a = \lambda/2$$

Holographic mask

Not as easy as it seems...



lattice with harmonic confinement



compensated optical lattice

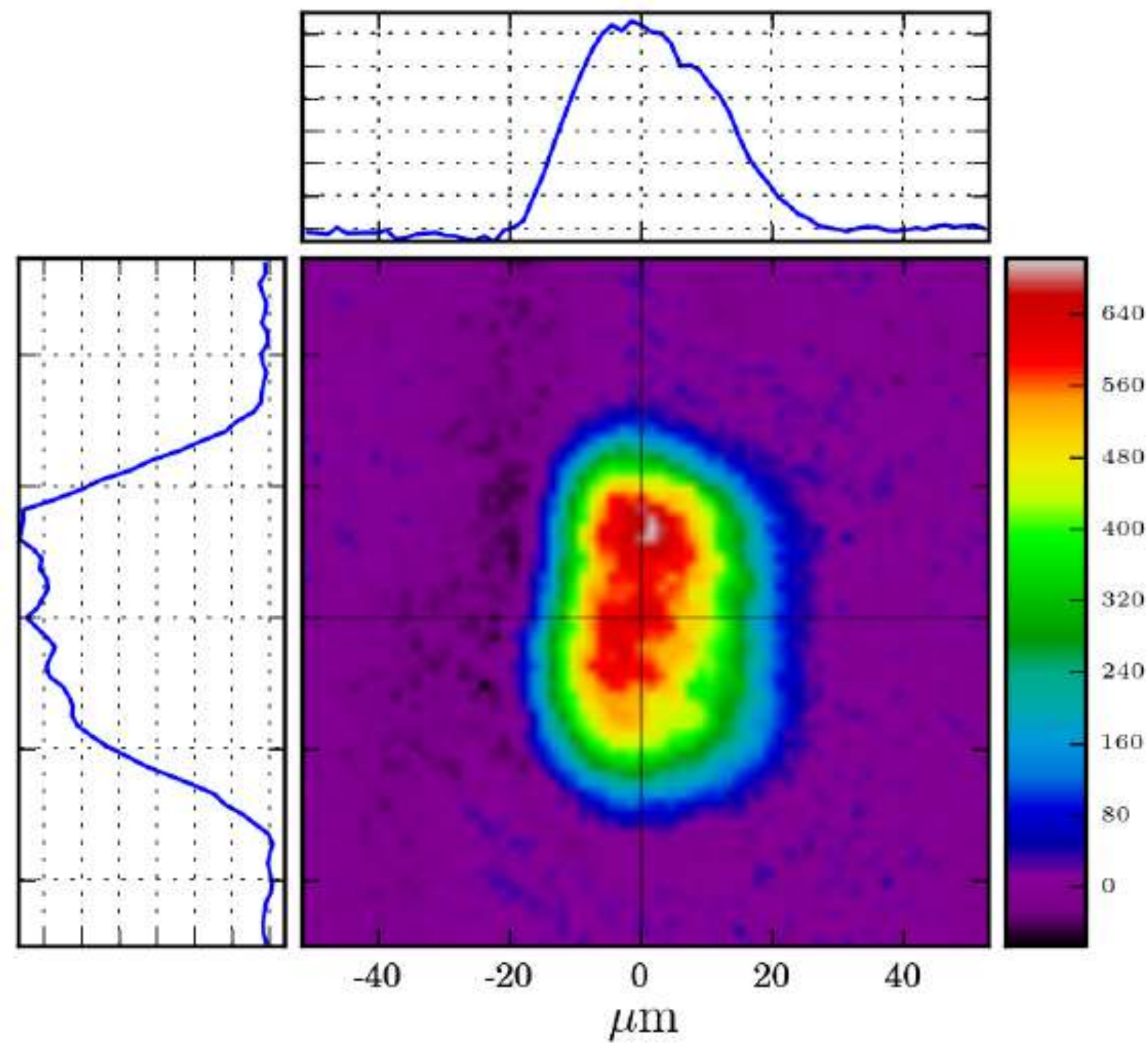
Inhomogeneity in the Hubbard parameters, tunneling and onsite interactions

→ enhanced entropy redistribution to the edges of the trap

Global chemical potential comes closer to the threshold for evaporation

→ possible evaporative cooling from the lattice

Challenge: trap is rather complex

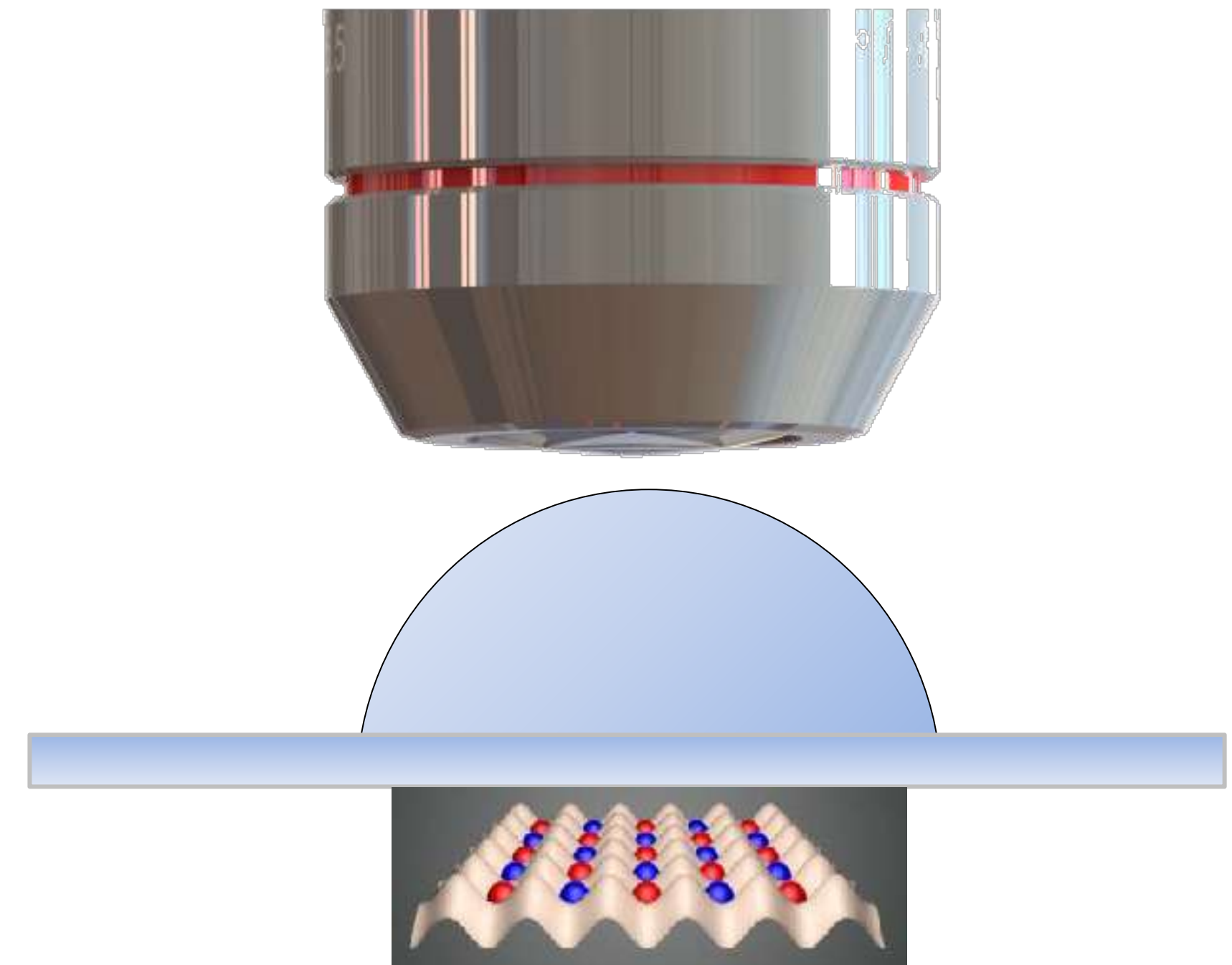


Density and **U** change
throughout the cloud

Advancement in the field

Atomic resolution

Quantum gas microscope



A quantum gas microscope for detecting single atoms in a Hubbard-regime optical lattice

Waseem S. Bakr¹, Jonathon I. Gillen¹, Amy Peng¹, Simon Fölling¹ & Markus Greiner¹

Bosons

Nature 2009

2009

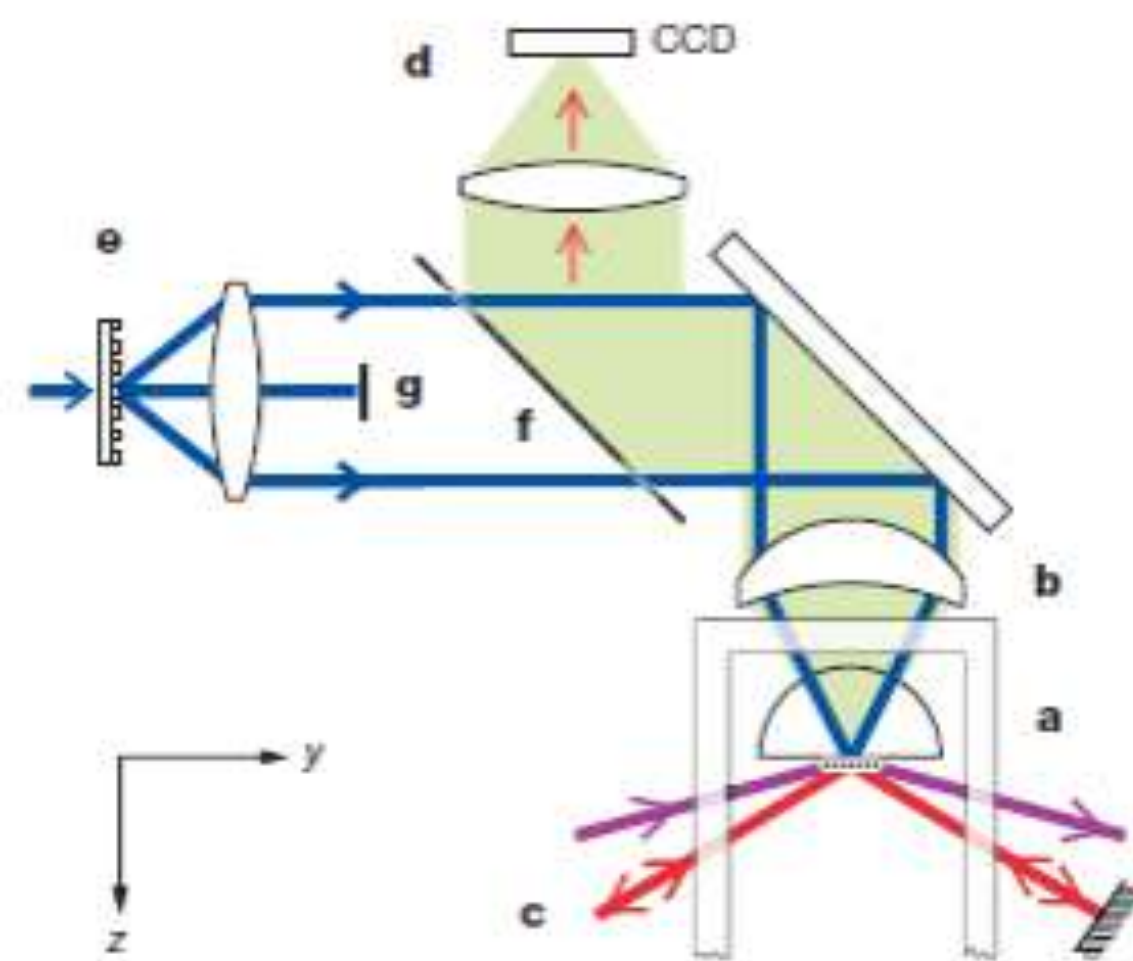


Figure 1 | Diagram of the quantum gas microscope. The two-dimensional atom sample (a) is located a few micrometres below the lower surface of a hemispherical lens inside the vacuum chamber. This lens serves to increase the numerical aperture (NA) of the objective lens outside the vacuum (b) by the index of refraction, from $NA = 0.55$ to $NA = 0.8$. The atoms are illuminated from the side by the molasses beams (c) and the scattered fluorescence light is collected by the objective lens and projected onto a CCD camera (d). A 2D optical lattice is generated by projecting a periodic mask (e) onto the atoms through the same objective lens via a beam splitter (f). The mask is a periodic phase hologram, and a beam stop (g) blocks the residual zeroth order, leaving only the first orders to form a sinusoidal potential.

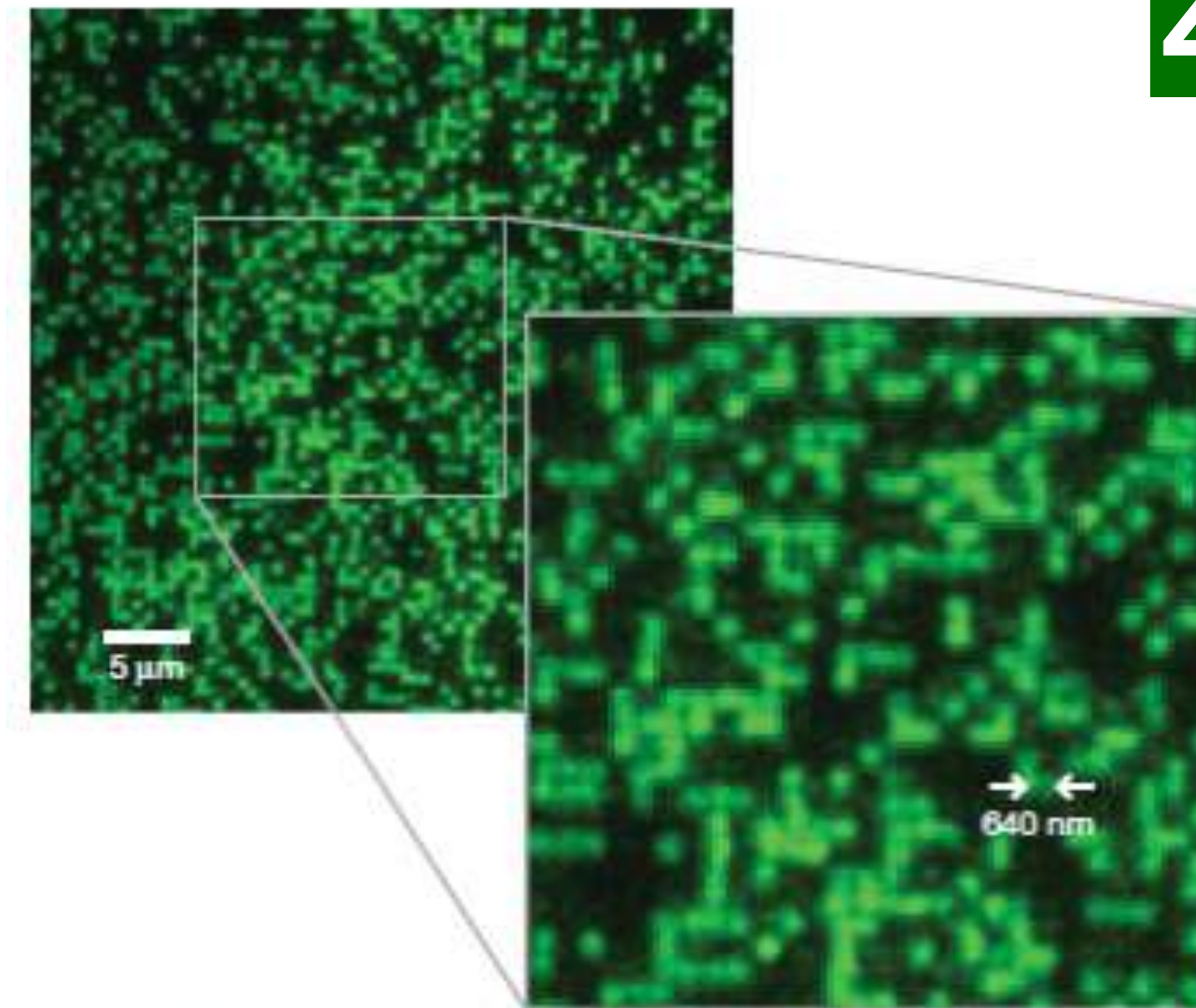


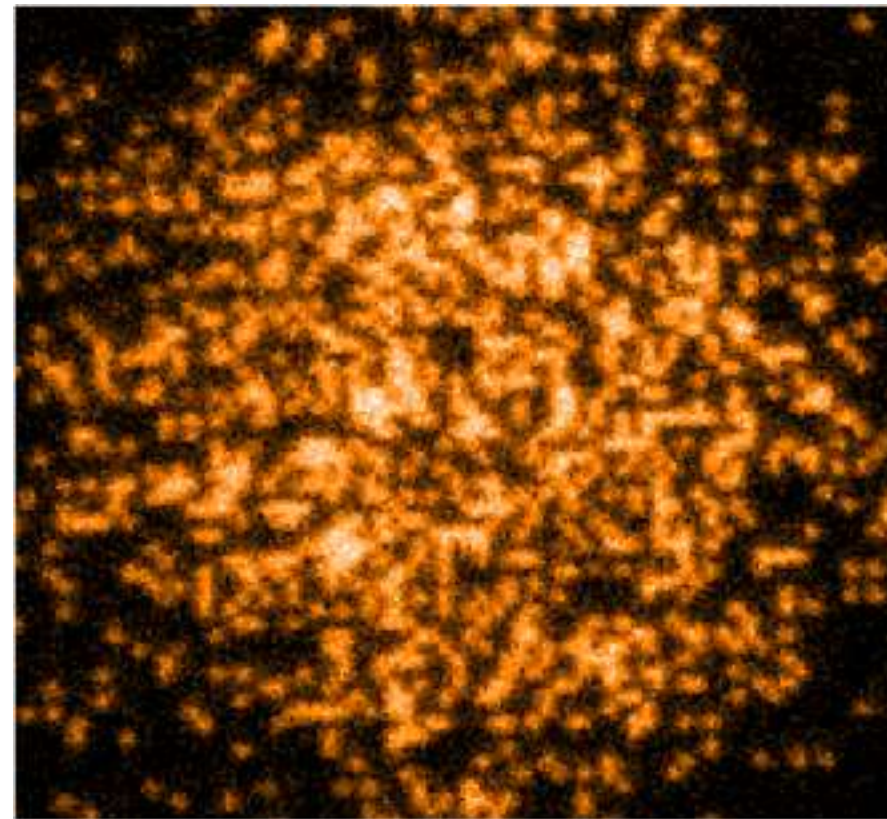
Figure 3 | Site-resolved imaging of single atoms on a 640-nm-period optical lattice, loaded with a high density Bose-Einstein condensate. Inset, magnified view of the central section of the picture. The lattice structure and the discrete atoms are clearly visible. Owing to light-assisted collisions and molecule formation on multiply occupied sites during imaging, only empty and singly occupied sites can be seen in the image.

Quantum gas microscope

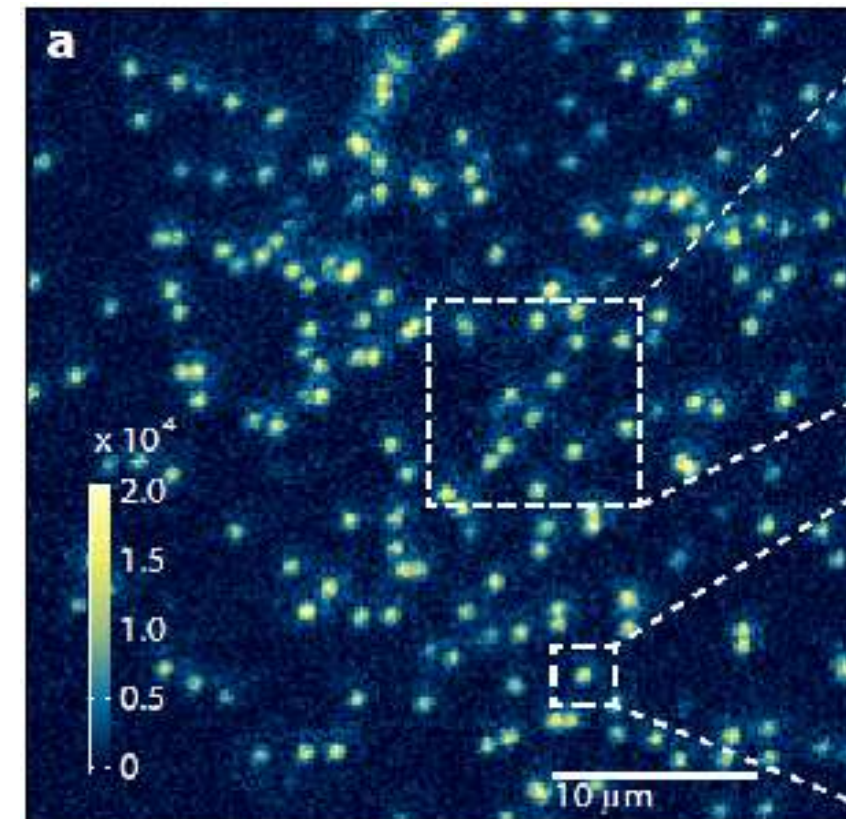
Fermions

2015

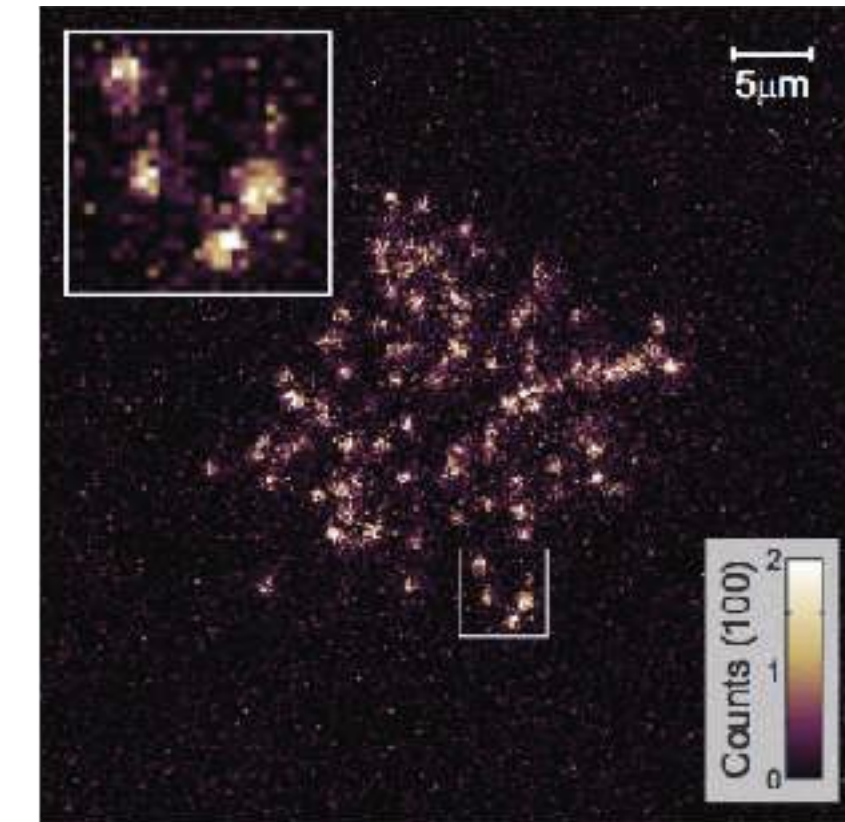
^{40}K



Zwierlen group, MIT
PRL 114, 193001 (2015)

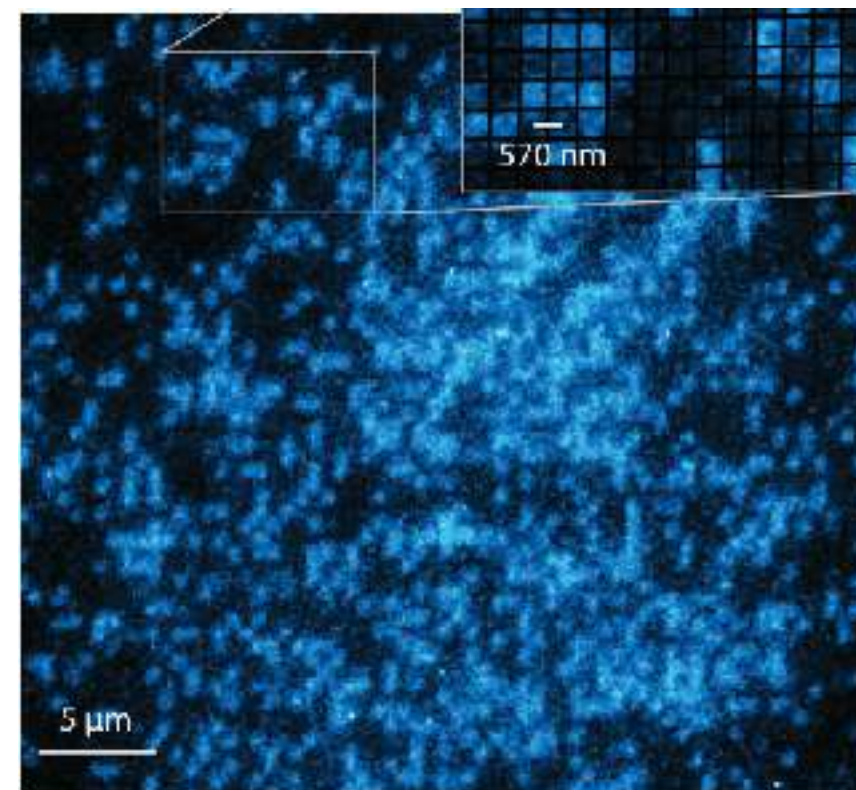


Kuhr group, Strathclyde
Nat. Phys. 11, 738 (2015)

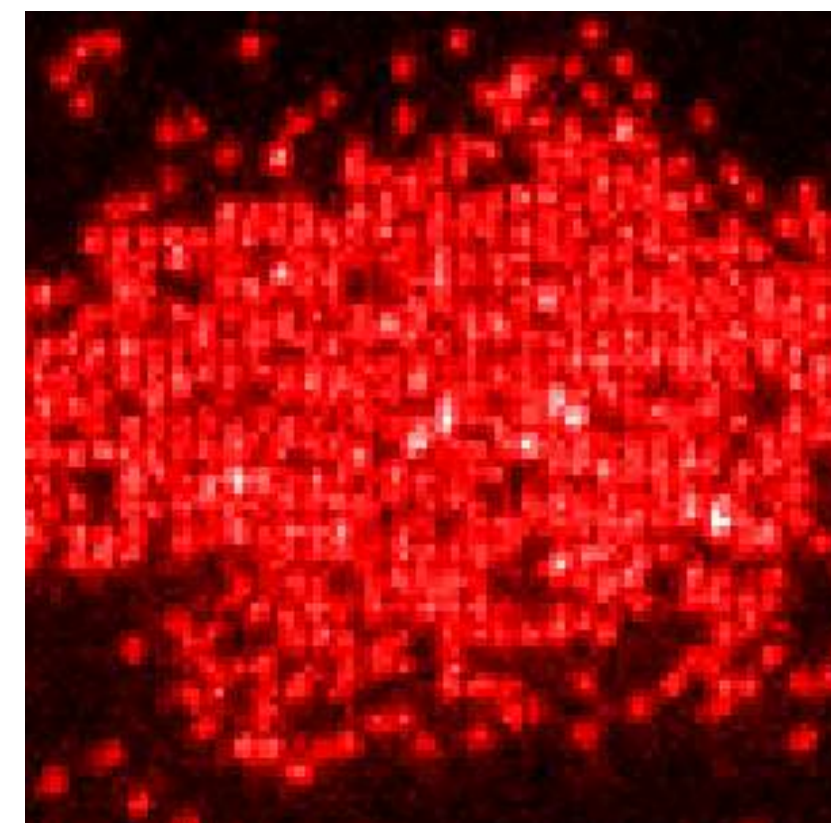


Thywissen group, Toronto,
PRA 92, 063406 (2015)

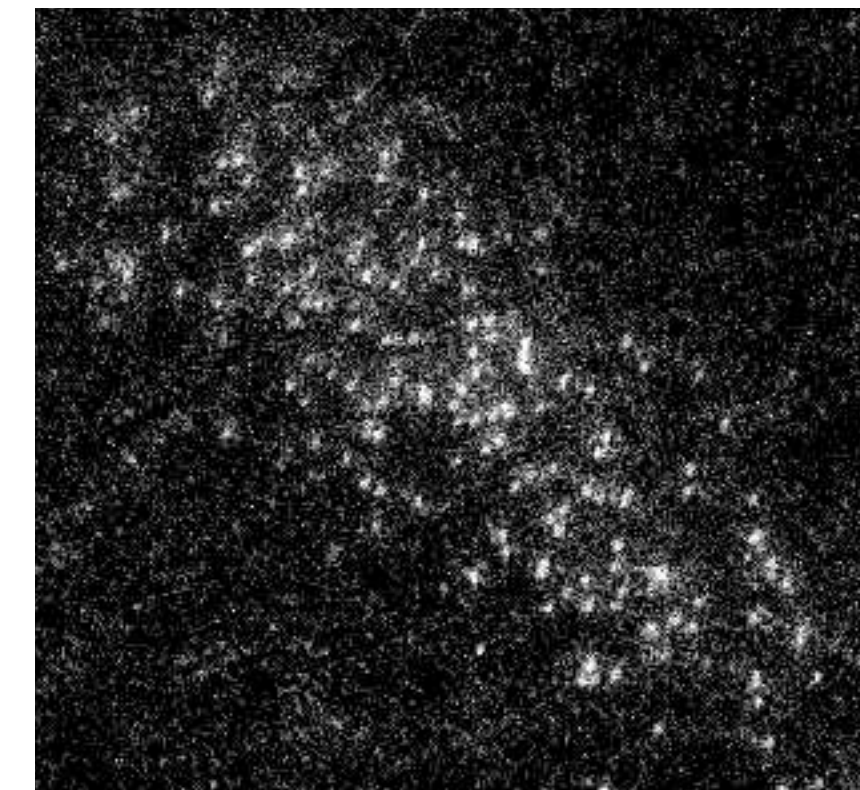
^6Li



Greiner group, Harvard
PRL 114, 213002 (2015)



Gross/Bloch group, MPQ
PRL 115, 263001 (2015)

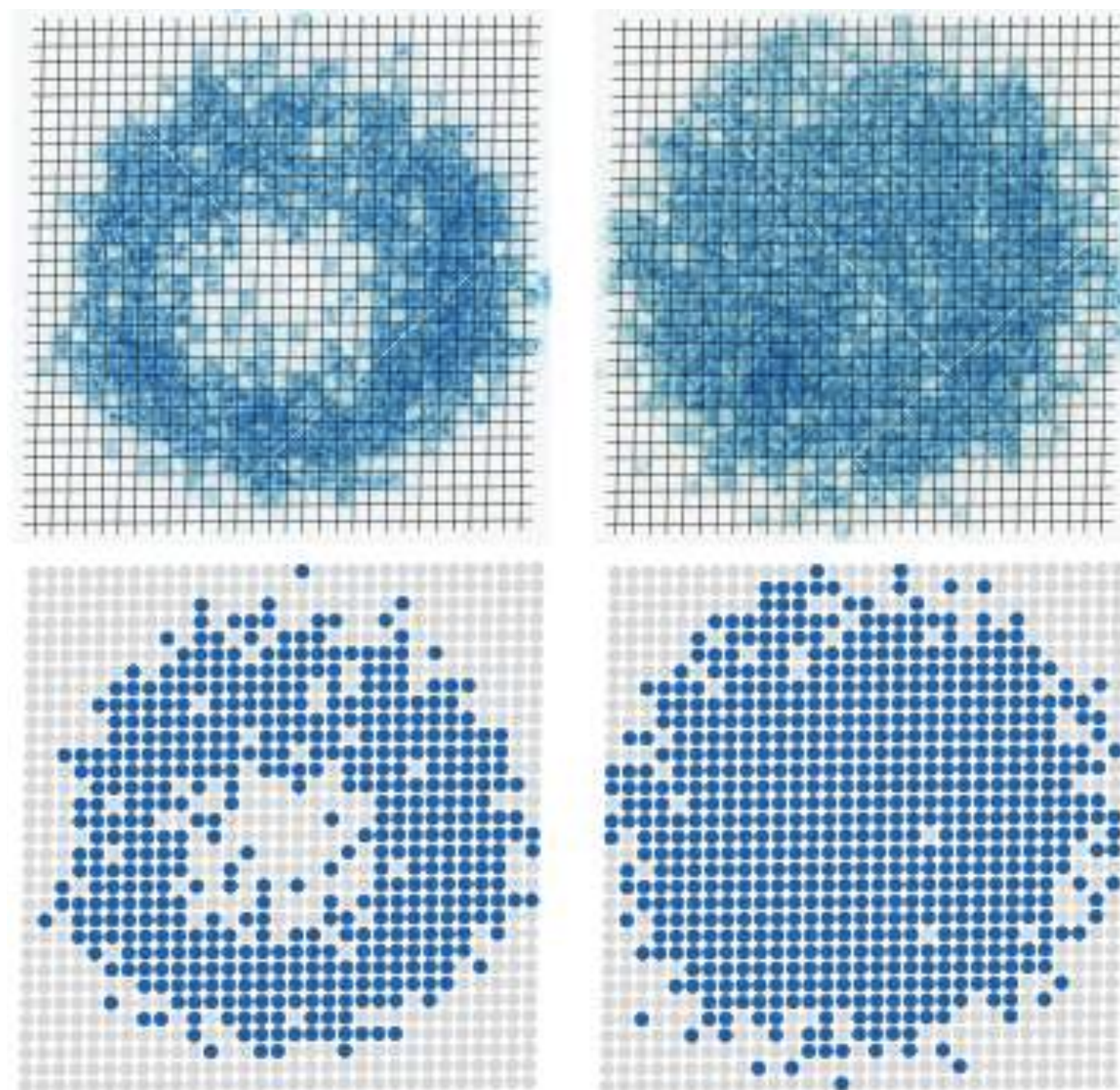


Bakr group, Princeton
PRL 114, 1193001 (2015)

Mott insulator

Site-resolved imaging of a
fermionic Mott insulator

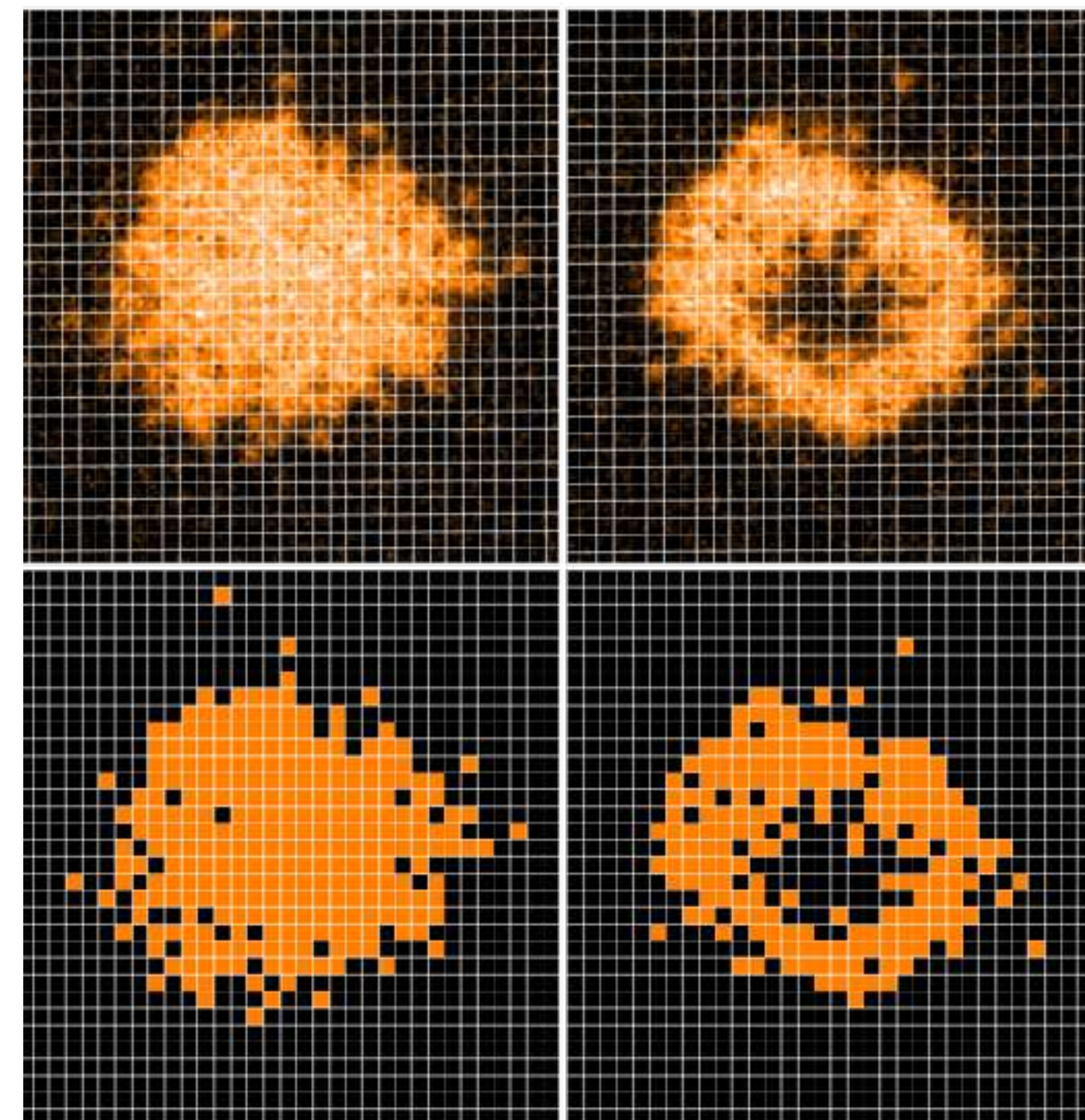
^6Li



Greif et al, Science (2016)
Greiner Group, Harvard

Observation of 2D fermionic
Mott insulators of ^{40}K with
single-site resolution

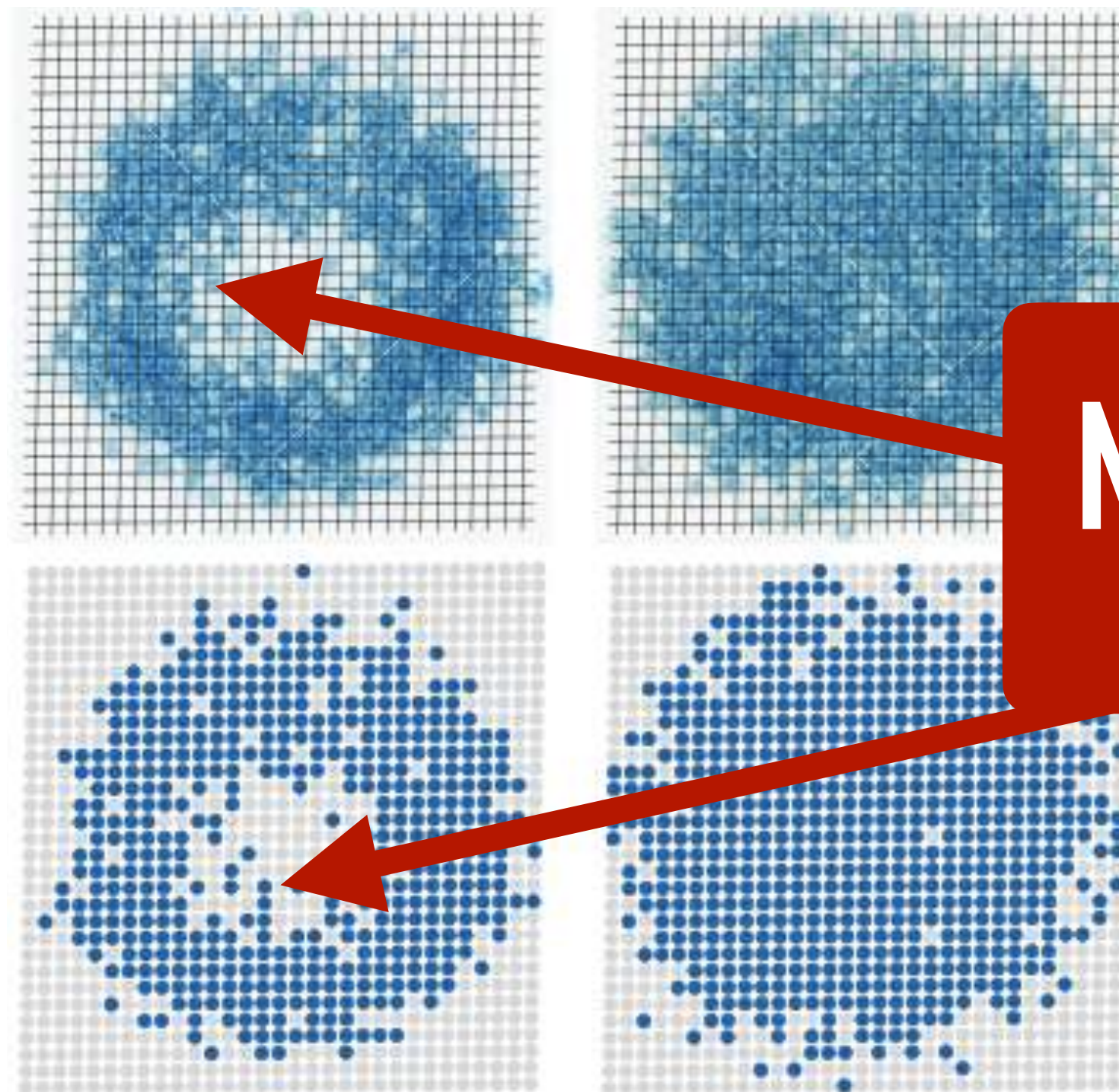
^{40}K



Cheuk et al, PRL (2016)
Zwierlein Group MIT

Site-resolved imaging of a
fermionic Mott insulator

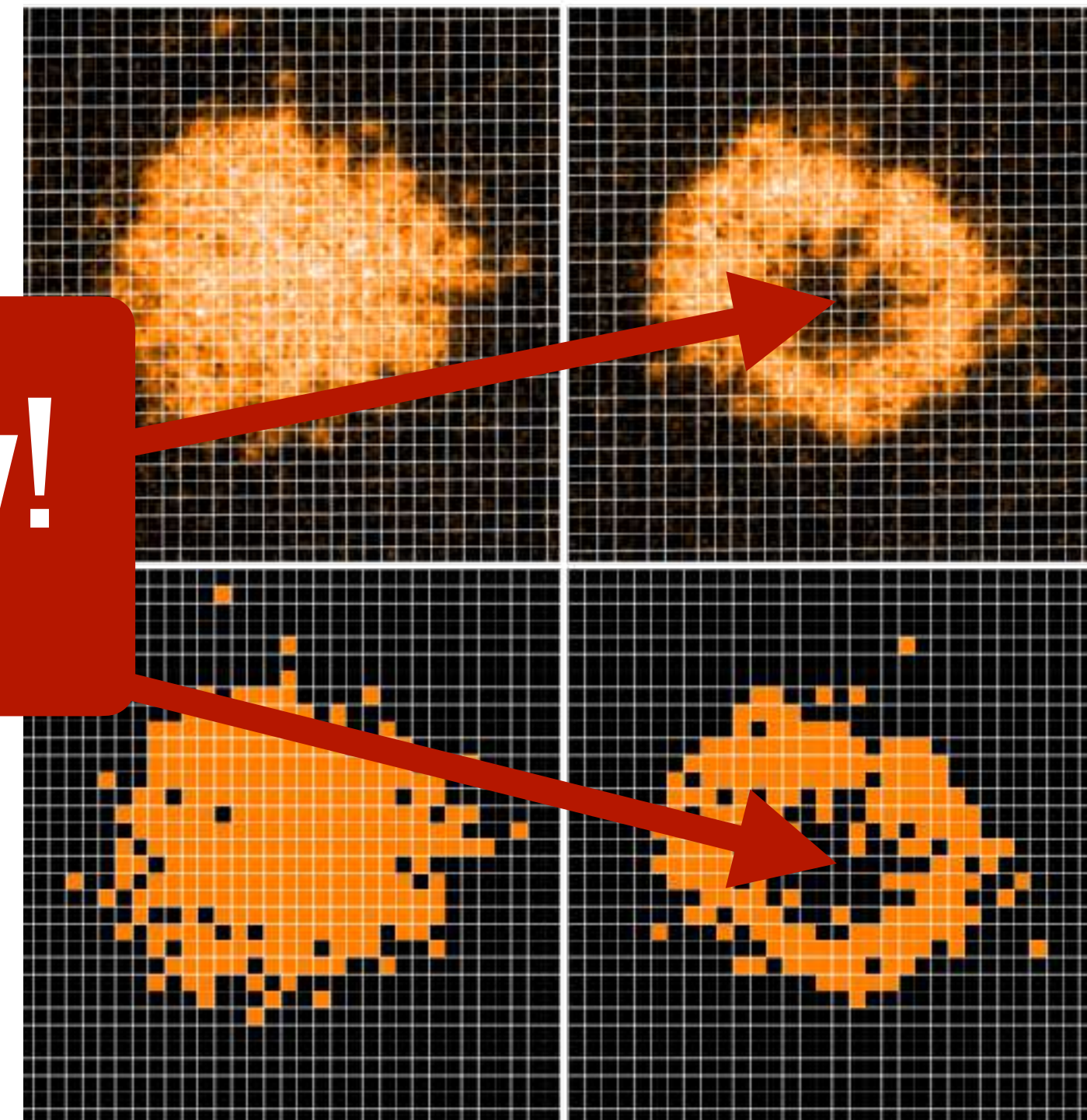
^6Li



Greif et al, Science (2016)
Greiner Group, Harvard

Observation of 2D fermionic
Mott insulators of ^{40}K with
single-site resolution

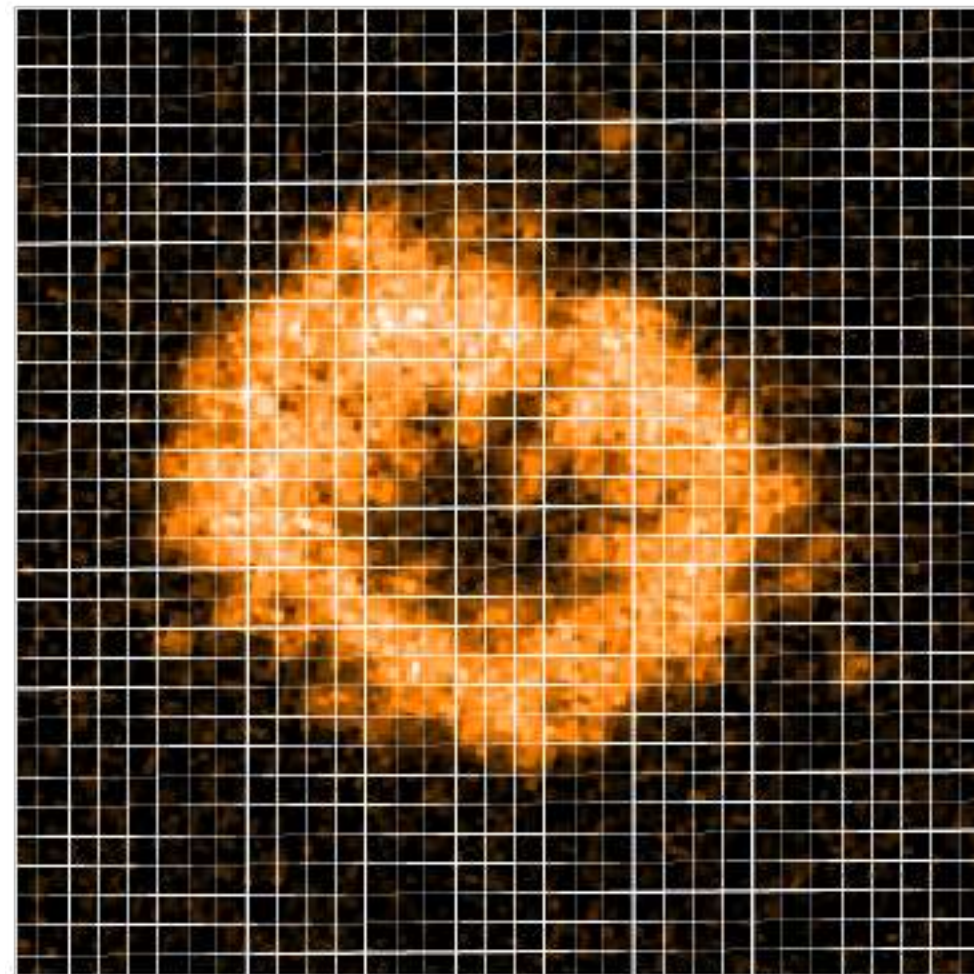
^{40}K



Cheuk et al, PRL (2016)
Zwierlein Group MIT

Not empty!

Fluorescence imaging



Atom pairs from the same site are lost due to collisions during light assisted imaging

Singly occupied sites

Local moment

$$\langle \hat{m}_{z,i}^2 \rangle = \langle (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 \rangle$$

Atomic resolution for fermions



Mott insulator



Real space antiferromagnetism

Quantum simulation

Site-resolved measurement of the spin-correlation function in the Fermi-Hubbard model

Maxwell F. Parsons, Anton Mazurenko, Christie S. Chiu, Geoffrey Ji, Daniel Greif, Markus Greiner*

Science 353,1253 (2016)

Spin- and density-resolved microscopy of antiferromagnetic correlations in Fermi-Hubbard chains

Martin Boll,^{1*} Timon A. Hilker,^{1*} Guillaume Salomon,^{1*} Ahmed Omran,¹ Jacopo Nespolo,² Lode Pollet,² Immanuel Bloch,^{1,2} Christian Gross^{1†}

Science 353,1257 (2016)

Observation of spatial charge and spin correlations in the 2D Fermi-Hubbard model

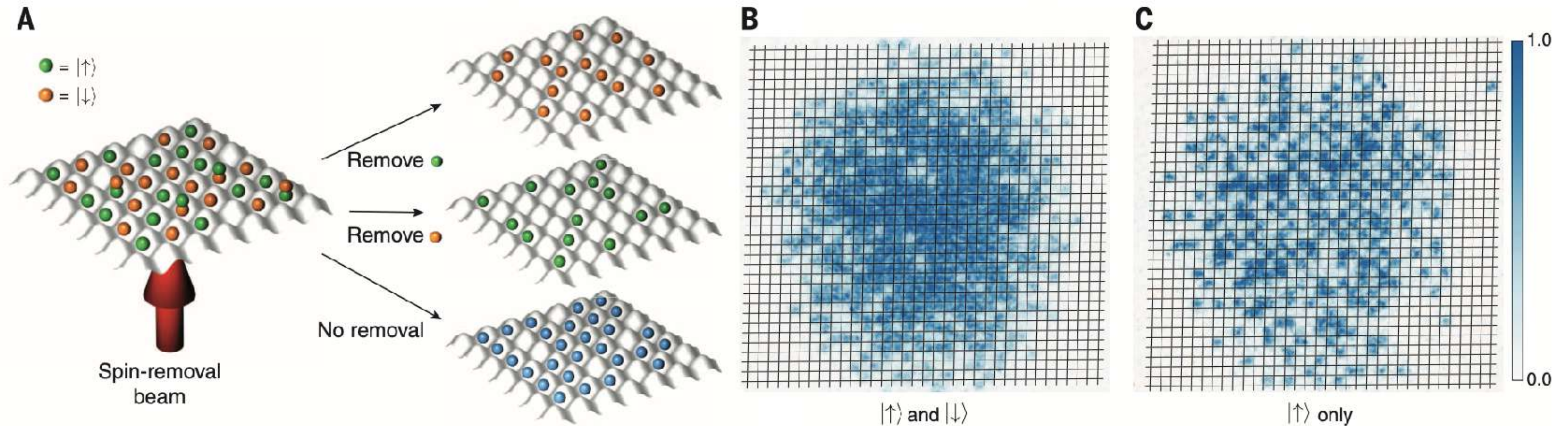
Lawrence W. Cheuk,^{1*} Matthew A. Nichols,^{1*} Katherine R. Lawrence,¹ Melih Okan,¹ Hao Zhang,¹ Ehsan Khatami,² Nandini Trivedi,² Thereza Paiva,⁴ Marcos Rigol,⁵ Martin W. Zwierlein^{1†}

Science 353,1260 (2016)

Site-resolved measurement of the spin-correlation function in the Fermi-Hubbard model

${}^6\text{Li}$

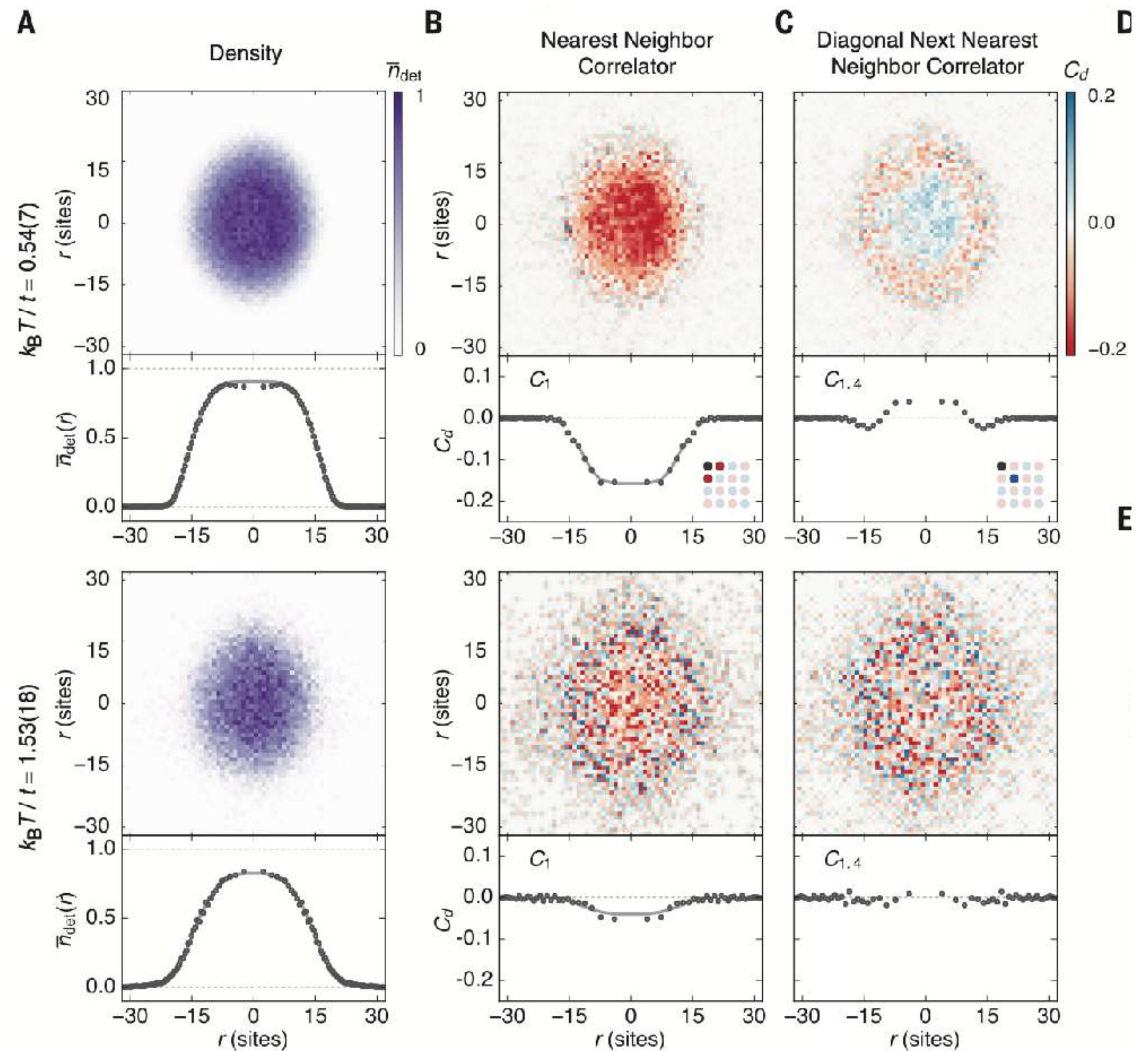
Maxwell F. Parsons, Anton Mazurenko, Christie S. Chiu, Geoffrey Ji,
Daniel Greif, Markus Greiner*



Nearest-neighbor and next-nearest neighbor spin-spin correlation functions

$U/t=8.0(1)$

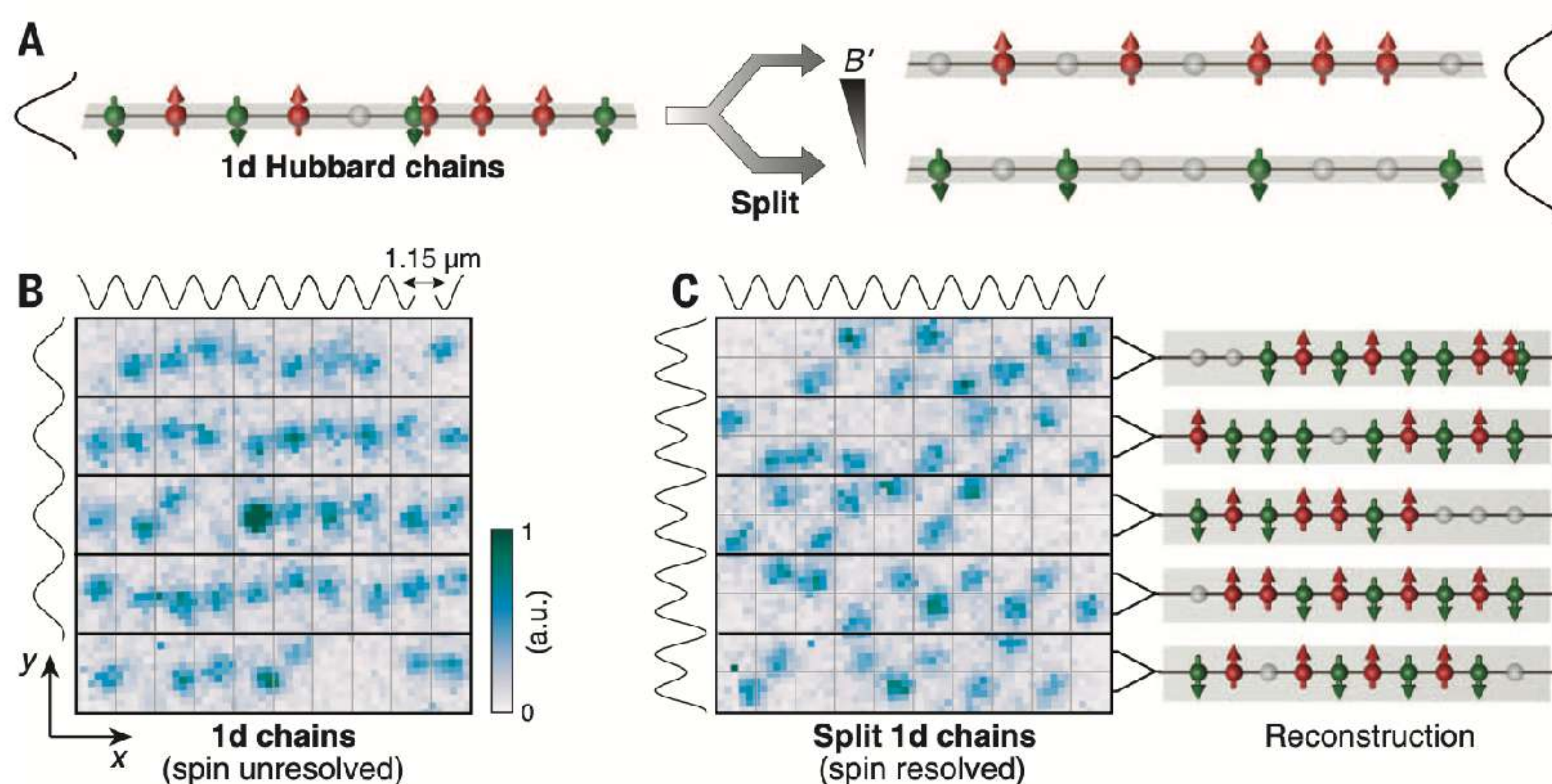
${}^6\text{Li}$



Spin- and density-resolved microscopy of antiferromagnetic correlations in Fermi-Hubbard chains

^6Li

Martin Boll,^{1*} Timon A. Hilker,^{1*} Guillaume Salomon,^{1*} Ahmed Omran,¹
Jacopo Nespolo,² Lode Pollet,² Immanuel Bloch,^{1,2} Christian Gross^{1†}



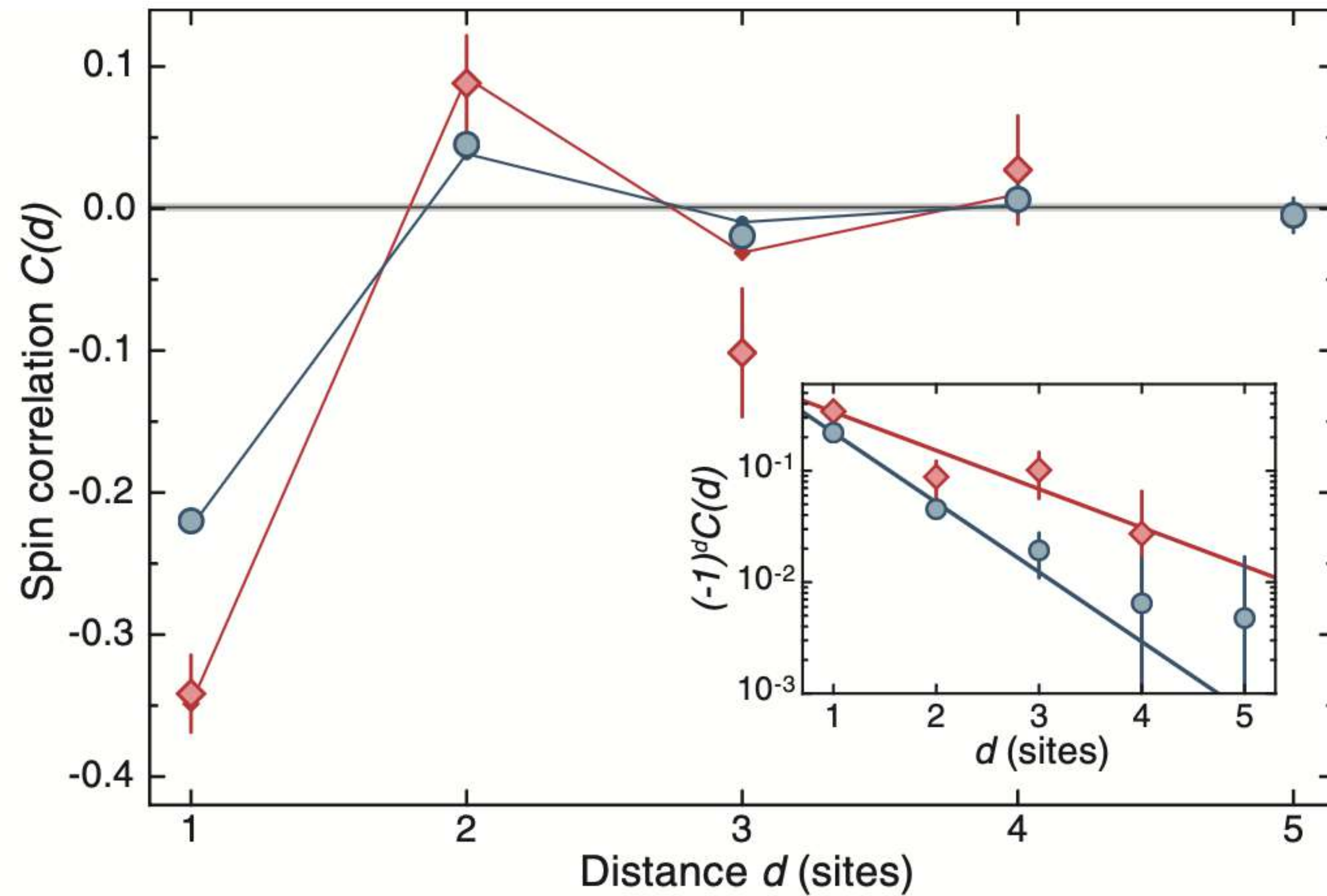
$U/t=12.6$

At half-filling

$S/N = 0.51(5)$

$S/N = 0.61(1)$

${}^6\text{Li}$



Observation of spatial charge and spin correlations in the 2D Fermi-Hubbard model

40K

Lawrence W. Cheuk,^{1*} Matthew A. Nichols,^{1*} Katherine R. Lawrence,¹ Melih Okan,¹
Hao Zhang,¹ Ehsan Khatami,² Nandini Trivedi,³ Thereza Paiva,⁴
Marcos Rigol,⁵ Martin W. Zwierlein^{1†}

SPIN

$$C_s(1) = \sum_{j \in \text{nn}_i} \left(\langle \hat{S}_{z,i} \hat{S}_{z,j} \rangle - \langle \hat{S}_{z,i} \rangle \langle \hat{S}_{z,j} \rangle \right)$$

CHARGE

$$C_m(1) = \frac{1}{4} \sum_{j \in \text{nn}_i} \left(\langle \hat{m}_{z,i}^2 \hat{m}_{z,j}^2 \rangle - \langle \hat{m}_{z,i}^2 \rangle \langle \hat{m}_{z,j}^2 \rangle \right)$$

CHARGE

$$\langle (m_i^z)^2 \rangle = \langle S_i^z S_i^z \rangle = \langle (n_{i,\uparrow} - n_{i,\downarrow})^2 \rangle \quad \rightarrow \quad cccc$$

$$C_m(1) = \frac{1}{4} \sum_{j \in \text{nn}_i} (\langle \hat{m}_{z,i}^2 \hat{m}_{z,j}^2 \rangle - \langle \hat{m}_{z,i}^2 \rangle \langle \hat{m}_{z,j}^2 \rangle) \quad \rightarrow \quad ccccccccc$$

Use Wick's theorem to write in terms of single-particle Green's function

CHARGE

$$\langle (m_i^z)^2 \rangle = \langle S_i^z S_i^z \rangle = \langle (n_{i,\uparrow} - n_{i,\downarrow})^2 \rangle \quad \rightarrow \quad cccc$$

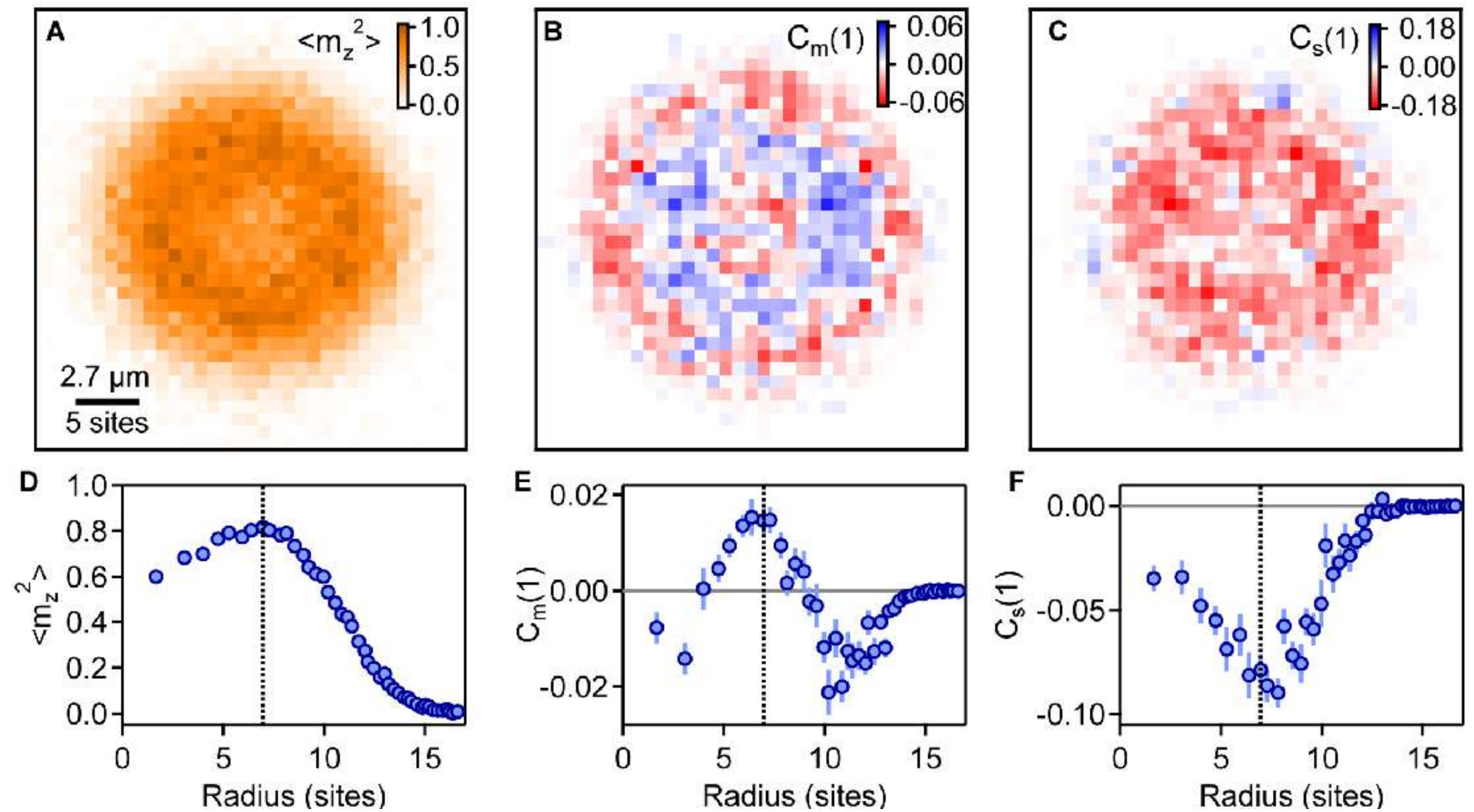
$$C_m(1) = \frac{1}{4} \sum_{j \in \text{nn}_i} (\langle \hat{m}_{z,i}^2 \hat{m}_{z,j}^2 \rangle - \langle \hat{m}_{z,i}^2 \rangle \langle \hat{m}_{z,j}^2 \rangle) \quad \rightarrow \quad ccccccccc$$

Use Wick's theorem to write in terms of
single-particle Green's function

Many pages of calculations....

No assumption
about trap shape

$$U/t=7.2(1)$$



$$\langle \hat{m}_{z,i}^2 \rangle = \langle (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 \rangle$$



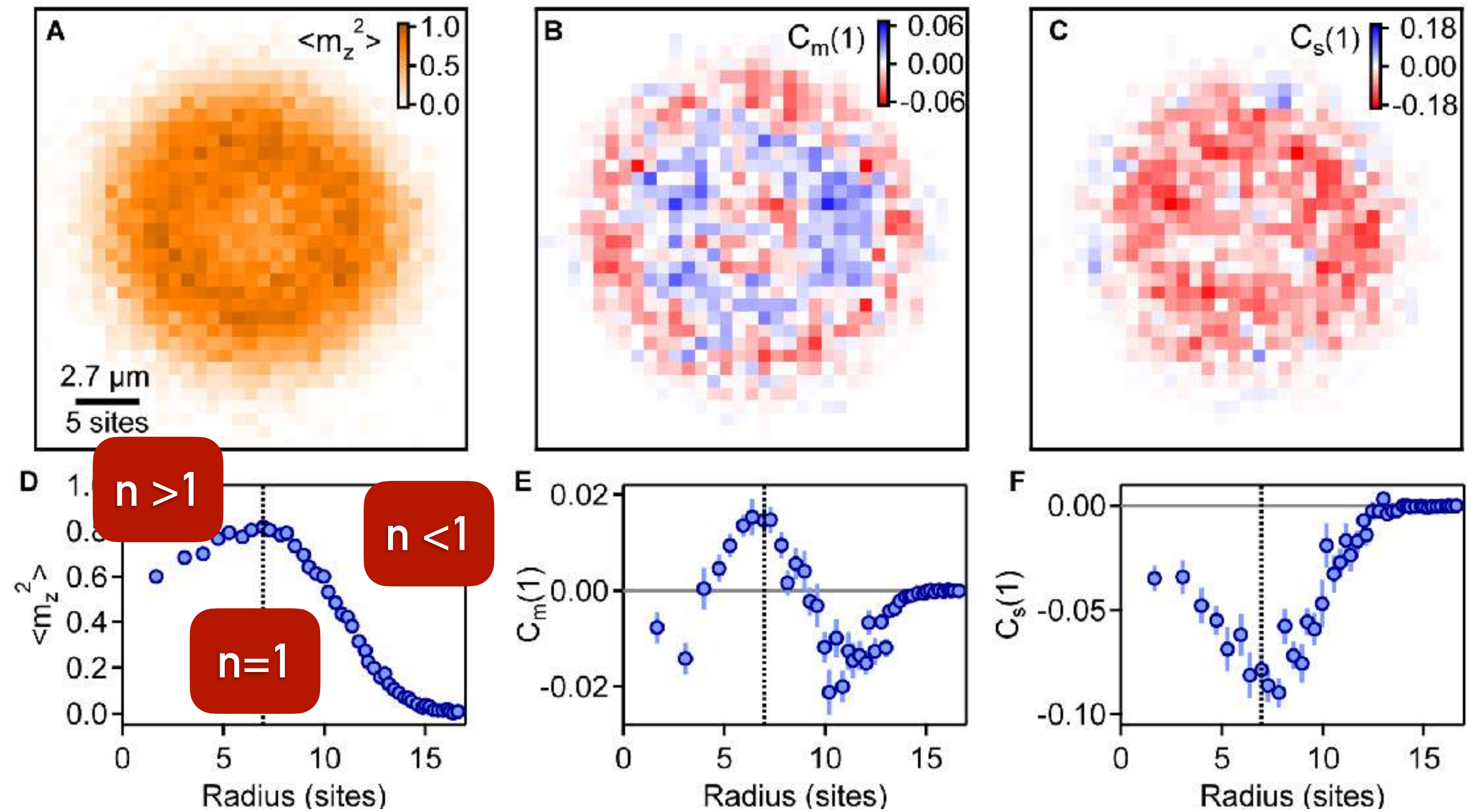
Charge



Spin

No assumption
about trap shape

$$U/t=7.2(1)$$



$$\langle \hat{m}_{z,i}^2 \rangle = \langle (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 \rangle$$

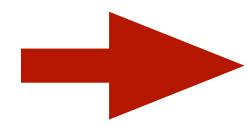


Charge



Spin

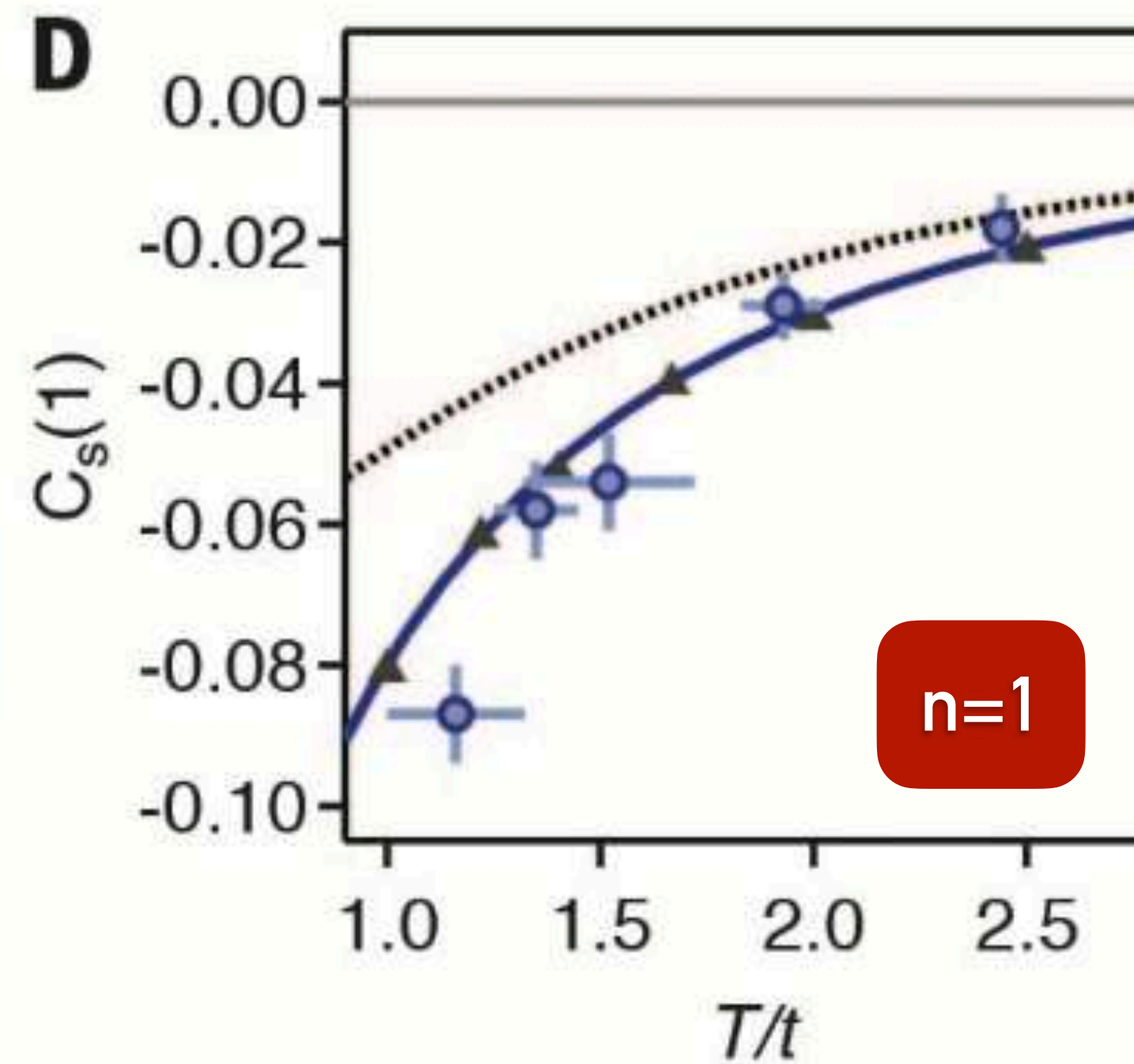
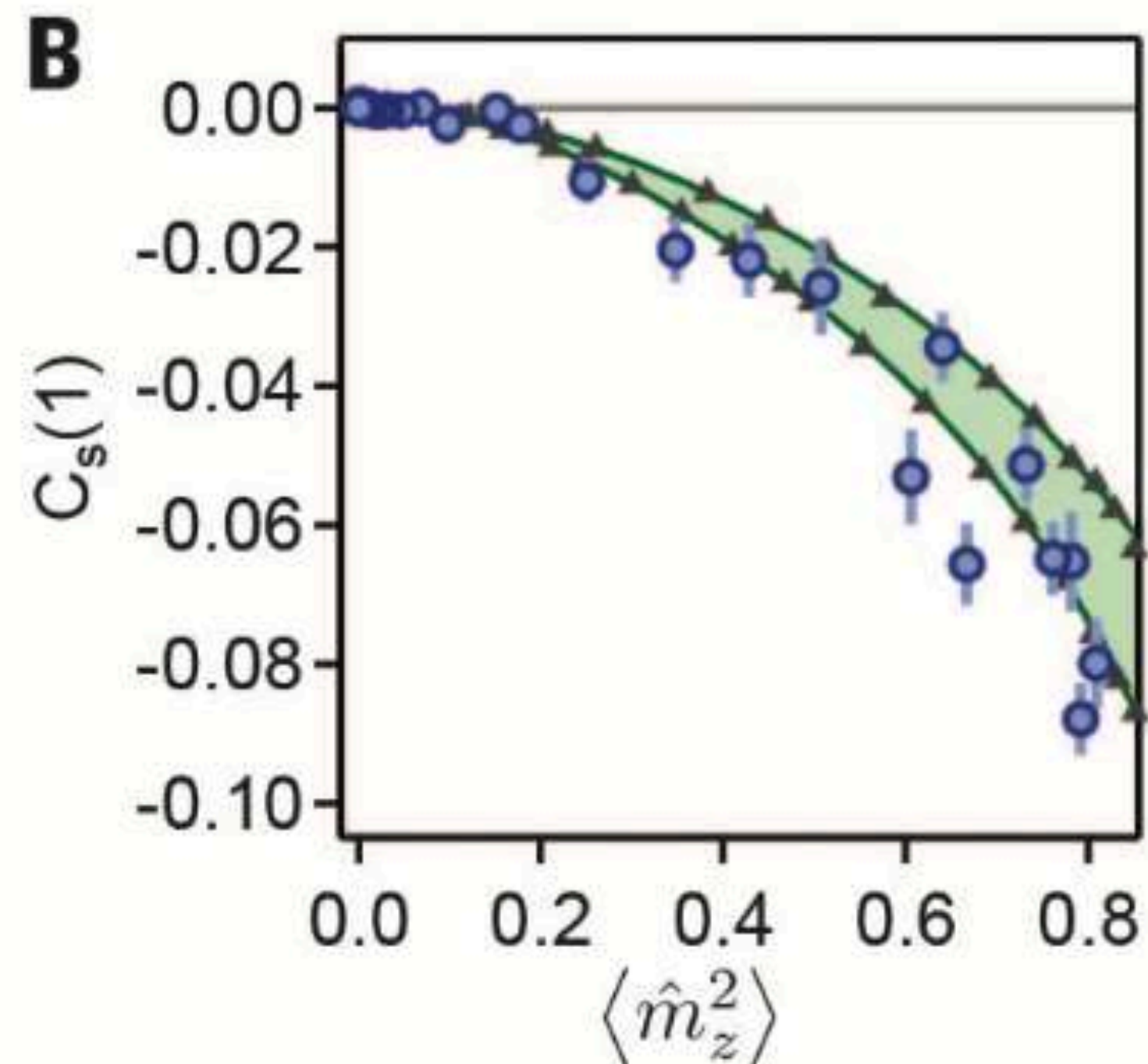
No assumption
about trap shape



Local moment

$$\langle \hat{m}_{z,i}^2 \rangle = \langle (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 \rangle$$

Spin



Green area
 $0.89 < T/t < 1.22$

Dotted line $U=0$

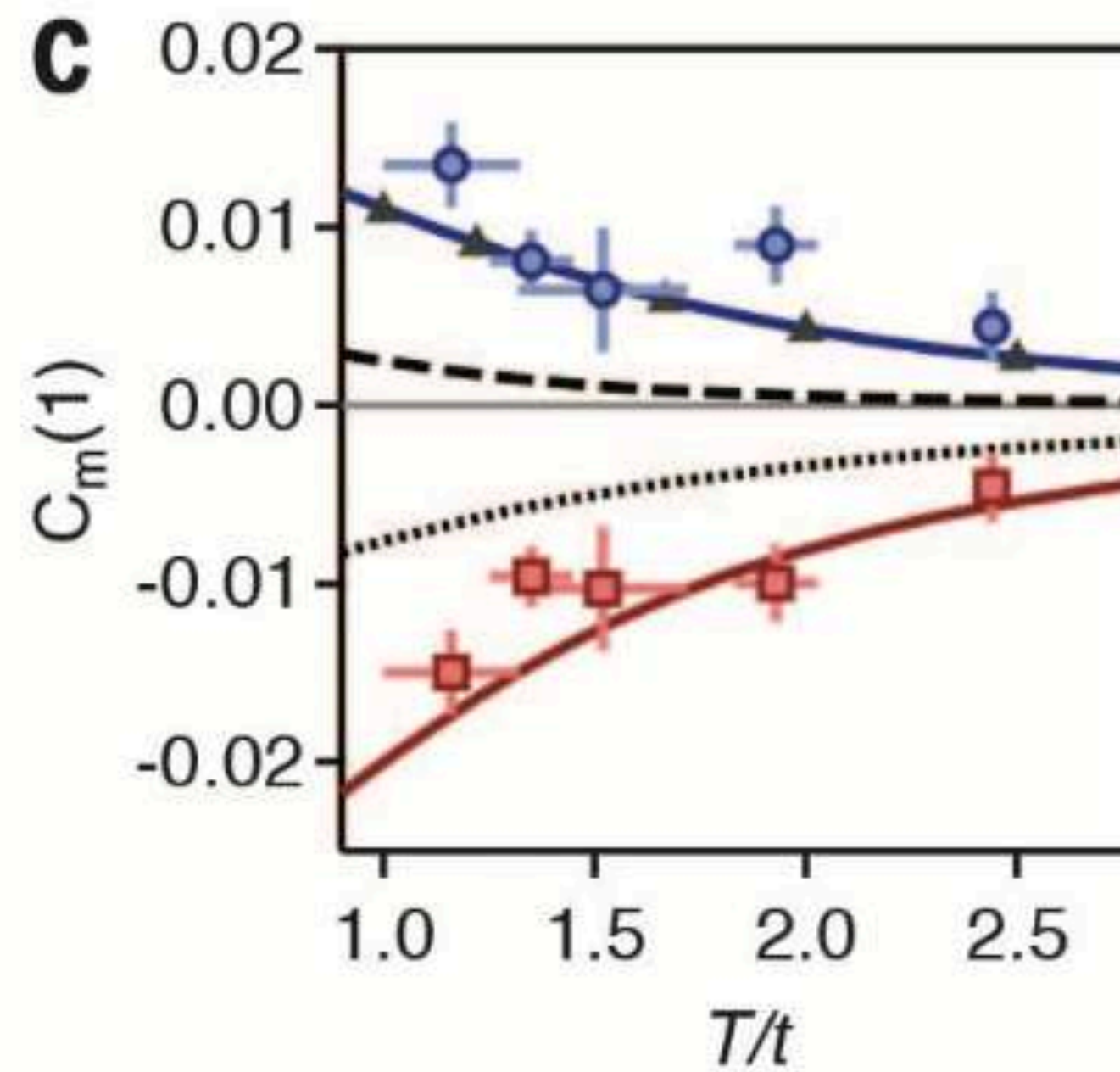
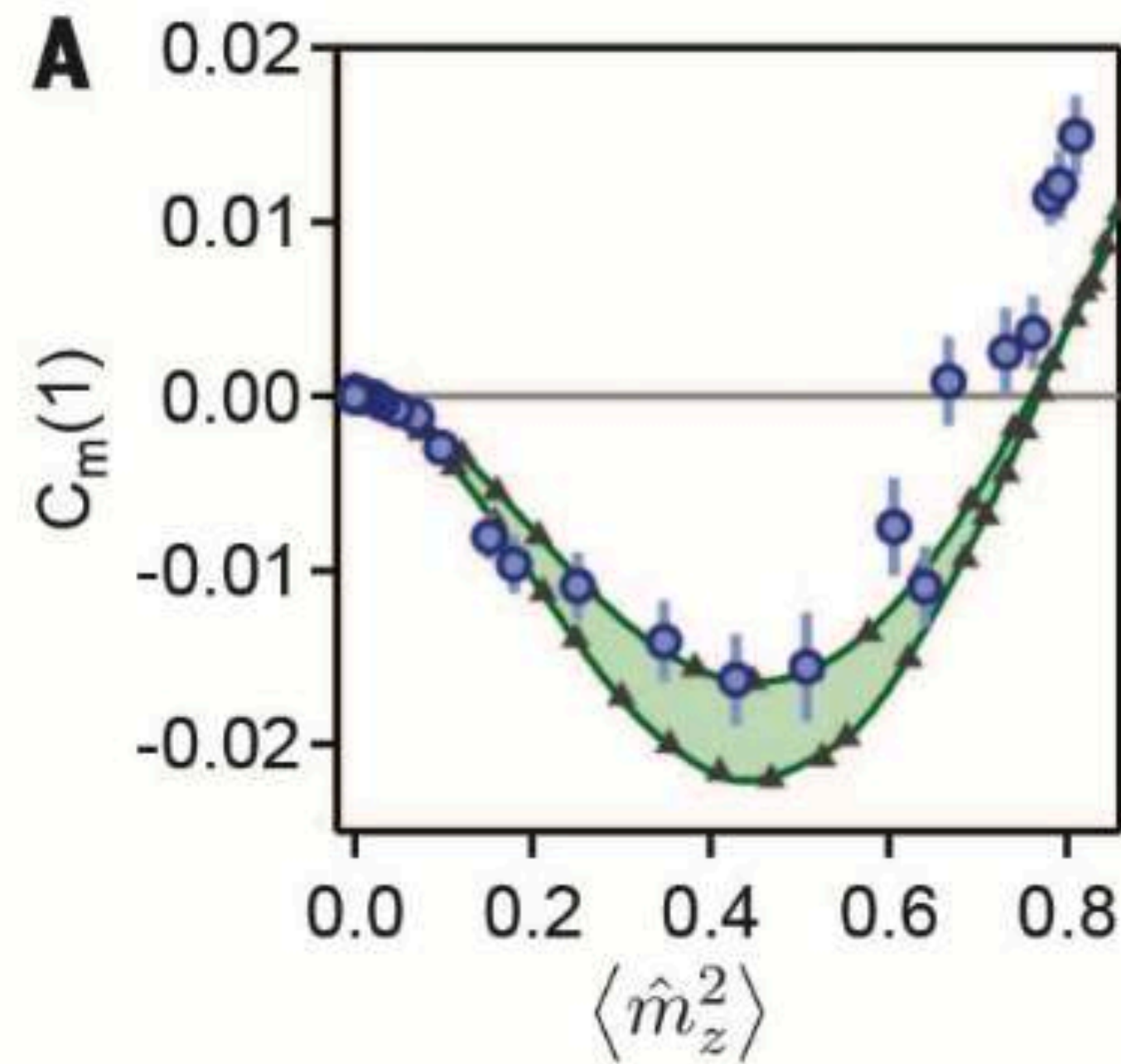
$U/t=7.2(1)$

Spin correlations increase close to half-filling

$C_s(1) < 0$ even when $U=0$ due to Pauli blocking

Correlations increase the effect

Charge



Green area
 $0.89 < T/t < 1.22$

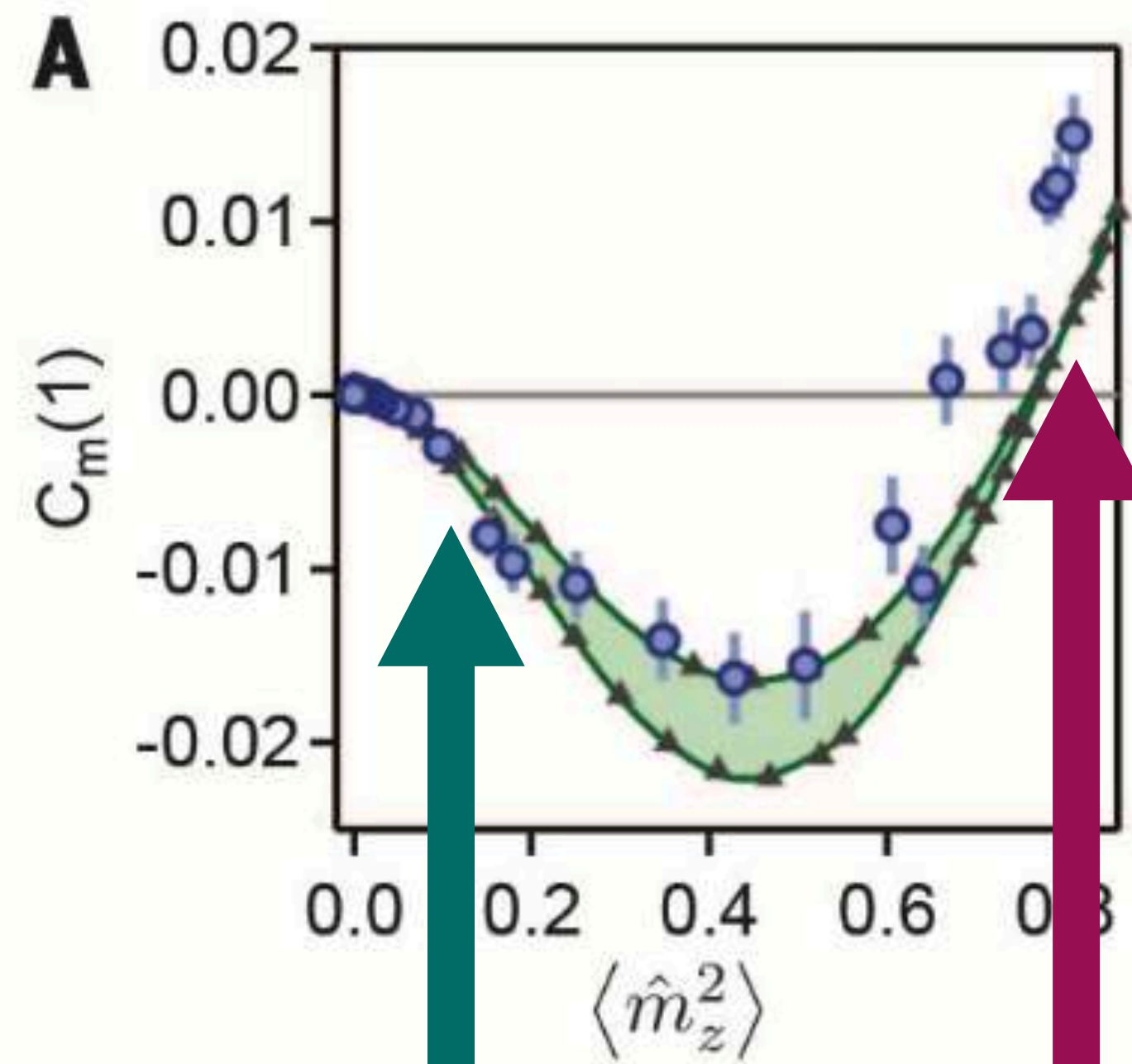
Dotted line $U=0$

$U/t=7.2(1)$

Maxima $n=1$

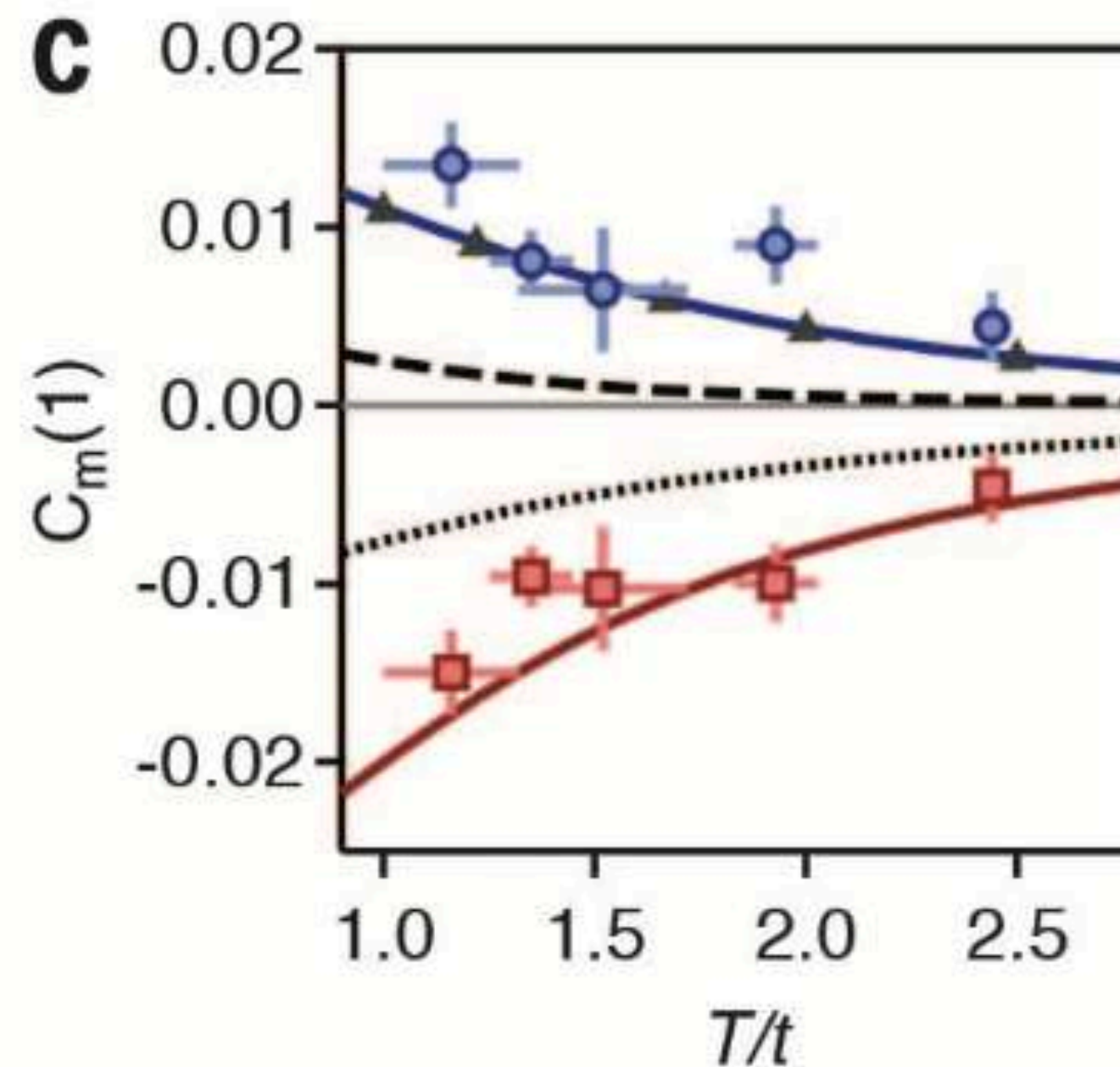
Minima

Charge



Anti-bunching

Repulsive



Bunching

Attractive

Green area
 $0.89 < T/t < 1.22$

Dotted line $U=0$

$U/t=7.2(1)$

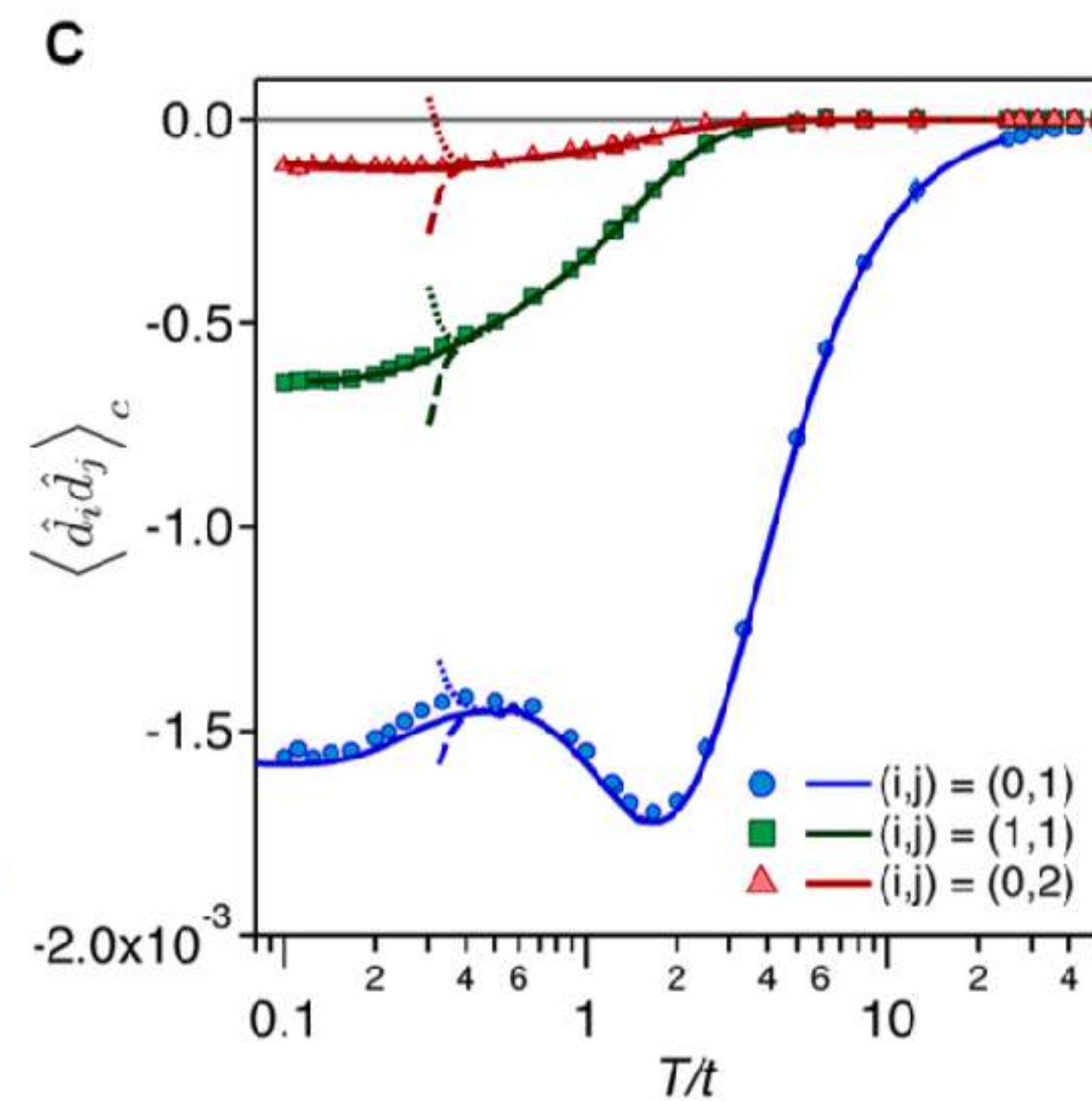
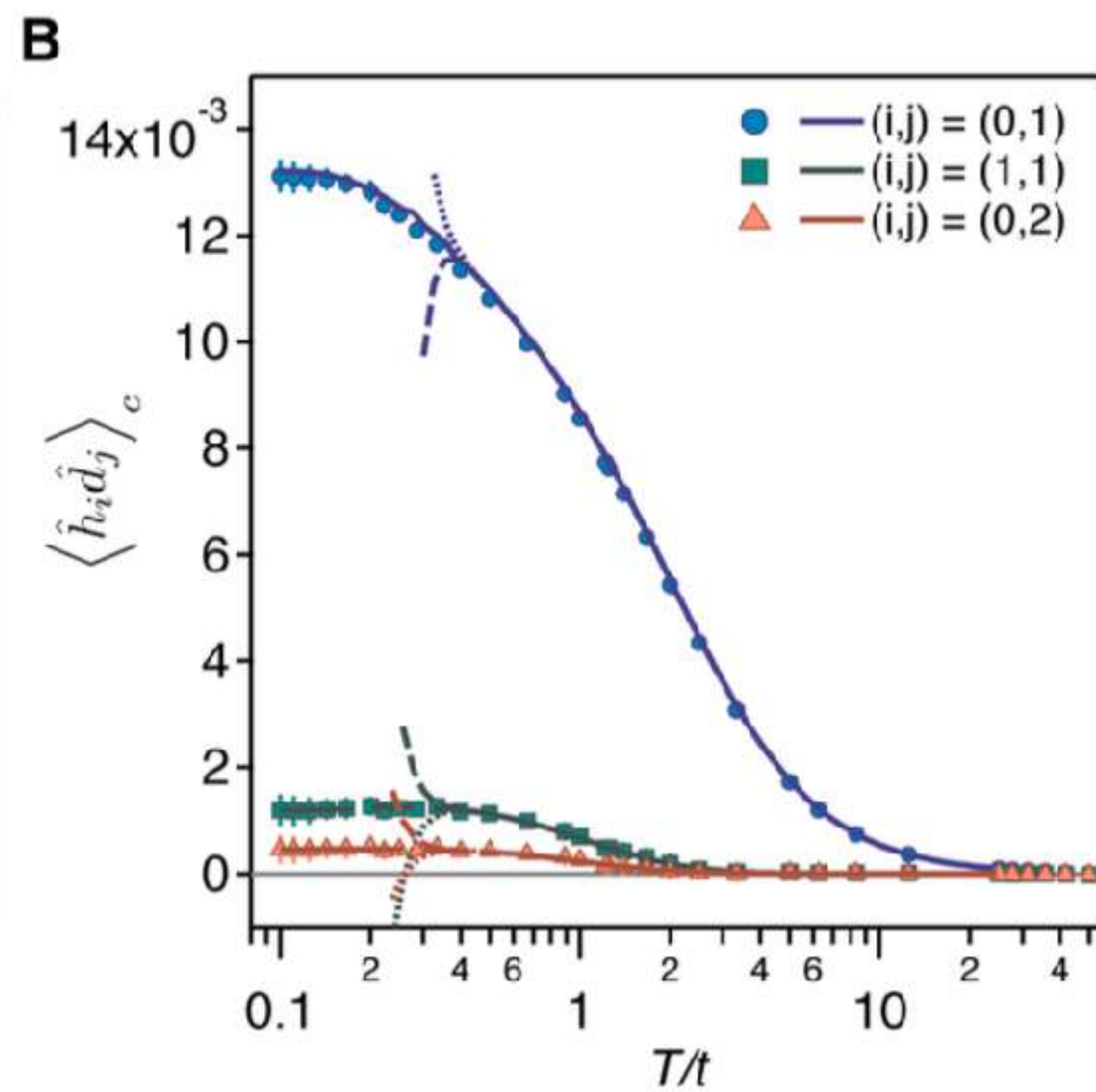
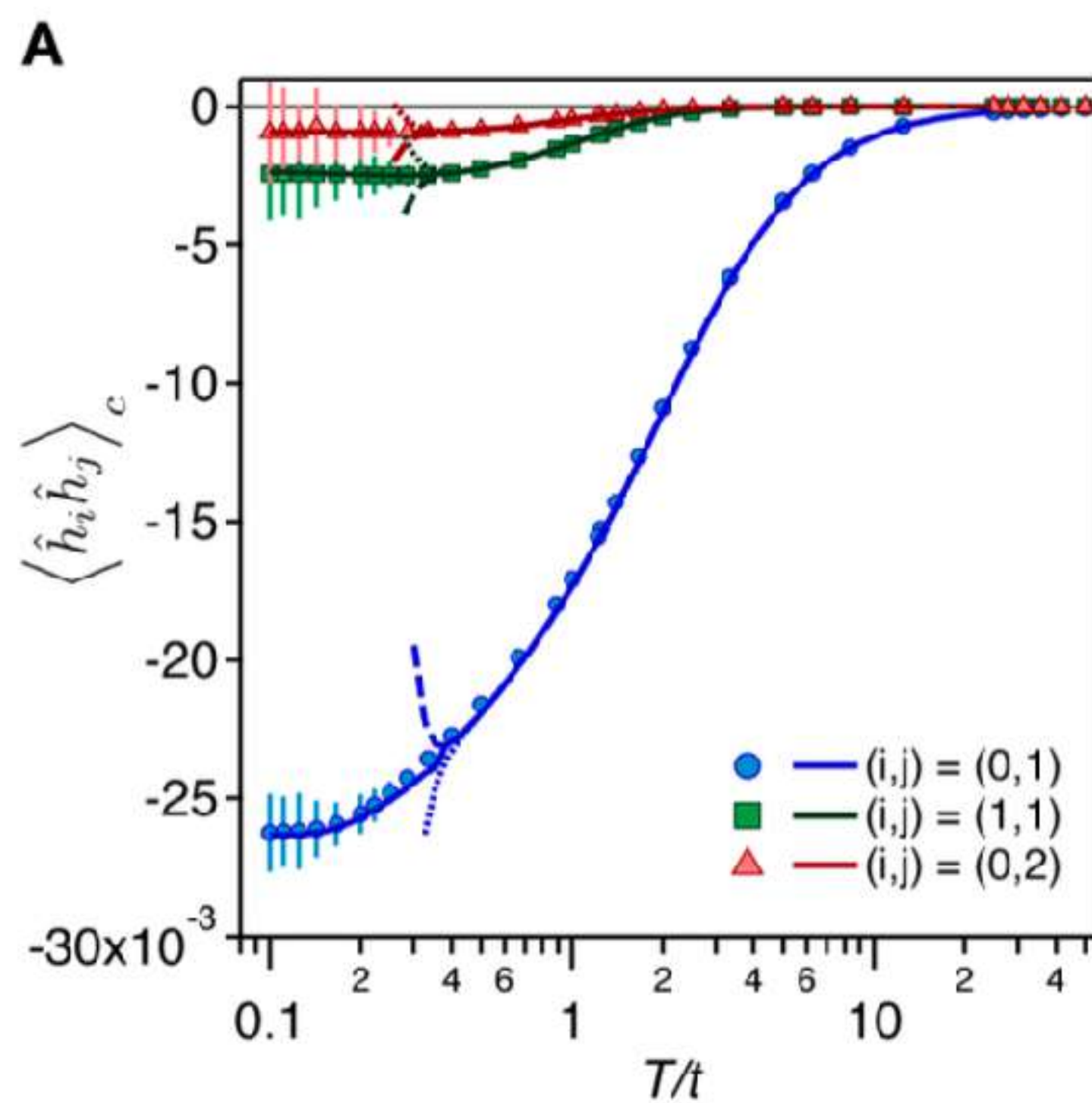
Maxima $n=1$

Minima

Hole-hole

Hole-doublon

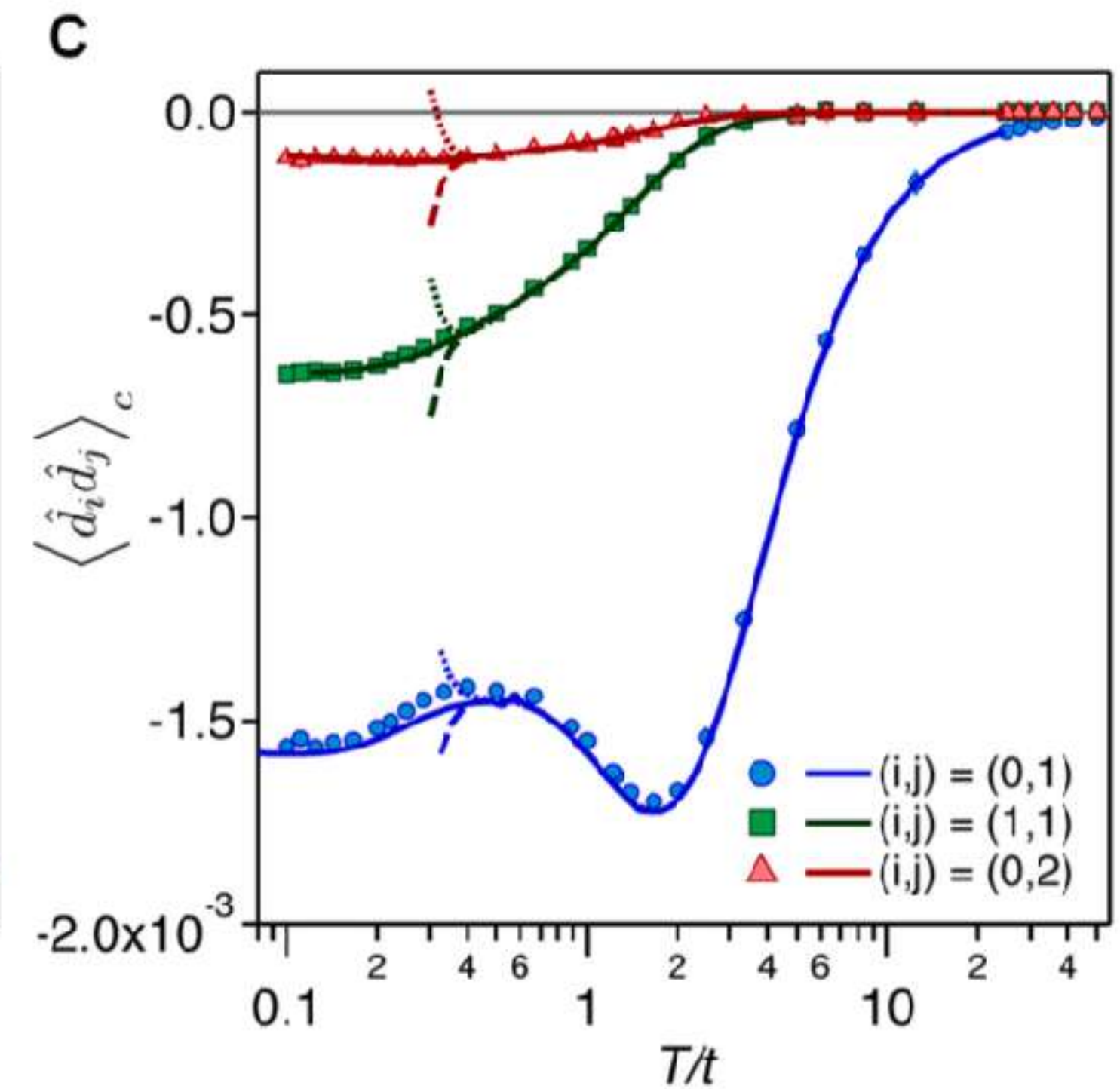
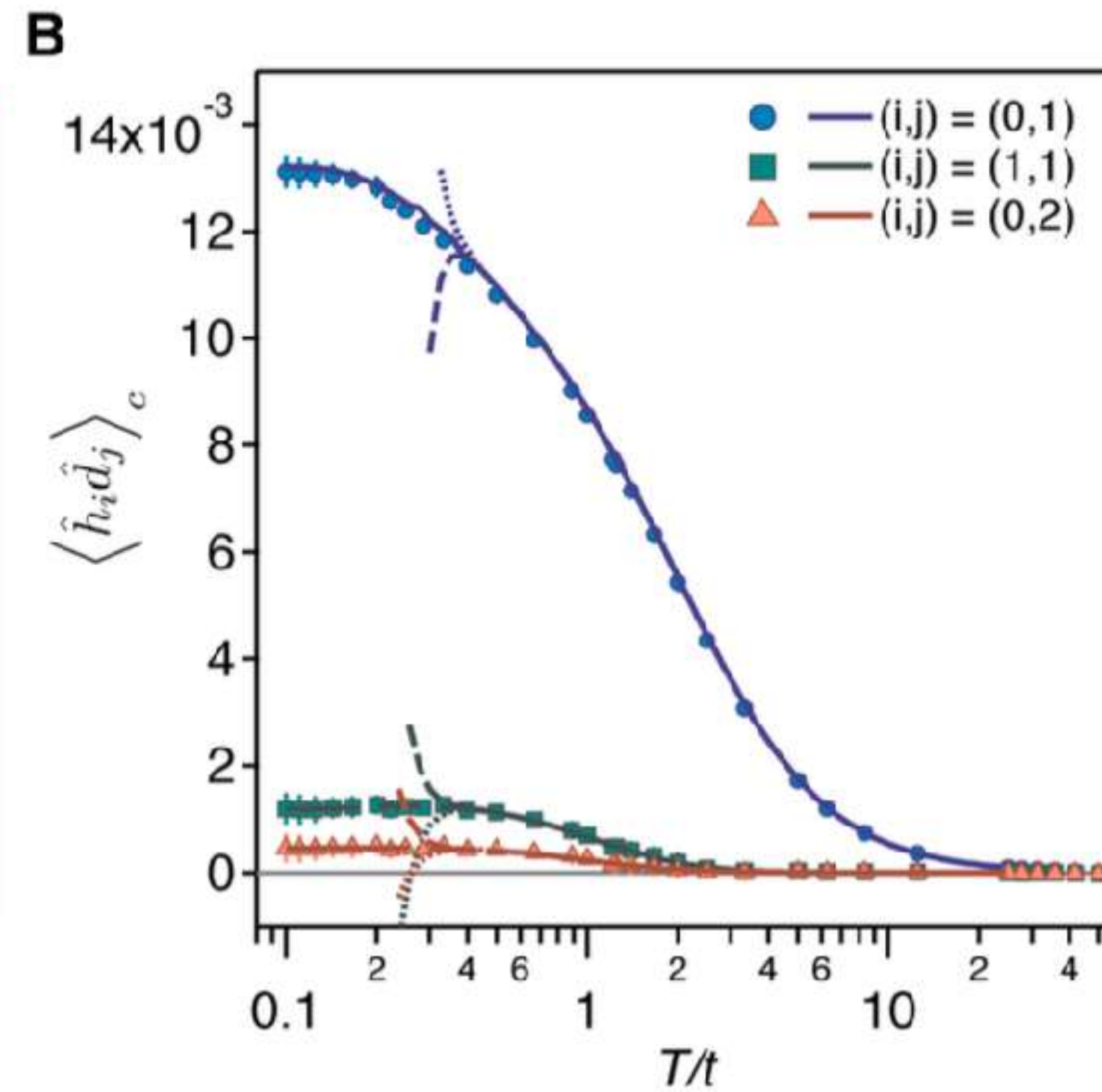
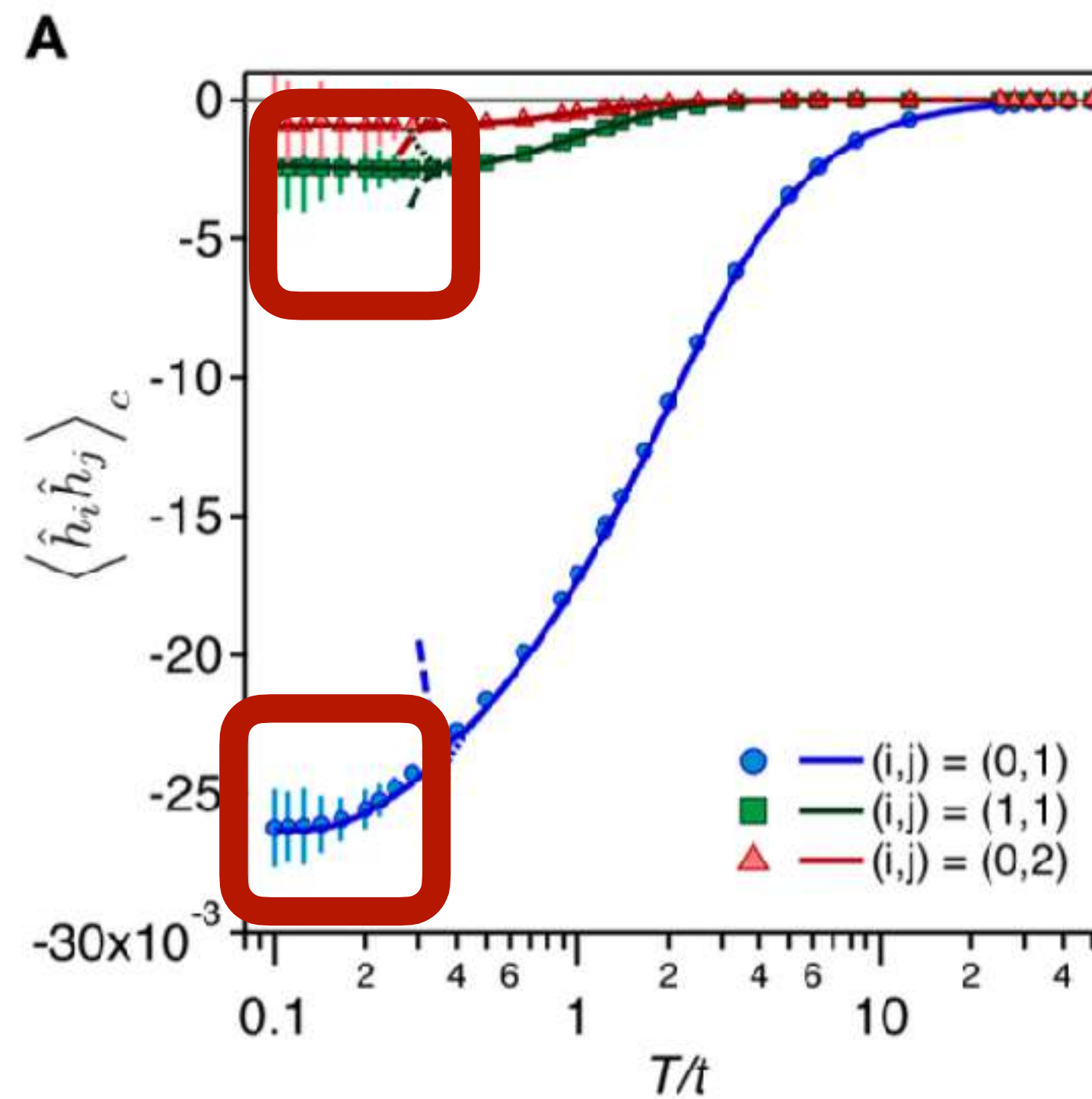
Doublon-doublon



Hole-hole

Hole-doublon

Doublon-doublon

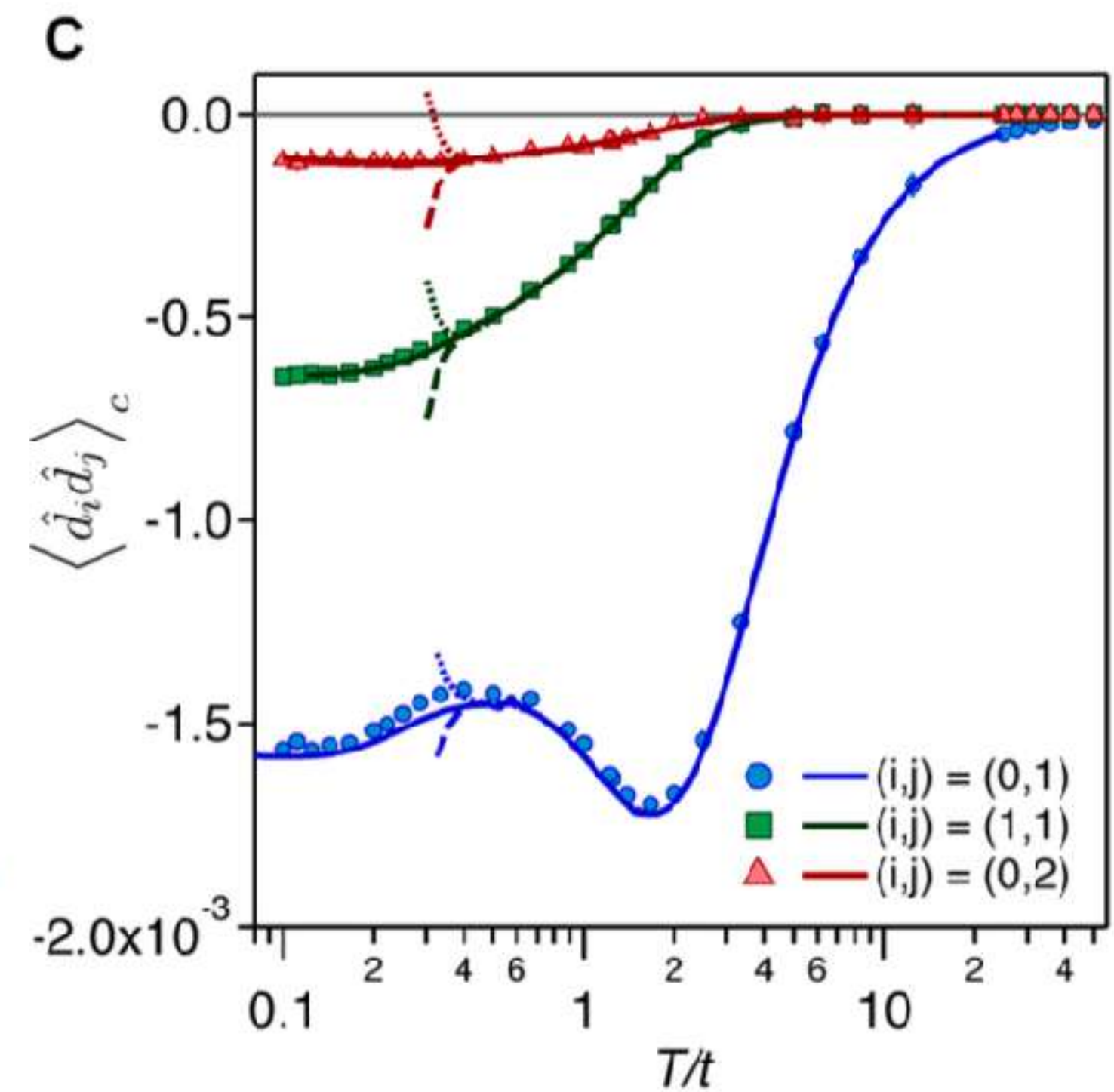
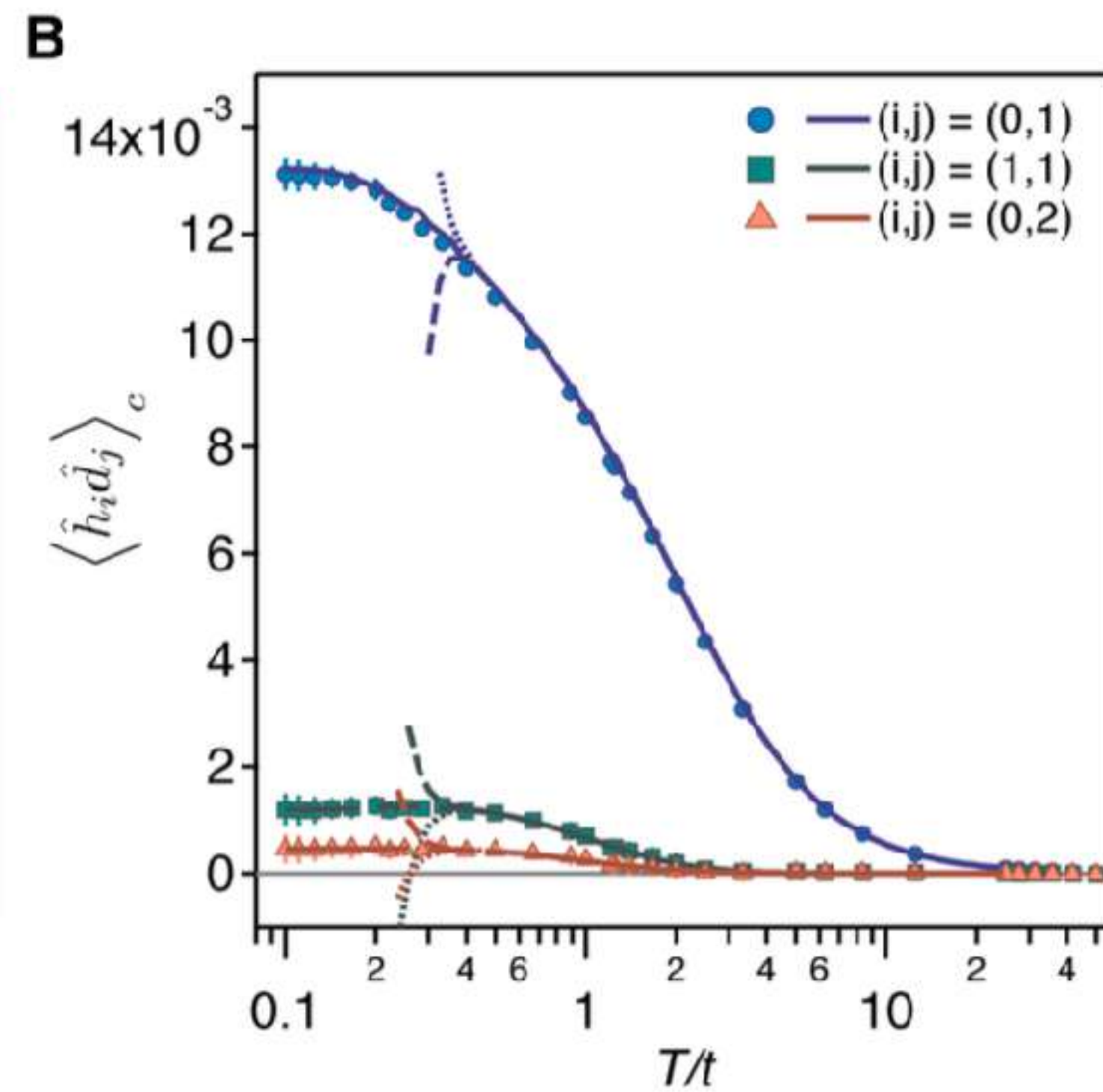
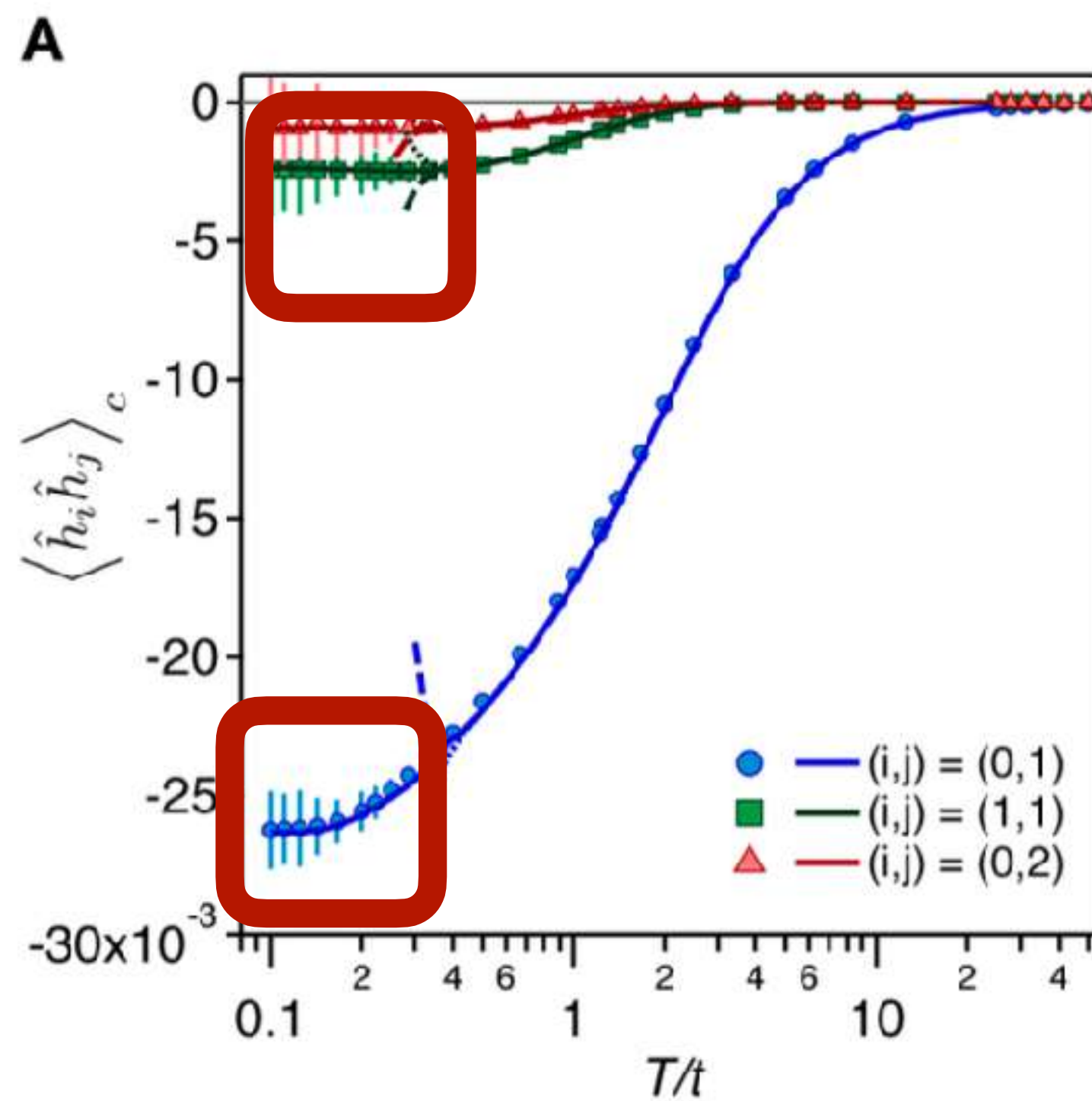


Big error bars: statistics?

Hole-hole

Hole-doublon

Doublon-doublon



Big error bars: statistics?

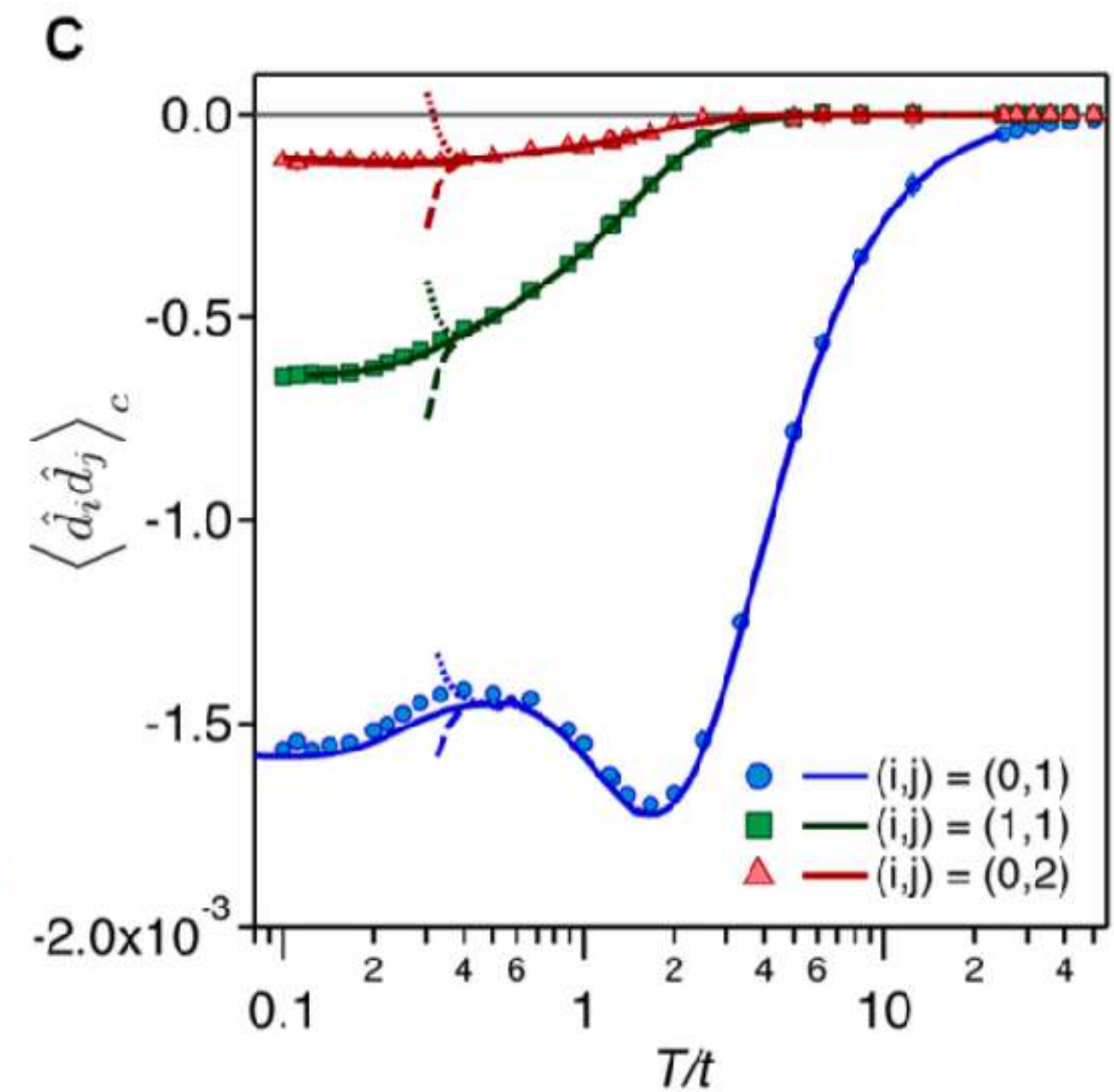
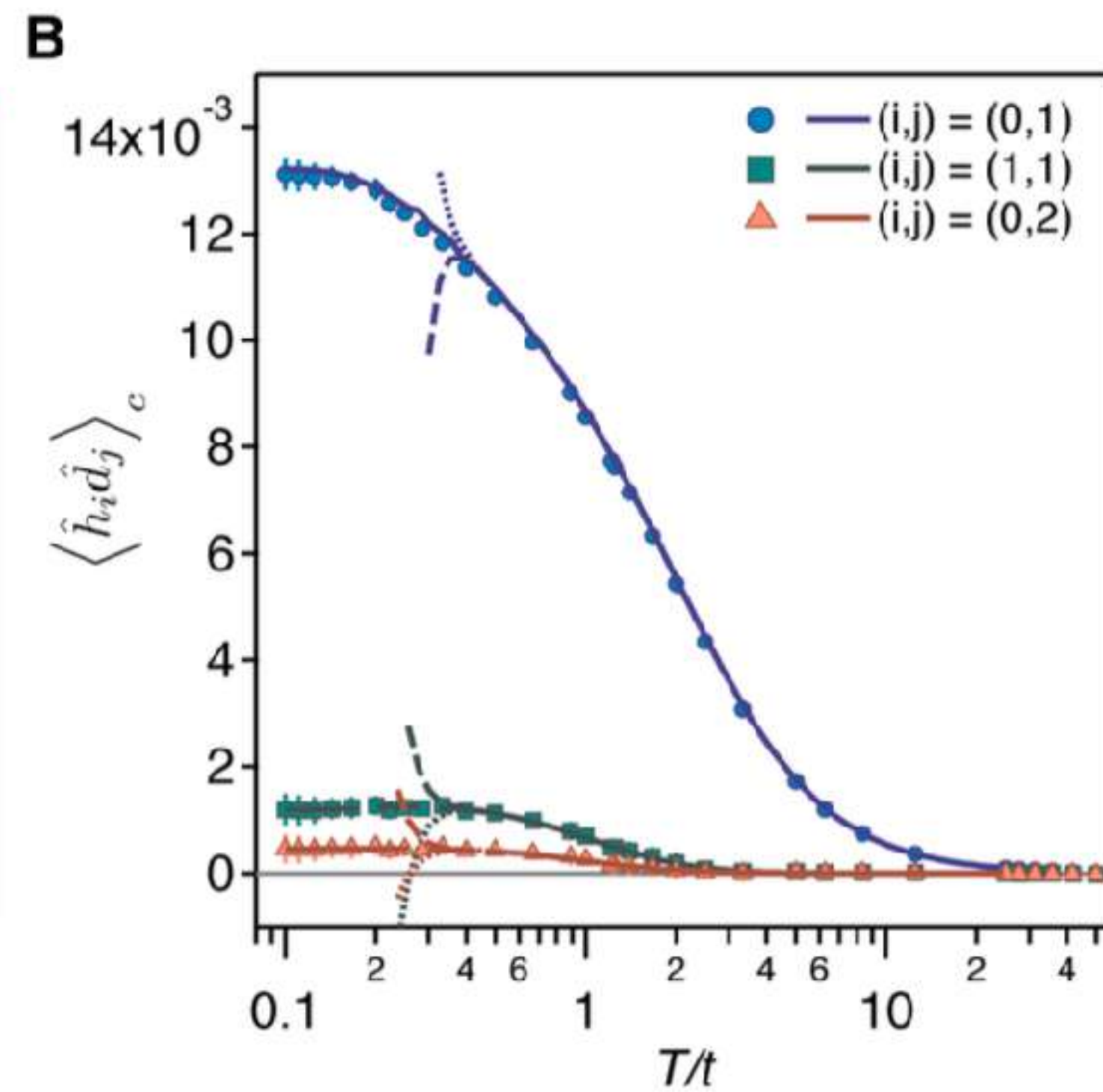
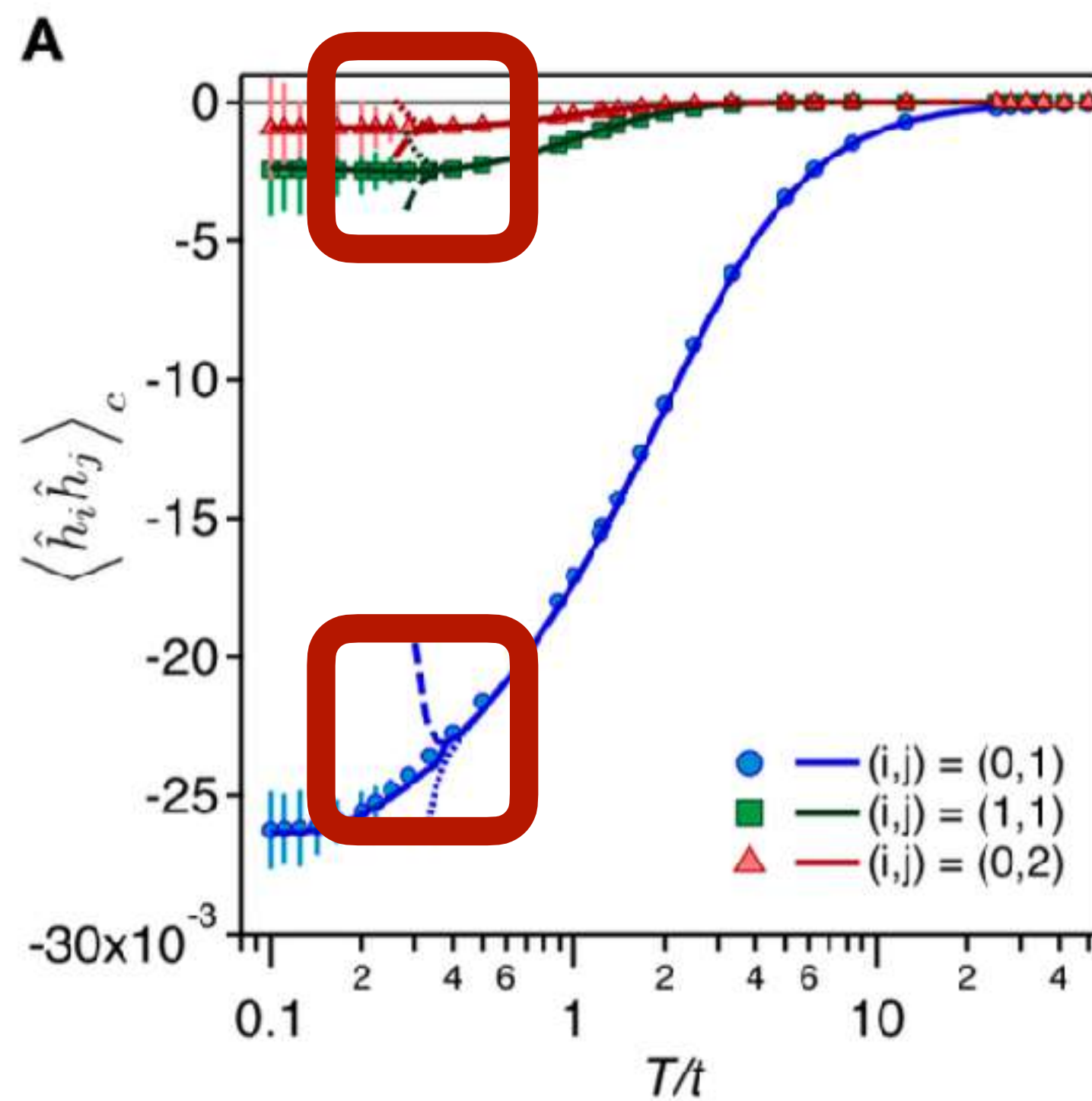


cccccccc

Hole-hole

Hole-doublon

Doublon-doublon



Convergence of NLCE

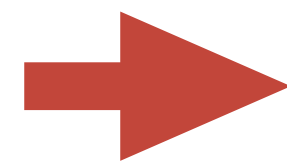
Spin-imbalance in a 2D Fermi-Hubbard system

Peter T. Brown,¹ Debayan Mitra,¹ Elmer Guardado-Sanchez,¹ Peter Schauß,¹
 Stanimir S. Kondov,^{1*} Ehsan Khatami,² Thereza Paiva,³ Nandini Trivedi,⁴
 David A. Huse,¹ Waseem S. Bakr^{1†}

⁶Li

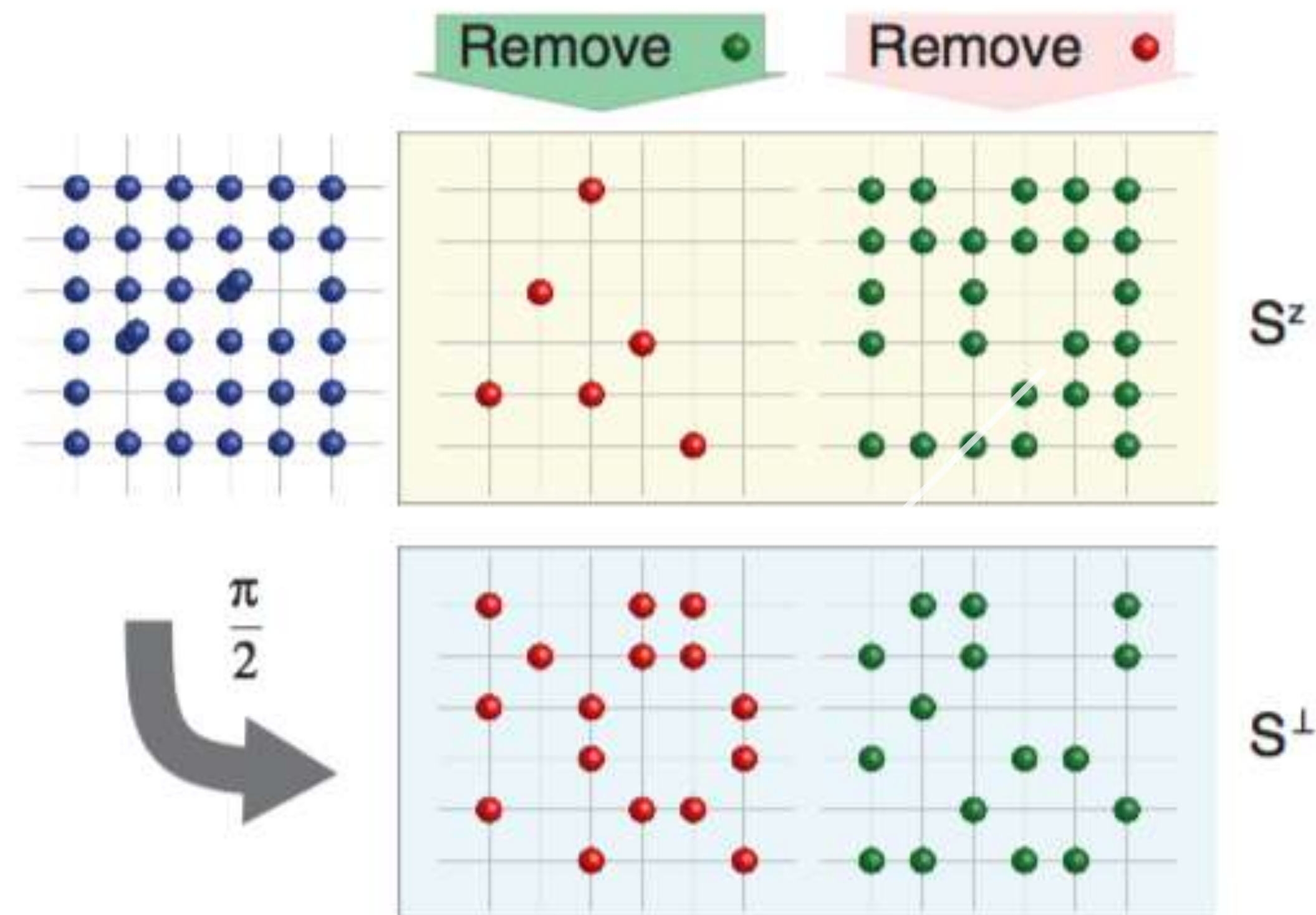
$U/t=8.0(5)$

Spin impalance



$$P = \frac{N \begin{array}{|c|} \hline \uparrow \\ \hline \end{array} - N \begin{array}{|c|} \hline \downarrow \\ \hline \end{array}}{N \begin{array}{|c|} \hline \uparrow \\ \hline \end{array} + N \begin{array}{|c|} \hline \downarrow \\ \hline \end{array}}$$

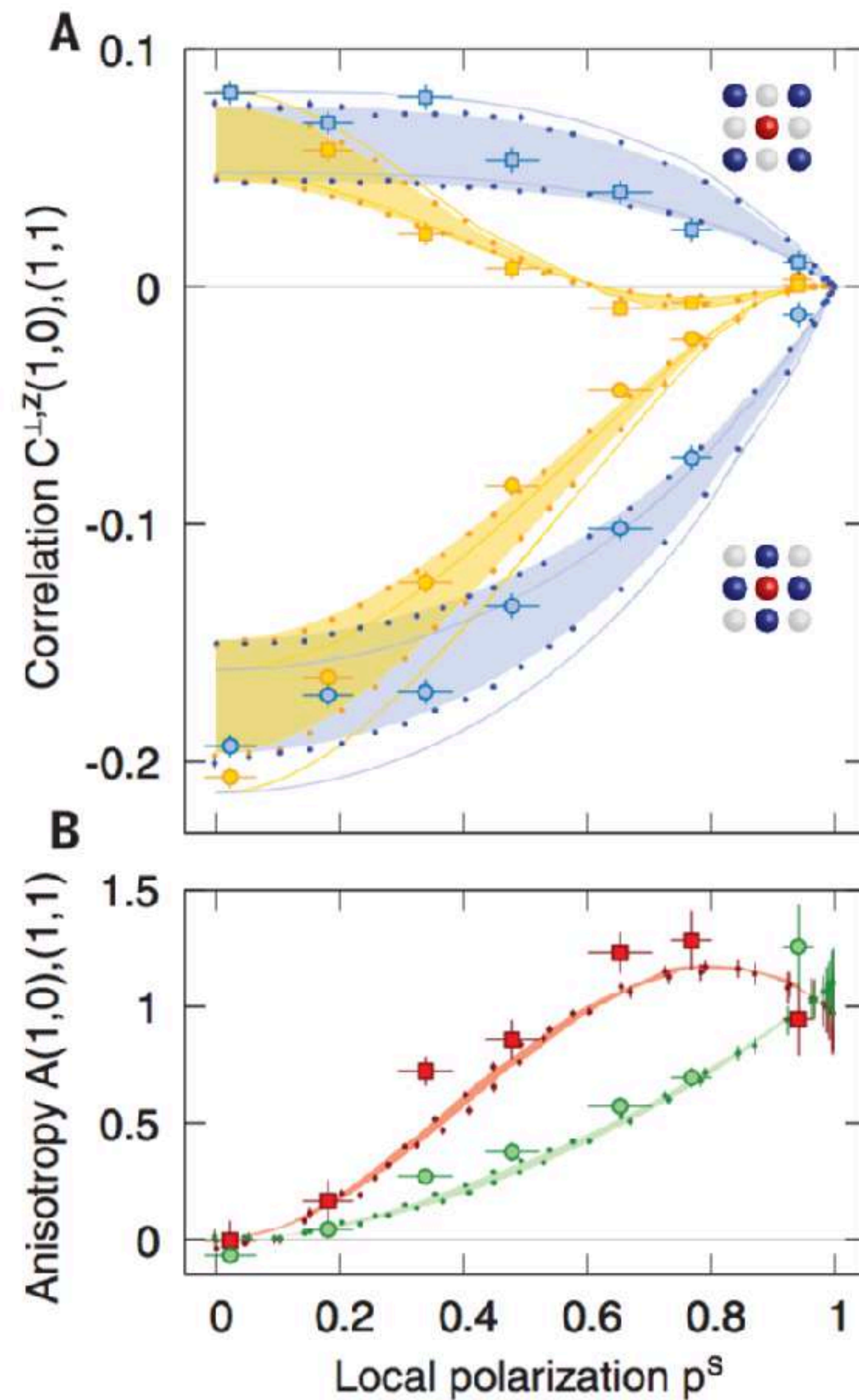
$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} (c_{i, \sigma}^\dagger c_{j, \sigma} + c_{j, \sigma}^\dagger c_{i, \sigma}) + U \sum_i n_{i, \uparrow} n_{i, \downarrow} - \bar{\mu} \sum_i (n_{i, \uparrow} + n_{i, \downarrow}) - 2h \sum_i S_i^z$$



Spin components

Along z C^z

Perpendicular to z $C^\perp$



$$0.38 \leq T/t \leq 0.53$$

$$8.4 \text{ nK} \leq T \leq 12.7 \text{ nK}$$

Along z C^z

Perpendicular to z $C^\perp$

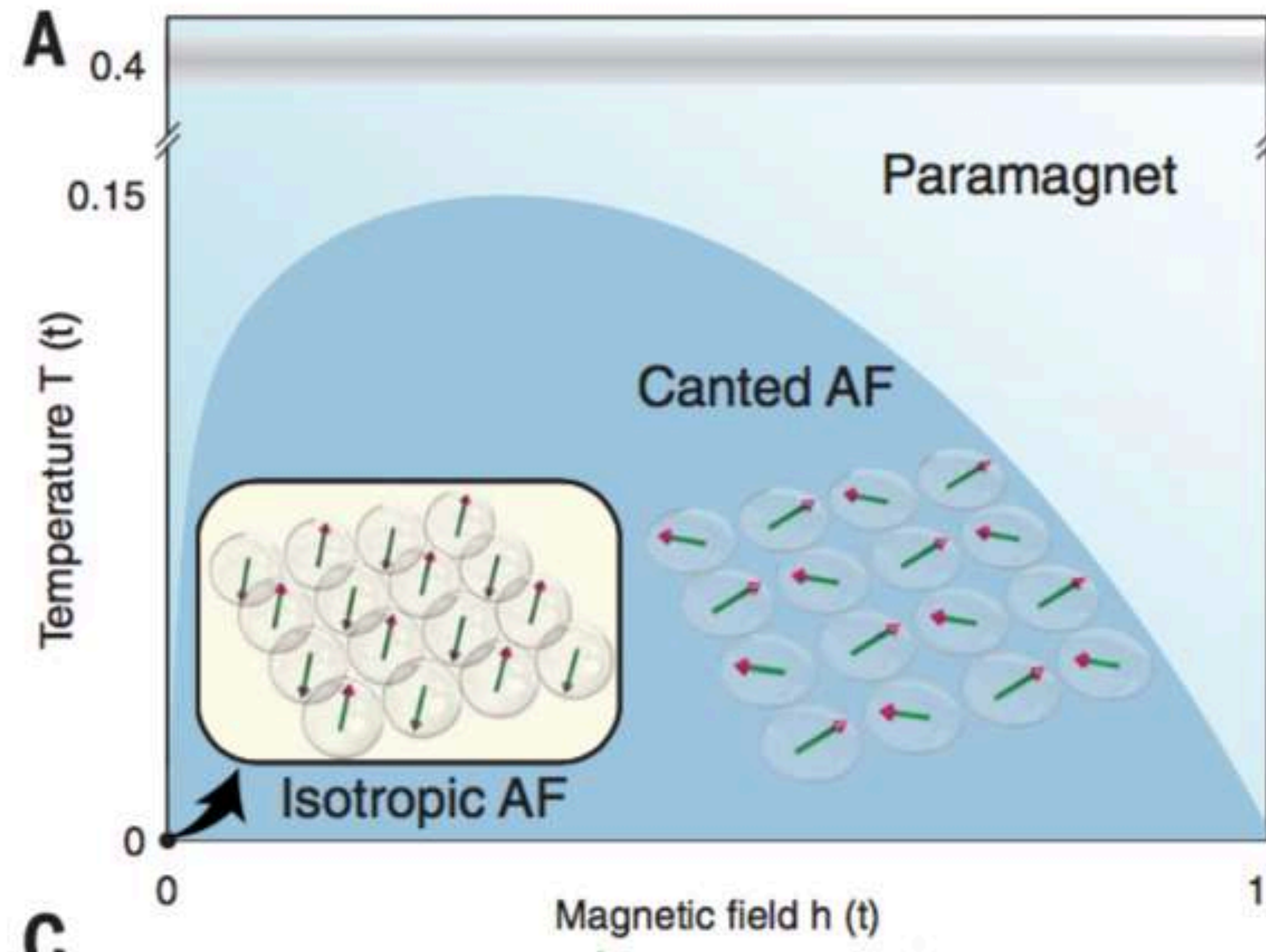
spin-spin
correlation
functions

$$A = 1 - C^z(1,0) / C^\perp(1,0)$$

$$A = 1 - C^z(1,1) / C^\perp(1,1)$$

Anisotropy

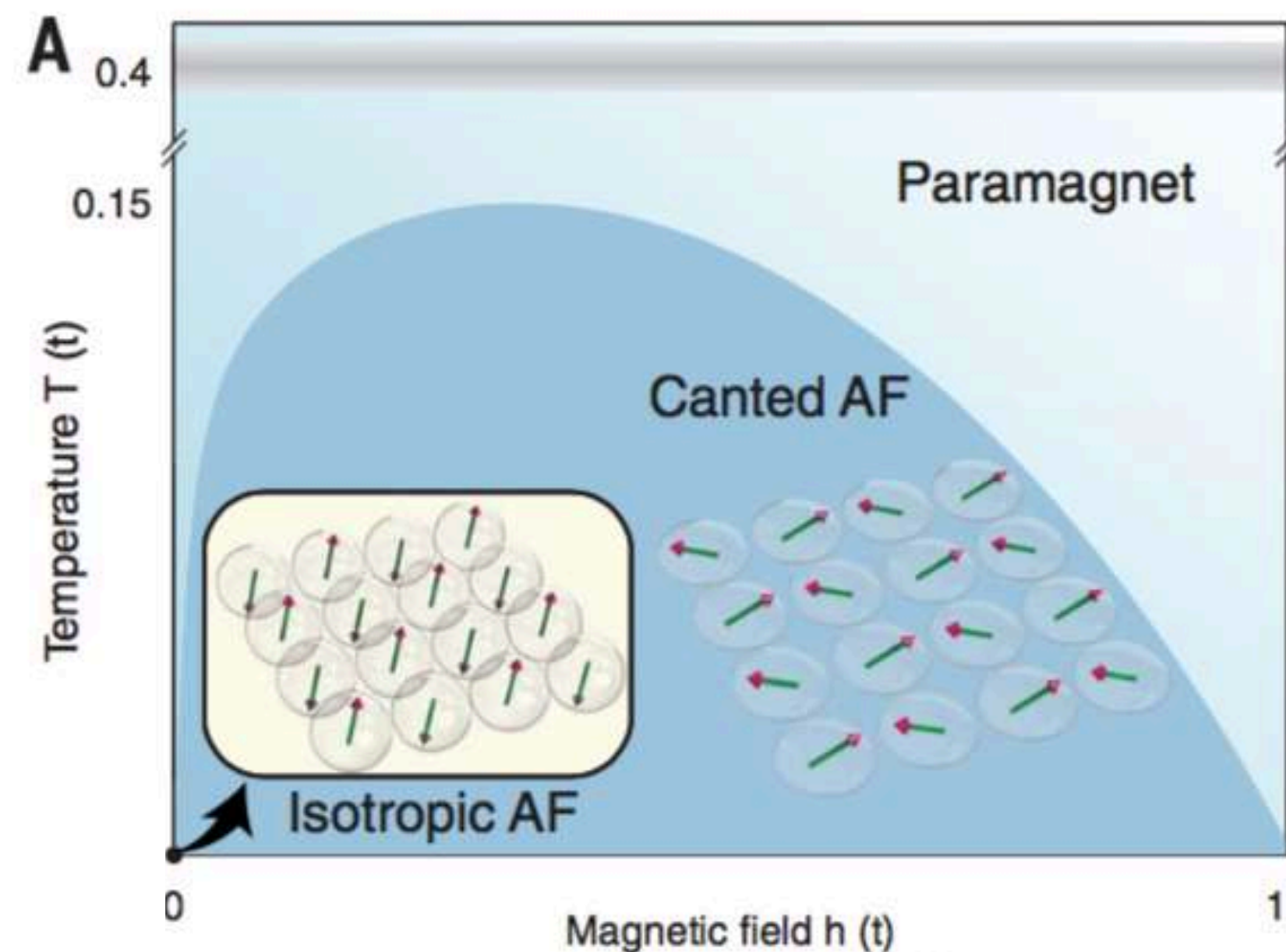
Canted antiferromagnetism



Spin-imbalance in a 2D Fermi-Hubbard system

P. Brown et. al, Science (2017)

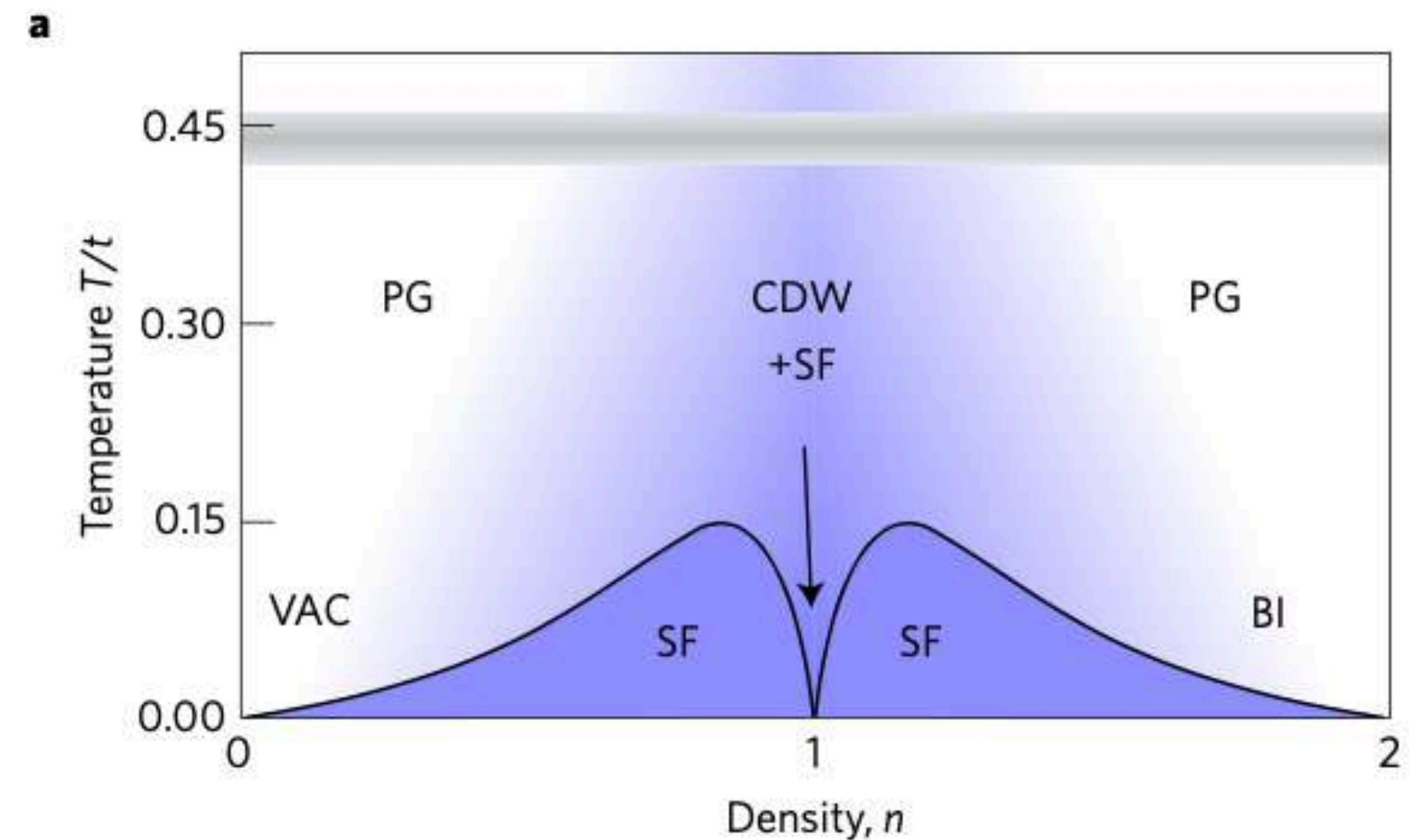
Repulsive Hubbard model with field h



Quantum gas microscopy of an attractive Fermi-Hubbard system

Mitra et al., Nat. Physics (2018)

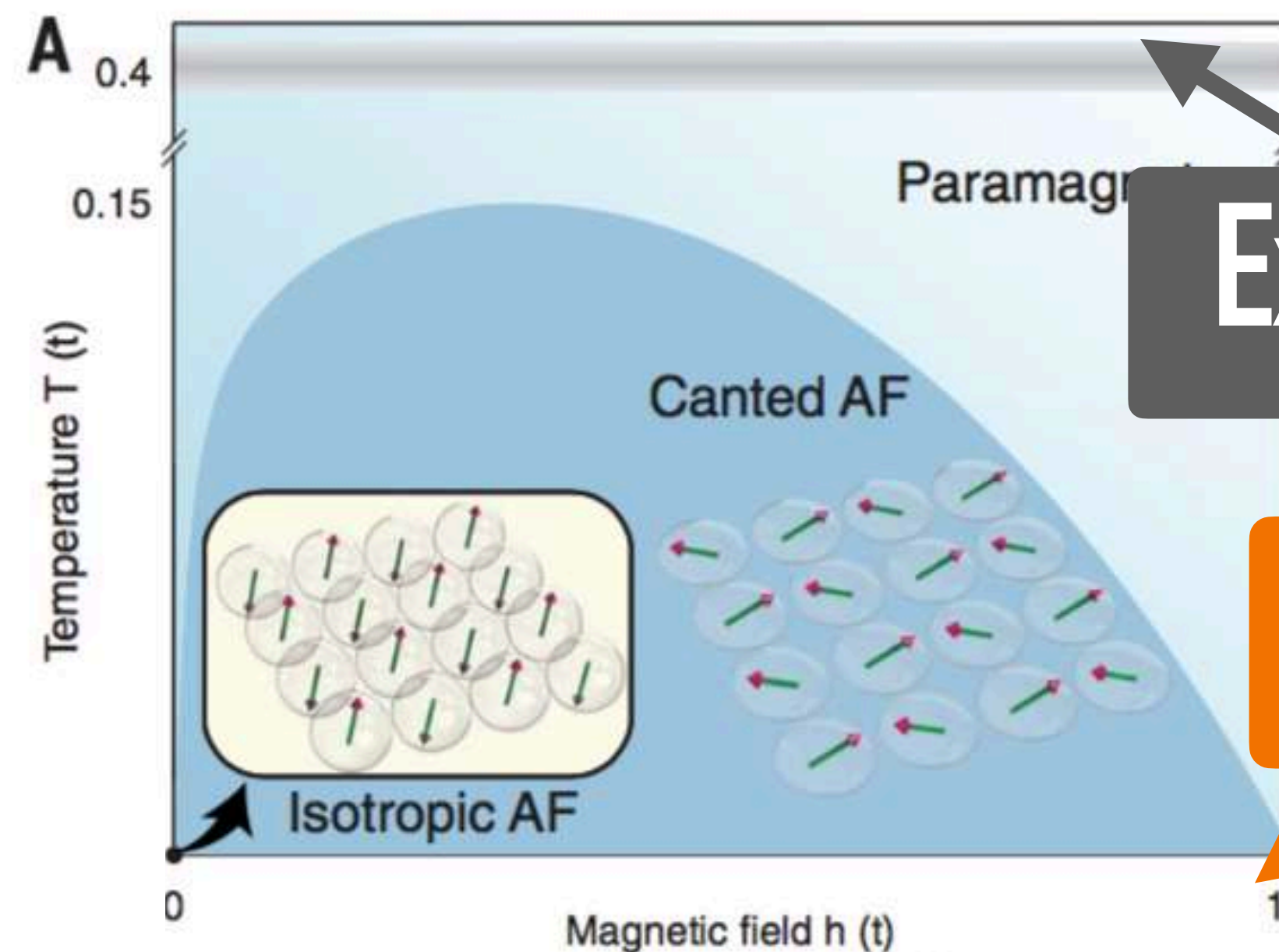
Attractive Hubbard model with doping n



Spin-imbalance in a 2D Fermi-Hubbard system

P. Brown et. al, Science (2017)

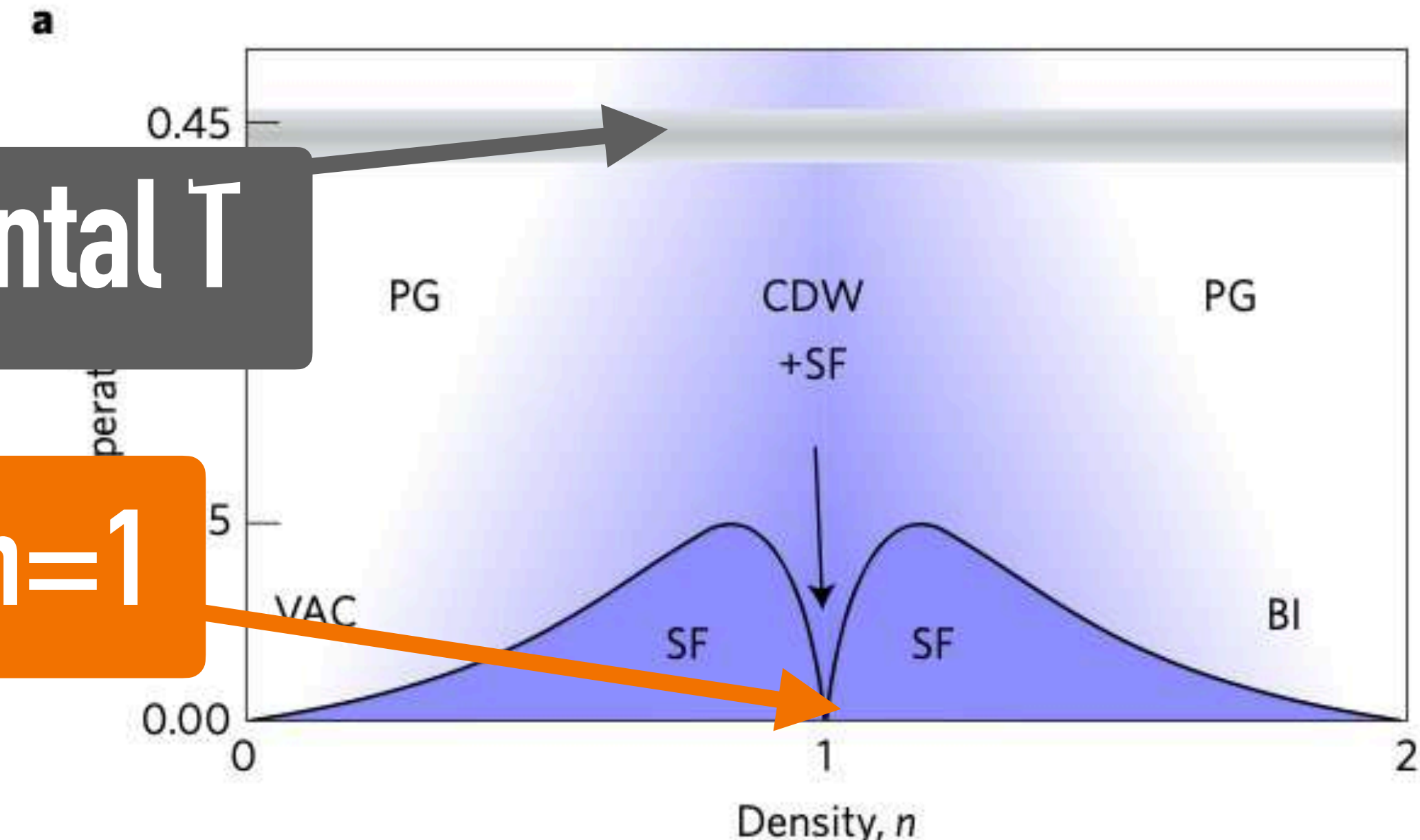
Repulsive Hubbard model with field h



Quantum gas microscopy of an attractive Fermi-Hubbard system

Mitra et al., Nat. Physics (2018)

Attractive Hubbard model with doping n



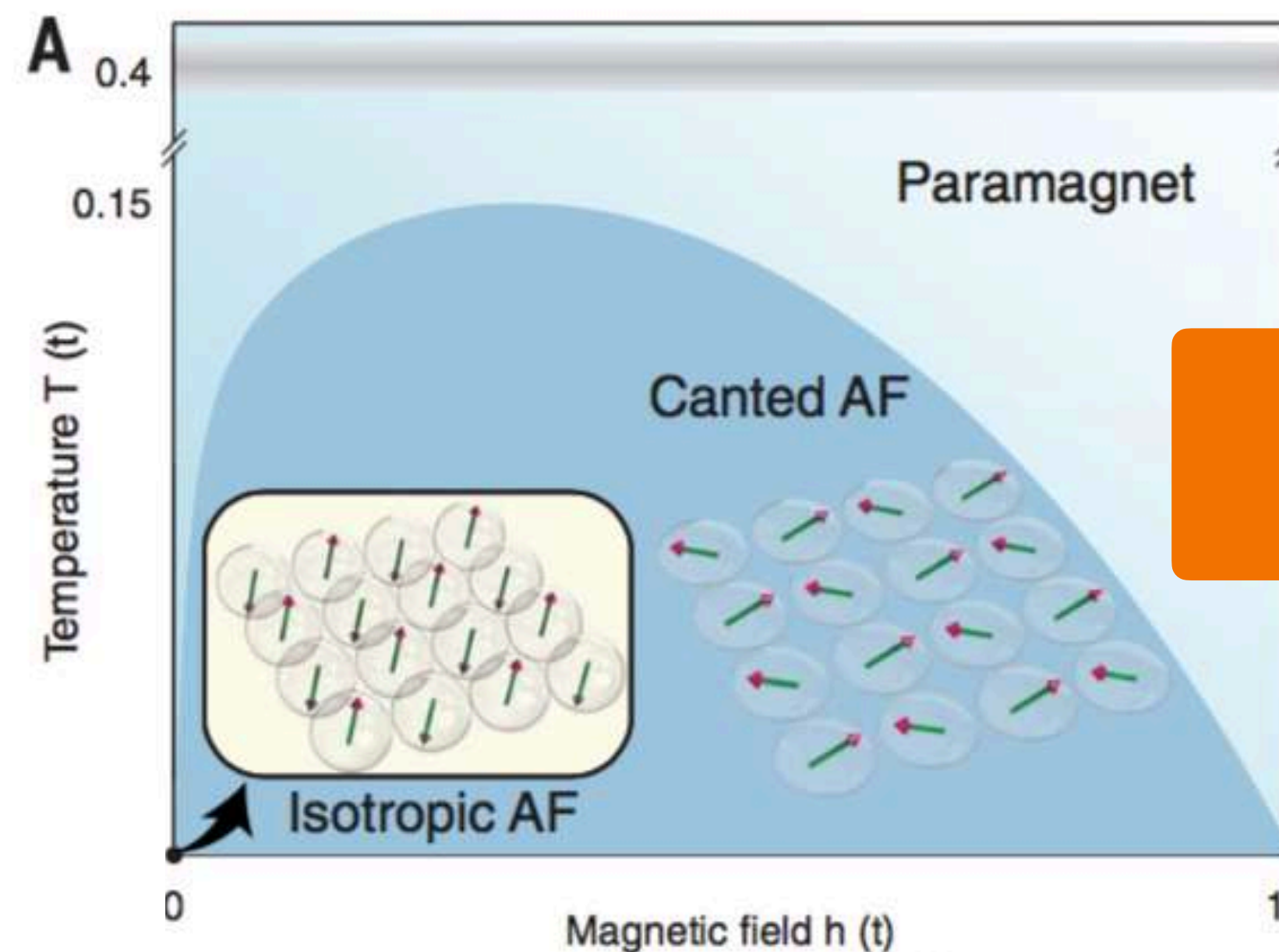
Experimental T

$T_c = 0$ at $n = 1$

Spin-imbalance in a 2D Fermi-Hubbard system

P. Brown et. al, Science (2017)

Repulsive Hubbard model with field h

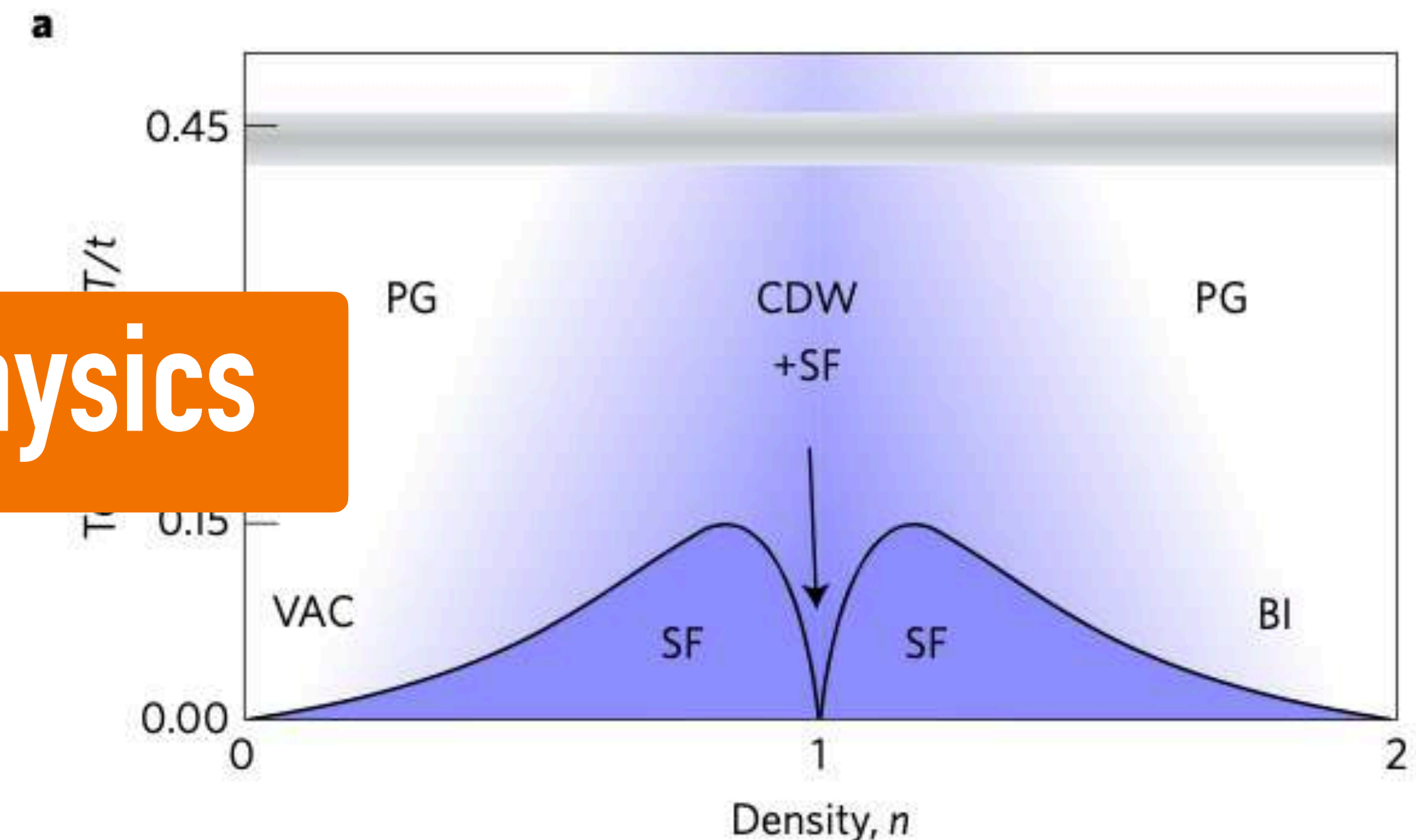


Same physics

Quantum gas microscopy of an attractive Fermi-Hubbard system

Mitra et al., Nat. Physics (2018)

Attractive Hubbard model with doping n



Spin-down particle-hole transformation

$$c_{j\uparrow} \rightarrow \bar{c}_{j\uparrow} \quad c_{j\downarrow} \rightarrow \bar{c}_{j\downarrow}^\dagger = (-1)^j c_{j\downarrow}$$

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} \right) + U \sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) - h \sum_i (\bar{n}_{i\uparrow} - \bar{n}_{i\downarrow}) - \mu N_s ,$$

$$+U \rightarrow -U$$

$$h \rightarrow \mu$$

$$\mu = 0 \quad h = 0$$

$$n = 1$$

$$\text{SU}(2)$$

$$\bar{\mathcal{H}} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \alpha_{ij}^{\sigma} \left(\bar{c}_{i\sigma}^\dagger \bar{c}_{j\sigma} + \text{H.c.} \right) - U \sum_i (\bar{n}_{i\uparrow} - \frac{1}{2})(\bar{n}_{i\downarrow} - \frac{1}{2}) - \mu \sum_{i,\sigma} n_{i\sigma} \left(\bar{c}_{i\sigma}^\dagger \bar{c}_{j\sigma} + \text{H.c.} \right)$$

$$\mu \neq 0 \rightarrow n \neq 1$$

or

$$h \neq 0 \rightarrow P \neq 1$$

Recently probed in experiments

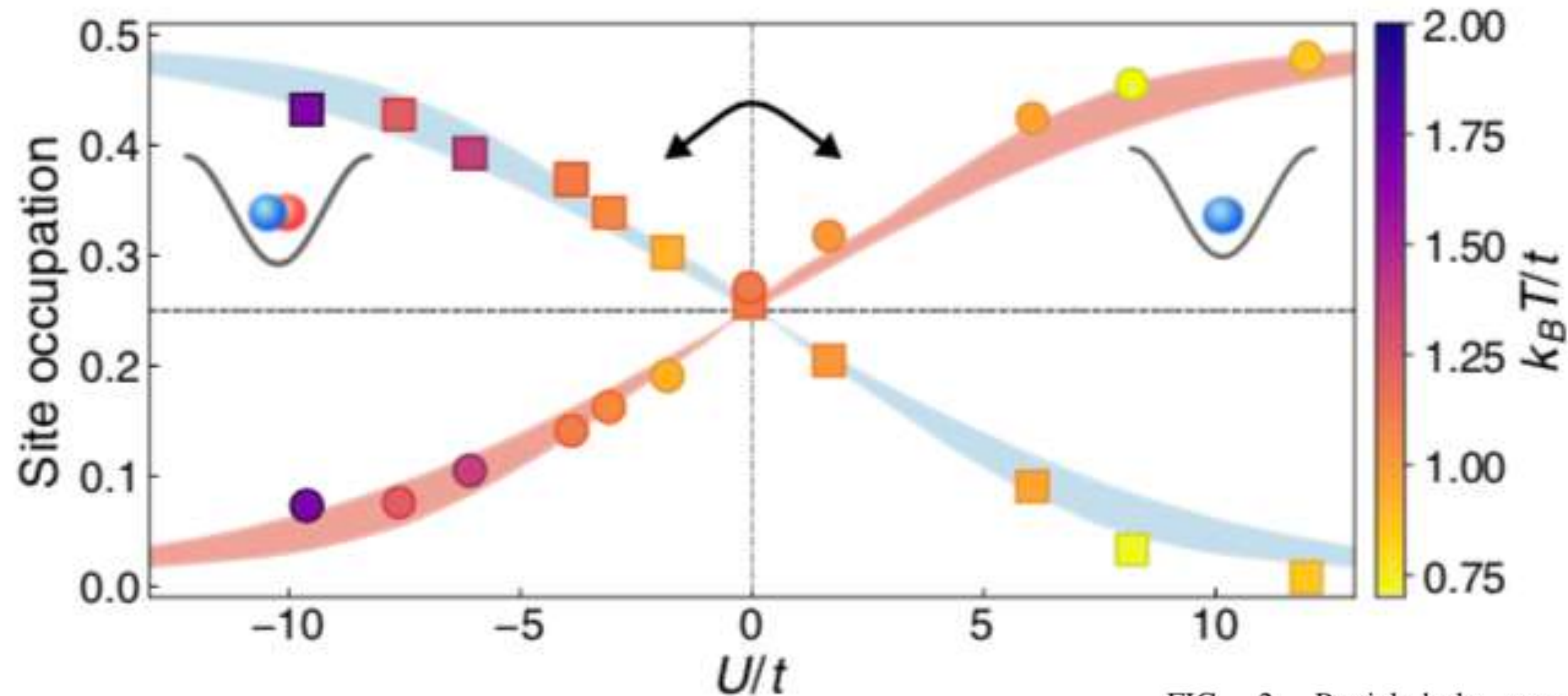


FIG. 2. Particle-hole symmetry for various interaction strengths. Doubles (squares) and singles (circles) site occupation at $\mu = h = 0$ vs U/t . For each interaction, we show the lowest temperature reached in our datasets. The red (blue) shaded regions show the results of the DQMC numerical calculations over $0.8 \leq k_B T/t \leq 2.0$.

M. Gall et al PRL (2020)

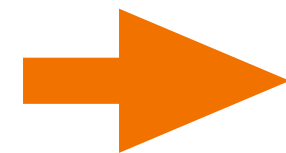
Mermin-Wagner Theorem

$$d \leq 2$$

2d systems

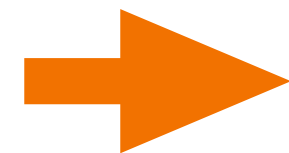
components of the order parameter $\rightarrow n$

$$d > n$$



$$T_c \neq 0$$

$$d < n$$

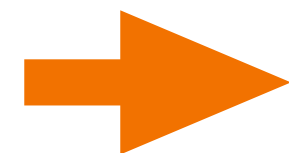


$$T_c = 0$$

SU(2)

half-filling, spin balanced $\mu = 0$ and $h = 0$

$$d = n$$



$$T_{KT} \neq 0$$

$$\left\{ \begin{array}{ll} -U & \mu \neq 0 \rightarrow n \neq 1 \\ +U & h \neq 0 \rightarrow P \neq 1 \end{array} \right.$$

Superfluid

anisotropic AF

Spin-down particle-hole transformation

$$c_{j\uparrow} \rightarrow \bar{c}_{j\uparrow}$$



unchanged

$$n_{j\uparrow} \rightarrow \bar{n}_{j\uparrow}$$

$$c_{j\downarrow} \rightarrow \bar{c}_{j\downarrow}^\dagger = (-1)^j c_{j\downarrow}$$



particle-hole transformation

$$n_{j\downarrow} \rightarrow \bar{n}_{j\downarrow} = 1 - n_{j\downarrow}$$

$$n_j \equiv n_{j\uparrow} + n_{j\downarrow} \rightarrow \bar{m}_j \equiv \bar{n}_{j\uparrow} - \bar{n}_{j\downarrow} = n_j - 1$$

$$m_j \rightarrow \bar{n}_j = 1 + m_j$$

$S_z \rightarrow$ charge

$S_{+-} \rightarrow$ SUC

charge and spin
degrees of freedom
are exchanged

End of third class