Phase diagrams of the attractive extended Bose-Hubbard model with three-body constraint

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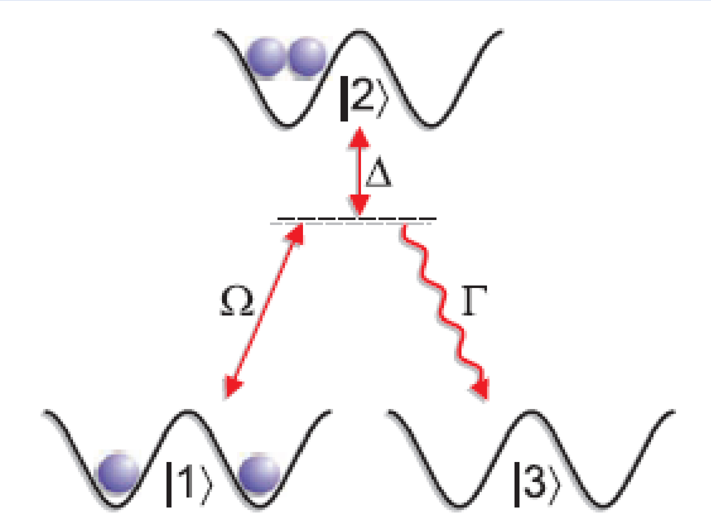
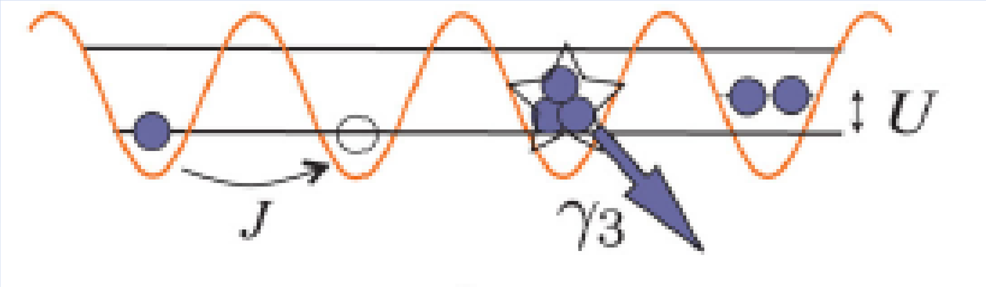
1. Syassen *et al.* (Science **320**, 1329 (2008)) showed that a strong two-body loss process (inelastic collision) for molecules in an optical lattice could produce an effective hard-core repulsion and thus a Tonks gas in 1D.
2. A large loss dynamically suppresses process creating two–body occupation on a particular site.



1. Daley *et al.* (PRL **102**, 040402 (2009)) proposed that the large three-body combination loss process (via triatomic Efimov resonance [Kraemer *et al.* Nature 440, 315 (2006)]) can leads to an effective three-body interactions – a three-body hard-core constraint.

2. This constraint stabilizes the attractive bosonic system (U<0) from collapse.

$$a_i^{+3} \equiv 0$$



If U>0, the ground states are either Mott insulator or atomic superfluid phases of Bose-Hubbard model.

The system is described by the attractive Bose-Hubbard Hamiltonian:

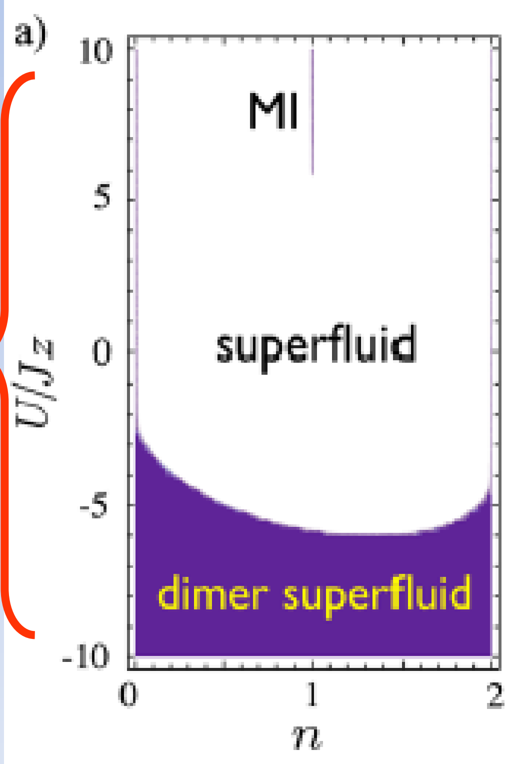
$$H = -t\sum_{\langle i,j\rangle} a_i^+ a_j + \frac{U}{2}\sum_i n_i(n_i - 1) - \mu\sum_i n_i$$

U<0

with the constraint $a_i^{3+} \equiv 0$

note that there is no hopping of dimers in *H*.

$$\langle a^2 \rangle \neq 0$$



atomic superfluid (ASF)

$$\langle a \rangle \neq 0$$

dimer superfluid DSF

$$\langle a \rangle = 0$$

Mean field result for one dimensional chain:

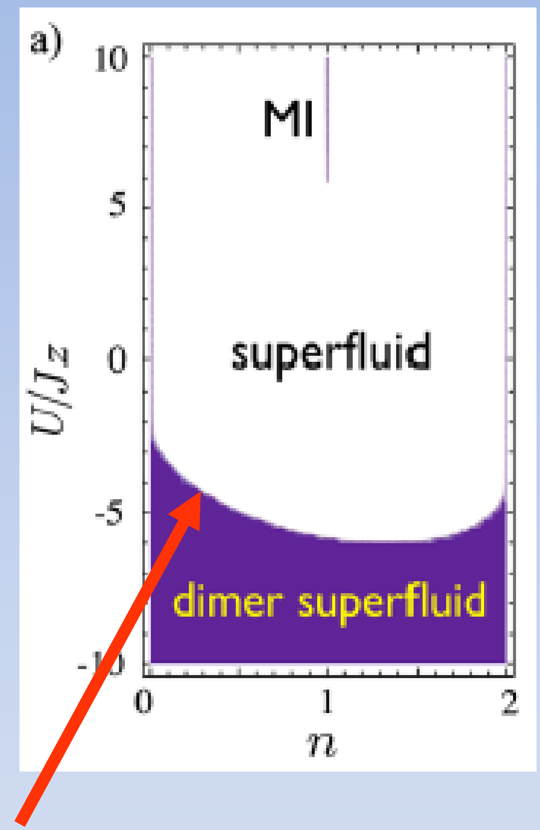
Daley *et al.* (PRL **102**, 040402 (2009))

1. The DSF order parameter transforms with the double phase ~ exp(2iθ) compared to the ASF order parameter ~ exp(iθ).

2. The symmetry θ-> θ+π exhibited by the DSF is broken when reaching the ASF phase.

3. A spontaneous breaking of a discrete Z_2 symmetry, reminiscent of an Ising transition

4. ASF and DSF can be expt. distinguished by measuring the momentum distribution, which has zero momentum peak for ASF state but not for DSF.



2nd order is expected

Daley *et al.* (PRL **102**, 040402 (2009))

- However this result is revised by the group Diehl *et al.* (PRL **04**, 165301 (2010)).
- One reason to question the MF result is the presence of two interacting soft modes (related to <a> and <a^2>) close to the phase transition.
- Quantum fluctuations can turn this transition into a 1st order one due to the Coleman-Weinberg mechanism.

$$S_{\mathrm{eff}}[\varphi,\pi] = \int_x \{\tfrac{1}{2}\varphi(-Z_\varphi\partial_\tau^2 - \xi_+^2\Delta + m_+^2)\varphi + \lambda\varphi^4 + \tfrac{1}{2}\pi(-Z\partial_\tau^2 - \xi^2\Delta)\pi + i\kappa\varphi^2\partial_\tau\pi\}.$$

Fluctuation induced 1^{st} order

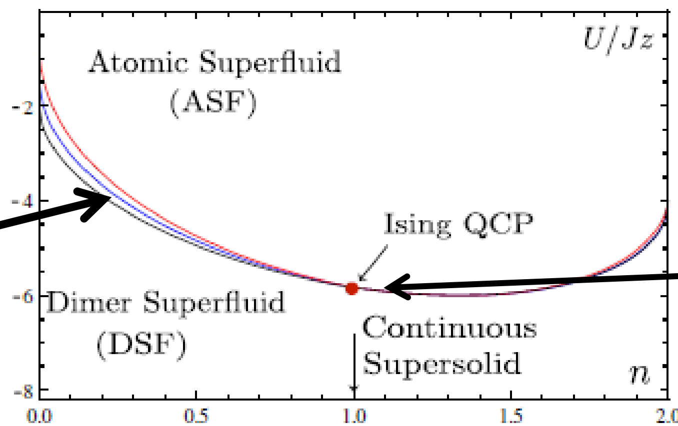


FIG. 1 (color online). Phase diagram for the Bose-Hubbard model with a three-body hard-core constraint, and $U < 0$. The black curve represents the mean field phase border, while red (light gray) and blue (dark gray) curves include shifts due to quantum fluctuations in $d = 2, 3$.

At n=1, coupling vanished; it is 2^{nd} order transition of Ising type

Our model:

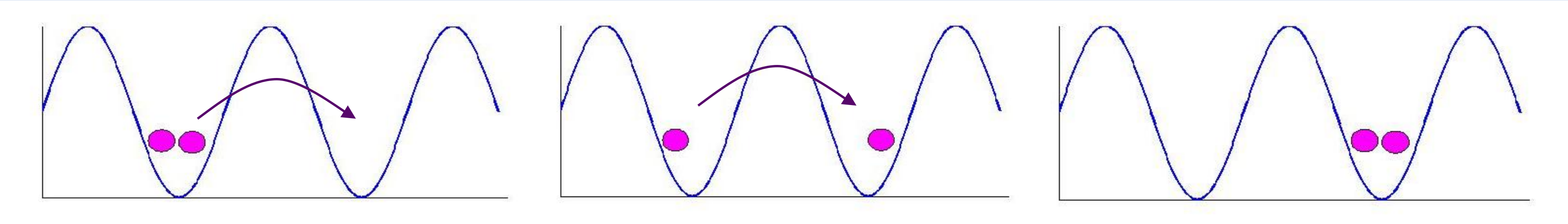
In order to enlarge the DSF regime, we add a nn repulsive term V in the Hamiltonian:

$$H = -t\sum_{\langle i,j\rangle} a_i^+ a_j + \frac{U}{2}\sum_i n_i(n_i - 1) + V\sum_{\langle i,j\rangle} n_i n_j - \mu\sum_i n_i$$

U<0 but V>0 (V can arise from dipole-dipole interactions)

For illustration, μ=-0.55, |U|=1, and V=0.25

- Again, there is no hopping of dimers in *H*.
- the hopping of dimers is a second order effect.
- DSF occurs only in low T < t^2



We try to study numerically the DSF phase using SSE (stochastic series expansion) method.

Order parameters:

Superfluidity (spin stiffness) ρ is related to the winding number (W) fluctuations in the simulation.

$$\rho_{even(odd)} = mT\left\langle W^2_{even(odd)} \right\rangle$$

$$m \equiv 1/2t$$

m is the effective mass in square lattice

1. To identify the ASF and DSF, we measure the odd and even winding number separately.
2. In the ASF phase, both ρ_{odd} and ρ_{even} are finite.
3. While the DSF phase, ρ_{even} is finite but $\rho_{\text{odd}}=0$ (two bosons move together) .

Basic idea of Stochastic Series Expansion (SSE)

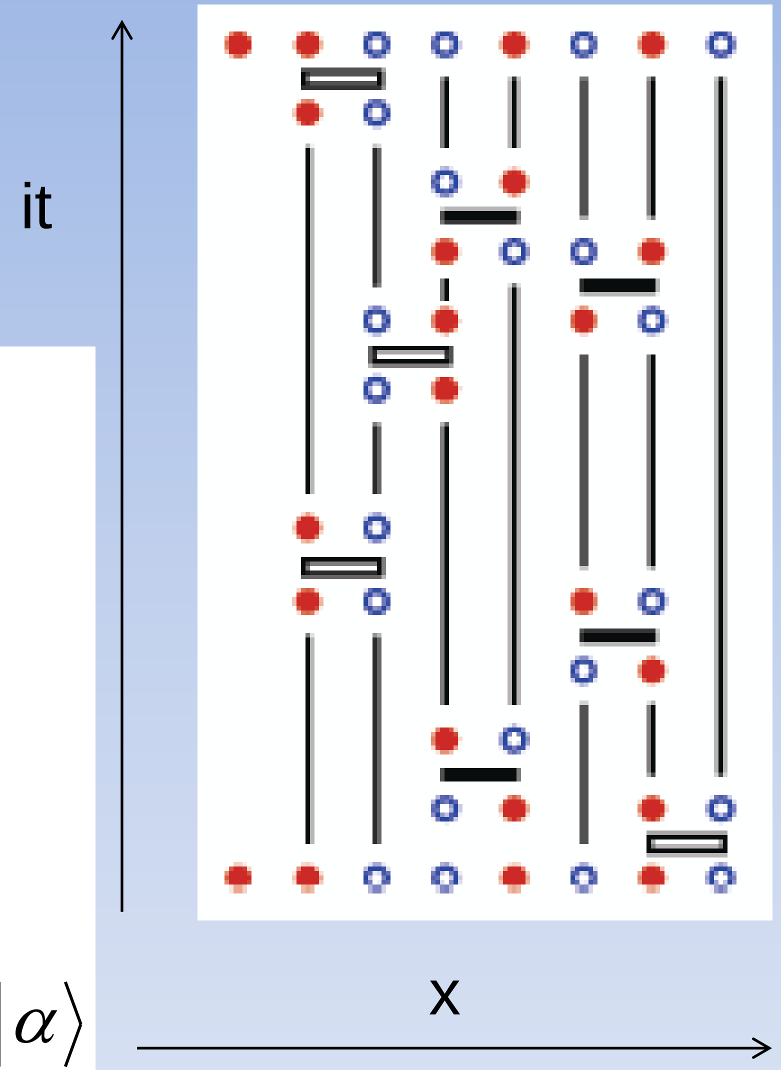
Thermal expectation value

$$\langle A \rangle = \frac{1}{Z} Tr\left[A e^{-\beta H} \right], \quad Z = Tr\{ e^{-\beta H} \}$$

$$Z = \sum_{\alpha} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle \alpha | (-H)^n | \alpha \rangle$$

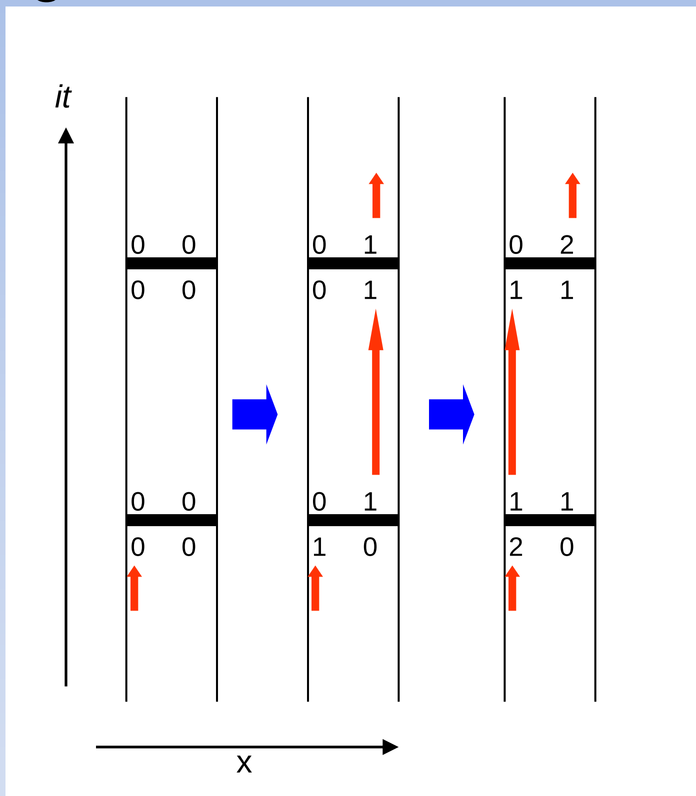
$$H = -\sum_{a,b} H_{a,b}$$

$$Z = \sum_{\alpha} \sum_{\{H_{ab}\}} \frac{\beta^n (M-N)!}{M!} \langle \alpha | \prod_{i=1}^{M} H_{a(i),b(i)} | \alpha \rangle$$



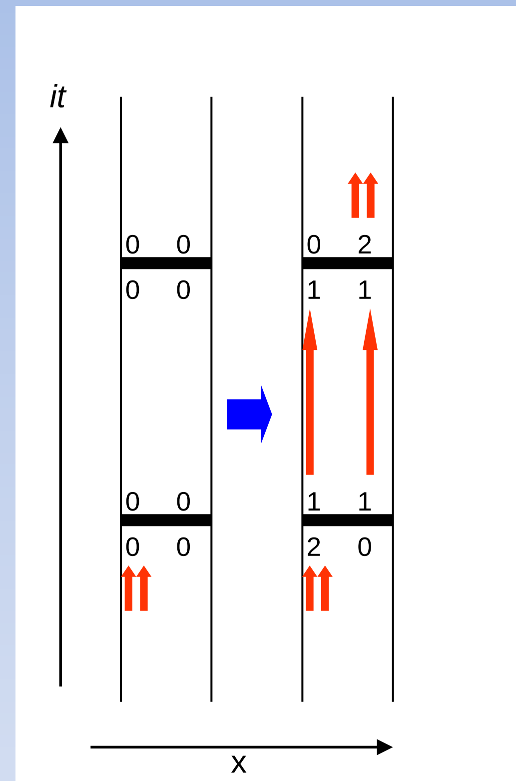
Examples of dimer hopping

Conventional one loop algorithm



This two steps hopping is very ineffective, especially in large lattice size.

Two loops algorithm

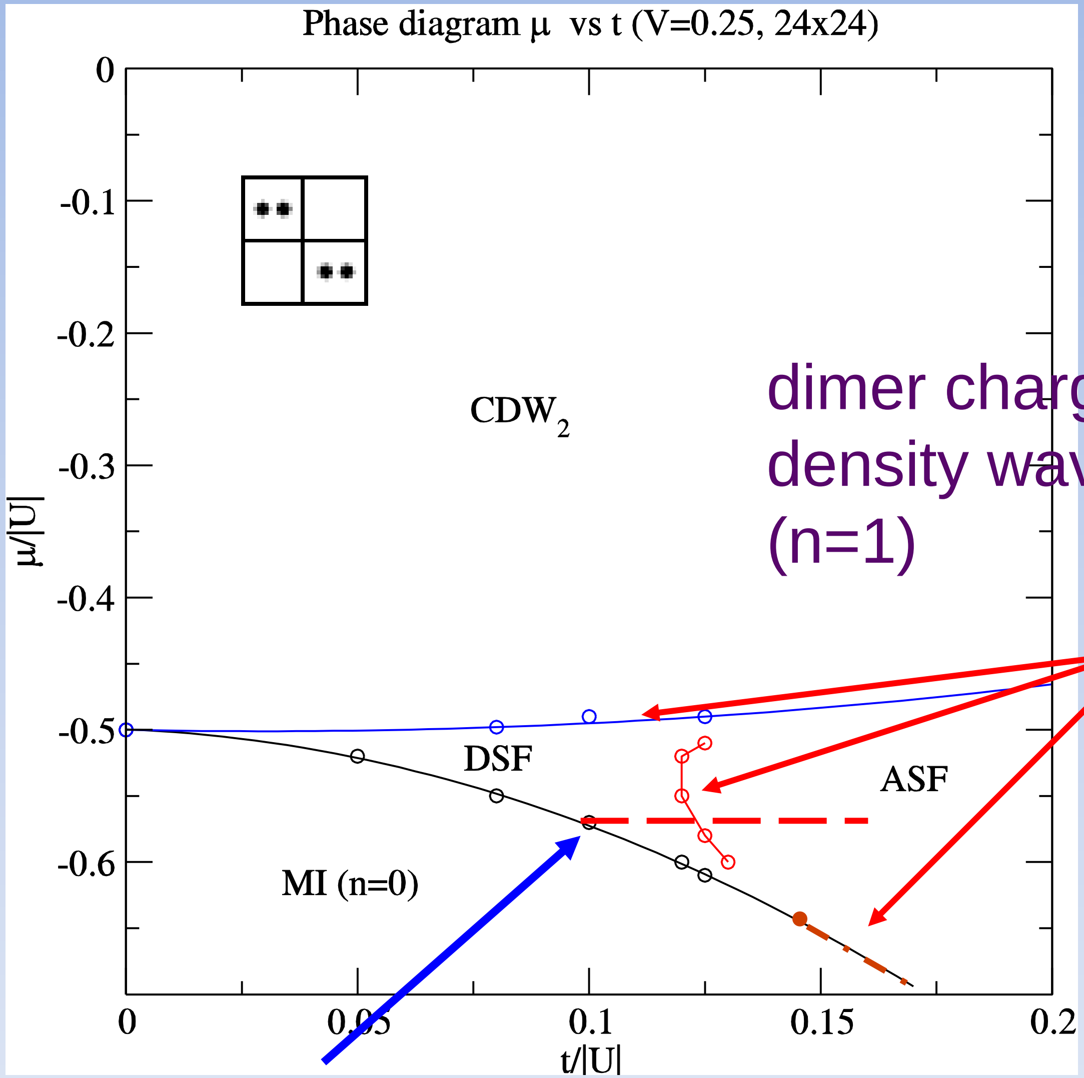


The dimer hopping always lead to even winding number.

Ground state phase diagrams:

T/|U|=0.001

n <= 1



dimer charge density wave (n=1)

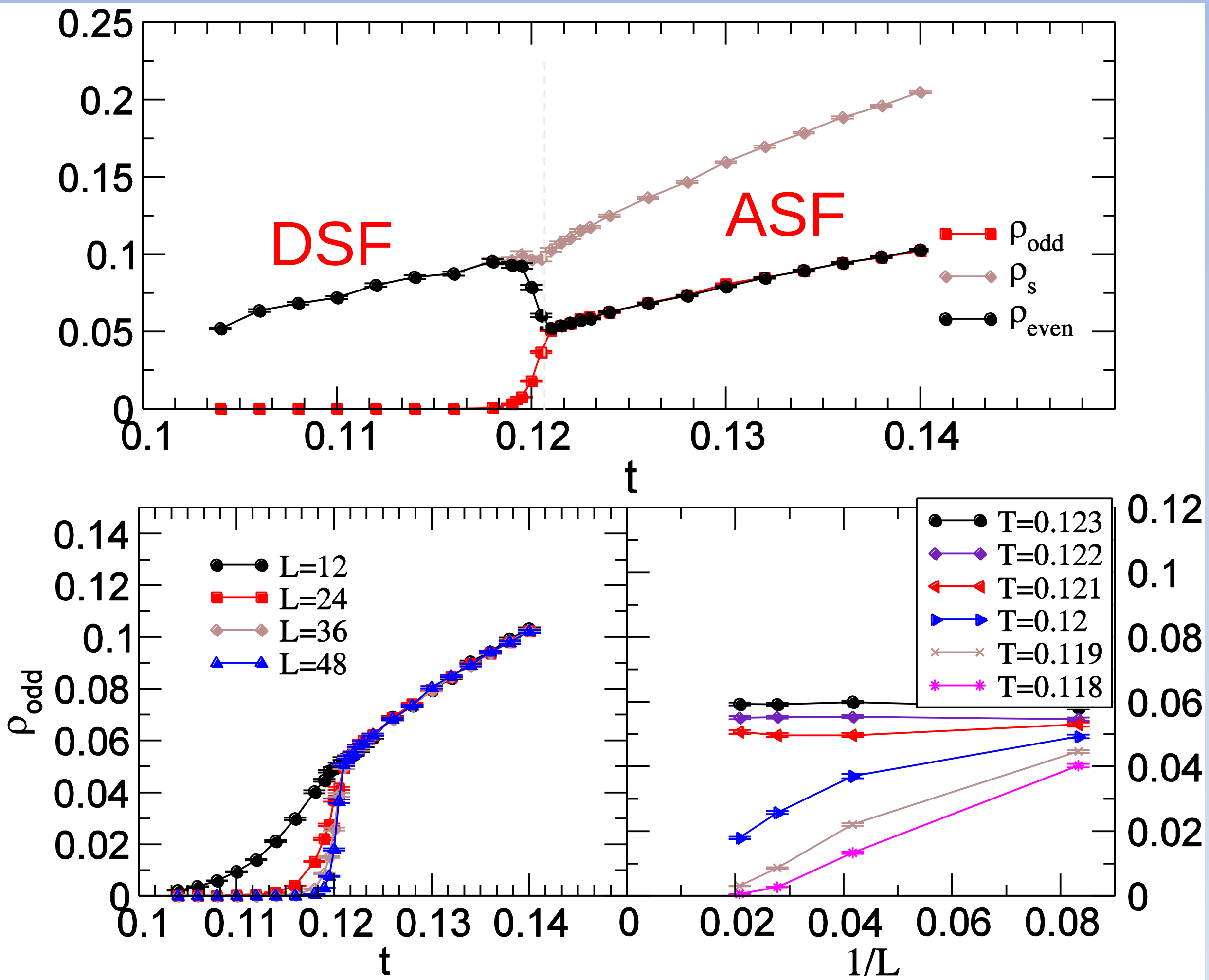
1st order

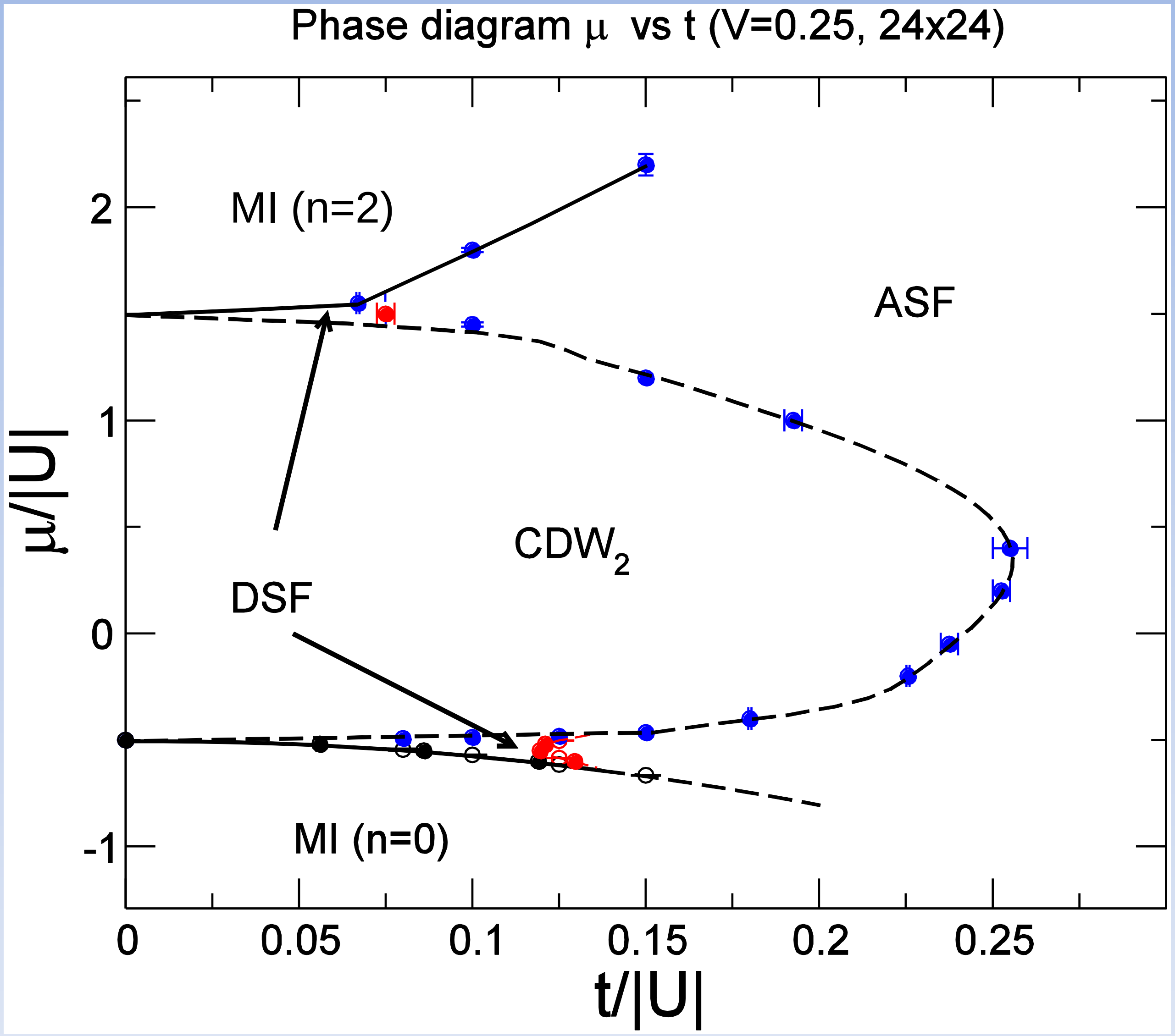
2nd order

DSF-ASF 1st order transition

(48x48 at T=0.005)

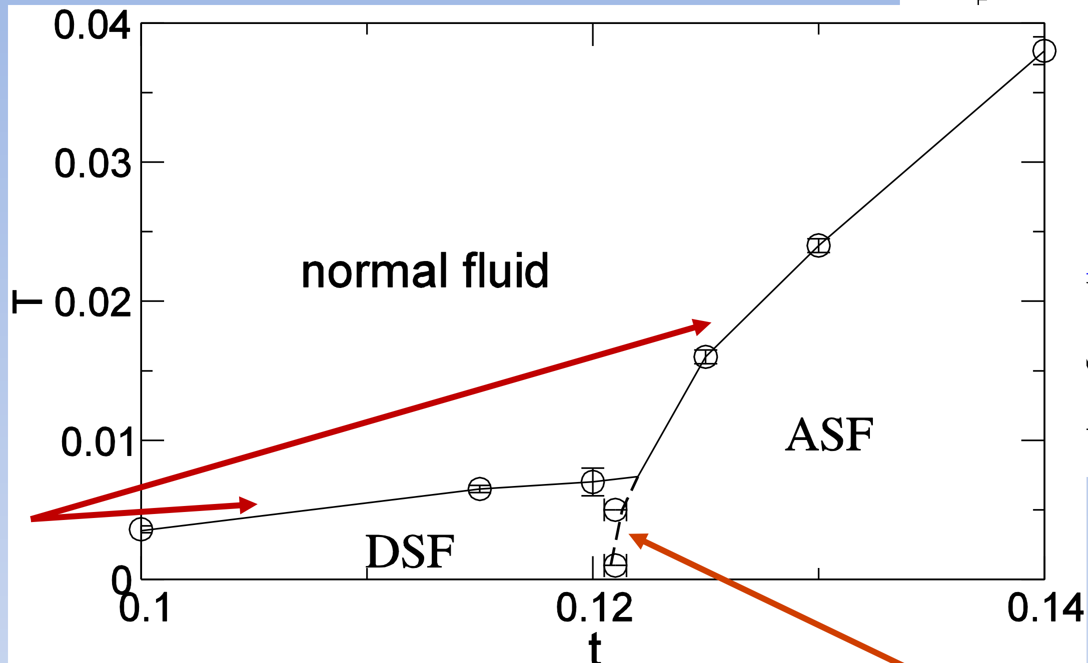
Finite size analysis

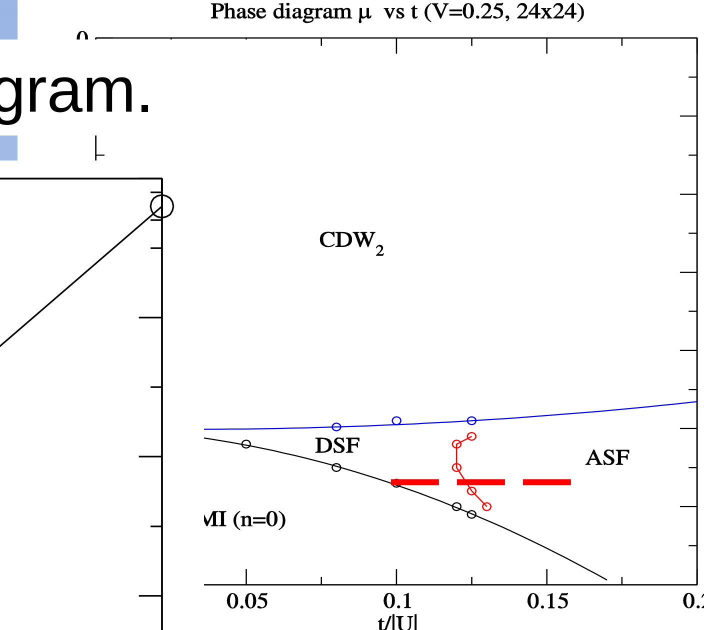




Phase diagram μ vs t (V=0.25, 24x24)
MI (n=2)
ASF
CDW2
DSF
MI (n=0)
2
1
0
-1
0
0.05
0.1
0.15
0.2
0.25
μ/|U|
t/|U|

Finite temperature phase diagram.





KT type

1st order

- Both of continuous KT (Kosterlitz-Thouless) type, but with distinct characters.
- universal stiffness jump of DSF is 4 times larger than that of ASF
- DSF-N transition is driven by the unbinding of half-vortices.

- the underlying Coleman-Weinberg mechanism is not spoiled by the thermal fluctuations.

The universal jump is given by:

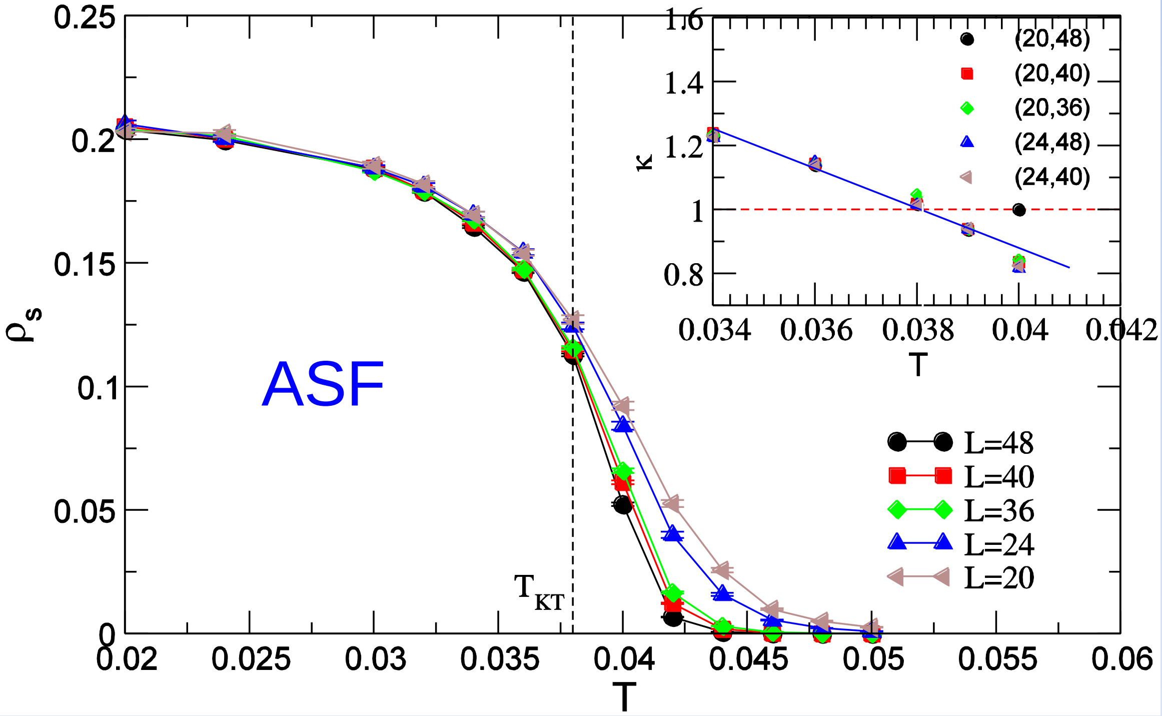
$$\rho_s = \frac{2mT_{KT}}{\pi v^2}$$

The vorticity v=±1 for conventional KT transition.

KT renormalization group integral equantion:

$$4\ln(L_2/L_1) = \int_{R_2}^{R_1} \frac{dt}{t^2(\ln(t)-\kappa)+t}$$

$$R(L) \equiv \pi v^2 \rho_s(L)/2mT$$



1. data of pairs of sizes collapse into a straight line.
2. T_{KT} is given at κ=1.

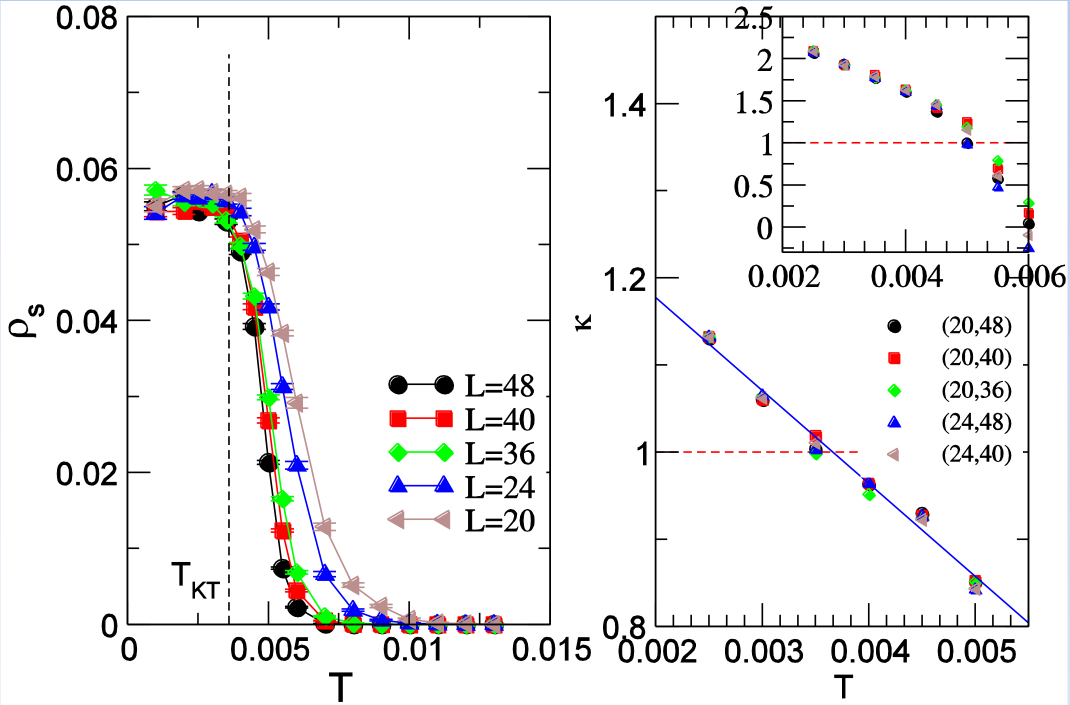
Weber and Minnhagen (1988)

Boninsegni and Prokofev (2005)

t=0.14

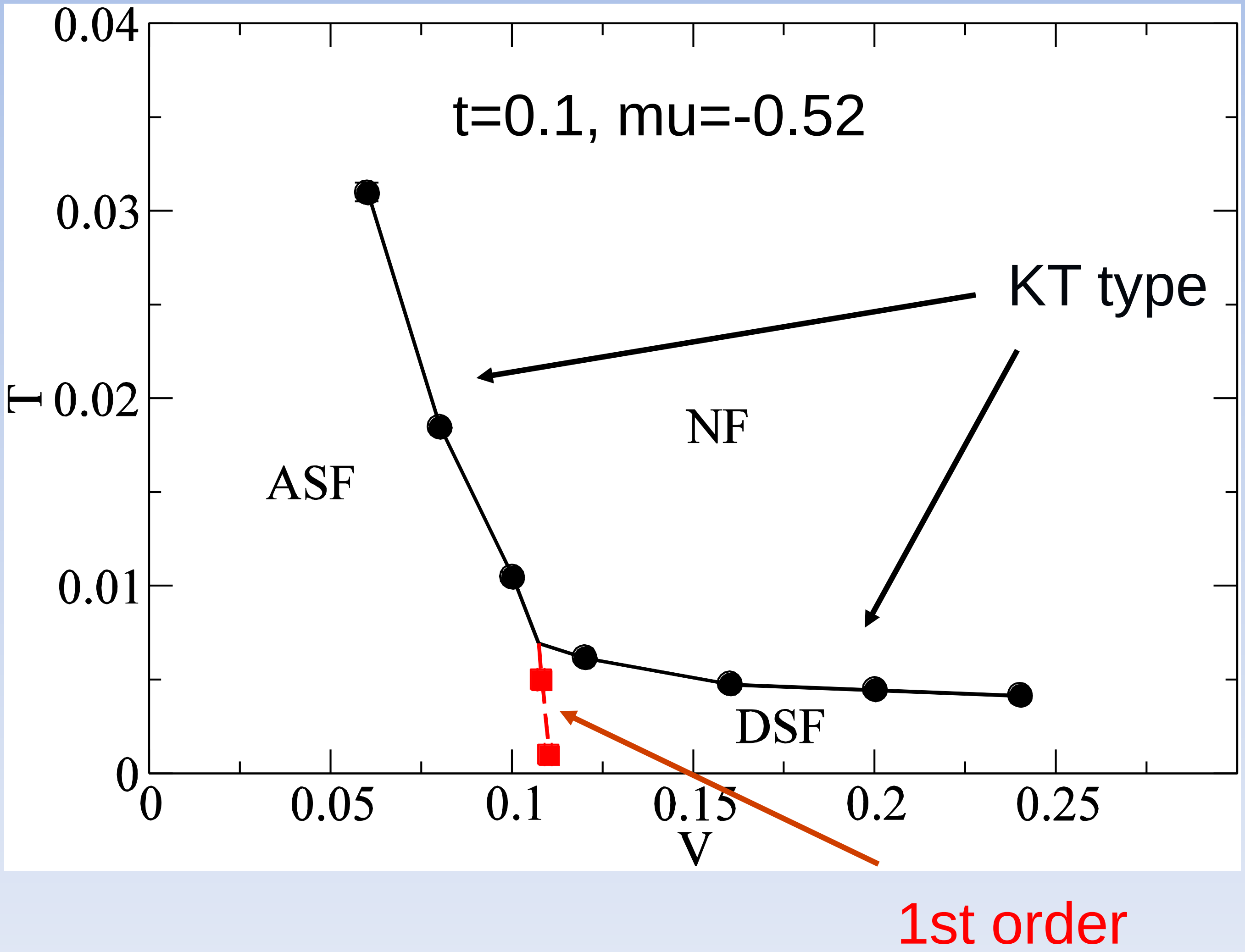
1. For the DSF, it preserves the π phase-rotation symmetry as exp(2iθ)
2. the vorticity v is ±1/2 instead of ±1.
3. the unversial jump is then $\rho_s = \frac{8mT_{KT}}{\pi}$

4 times larger than conventional case



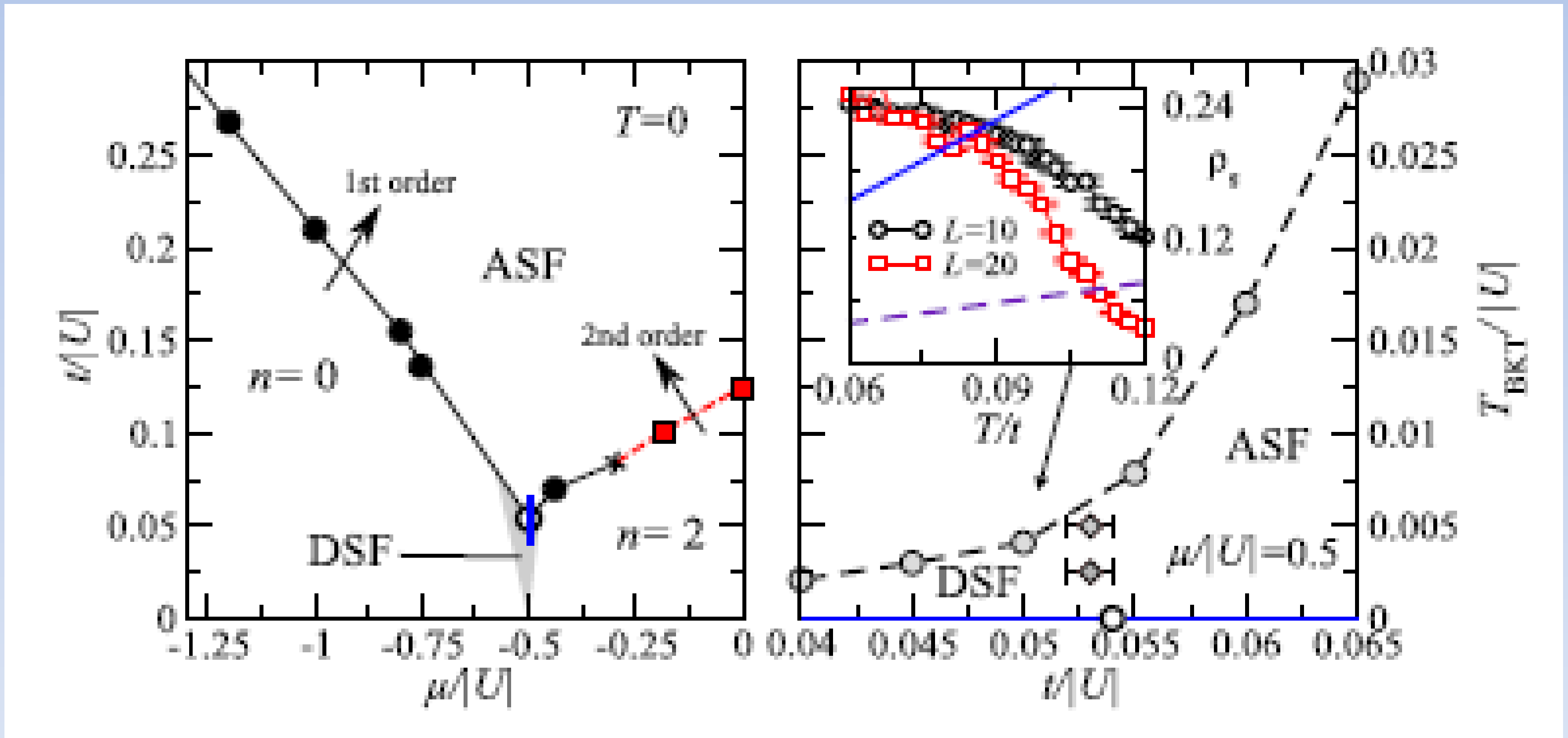
t=0.1

• The nn repulsive interaction enhances the formation of DSF



Similar works:

L. Bonnes and S. Wessel, PRL **106**, 185302 (2011).
arXiv: 1101.5991



Histograms of condensate density show a power-law decay s.t. variance does not exist, central limit theorem for the mean value doesn’t hold

- To overcome this, a dimer hopping t’ term is added,
- but one has to extrapolate to t’=0.
- it is inefficient.

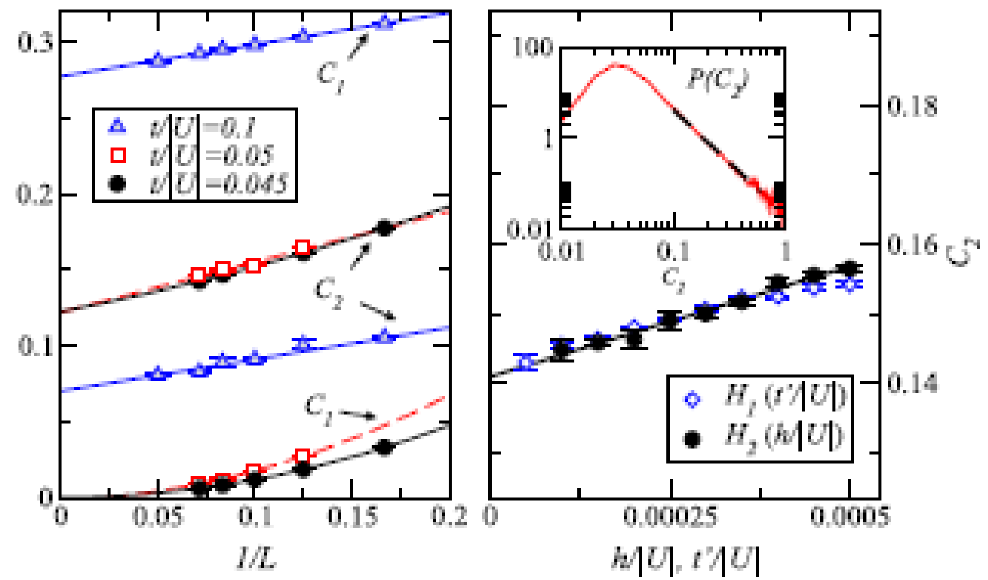


FIG. 2 (color online). Left-hand panel: Finite-size scaling of C_1 and C_2 for different values of $t/|U|$ from simulations at $T/|U| = 0.01/L$. Right-hand panel: Extracting C_2 from simulations of H_1 and H_2. Inset: Histogram $P(C_2)$ from simulations of H, with a power-law fit $P(C_2) \propto (C_2)^\alpha$, $\alpha = -2.2$ (dashed line) to the fat tail at $t/|U| = 0.045$, $\mu/|U| = -0.5$, $L = 14$, and $T/|U| = 0.002$.

Summary:

1. Using the two-loops algorithm, the finite temperature phase diagram for DSF and ASF phases is studied.

2. DSF-ASF transitions are fluctuation induced 1st order as predicted by Diehl *et al.*, and preserved at finite temperature.

3. KT transitions observed for ASF-N and DSF-N transitions, but with distinct characteristics: DSF-N is driven by unbinding of half-vortices.

4. The anomalous KT transition can be served as a signature for the DSF in real experiments.