

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

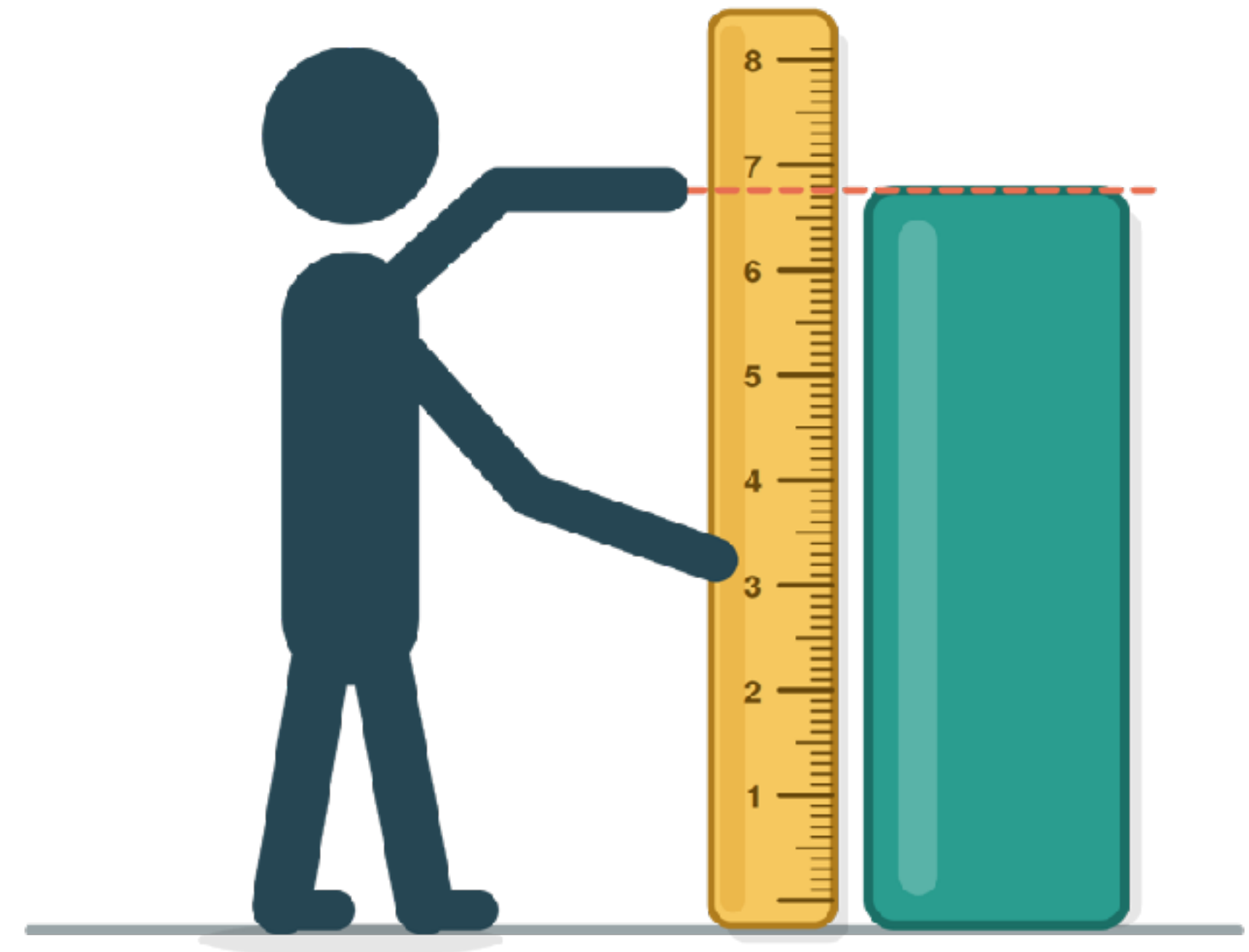
- 1 – Classical Monte Carlo
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Summary

Measurements in QMC II

QMC implementations

Measurements in QMC II



Measurements in QMC

Metal, Insulator, Superconductor

Superconducting correlations

Thermodynamic properties

**Metal, insulator,
superconductor**

The criteria

Insulator, metal, or superconductor: The criteria

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The appropriate infinite-wavelength $q_i \rightarrow 0$ and zero-frequency $\omega \rightarrow 0$ limits of the paramagnetic current-current correlation function provide criteria for determining whether a system is insulating, metallic, or superconducting. Here we discuss these criteria for lattice models and present Monte Carlo data for the two-dimensional positive- and negative- U Hubbard models that imply that the ground state of the half-filled positive- U Hubbard model is an insulator, the doped state is a metal, and the negative- U Hubbard model is a superconductor.

Superfluid density (D_s) and Drude weight (D)

Superfluid Density and the Drude Weight of the Hubbard Model

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Download

(24 February 1992)

We study the superfluid density and the Drude weight of the Hubbard model by investigating two different limiting behaviors of the current-current correlation function. These quantities provide criteria which allow one to distinguish between superconducting, metallic, and insulating ground states of an interacting many-body system. Monte Carlo calculations are performed to study these quantities.

Probe the response, not an order parameter

Two limits of **one** correlation function decide the ground state.

No need to guess the pairing symmetry or the right pair-field operator.

GROUND STATE

	D	D_s
● Insulator	0	0
● Metal	finite	0
● Superconductor	finite	finite

$D \rightarrow$ Drude weight $\rightarrow$ from the optical conductivity,

$D_s \rightarrow$ Superfluid density $\rightarrow$ from the London penetration depth λ .

Kinetic energy

$$K = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j,\sigma} + h.c.)$$

Current response in the presence of a vector potential

$$A_x(l, t) = A_x(\mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{l} - i\omega t}$$

Peirls phase-factors $\rightarrow$
$$K = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j,\sigma} e^{iA_x} + h.c.)$$

Expand in second order in A

$$e^{\pm ieA} \simeq 1 \pm ieA - \frac{1}{2}e^2 A^2$$

applied to one x-bond:

$$-t \left(e^{ieA_x} c_{l+\hat{x}}^\dagger c_l + e^{-ieA_x} c_l^\dagger c_{l+\hat{x}} \right) = -t \left(c_{l+\hat{x}}^\dagger c_l + \text{h.c.} \right) - eA_x j_x^p(l) - \frac{e^2}{2} A_x^2 k_x(l) + \mathcal{O}(A^3)$$

$$K_A = K - \sum_l \left[e j_x^p(l) A_x(l) + \frac{e^2 k_x(l)}{2} A_x^2(l) \right]$$

Where $j_x^p(l) = it \sum_s \left(c_{l+\hat{x},s}^\dagger c_{l,s} - c_{l,s}^\dagger c_{l+\hat{x},s} \right)$ and $k_x(l) = -t \sum_s \left(c_{l+\hat{x},s}^\dagger c_{l,s} + c_{l,s}^\dagger c_{l+\hat{x},s} \right)$

Linear response

$$j_x(l) = -\frac{\delta K_A}{\delta A_x(l)} = \underbrace{e j_x^p(l)}_{\text{paramagnetic}} + \underbrace{e^2 k_x(l) A_x(l)}_{\text{diamagnetic}}$$

$$\langle j_x(\mathbf{q}, \omega) \rangle = -e^2 [\langle -k_x \rangle - \Lambda_{xx}(\mathbf{q}, \omega)] A_x(\mathbf{q}, \omega)$$

Current-current correlation functions

$$j_x(\ell, \tau) = e^{\mathcal{H}\tau} \left[it \sum_{\sigma} \left(c_{\ell+\hat{x},\sigma}^{\dagger} c_{\ell,\sigma} - c_{\ell,\sigma}^{\dagger} c_{\ell+\hat{x},\sigma} \right) \right] e^{-\mathcal{H}\tau} \quad \Rightarrow \quad \text{Current density}$$

$$\Lambda_{xx}(\ell, \tau) = \langle j_x(\ell, \tau) j_x(0, 0) \rangle \quad \Rightarrow \quad \text{Current-current correlation function}$$

$$\Lambda_{xx}(\mathbf{q}, \omega_n) = \sum_{\ell} \int_0^{\beta} d\tau e^{i\mathbf{q} \cdot \ell} e^{i\omega_n \tau} \Lambda_{xx}(\ell, \tau) \quad \text{where} \quad \omega_n = 2n\pi T$$

Different order of limits

$$\Lambda^L \equiv \lim_{q_x \rightarrow 0} \Lambda_{xx}(q_x, q_y = 0, \omega_n = 0)$$

$$\Lambda^T \equiv \lim_{q_y \rightarrow 0} \Lambda_{xx}(q_x = 0, q_y, \omega_n = 0)$$

Longitudinal static limit ($\mathbf{q} \parallel \mathbf{A}$): a pure gauge, so there is no current in any phase.

$$\langle -k_x \rangle - \Lambda_{xx}(q_x \rightarrow 0, q_y = 0, i\omega_m = 0) = 0$$

$$\langle -k_x \rangle = \Lambda^L$$

Gauge invariance: must hold,
nontrivial test of the numerics

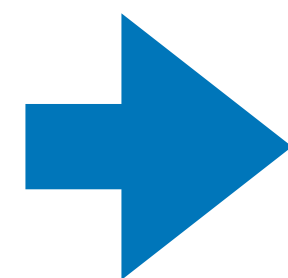
Meissner effect: $\omega = 0$ first, then $q \rightarrow 0$

London: a static, transverse ($q \cdot A = 0$) field is screened. Take $A \parallel x$ and $q \parallel y$.

$$\langle j_x(q_y) \rangle = -\frac{1}{4\pi\lambda^2} A_x(q_y), \quad \frac{1}{\lambda^2} = \frac{4\pi n_s e^2}{mc^2}$$

$$\frac{D_s}{\pi e^2} = \langle -k_x \rangle - \Lambda_{xx}(q_x = 0, q_y \rightarrow 0, i\omega_m = 0) = \left(\frac{n_s}{m}\right)^*$$

**Superfluid
density**



$$\frac{D_s}{\pi e^2} = \Lambda^L - \Lambda^T$$

Zero resistance: a δ -function in $\sigma(\omega)$

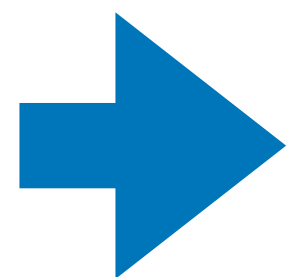
Take $q = 0$ first and an electric field $E_x(\omega) = i \omega A_x(\omega)$:

$$\sigma_{xx}(\omega) = -e^2 \frac{\langle -k_x \rangle - \Lambda_{xx}(\mathbf{q} = 0, \omega)}{i(\omega + i\delta)}$$

$$\text{Re } \sigma_{xx}(\omega) = D \delta(\omega) + \sigma_{xx}^{\text{reg}}(\omega)$$

$$\frac{D}{\pi e^2} = \langle -k_x \rangle - \text{Re } \Lambda_{xx}(\mathbf{q} = 0, \omega \rightarrow 0) = \left(\frac{n}{m} \right)^*$$

Drude
weight



$$\omega_n = 2n\pi T$$

$$\frac{D}{\pi e^2} = \lim_{T \rightarrow 0} [\Lambda^L - \Lambda(\mathbf{q} = 0, i\omega_m)]$$

Zero resistance: a δ -function in $\sigma(\omega)$

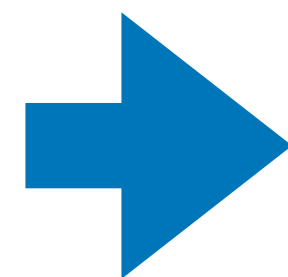
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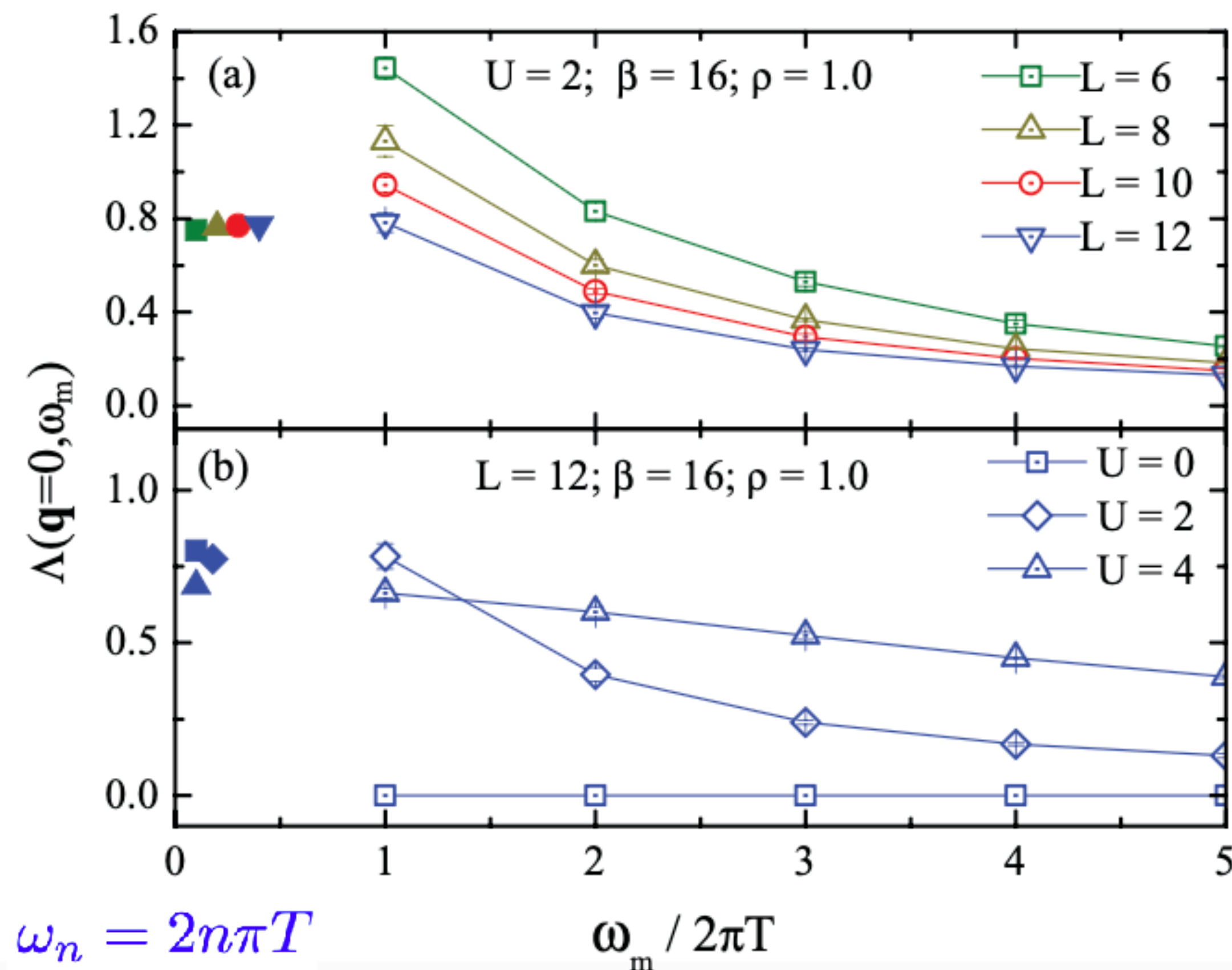
$$\frac{D}{\pi e^2} = \langle -k_x \rangle - \text{Re } \Lambda_{xx}(\mathbf{q} = 0, \omega \rightarrow 0) = \left(\frac{n}{m} \right)^*$$

Drude
weight



Less used: compressibility, density
of states, conductivity

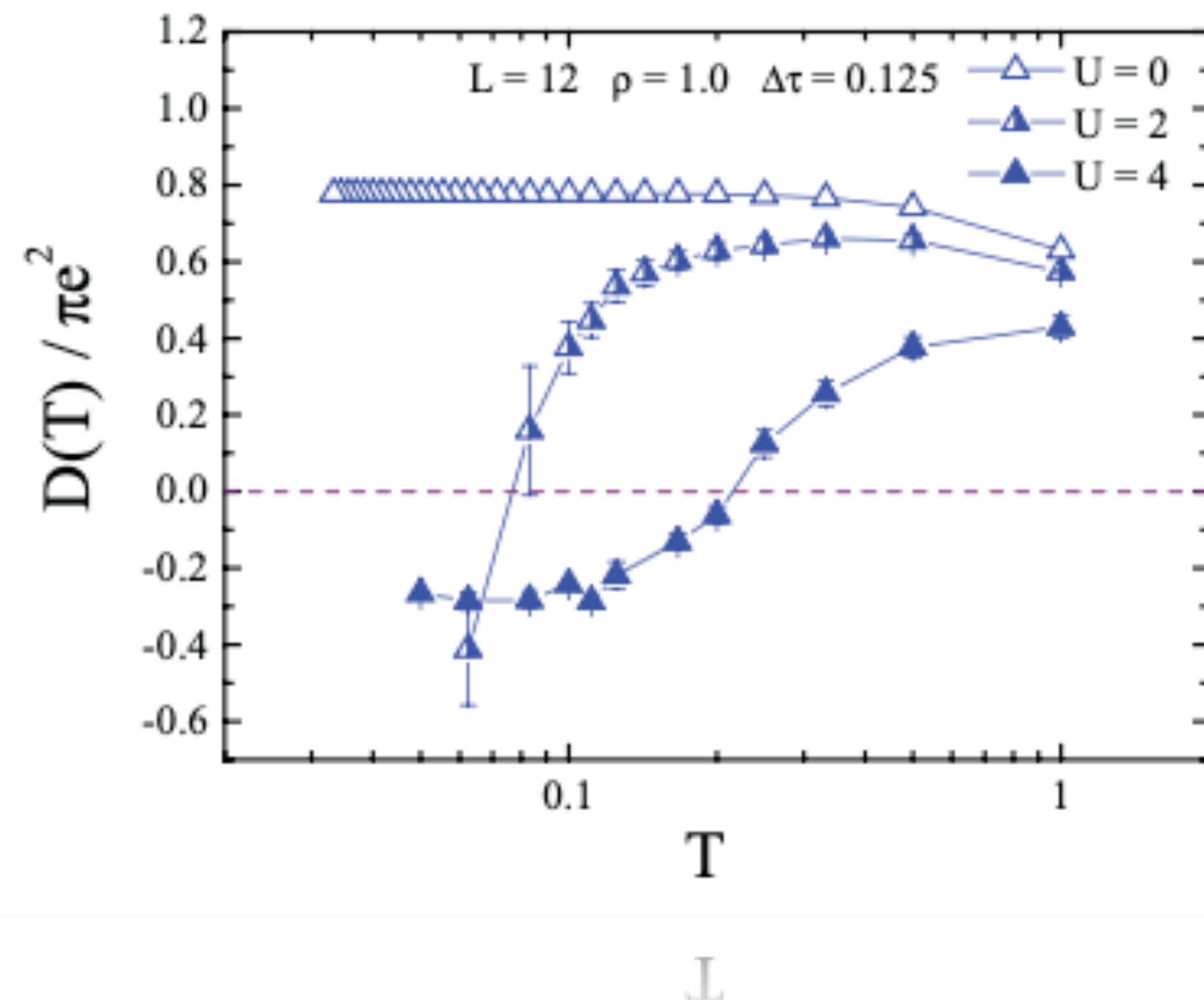
Drude weight



$$\frac{D}{\pi e^2} = \langle -k_x \rangle - \text{Re} \Lambda_{xx}(\mathbf{q} = 0, \omega \rightarrow 0) = \left(\frac{n}{m} \right)^*$$

PRB 2012 Mondaini et al

Drude weight



$$\lim_{T, m \rightarrow 0} \tilde{D}_m \equiv \lim_{T \rightarrow 0} D(T) = D$$

PRB 2012 Mondaini et al

Same functions, different order of limits

Gauge check

$\omega_m = 0$ first, then $q_x \rightarrow 0$ (longitudinal)

$$\langle -k_x \rangle = \Lambda^L$$

Superfluid weight D_s

$\omega_m = 0$ first, then $q_y \rightarrow 0$ (transverse)

$$\frac{D_s}{\pi e^2} = \Lambda^L - \Lambda^T$$

Drude weight D

$q = 0$ first, then $\omega_m \rightarrow 0$

$$\frac{D}{\pi e^2} = \lim_{T \rightarrow 0} [\Lambda^L - \Lambda(\mathbf{q} = 0, i\omega_m)]$$

The Criteria

Insulator

$$D = 0, D_S = 0$$

Resistance and no Meissner effect

Metal

$$D > 0, D_S = 0$$

Zero resistance but no Meissner effect

Superconductor

$$D > 0, D_S > 0$$

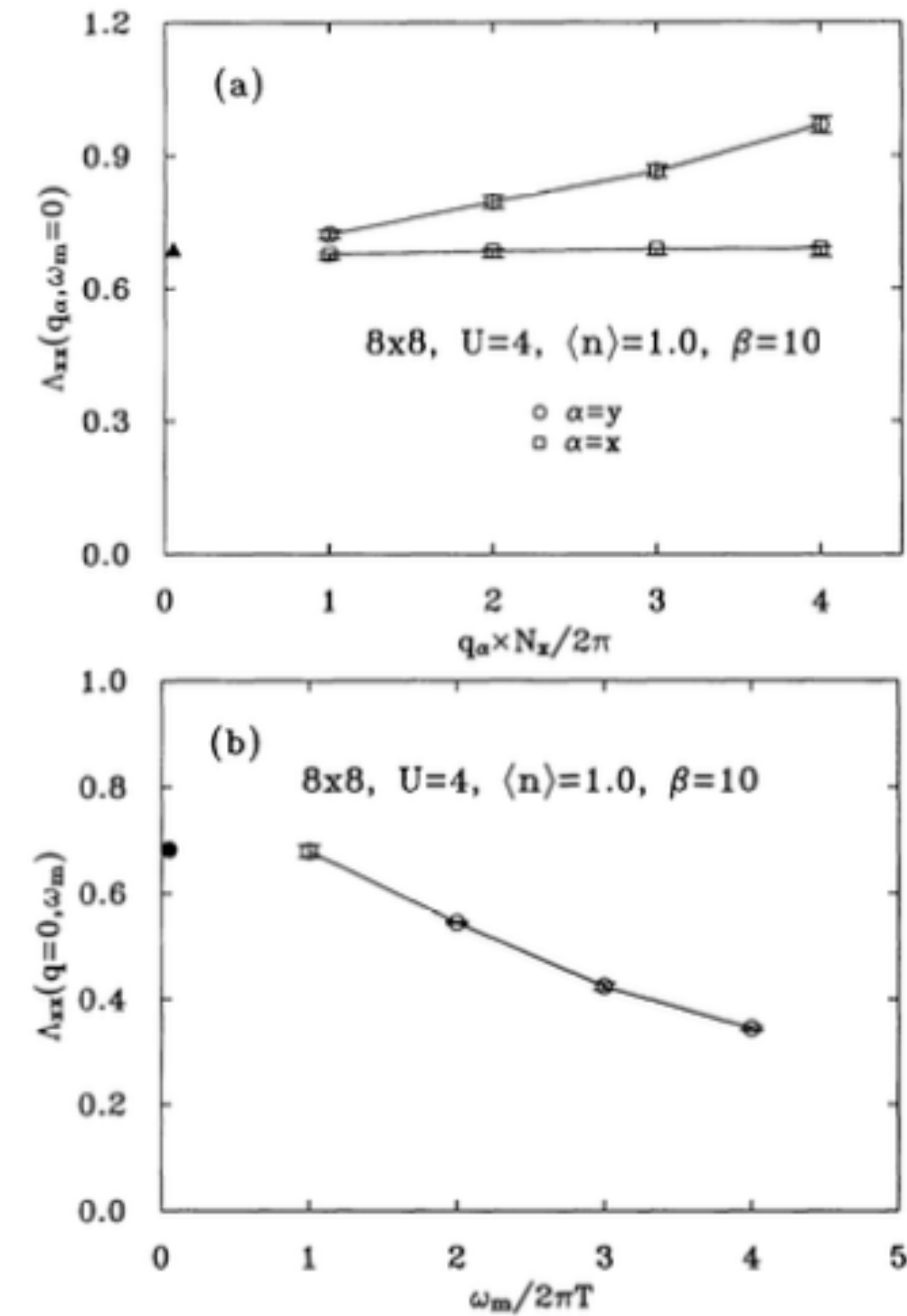
Zero resistance and Meissner effect

Insulator

$$D = 0, D_S = 0$$

Resistance and no Meissner effect

PRL 1992 Scalapino, White and Zhang

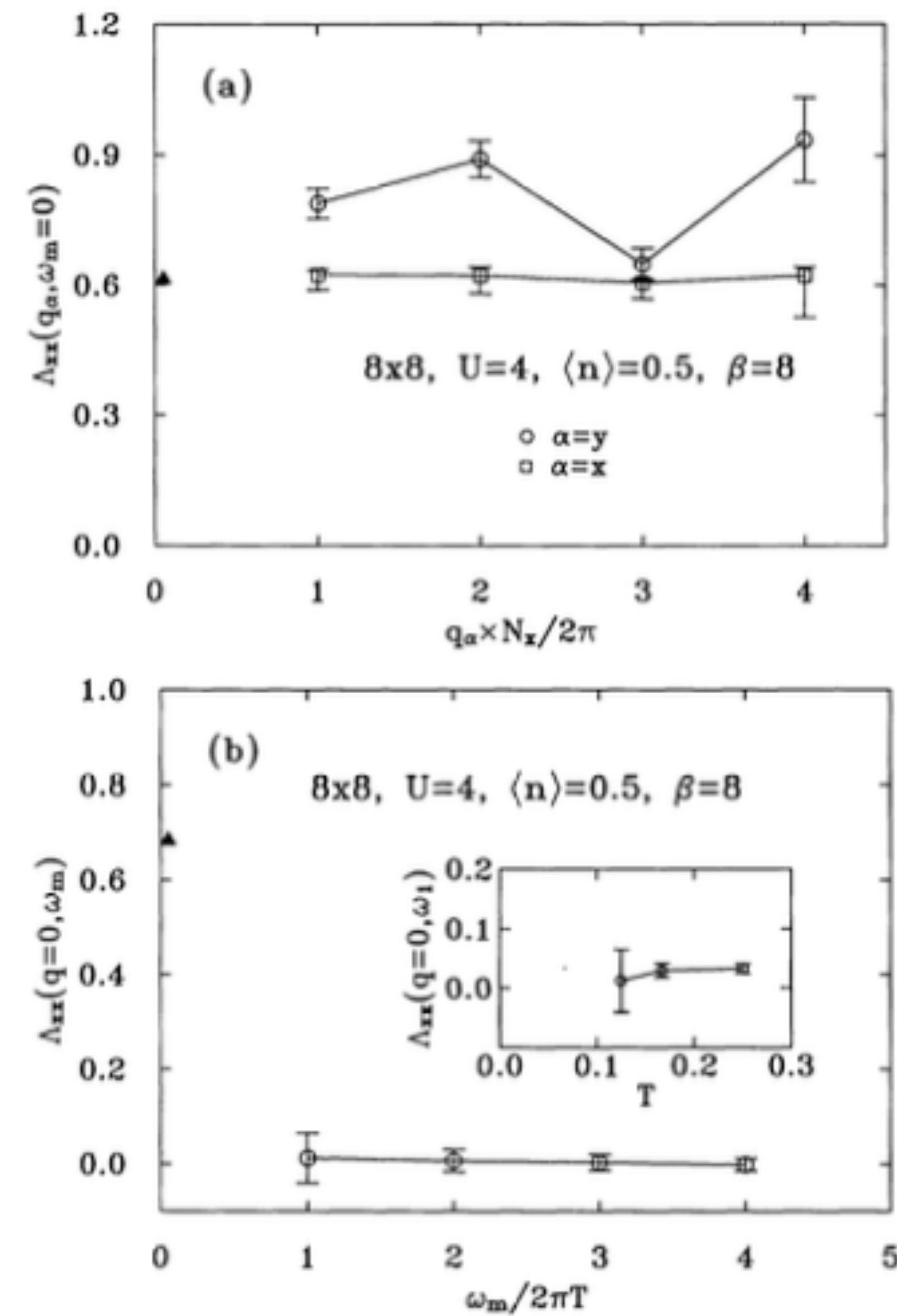


Metal

$$D > 0, D_S = 0$$

Zero resistance but no Meissner effect

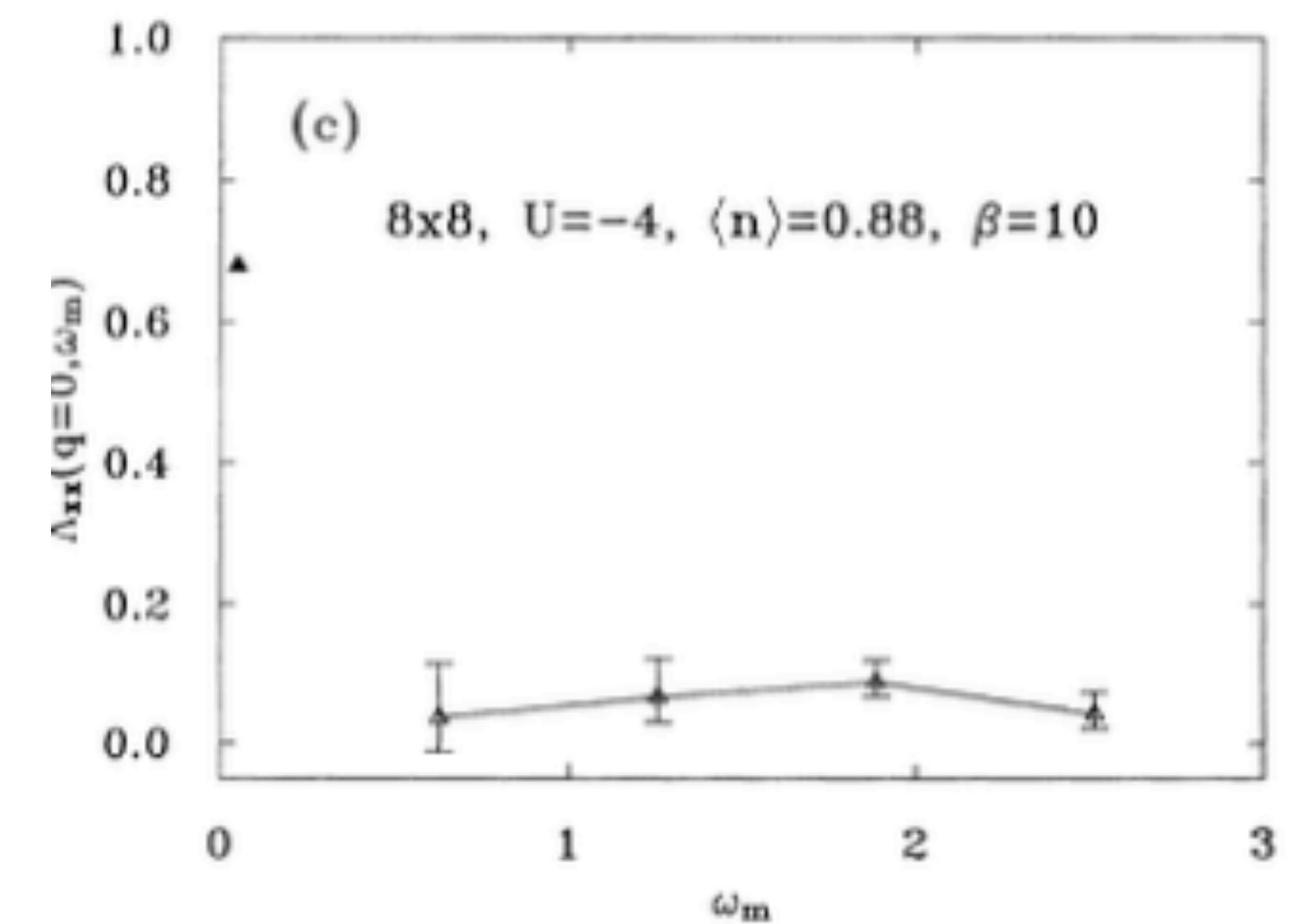
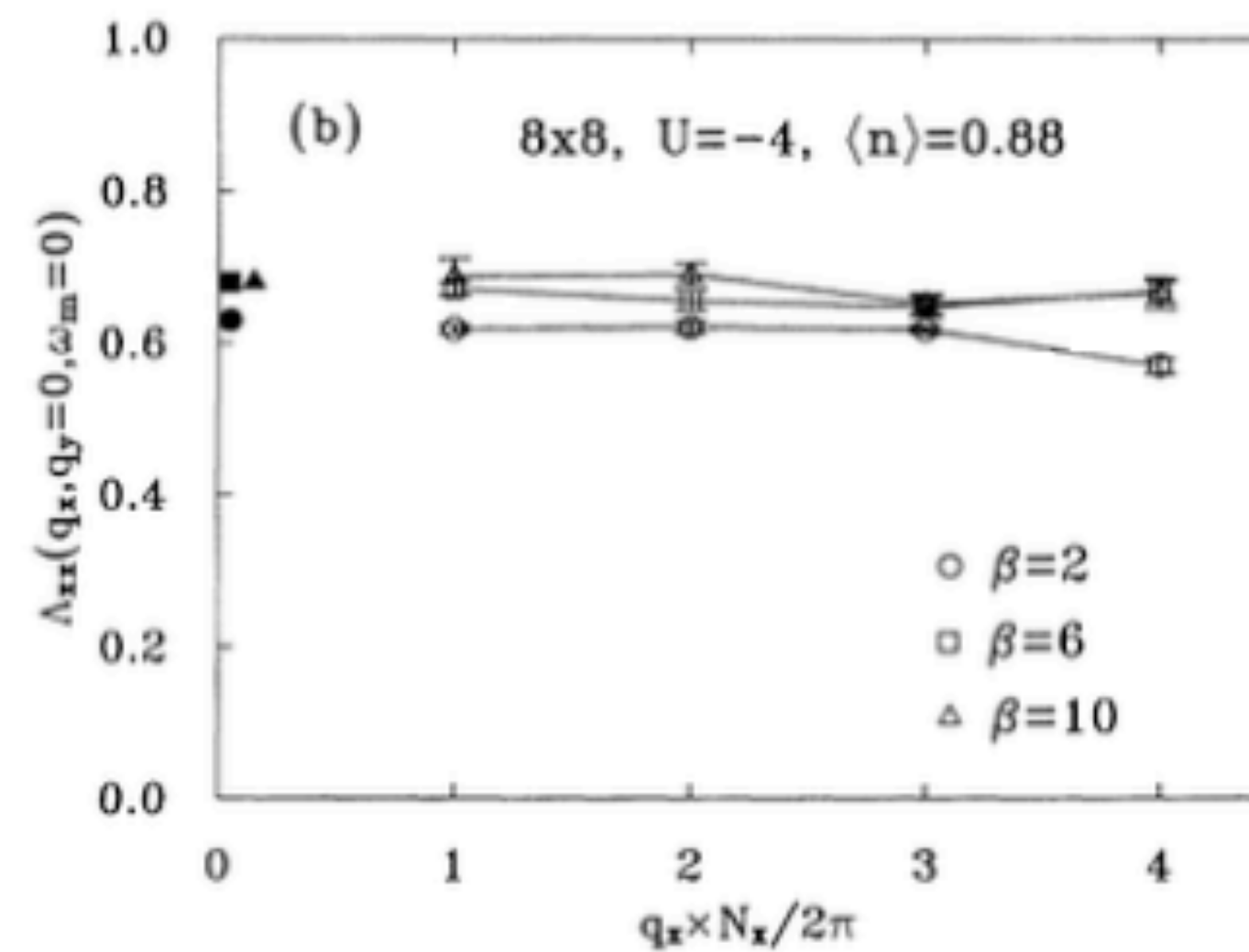
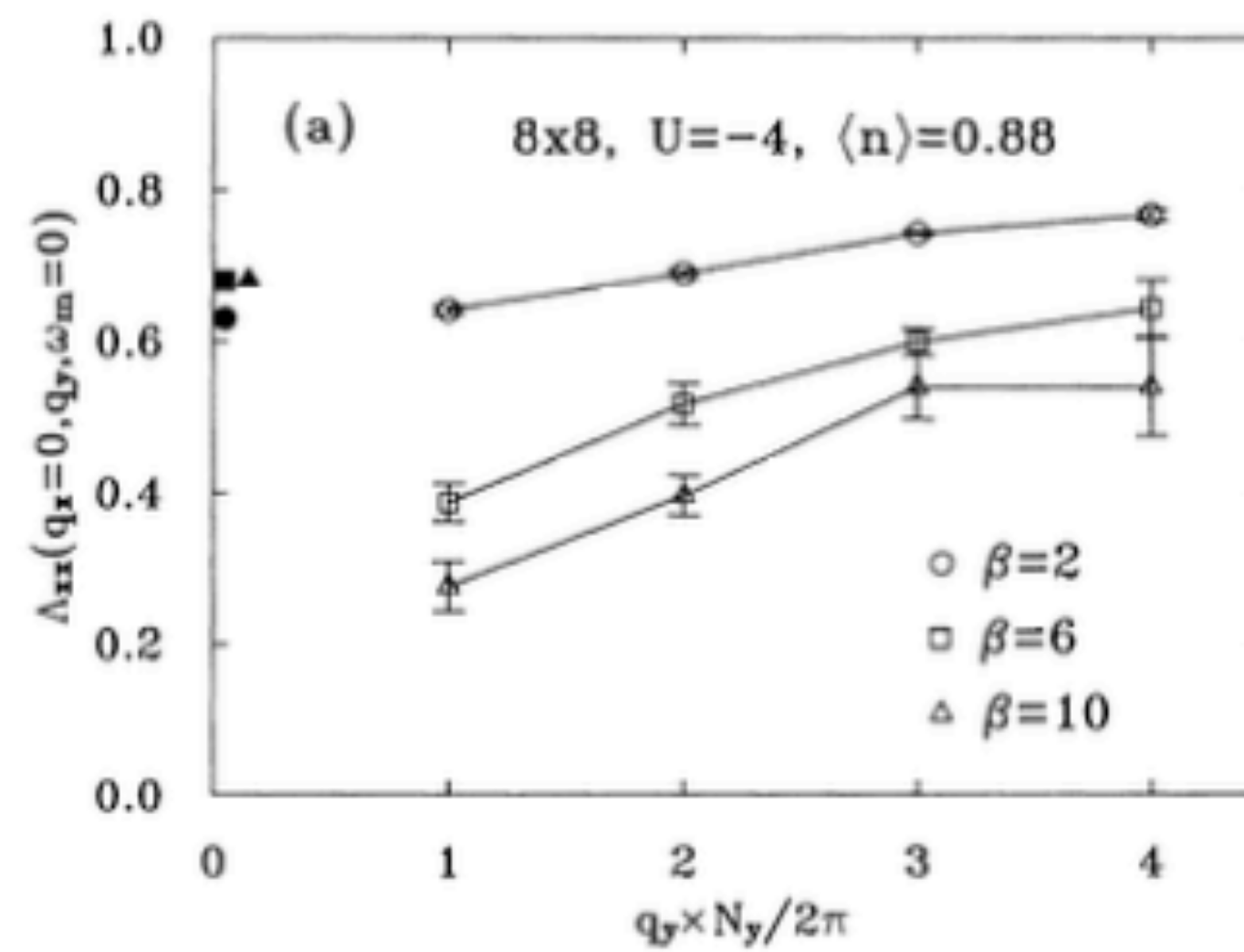
PRL 1992 Scalapino, White and Zhang



Superconductor

$$D > 0, D_S > 0$$

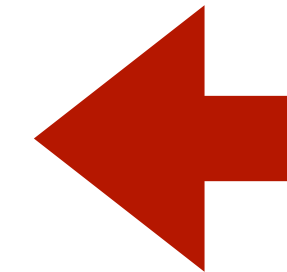
Zero resistance and Meissner effect



Conductivity and Density of states

Current-current correlation functions

$$\Lambda(\mathbf{q} = 0, \tau) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{e^{-\omega\tau}}{1 - e^{-\beta\omega}} \text{Im } \Lambda(\mathbf{q} = 0, \omega)$$



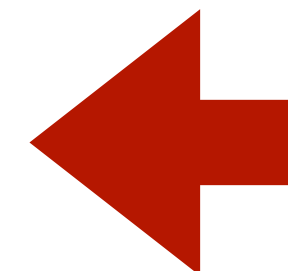
Laplace inversion to
get the conductivity

Linear response theory

$$\text{Im } \Lambda(\mathbf{q} = 0, \omega) = \omega \text{Re } \sigma(\omega)$$

Similarly for the Green's function

$$G(\mathbf{r} = 0, \tau) = \int_{-\infty}^{\infty} d\omega \frac{e^{-\omega\tau}}{1 + e^{-\beta\omega}} N(\omega)$$



Laplace inversion to get
the density of states

Is there a way not to do the Laplace inversion?

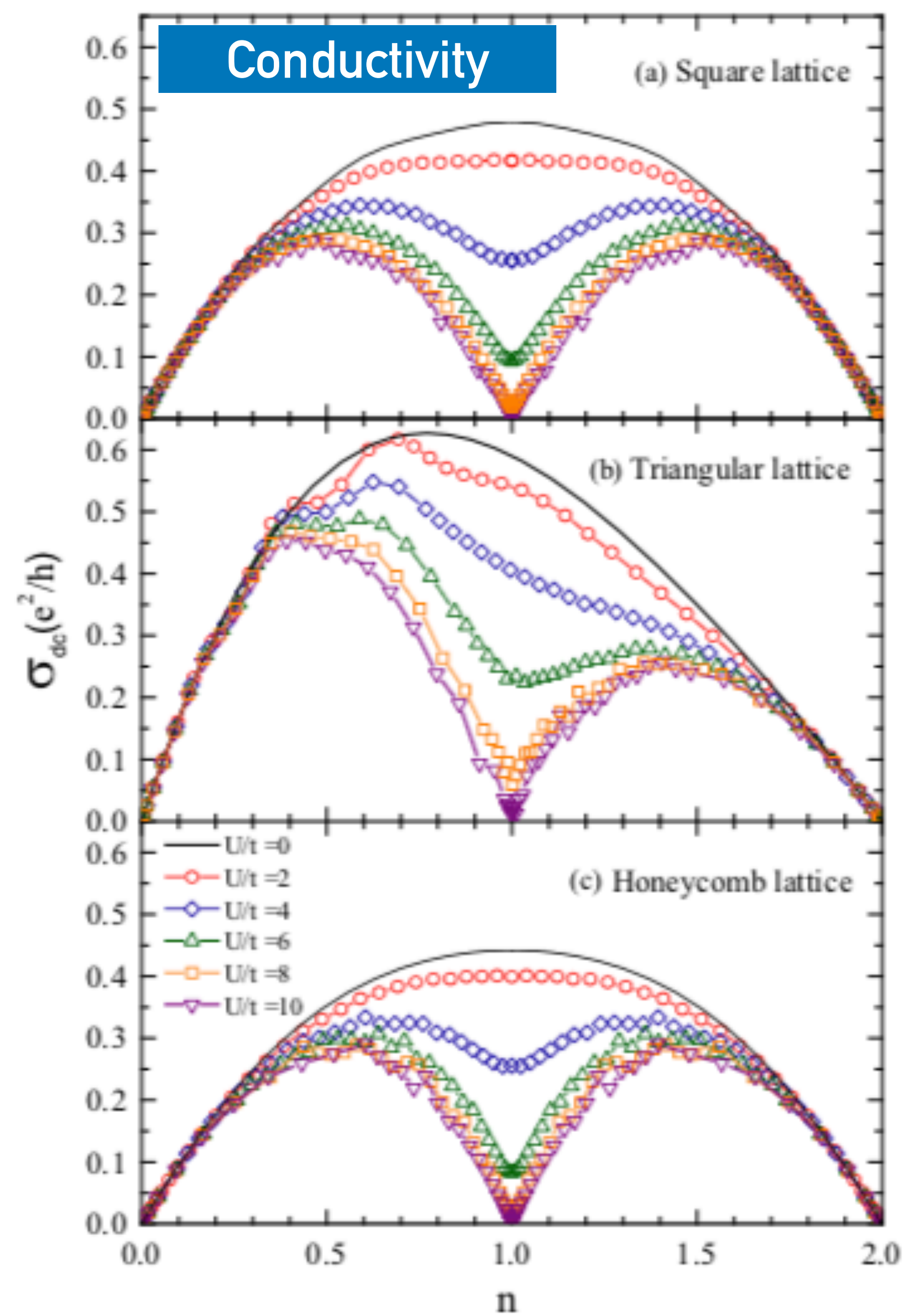
Conductivity

$$\sigma_{dc} \approx \frac{\beta^2}{\pi} \Lambda_{xx}(\mathbf{q} = \mathbf{0}, \tau = \beta/2)$$

Density of states

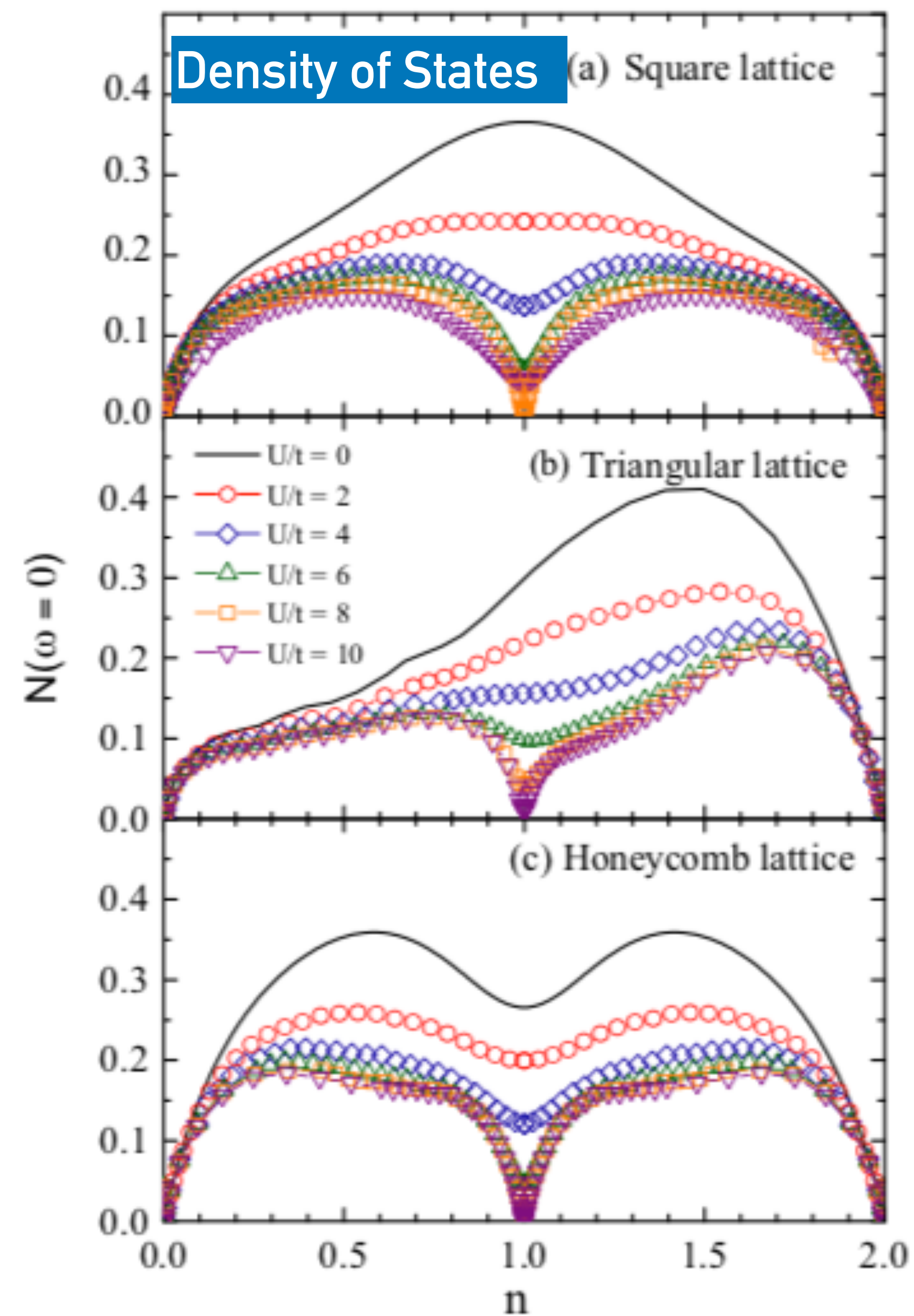
$$N(\omega = 0, T) = \frac{dn}{d\mu} = n^2 \kappa(T)$$

Conductivity



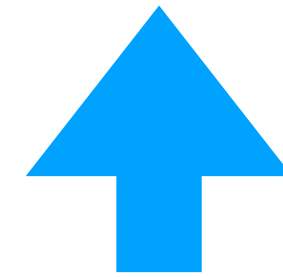
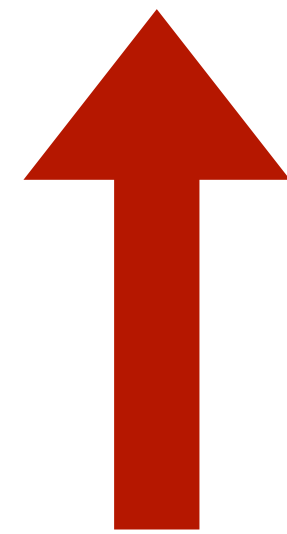
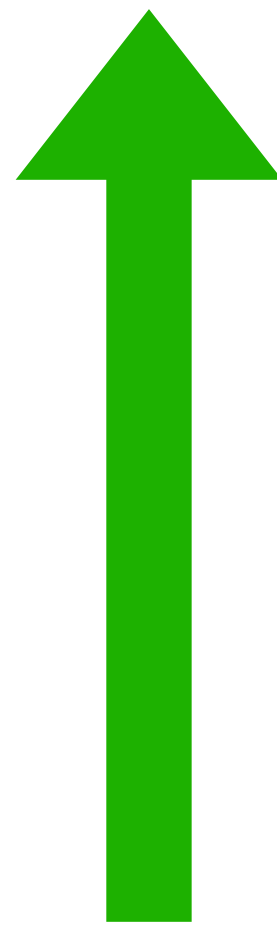
$T/t=0.5$

Density of States



Single particle excitation gap

$$G(\mathbf{q}_F, \tau) \sim e^{-\Delta_{sp}(\mathbf{q}_F)\tau}$$



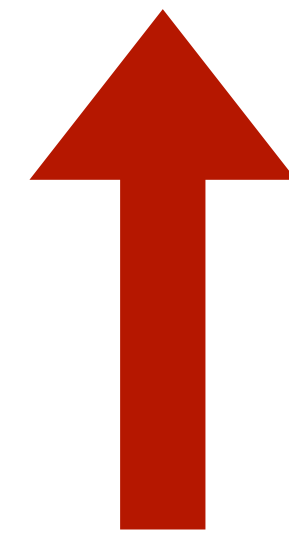
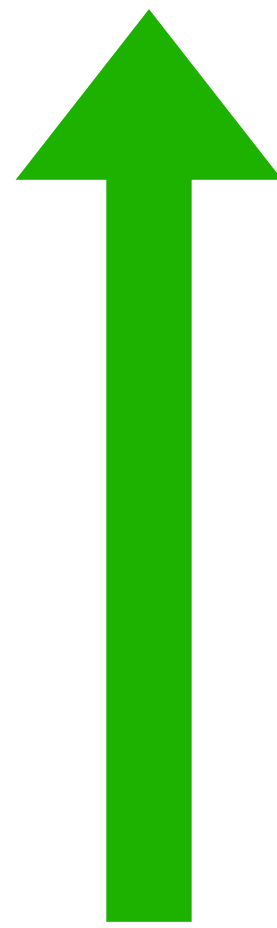
Single particle excitation gap

Fermi vector

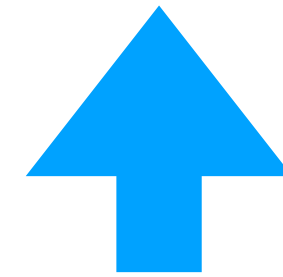
Imaginary-time-dependent Green's function

Single particle excitation gap

$$G(\mathbf{q}_F, \tau) \sim e^{-\Delta_{sp}(\mathbf{q}_F)\tau}$$



Fermi vector



Single particle excitation gap

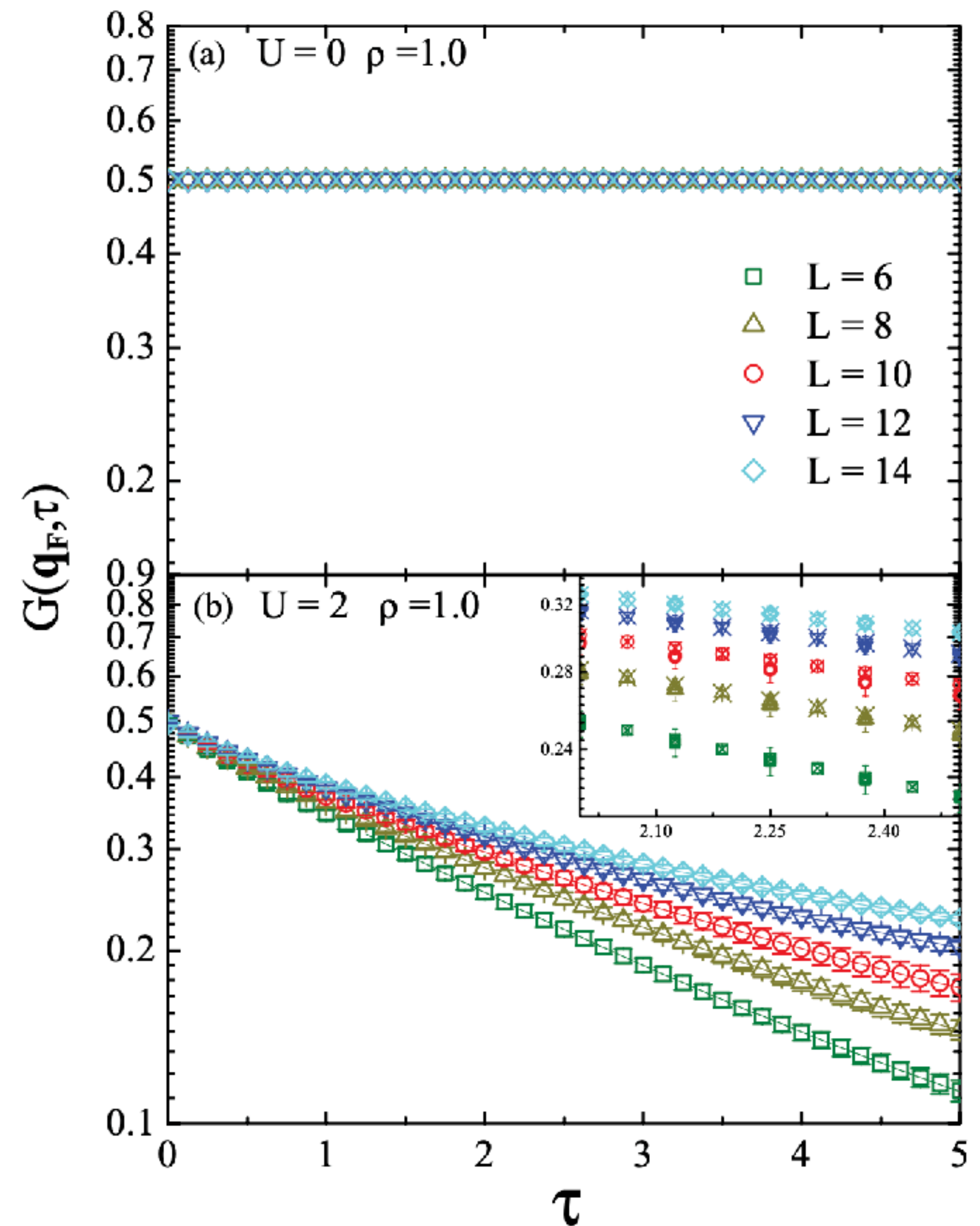
Minimum energy necessary to extract one Fermion from the system: related to gap measured in photoemission experiments

Imaginary-time-dependent Green's function

$$G(\mathbf{q}_F, \tau) \sim e^{-\Delta_{sp}(\mathbf{q}_F)\tau}$$

Exponential behavior for large τ

Mondaini et al PRB 2012

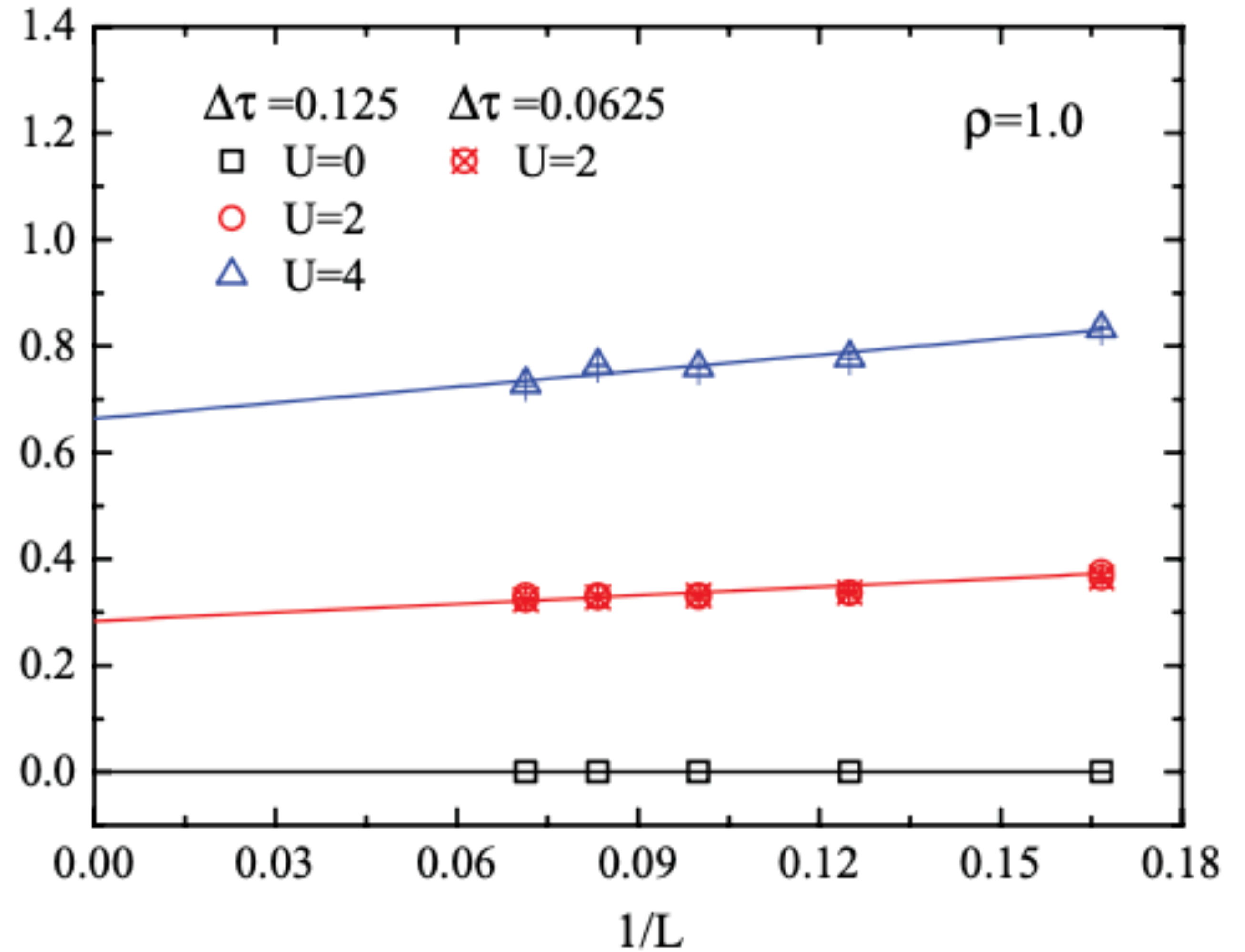


Metal-Insulator transition through single particle excitation gap measurements

Insulator

Metal

$$\Delta_{sp}(q=q_F)$$



Mondaini et al PRB 2012

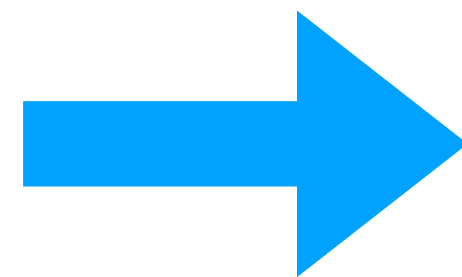
Superconducting correlations

Superconducting correlations

Imaginary time singlet pair-field operator Inspired in BCS gap function

$$\Delta_{\zeta}(\tau) \equiv \frac{1}{\sqrt{N_s}} \sum_{\mathbf{k}} f_{\zeta}(\mathbf{k}) c_{\mathbf{k}\uparrow}(\tau) c_{-\mathbf{k}\downarrow}(\tau),$$

Form factor:



Symmetry of the
pairing state

$$s - \text{wave} : f_s(\mathbf{k}) = 1,$$

$$\text{extended } s - \text{wave} : f_{s^*}(\mathbf{k}) = \cos k_x + \cos k_y,$$

$$d_{x^2-y^2} - \text{wave} : f_{d_{x^2-y^2}}(\mathbf{k}) = \cos k_x - \cos k_y,$$

$$d_{xy} - \text{wave} : f_{d_{xy}}(\mathbf{k}) = \sin k_x \sin k_y,$$

Equal time pairing correlation functions

$$P_{\zeta}(\mathbf{i}, \mathbf{j}) = \langle \Delta_{\zeta}^{\dagger}(\mathbf{i}) \Delta_{\zeta}(\mathbf{j}) + \text{H.c.} \rangle,$$

Uniform ($q=0$) Fourier transform

$$\tilde{P}_{\zeta} = \frac{1}{N_s} \sum_{\mathbf{i}, \mathbf{j}} \langle \Delta_{\zeta}^{\dagger}(\mathbf{i}) \Delta_{\zeta}(\mathbf{j}) + \text{H.c.} \rangle,$$

Superconducting pairing symmetry in the kagome-lattice Hubbard model

Chenyue Wen,^{1,*} Xingchuan Zhu^{2,*}, Zhisong Xiao¹, Ning Hao,³ Rubem Mondaini⁴,
 Huaiming Guo,^{1,4,†} and Shiping Feng⁵

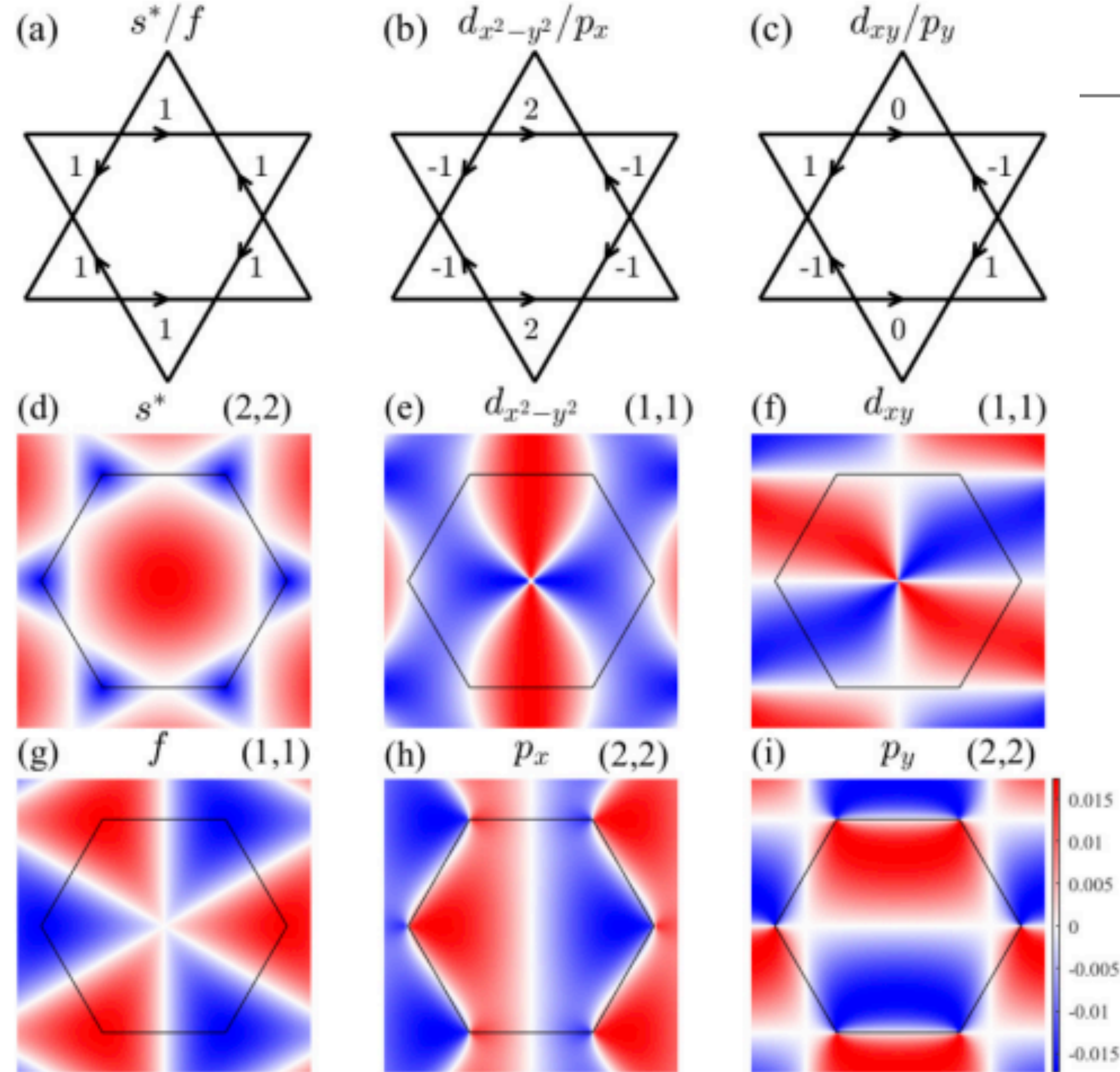


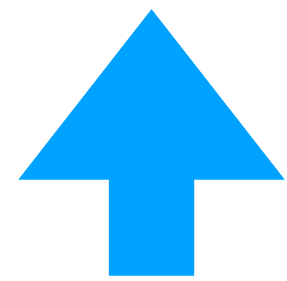
FIG. 2. The pairing symmetries allowed by the point group of the kagome lattice: (a) s^* and f wave, (b) $d_{x^2-y^2}$ and p_x wave, and (d) d_{xy} and p_y wave. For triplet pairing, there is an additional sign when the pairing is along the opposite direction of the arrow. The momentum dependence of the intraband pairing function for (d) s^* , (e) $d_{x^2-y^2}$, (f) d_{xy} , (g) f , (h) p_x , and (i) p_y pairing channels.

Unequal time uniform pairing susceptibility

$$\chi^\alpha = \frac{1}{N} \int_0^\beta d\tau \sum_{ij} \langle \Delta_i^\alpha(\tau) \Delta_j^{\alpha\dagger}(0) \rangle$$

$$\Delta_i^\alpha(\tau) = \sum_j f_{ij}^\alpha e^{\tau H} c_{i\uparrow} c_{j\downarrow} e^{-\tau H}$$

$$\chi_{eff}^\alpha = \chi^\alpha - \chi_0^\alpha$$



Subtracting the uncorrelated part

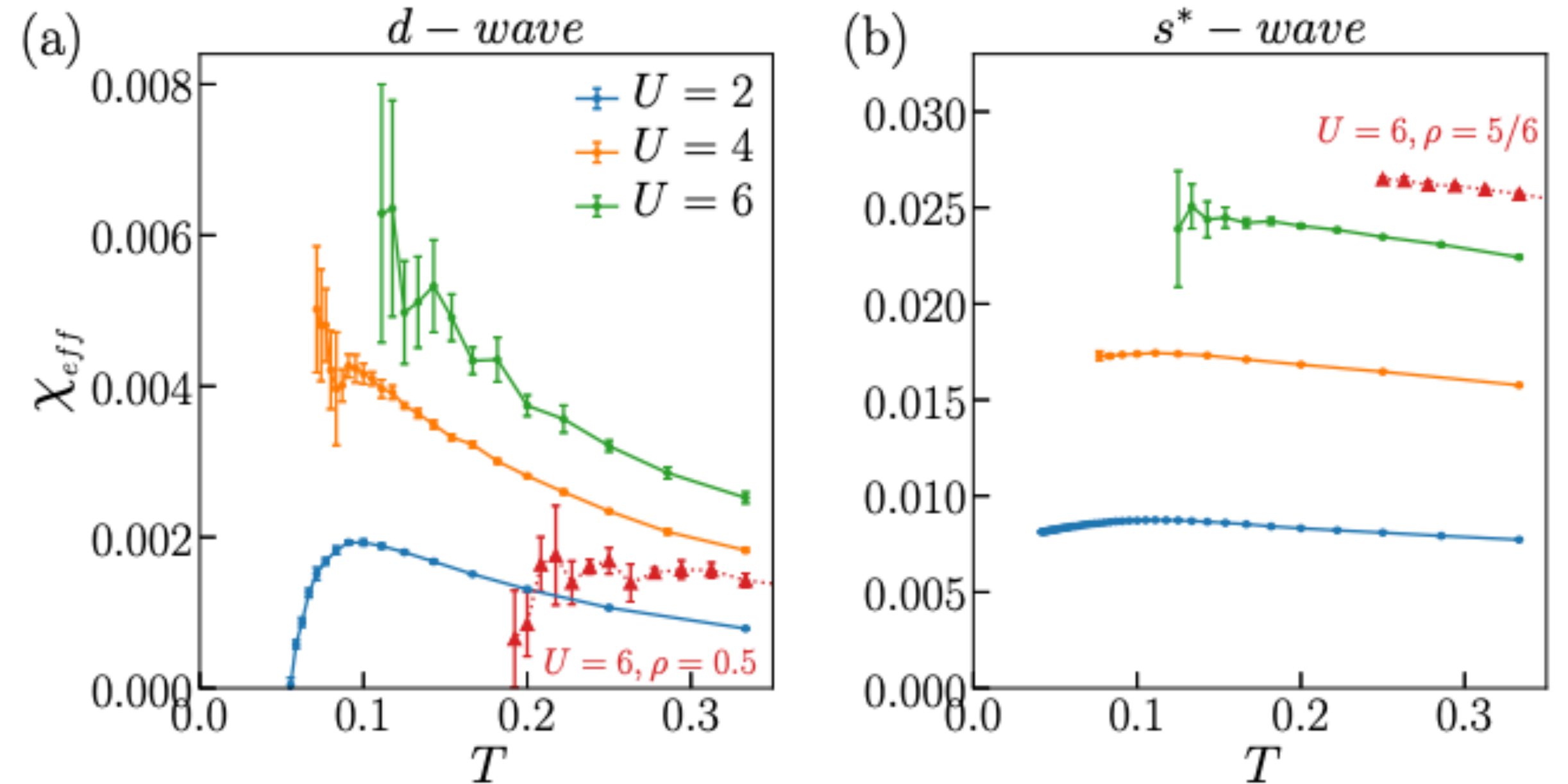
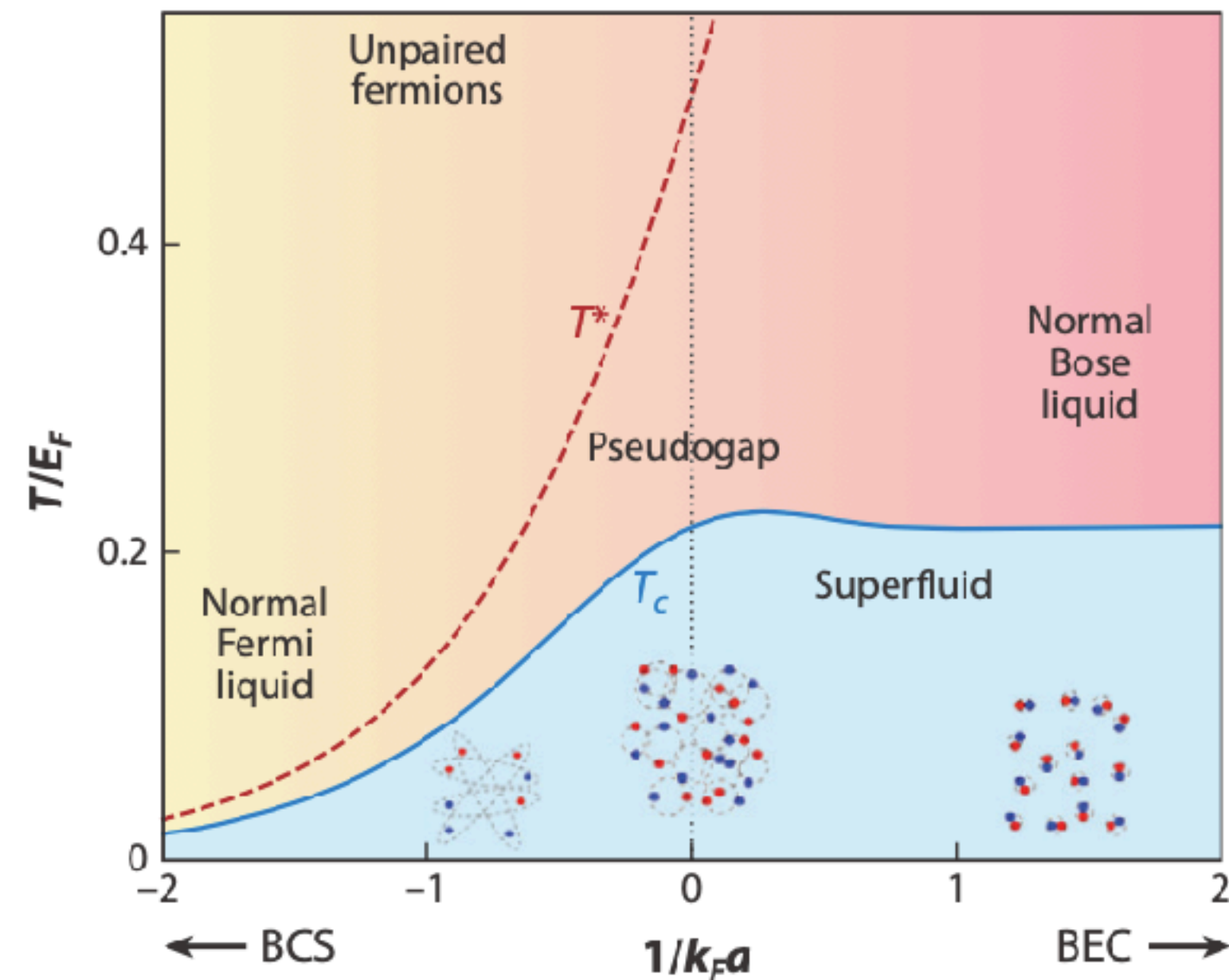


FIG. 4. The effective susceptibility of the dominating pairing channel as a function of temperature for several values of U : (a) d wave at $\rho_1 = 0.62$ and (b) s^* wave at $\rho_2 = 0.713$. Here ρ_1 and ρ_2 are symmetric to the Dirac points and correspond to hole and electron dopings, respectively. χ_{eff}^d ($\chi_{eff}^{s^*}$) at the lower (upper) VHS is also plotted in (a) [(b)] to demonstrate the evolution with doping.

Attractive interactions in Fermionic systems

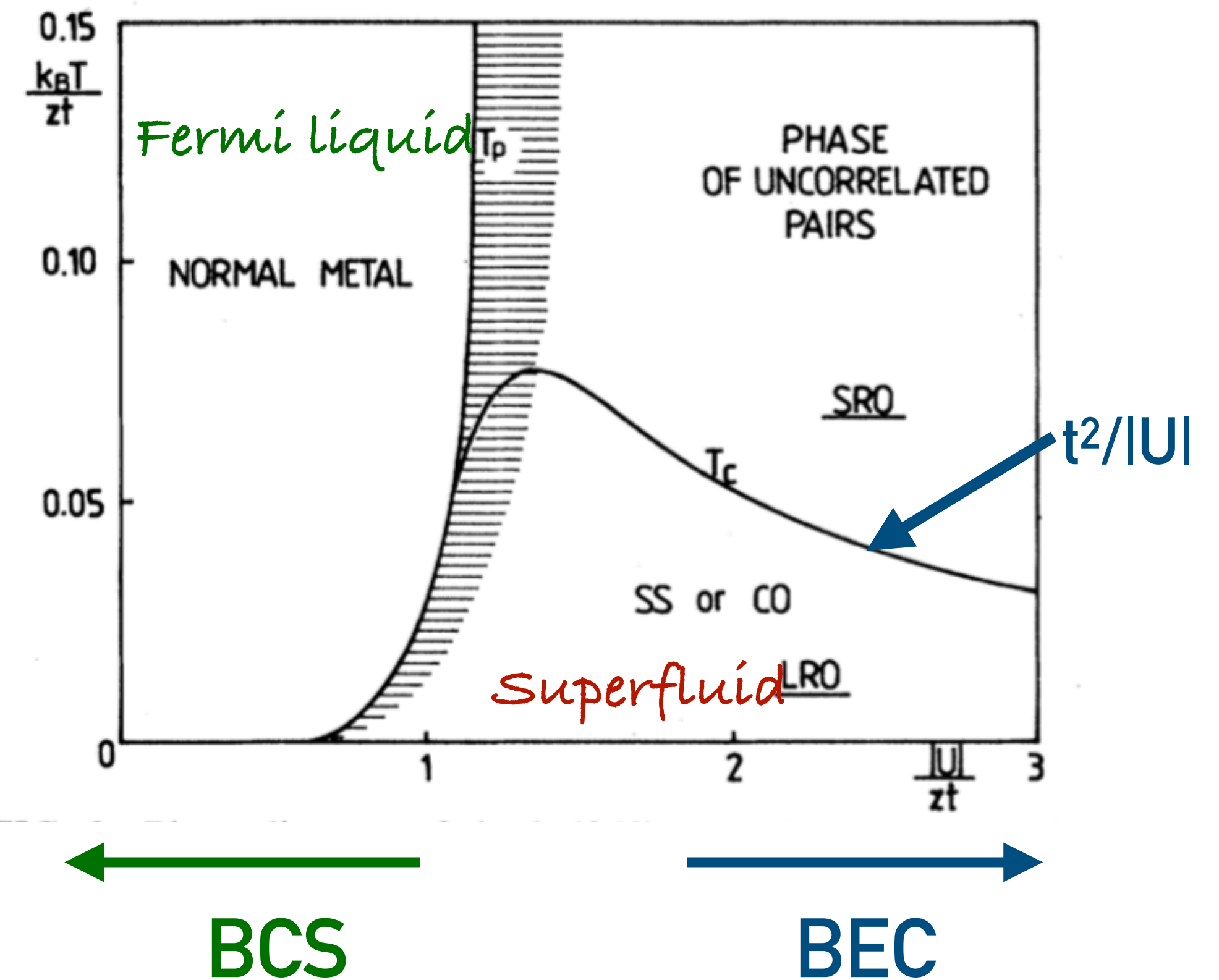
Continuum



M Randeria and E. Taylor, Annu. Rev. Condens. Matter Phys (2014)

C. A. R. Sá de Melo, M Randeria and J. R. Engelbrecht, Phys. Rev. Lett. (93)

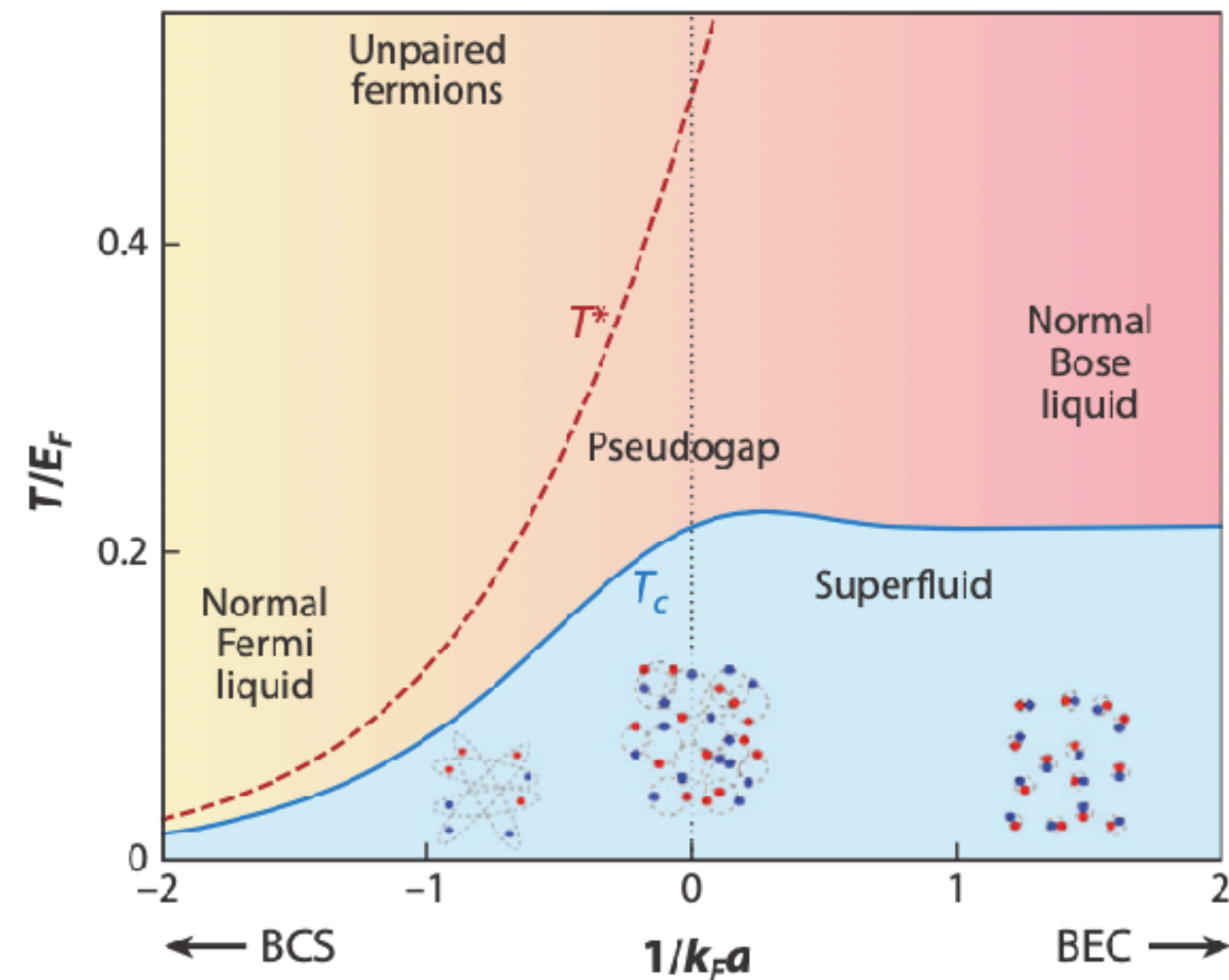
Lattice



Micnas et al, Rev Mod Phys 62, 113(90)

Attractive interactions in Fermionic systems

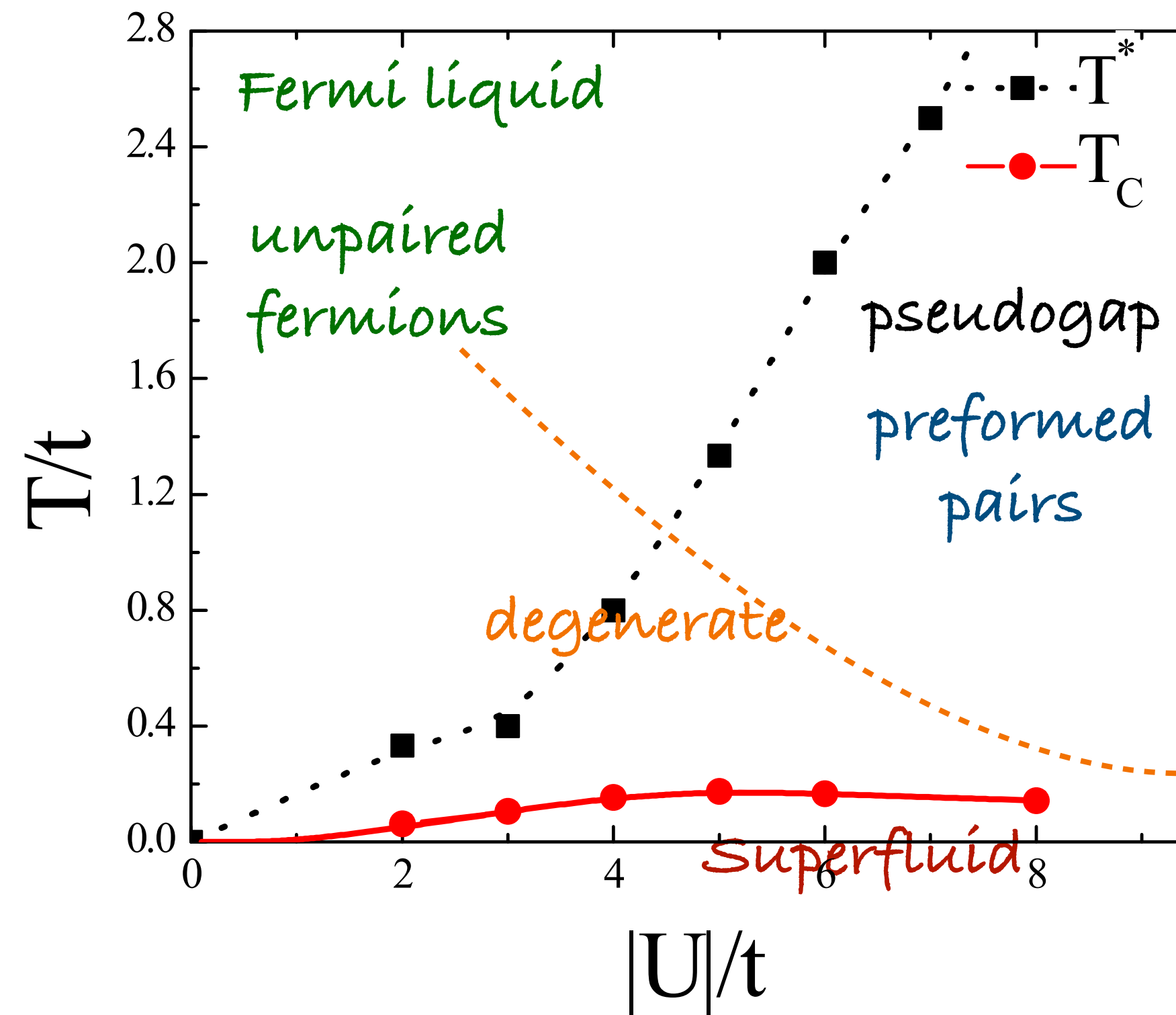
Continuum



M Randeria and E. Taylor, Annu. Rev. Condens. Matter Phys (2014)

C. A. R. Sá de Melo, M Randeria and J. R. Engelbrecht, Phys. Rev. Lett. (93)

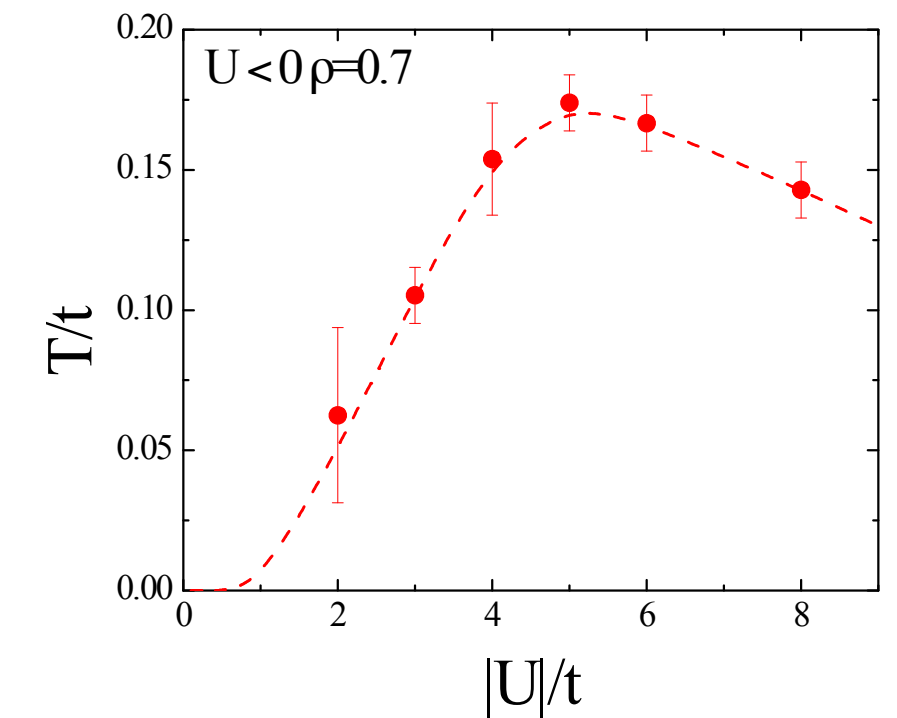
Lattice



Paiva et al, PRL (10)

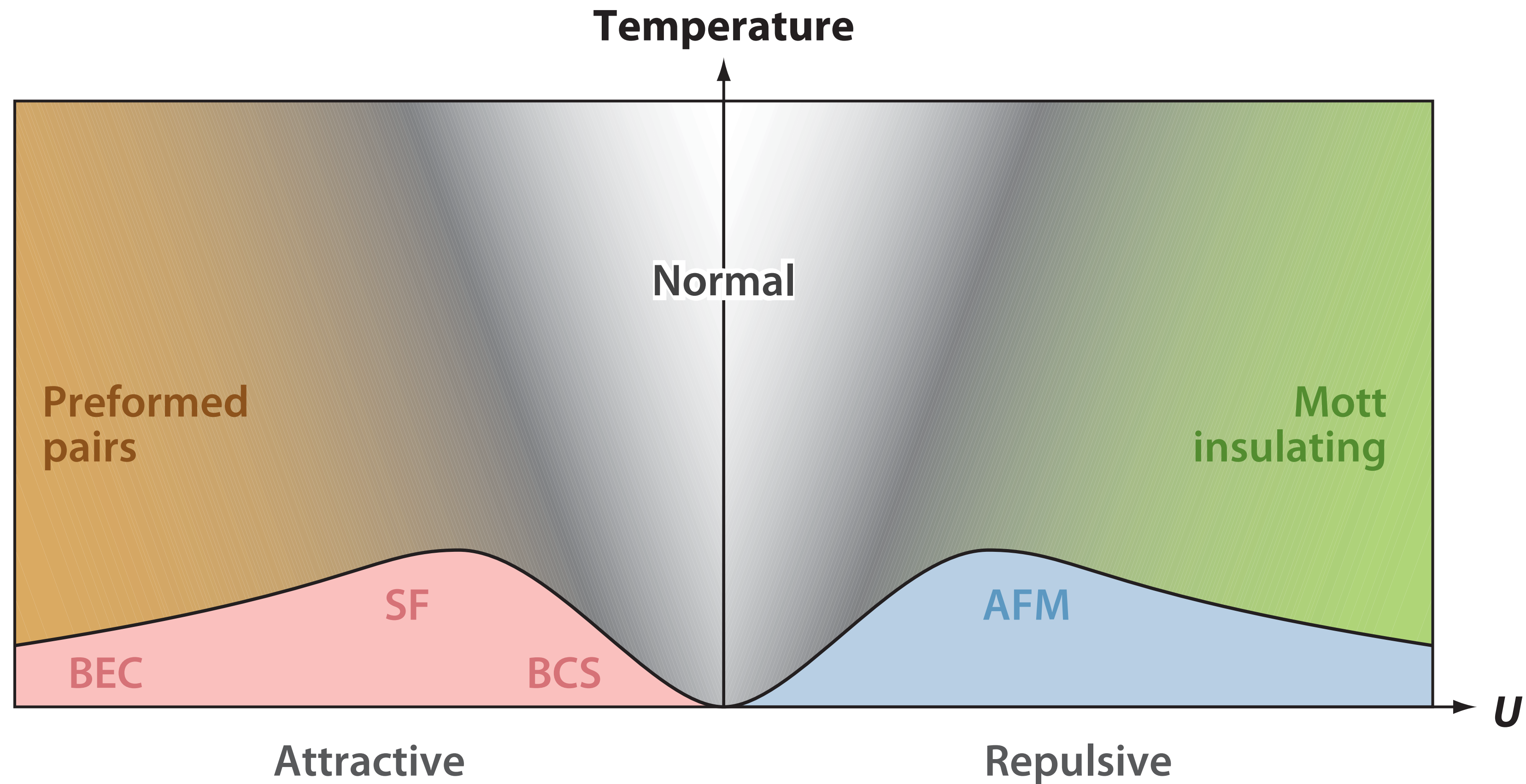
$t^2/|U|$

behavior for large $|U|$



$n=0.7$

Relation between repulsive and attractive models



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

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

Fontenele's thesis

Two-dimensional attractive Hubbard model and the BCS-BEC crossover

Rodrigo A. Fontenele ¹, Natanael C. Costa ^{1,2}, Raimundo R. dos Santos ¹, and Thereza Paiva ¹

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²*International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy*

PRB 105, 184502 (2022)

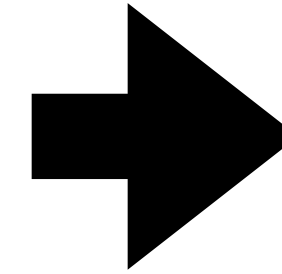
Increasing superconducting T_c by layering in the attractive Hubbard model

Rodrigo A. Fontenele , Natanael C. Costa , Thereza Paiva , and Raimundo R. dos Santos 

Instituto de Física, Universidade Federal do Rio de Janeiro Cx.P. 68.528, 21941-972 Rio de Janeiro, Brazil

PRA 110, 053315 (2024)

Pairing correlation functions



$$C_{ij}^{\Delta} \equiv \langle b_i^{\dagger} b_j + \text{H.c.} \rangle$$

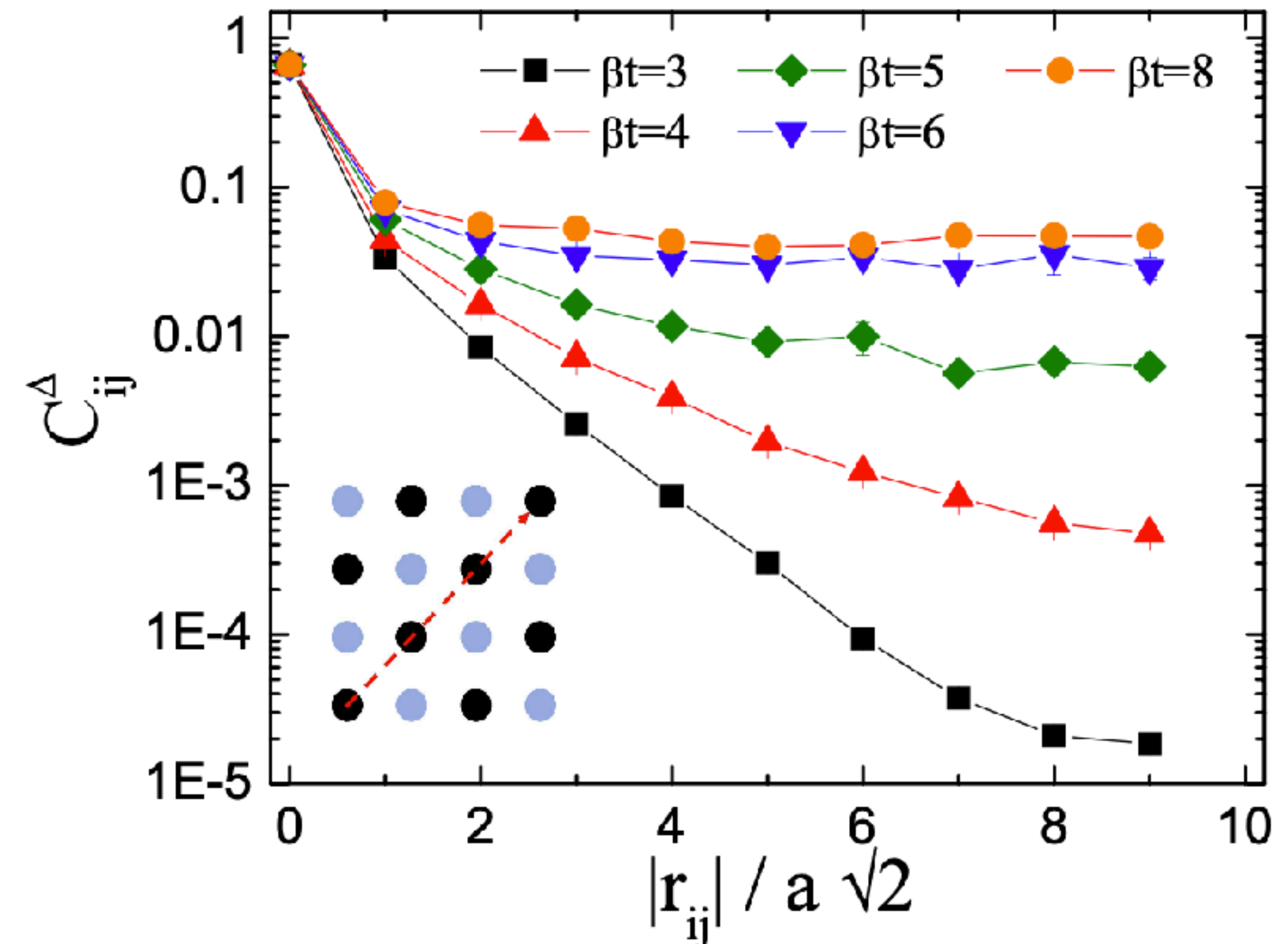
$$b_i \equiv c_{i\downarrow} c_{i\uparrow} \quad b_i^{\dagger} \equiv c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger}$$

$$r_{ij} \equiv |\mathbf{i} - \mathbf{j}|$$

$U/t = -5$
 $n = 0.5$
 18 x 18 lattice

$$\beta = \frac{1}{k_B T}$$

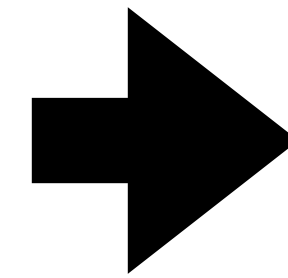
If $\lim_{|\mathbf{i}-\mathbf{j}| \rightarrow \infty} C_{ij}^{\Delta} \sim \text{const} \Rightarrow \text{order}$



Attractive Hubbard Model

Free from fermionic sign problem

Pairing correlation functions



$$C_{ij}^{\Delta} \equiv \langle b_i^{\dagger} b_j + \text{H.c.} \rangle$$

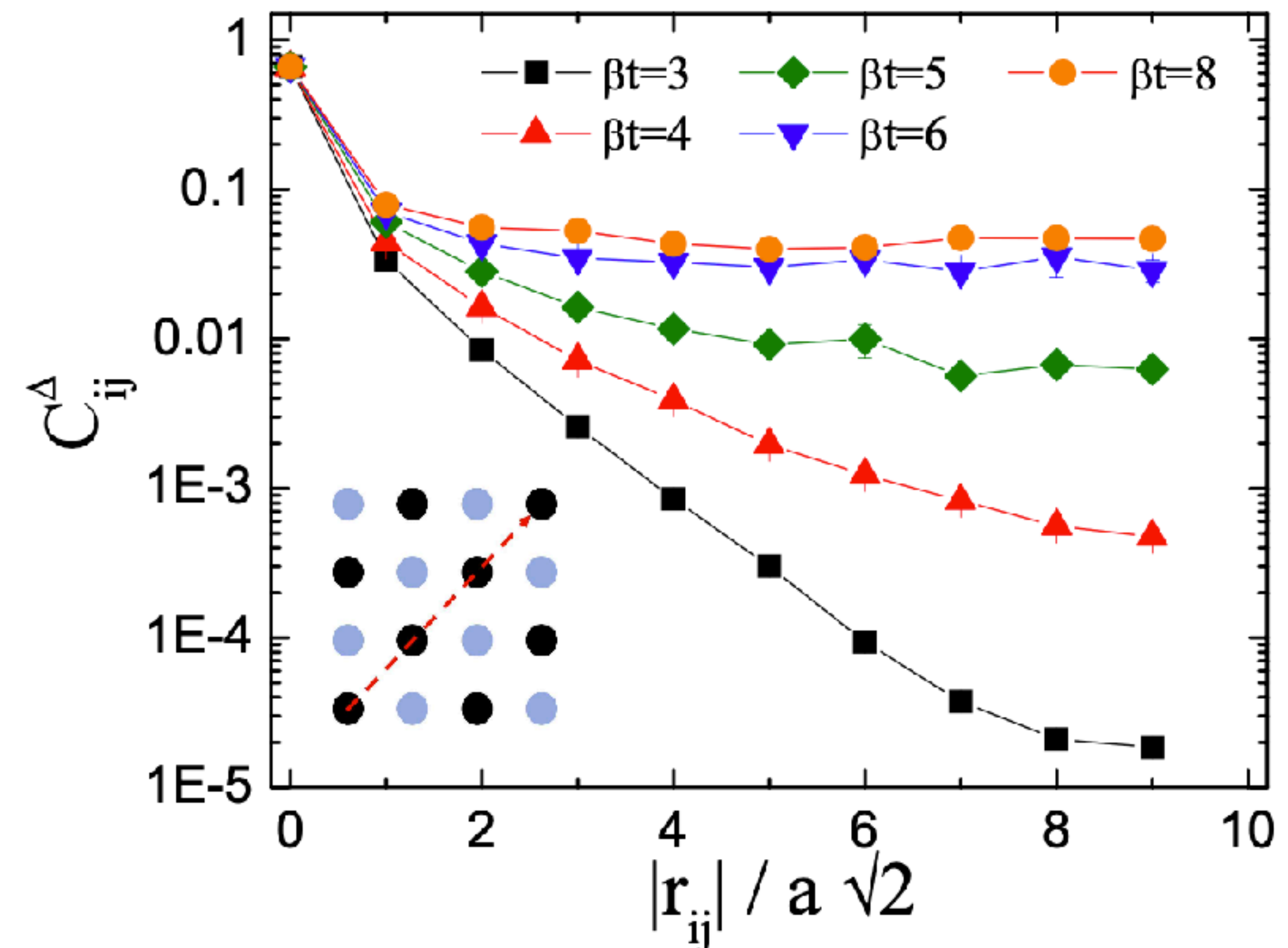
$$b_i \equiv c_{i\downarrow} c_{i\uparrow} \quad b_i^{\dagger} \equiv c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger}$$

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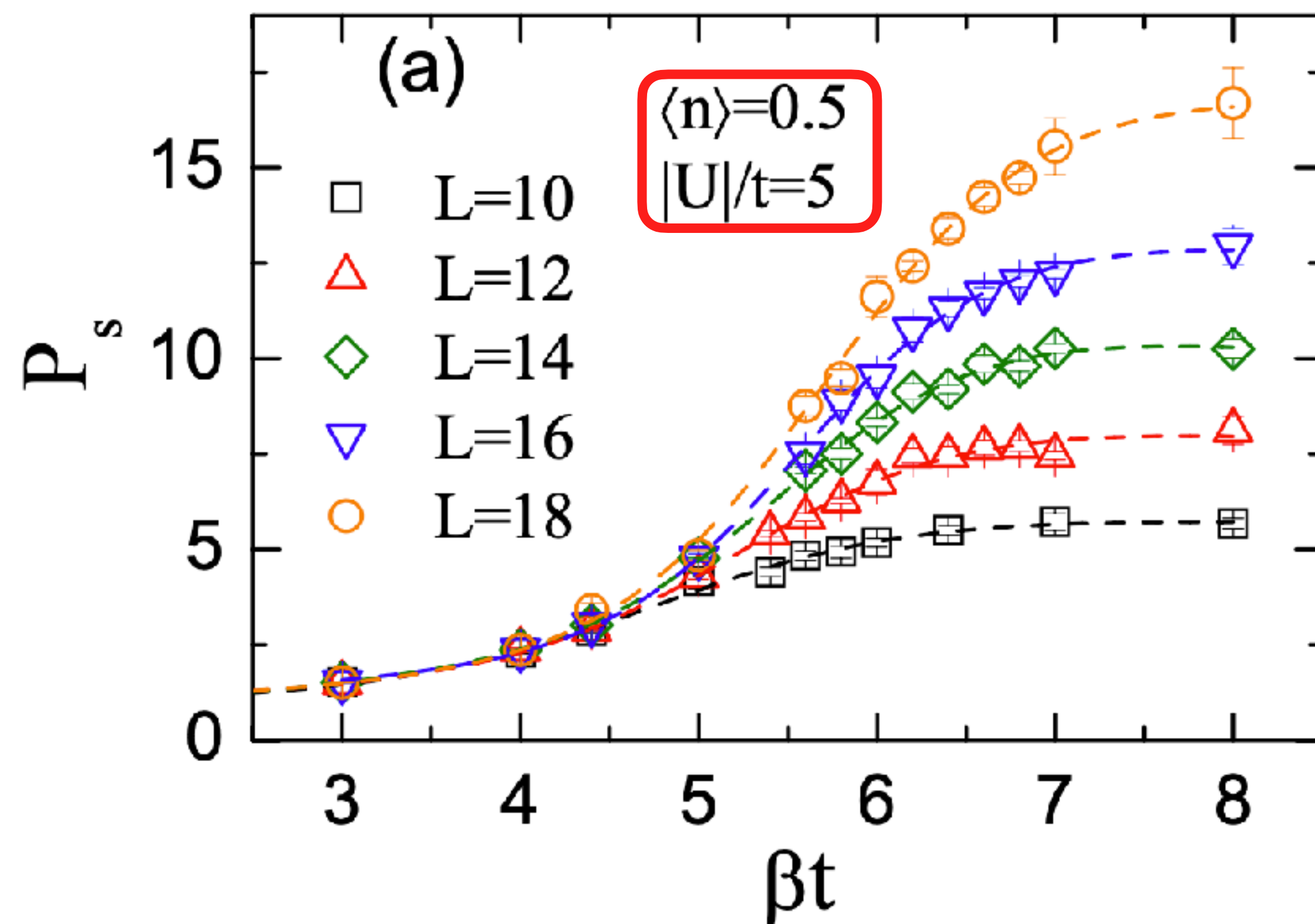
$$\beta = \frac{1}{k_B T}$$

If $\lim_{|\mathbf{i}-\mathbf{j}| \rightarrow \infty} C_{ij}^{\Delta} \sim \text{const} \Rightarrow \text{order}$



Critical temperature

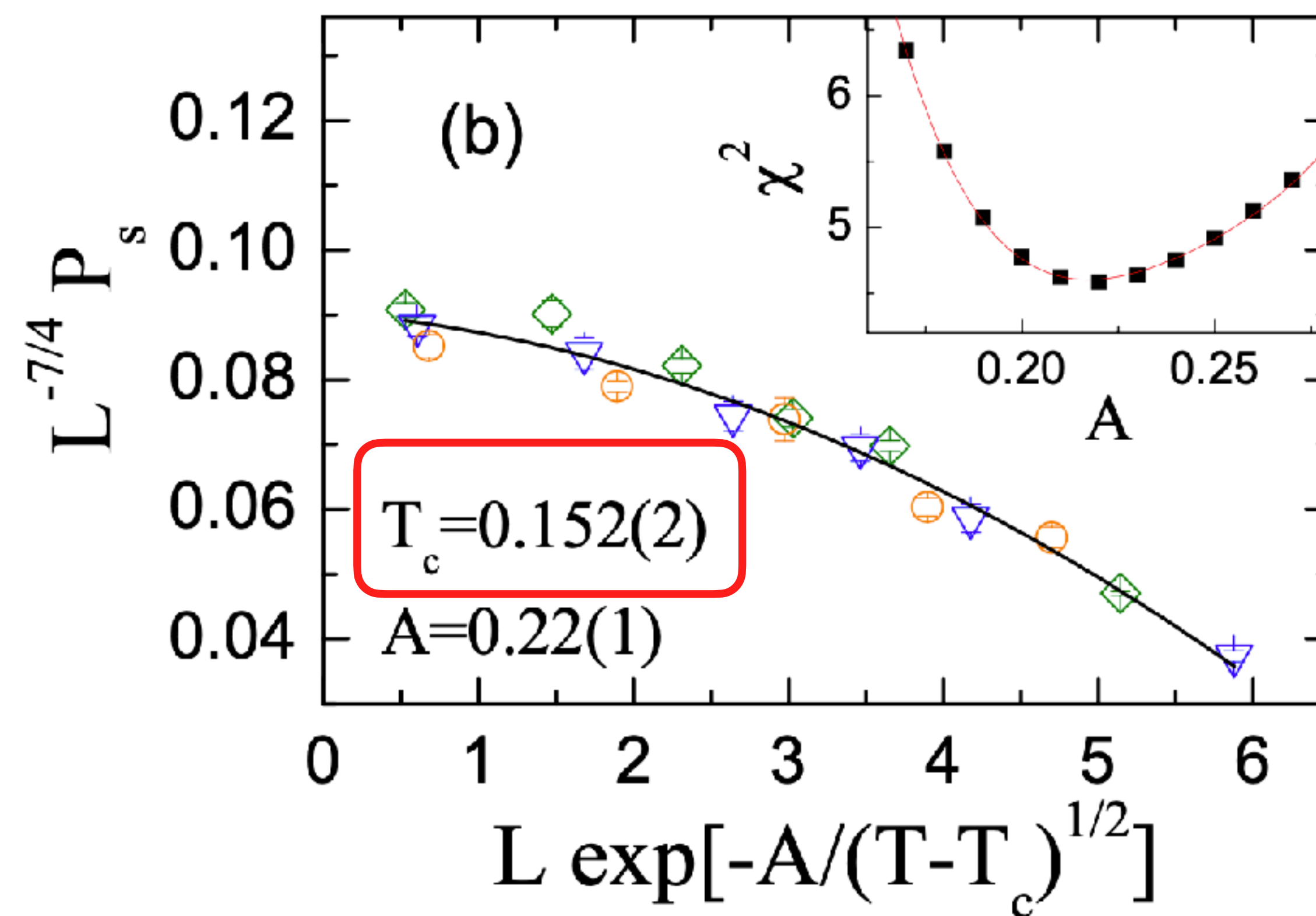
$$P_s = \langle \Delta^\dagger \Delta + \Delta \Delta^\dagger \rangle \quad \Delta^\dagger = \frac{1}{\sqrt{N}} \sum_i b_i^\dagger$$



Finite-size scaling for a Kosterlitz-Thouless transition

$$P_s = L^{2-\eta(T_c)} f(L/\xi), \quad L \gg 1, T \rightarrow T_c^+$$

$$\xi \sim \exp \left[\frac{A}{(T - T_c)^{1/2}} \right] \quad \eta = 1/4$$

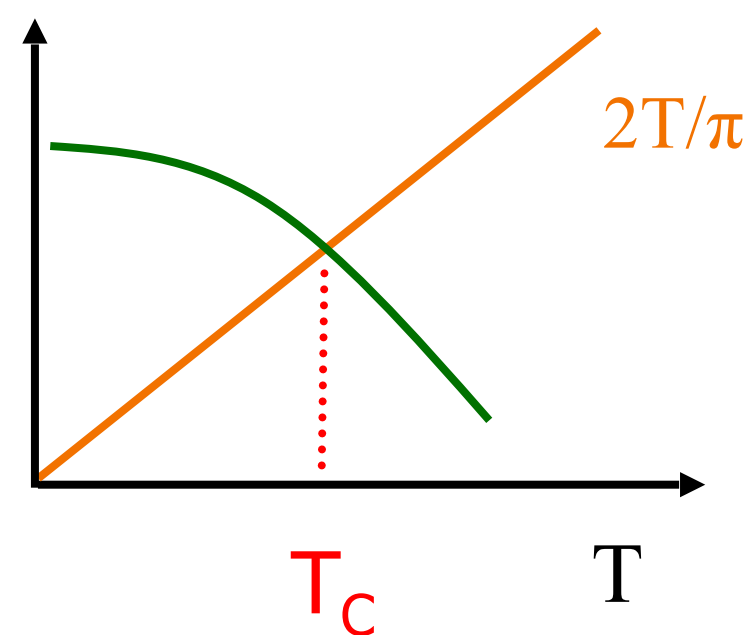


How do we find T_c

$$T_c = \frac{\pi}{2} \rho_s^-$$

helicity modulus just below T_c

Jump in superfluid
helicity modulus



$$\rho_s = \frac{D_s}{4\pi e^2} = \frac{1}{4}[\Lambda^L - \Lambda^T]$$

$$\left\{ \begin{array}{l} \Lambda^L \equiv \lim_{q_x \rightarrow 0} \Lambda_{xx}(q_x, q_y = 0, \omega_n = 0) \\ \Lambda^T \equiv \lim_{q_y \rightarrow 0} \Lambda_{xx}(q_x = 0, q_y, \omega_n = 0) \end{array} \right.$$

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we start with the x-
component of the current
density operator

$$j_x(\ell, \tau) = e^{\mathcal{H}\tau} \left[it \sum_{\sigma} \left(c_{\ell+\hat{x},\sigma}^{\dagger} c_{\ell,\sigma} - c_{\ell,\sigma}^{\dagger} c_{\ell+\hat{x},\sigma} \right) \right] e^{-\mathcal{H}\tau}$$

$$\Lambda_{xx}(\ell, \tau) = \langle j_x(\ell, \tau) j_x(0, 0) \rangle$$

$$\Lambda_{xx}(\mathbf{q}, \omega_n) = \sum_{\ell} \int_0^{\beta} d\tau e^{i\mathbf{q} \cdot \ell} e^{i\omega_n \tau} \Lambda_{xx}(\ell, \tau) \quad \text{where} \quad \omega_n = 2n\pi T$$

How do we find T_c

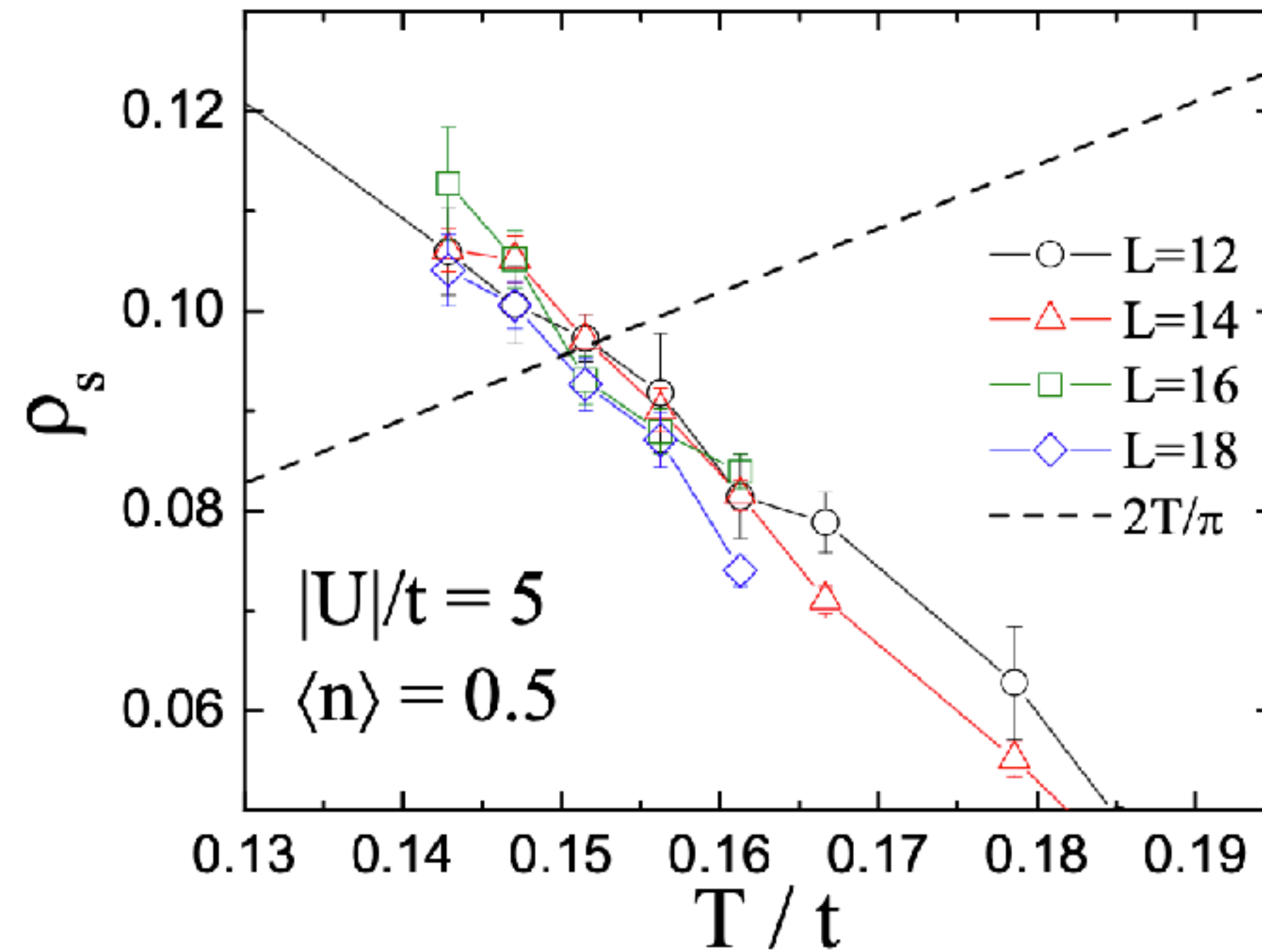
Finite-size scaling for a Kosterlitz-Thouless transition

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How do we find T_c

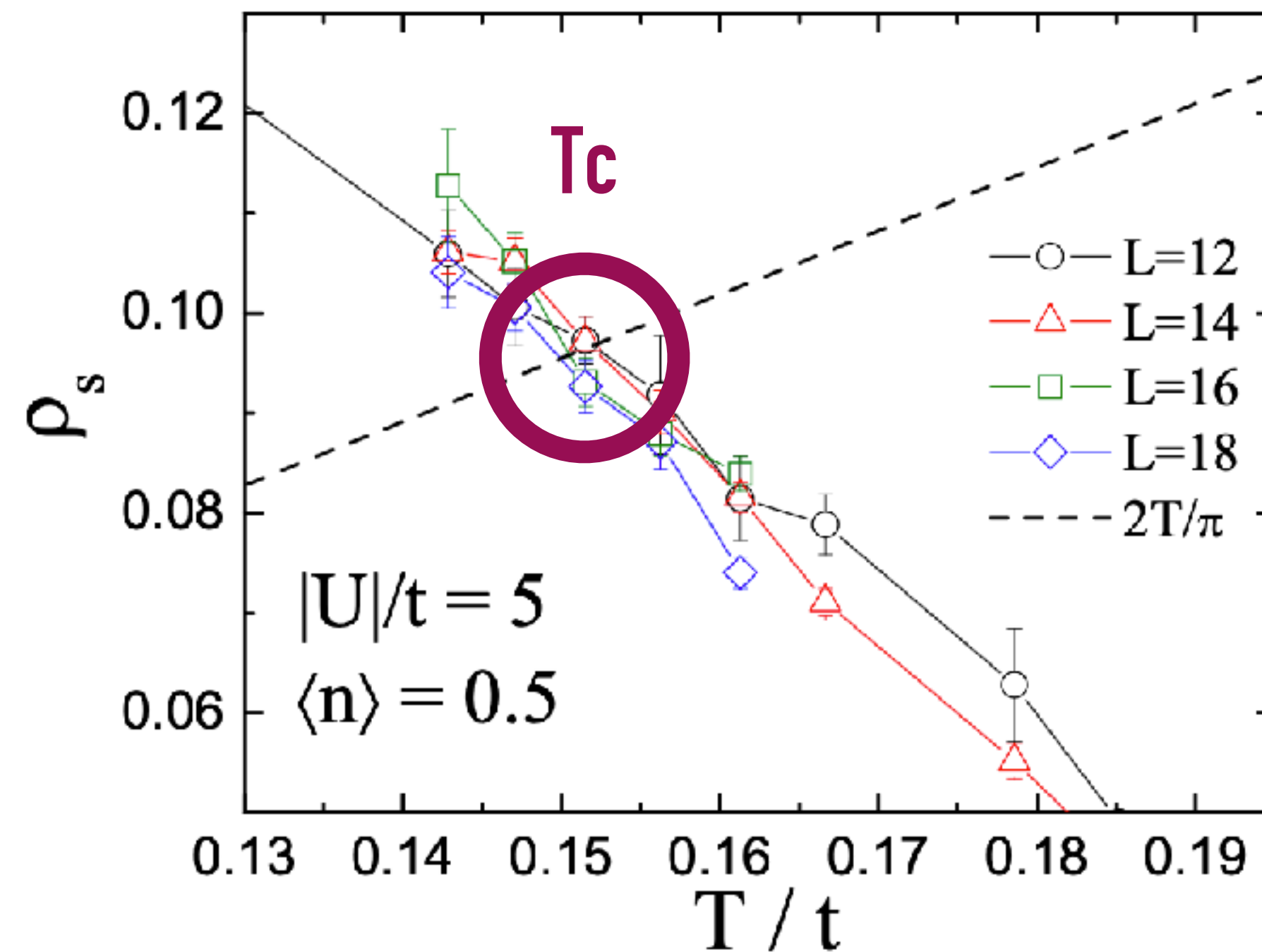
Finite-size scaling for a Kosterlitz-Thouless transition

$$T_c = \frac{\pi}{2} \rho_s^-$$

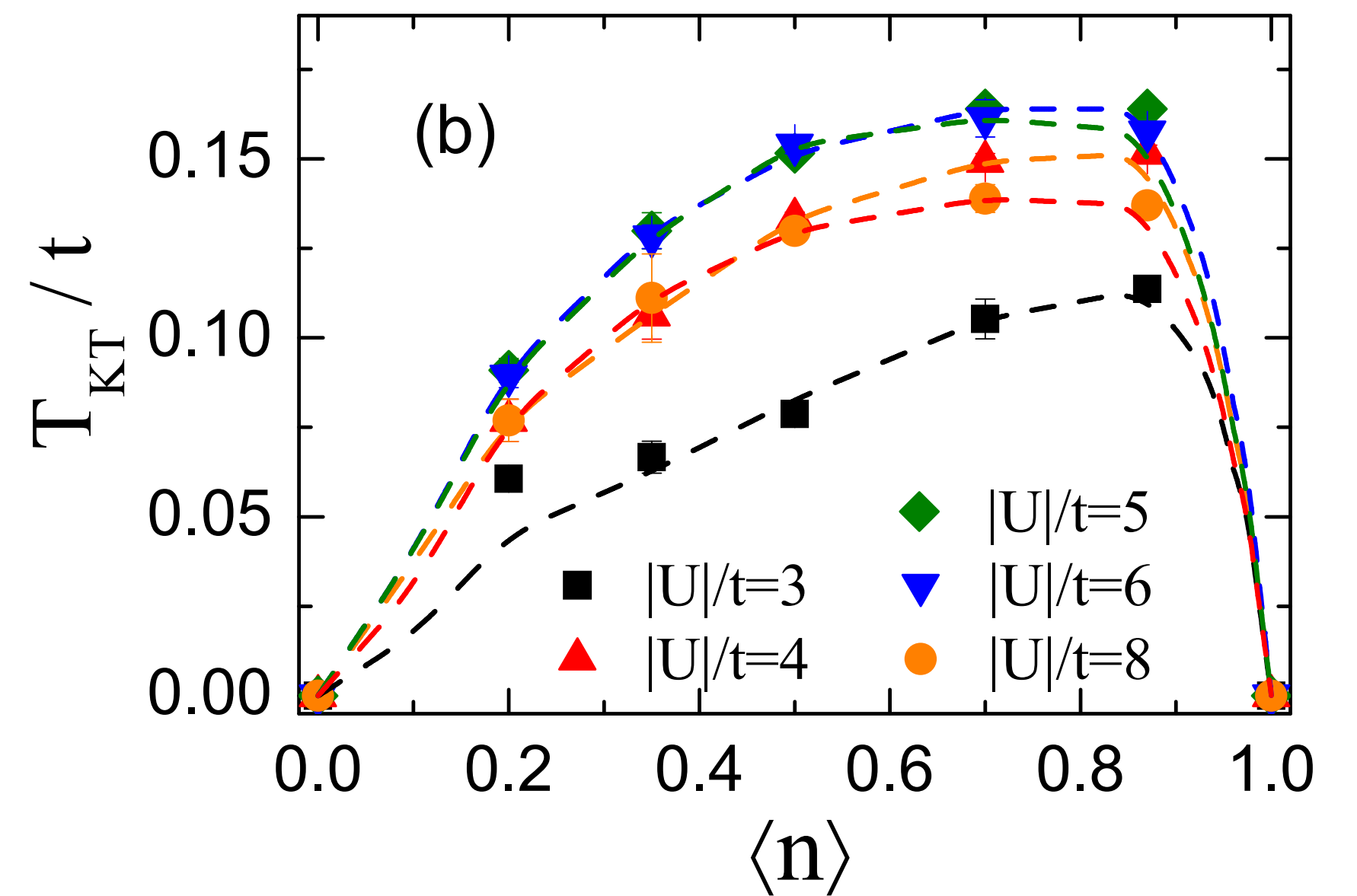
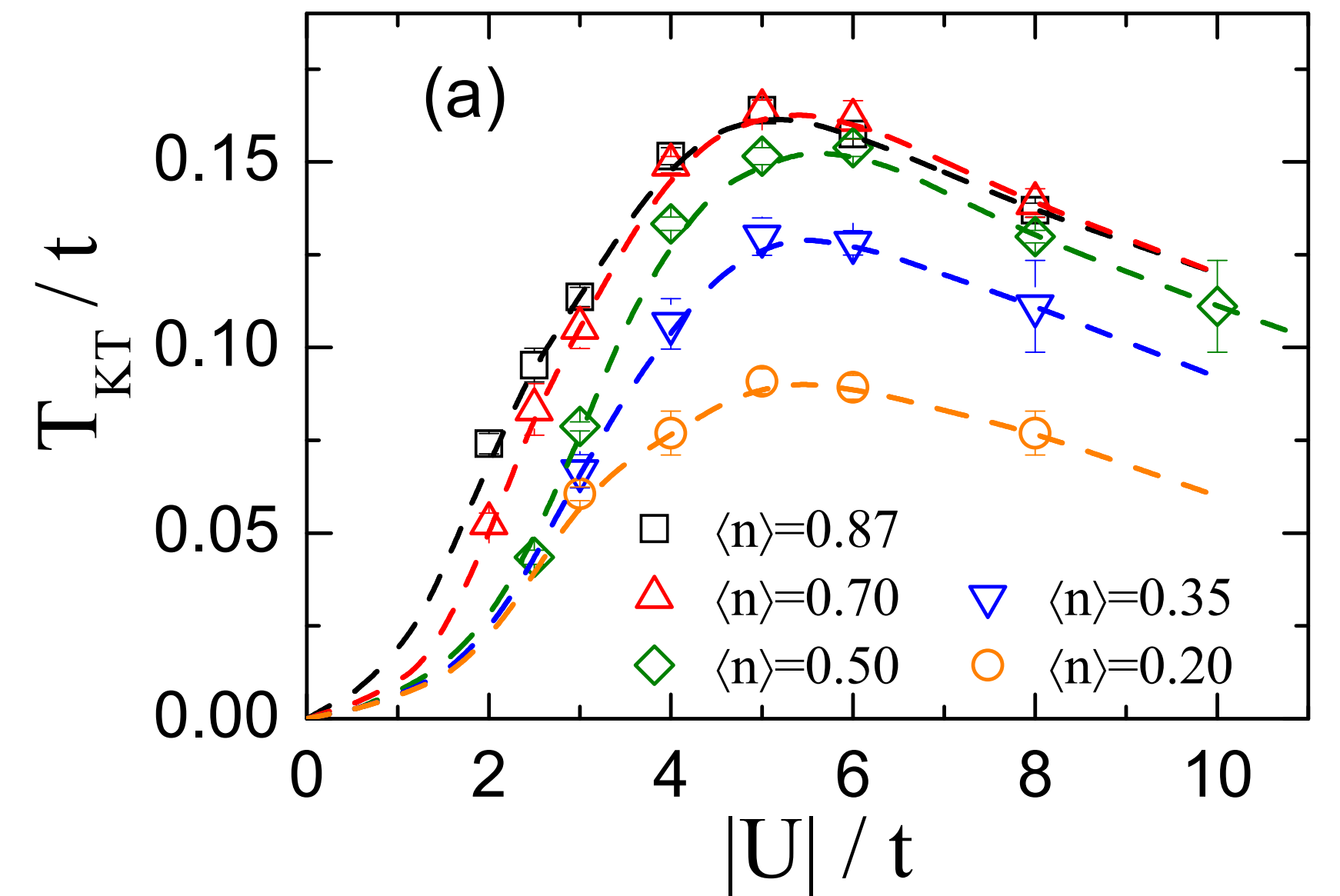
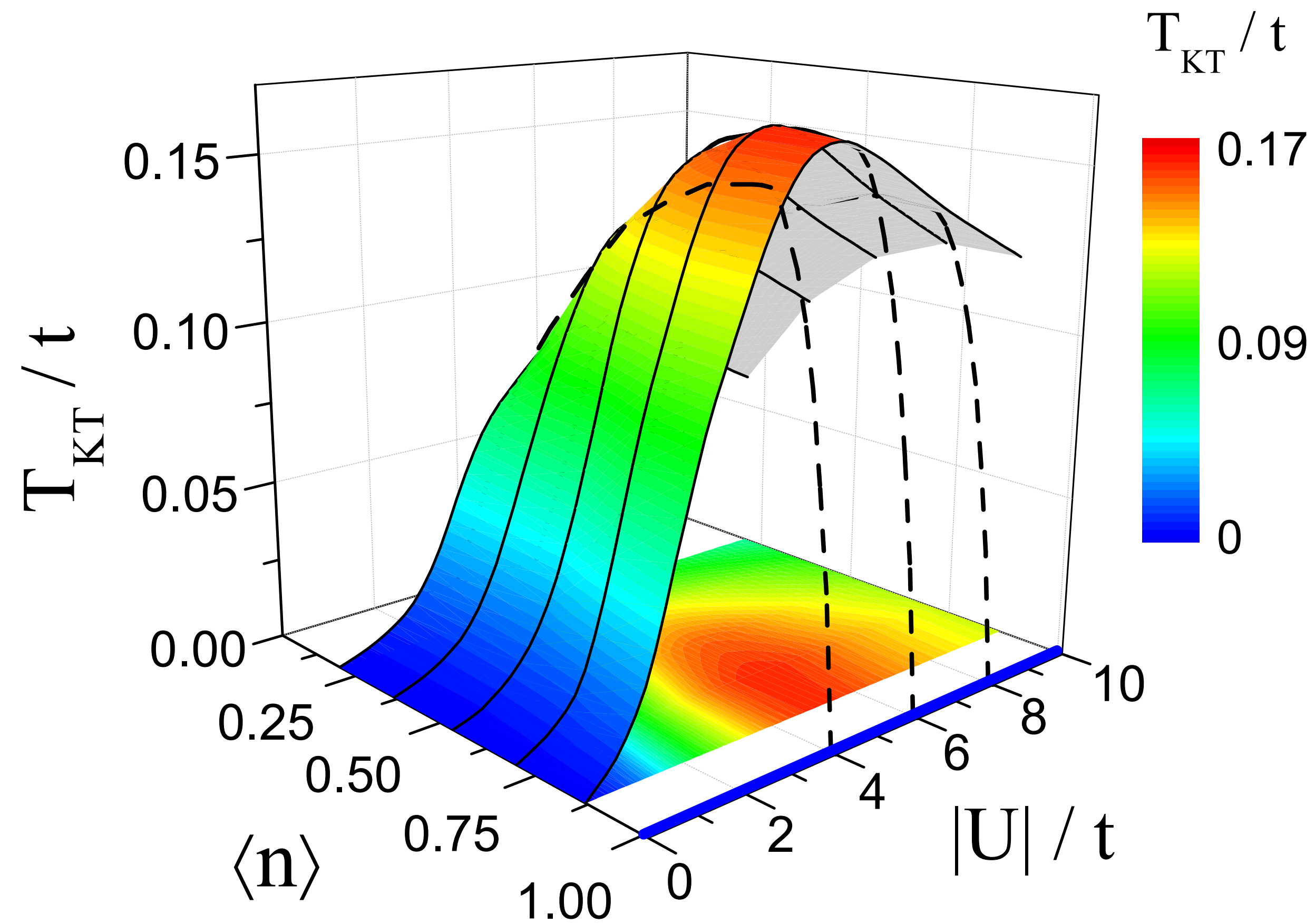
helicity modulus just below T_c

Jump in superfluid
helicity modulus

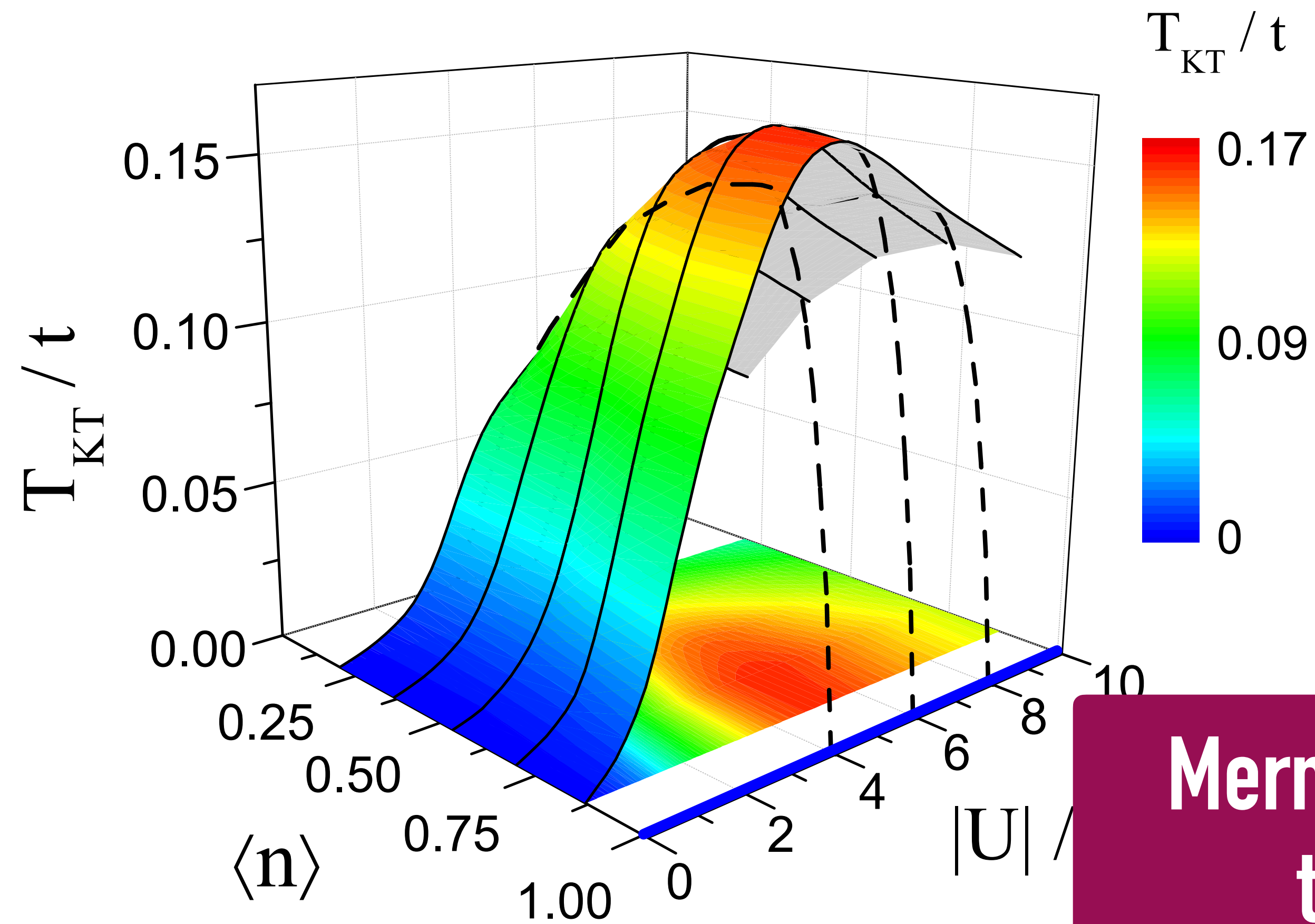
$$\rho_s = \frac{D_s}{4\pi e^2} = \frac{1}{4}[\Lambda^L - \Lambda^T]$$



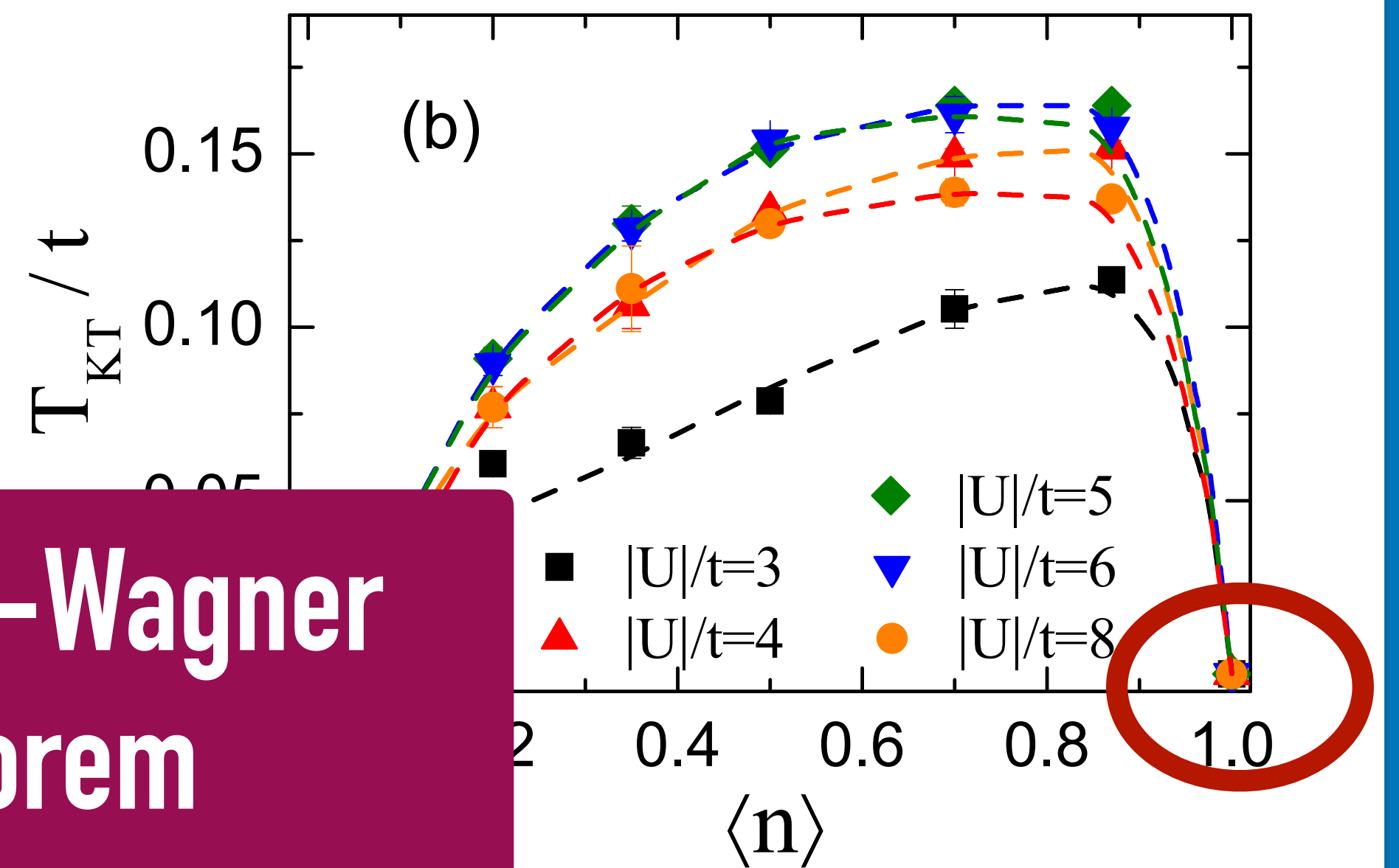
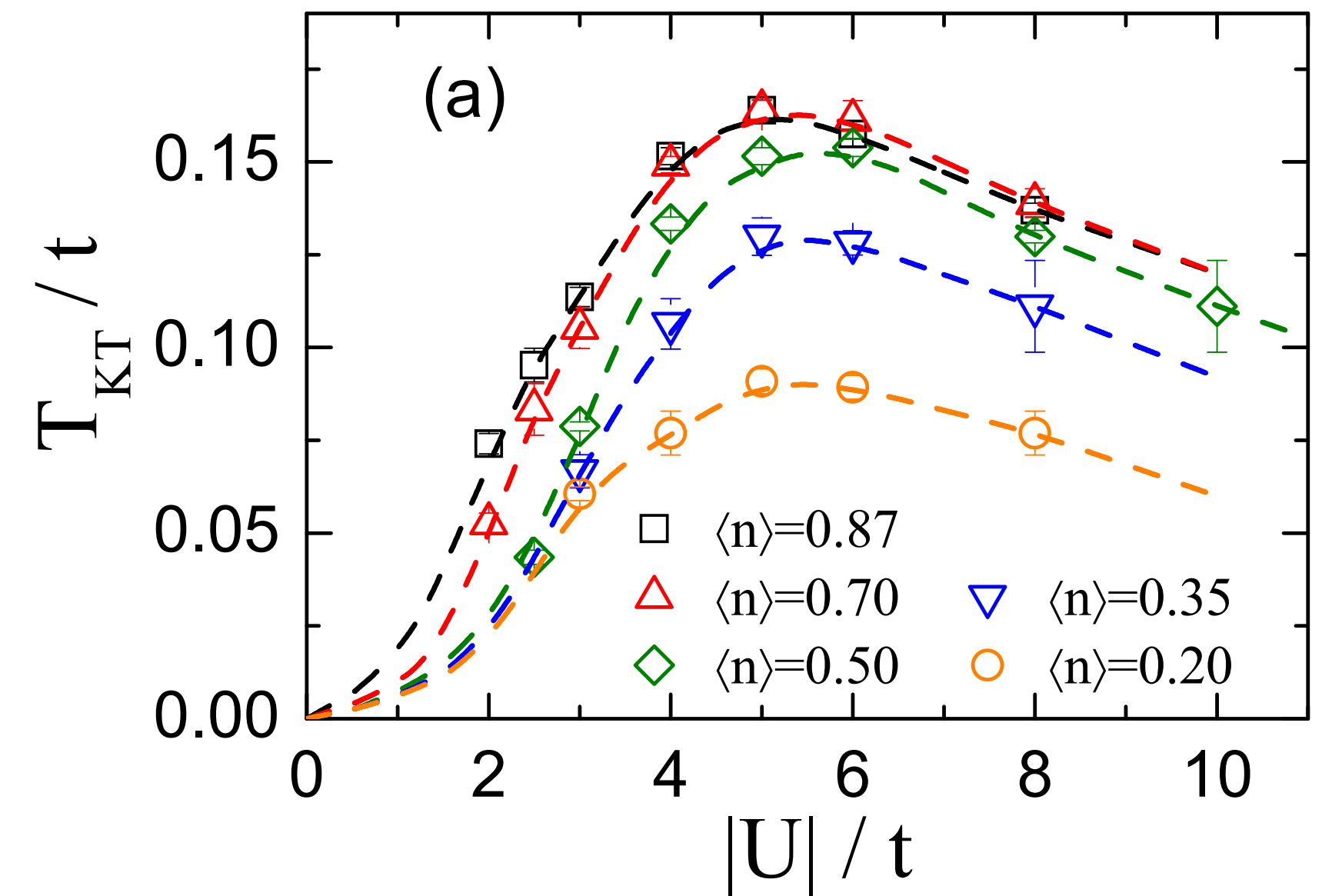
Critical temperature



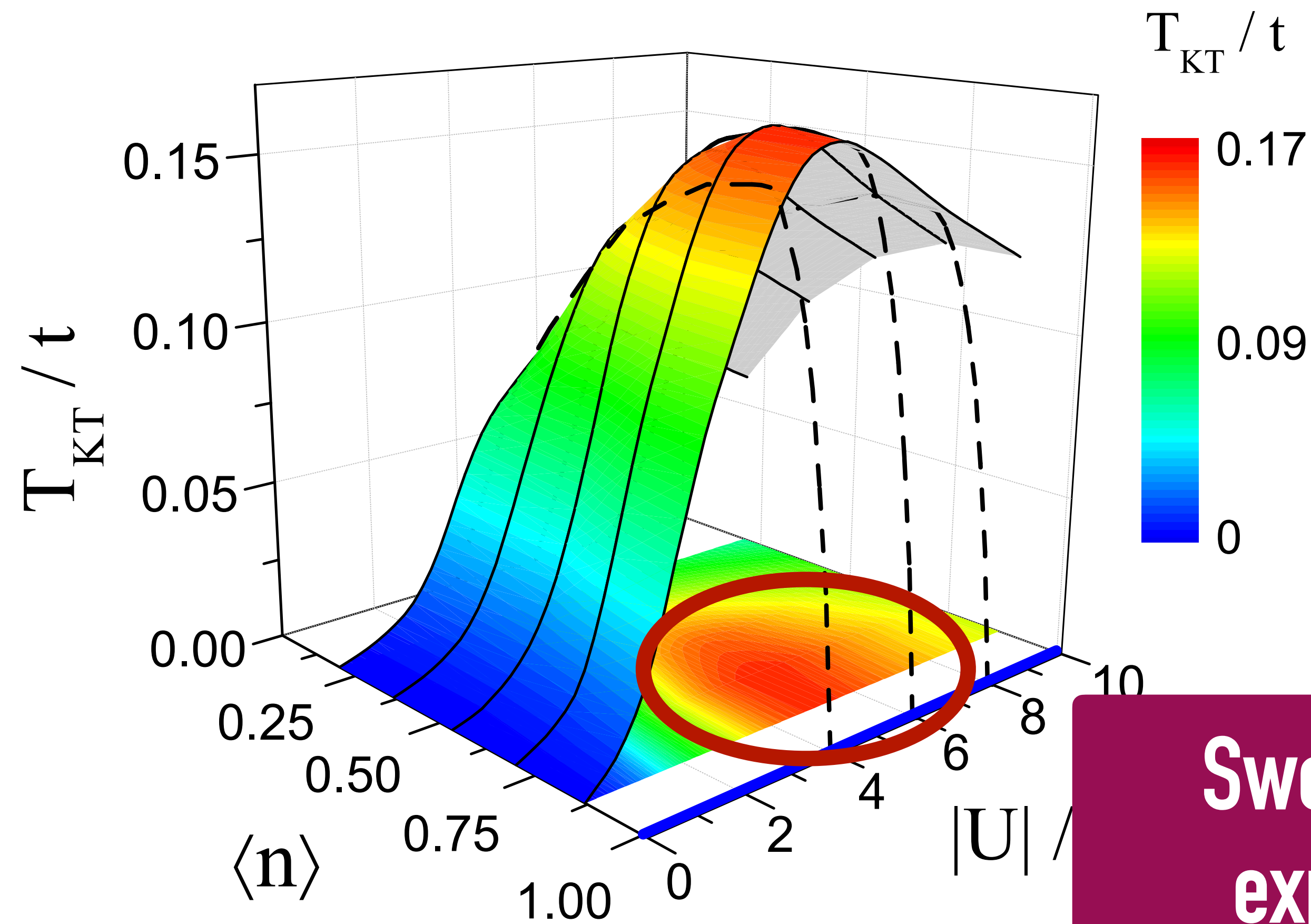
Critical temperature



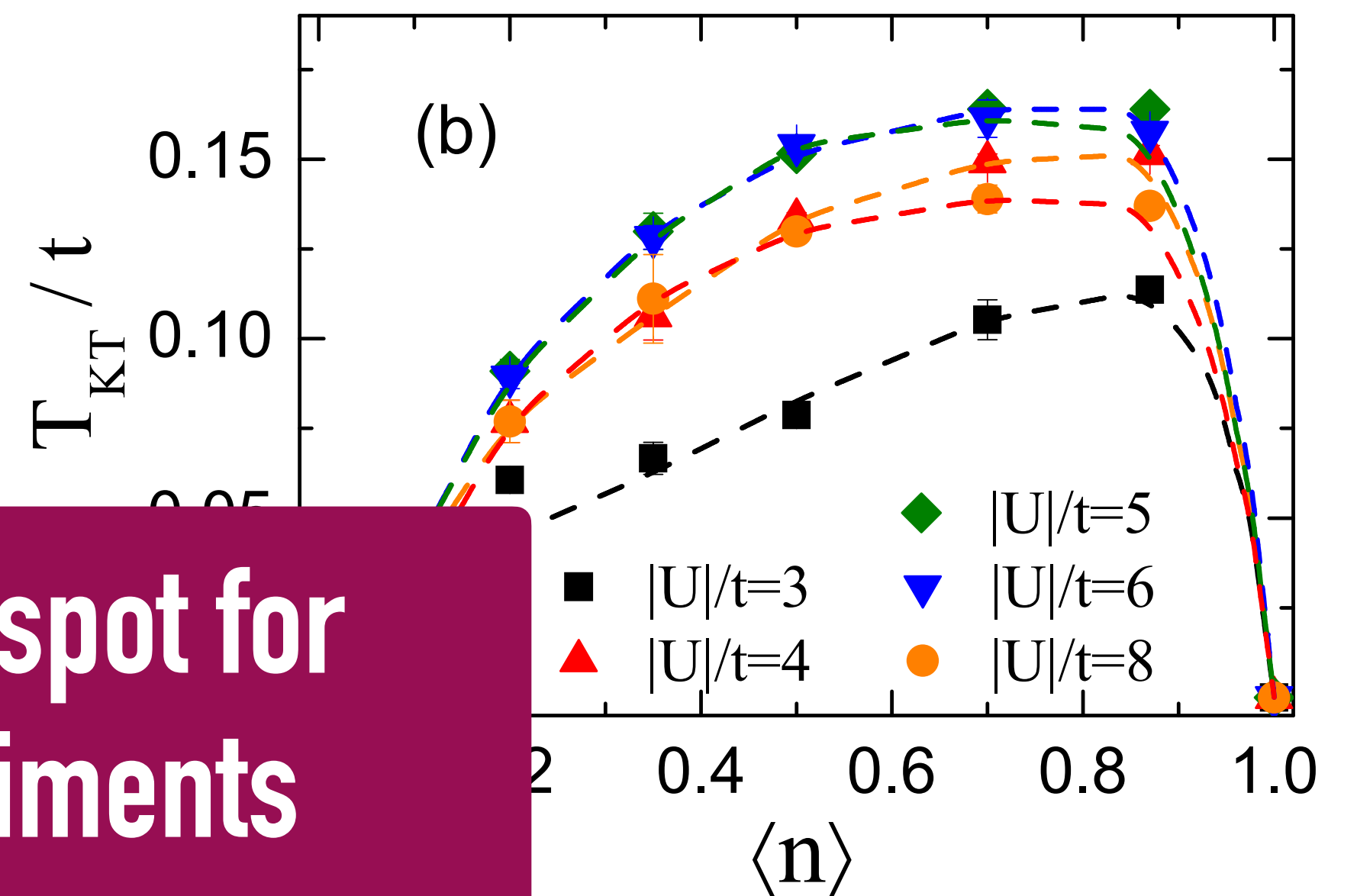
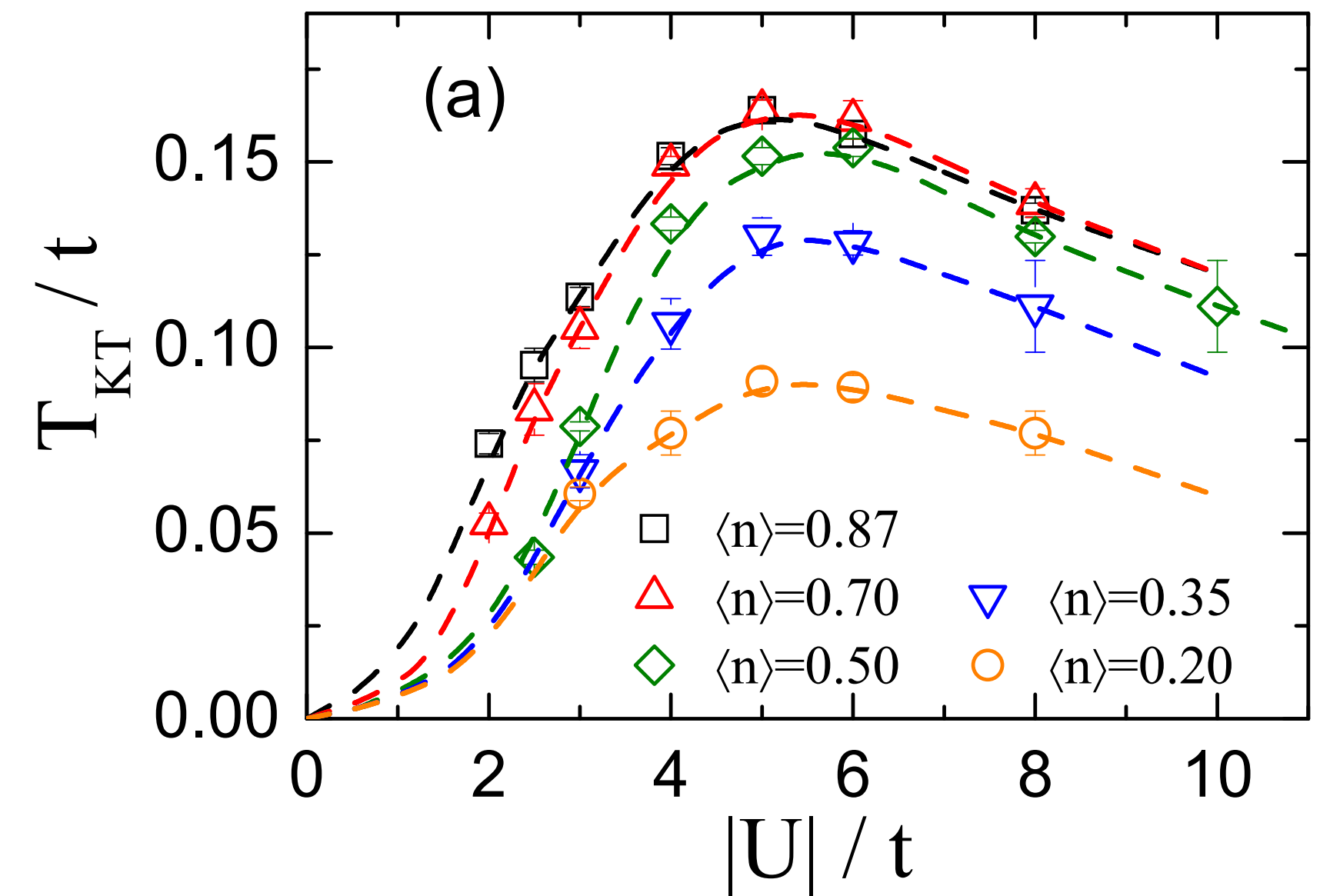
Mermin-Wagner
theorem



Critical temperature

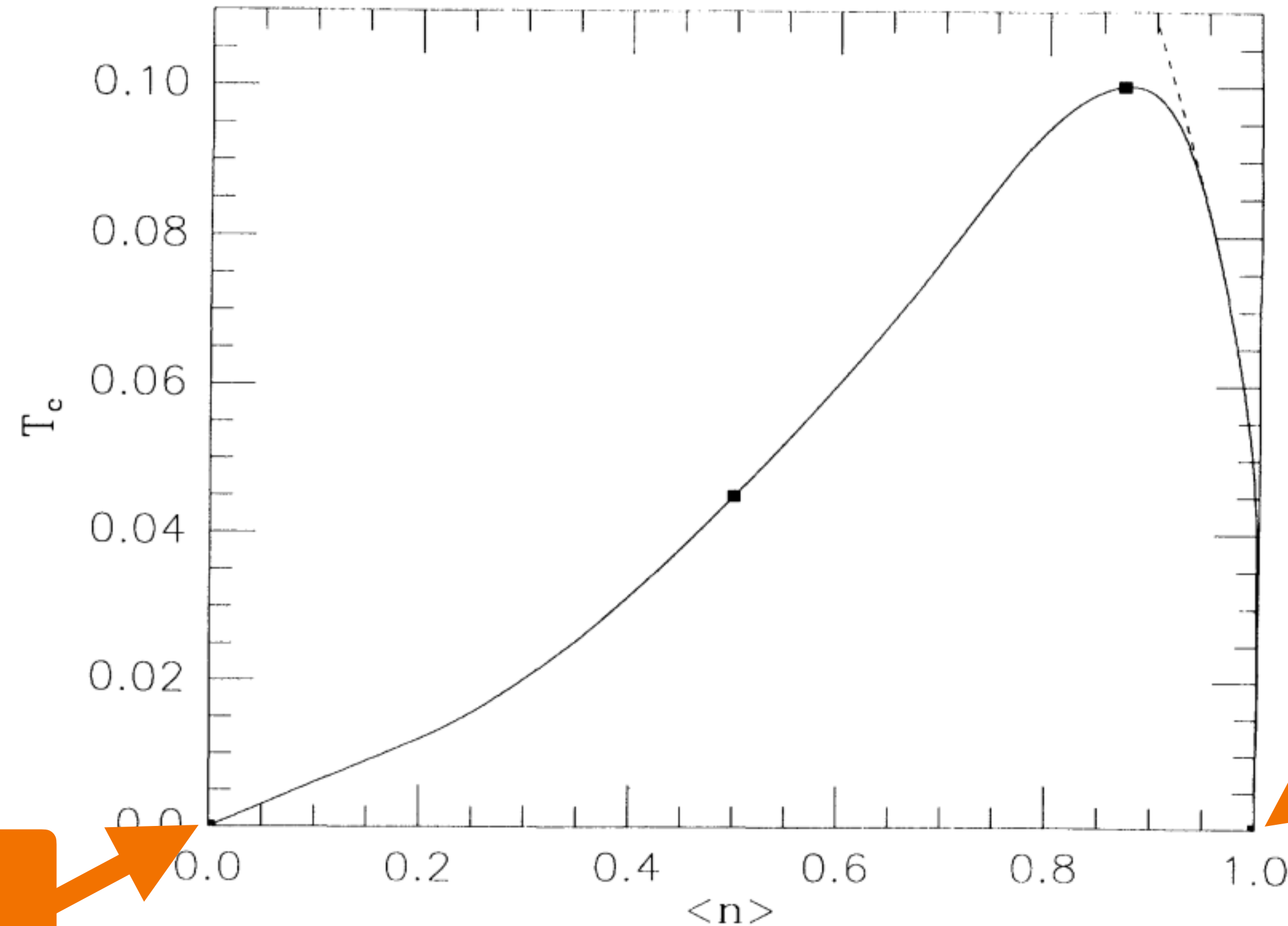


Sweet spot for experiments



Size effects again...

Critical temperature

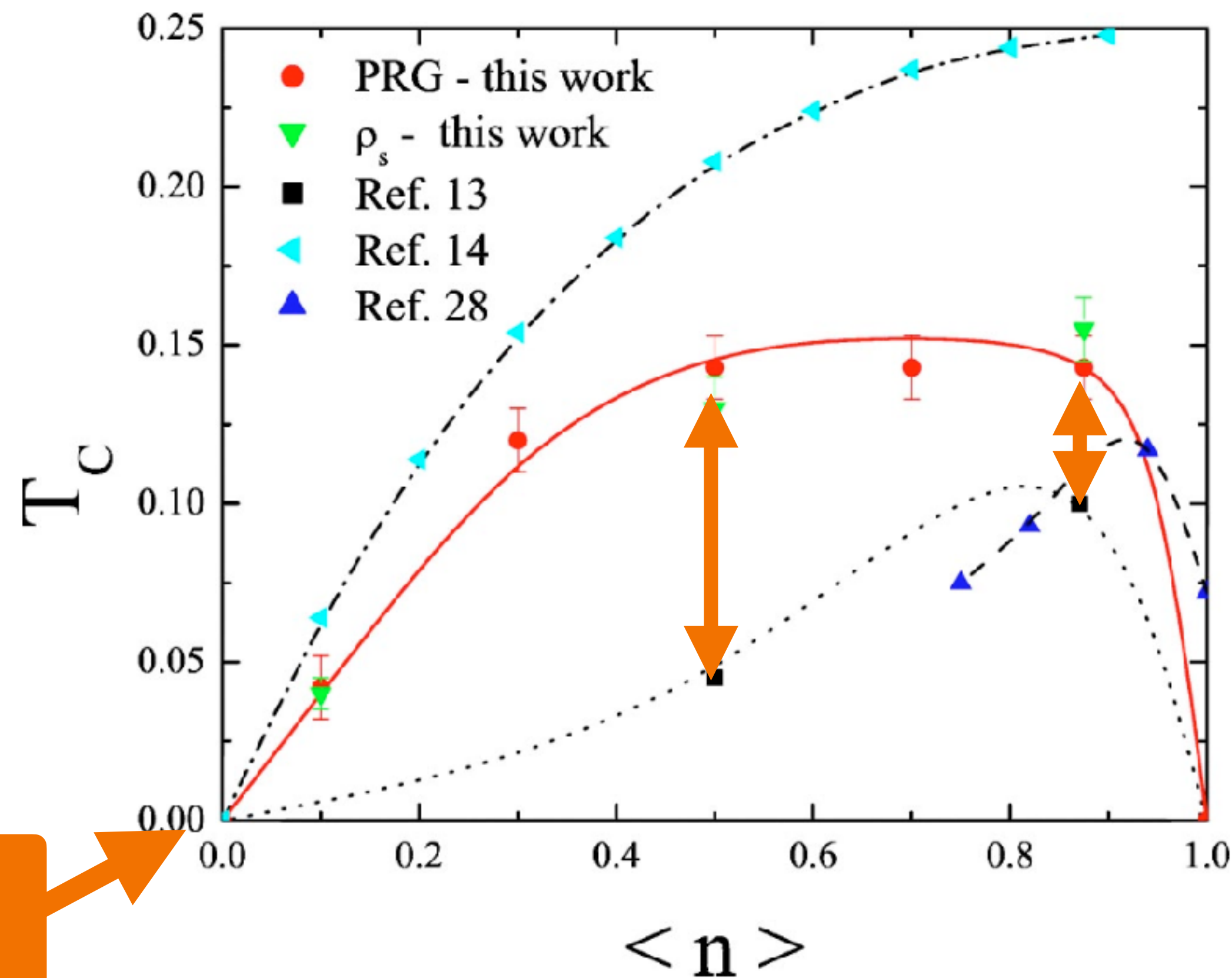


CDW and SUC are
degenerated at half-
filling

Empty
system

Moreo and Scalapino PRL 91

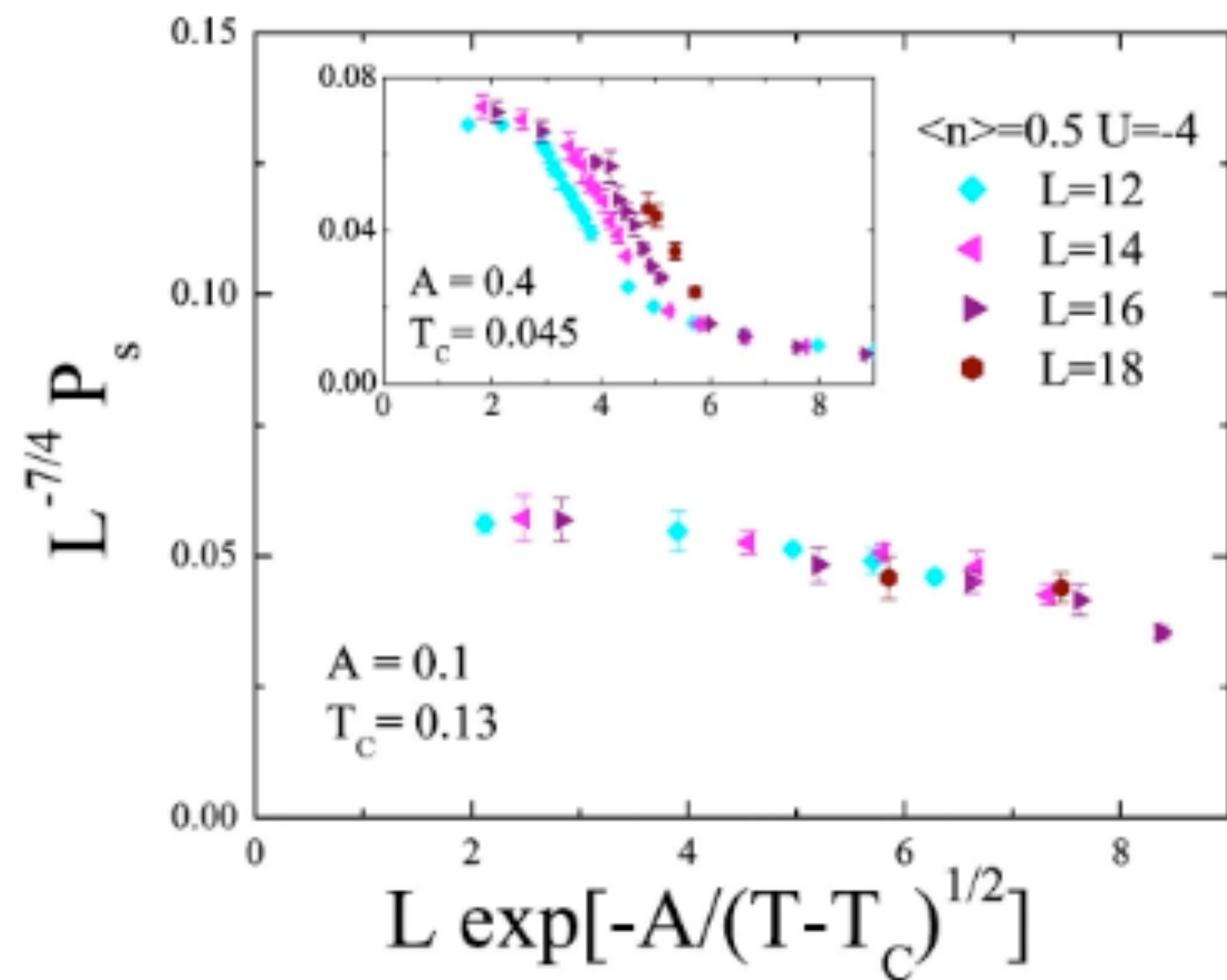
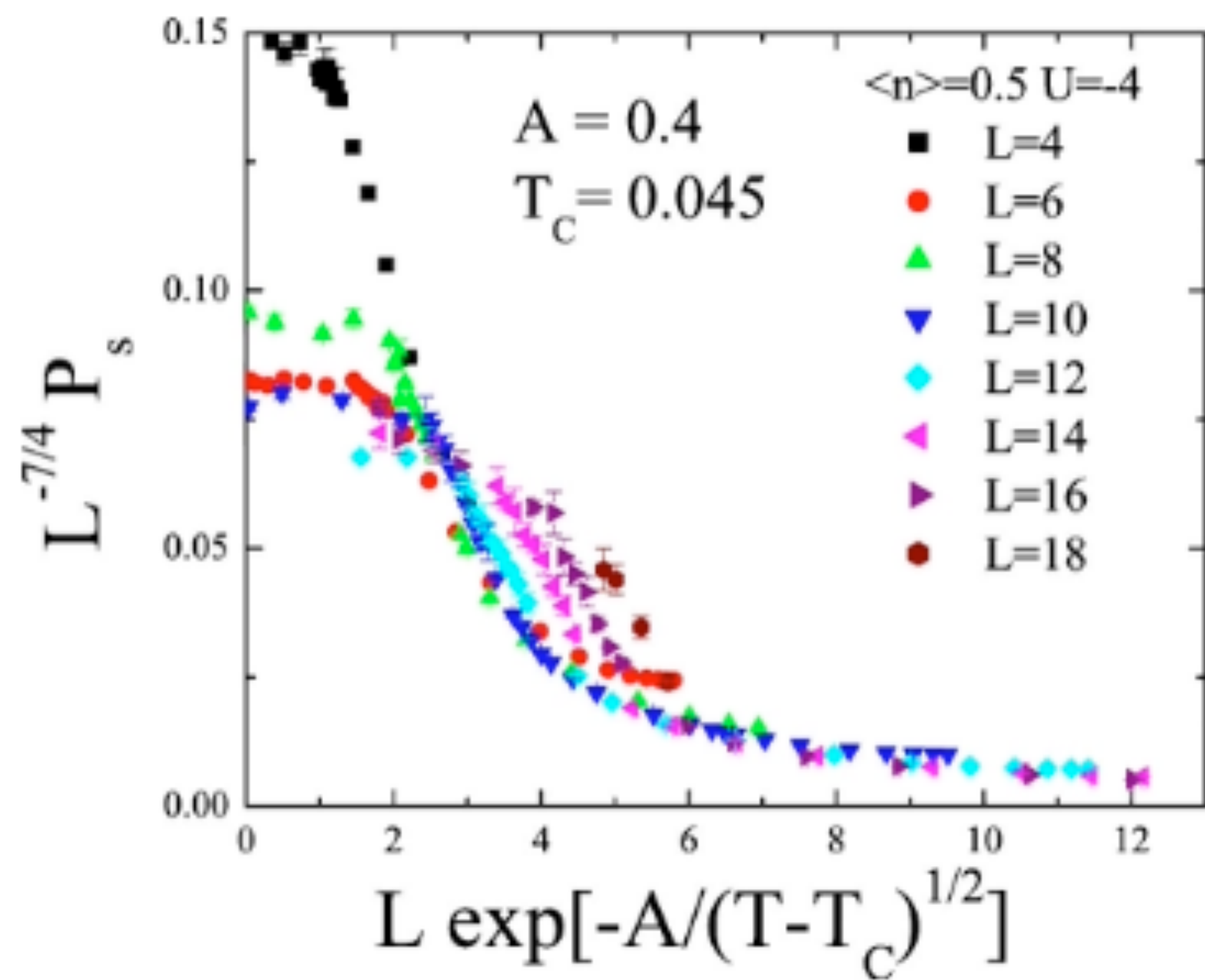
Critical temperature

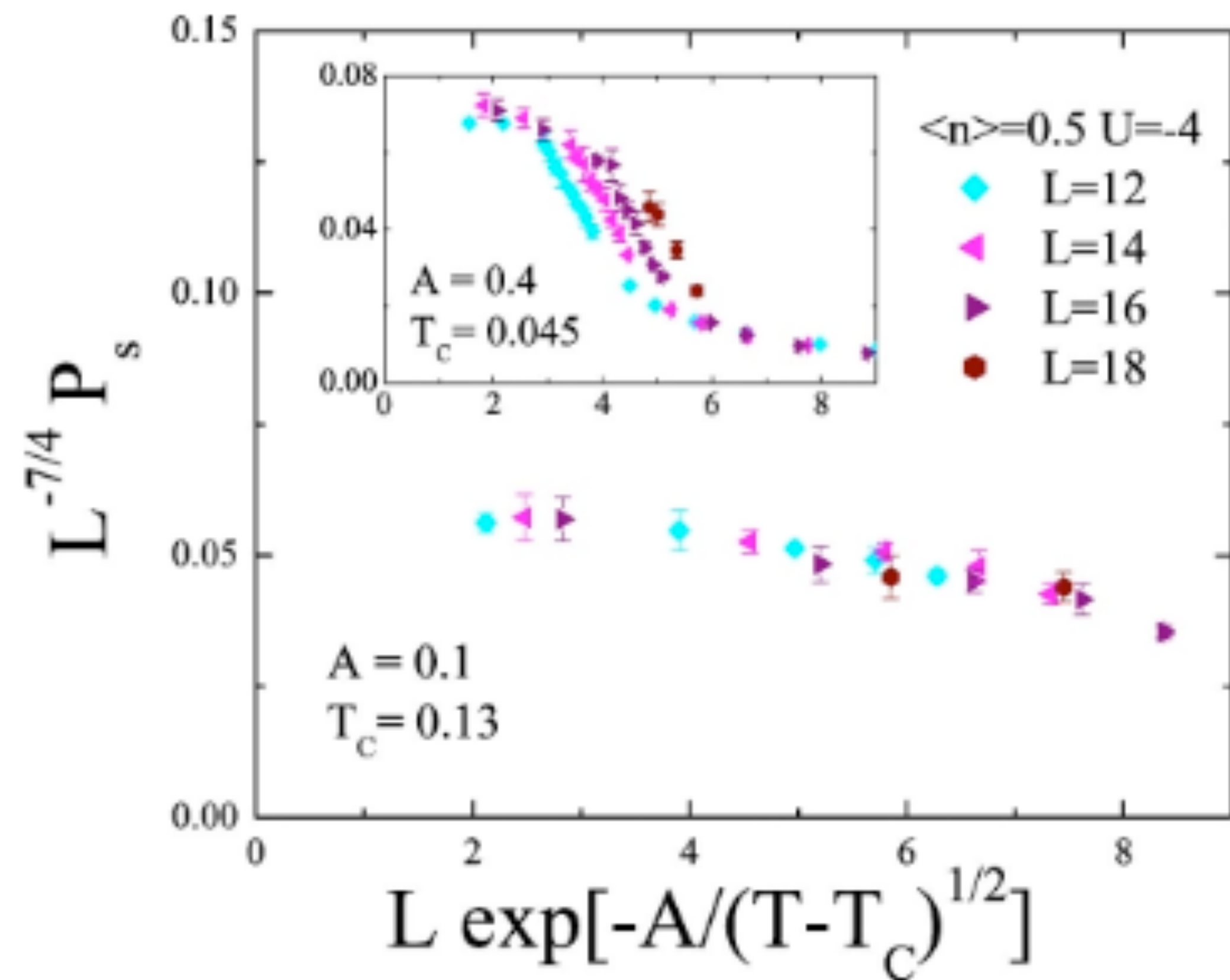
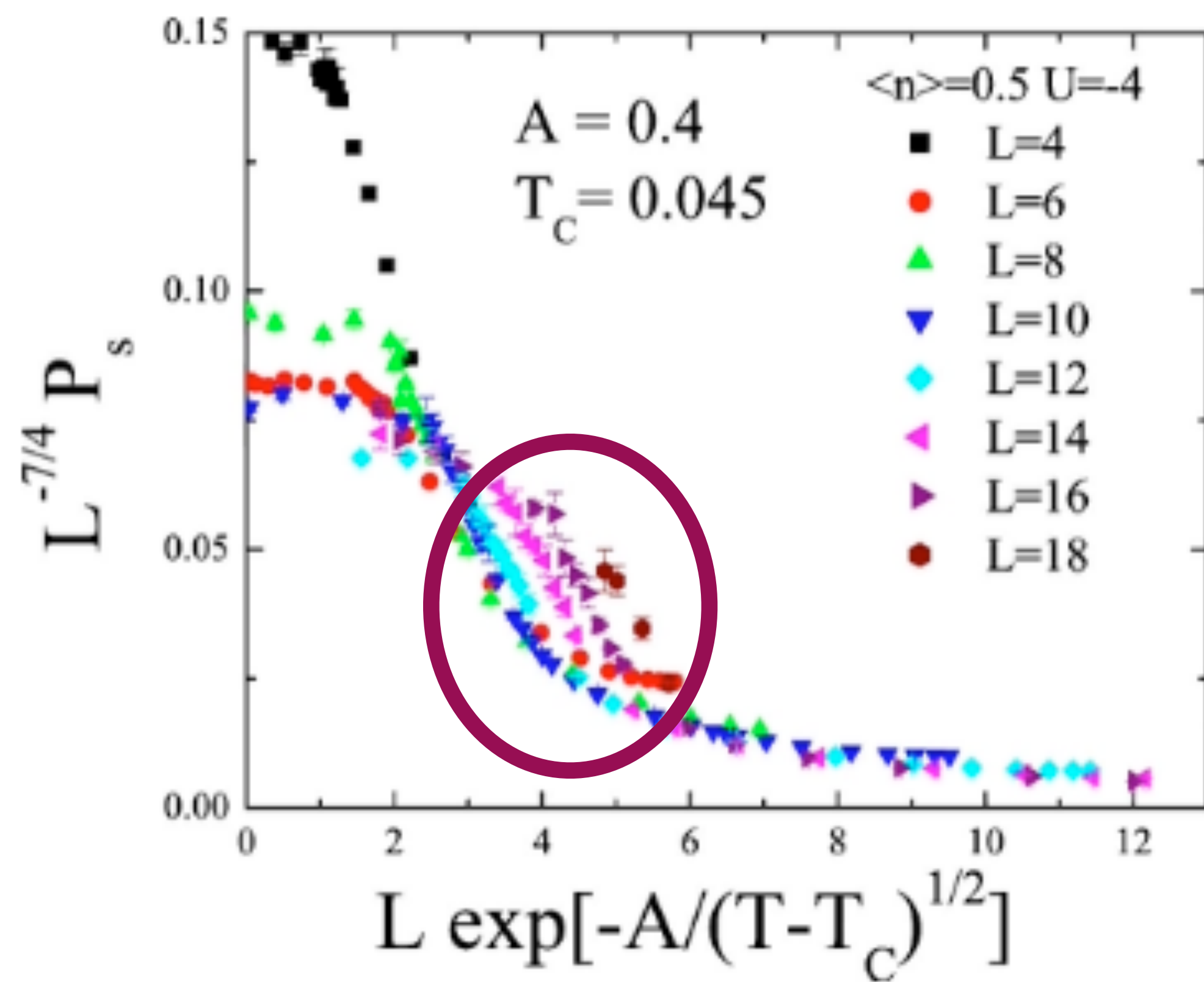


CDW and SUC are degenerated at half-filling

Empty system

Paiva et al PRB 2004





Collapse for larger system sizes: different T_c

Superconducting correlations for the repulsive Hubbard Model

For the repulsive Hubbard model

d-wave correlations

$$c_{\text{spin}}(\mathbf{i}) = \langle S_{\mathbf{j}+\mathbf{i}}^- S_{\mathbf{j}}^+ \rangle, \quad S_{\mathbf{j}}^+ = c_{\mathbf{j}\uparrow}^\dagger c_{\mathbf{j}\downarrow}$$

$$c_{d\text{ pair}}(\mathbf{i}) = \langle \Delta_{d\mathbf{j}+\mathbf{i}} \Delta_{d\mathbf{j}}^\dagger \rangle,$$

$$\Delta_{d\mathbf{j}}^\dagger = c_{\mathbf{j}\uparrow}^\dagger (c_{\mathbf{j}+\hat{x}\downarrow}^\dagger - c_{\mathbf{j}+\hat{y}\downarrow}^\dagger + c_{\mathbf{j}-\hat{x}\downarrow}^\dagger - c_{\mathbf{j}-\hat{y}\downarrow}^\dagger).$$

$$c_{d\text{ pair}}(\mathbf{i}, \tau) = \langle \Delta_{d\mathbf{j}+\mathbf{i}}(\tau) \Delta_{d\mathbf{j}}^\dagger(0) \rangle,$$

$$\Delta_{d\mathbf{j}}^\dagger(\tau) = e^{\tau H} \Delta_{d\mathbf{j}}^\dagger(0) e^{-\tau H},$$

$$P_d = \sum_{\mathbf{i}} \int_0^\beta c_{d\text{ pair}}(\mathbf{i}, \tau) d\tau.$$

Pair-field susceptibility

Vertex $\Gamma_d = \frac{1}{P_d} - \frac{1}{\overline{P}_d}.$ If $\Gamma_d \overline{P}_d < 0,$

$$P_d = \frac{\overline{P}_d}{1 + \Gamma_d \overline{P}_d} \quad \Gamma_d \overline{P}_d \rightarrow -1$$

Signals a superconducting instability, similar to Stoner criteria

Mondaini et al, PRB 86 184506 (12)

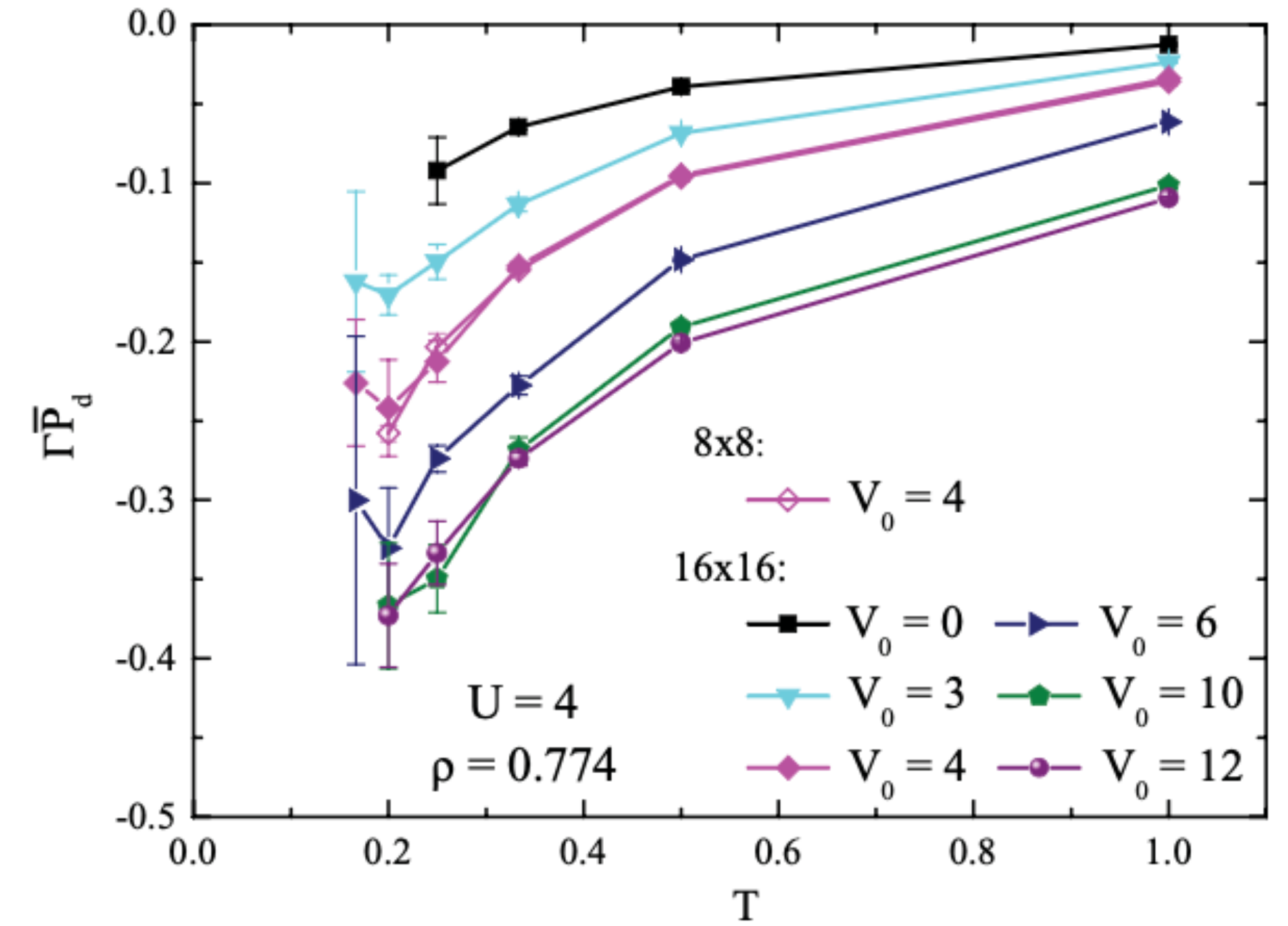


FIG. 10. (Color online) The d -wave pairing vertex is shown as a function of temperature for $U = 4$, $\rho = 0.774$, and different values of the externally imposed stripe potential V_0 . For the homogeneous system $V_0 = 0$, and small V_0 generally, $|\Gamma \bar{P}_d| \lesssim 0.10$. For larger V_0 , $|\Gamma \bar{P}_d|$ exceeds 0.3 in magnitude. A superconducting instability is signaled by $\Gamma \bar{P}_d \rightarrow -1$. Data for 8×8 lattice ($V_0 = 4$, open symbols) show finite-size effects are negligible.

Sign problem

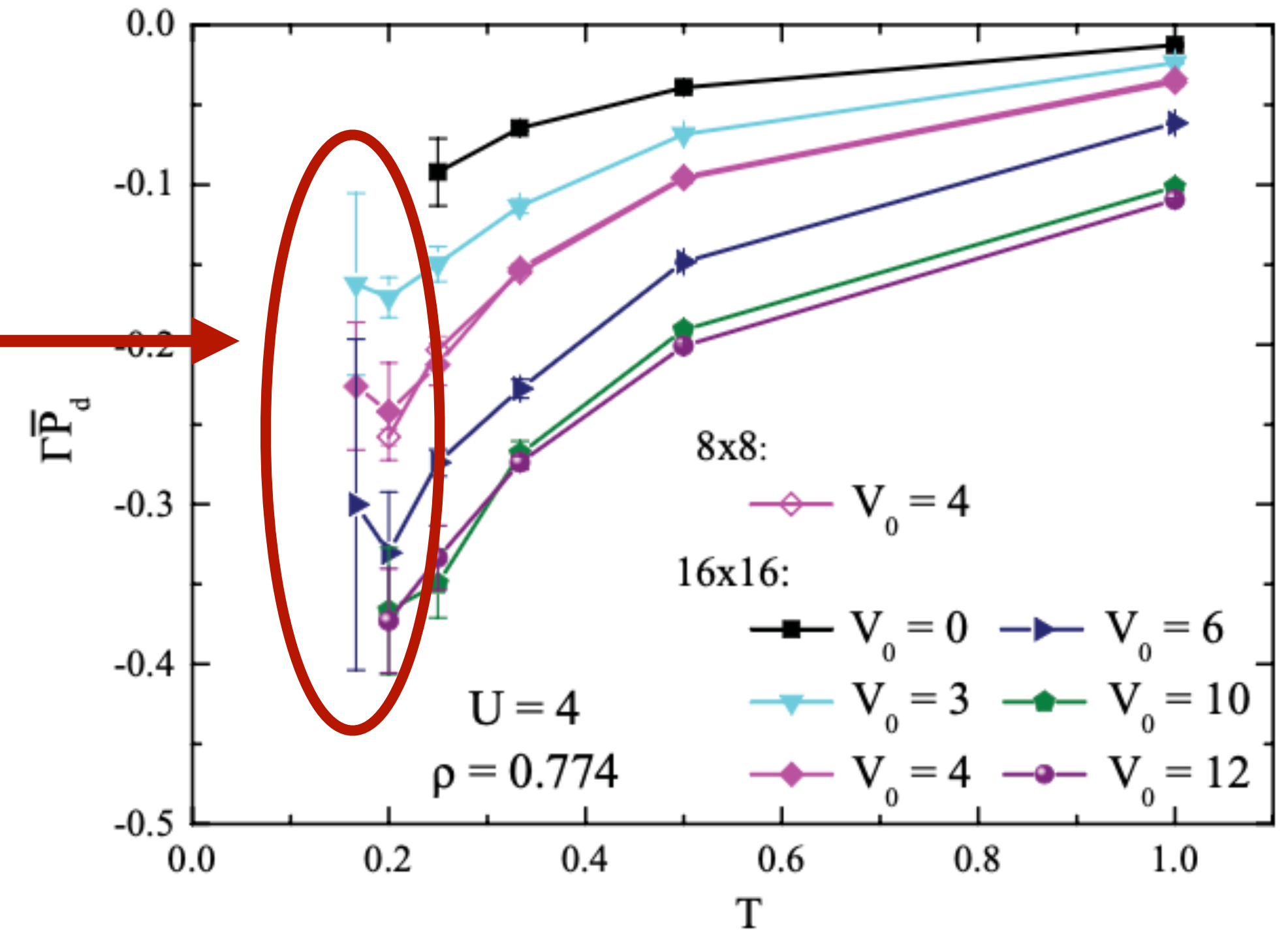


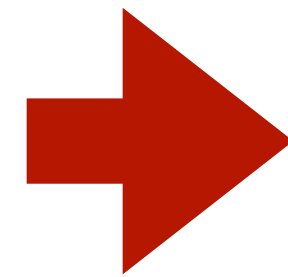
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Mondaini et al, PRB 86 184506 (12)

Thermodynamic correlations

Specific heat

$$C = \beta \left(\langle E^2 \rangle - \langle E \rangle^2 \right)$$

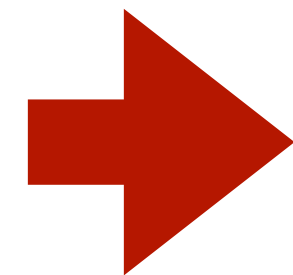


Used in classical Monte Carlo

Specific heat

$$C = \beta \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \quad \rightarrow \quad \text{Used in classical Monte Carlo}$$

QMC

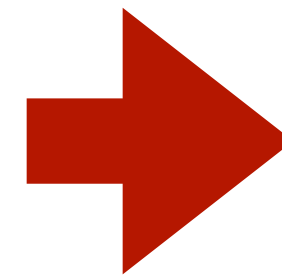


Product of 6 and 8 fermion operators

Large fluctuations

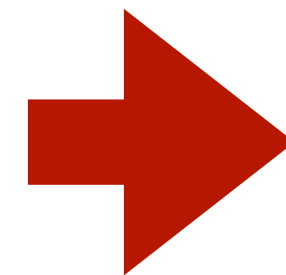
Specific heat

$$C = \beta \left(\langle E^2 \rangle - \langle E \rangle^2 \right)$$



Used in classical Monte Carlo

QMC



Products

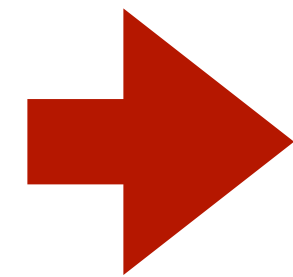
Large

AVOID

S

Specific heat

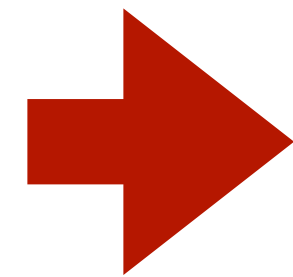
$$C = \frac{dE}{dT}$$



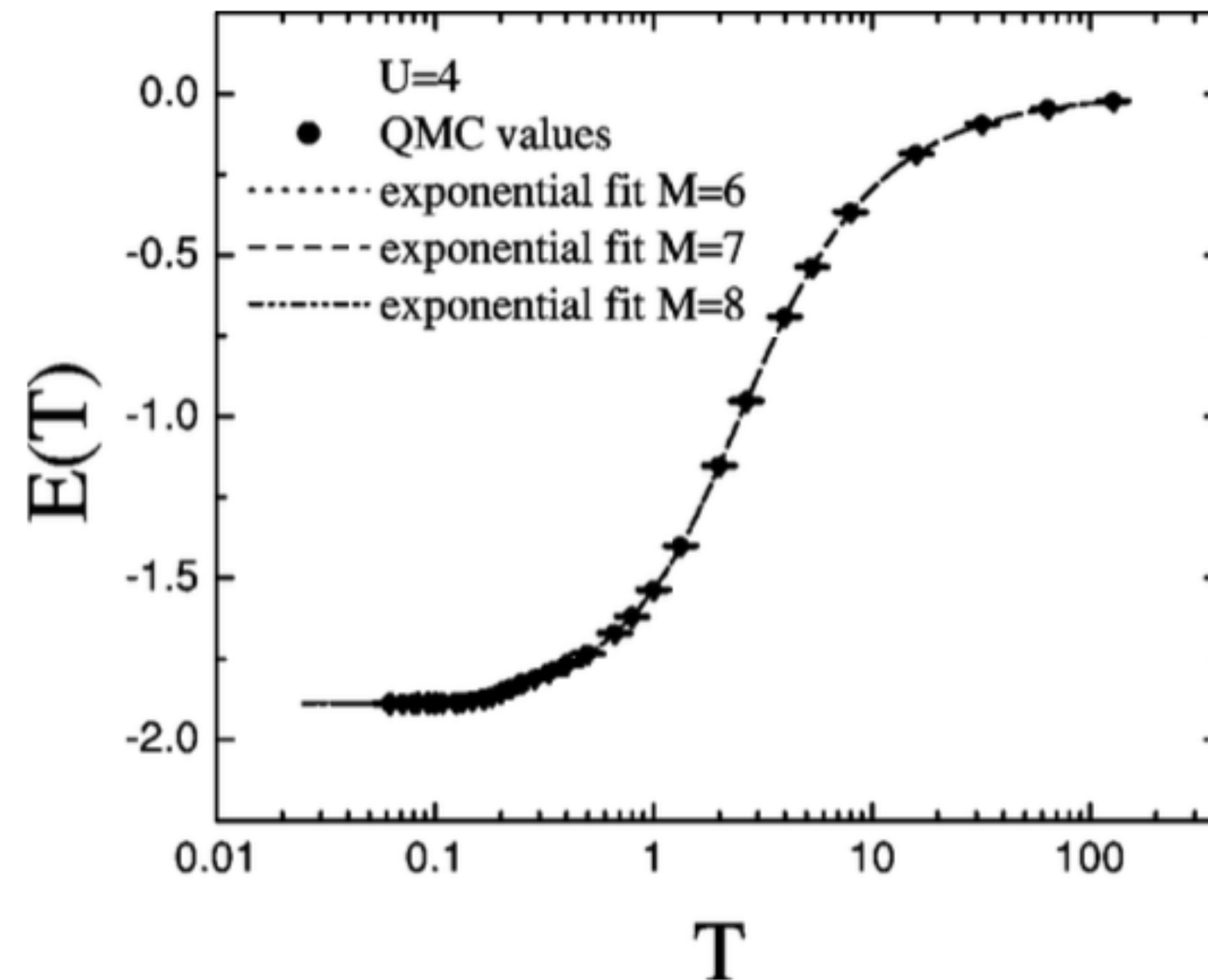
Obtain E in a very fine grid

Specific heat

$$C = \frac{dE}{dT}$$

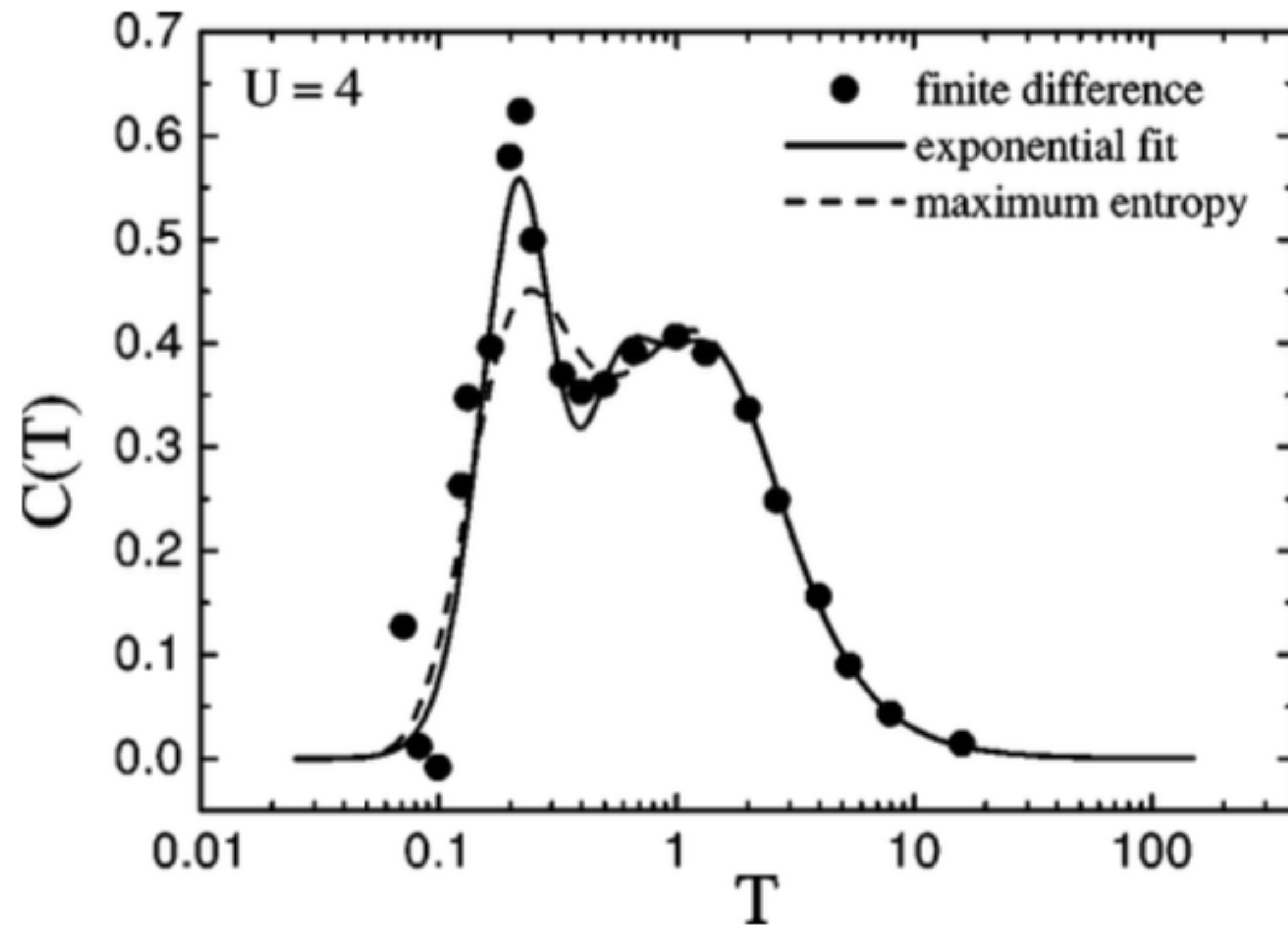


Obtain E in a very fine grid



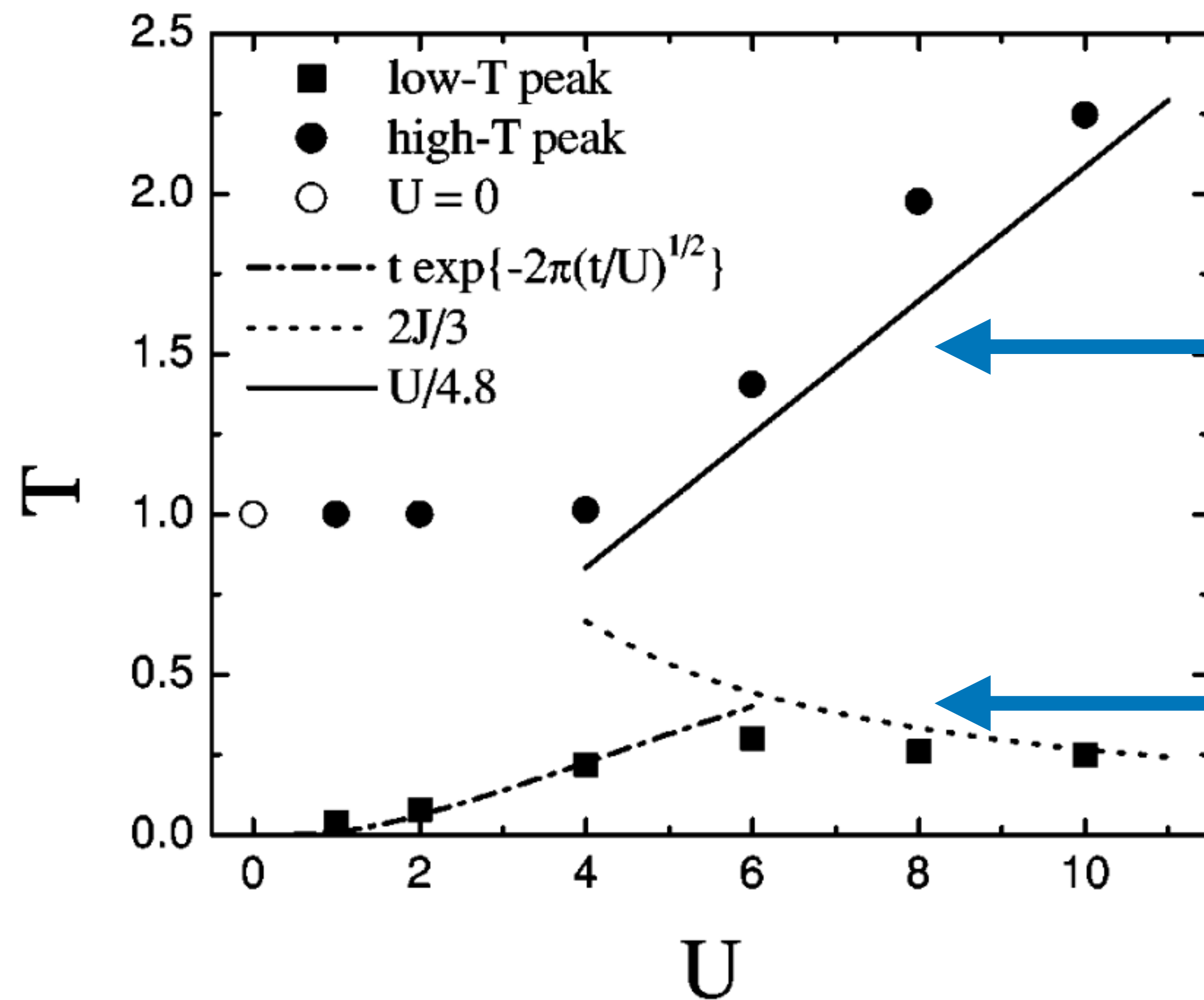
Paiva et al PRB 2001

2D: peak of the specific heat



2D: peak of the specific heat

AF at $T=0$
(Mermin-Wagner theorem)



Charge fluctuations

Large U

Spin fluctuations

3D: peak of the specific heat $\rightarrow T_{\text{Neel}}$

R. Staudt, M. Dzierzawa, and A. Muramatsu, Eur. Phys. J. B 17, 411 (2000).

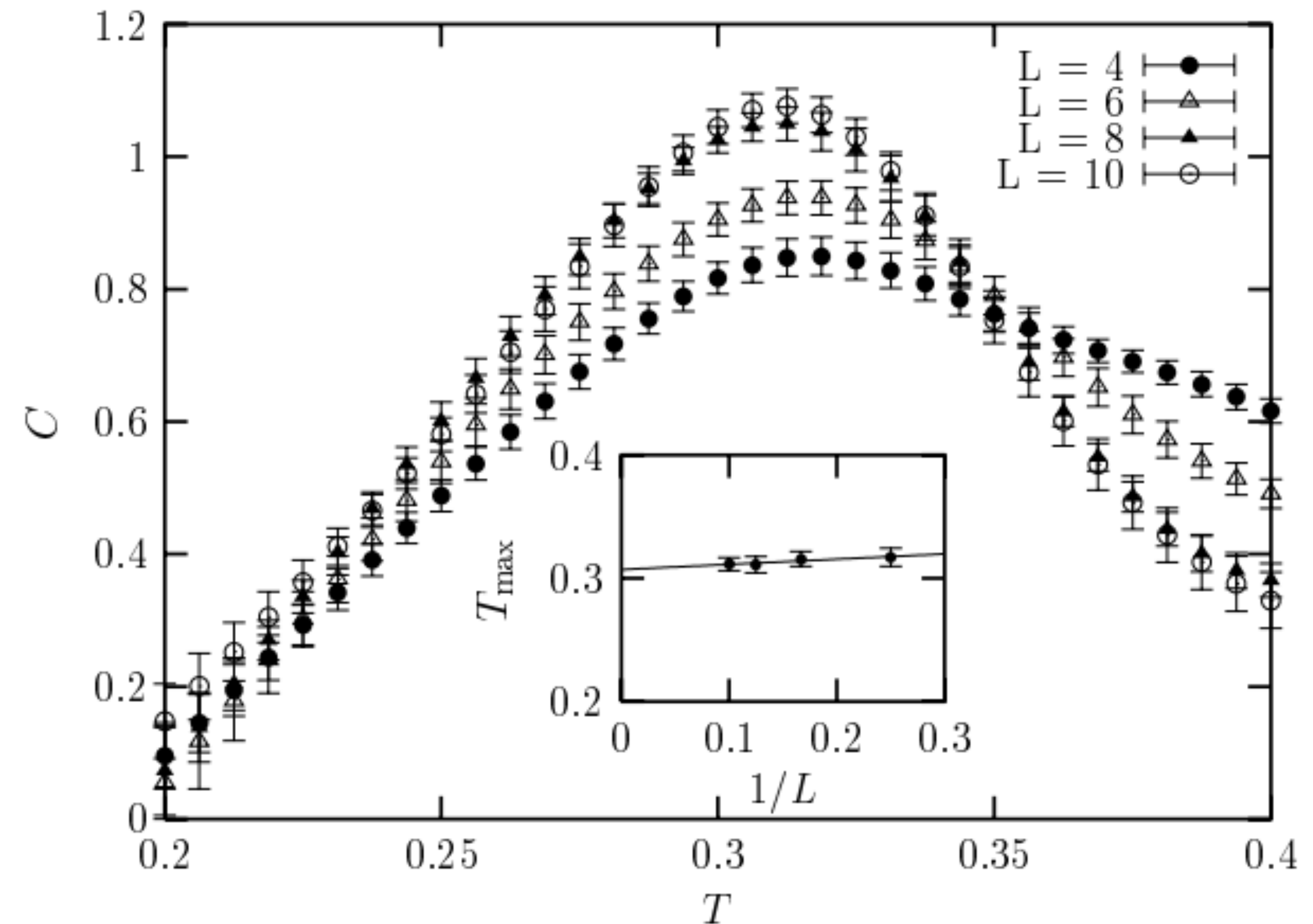
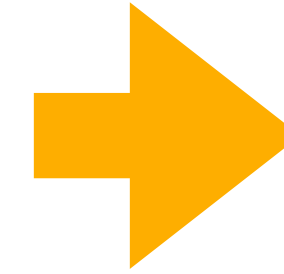
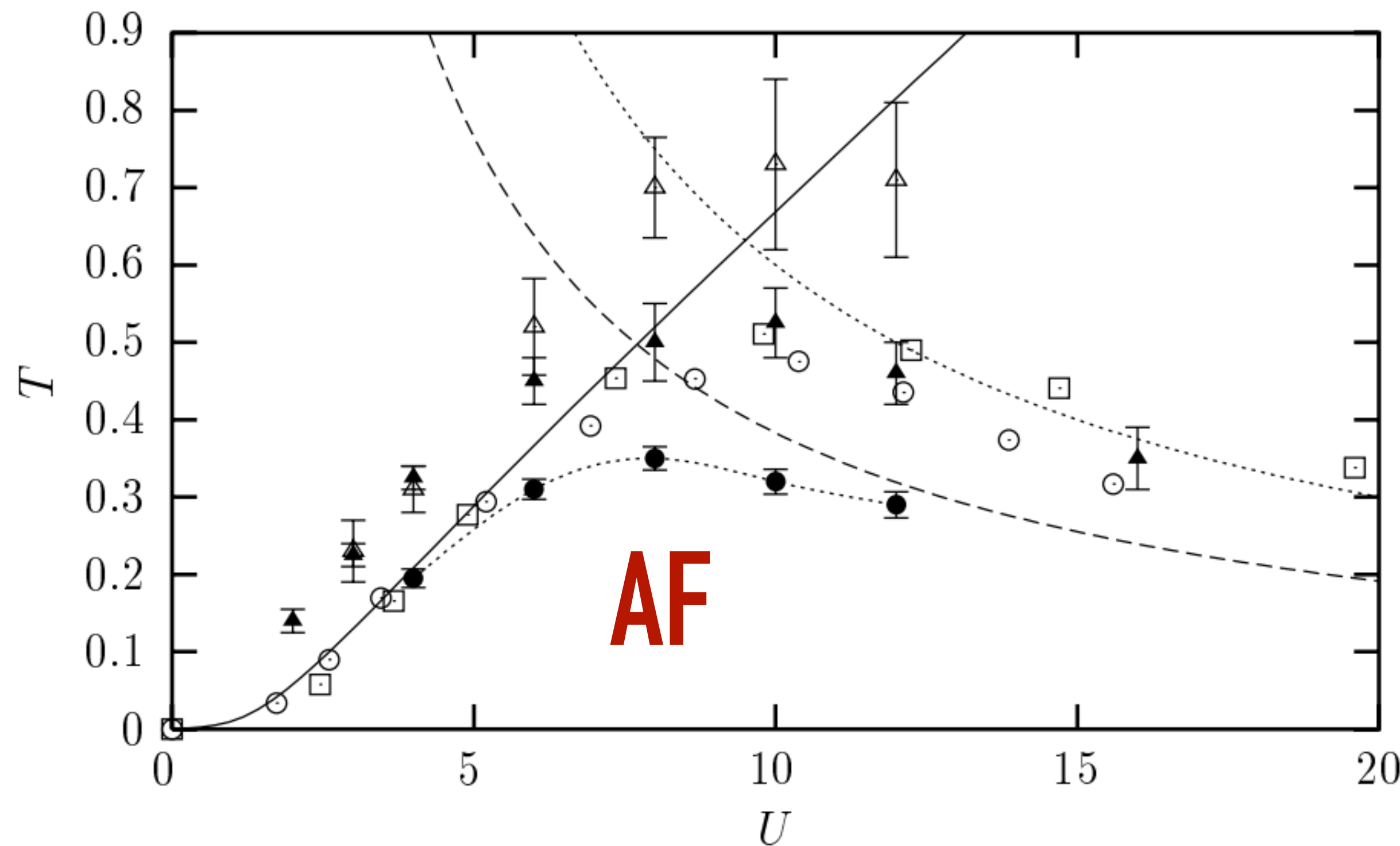


Fig. 2. Specific heat as function of temperature for $U = 6$ and $L = 4, 6, 8, 10$. The inset shows the position of the maximum of the specific heat *vs.* $1/L$.

3D: peak of the specific heat



T_{Neel}



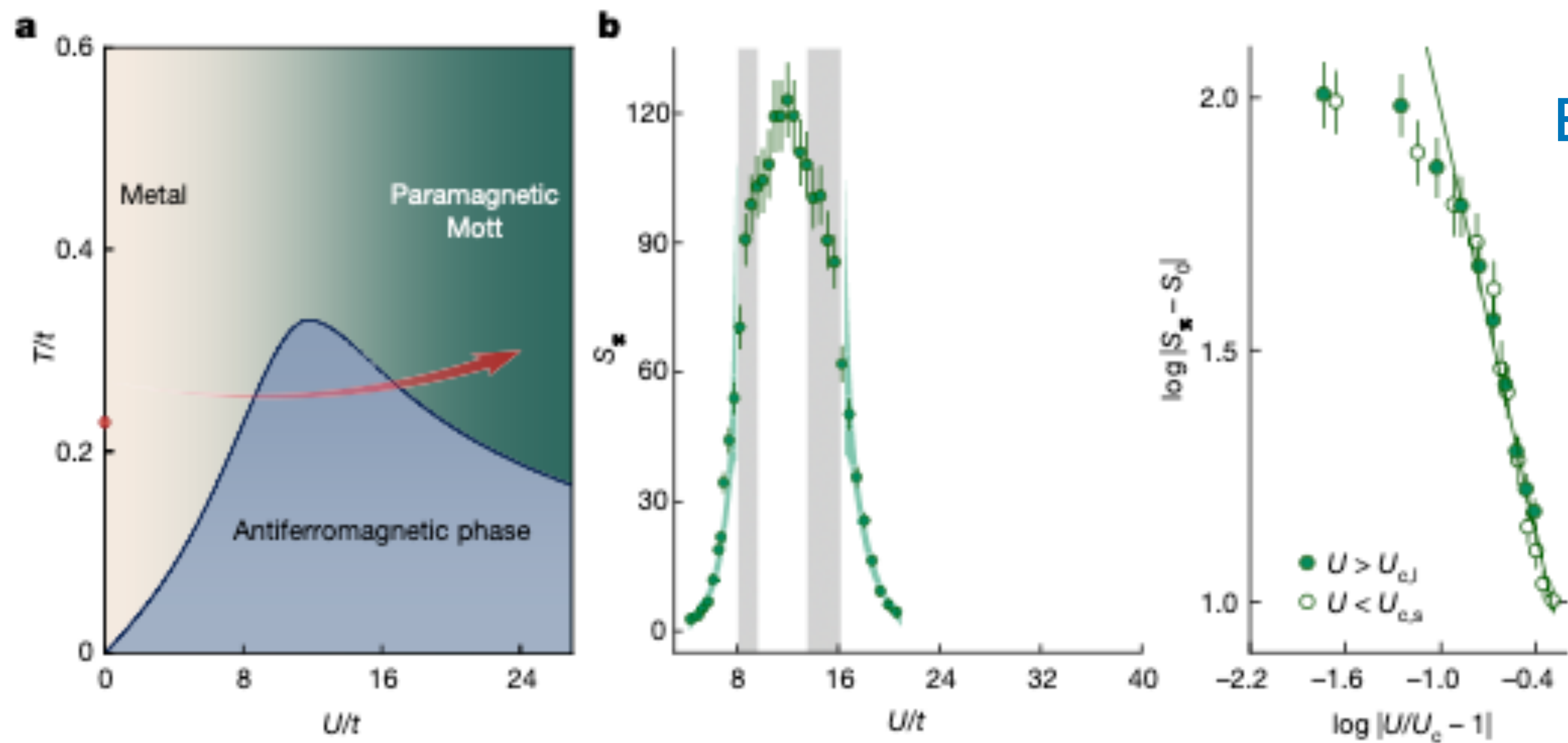
R. Staudt, M. Dzierzawa, and A. Muramatsu, Eur. Phys. J. B 17, 411 (2000).

Fig. 4. Magnetic phase diagram of the half-filled Hubbard model. Néel temperature T_N as function of U from various approaches: QMC, this work (filled circles; dots are meant as a guide to the eye only), QMC [4] (open triangles), QMC [5] (filled triangles), DMFT [10] (open circles), DMFT [12] (open squares), modified Hartree-Fock theory [8] (solid curve), Heisenberg limit from high temperature expansions, $T_N = 3.83t^2/U$ [15] (dashed curve), Weiss molecular field theory, $T_N^{\text{mf}} = 6t^2/U$ (dotted curve).

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}



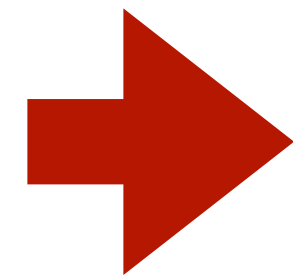
Bragg scattering

$T/t=0.229(2)$

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

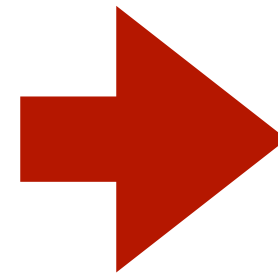
Entropy

$$C = \frac{dE}{dT}$$



Obtain E in a very fine grid

$$S(T) = \int_0^T \frac{C(T')}{T'} dT'$$



Integrate the specific heat

C away from half-filling

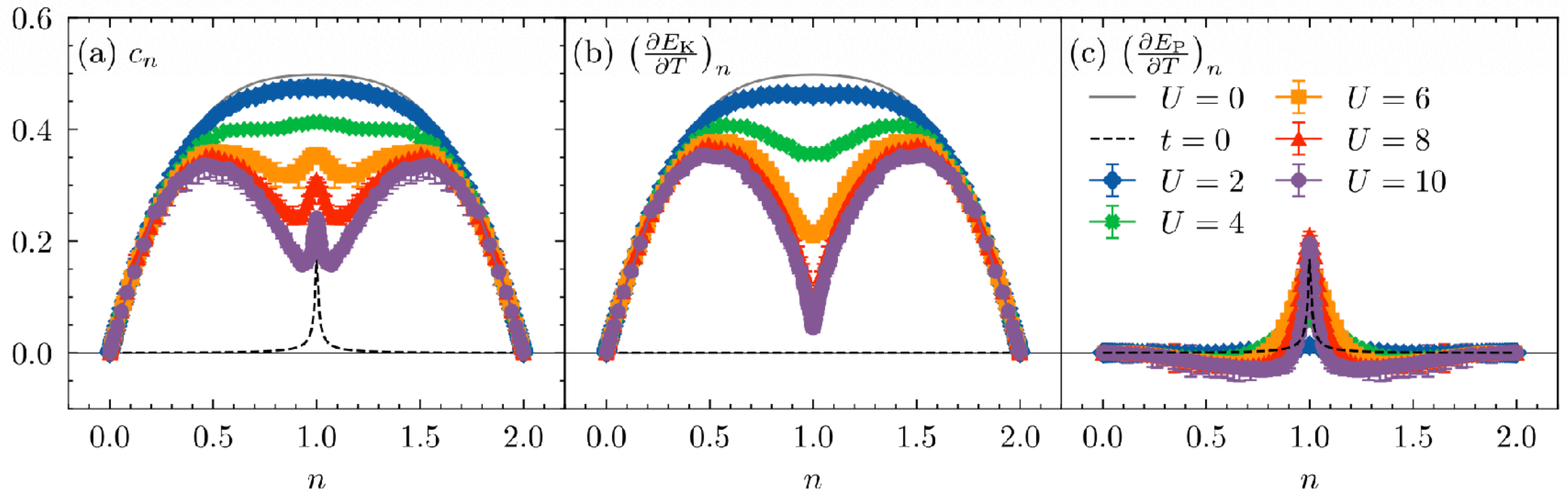
$$c_n = c_\mu - \left(\frac{\partial E}{\partial \mu} \right)_T \frac{\alpha_\mu}{n^2 \kappa_T},$$

$$c_\mu = \left(\frac{\partial E}{\partial T} \right)_\mu \quad \rightarrow \quad \text{Obtain } E \text{ in a very fine grid}$$

$$\alpha_\mu = \left(\frac{\partial n}{\partial T} \right)_\mu \quad \rightarrow \quad \text{Thermal expansion coefficient}$$

$$\kappa_T = \frac{1}{n^2} \left(\frac{\partial n}{\partial \mu} \right)_T \quad \rightarrow \quad \text{Compressibility}$$

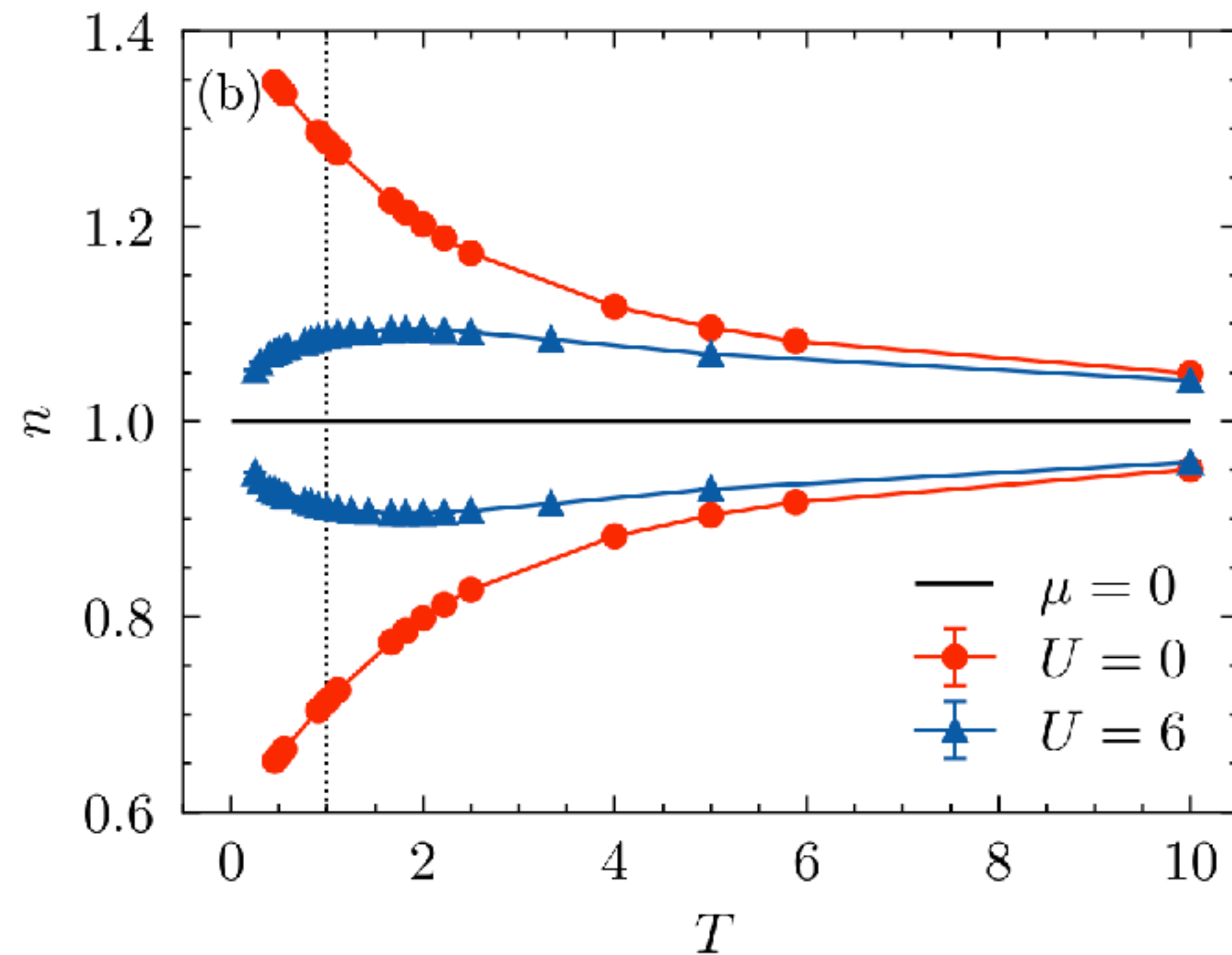
T=t 10x10 square lattice



PRB 2026 Habitzreuter

Thermal expansion coefficient

$$\alpha_{\mu} = \left(\frac{\partial n}{\partial T} \right)_{\mu}$$

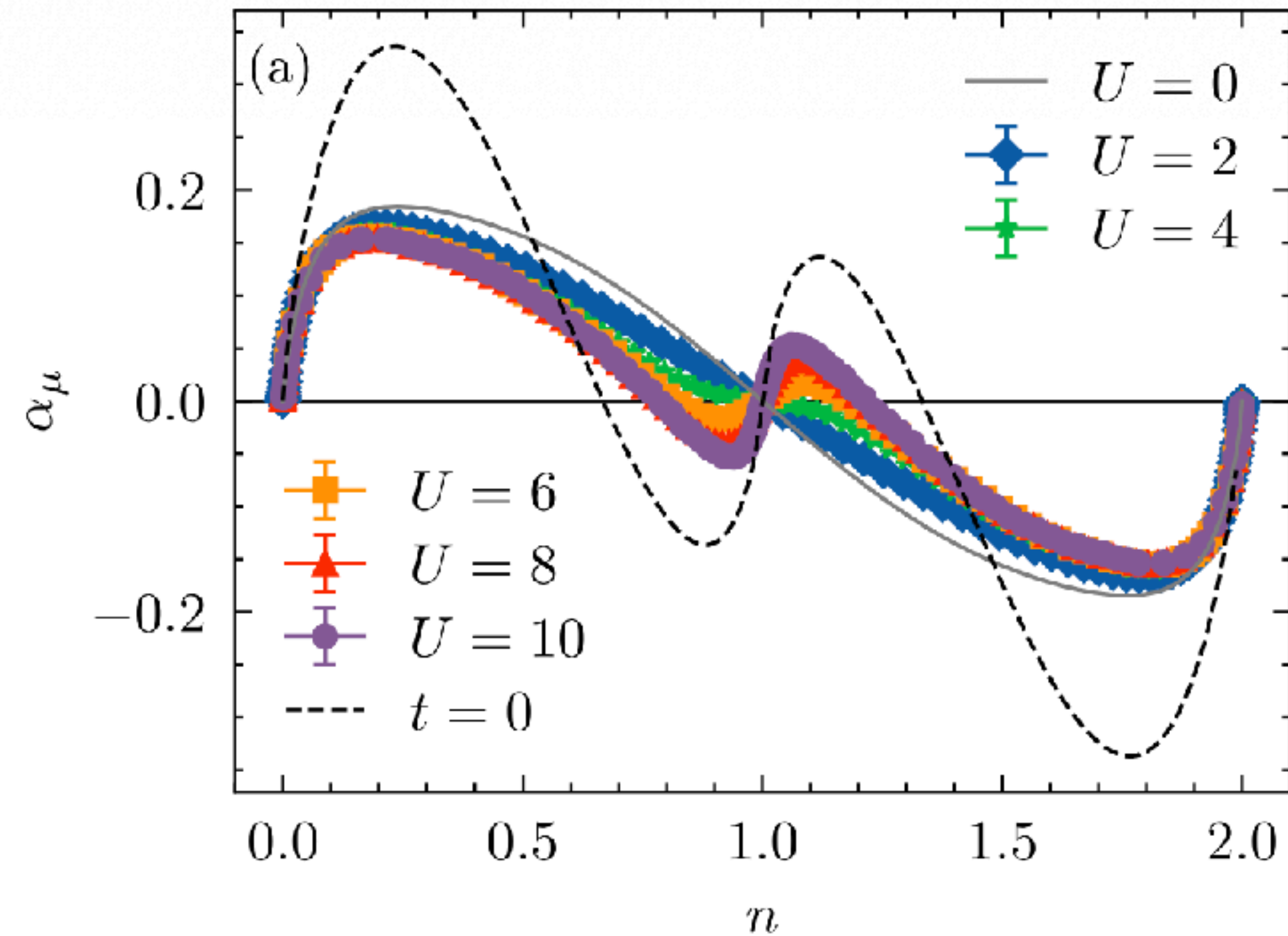
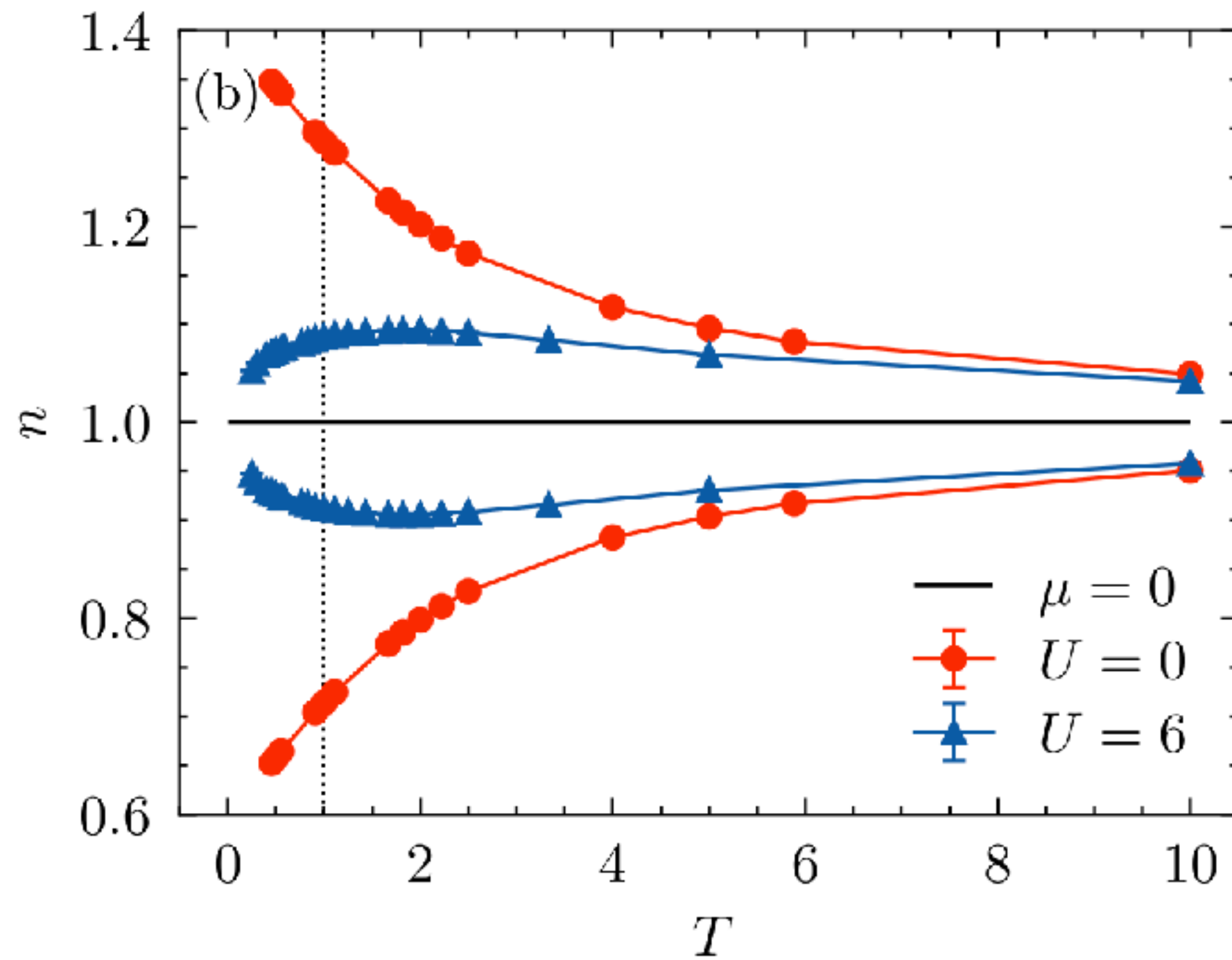


Anomalous behavior for $U=6$

PRB 2026 Habitzreuter

Thermal expansion coefficient

$$\alpha_{\mu} = \left(\frac{\partial n}{\partial T} \right)_{\mu}$$

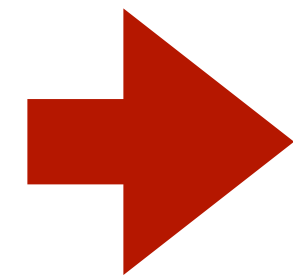


Anomalous behavior for $U=6$

PRB 2026 Habitzreuter

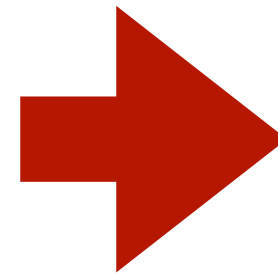
Entropy

$$C = \frac{dE}{dT}$$



Obtain E in a very fine grid

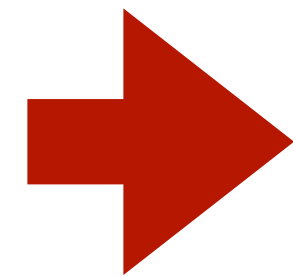
$$S(T) = \int_0^T \frac{C(T')}{T'} dT'$$



Integrate the specific heat

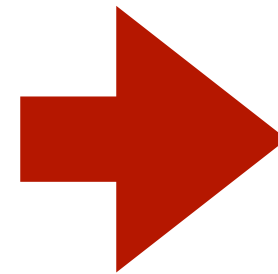
Entropy

$$C = \frac{dE}{dT}$$



Obtain E in a very fine grid

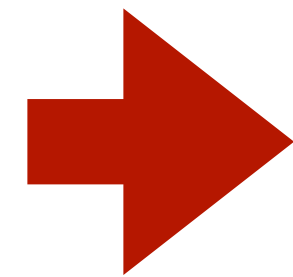
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Integrate the specific heat

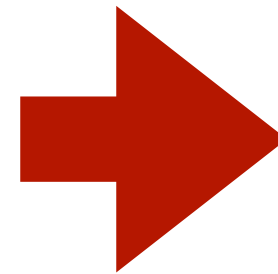
Entropy

$$C = \frac{dE}{dT}$$



Obtain E in a very fine grid

$$S(T) = \int_0^T \frac{C(T')}{T'} dT'$$



Integrate the specific heat



Integration limits

Entropy

up-down

$$s(T, U) = s(0, U) + \int_0^T e(T', U) dT'$$



Residual entropy

Entropy

up-down

$$s(T, U) = s(0, U) + \int_0^T e(T', U) dT'$$

down-up

A-M Daré et al PRB 2007

$$s(\beta, U) = \ln 4 + \beta e(\beta, U) - \int_0^\beta e(\beta', U) d\beta'$$

Download



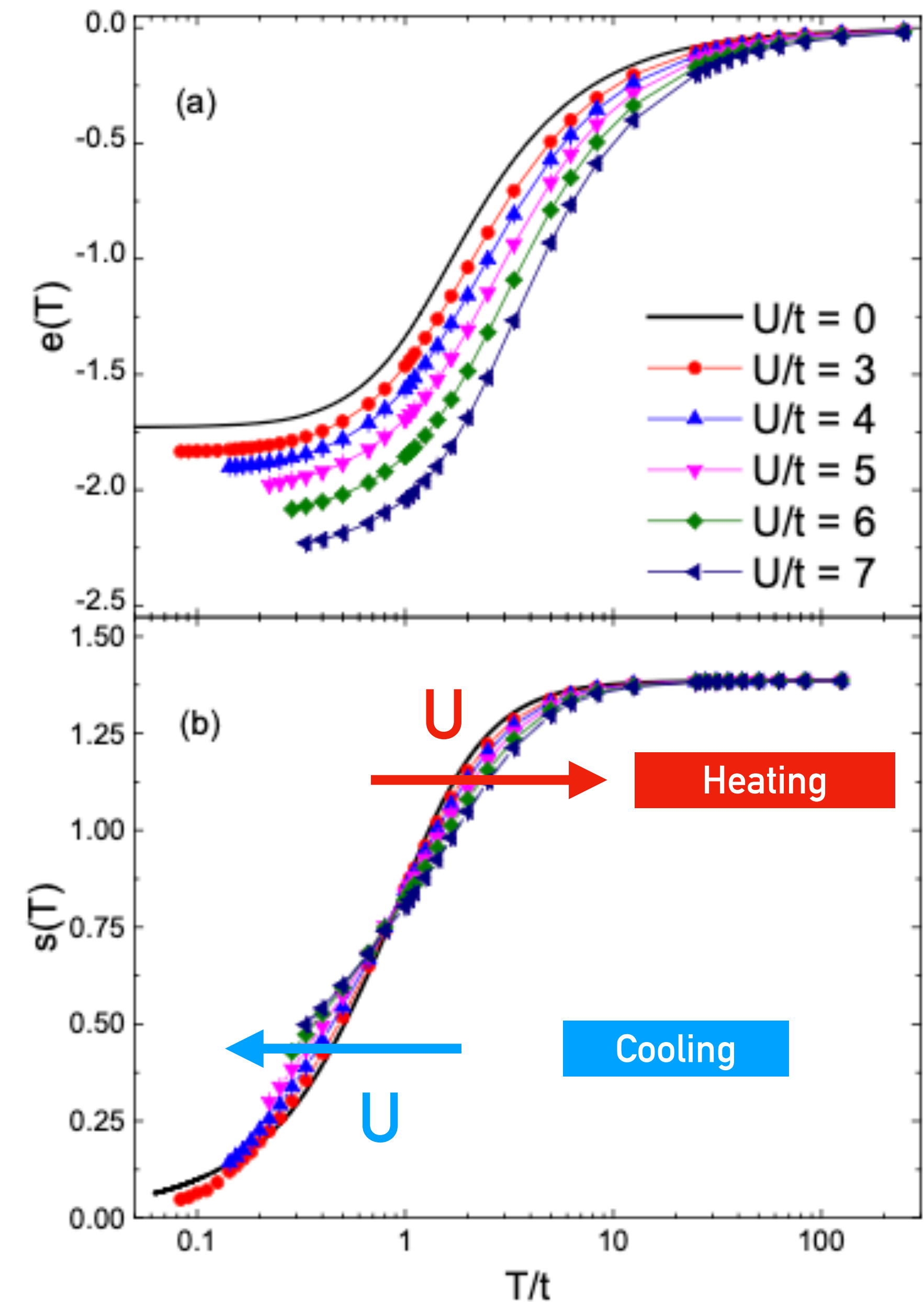
$n=1$

$$s(\beta = 0) = 2\ln 2 - n\ln n - (2 - n)\ln(2 - n)$$

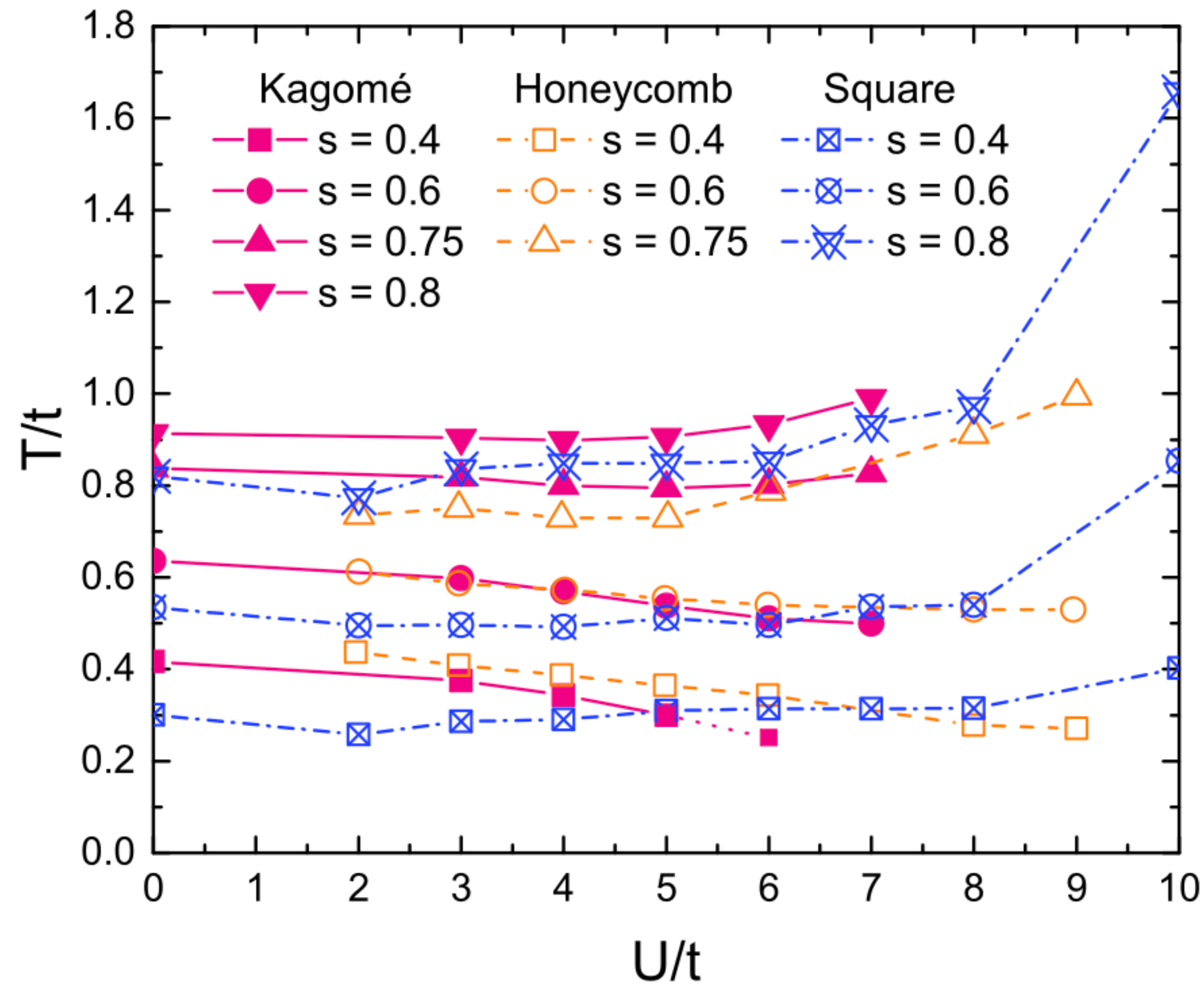
Entropy

Hubbard model on the Kagome lattice

Medeiros-Silva PRB 23



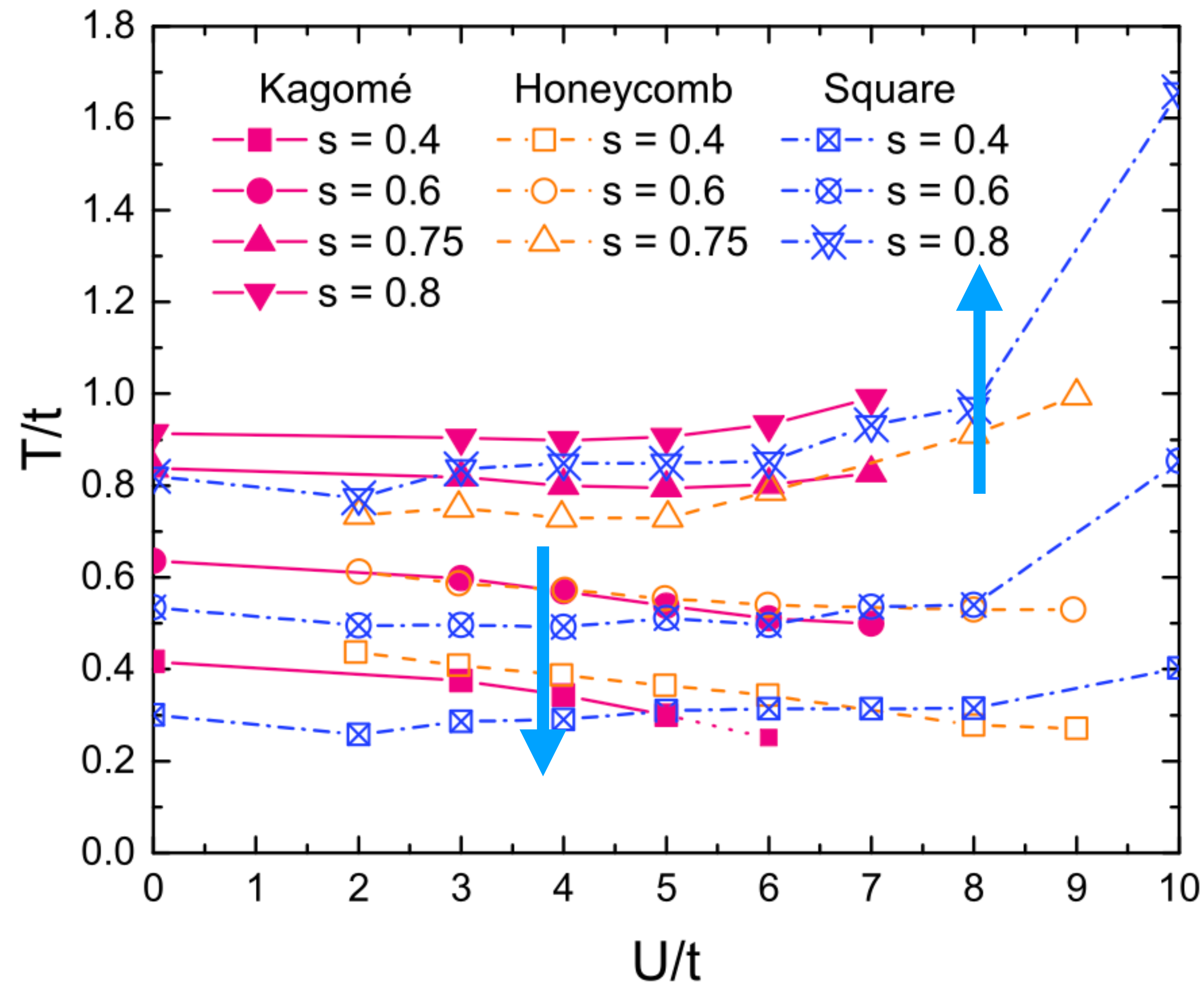
Adiabatic cooling



Important for cold
atom experiments

PRB 2023,
Medeiros-Silva et al

Adiabatic cooling



Important for cold
atom experiments

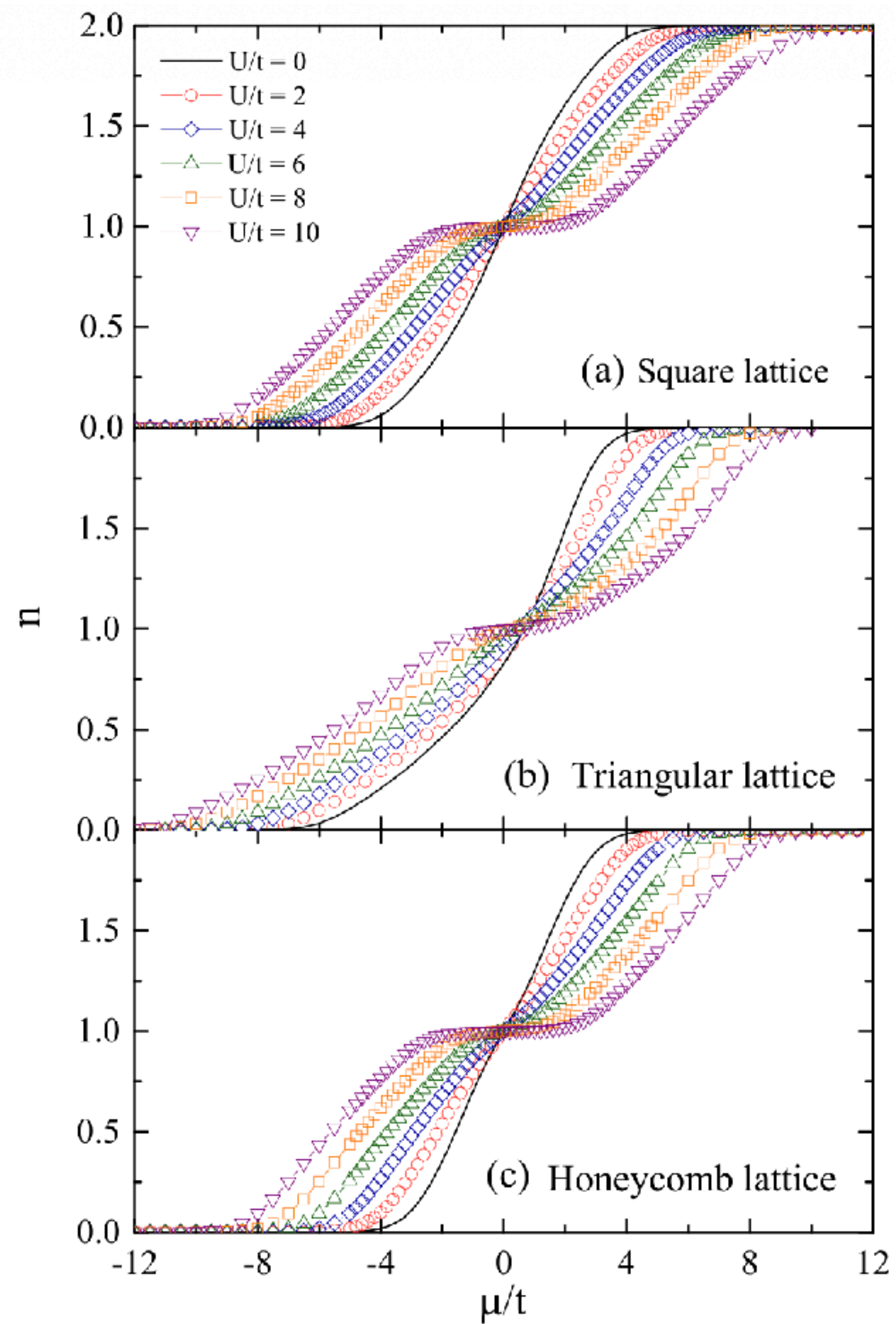
PRB 2023,
Medeiros-Silva et al

Another way to extract the entropy

$$s(\mu, T) = \int_{-\infty}^{\mu} d\mu' \left. \frac{\partial n}{\partial T} \right|_{\mu'}$$

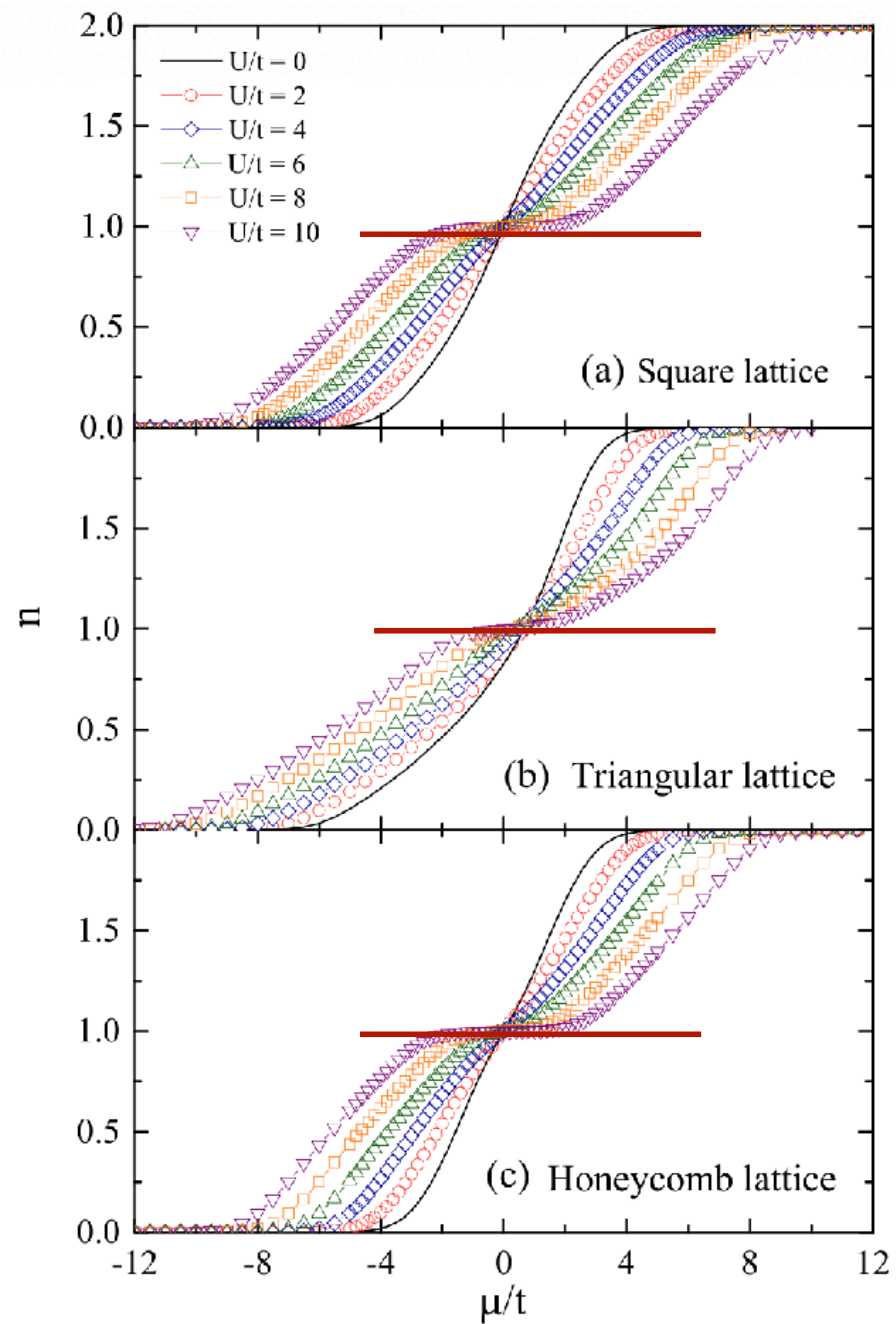
➡ Obtain $\partial n / \partial T$ for $n=0$ to $n=2$ in a fine grid of chemical potentials

➡ Integrate in μ



$T/t=0.5$

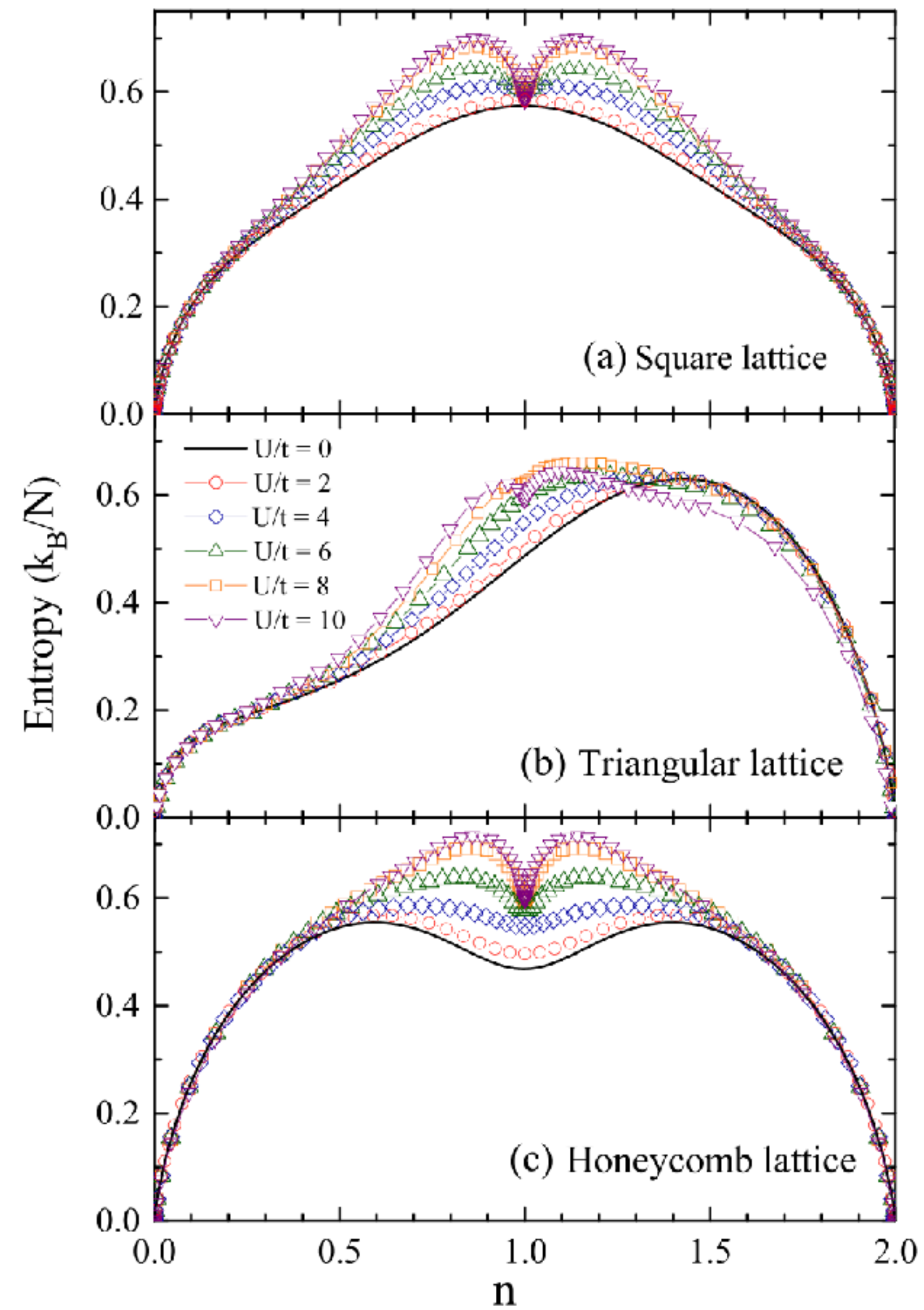
Freitas Silva PRB 2023



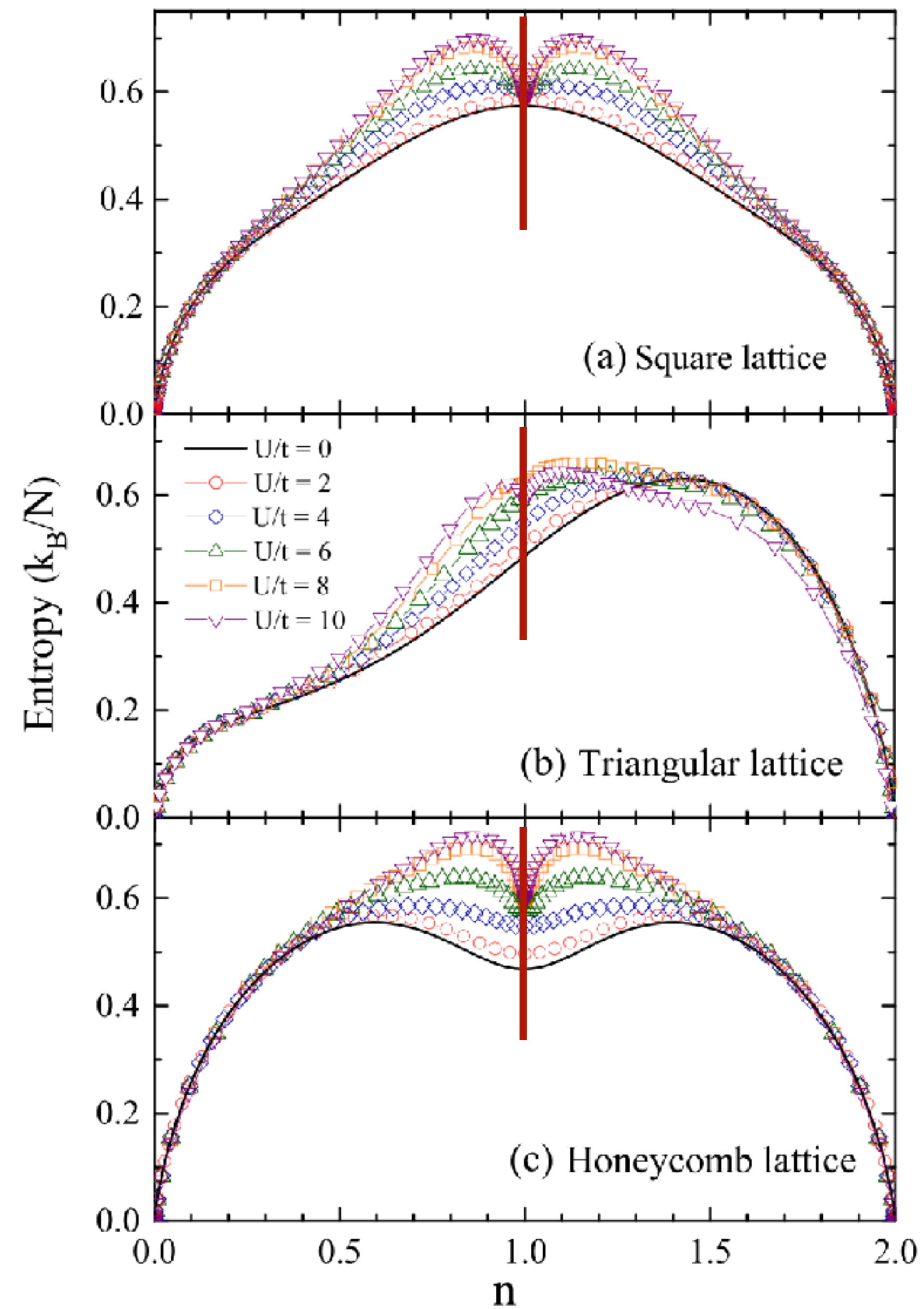
$T/t=0.5$

Mott plateau

Freitas Silva PRB 2023



Freitas Silva PRB 2023



Mott plateau

Freitas Silva PRB 2023

Other quantities

Seebeck coefficient

$$S_{Kelvin} = -\frac{1}{e} \frac{\partial \mu}{\partial T} \Big|_{V,n} = \frac{\partial s}{\partial n} \Big|_{T,V}$$

Peterson and Shastry,
PRB 2010

Low frequency: $\hbar\omega < U$

Sign is related to carrier

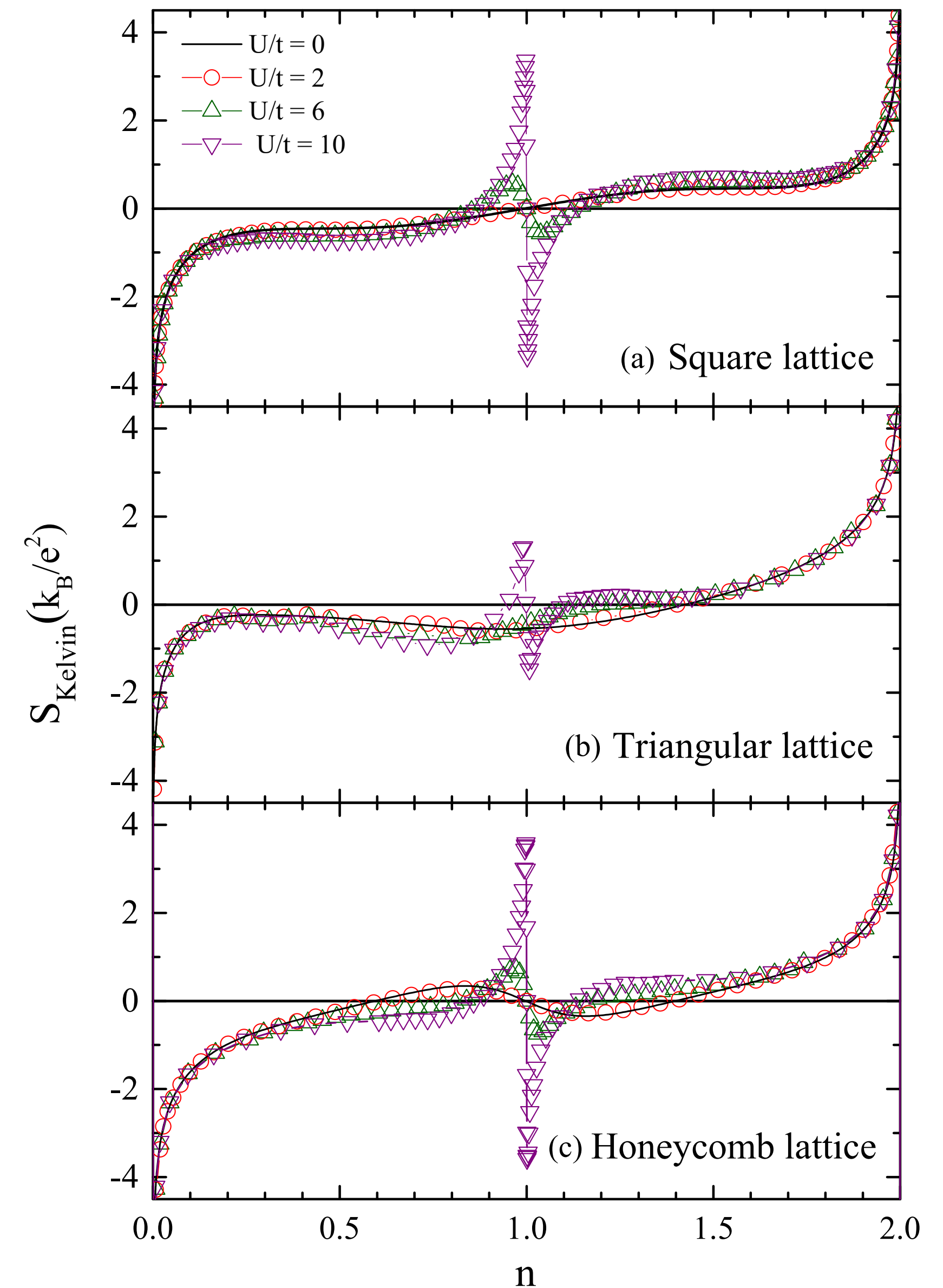
Seebeck coefficient

Sign is related to carrier

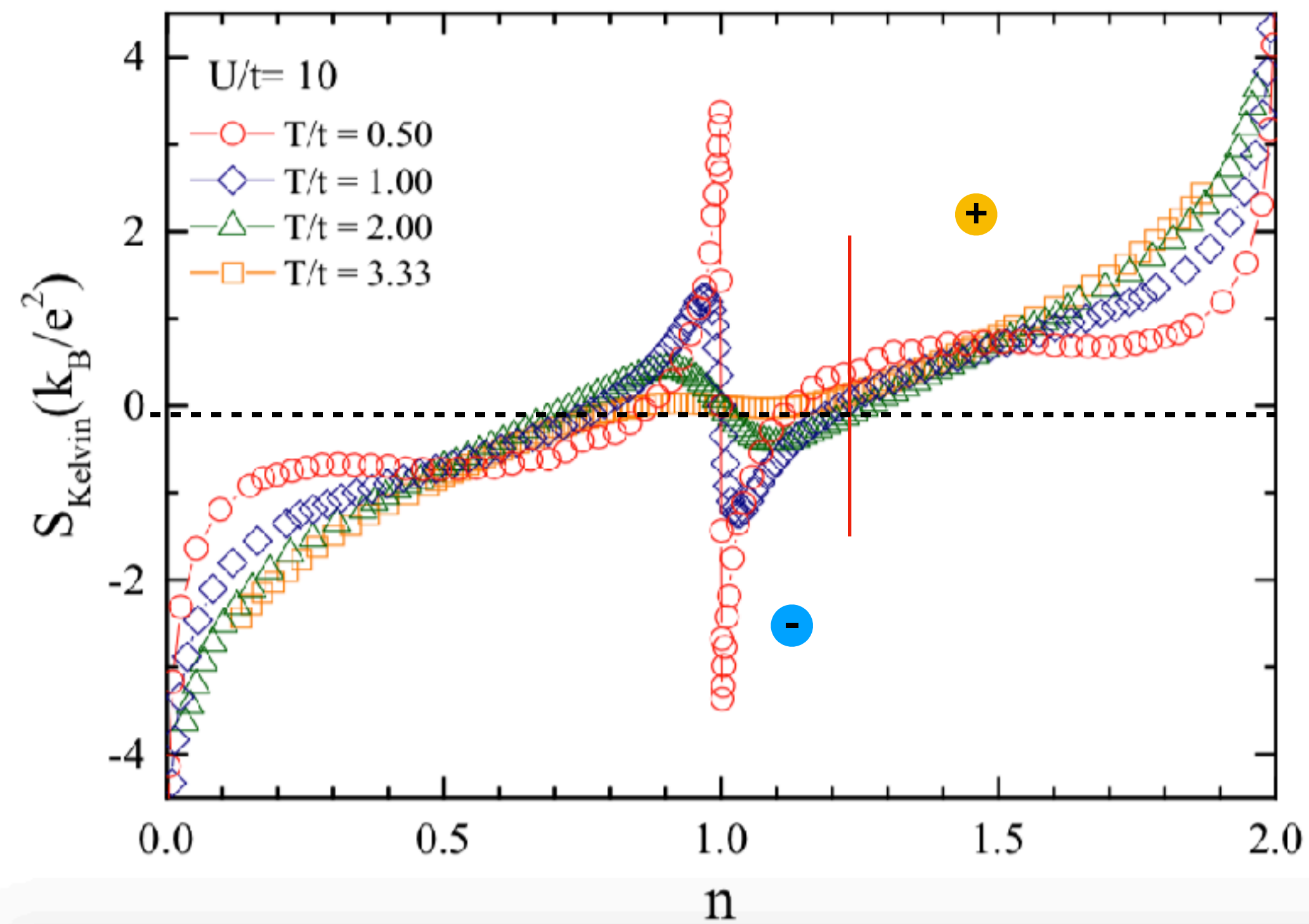
Anomalous behavior as U increases

Additional sign changing densities

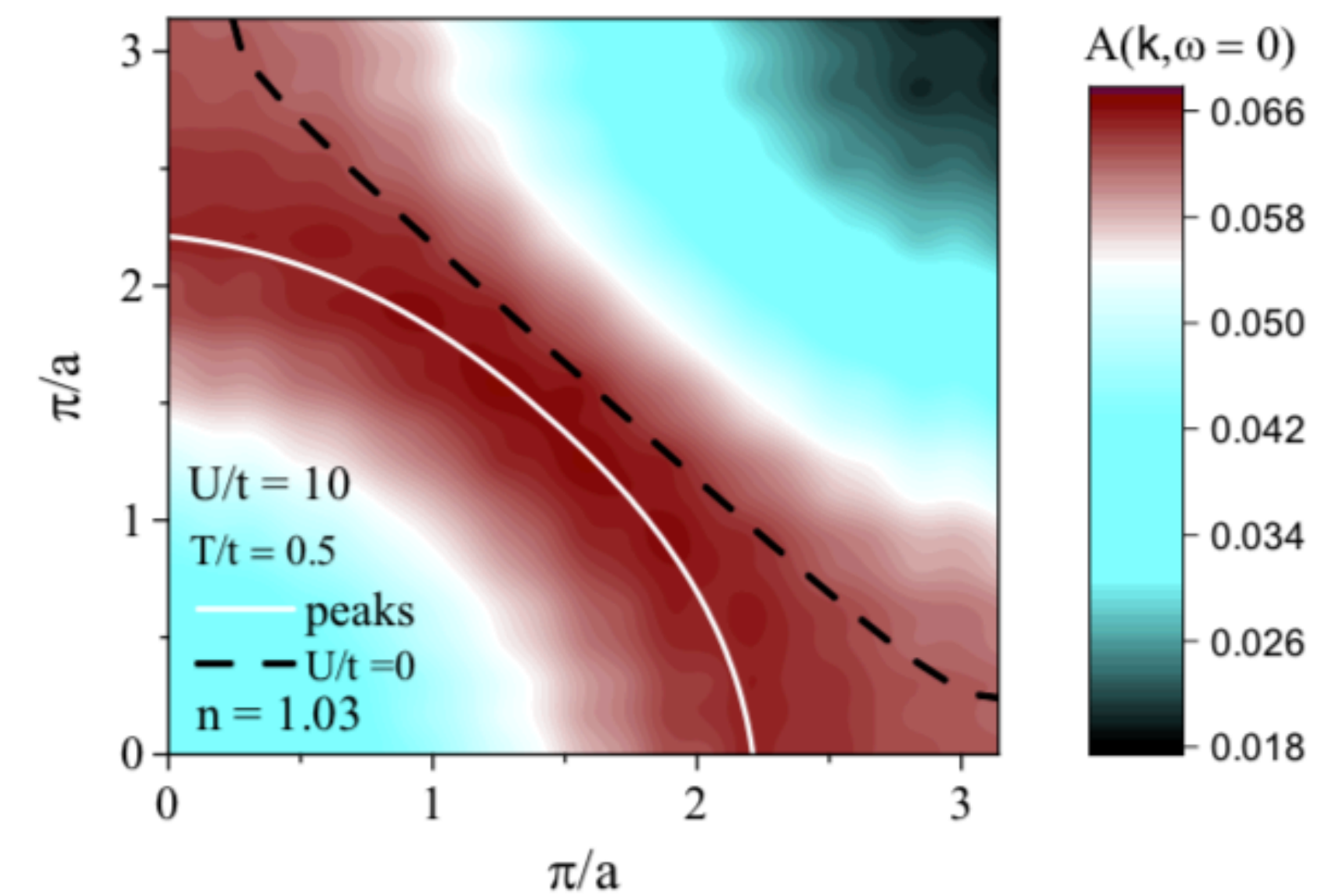
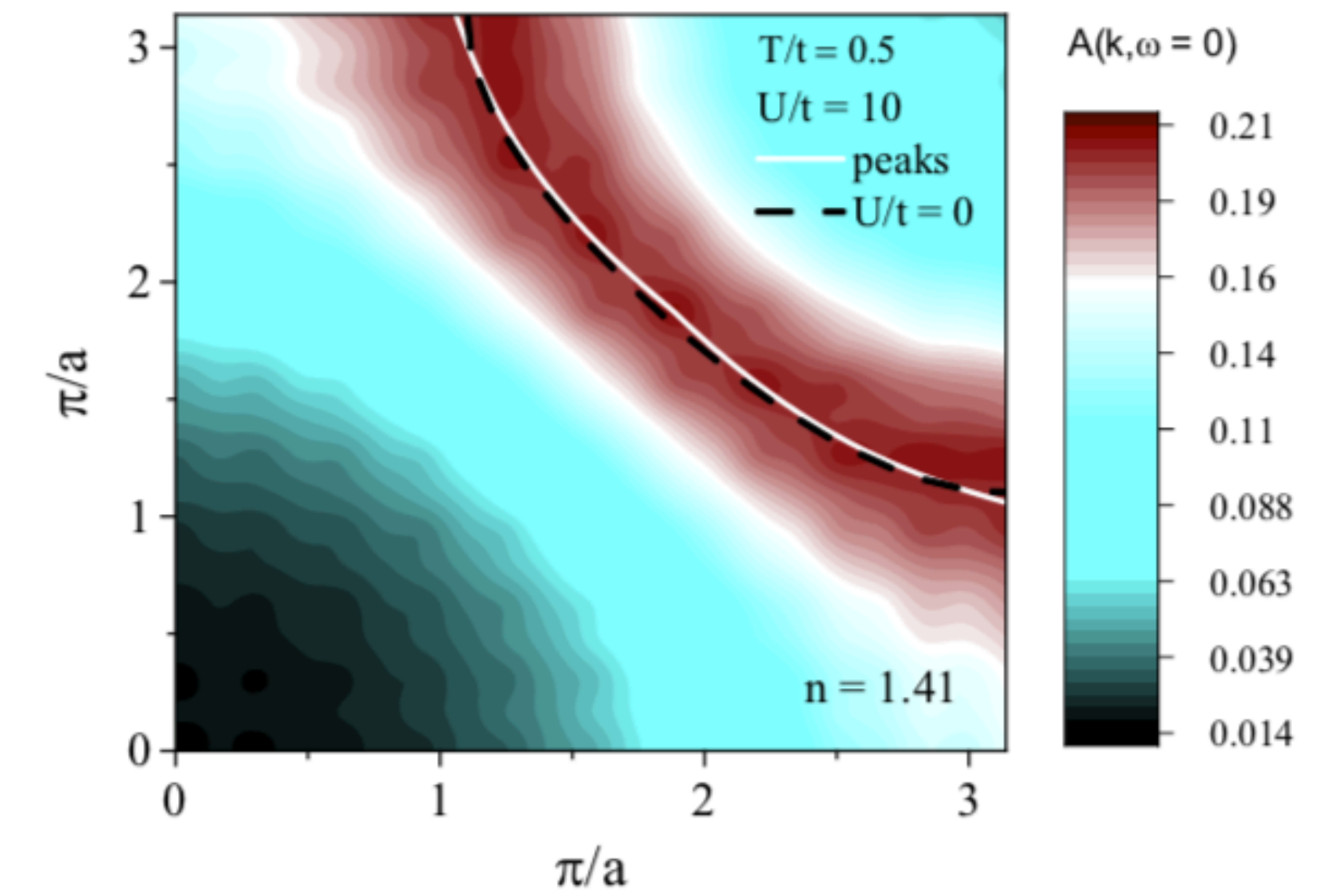
Freitas Silva PRB 2023



Fermi surface restructuring



Sign is related to carrier



QMC Implementations

DQMC

Others

DQMC

Legacy codes

QUEST

ALF

SmoQyDQMC

ALPS

Legacy codes

PHYSICAL REVIEW D

VOLUME 24, NUMBER 8

15 OCTOBER 1981

Monte Carlo calculations of coupled boson-fermion systems. I

R. Blankenbecler*

Laboratoire de Physique Théorique et Hautes Energies, University of Paris XI, 91405, Orsay, France

D. J. Scalapino and R. L. Sugar

Institute for Theoretical Physics and Department of Physics, University of California, Santa Barbara, California 93106

(Received 15 June 1981)

Variations of the codes produced by this group and their students

UC Santa Barbara

Legacy codes

PHYSICAL REVIEW B

VOLUME 28, NUMBER 7

RAPID COMMUNICATIONS

1 OCTOBER 1983

Discrete Hubbard-Stratonovich transformation for fermion lattice models

J. E. Hirsch

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

(Received 16 June 1983)

We discuss a new functional-integral formulation of interacting fermion systems on a lattice such as the Anderson or Hubbard models: the fermion-fermion interaction is eliminated by introducing auxiliary Ising variables. The resulting model for a d -dimensional quantum system is a $(d+1)$ -dimensional Ising model with complicated interactions. The new transformation is particularly useful for performing numerical studies of these models using Monte Carlo techniques. We study its convergence properties and compare it with the usual Gaussian formulation for the case of the Hubbard model.

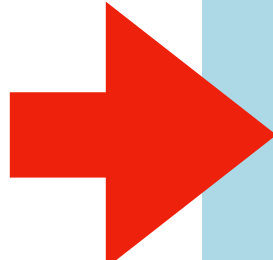
Modifications by different groups

Legacy codes

- One code for each geometry
- Different code for $U > 0$ and $U < 0$
- F77

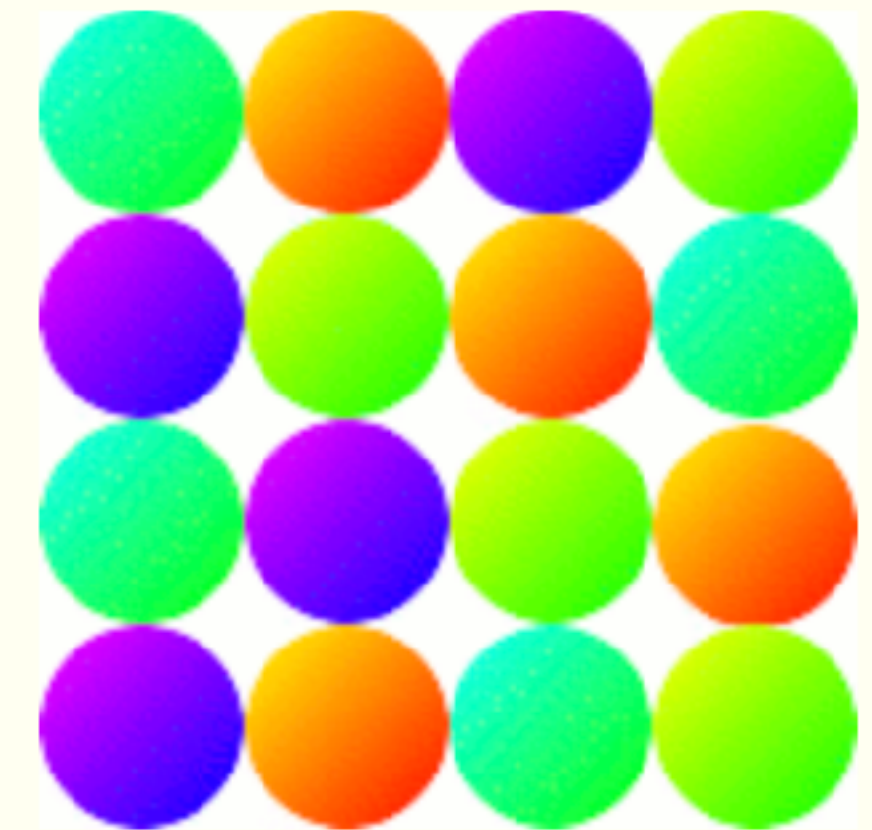
Main advantage: easy to make changes (for older people that are used to Fortran)

QUEST: QUantum Electron Simulation Toolbox



- Home
- User's Guide
- Download
- ADEPT
- Documentation
- Publications
- Developers

QUantum Electron Simulation Toolbox (QUEST) is a Fortran 90/95 package that implements the Determinant Quantum Monte Carlo (DQMC) method for quantum electron simulations. The original versions of DQMC programs, developed by the condensed matter theory group at UCSB including R. L. Sugar, D. J. Scalapino, S. R. White, and E. Y. Loh, and maintained by R. Scalettar, have been extensively used to study magnetism, metal-insulator transitions, and superconductivity by the Hubbard model. QUEST, the new version of DQMC simulations, serves three purposes.



<https://www.cs.ucdavis.edu/~bai/QUEST/index.html>

QUEST: QUantum Electron Simulation Toolbox

Richard Scalettar - Dept of Physics

Zhaojun Bai - Dept of Computer Science and Mathematics

et. al

UC Davis

<https://www.cs.ucdavis.edu/~bai/QUEST/index.html>

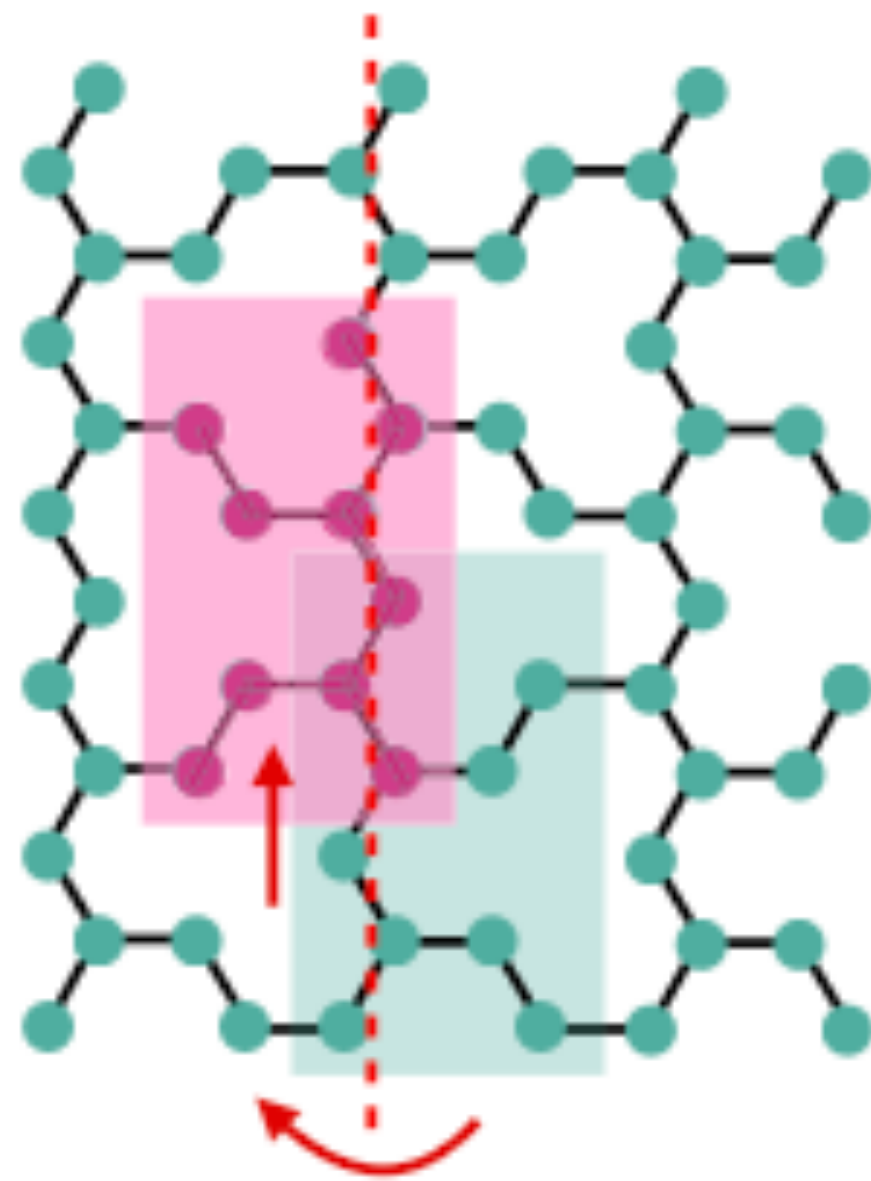
QUEST: QUantum Electron Simulation Toolbox

- Same code for positive and negative U and different geometries
- F90
- Hubbard Model

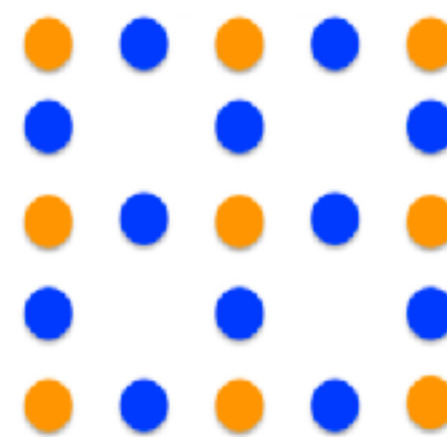
Main advantage: easy to use and easy to implement different geometries, including disorder

Square, triangle, honeycomb...

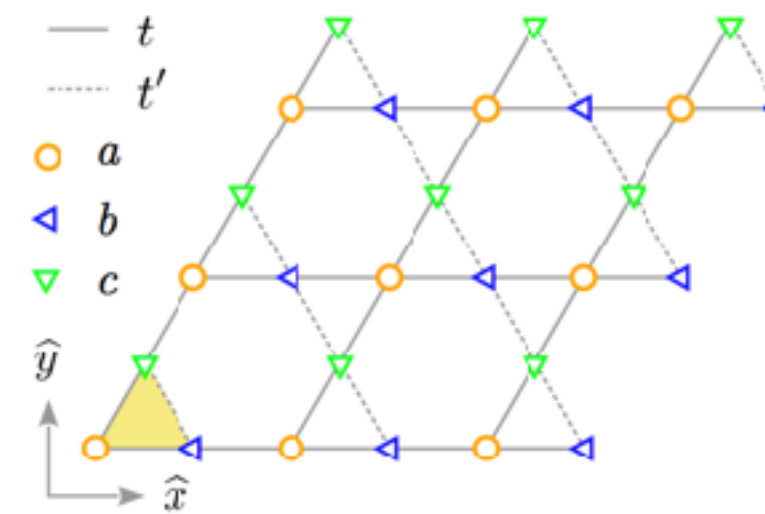
Decorated honeycomb



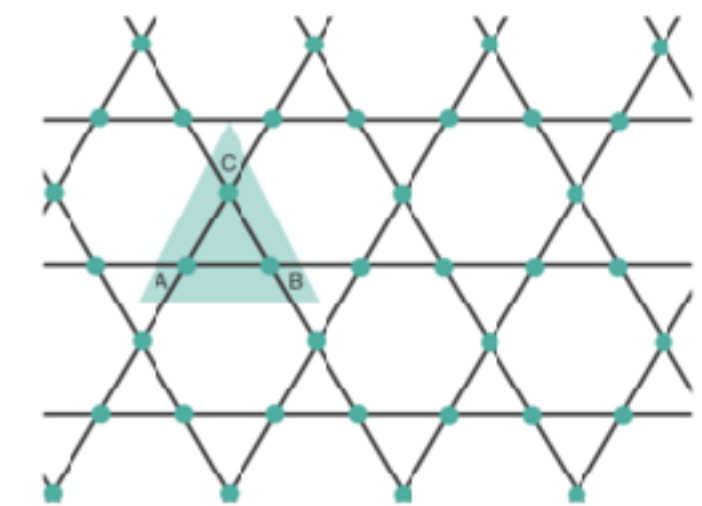
Lieb



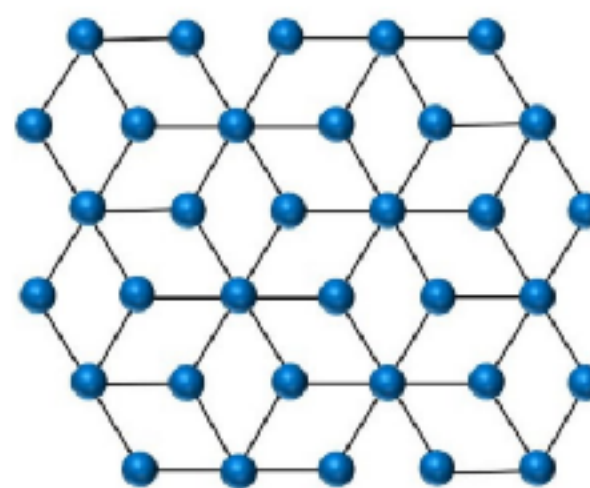
Anisotropic kagome



Kagome



Dice





What's ALF

Auxiliary-field quantum Monte Carlo package

The *Algorithms for Lattice Fermions* package provides a general code for auxiliary-field quantum Monte Carlo simulations.

<https://alf.physik.uni-wuerzburg.de/page/about/>

General Hamiltonian

ALF simulates *any model* that can be written (see below) in terms of sums of:

- single-body operators,
- squares of single-body operators, and
- single-body operators coupled to an Ising field with given dynamics.

Ease of Use

The package capabilities are made easily accessible through:

- its Python interface, [pyALF](#),
- extensive [documentation](#) and a short [tutorial](#), as well as
- a large set of Predefined Structures that substantially simplify extending the code.

ALF Hamiltonians

SU(N), Spin S antiferromagnet

Extended Hubbard model

Hubbard model in canonical ensemble.

Kitaev-Heisenberg model

SU(2) Kondo and Anderson impurities.

Nematic Quantum Criticality in Dirac Systems

QSH $t - \lambda$ model

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ALF Hamiltonians

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SU(2) Kondo and Anderson impurities.

Nematic Quantum Criticality in Dirac Systems

QSH $t - \lambda$ model

**The *ALF* (Algorithms for *L*attice *F*ermions)
project release 2.4**

Documentation for the auxiliary-field quantum Monte Carlo code

The **ALF Collaboration**^{*}: F. F. Assaad^{1,4}, M. Bercx¹, F. Goth¹, A. Götz¹, J. S. Hofmann²,
E. Huffman³, Z. Liu¹, F. Parisen Toldin¹, J. S. E. Portela¹, J. Schwab¹

1 Institut für Theoretische Physik und Astrophysik, Universität Würzburg,
97074 Würzburg, Germany

2 Department of Condensed Matter Physics, Weizmann Institute of Science,
Rehovot, 76100, Israel

3 Perimeter Institute for Theoretical Physics,
Waterloo, Ontario N2L 2Y5, Canada

4 Würzburg-Dresden Cluster of Excellence ct.qmat,
Am Hubland, 97074 Würzburg, Germany

^{*}alf@physik.uni-wuerzburg.de

October 1, 2025

<https://arxiv.org/pdf/2012.11914>



*Algorithms
Lattice
Fermions*

- Fortran and python interface
- Not so easy to use

Main advantage: Different hamiltonians, $T=0$ and $T \neq 0$

SmoQyDQMC

We introduce version 2.0 of the [SmoQyDQMC.jl](https://github.com/SmoQySuite/SmoQyDQMC.jl) package, a Julia implementation of the determinant quantum Monte Carlo algorithm. [SmoQyDQMC.jl](https://github.com/SmoQySuite/SmoQyDQMC.jl) supports generalized tight-binding Hamiltonians with local and extended Hubbard and generalized electron-phonon (*e*-ph) interactions, including non-linear *e*-ph coupling and anharmonic lattice potentials. Our implementation uses an optimized hybrid Monte Carlo method with exact forces to efficiently sample the phonon fields, enabling the simulation of low-energy phonon branches, including acoustic phonons. The [SmoQyDQMC.jl](https://github.com/SmoQySuite/SmoQyDQMC.jl) package also uses a flexible scripting interface, allowing users to adapt it to different workflows and interface with other software packages in the Julia ecosystem. The code for this package can be downloaded from our GitHub repository at <https://github.com/SmoQySuite/SmoQyDQMC.jl> or installed using the Julia package manager. The online documentation, including examples, is found at <https://smoqysuite.github.io/SmoQyDQMC.jl/stable/>.

<https://smoqysuite.github.io/SmoQyDQMC.jl/stable/#SmoQyDQMC>

SmoQyDQMC.jl: A flexible implementation of determinant quantum Monte Carlo for Hubbard and electron-phonon interactions (version 2.0 release)

Benjamin Cohen-Stead^{1,2} , Shruti Agarwal^{1,2} , Sohan Malkaruge Costa^{1,2} ,
James Neuhaus^{1,2} , Andy Tanjaroon Ly^{1,2} , Yutan Zhang³ , Richard Scalettar³ ,
Kipton Barros⁴ , and Steven Johnston^{1,2,*} 

1 Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996, USA

2 Institute for Advanced Materials and Manufacturing, The University of Tennessee, Knoxville, Tennessee 37996, USA

3 Department of Physics and Astronomy, University of California, Davis, California 95616, USA

4 Theoretical Division and CNLS, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

* sjohn145@utk.edu

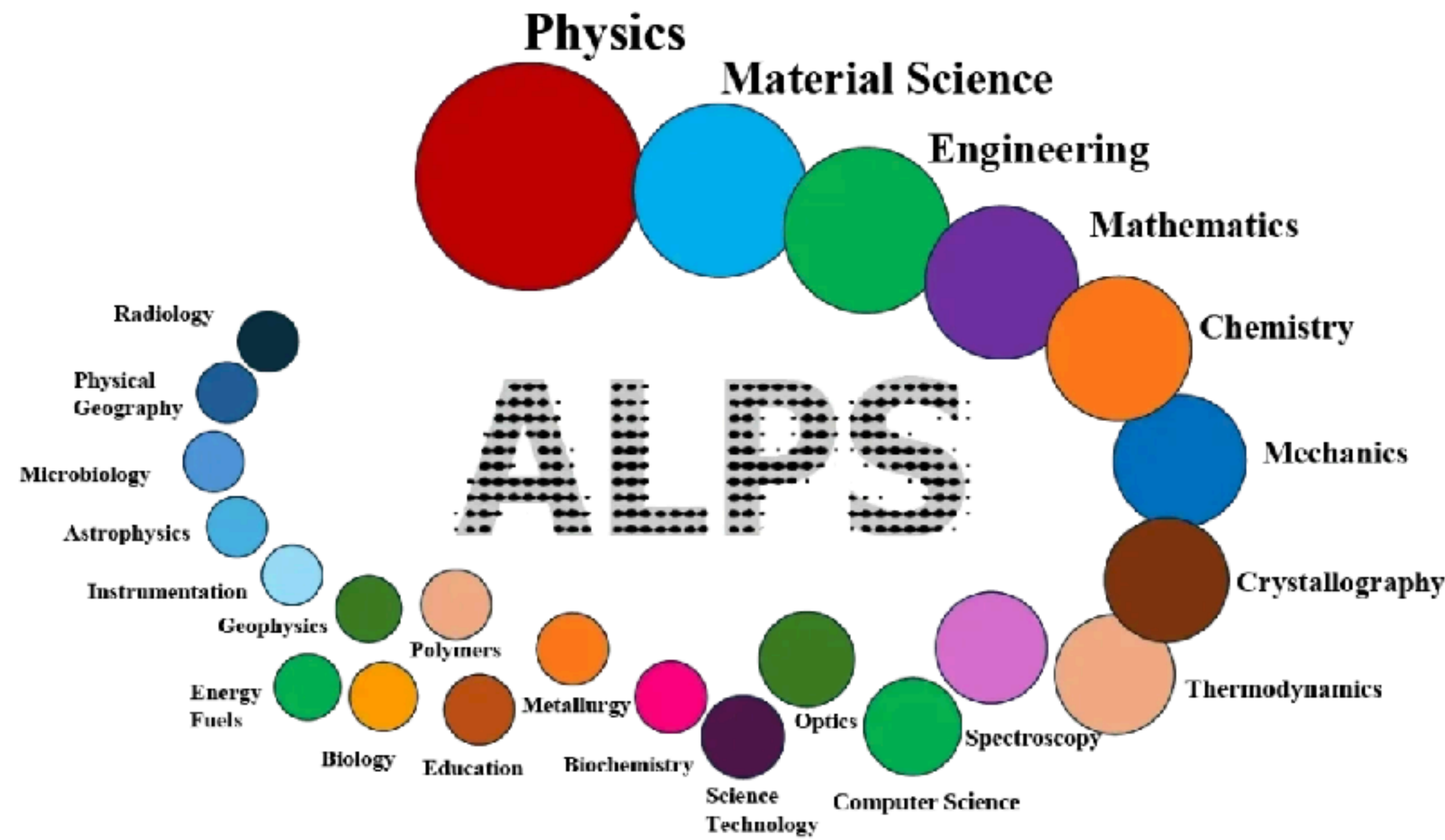
March 30, 2026

<https://arxiv.org/abs/2311.09395>

SmoQyDQMC

- Julia implementation of DQMC
- Different hamiltonians - Hubbard, extended Hubbard, e-ph

Main advantage: very easy to instal and use

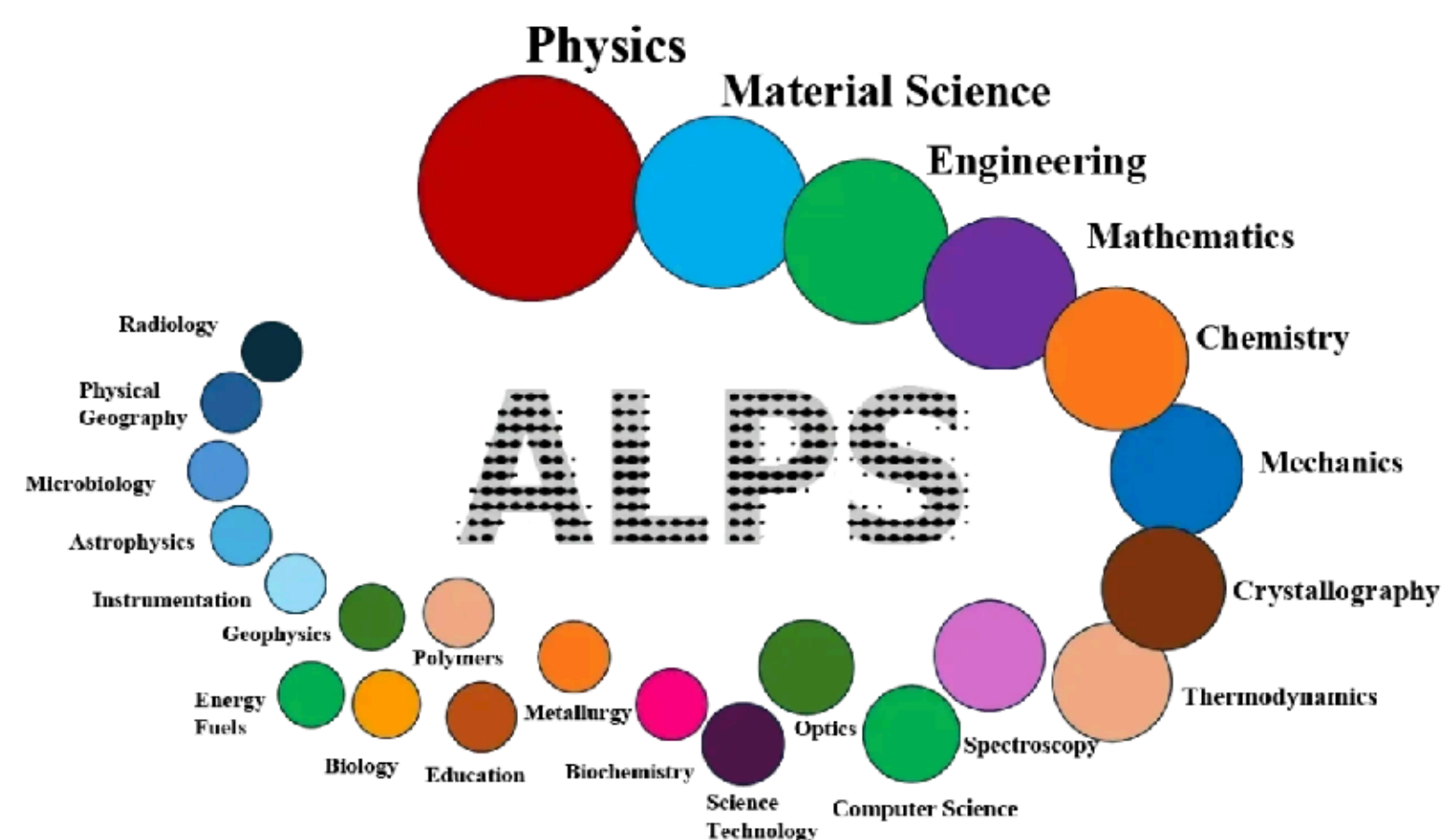


alps.comp-phys.org/

Welcome to the ALPS Software Package

ALPS (Algorithms and Libraries for Physics Simulations) is an open-source package for numerical simulations of quantum and classical condensed matter systems. It provides production-ready implementations of leading quantum algorithms for spin, bosonic, and fermionic lattice models. A Python interface and standardized file formats make it straightforward to set up simulations, run them on a laptop or HPC cluster, and analyse the results.

Since its inception, ALPS has been used by hundreds of researchers across at least 52 countries, has underpinned thousands of publications, and has been applied to more than 20 research disciplines.



 [Get Started](#)

[< > GitHub Source](#)

[📅 Events](#)

[⬇️ Installation](#)

[🐛 Issues](#)

[🏛️ Governance](#)

[🎓 Tutorials](#)

[🔬 Models](#)

[💬 Discord](#)

[❓ FAQ](#)

[📄 Publication Link](#)

[🗒️ Cite](#)

[👥 Contributors](#)

ALPSCore

Applications and Libraries for Physics Simulations Core libraries

The ALPS Core libraries aim to provide a set of well tested, robust, and standardized components for numerical simulations of condensed matter systems, in particular systems with strongly correlated electrons. The ALPS project, including legacy application codes not contained in the core libraries, is currently being worked on at alps.comp-phys.com.

 Install

 Cite

 Use

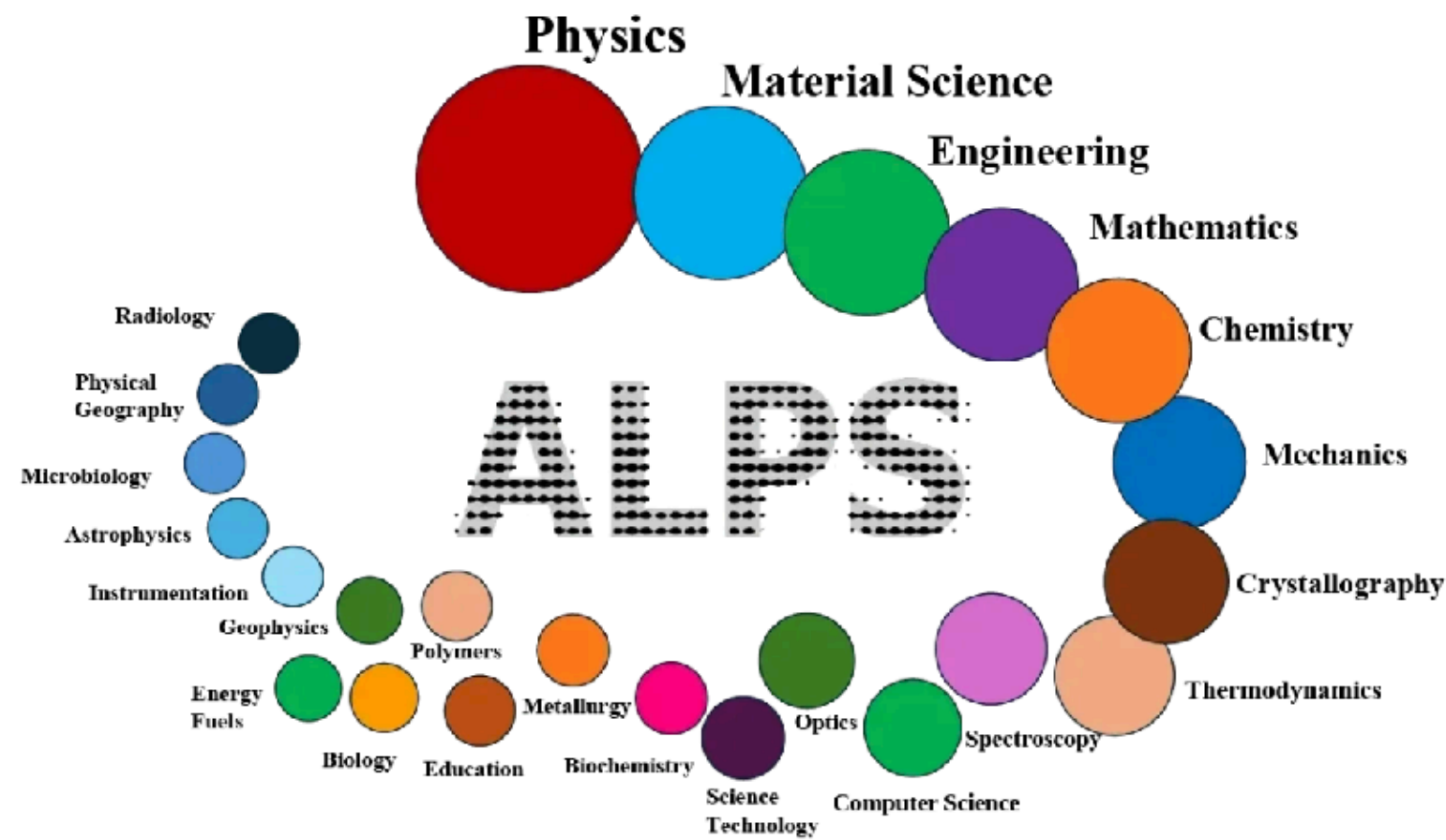
 Contribute

alpscore.org

The ALPS project release 3.0: open source software for strongly correlated systems

E. Alet¹, T. Chen², A. Feiguin³, E. Gull^{4,5}, S. Isakov⁴, J. P. F. LeBlanc⁶, F. Lin⁷,
A. Mirmira¹¹, G. Möller⁸, L. Pollet⁹, M. Rosales⁷, V. W. Scarola^{7*}, H. Shinaoka¹⁰,
H. Terletska¹¹, S. Todo¹², M. Troyer¹³, M. Wallerberger¹⁴, P. Werner¹⁵ and T. M. R. Wolf⁷

(for the ALPS collaboration)



- 1 Univ Toulouse, CNRS, Laboratoire de Physique Théorique, Toulouse, France
- 2 Department of Physics and Engineering, West Chester University, Pennsylvania, USA
- 3 Department of Physics, Northeastern University, Boston, Massachusetts, USA
- 4 Department of Physics, University of Michigan, Ann Arbor, Michigan, USA
- 5 Department of Physics, University of Warsaw, Warsaw, Poland
- 6 Department of Physics and Physical Oceanography, Memorial University of Newfoundland, St. John's, Newfoundland, Canada
- 7 Department of Physics, Virginia Tech, Blacksburg, Virginia, USA
- 8 School of Engineering, Mathematics and Physics, University of Kent, Canterbury, UK
- 9 Arnold Sommerfeld Center for Theoretical Physics, Department of Physics, Ludwig-Maximilians-Universität München, Munich, Germany
- 10 Department of Physics, Saitama University, Saitama, Japan
- 11 Department of Physics and Astronomy, Middle Tennessee State University, Murfreesboro, Tennessee, USA
- 12 Department of Physics, University of Tokyo, Tokyo, Japan
- 13 Microsoft Quantum, Redmond, Washington, USA
- 14 TU Wien, Institute of Solid State Physics, Austria
- 15 Department of Physics, University of Fribourg, Switzerland

arxiv.org/pdf/2610.03884

ALPS 3.0

- Python interface
- Different numerical methods: Classical MC, QMC, DMRG

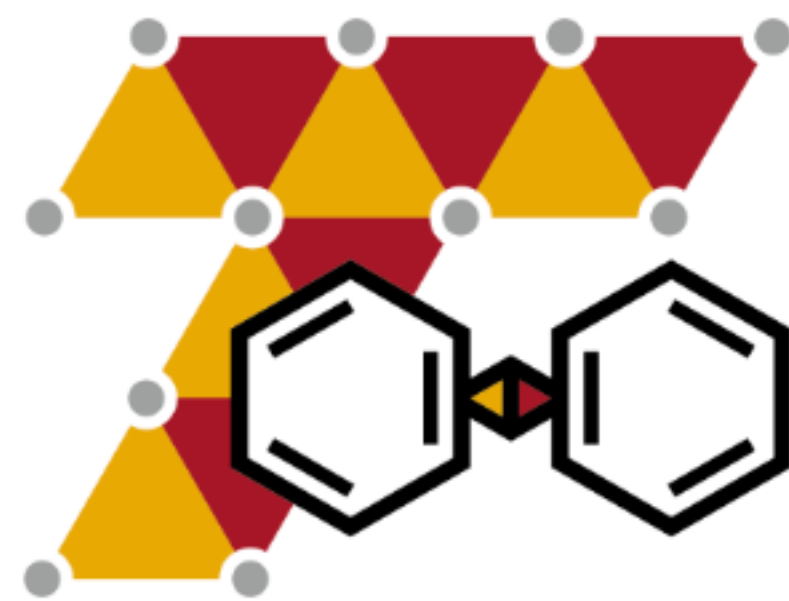
Other
implementations

Variational QMC

Diffusion QMC



QMCPACK

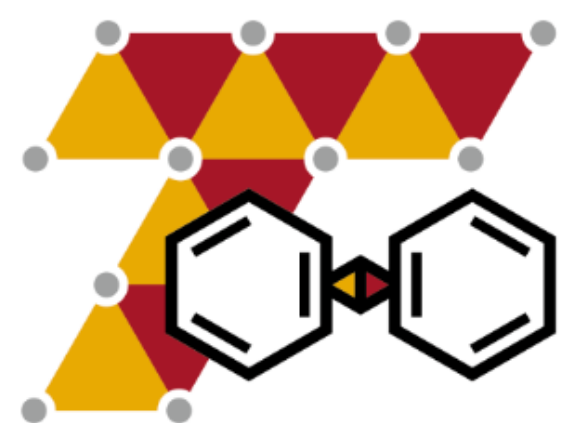


TurboRVB
Quantum Monte Carlo Package **SISSA**

SISSA Quantum Monte Carlo package

**Sandro Sorella and Michele Casula
and others along 20 years**

<https://github.com/sissaschool/turborvb>



TurboRVB
Quantum Monte Carlo Package **SISSA**

Variational QMC

Diffusion QMC

RESEARCH ARTICLE | MAY 29 2020

TURBORVB: A many-body toolkit for *ab initio* electronic simulations by quantum Monte Carlo

Special Collection: [Electronic Structure Software](#) , [Chemical Physics Software Collection](#)

Kousuke Nakano ; Claudio Attaccalite ; Matteo Barborini ; Luca Capriotti ; Michele Casula ; Emanuele Coccia ; Mario Dagrada; Claudio Genovese ; Ye Luo ; Guglielmo Mazzola ; Andrea Zen ; Sandro Sorella



J. Chem. Phys. 152, 204121 (2020)

<https://doi.org/10.1063/5.0005037>

QMCPACK

Variational QMC

Background

QMCPACK, is a modern high-performance open-source Quantum Monte Carlo (QMC) simulation code. Its main applications are electronic structure calculations of molecular, quasi-2D and solid-state systems. Variational Monte Carlo (VMC), diffusion Monte Carlo (DMC) and a number of other advanced QMC algorithms are implemented. Orbital space auxiliary field QMC (AFQMC) has recently been added. By directly solving the Schrodinger equation, QMC methods offer greater accuracy than methods such as density functional theory, but at a trade-off of much greater computational expense.

QMCPACK is written in C++ and designed with the modularity afforded by object-oriented programming. It makes extensive use of template metaprogramming to achieve high computational efficiency. Due to the modular architecture, the addition of new wavefunctions, algorithms, and observables is relatively straightforward. For parallelization QMCPACK utilizes a fully hybrid (OpenMP,CUDA)/MPI approach to optimize memory usage and to take advantage of the growing number of cores per SMP node or GPUs. High parallel and computational efficiencies are achievable on the largest supercomputers. Finally, QMCPACK utilizes standard file formats for input and output in XML and HDF5 to facilitate data exchange.

<https://qmcpack.org/>

QMC PACK: an open source *ab initio* quantum Monte Carlo package for the electronic structure of atoms, molecules and solids

Jeongnim Kim¹, Andrew D Baczewski², Todd D Beaudet³, Anouar Benali^{4,5}, M Chandler Bennett⁶, Mark A Berrill⁷, Nick S Blunt⁸, Edgar Josué Landinez Borda⁹, Michele Casula¹⁰, David M Ceperley¹¹, Simone Chiesa¹¹, Bryan K Clark¹¹, Raymond C Clay III², Kris T Delaney¹², Mark Dewing⁵, Kenneth P Esler¹³, Hongxia Hao¹⁴, Olle Heinonen^{15,16}, Paul R C Kent^{17,18}, Jaron T Krogel¹⁹, Ilkka Kylänpää¹⁹, Ying Wai Li²⁰, M Graham Lopez⁷, Ye Luo^{4,5}, Fionn D Malone⁹, Richard M Martin¹¹, Amrita Mathuriya¹, Jeremy McMinis⁹, Cody A Melton⁶, Lubos Mitas⁶, Miguel A Morales⁹, Eric Neuscamman^{21,22}, William D Parker²³, Sergio D Pineda Flores²¹, Nichols A Romero^{4,5}, Brenda M Rubenstein¹⁴, Jacqueline A R Shea²¹, Hyeondeok Shin⁵, Luke Shulenburger², Andreas F Tillack²⁰, Joshua P Townsend², Norm M Tubman²¹, Brett Van Der Goetz²¹, Jordan E Vincent¹¹, D ChangMo Yang²⁴, Yubo Yang¹¹, Shuai Zhang⁹ and Luning Zhao²¹

RESEARCH ARTICLE | MAY 04 2020

QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion quantum Monte Carlo

Special Collection: [Electronic Structure Software](#) , [Chemical Physics Software Collection](#)

P. R. C. Kent   ; Abdulgani Annaberdiyev  ; Anouar Benali  ; M. Chandler Bennett  ;
Edgar Josué Landinez Borda  ; Peter Doak  ; Hongxia Hao  ; Kenneth D. Jordan  ; Jaron T. Krogel  ;
Ilkka Kylänpää  ; Joonho Lee  ; Ye Luo  ; Fionn D. Malone  ; Cody A. Melton  ; Lubos Mitas  ;
Miguel A. Morales; Eric Neuscamman  ; Fernando A. Reboredo; Brenda Rubenstein  ; Kayahan Saritas  ;
Shiv Upadhyay  ; Guangming Wang  ; Shuai Zhang  ; Luning Zhao 



J. Chem. Phys. 152, 174105 (2020)

<https://doi.org/10.1063/5.0004860>

 CHORUS

End of fourth class