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Workshop on Supersolid 2008

18 - 22 August 2008

Supersolids bosons on frustrated lattices

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Supersolid Bosons on Frustrated Lattices

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Institute for Theoretical Physics

Stuttgart University

Overview

- Ultracold atoms on optical lattices

- Triangular lattice
- Supersolid

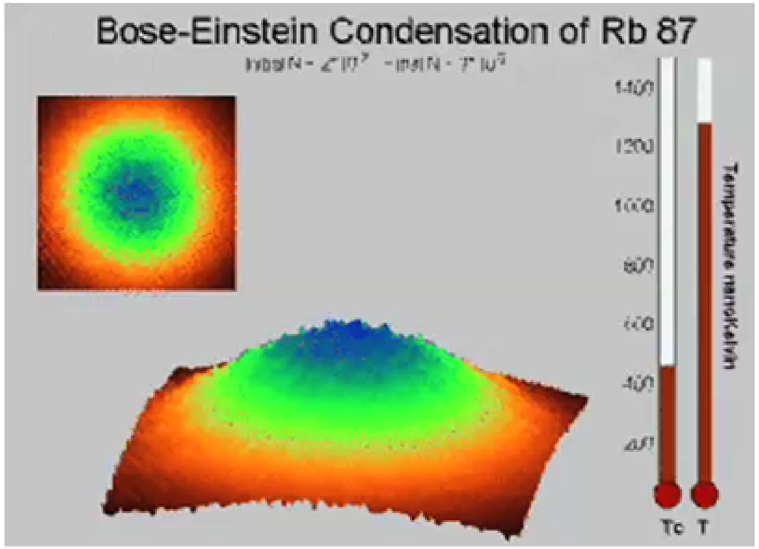
- Kagome lattice
- No supersolid - a valence bond solid

- Polar molecules on optical lattices
- New route to supersolids

- Summary

Ultracold Atoms on Optical Lattices

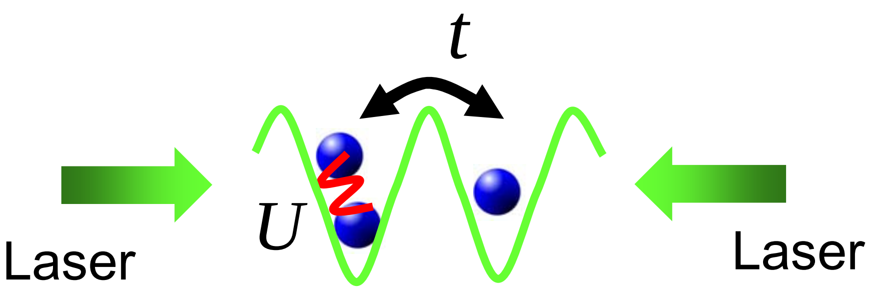
movie



Optical lattice

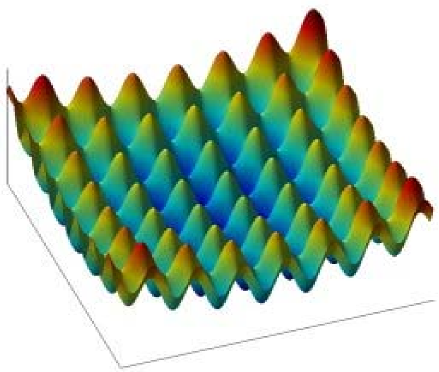
→ Dense quantum gas

→ Increased correlations



- Effective Boson Hubbard model

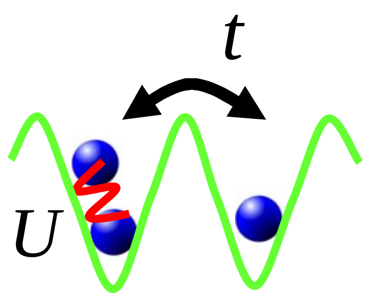
$$H = -t\sum_{\langle i,j\rangle}\left(b_i^\dagger b_j + h.c.\right) + \frac{U}{2}\sum_i n_i(n_i - 1)$$



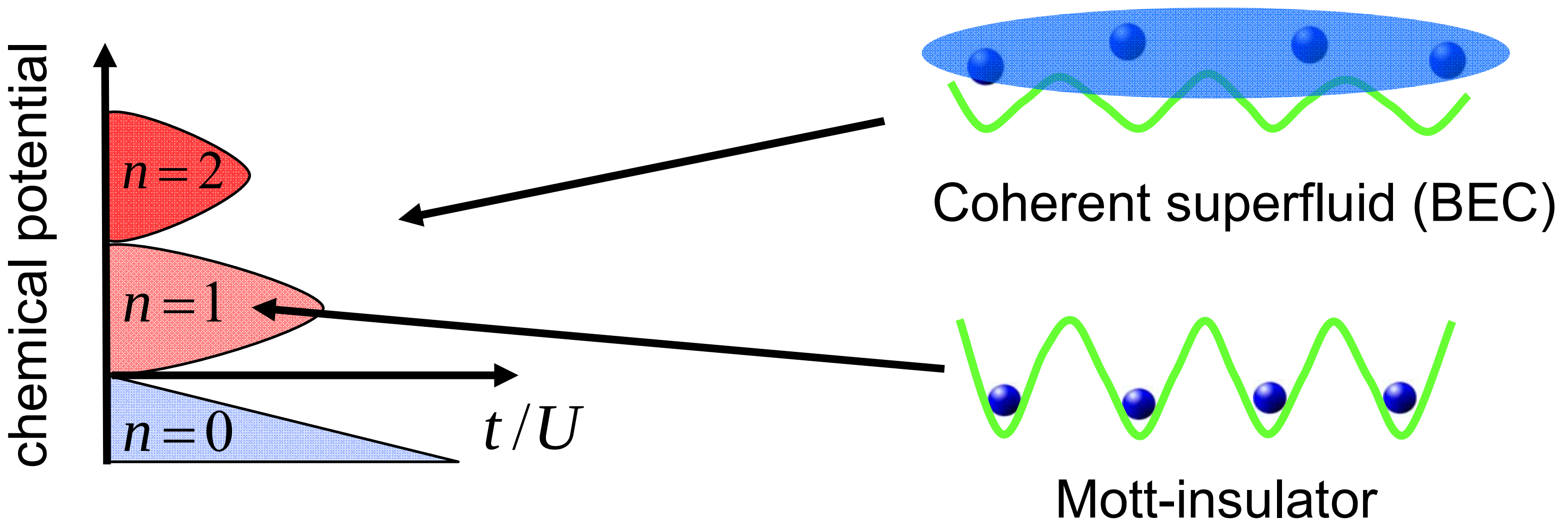
The Boson Hubbard Model

Describes bosons on an optical lattice

$$H = -t \sum_{\langle i,j \rangle} \left(b_i^\dagger b_j + h.c. \right) + \frac{U}{2} \sum_i n_i (n_i - 1)$$



Phase diagram:



Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms

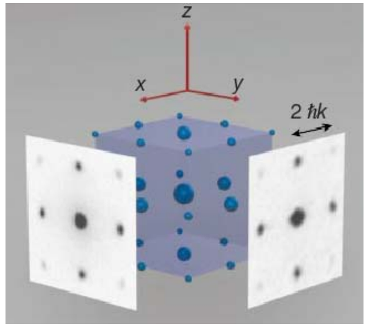
Markus Greiner*, Olaf Mandel*, Tilman Esslinger†, Theodor W. Hänsch* & Immanuel Bloch*

* *Sektion Physik, Ludwig-Maximilians-Universität, Schellingstrasse 4/III, D-80799 Munich, Germany, and Max-Planck-Institut für Quantenoptik, D-85748 Garching, Germany*

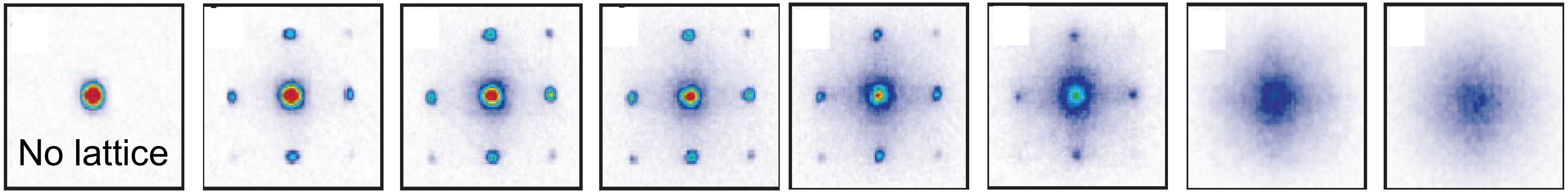
† *Quantenelektronik, ETH Zürich, 8093 Zurich, Switzerland*

Nature 415, 39 (2002)

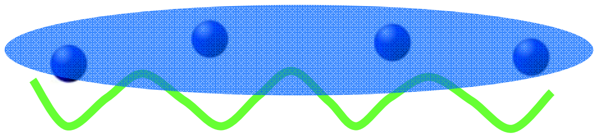
Time-of-flight interference pattern



Increasing the lattice depth:

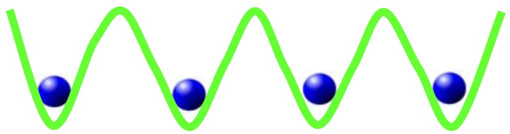


$t >> U$ → $U >> t$



Lattice depth

U / t

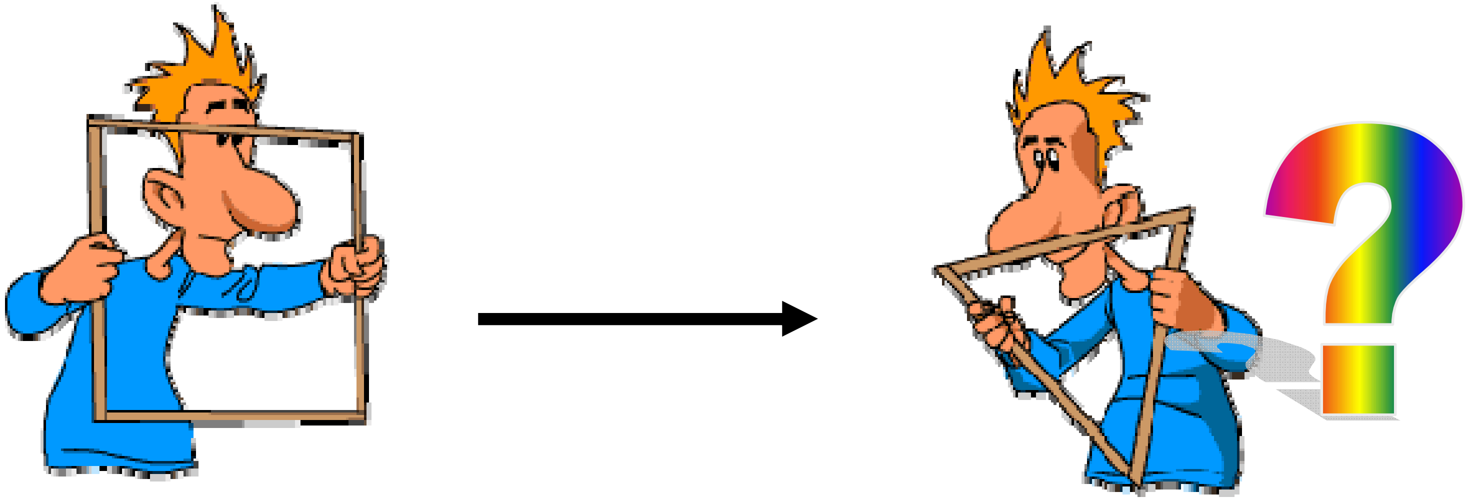


Coherent superfluid (BEC)

Mott-insulator

2D square lattice: I. B. Spielman, et al., PRL 98, 080404 (2007)

Beyond Square Lattice Geometry



Bosons on the Triangular Lattice

Frustrated lattice geometry

Nearest neighbor repulsion

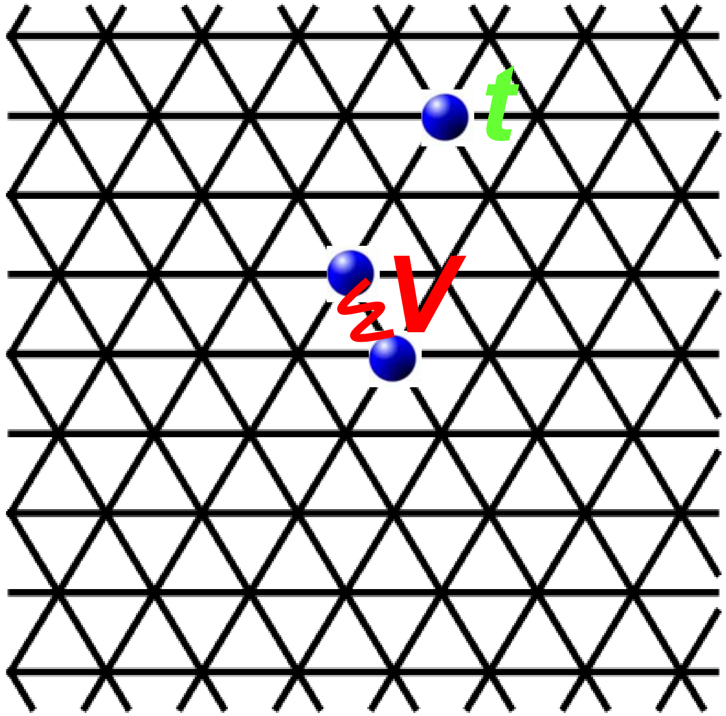
Possible novel phases

Consider first hardcore limit $(U \to \infty)$

$$H = -t \sum_{\langle i,j \rangle} \left(a_i^\dagger a_j + a_j^\dagger a_i \right)$$

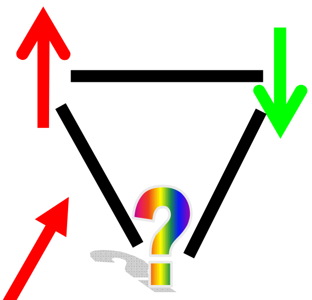
$$+ V \sum_{\langle i,j \rangle} n_i n_j - \mu \sum_i n_i$$

Nearest neighbor repulsion



Frustrated Quantum Spins

Equivalent to a quantum spin model



$$H = -J_{xy} \sum_{\langle i,j \rangle} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + J_z \sum_{\langle i,j \rangle} S_i^z S_j^z - h \sum_i S_i^z$$

Large-scale quantum Monte-Carlo simulations possible

Effects of quantum fluctuations on
frustrated classical spin models

Quantum Monte Carlo

High-Temperature Expansion

$$Z = \mathrm{Tr}\, e^{-\beta H} = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \mathrm{Tr}\,(-H)^n$$

$$= \sum_{n=0}^{\infty} \sum_{|s\rangle} \underbrace{\frac{\beta^n}{n!} \langle s | (-H)^n | s \rangle}_{\text{Statistical weight}}$$

→ Stochastic Series Expansion (SSE)

O.F. Syljuåsen and A.W. Sandvik, PRE 66, 046701 (2002)

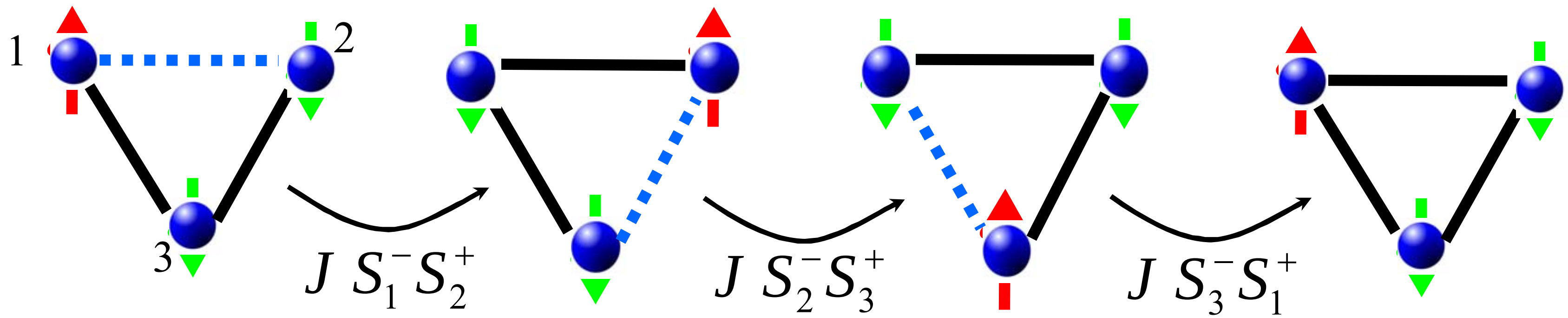
F. Alet, S. W., and M. Troyer, PRE 71, 036706 (2005)

The Sign-Problem

$$Z = \sum_{n=0}^{\infty} \sum_{|s\rangle} \underbrace{\frac{\beta^n}{n!} \langle s | (-H)^n | s \rangle}_{\text{Statistical weight should be} \geq 0\text{ !}}$$

Statistical weight should be ≥ 0 !

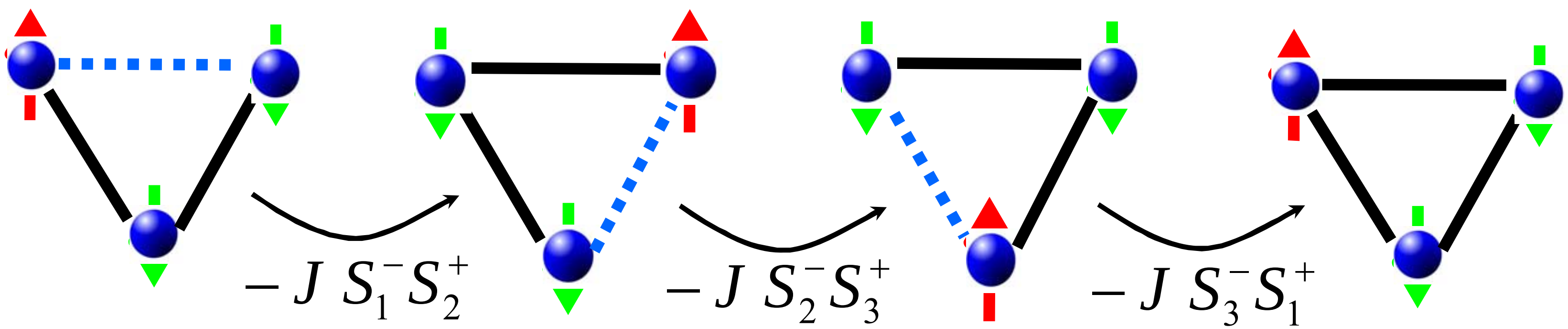
Geometrical frustration:



Statistical weight: $\propto (-J)(-J)(-J) < 0$

Frustration Without Sign-Problem?

$$H = -J_{xy} \sum_{\langle i,j \rangle} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + J_z \sum_{\langle i,j \rangle} S_i^z S_j^z - h \sum_i S_i^z$$



Statistical weight: $\propto (+J)(+J)(+J) > 0$

→ Quantum fluctuation on frustrated magnets

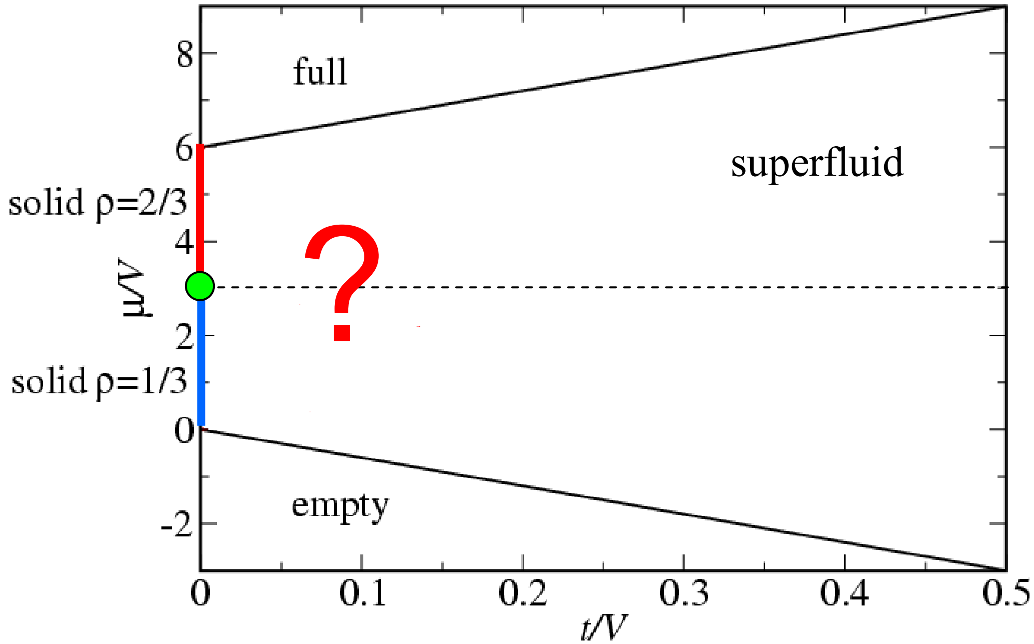
Poor Man´s Phase Diagram

Classical limit for $t = 0$: Ising model

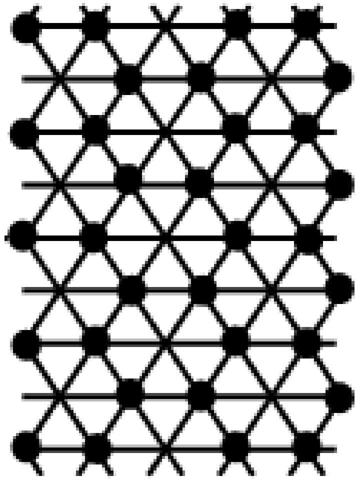
G. H. Wannier (1950)

- Two solid phases, **ρ=1/3** and **ρ=2/3**
- Extensive ground state entropy at **ρ=1/2**

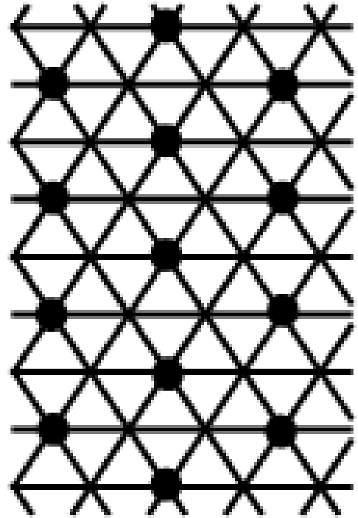
$$S / N \approx 0.323\, k_B$$



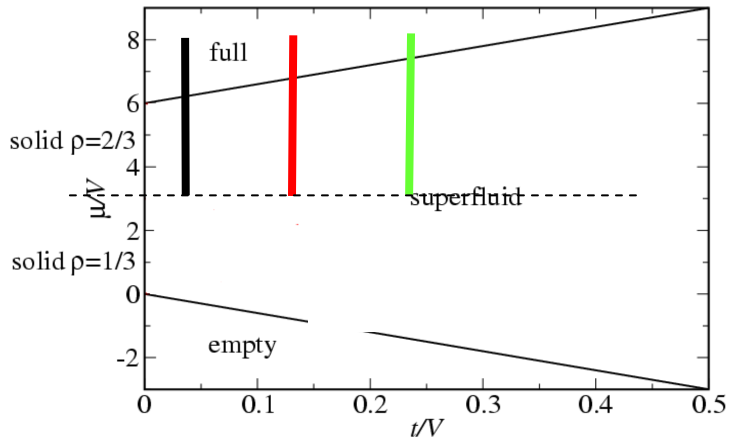
ρ=2/3

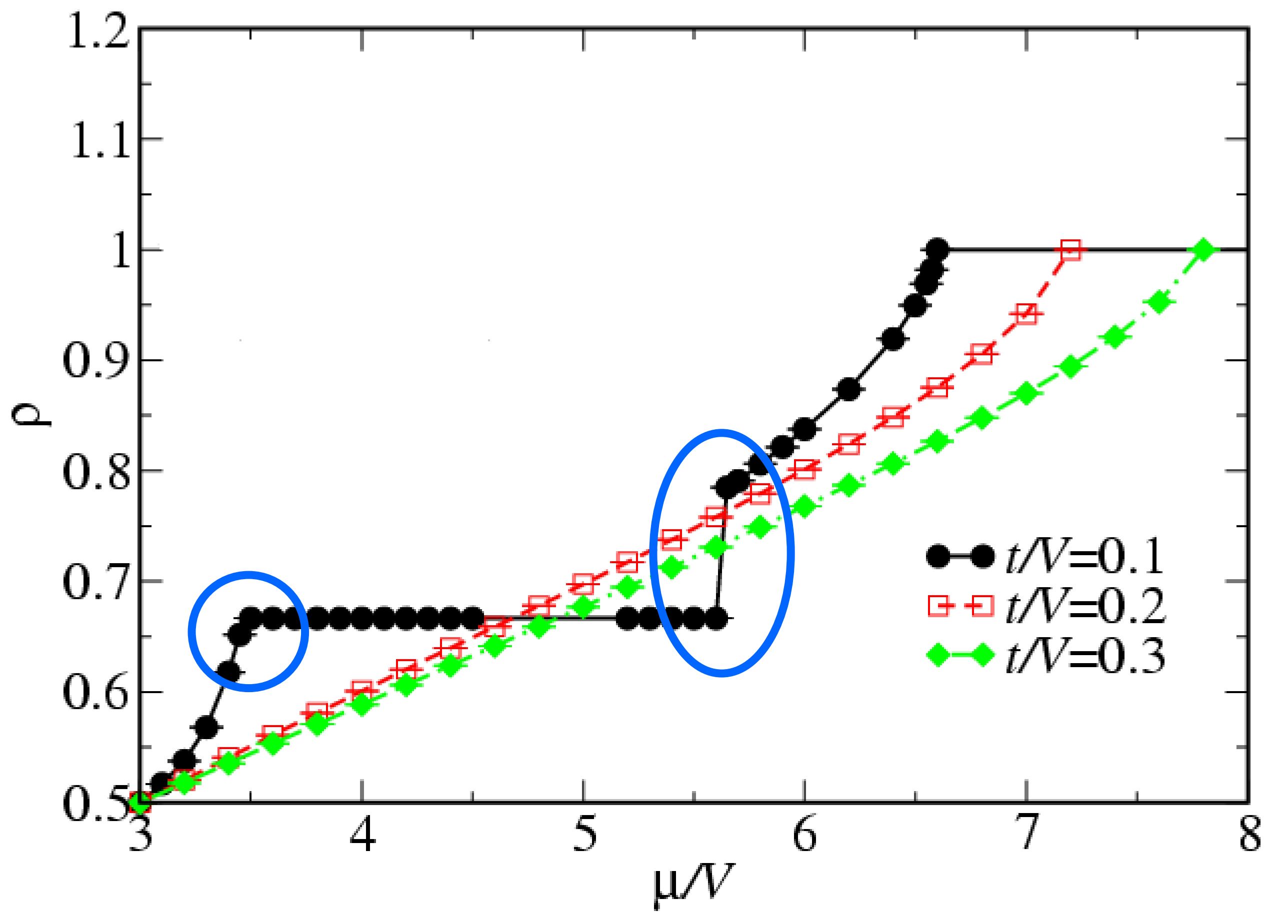


ρ=1/3



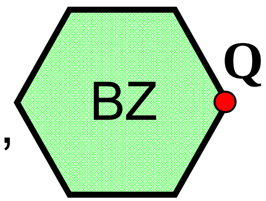
Density Profiles





Supersolid Order Parameters

- Density structure factor $S(\mathbf{Q})$,
- Superfluid density ρ_S



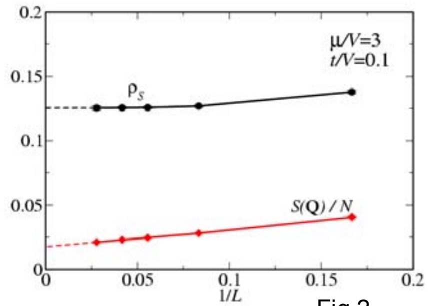


Fig.2

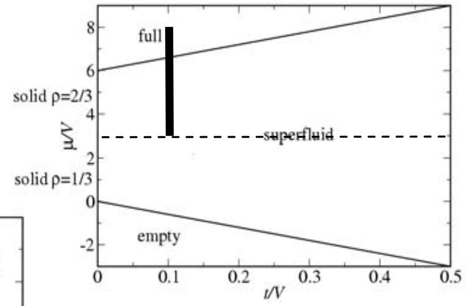
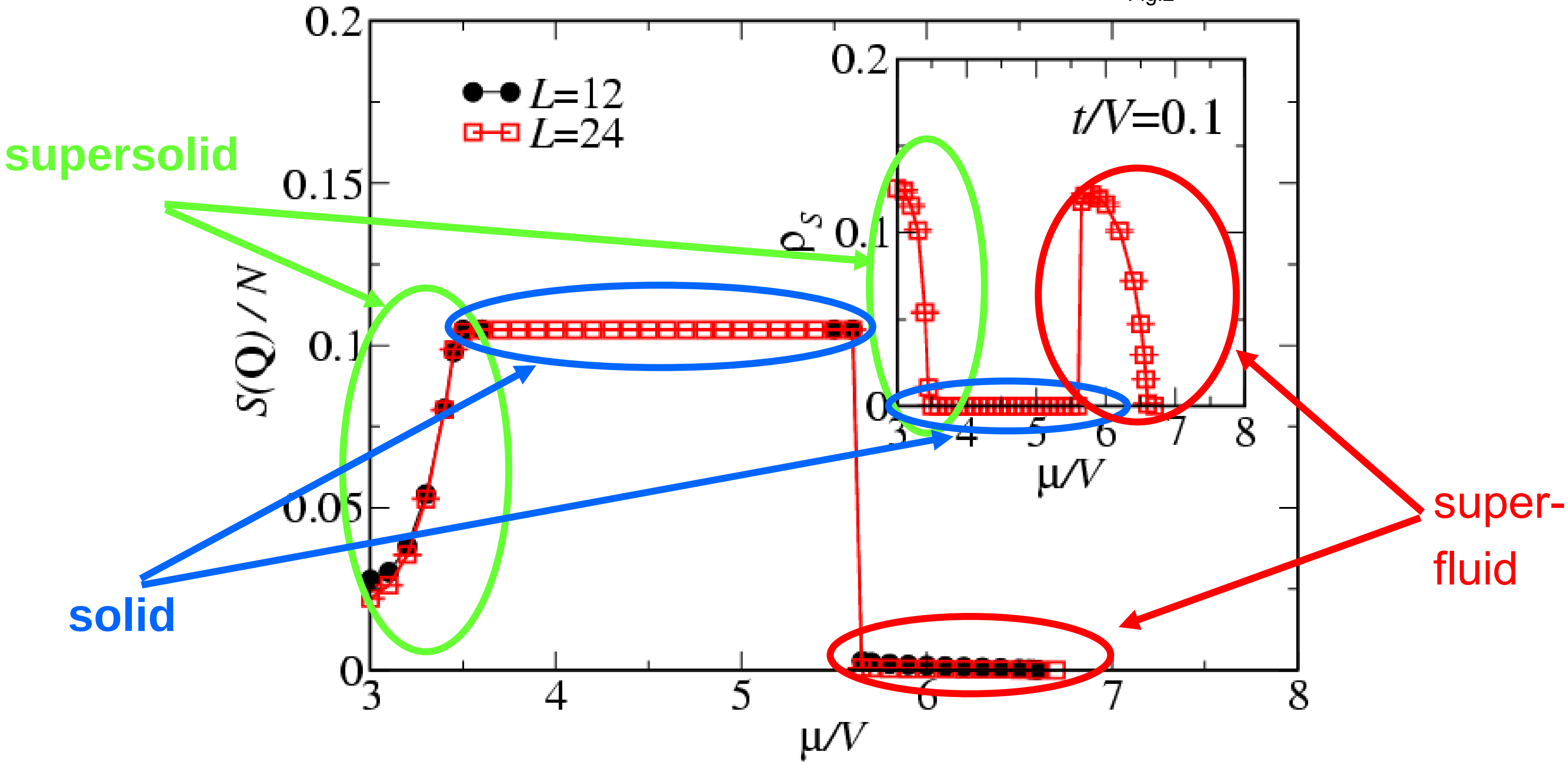


Fig.1



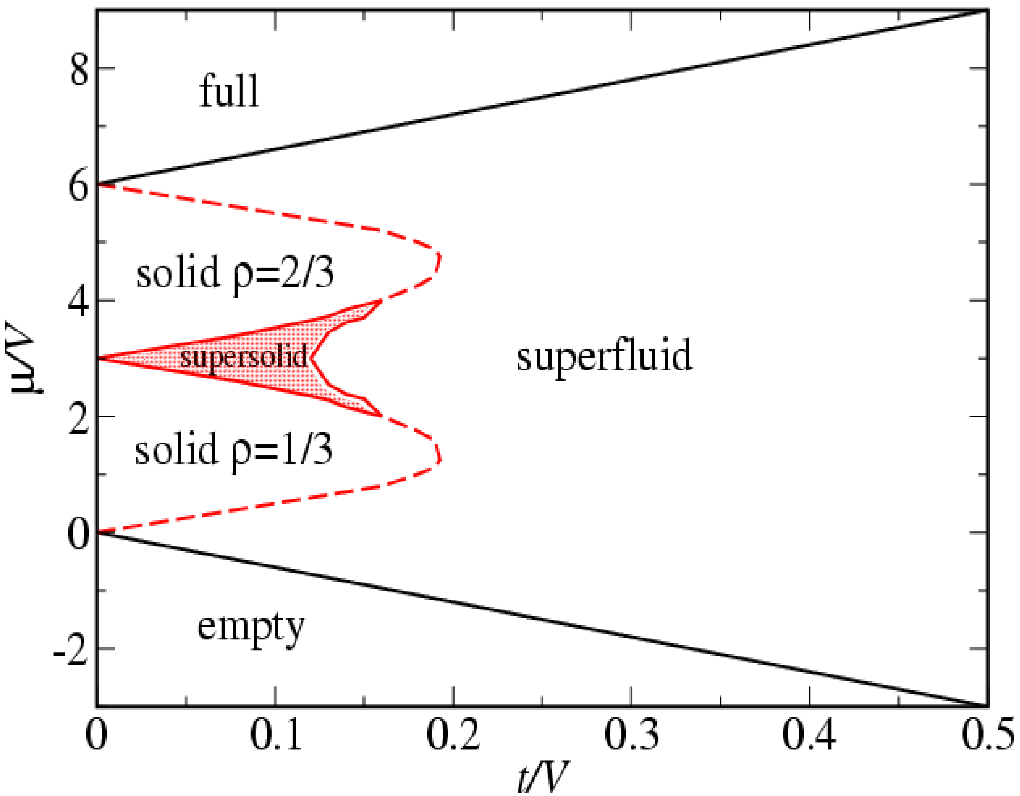
Phase Diagram

qualitative agreement with spin-wave theory

G. Murthy, D. Arovas, and A. Auerbach, Phys. Rev. B 55, 3104 (1997)

extends previous GF QMC

M. Boninsegni, J. Low Temp. Phys., 132, 39 (2003)



S. W. and M. Troyer,
PRL 95, 127205 (2005)

D. Heidarian and K. Damle,
PRL 95, 127206 (2005)

R. G. Melko, A. Paramekanti,
A.A. Burkov, A. Vishwanath,
D.N. Sheng, L. Balents,
PRL 95, 127207 (2005)

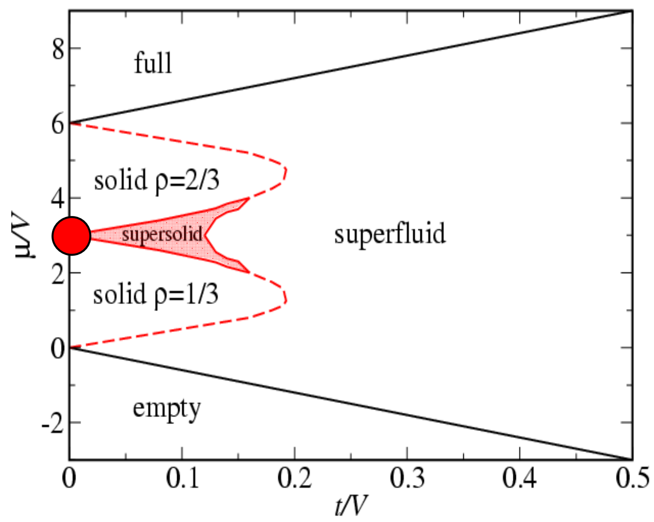
M. Boninsegni and N. Prokof’ev,
PRL 95, 237204 (2005)

Order-by-Disorder Effect

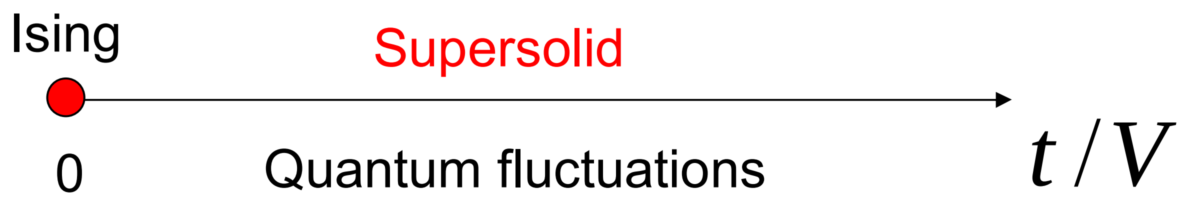
Classical limit: Frustrated Ising model

Extensive ground state entropy

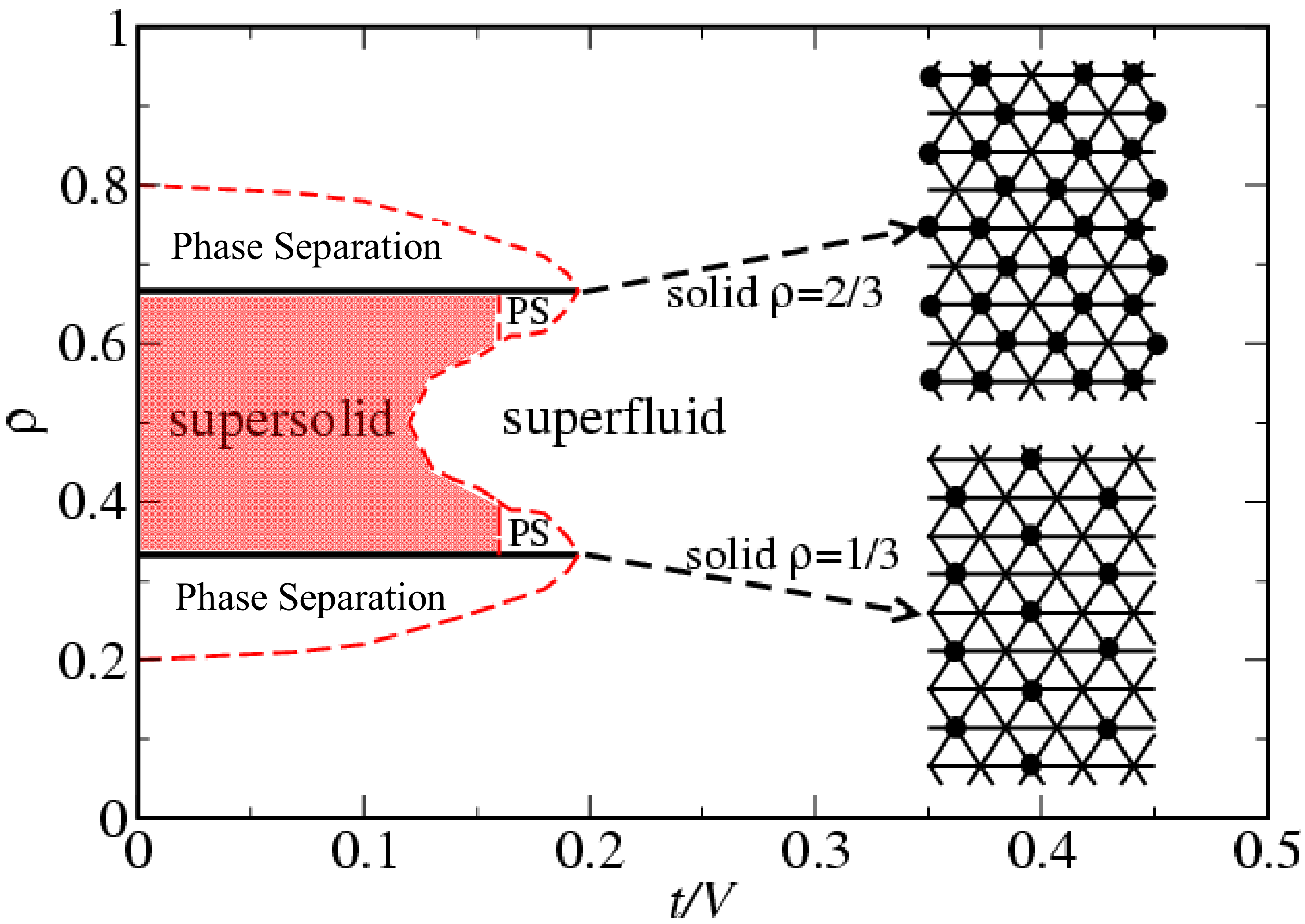
$$S / N \approx 0.323\, k_B$$



Degeneracy lifted by quantum fluctuations:

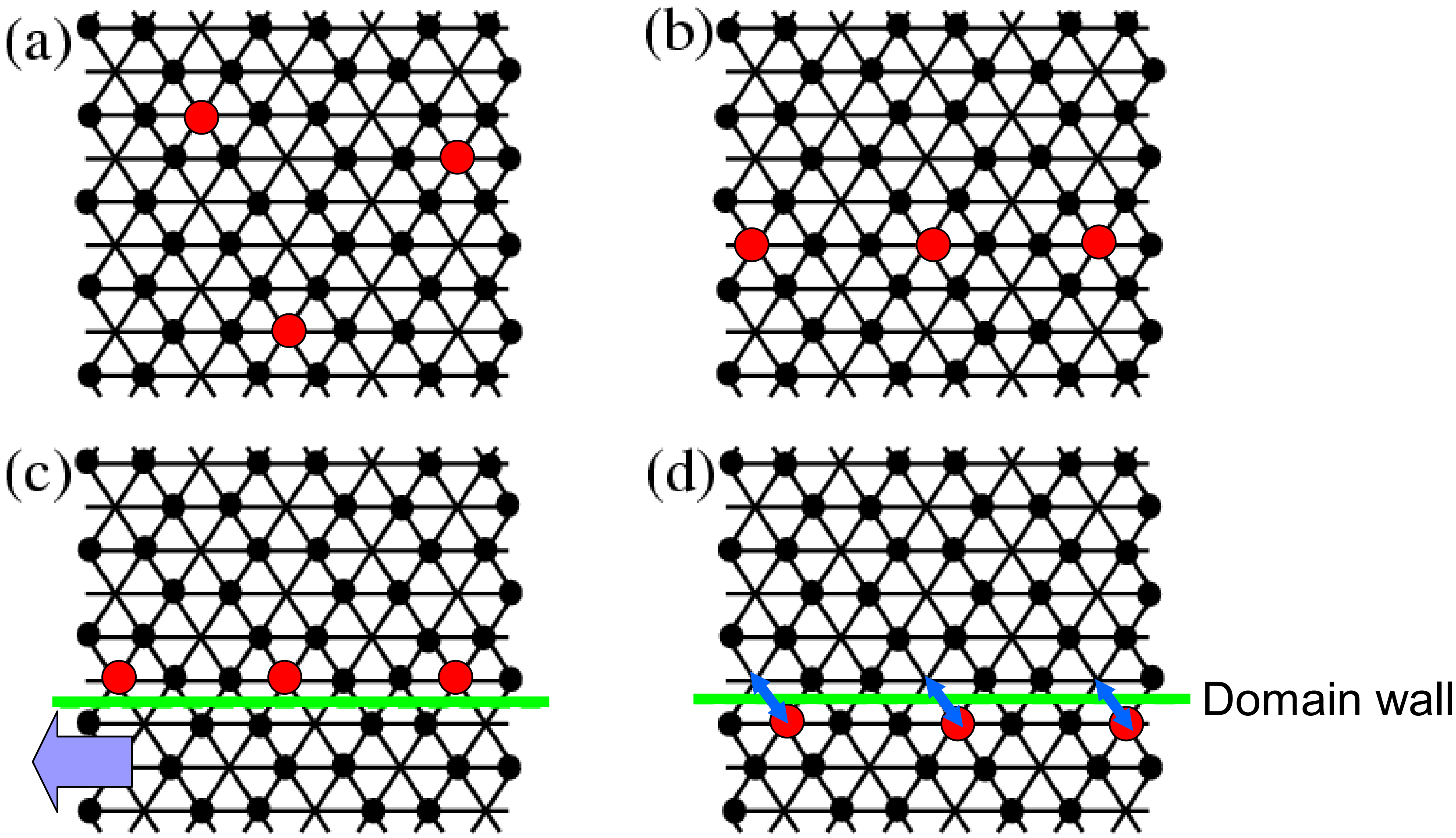


Canonical Phase Diagram

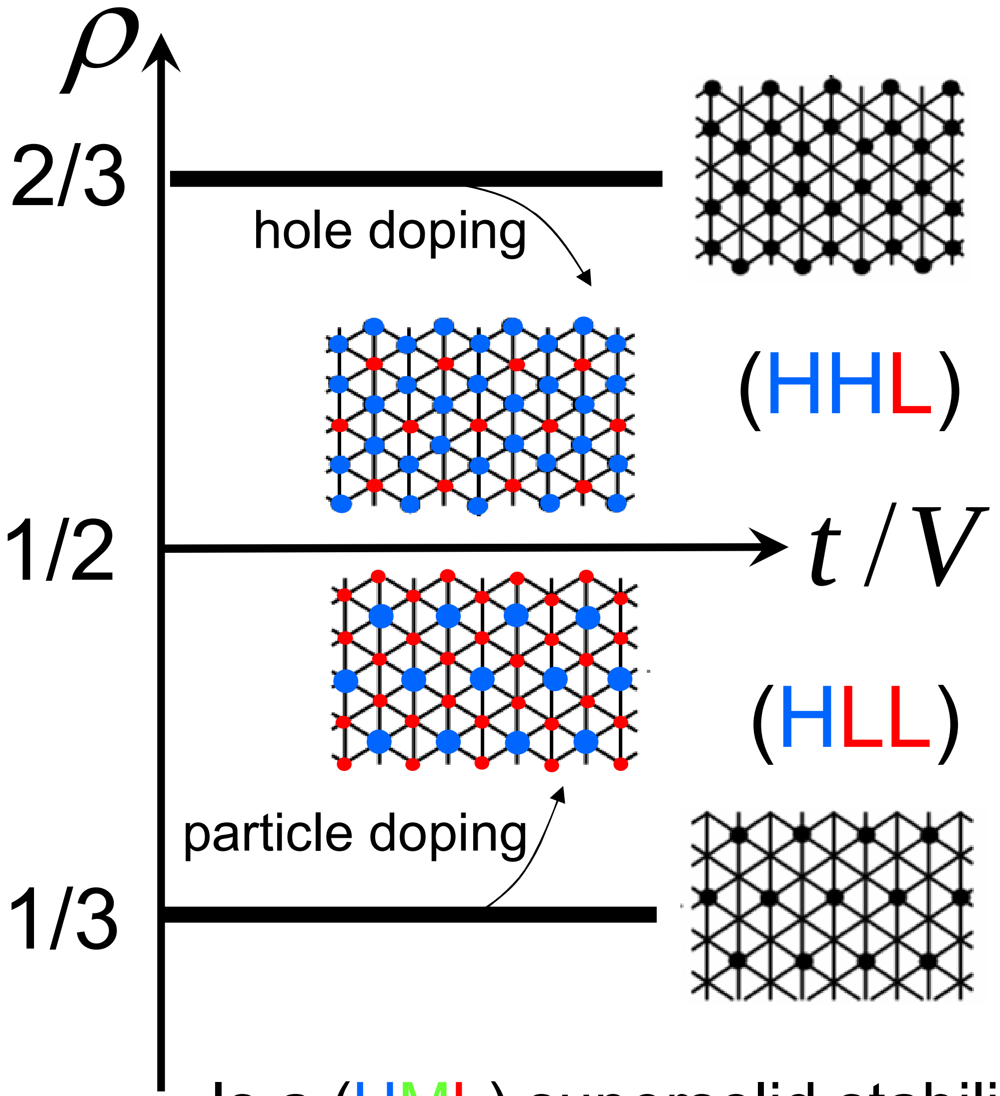


Extended supersolid phase

Competing Phase Separation



Structure of the Supersolid at Half-Filling

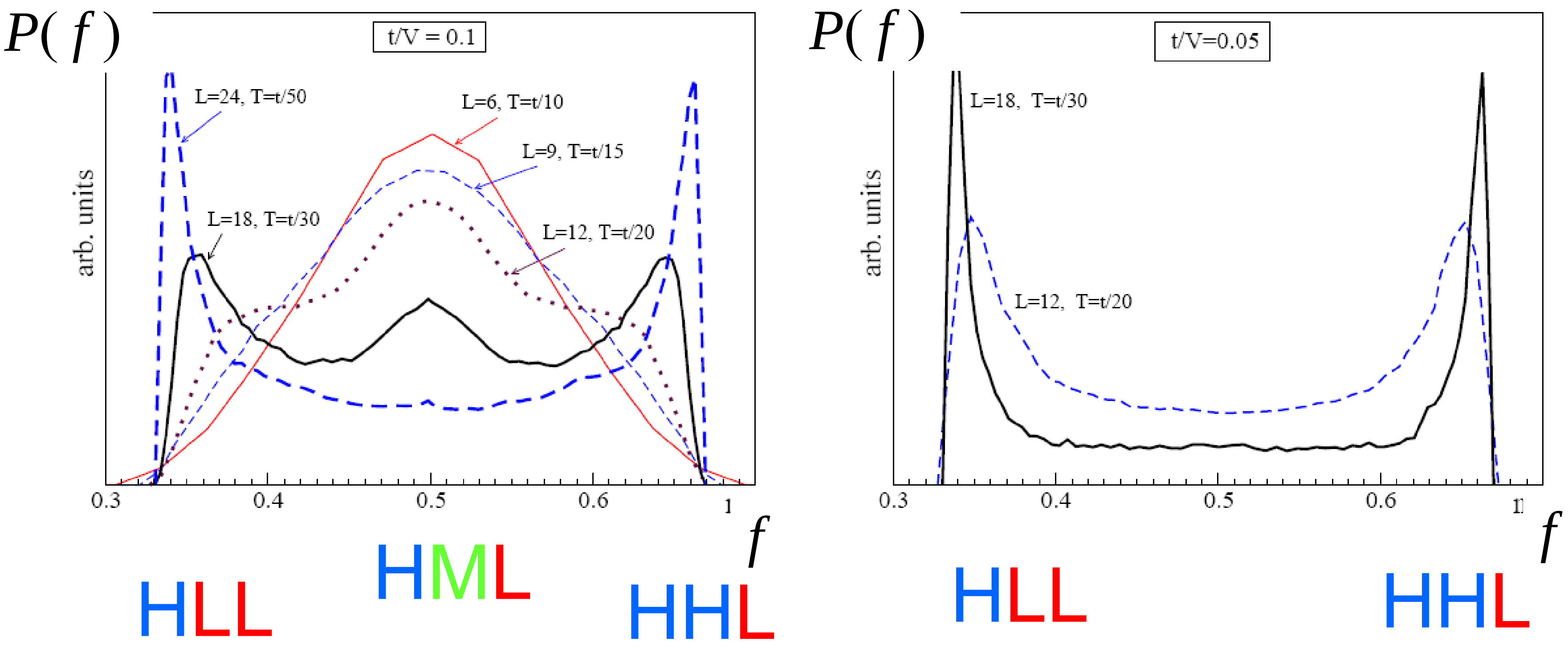


Discontinuous Supersolid-Supersolid transition across the half-filling line

Is a (HML) supersolid stabilized at half-filling?

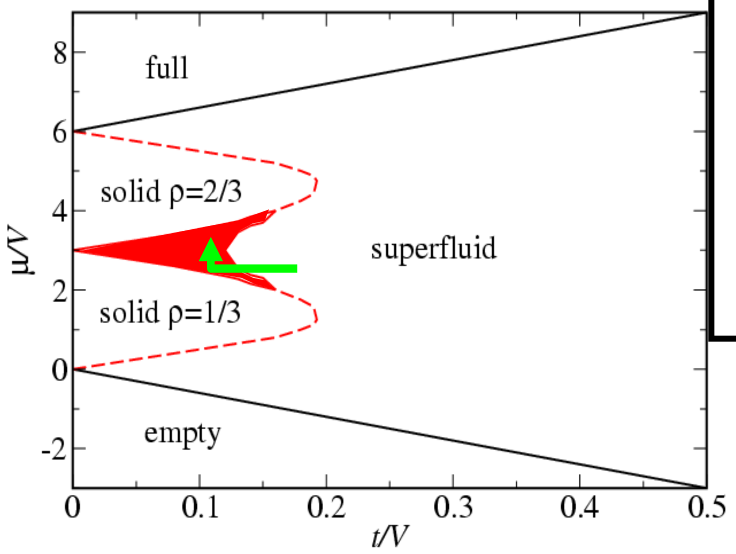
Supersolid-Supersolid Transition

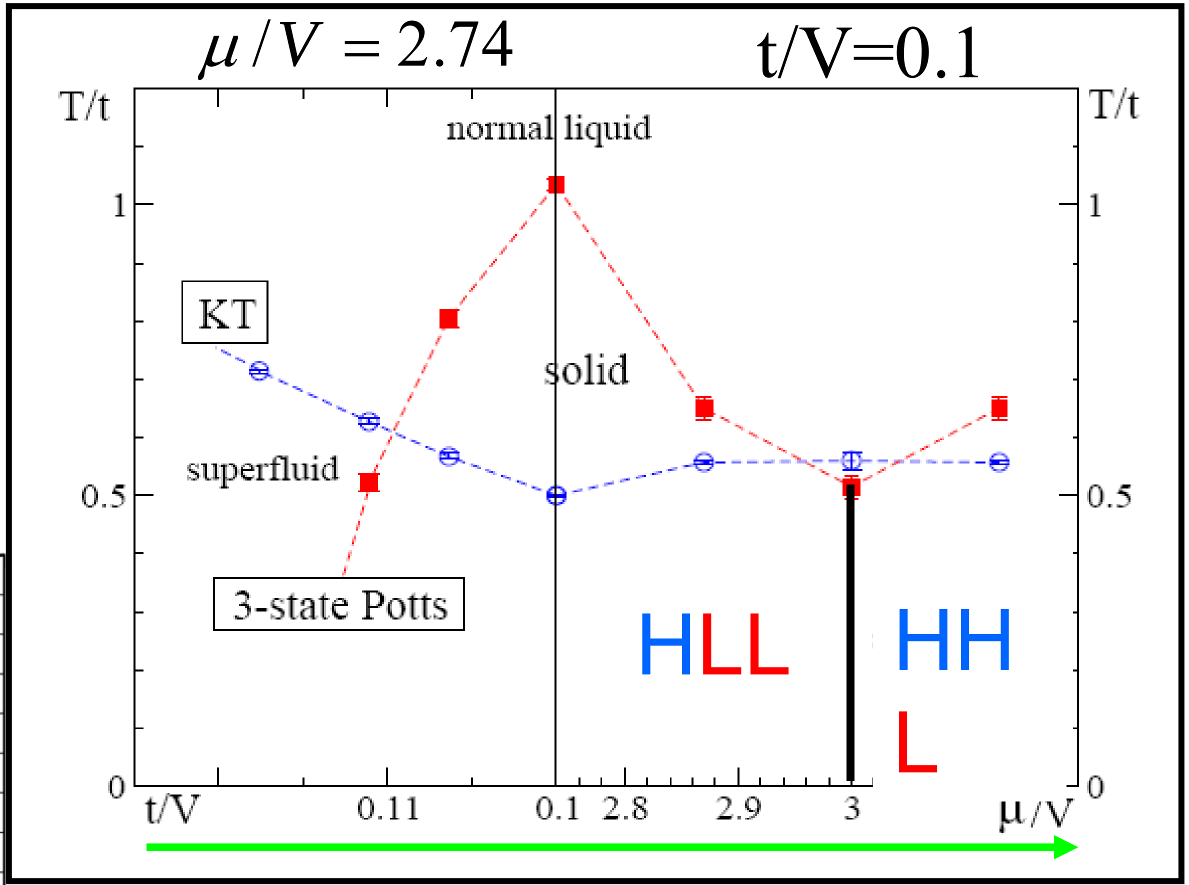
Histogram of the fraction f of sites with local density $n_i > 1/2$



M. Boninsegni and N. Prokof'ev, PRL 95, 237204 (2005)

Thermal Transitions



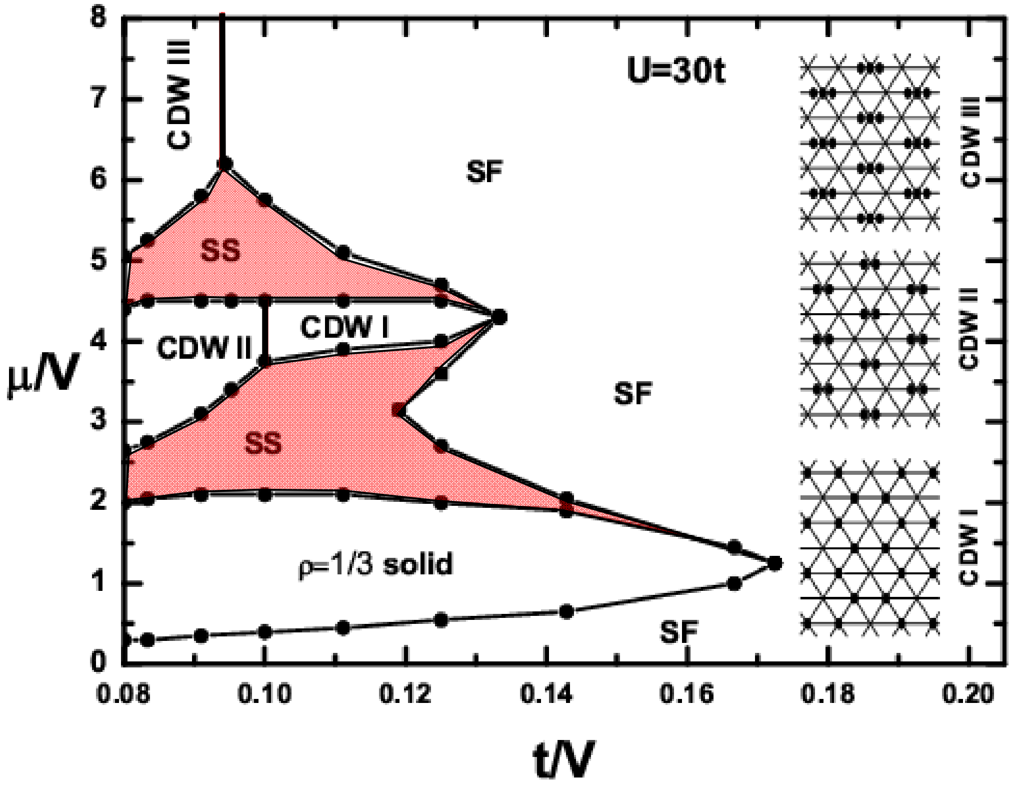


M. Boninsegni and N. Prokof'ev, PRL 95, 237204 (2005)

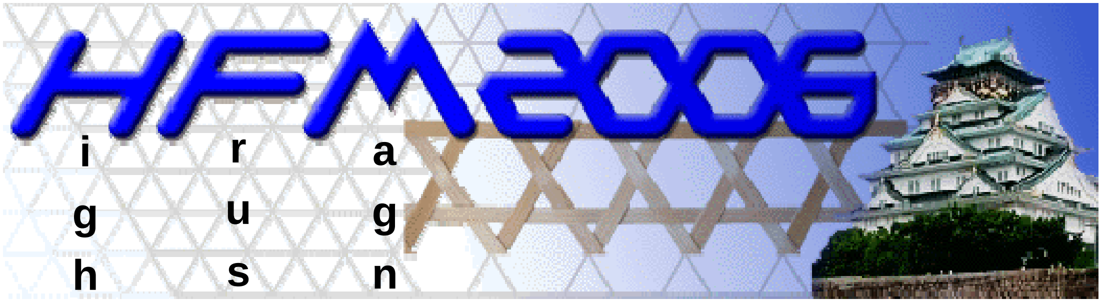
Stability of the Supersolid

with respect to

- a finite onsite repulsion U
  - J. Y. Gan, et al., Phys. Rev. B, 75, 094501 (2007)
- non-zero next-nearest-neighbor repulsion
  - R. G. Melko, et al., Phys. Rev. B 74, 214517 (2006)
- anisotropies from the lattice geometry
  - S. Isakov, et al., arXiv:0708.3084



Kagome Lattice



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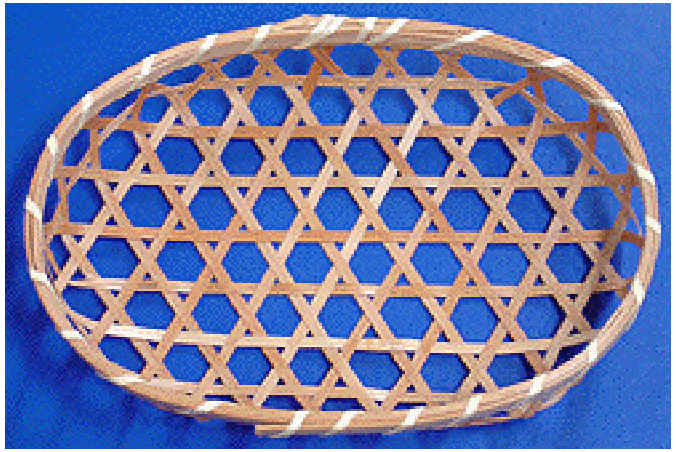
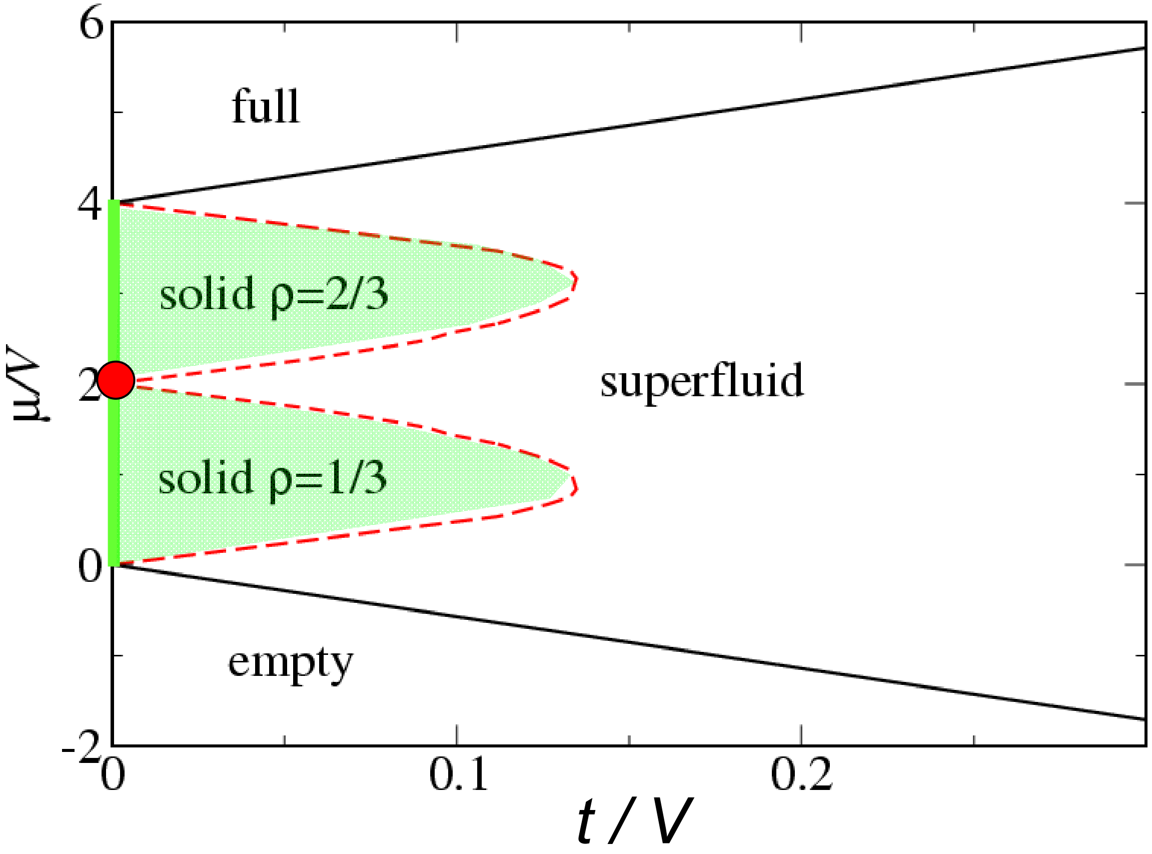
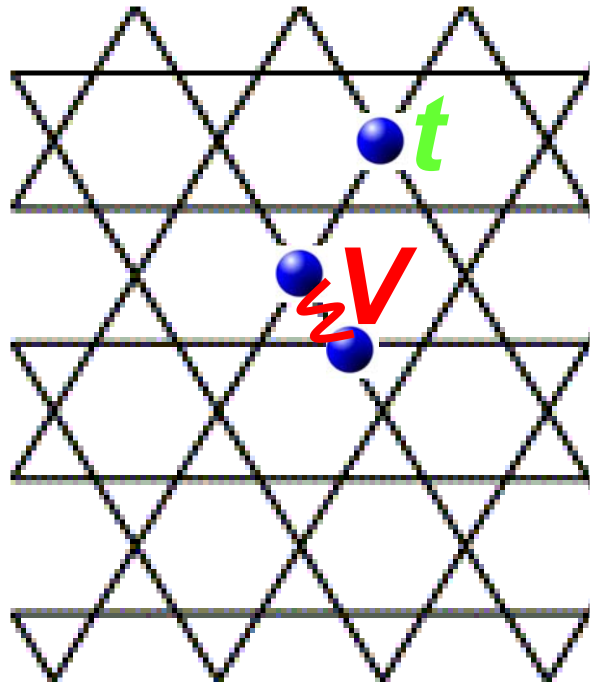


→ $ZnCu_3(OH)_6Cl_2$

Bosons on the Kagome Lattice

No supersolid phase emerges





S.V. Isakov, S.W., R.G. Melko, K. Sengupta, Y.B. Kim, Phys. Rev. Lett. 97, 147202 (2006).

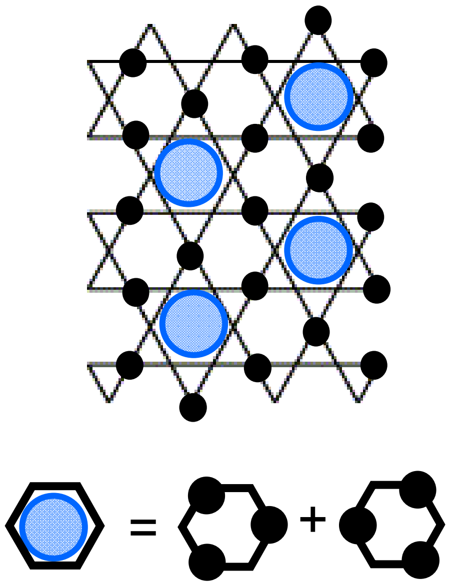
Degeneracy:

$S / N \approx 0.503\, k_B$

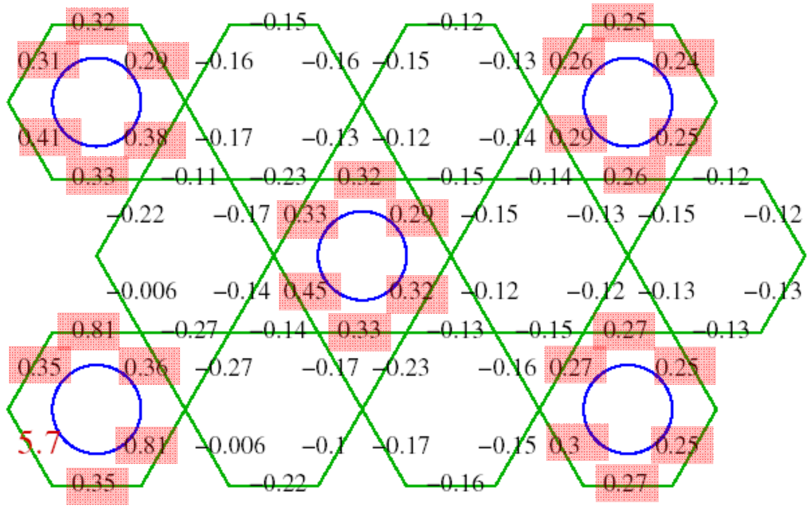
$S / N \approx 0.108\, k_B$

Valence Bond Solid

Local bosonic resonances



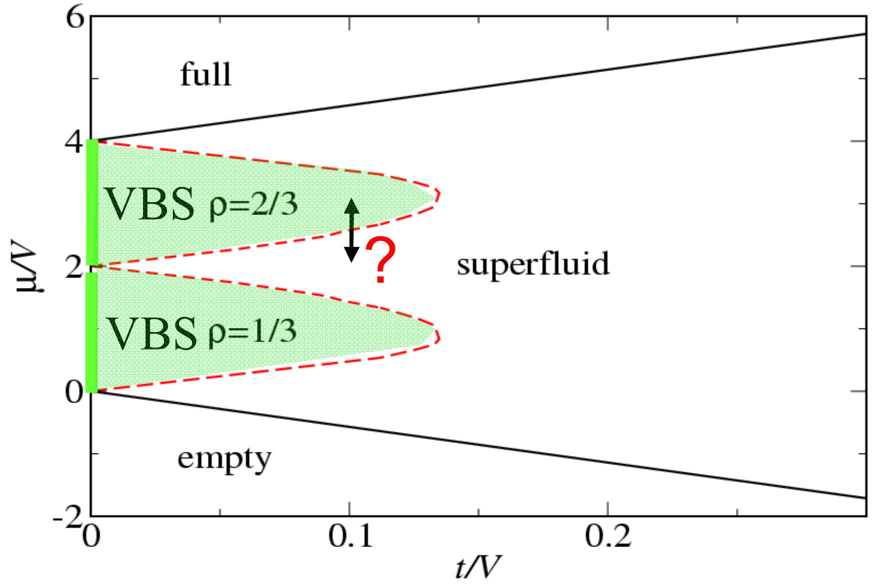
Bond-bond correlations

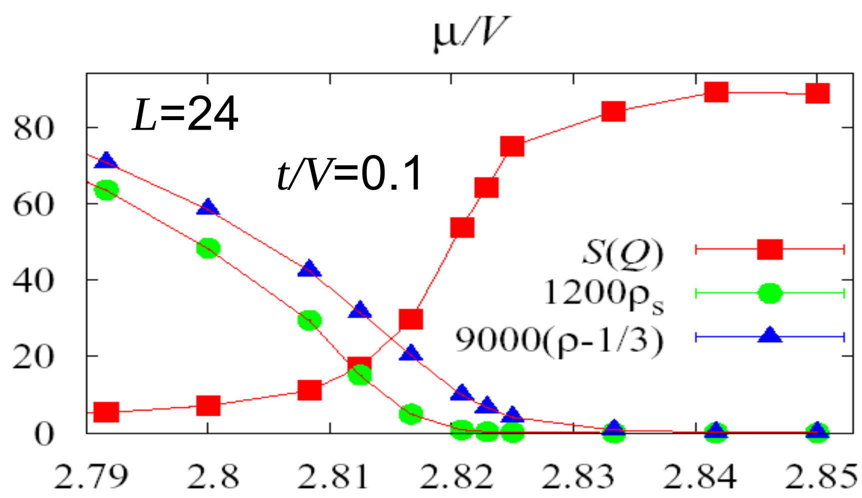


$V >> t \;\rightarrow$ Quantum dimer model on the honeycomb lattice

R. Moessner, S.L. Sondhi, and P. Chandra (2001).

Quantum Melting Transition

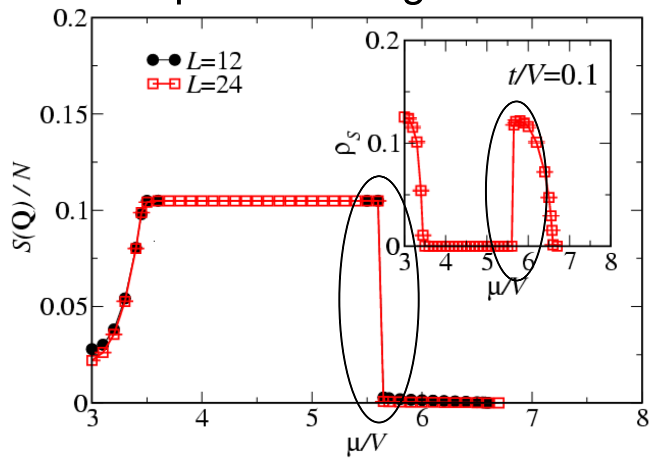




Different symmetries broken in SF and VBS phase (U(1) vs. space group):

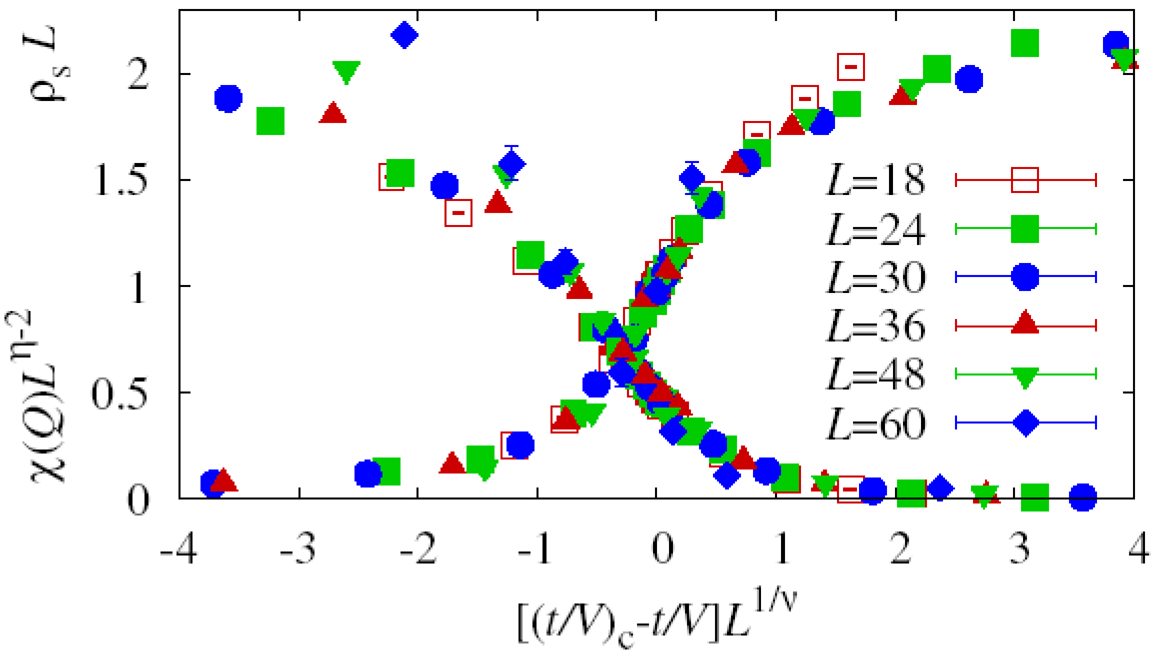
- Weakly first-order transition?
- Intermediate supersolid phase?
- Unconventional continuous quantum phase transition?

Compare to triangular lattice:



Unconventional Continuous QPT?

Finite size scaling analysis:

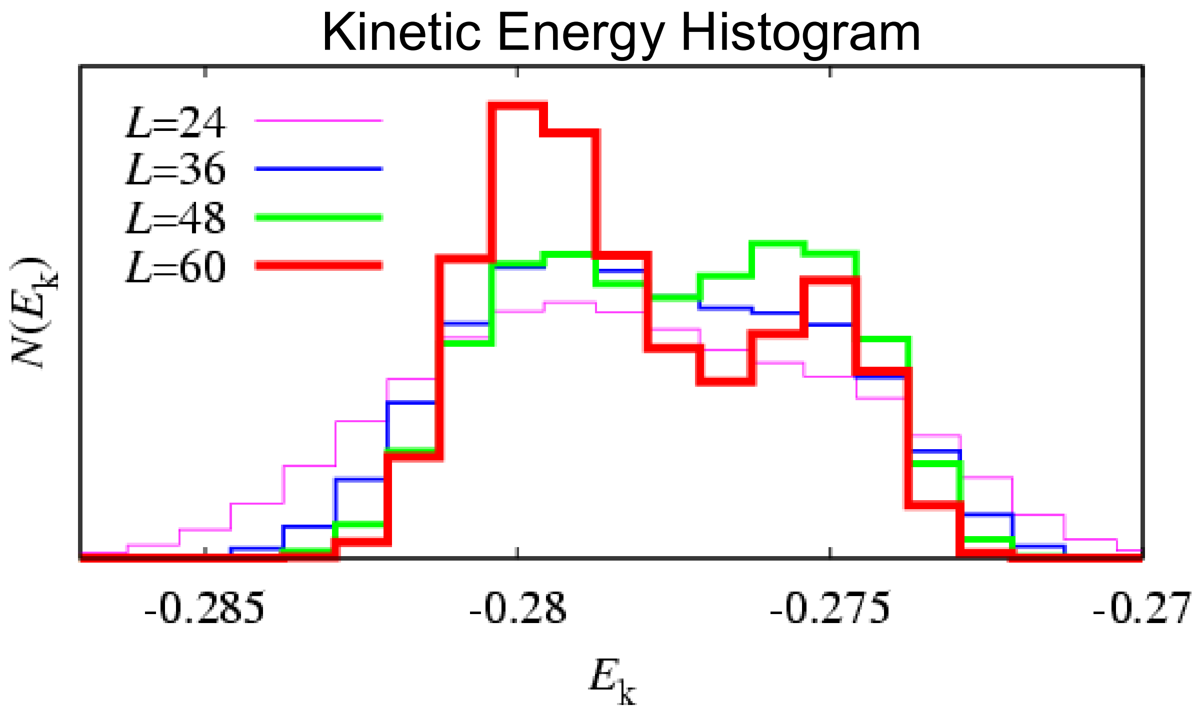


$$z = 1.0(2)$$

$$\nu = 0.44(1)$$

$$\eta = -0.50(2)$$

QMC Histogram Analysis

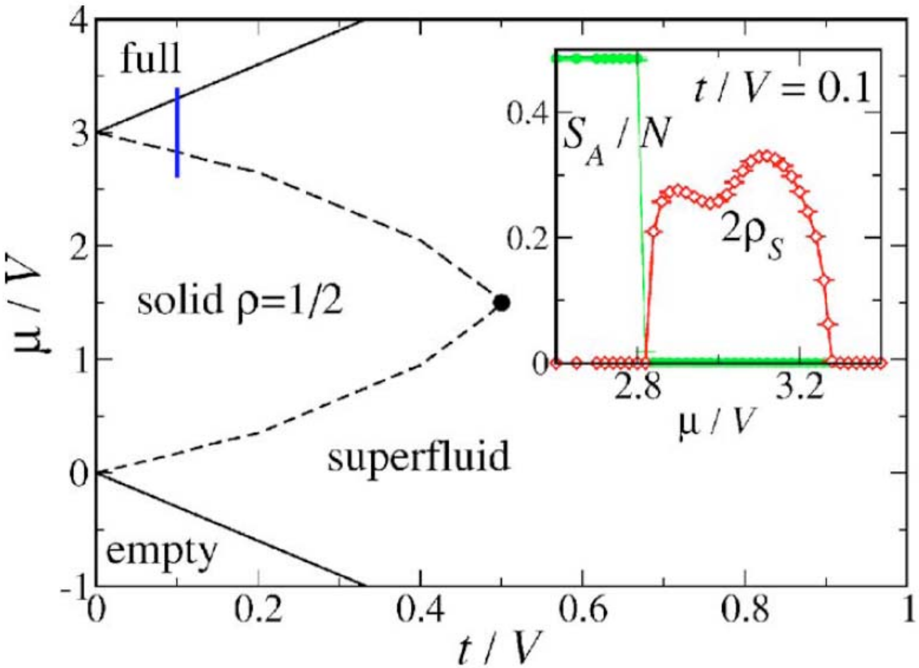


→ Weakly first-order generic quantum melting of the VBS

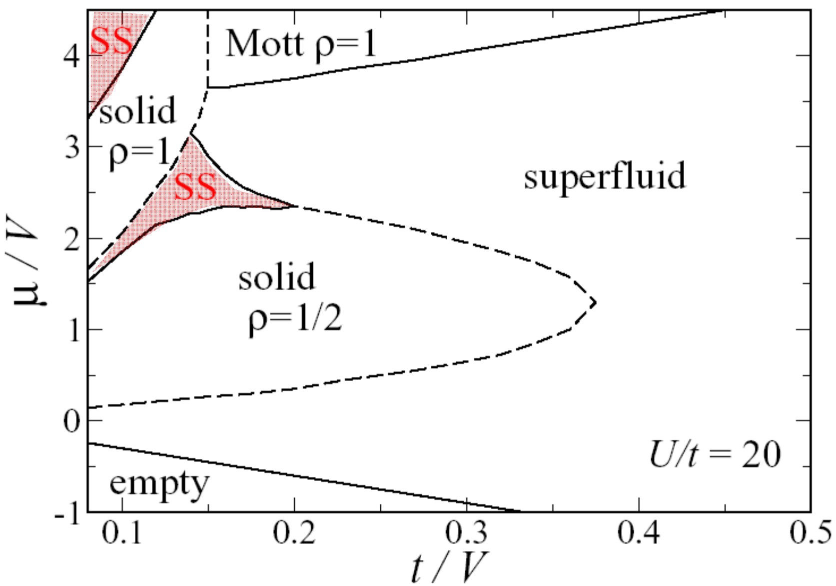
Is the transition through the tip of the VBS lobe special? – No!

Honeycomb Lattice

hard-core bosons



soft-core bosons



S.W., PRB 75, 174301 (2007)

Longer Ranged Interactions

- Dipolar gases
  - K. Goral, L. Santos, and M. Lewenstein, Phys. Rev. Lett. 88, 170406 (2002).
  - BEC of Chromium atoms:

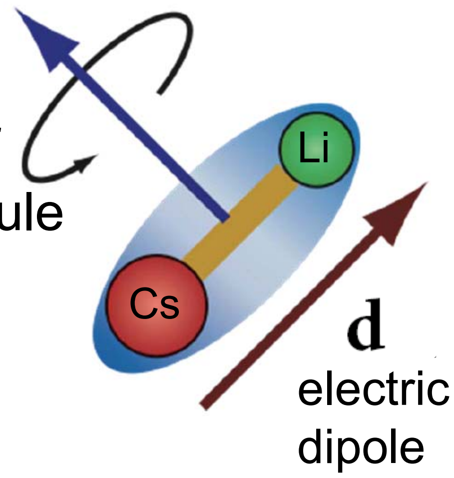
    A. Griesmaier et al., Phys. Rev. Lett. 94, 160401 (2005).

- Bose-Fermi mixtures
  - H. P. Büchler and G. Blatter, Phys. Rev. Lett. 91, 130404 (2003).

- Excited states in higher bands
  - V.W. Scarola and S. Das Sarma, Phys. Rev. Lett. 95, 03303 (2005).

- Polar molecules

Cold Polar Molecules



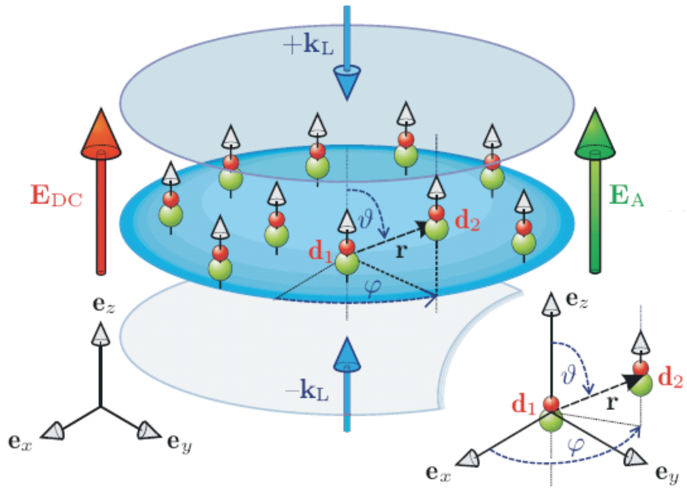
$X^1\Sigma(v = 0)$: Rigid rotor and electric dipole

E.g. LiCs: d = 6.3 Debye = 2.5 ea_B

Two molecules: dipole-dipole interactions

$$V_{\mathrm{d-d}}(\mathbf{r}_{ij}) = \frac{\mathbf{d}_i \mathbf{d}_j}{|\mathbf{r}_{ij}|^3} - \frac{3(\mathbf{r}_{ij}\mathbf{d}_i)(\mathbf{r}_{ij}\mathbf{d}_j)}{|\mathbf{r}_{ij}|^5}$$

Interaction engineering possible with static electric and microwave fields



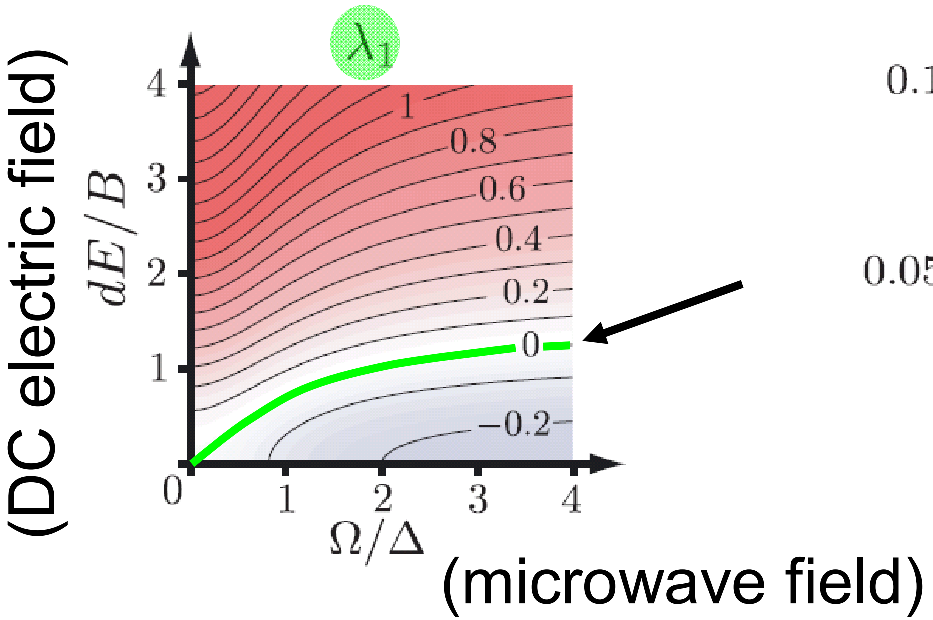
HP. Büchler, A. Micheli, P. Zoller, *Nature Physics* (2007)

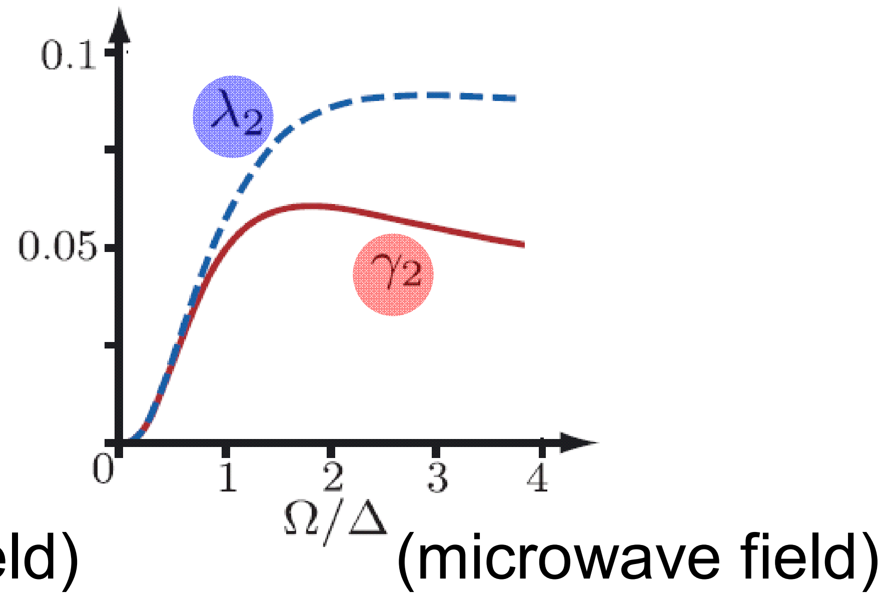
Interaction Engineering

$$V_{\text{eff}}(\{\mathbf{r}_i\}) = \sum_{i<j} V(\mathbf{r}_i - \mathbf{r}_j) + \sum_{i<j<k} W(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \cdots$$

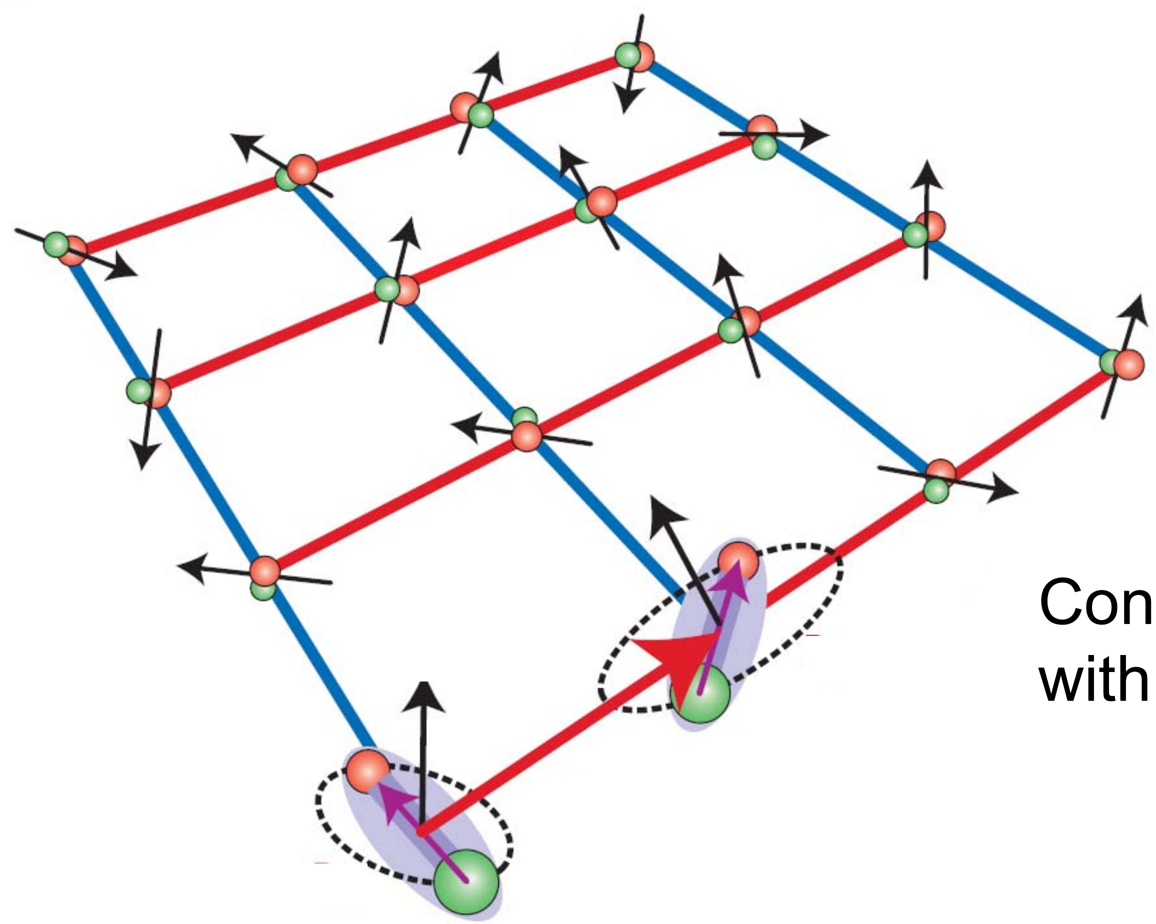
$$V(\mathbf{r}) = \lambda_1 D\,\nu(\mathbf{r}) + \lambda_2 D R_0^3\,[\nu(\mathbf{r})]^2 \qquad \nu(\mathbf{r}) = (1-3\cos^2\vartheta)/r^3$$

$$W(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \gamma_2 R_0^3 D\,[\nu(\mathbf{r}_{12})\nu(\mathbf{r}_{13}) + \nu(\mathbf{r}_{12})\nu(\mathbf{r}_{23}) + \nu(\mathbf{r}_{13})\nu(\mathbf{r}_{23})]$$





Polar Molecules on Optical Lattices



Condensed matter physics
with cold polar molecules

A. Micheli, G.K. Brenner, P. Zoller, *Nature Physics* (2006)

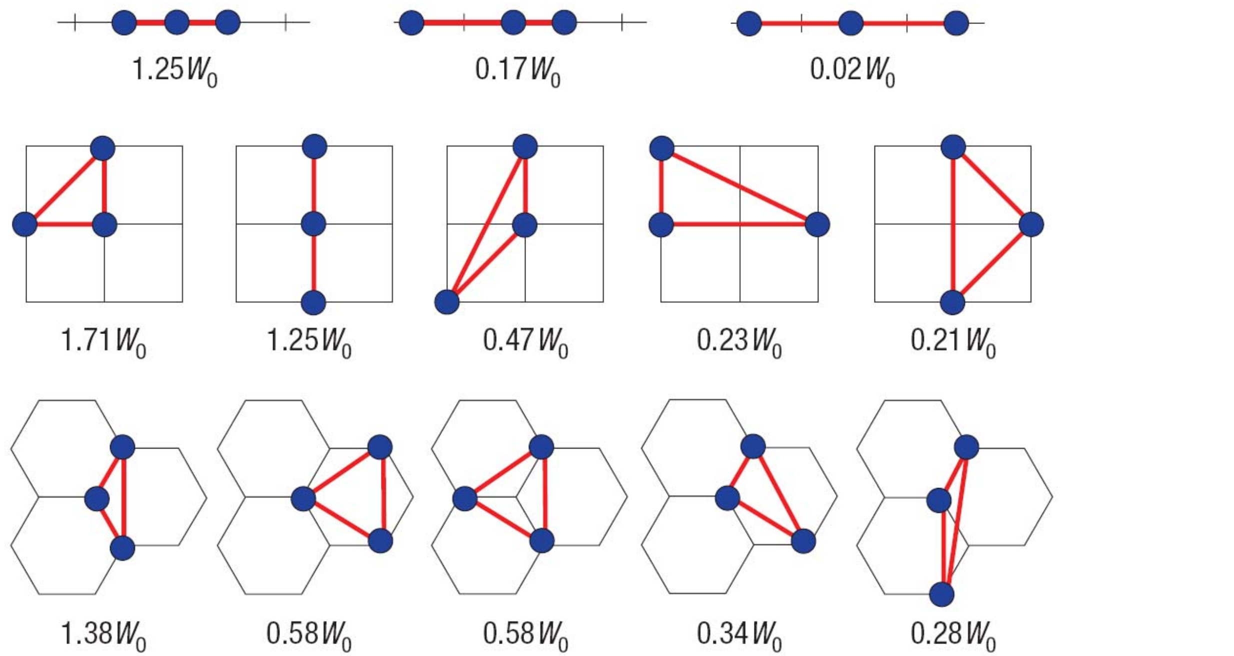
Three-Body Hubbard Model

$$H = -J\sum_{\langle ij\rangle} b_i^\dagger b_j + \sum_{i\neq j}\frac{U_{ij}}{2}n_i n_j + \sum_{i\neq j\neq k}\frac{W_{ijk}}{6}n_i n_j n_k$$

1D Chain:

2D Square:

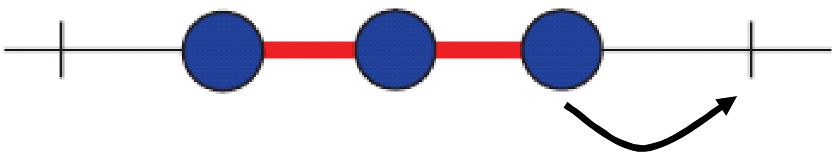
Honeycomb:



HP. Büchler, A. Micheli, P. Zoller, *Nature Physics* (2007)

Minimal Model in 1D

Dominant nearest-neighbor tree-body repulsions



$$H = -J \sum_i \left[b_i^\dagger b_{i+1} + b_i b_{i+1}^\dagger \right] + W \sum_i n_{i-1} n_i n_{i+1}$$

Low-energy phase diagram

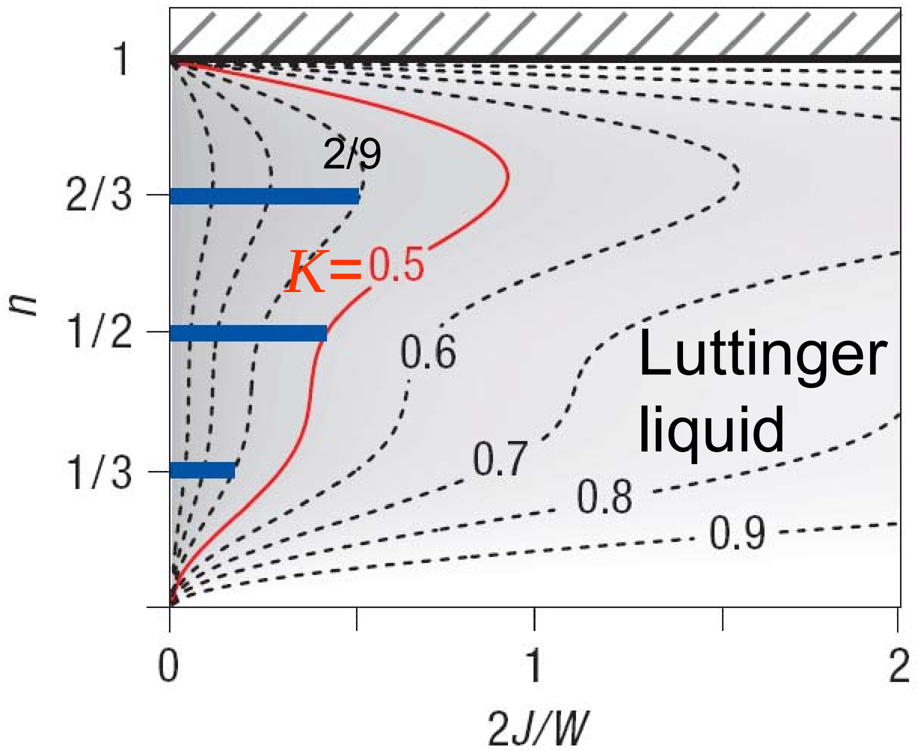
HP. Büchler, A. Micheli, P. Zoller, *Nature Physics* (2007)

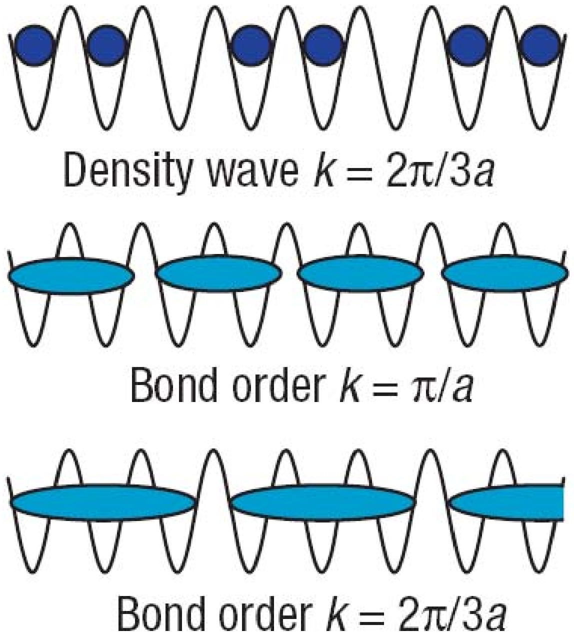
Sine-Gordon Theory

$$H = \frac{\hbar v}{2} \int dx \left\{ \left[K\Pi^2 + \frac{1}{K} \left(\partial_x \Phi\right)^2 \right] + \lambda \cos(\gamma \Phi) \right\}$$

Luttinger liquid parameter

Low energy phase diagram





QMC Results

Combined numerical study using

- Stochastic series expansion
- Worm algorithm path-integral approach

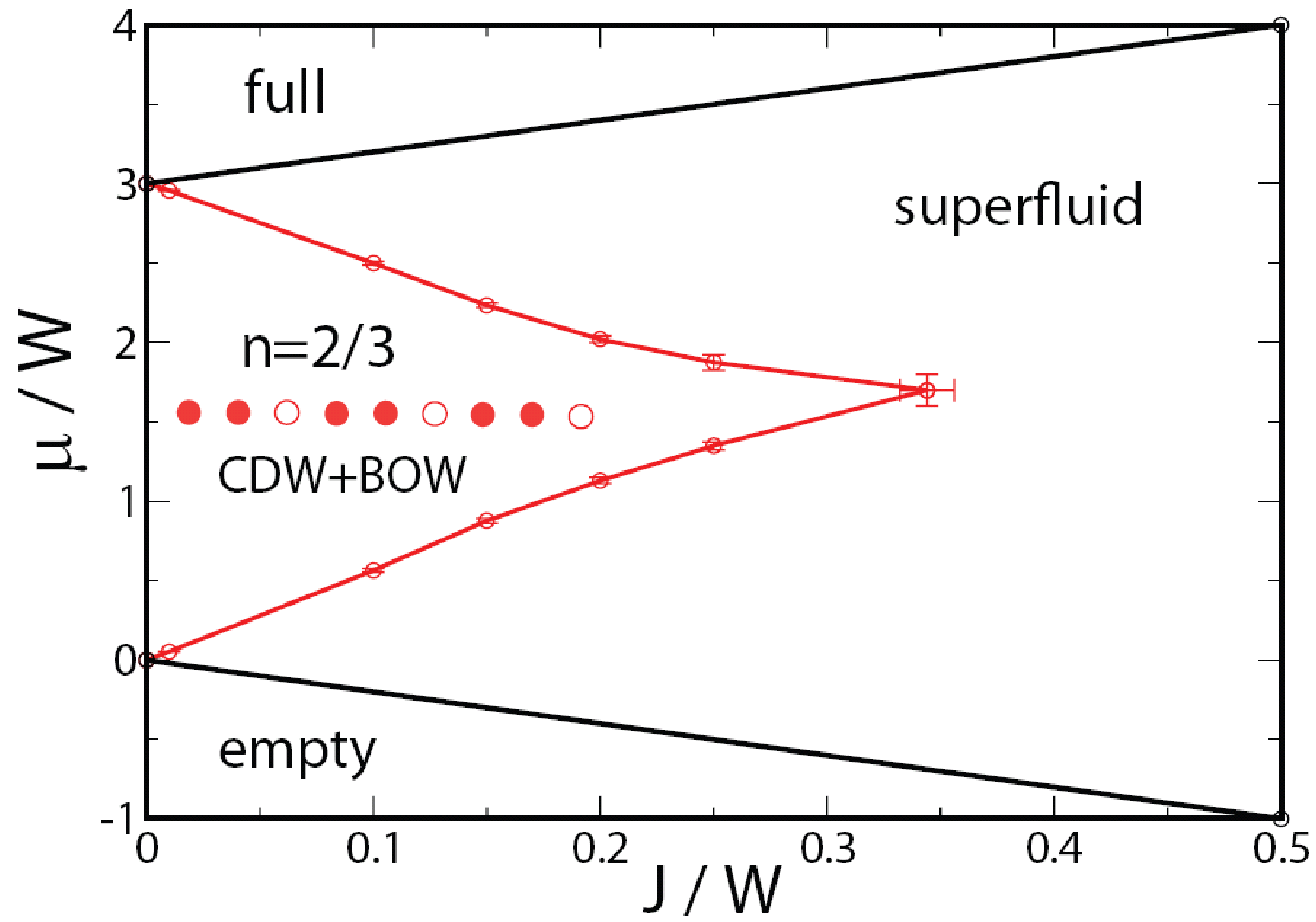
  N.V. Prokof'ev, S.V. Svistunov, I.S. Tupitsyn,

  Phys. Lett. A, JETP (1998)

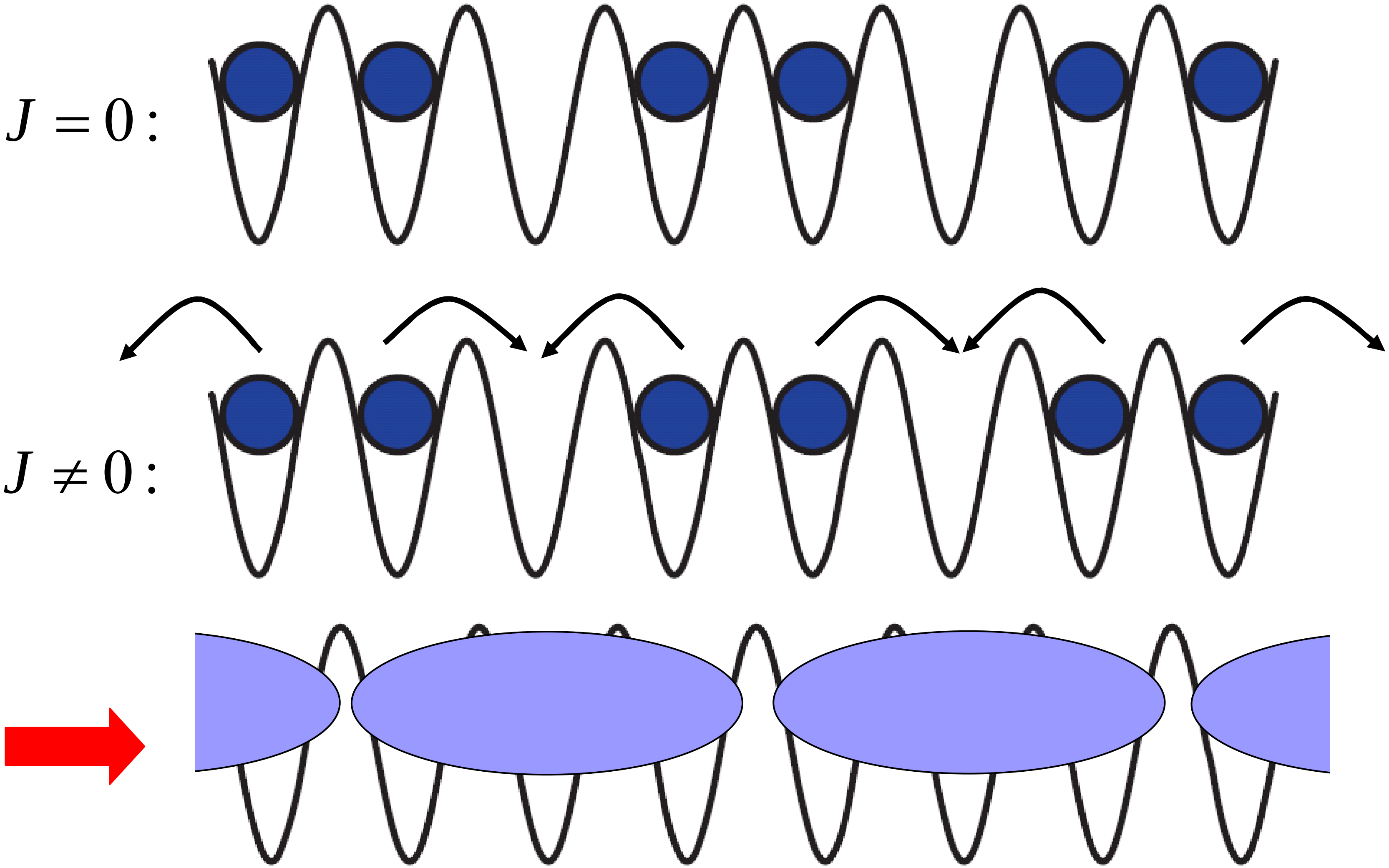
B. Capogrossa-Sansone, S. W., HP. Büchler,

P. Zoller, G. Pupillo, arXiv:0807.4563, subm. to Phys. Rev. Lett.

Quantum Phase Diagram

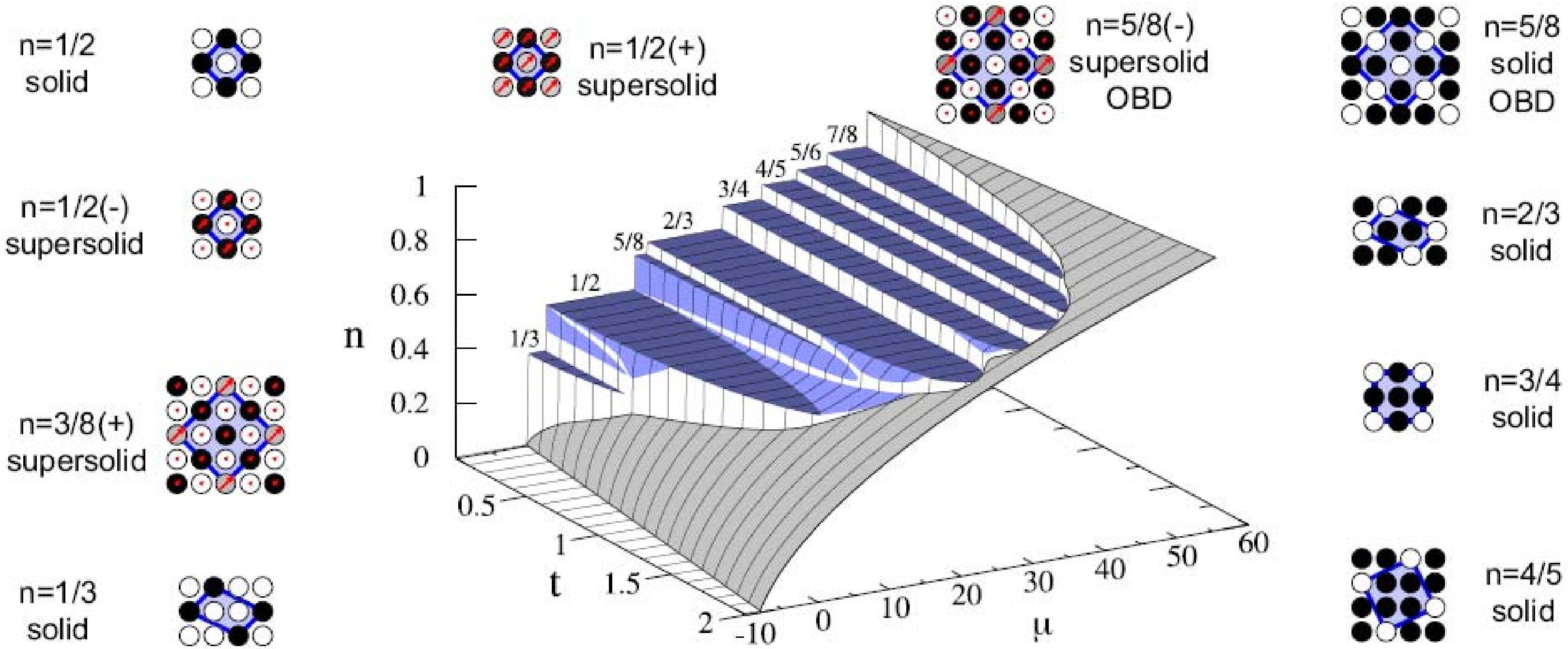


Schematic Picture



2D Square Lattice – Solids and Supersolids

Semi-classical approximation



K. P.Schmidt, J. Dorier, A. M. Läuchli, arXiv:0805.1408

Conclusions

Novel quantum phases accessible with
quantum gases on frustrated optical lattices

Realization of a supersolid phase on the triangular lattice in
the hard-core limit

A valence bond solid emerges on the Kagomé lattice
realizing a quantum dimer model

Three-body interactions can be driven to dominate polar molecules
a mixed BOW+CDW phase found in simplest 1D system

Study 2D models more carefully