Simulations and Emulations of Fermions in Optical Lattices

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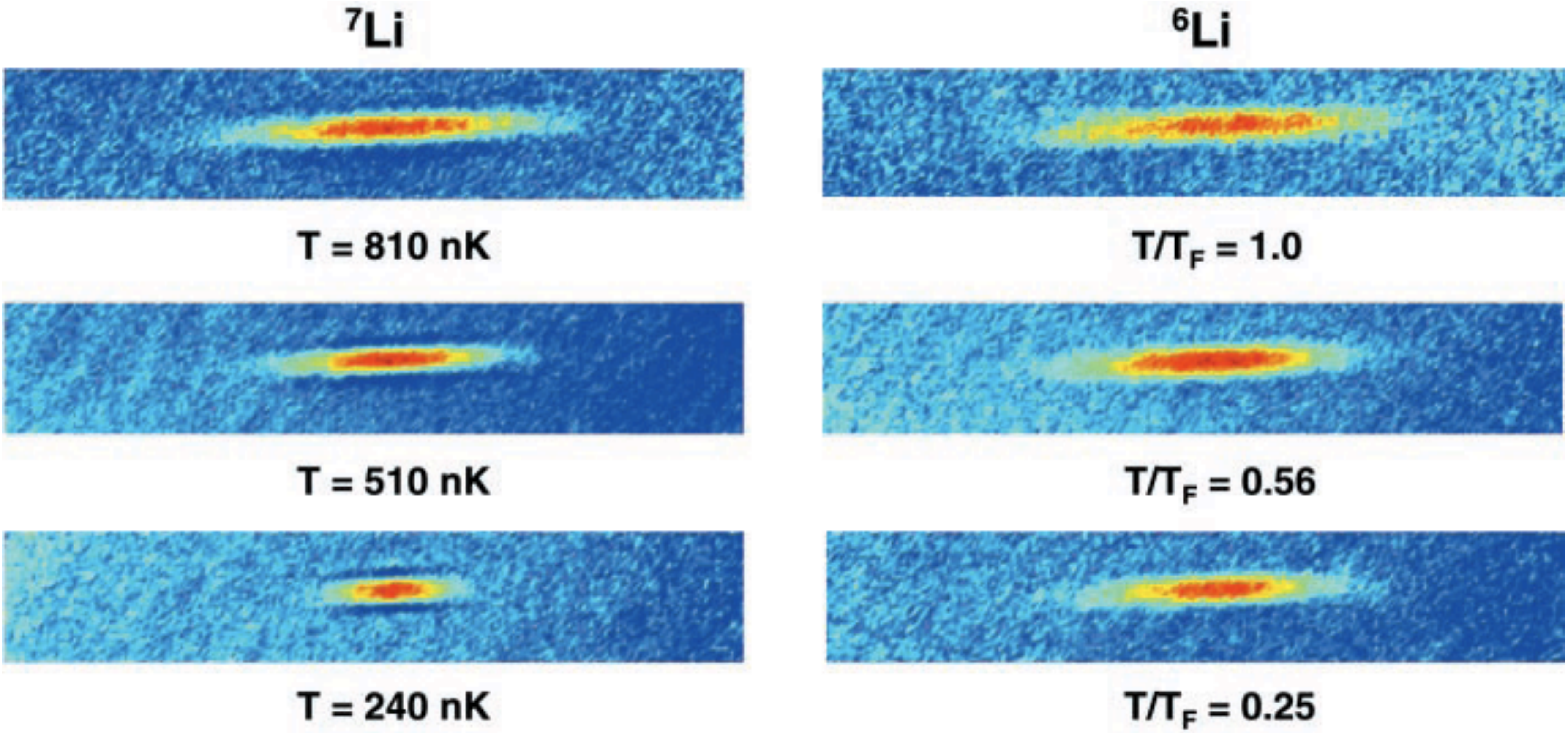
BOSONS vs FERMIONS



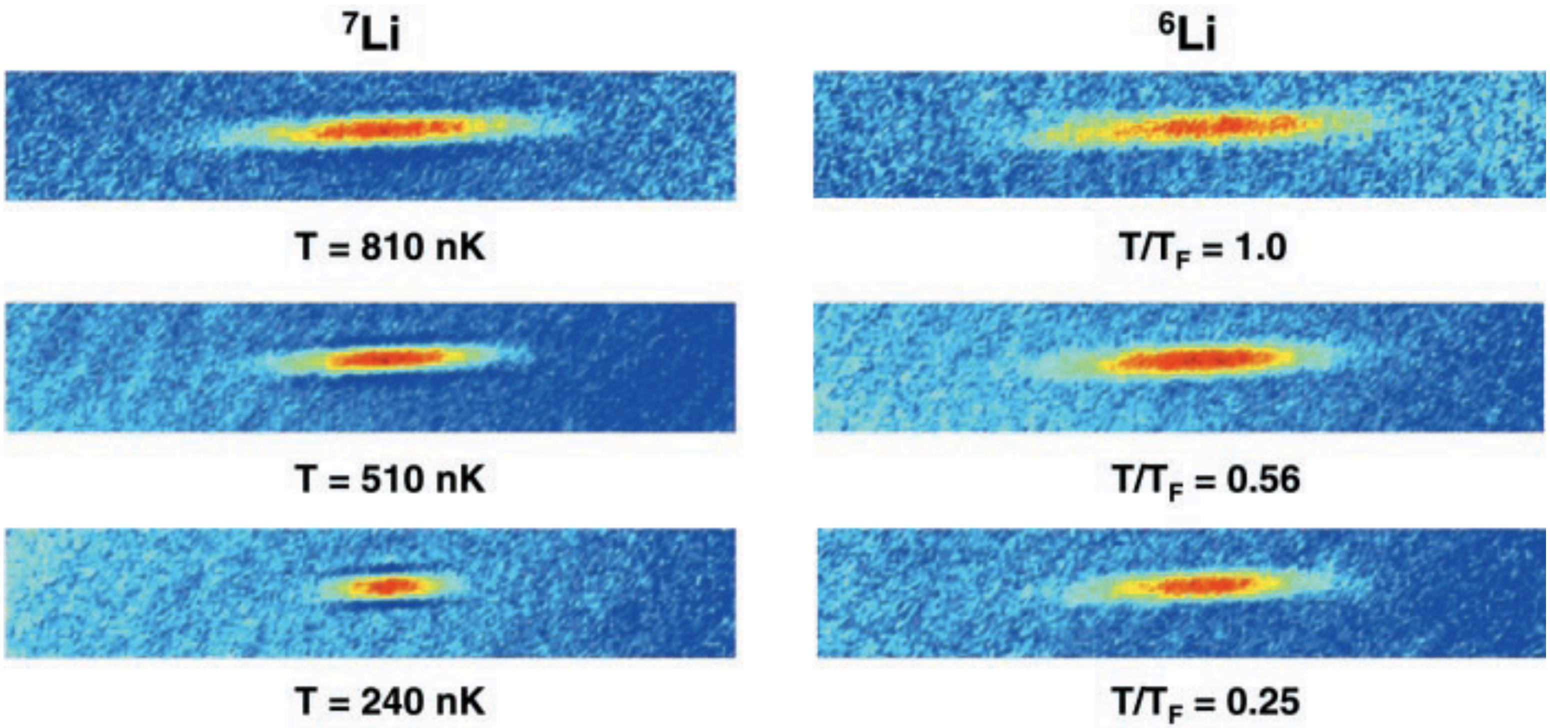
Observation of Fermi Pressure in a Gas of Trapped Atoms

Andrew G. Truscott, Kevin E. Strecker, William I. McAlexander,*
Guthrie B. Partridge, Randall G. Hulet†

Science 291, 2570 (2001)

What happened to the sign problem?

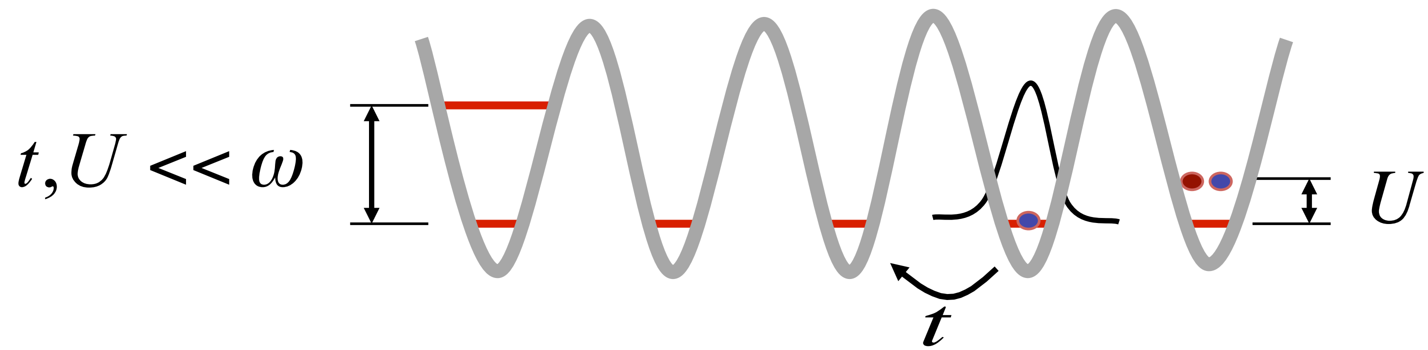
Nature seems to have no difficulty reaching the ground state of bosons or fermions!



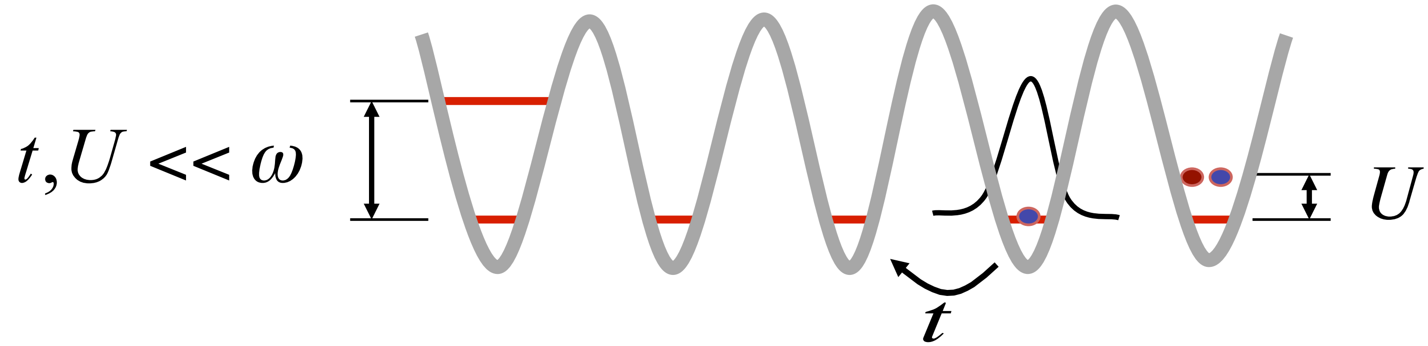
EMULATION vs SIMULATION

Truscott et al. Science 291, 2570 (2001)

Cold Atomic Gases in Optical Lattices → Hubbard Models



Cold Atomic Gases in Optical Lattices → Hubbard Models



$$H = -t \sum_{(i,j)\sigma} (c^{+}_{i\sigma} c_{j\sigma} + c^{+}_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) - h \sum_i (n_{i\uparrow} - n_{i\downarrow})$$

tunneling

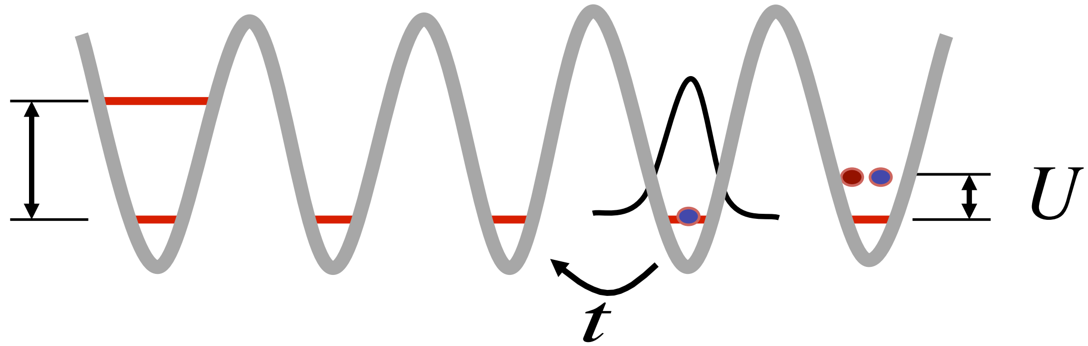
interaction

chemical potential

Zeeman field

Cold Atomic Gases in Optical Lattices → Hubbard Models

$t, U << \omega$



$$H = -t \sum_{(i,j)\sigma} (c_{i\sigma}^{+} c_{j\sigma} + c_{j\sigma}^{+} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) - h \sum_i (n_{i\uparrow} - n_{i\downarrow})$$

tunneling

interaction

chemical potential

Zeeman field

$\lambda \approx 1000nm$

$t \sim 10nK$

$U/t \sim 10$

$J = 4t^2/U \approx 4nK$

^{6}Li

$|F, m_F\rangle = \left|\frac{1}{2}, \frac{-1}{2}\right\rangle \equiv |\downarrow\rangle$

$|F, m_F\rangle = \left|\frac{1}{2}, \frac{1}{2}\right\rangle \equiv |\uparrow\rangle$

^{40}K

$|F, m_F\rangle = \left|\frac{9}{2}, \frac{-9}{2}\right\rangle \equiv |\downarrow\rangle$

$|F, m_F\rangle = \left|\frac{9}{2}, \frac{-7}{2}\right\rangle \equiv |\uparrow\rangle$

Schneider et al. Science 322, 1520 (2008)
Jordens et al Nature 455, 204 (2008)
Liao et al Nature 467, 567-569 (2010)

OUTLINE

I. Repulsively interacting fermions in 3D optical lattices:

What are the entropy constraints required to reach the AF phase with long range order?

Collaborators: Part I

Thereza Paiva
University Rio de Janeiro,
Brazil

Mohit Randeria
The Ohio State
University

Richard Scalettar
UC Davis

Fermions in 2D Optical Lattices: Temperature and Entropy Scales for Observing Antiferromagnetism and Superfluidity,
Paiva, Scalettar, Randeria, and Trivedi, Phys. Rev. Lett. 104, 066406 (2010).

3D work unpublished

Determinantal QMC: Equation of state $\rho(\mu, T, U/t)$

“exact” unbiased on finite systems and finite T

Determinantal QMC: Equation of state $\rho(\mu, T, U/t)$

"exact" unbiased on finite systems and finite T

$$Z = Tr e^{-\beta H} = Tr[(e^{-\Delta\tau H})^L] \approx Tr[(e^{-\Delta\tau K} e^{-\Delta\tau V})^L]$$

$$\langle A \rangle = Tr[A e^{-\beta H}]/Z$$

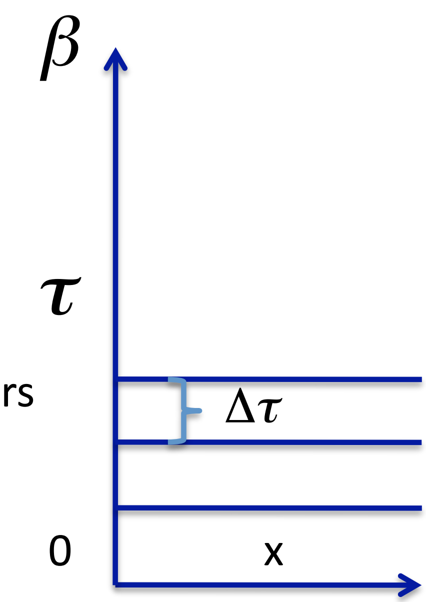
$$e^{-\Delta\tau V} = e^{-\Delta\tau U \sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2)} = \frac{1}{2} e^{-\frac{\Delta\tau U}{4}} \sum_{S(i)=\pm 1} e^{\Delta\tau S(i) \lambda (n_{i\uparrow} - n_{i\downarrow})}$$

Quadratic operators

$$Z = \sum_{S(i,\tau)} Det[M_\uparrow(S(i,\tau))] Det[M_\downarrow(S(i,\tau))]$$

At the cost of extra fields

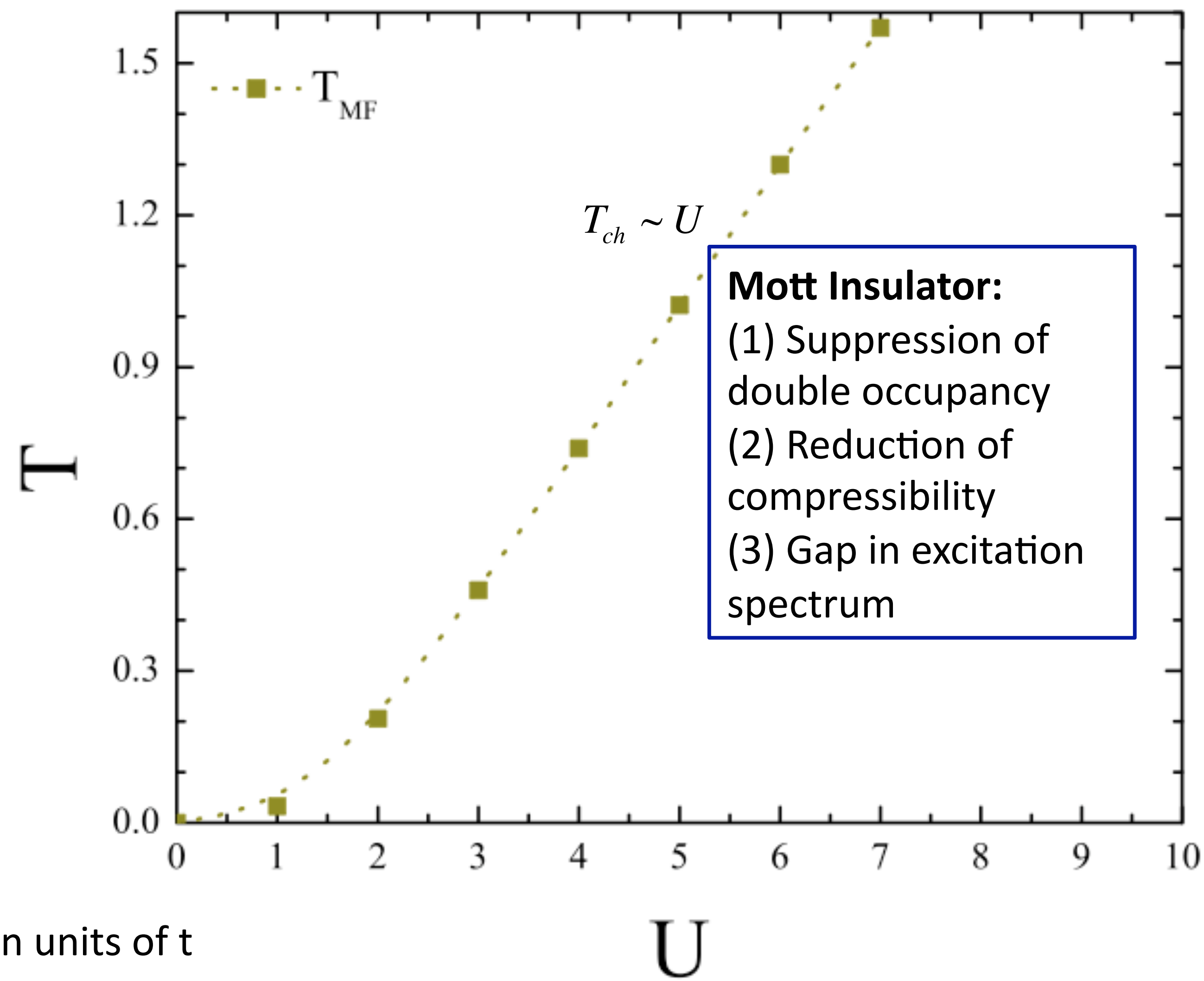
$$\langle A \rangle = \frac{\langle A \,\mathrm{sgn} \rangle\big|_{|\det M|}}{\langle \mathrm{sgn} \rangle\big|_{|\det M|}}$$



"Sign problem" at low $T \leq 0.1t$ but controlled by longer simulations

Repulsive U Hubbard model: Phase Diagram at Half Filing

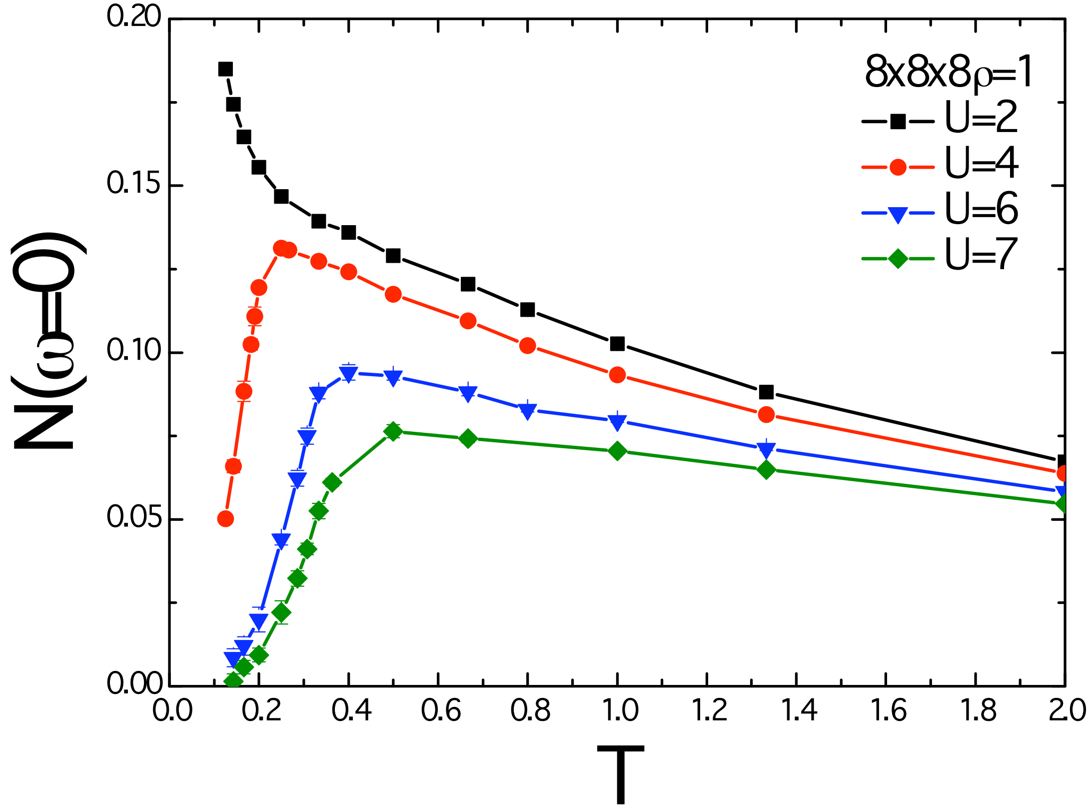
$$N_{\uparrow} = N_{\downarrow}; N_{fermions} = N_{sites}; d = 3$$



All energies in units of t

Mott Physics and Charge Gap

Density of states at the chemical potential



Appearance of gap in low energy excitation spectrum
Gap increases with U

Repulsive U Hubbard model: Phase Diagram at Half Filing

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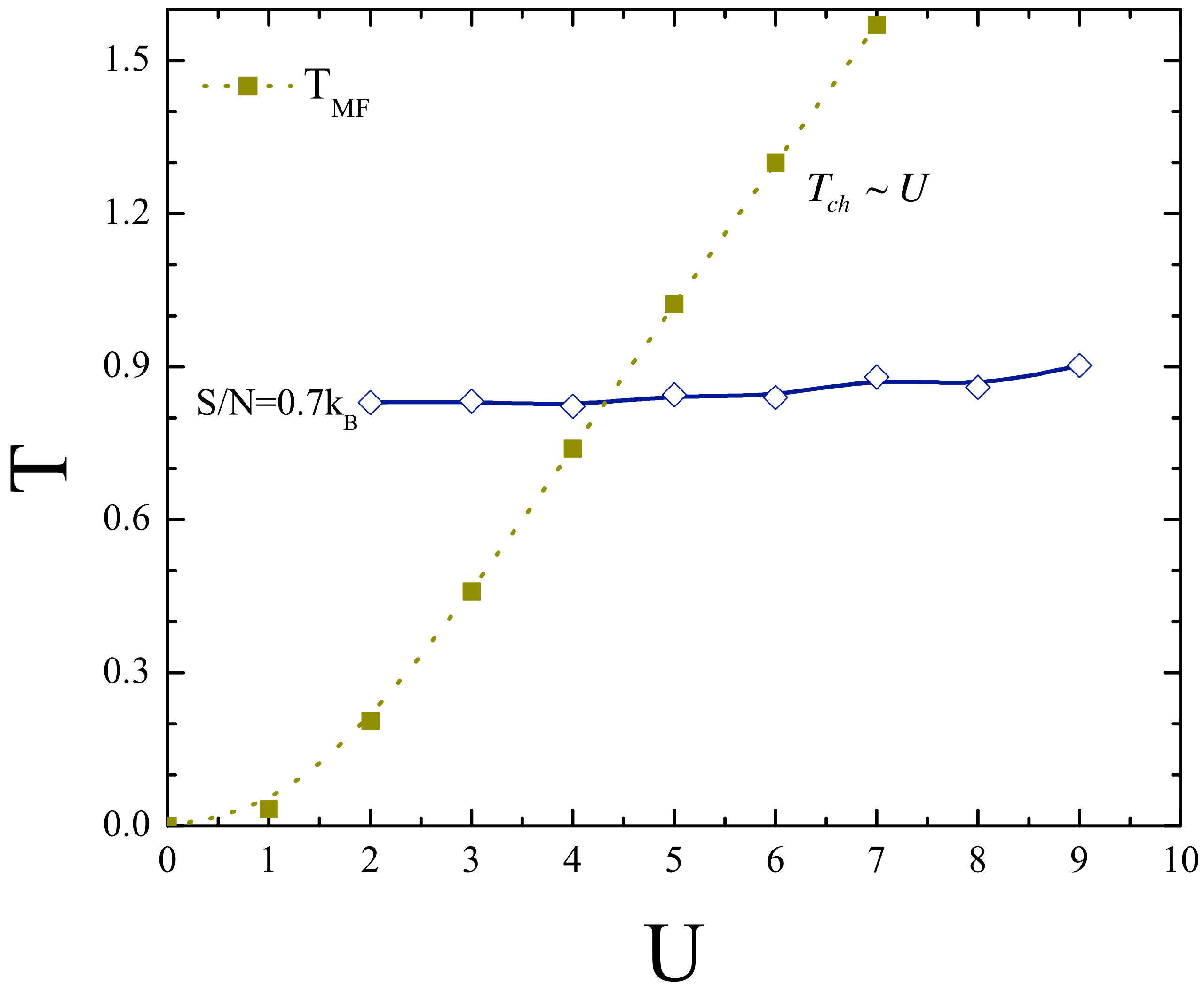


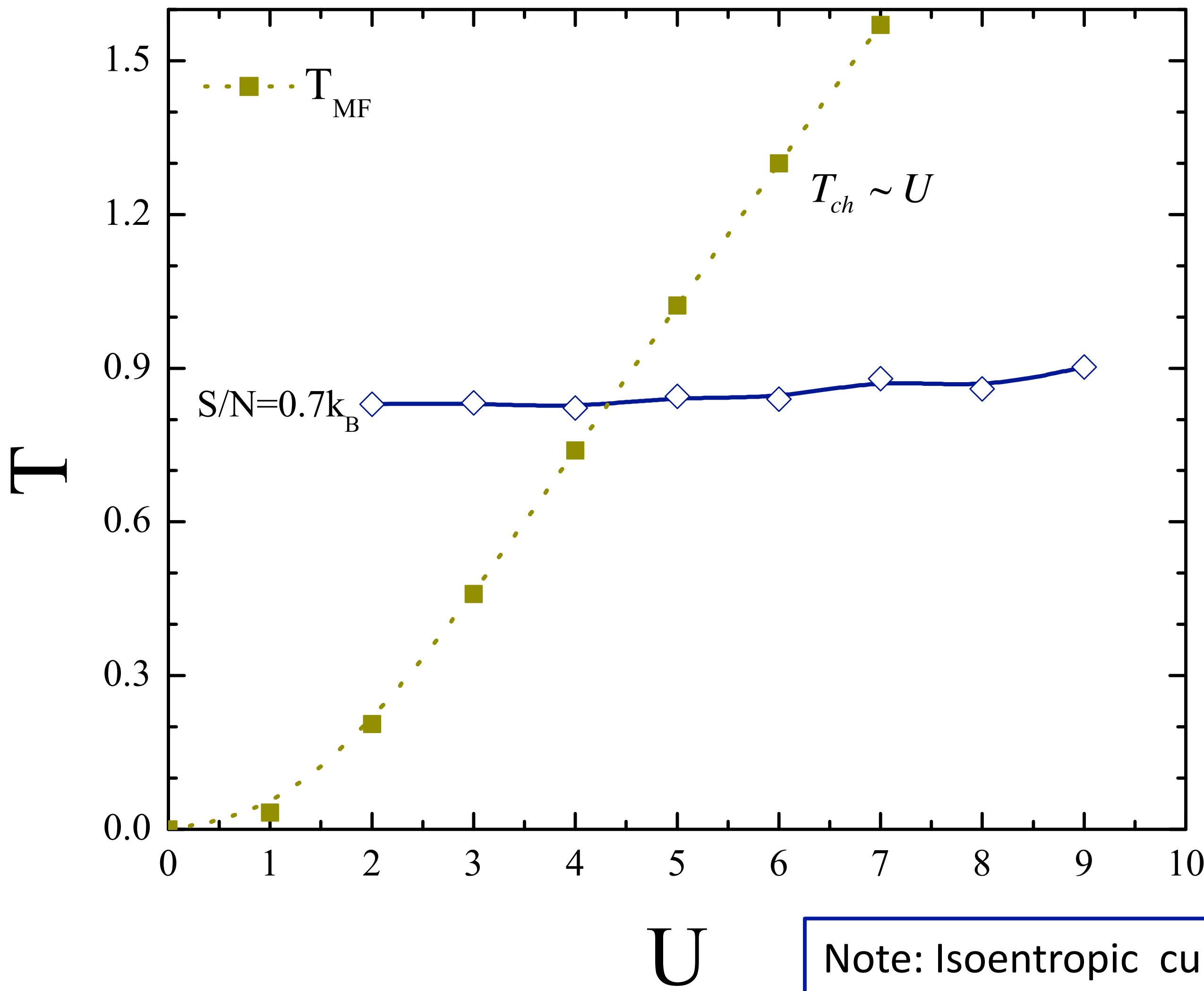
$S_{\max} / Nk_B = \ln(4) \approx 1.4$

$S_{\exp t} / Nk_B \approx 0.7 - 1$

All energies in units of t

Repulsive U Hubbard model: Phase Diagram at Half Filing

$N_{\uparrow} = N_{\downarrow}; N_{fermions} = N_{sites}; d = 3$



$S_{\max} / Nk_B = \ln(4) \approx 1.4$

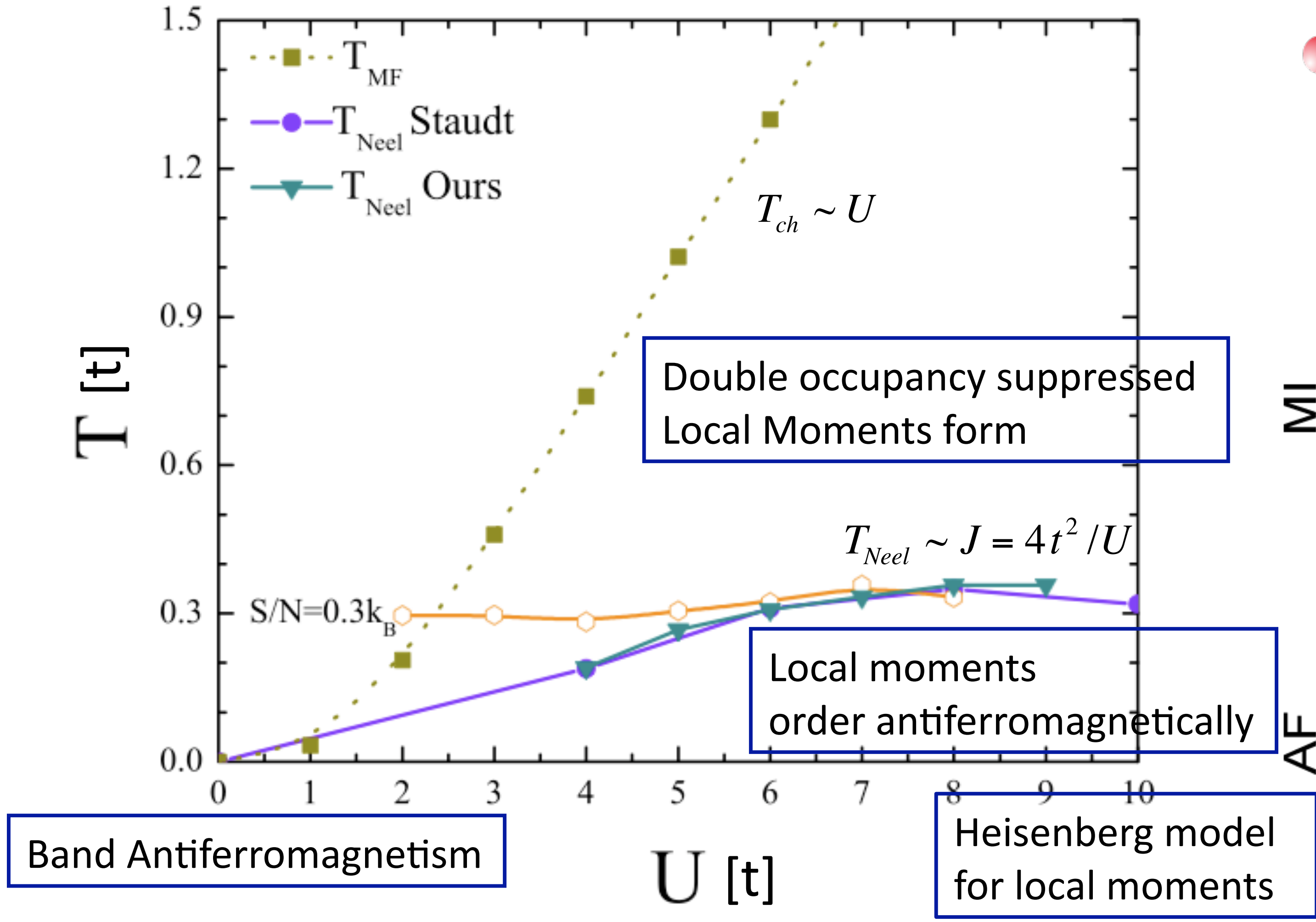
$S_{\exp t} / Nk_B \approx 0.7 - 1$

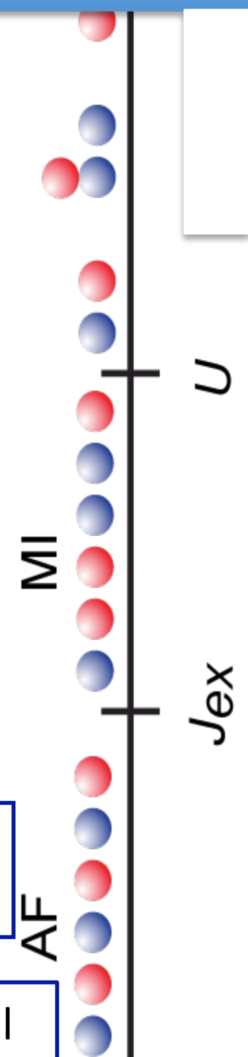
Note: Isoentropic curve is also an isothermal curve
As U is increases T remains rather constant

All energies in units of t

3D Repulsive U Hubbard model: QMC Phase Diagram

$N_{\uparrow} = N_{\downarrow}; N_{fermions} = N_{sites}; d = 3$

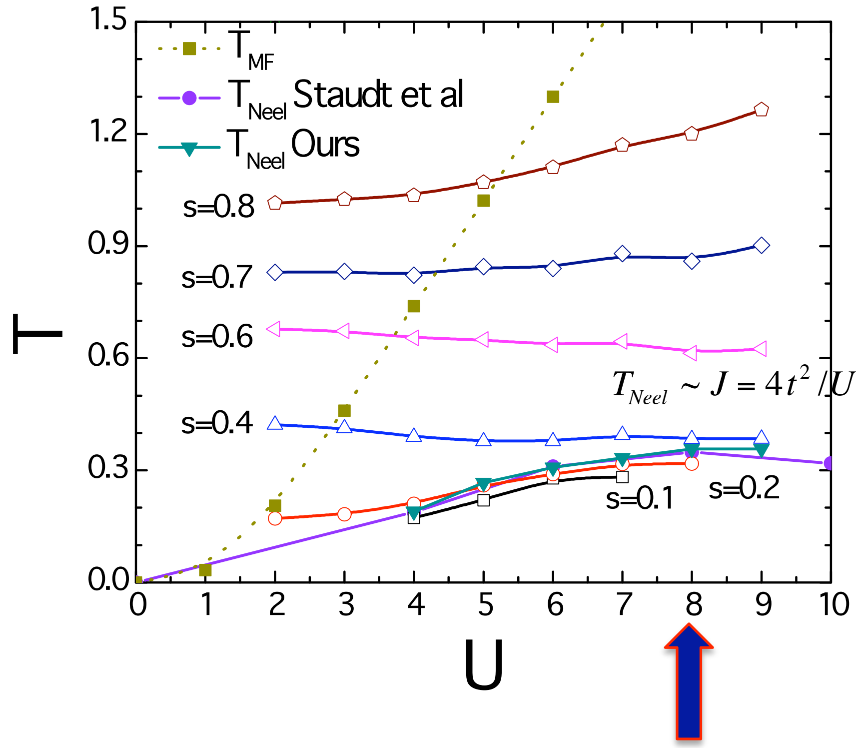




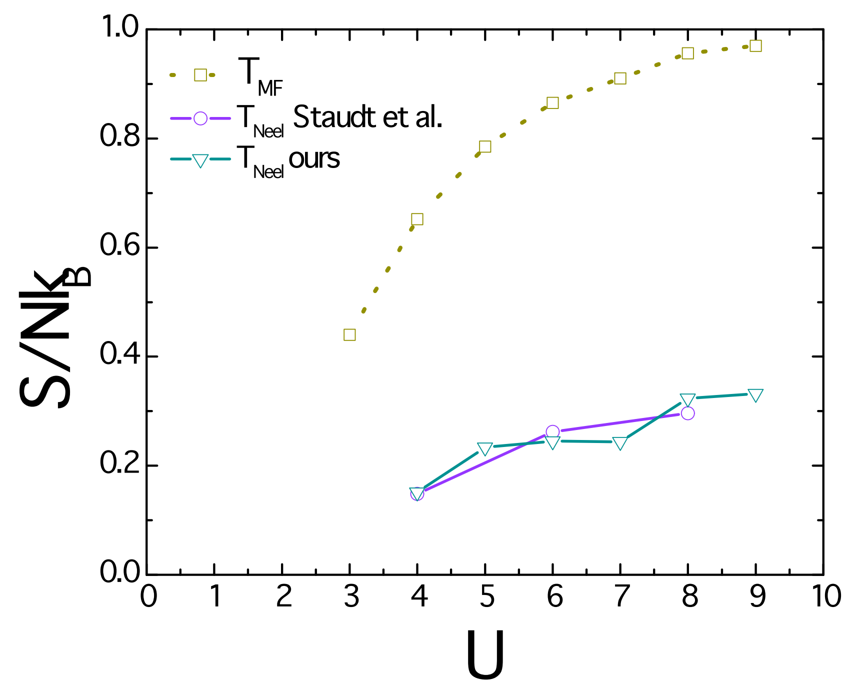
Energy in units of t

Staudt, Dzierzawa and Muramatsu EPJ B17, 411 (2000)

3D Hubbard Model at half filling: Isoentropic Curves (QMC)



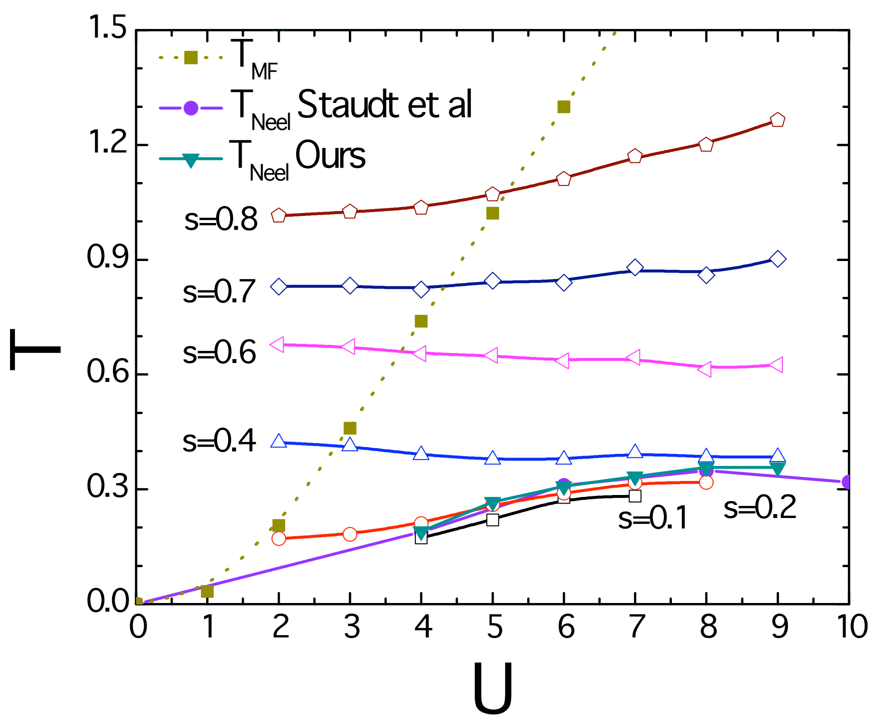
Critical Entropy vs U



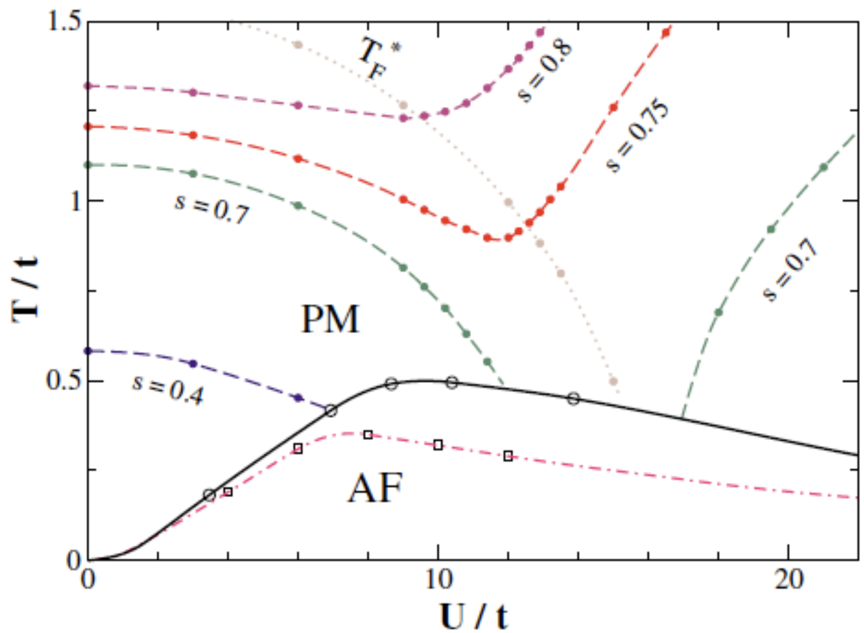
$S_{AF,Quantum}/Nk_B \approx 0.3$ ← Target entropy to see AF LRO in 3D Hubbard Model

$S_{expt}/Nk_B \approx 0.7 - 1$

QMC vs DMFT: No significant adiabatic cooling from QMC



QMC ("exact")
Adiabatic cooling not significant



Dynamical Mean Field Theory:
Werner, Parcollet, Georges, Hassan, PRL 95, 056401 (2005)

DMFT misses important singlet correlations even above T_{Neel}

Trap

3D Hubbard Quantum Simulations with a Trap

$$H = -t \sum_{(i,j)\sigma} (c^{+}_{i\sigma} c_{j\sigma} + c^{+}_{j\sigma} c_{i\sigma}) + U \sum_{i} (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2) - \mu \sum_{i} n_i$$

- Determinantal QMC for homogeneous system to calculate equation of state $\rho(\mu, T, U/t)$

  Particle-hole symmetry $\rho(-\mu) = 2 - \rho(\mu)$

3D Hubbard Quantum Simulations with a Trap

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- Determinantal QMC for homogeneous system to calculate equation of state $\rho(\mu, T, U/t)$

  Particle-hole symmetry $\rho(-\mu) = 2 - \rho(\mu)$

- Local density approximation to include the inhomogeneous distribution in trap

$$\mu(r) = \mu - \alpha \frac{r^2}{d^2}$$

$$N = \int dr^3 \rho(r) = \frac{4\sqrt{2}\pi}{(m\omega^2)^{3/2}} \int_{-\infty}^{\mu_0} d\mu \sqrt{\mu_0 - \mu}\, \rho(\mu)$$

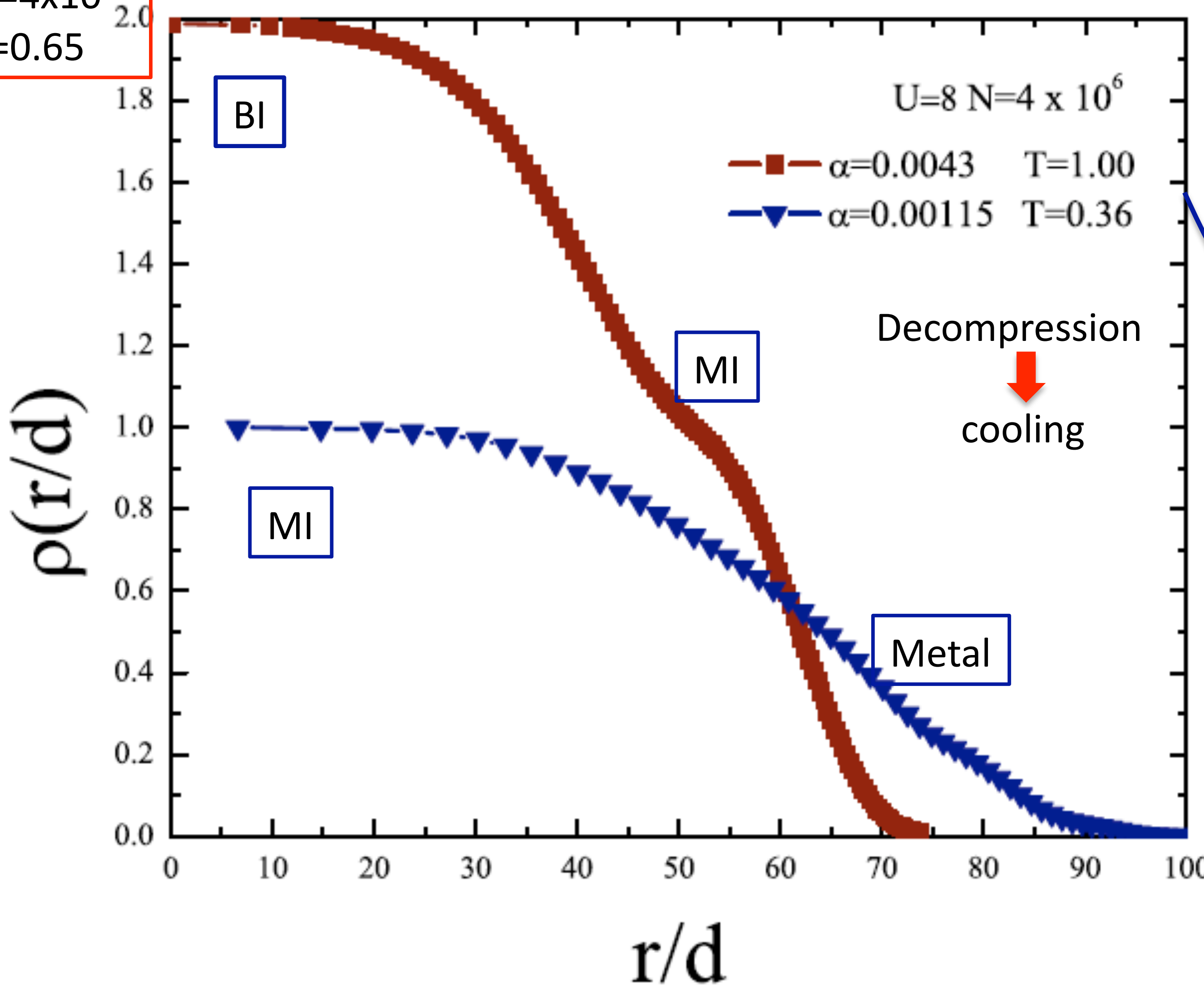
$$\left.\frac{\partial \rho}{\partial T}\right|_{\mu} = \left.\frac{\partial s}{\partial \mu}\right|_{T}$$

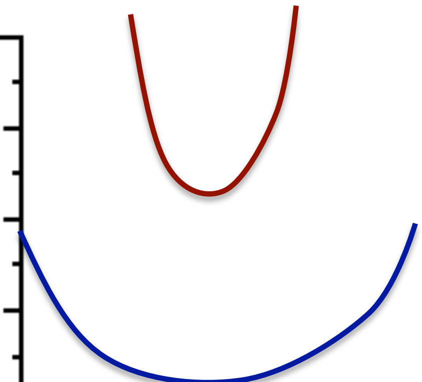
$$s(\mu) = \int_{-\infty}^{\mu} d\mu' \left.\frac{\partial \rho}{\partial T}\right|_{\mu'}$$

$$\nu = [20 - 120] Hz \Rightarrow \alpha = [0.0006 - 0.021] t$$

Inhomogeneous Distribution of Phases in a Trap

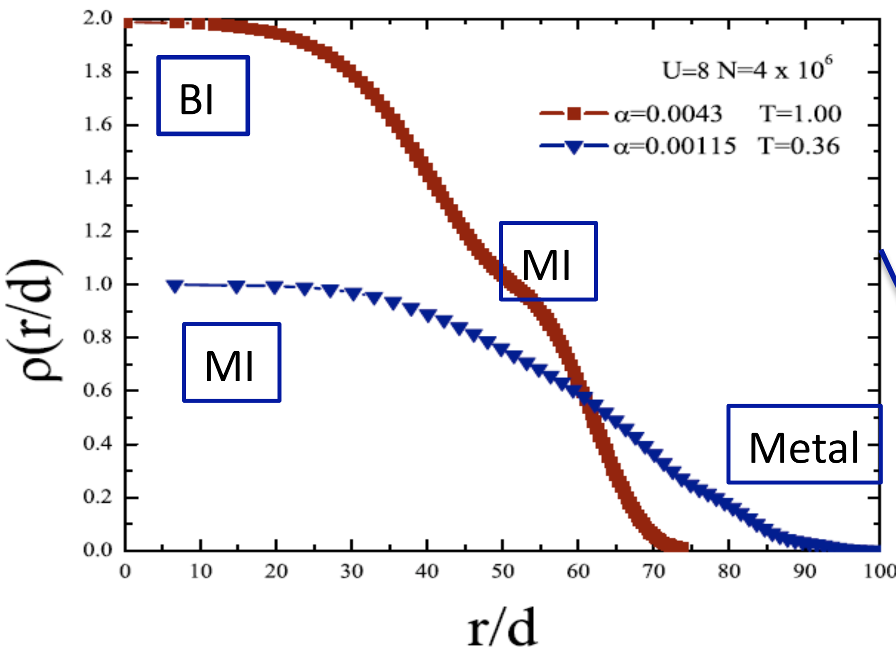
U=8 N=4x10^6
S/Nk$_B$=0.65

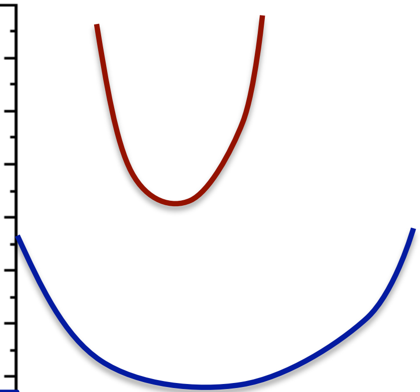




$\nu = [20 - 120]Hz \Rightarrow$

$\alpha = [0.0006 - 0.021]t$





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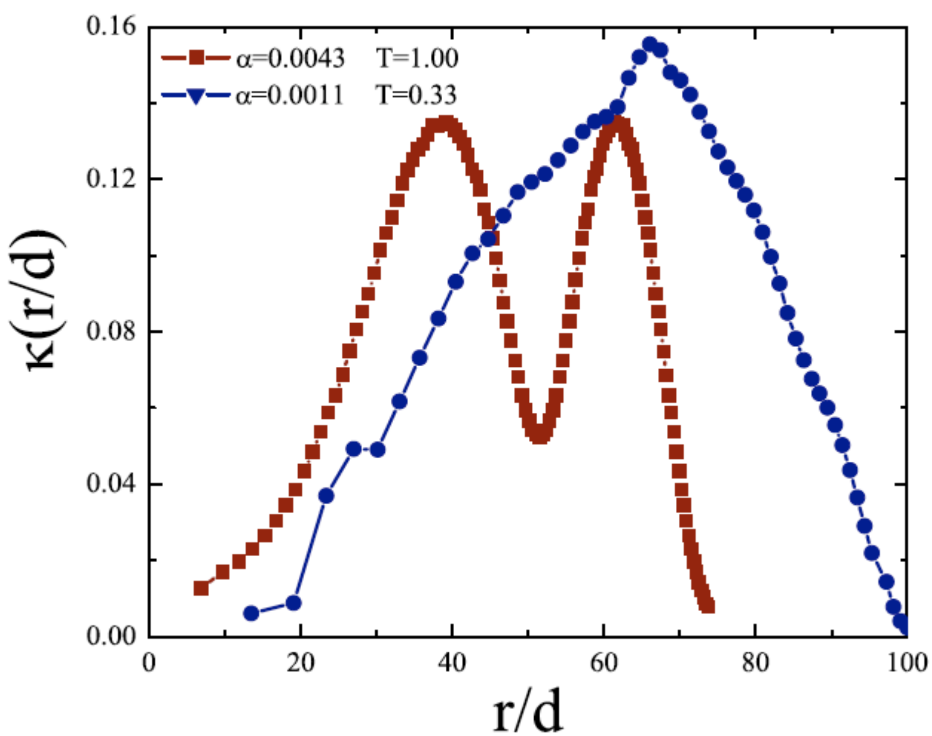
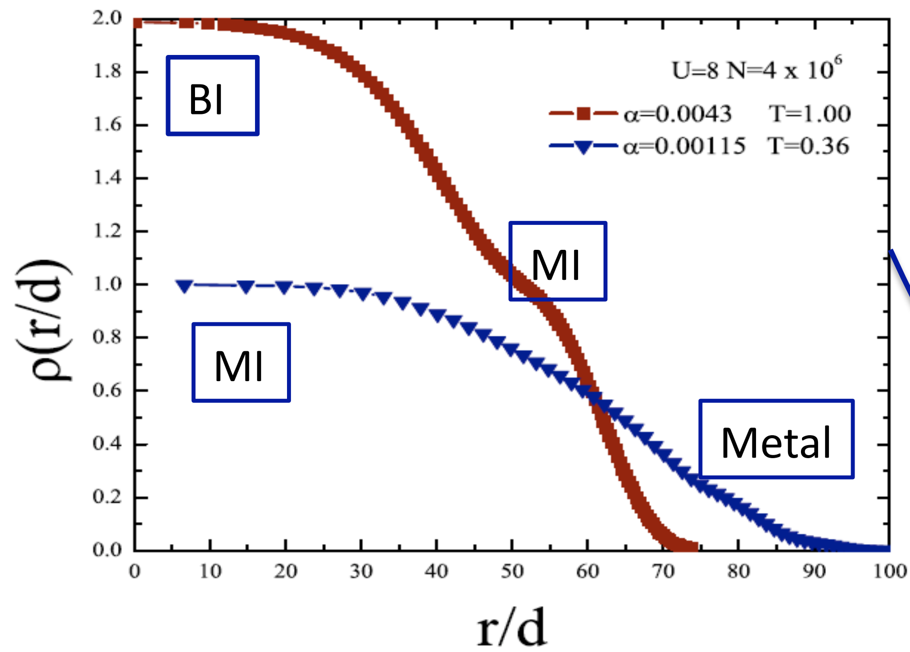
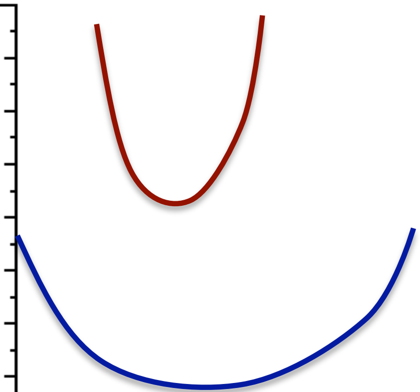


$$\kappa = \frac{1}{\rho}\frac{d\rho}{d\mu}$$

Compressibility suppressed in BI and MI





U=8 N=4x10^6
S/Nk$_B$=0.65

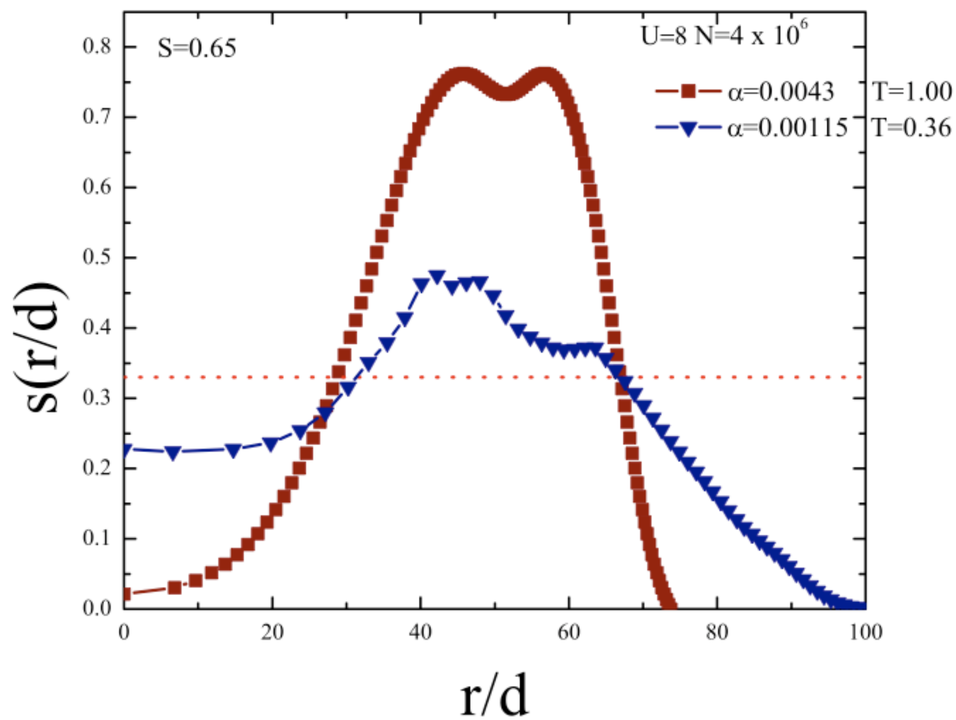
Entropy Distribution in Trap

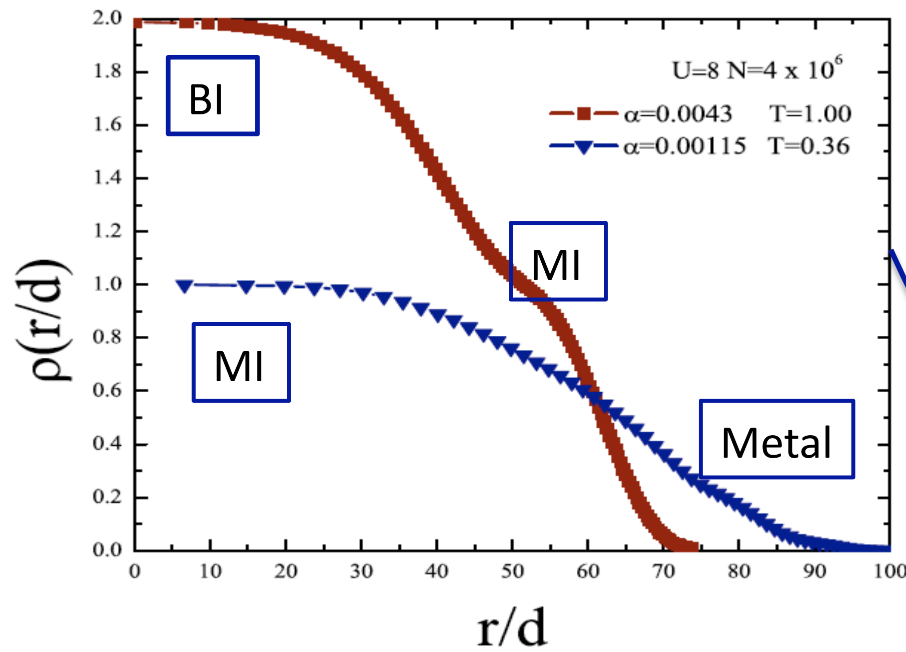
BI: entropy ~0

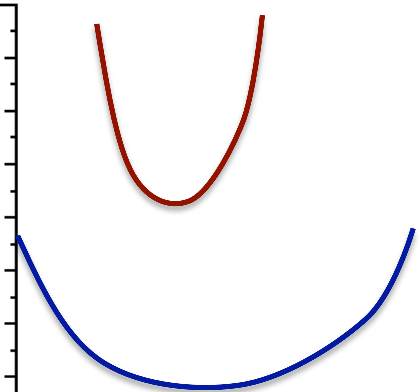
MI: low but finite entropy

because of spin waves

Metal: entropy sinks







U=8 N=4x10[6]
S/Nk_B=0.65

Entropy Distribution in Trap
BI: entropy ~0
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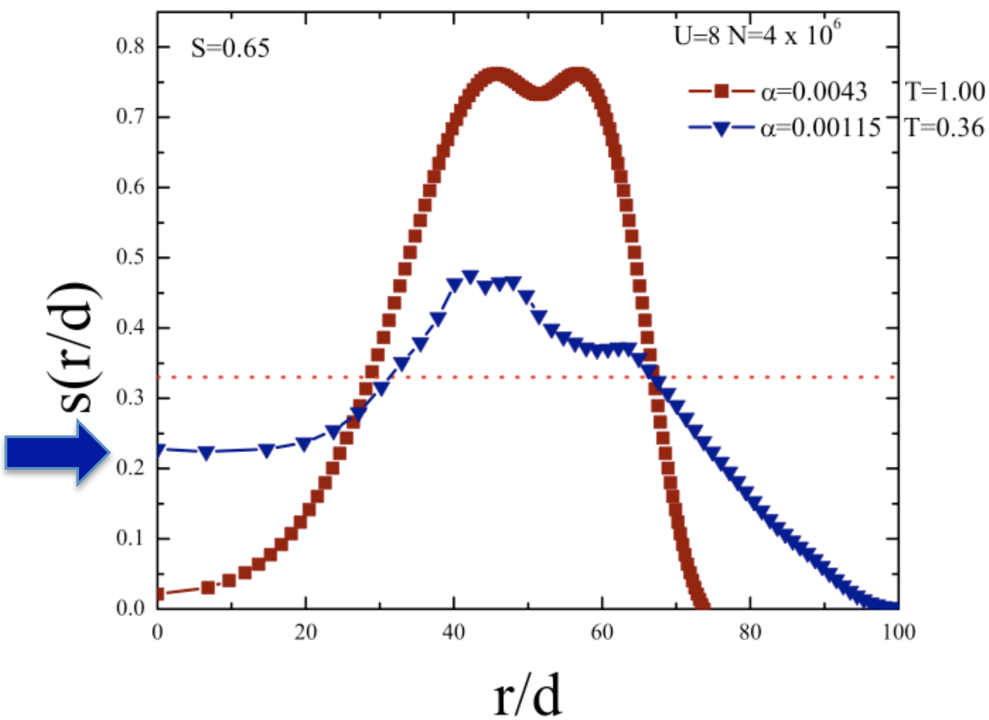
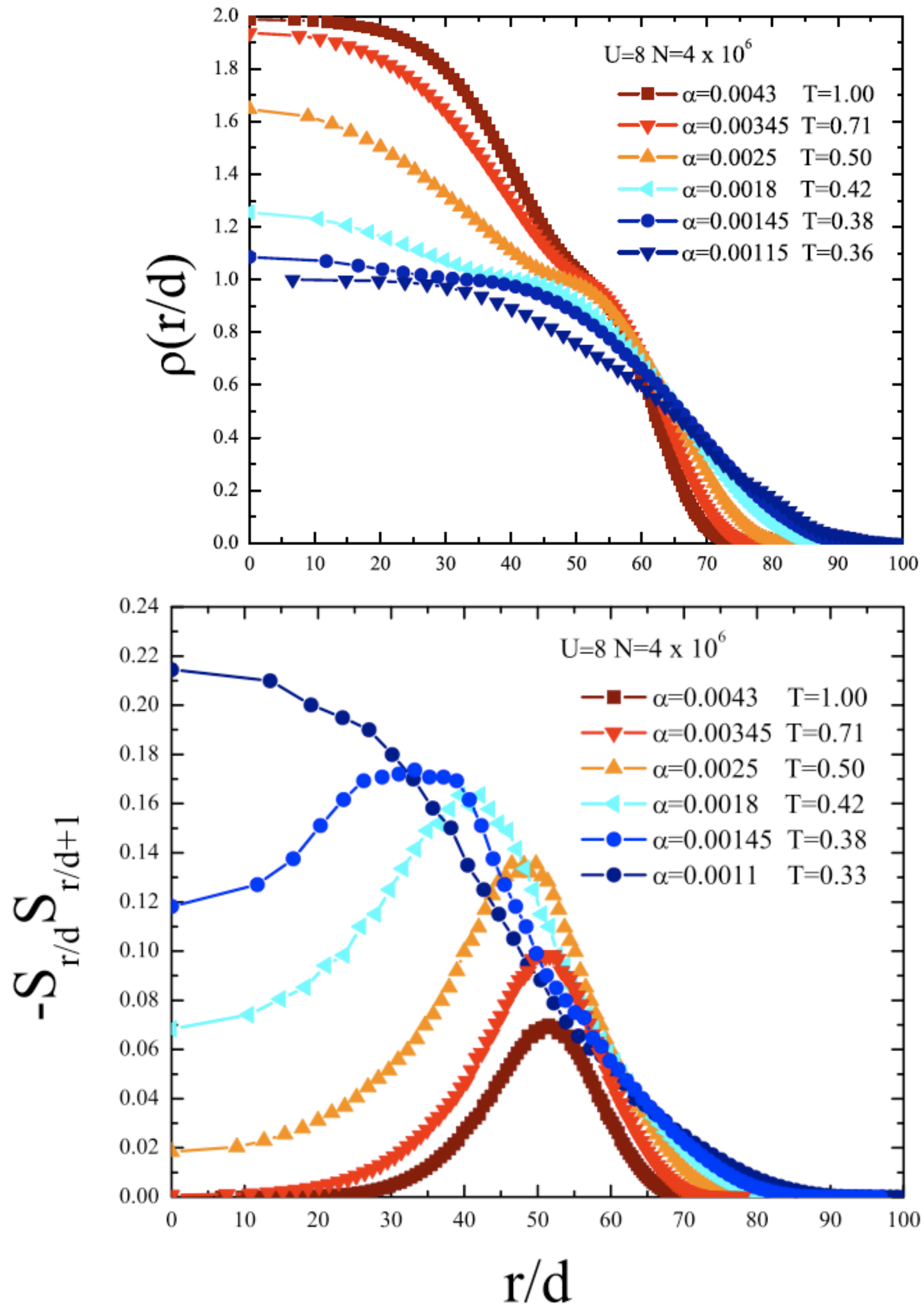


Even when the total entropy per site
is above the critical entropy to see
the AF phase in a homogeneous system,
in a trap the entropy in the center can drop
below $s_c \sim 0.3k_B$



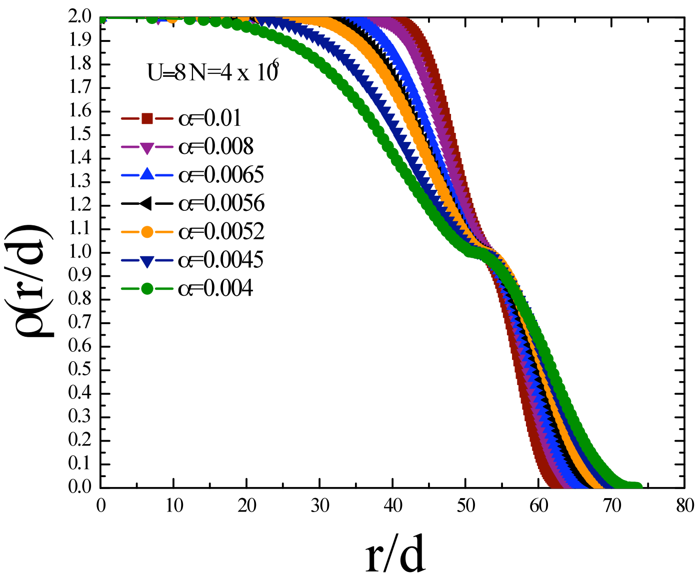
Nearest neighbor spin-spin correlation function

Grows as the trap opens up and tracks the Mott region

Lower entropy is not always a good thing!

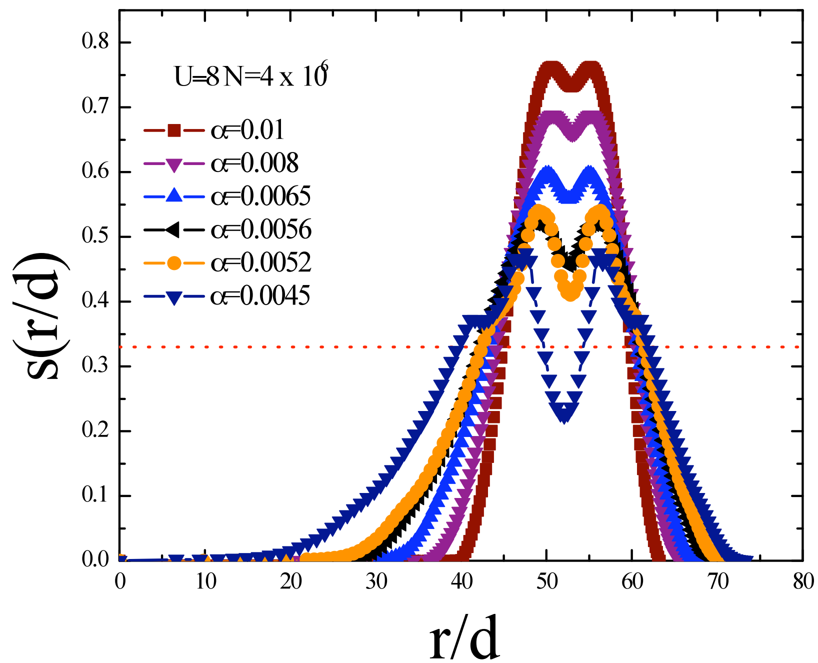
$U=8$ $N=4x10^6$
$S/Nk_B=0.3$

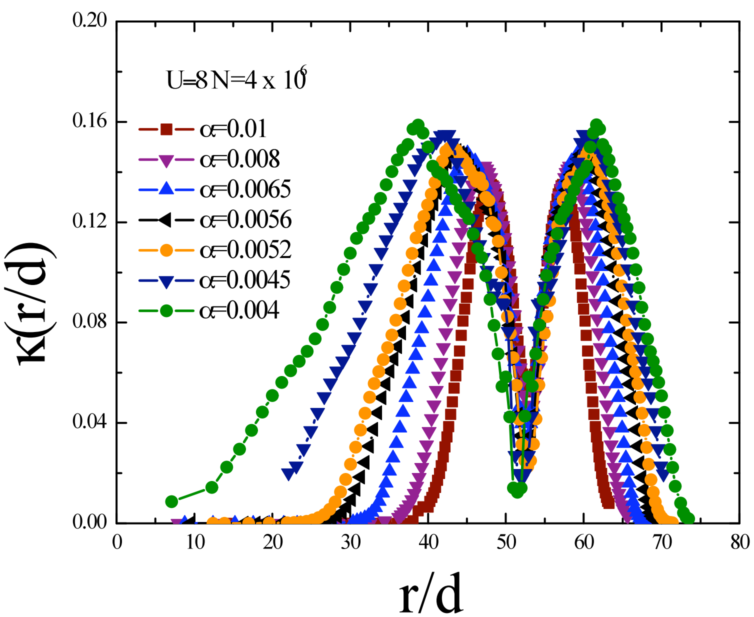
Lower entropy is not always a good thing!



U=8 N=4x10^6

S/Nk$_B$=0.3





If S is very low the system generates a large BI region in center

MI away from center which may be harder to find

Many other ideas for cooling…

Using a bosonic sympathetic species

[T.L. Ho and Q. Zhou, PNAS, 106, 6916 (2009)]

Using dimpled potentials [Ho & Zhou, arXiv:0911.5506]

Our proposal of "decompression cooling" here is really simple

To just judiciously utilize the trap to redistribute entropy

And most importantly the numbers work out

OUTLINE Part II: Modulated Superfluid Phases

Unequal fermion populations with attractive interactions:

Does the FFLO phase
(Superfluid phase with modulating order parameter) exist?
What are the observable signatures of such a phase?

Collaborators: Part II

- 3D Attractive Hubbard model with $N_\uparrow \neq N_\downarrow$ (BdG)

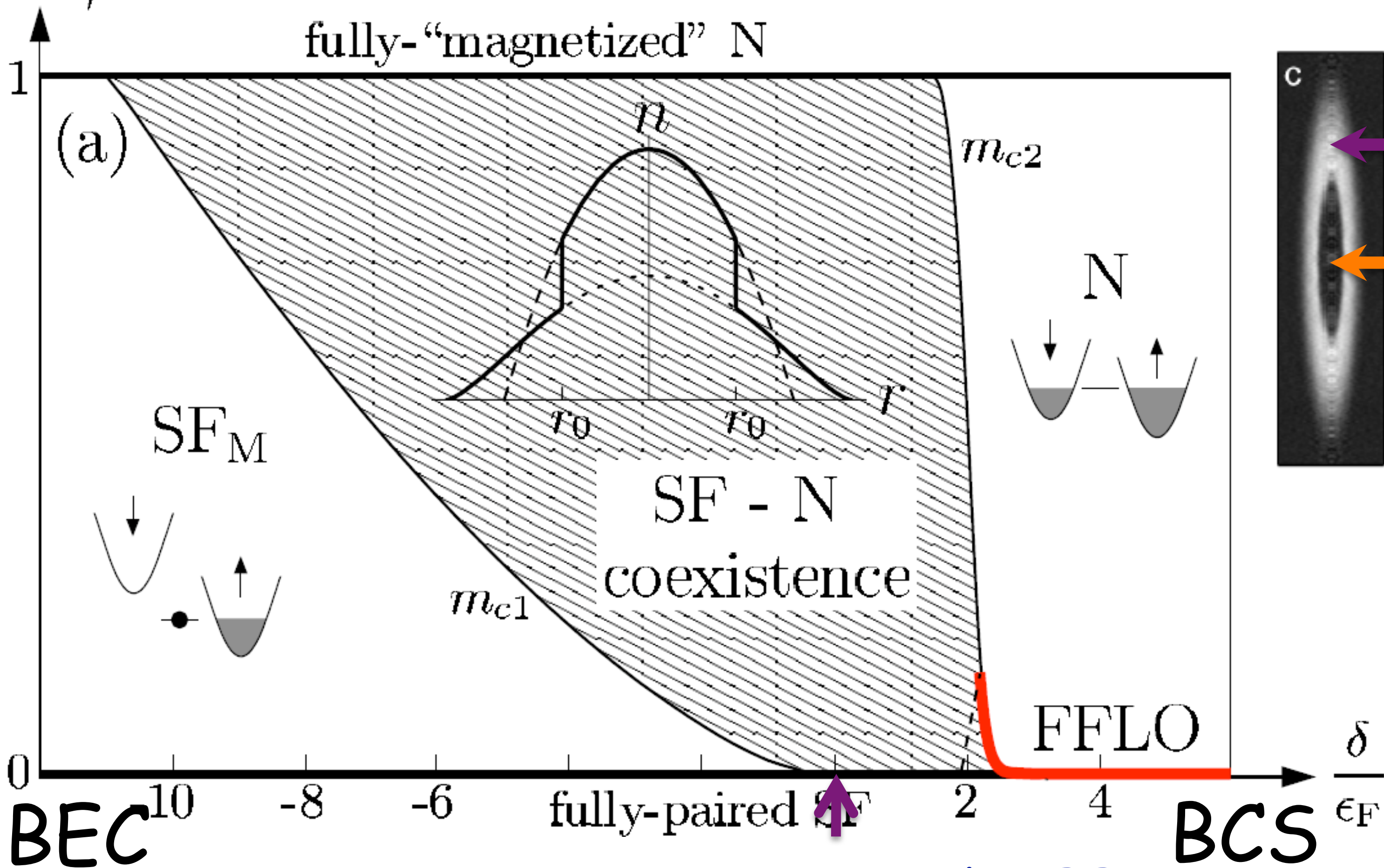
  Y. –L. Loh and NT PRL 104, 165302 (2010);

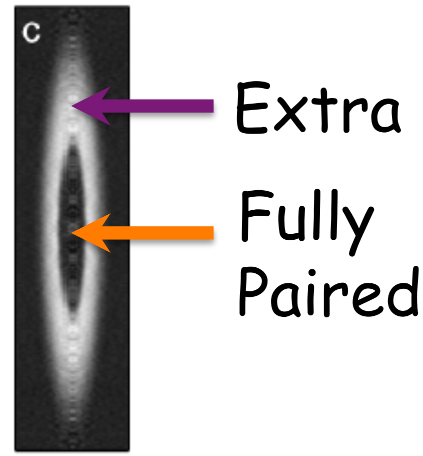
- 1D Spectral functions: Role of fluctuations (QMC)

  K. Bouadim, Y.-L Loh, R. Rousseau, NT (unpublished)

Tiny FFLO sliver in continuun

P= m/n





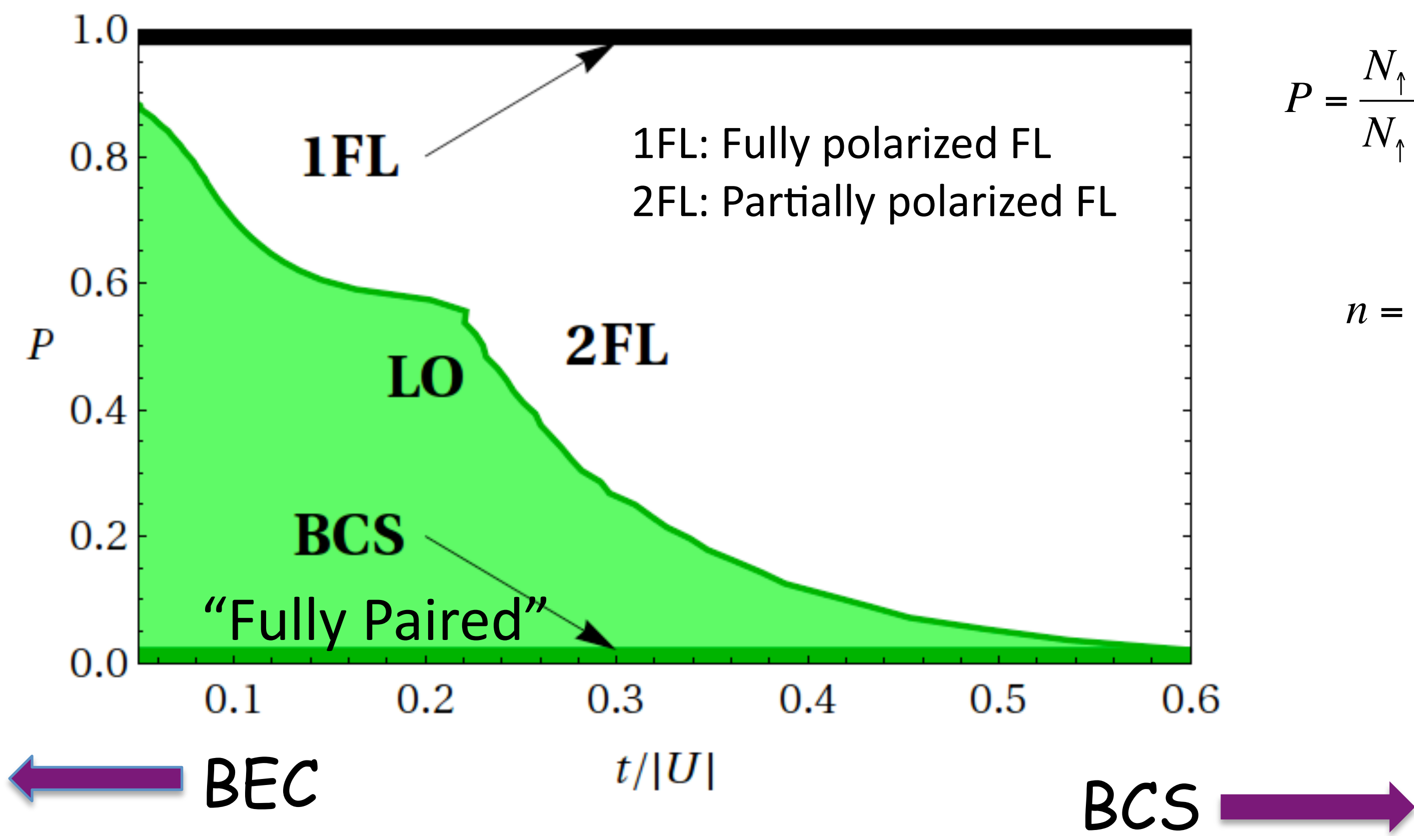
$1/k_F a$

At unitarity the FFLO phase disappears

Sheehy and Radzihovsky, PRL 96, 060401 (2006).

Large region of LO in a lattice

Phase separated region replaced by LO
Interactions further enhance the LO region

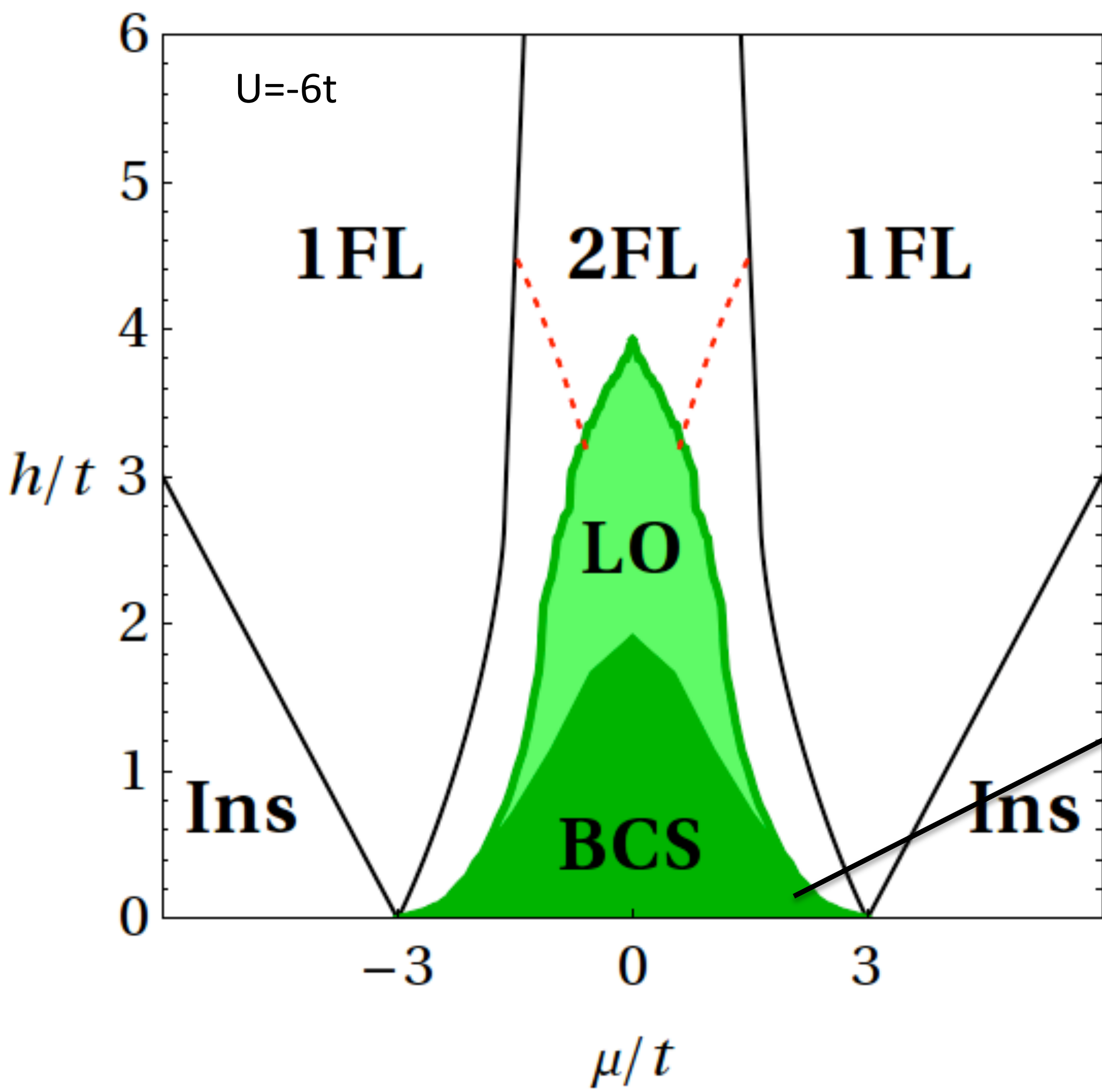


$$P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} = \frac{m}{n}$$

$$n = \frac{N_\uparrow + N_\downarrow}{N_{sites}}$$

3D Attractive Hubbard phase diagram for imbalanced gases

BdG-HF calculations in 3D



LO enhanced due to nesting in lattice and Hartree corrections

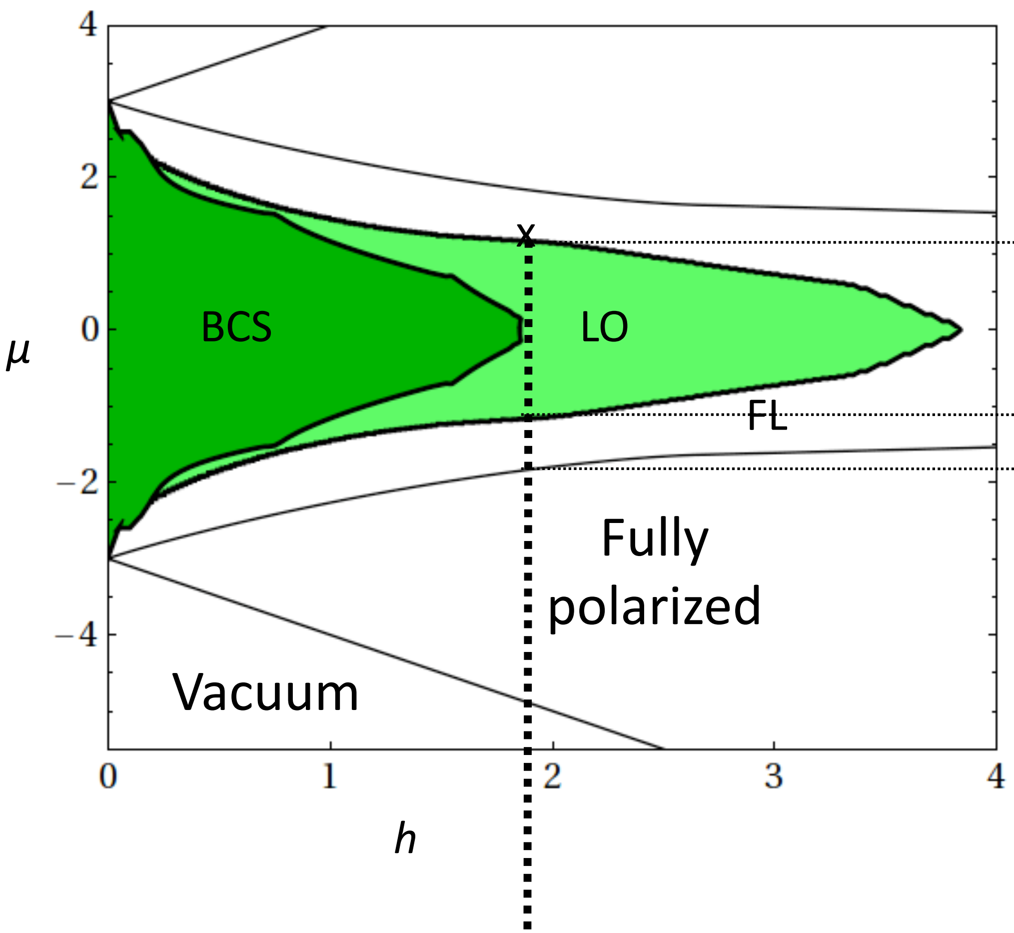
→ Size of LO region comparable to BCS!!

"continuum" results

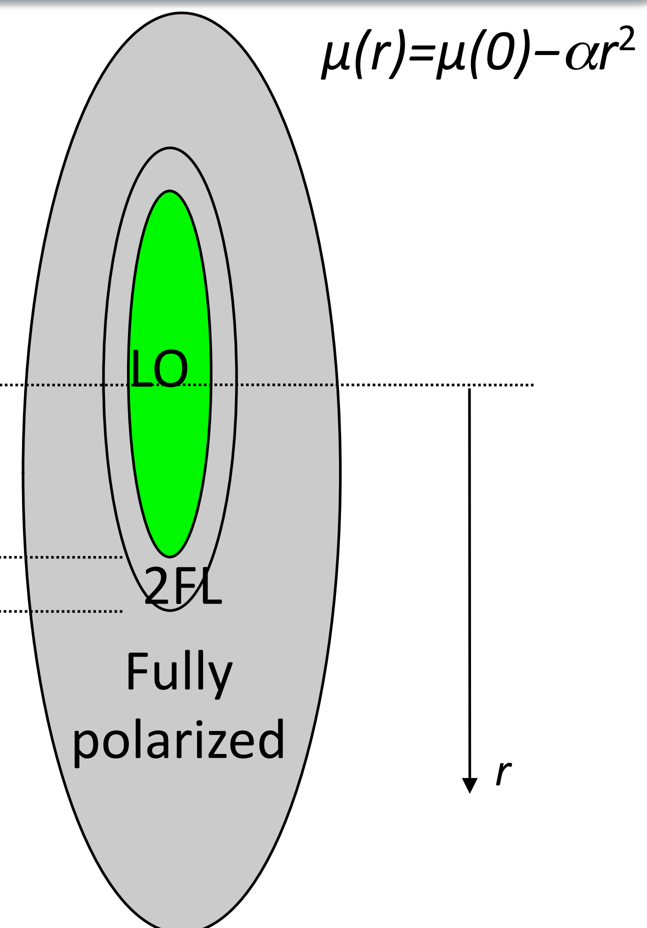
Also:Koponen-Paananen-Martikainen-Törmä PRL 99, 120403, 2007 studied Δ ~ exp iq·r

We find that Δ ~ cos q·r (or more complicated patterns) have significantly lower energy

Large LO phase in trap center: cannot be missed in lattice!



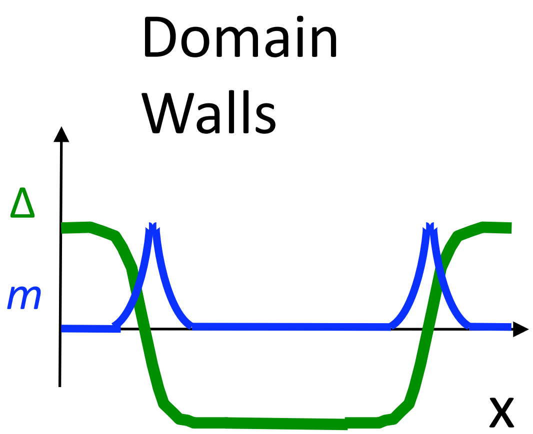
Constant-*h* slice

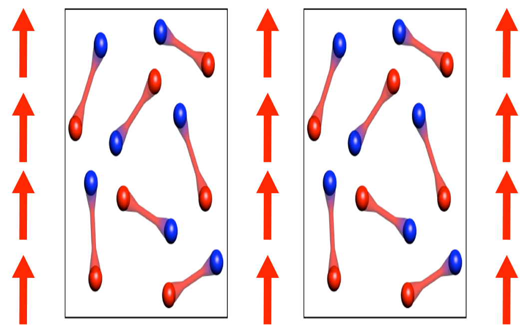


80% of atoms in
LO phase at trap center!
P=0.37 U=-6t

BdG + LDA with trap

LO phase and Domain Walls



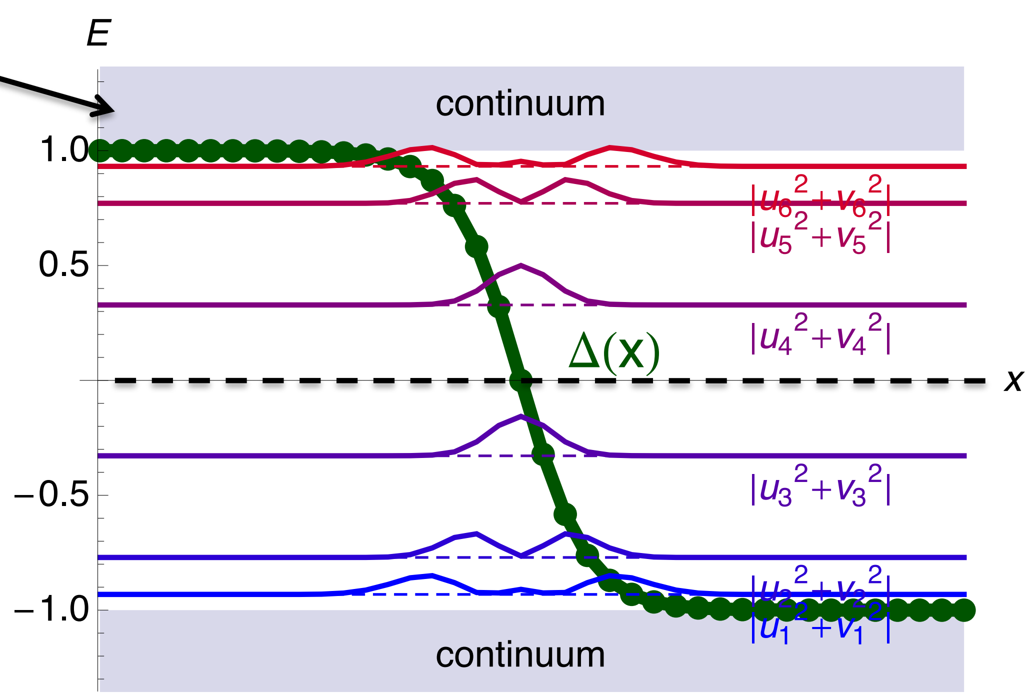


Microscale
Phase separation

Order parameter changes sign
Excess fermions piled up in the regions
where the order parameter crosses zero

Domain Walls and Andreev Bound States

pairing amplitude



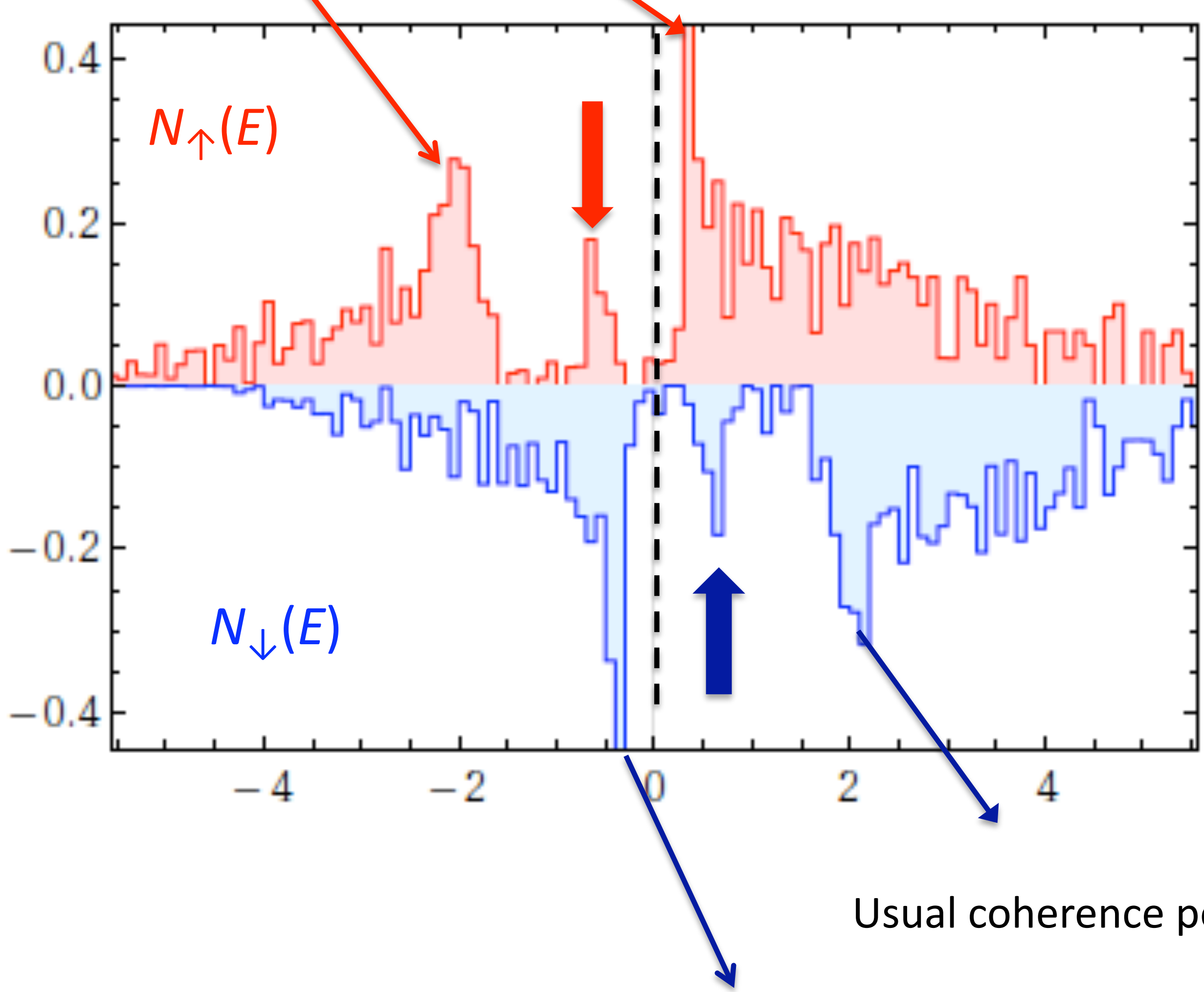
$$H = \begin{pmatrix} K & \Delta \\ \Delta^* & -K \end{pmatrix}$$

Bound state energies within gap

Bound state wavefunctions localized in vicinity of domain wall

Spectroscopic Signatures of Andreev Bound States

Usual coherence peaks in a superfluid



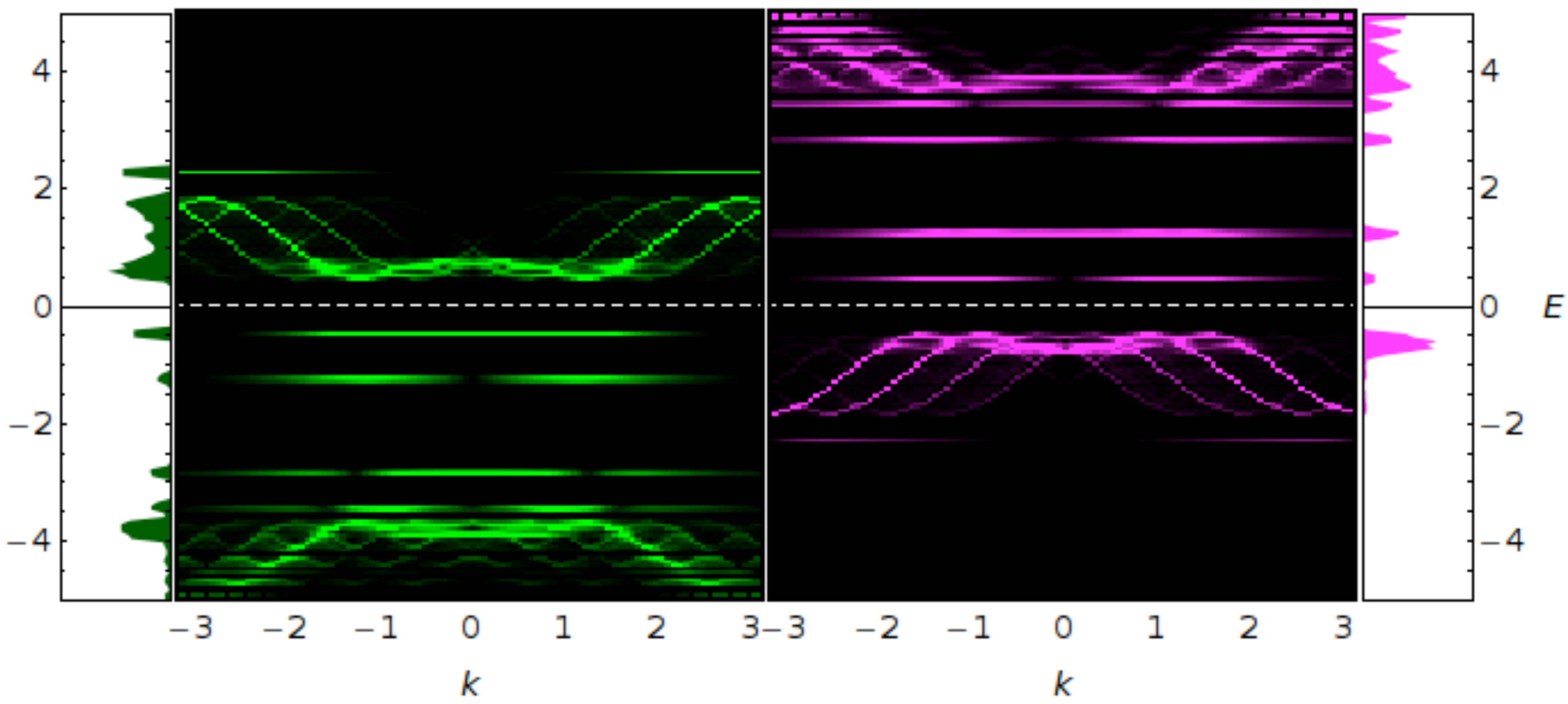
Andreev bound states (ABS) within gap

Increase gap using U to better separate ABS

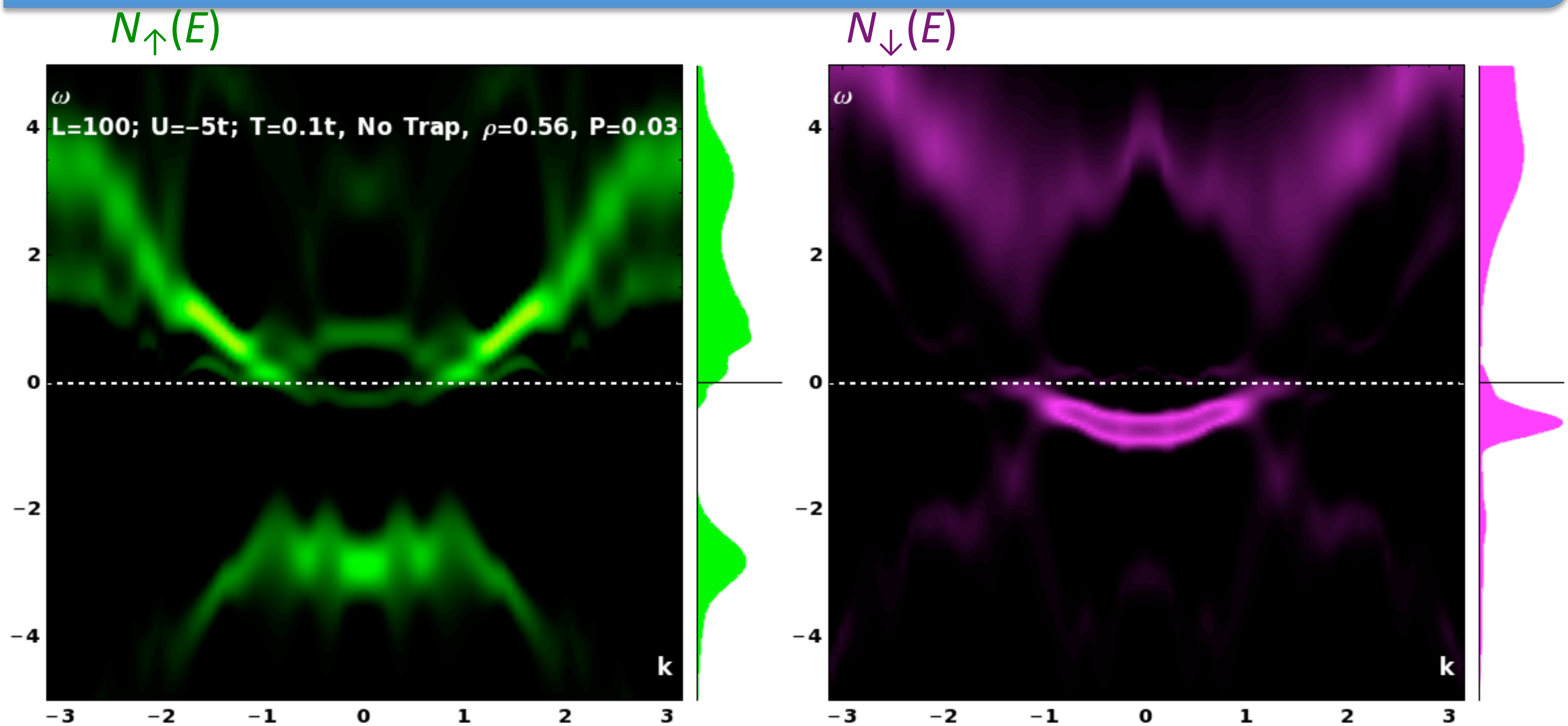
Usual coherence peaks in a superfluid

Spectroscopic Signatures of Andreev Bound States

Density of states for 1D LO: BdG



LO Density of States in 1D lattice (QMC)



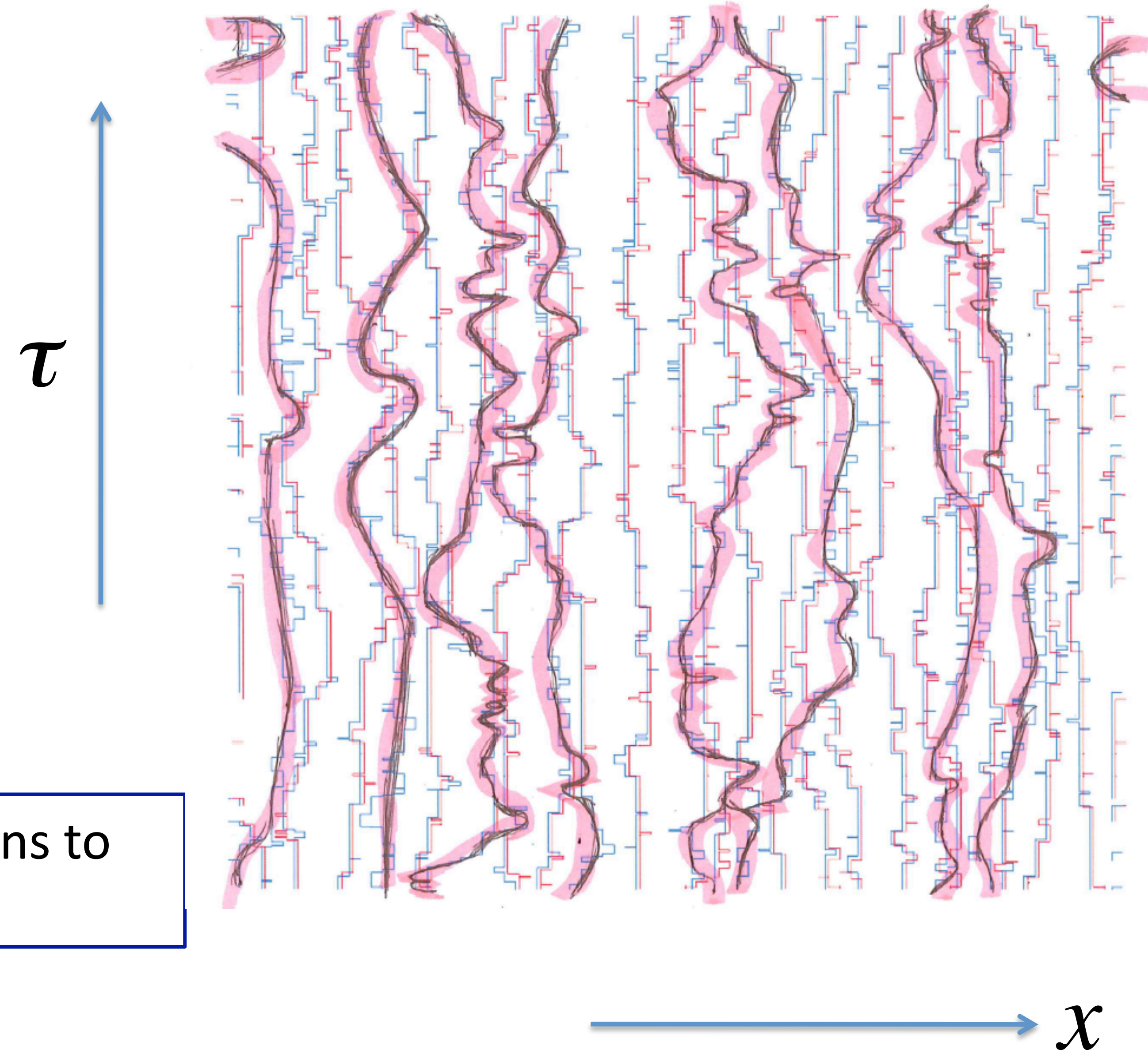
Determinantal QMC + Maximum Entropy methods for analytic continuation

Note: compared to BdG the Andreev “bound” states are not so well defined and merge with continuum

See also DMRG: Feiguin and Huse PRB 79, 100507 (2009)

Fluctuating Domain Walls in 1D

L=80
U=-4t
$N_\uparrow$=24
$N_\downarrow$=16



Next: Coupled chains to stabilize LO state

CONCLUSIONS

I. Repulsively interacting fermions in optical lattices:

In a homogeneous system must go below $S/Nk_B \approx 0.3$
to see an AF phase

In a trap can start with high entropy e.g. $S/Nk_B \approx 0.7$
Decompress
Entropy redistributed over a larger region
Can achieve low temperatures to see AF /Mott

Decompressional Cooling

In fact starting with very low entropy may be detrimental!

II. Attractive fermions in optical lattices:

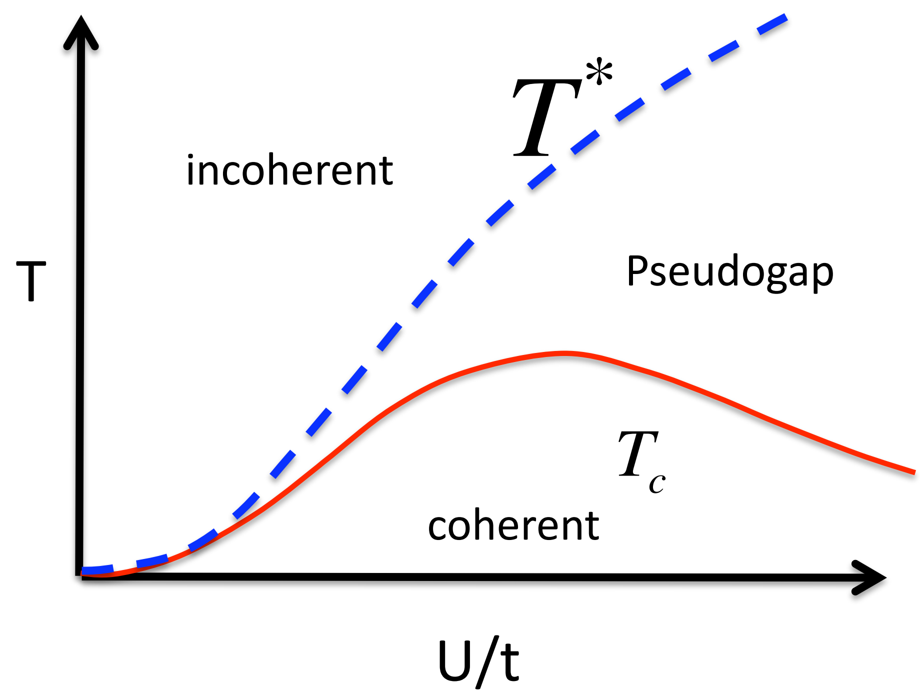
LO phase enhanced by lattice effects; low dimensions
Control fluctuations using coupling between ladders
Spectroscopic signatures within gap and
pair momentum enhancement at q_{LO}

Explore "Pseudogap" Region in All Hubbard models

We understand the phases…

Explore the intermediate temperature scale where the incoherent degrees of freedom organize themselves into a coherent phase

$$T_c < T < T^*$$



end