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Workshop on Supersolid 2008

18 - 22 August 2008

Supersolid phases of hard core bosons in optical lattices

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Supersolid phases of hard core bosons in optical lattices

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Workshop "Supersolid 2008"
ICTP
Trieste, Italy August 2008

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Funding

What's the point of lattice models ?

- Motivation: Basic many-body and condensed matter physics → *Optical Lattices* (also, *adsorbed ^{4}He films*)

- Search for *exotic* phases matter in simplified setting

  Some "old" problems, until now of "academic" interest only

  → **Supersolid** phase

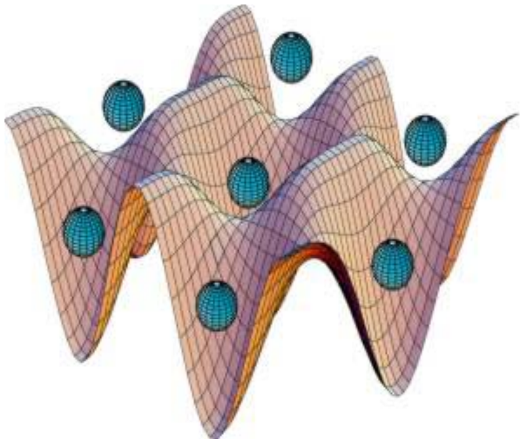
- Theoretical studies: Quantum Monte Carlo simulations

- Physical Issues:

  Vacancy and interstitial based supersolidity

  Generic supersolid phase diagram

Optical lattices (OL)



Interfering laser beams can hold atoms at precisely defined spatial (lattice) positions

- **Spatially confined** assemblies of *laser cooled* gases
- **Optical potential**: standing wave light field formed at intersection of *four* laser beams → *crystal lattice pattern*

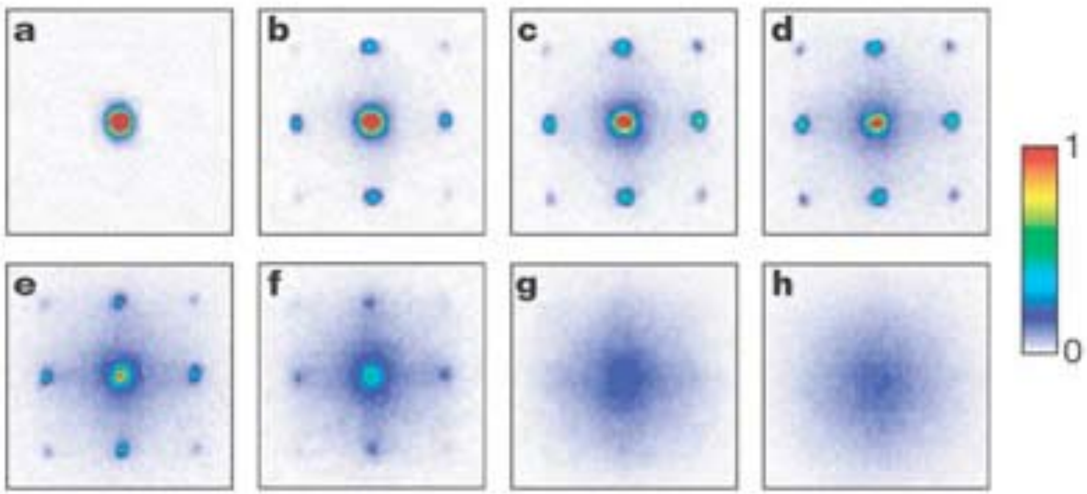
  G. Birkl, *et al*. Phys. Rev. Lett. **75**, 2823 (1995)
- **Atomic dynamics** in OL studied experimentally

  http://physics.nist.gov
- **Physical realization** of many-body systems long regarded as mostly *academically* interesting (Hubbard model)

Quantum Phase Transitions in Optical Lattices

- Observation of loss of superfluid coherence as system enters Mott insulator regime, through measurement of the *momentum distribution of trapped cold atoms*

M. Greiner *et al.*, **Nature** 415, 39 (2002)



U/t increases from (a) to (h)
Systems evolves from ***Superfluid***
to ***Mott insulator***

Supersolid (SS)

- Phase of matter displaying simultaneously

  Delocalization, dissipationless flow, off-diagonal long-range order, Bose condensate, broken gauge symmetry...

  Localization, shear modulus, diagonal long-range order, broken translational symmetry...

- One of "holy grails" of quantum many-body physics

  Vacancy scenario (Andreev and Lifshits, 1967)

  Long sought experimentally in solid ^{4}He *without* success (.. that is, until recently...*maybe*...)

  E. Kim and M. H.W. Chan, Science **305**, 1941 (2004)

Adsorbed ^{4}He films

- **Subject of experimental and theoretical research** for decades of *laser*

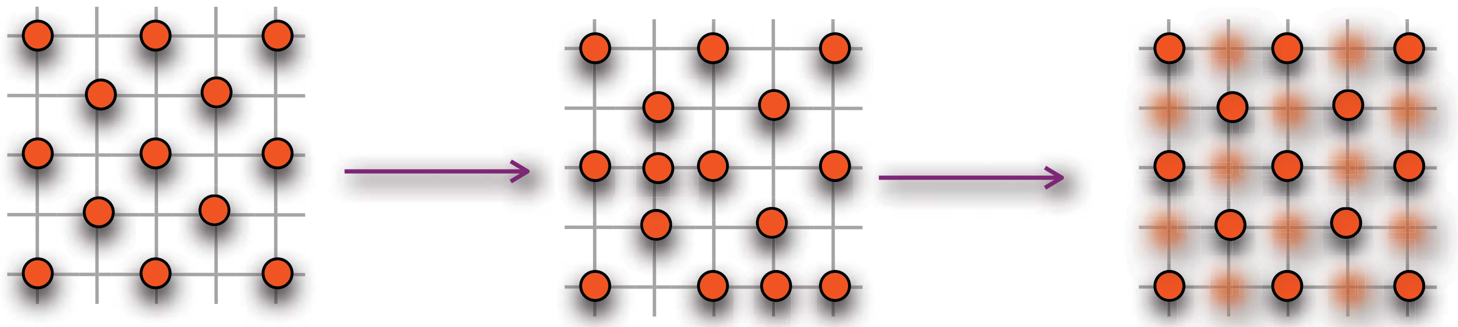
- Phase diagram of ^{3}He adorbed on graphite displays *dazzling* variety of phases (Bretz, Dash, 1973)

- Recent interest in possible realization of supersolid phase of ^{4}He on the same substrate (Saunders, 2008)

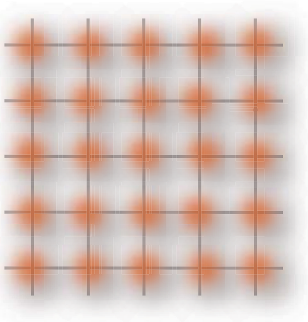
- Lattice model with correct geometry and even rather basic interactions may capure *essential* physical ingredients

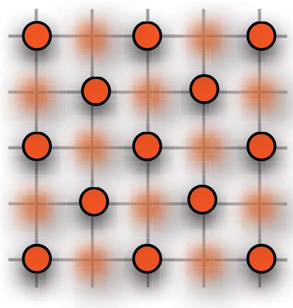
Search for SS phase on lattices

Strong on-site and nearest-neighbor repulsion → ***crystalline order***

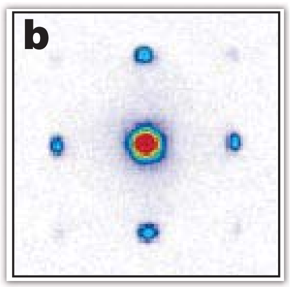


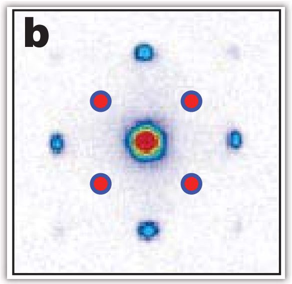
Crystal at half-filling **Doped** solid away from half-filling **Supersolid ?**



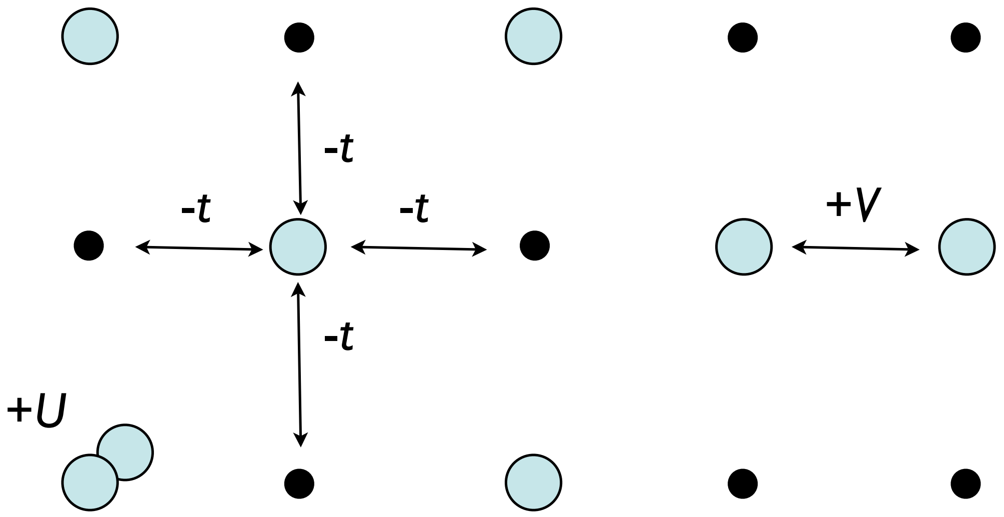


SS detectable experimentally through occurrence of peak associated to doubled unit cell





Models of Lattice Bosons



"Extended" Hubbard Model

$$\hat{H} = -t \sum_{\langle ij \rangle} \left(\hat{a}_i^\dagger \hat{a}_j + h.c. \right) + U \sum_i \hat{n}_i (\hat{n}_i - 1) + V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j$$

$$\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$$

- **Minimal** model of, e.g., ultracold gas of **bosonic** atoms in OL

U (energy cost of double occupation)
Nearest-neighbor potential ***V*** arising from strong *dipolar* interactions
Both *U and V "tunable"*

Hard Core limit

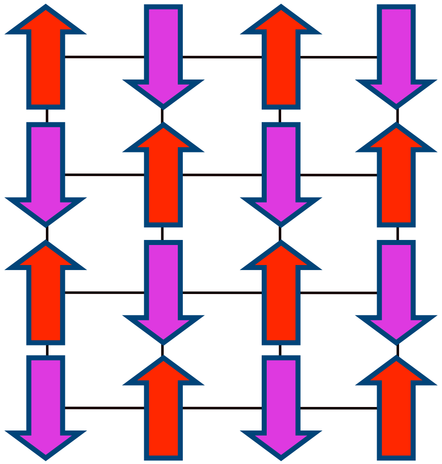
- $U \rightarrow \infty$, **no** double occupancy: analogy with *spin systems*

$$\hat{H} = -t \sum_{\langle ij \rangle} \left(\hat{a}_i^\dagger \hat{a}_j + h.c. \right) + V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j$$

boson language

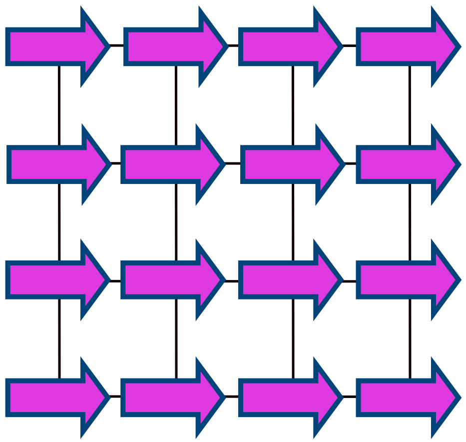
$$\hat{H} = -J_\perp \sum_{\langle ij \rangle} \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y \right) + J_z \sum_{\langle ij \rangle} \hat{S}_i^z \hat{S}_j^z$$

spin language



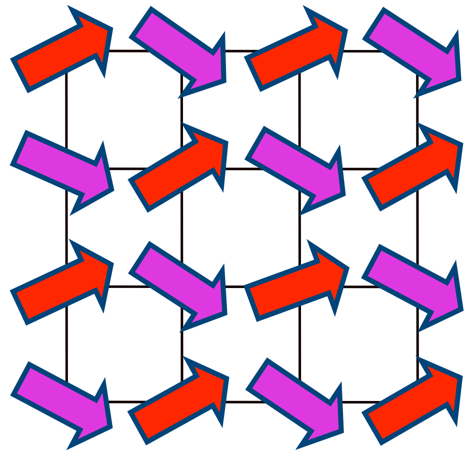
Crystal: $\mathbf{S}_Z \Leftrightarrow n$ order

breaks lattice symmetry



Superfluid: $\mathbf{S}_x \Leftrightarrow \langle \hat{a} \rangle$ order

breaks phase rotational symmetry



Supersolid: breaks both symmetries

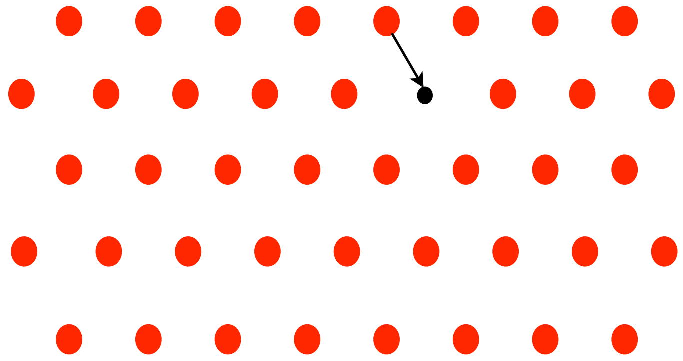
Phase diagram of lattice hard core bosons: theoretical approaches

- *Analytical*: mostly based on analogy with quantum spin systems
  mean-field theories
  spin-wave approximation
  series expansions
  variational calculations

- *Numerical*: mostly Quantum Monte Carlo
  T=0: Green Function Monte Carlo (GFMC)
  Finite T: Stochastic Series Expansion (SSE), Sandvik (1999)
  Worm Algorithm (WA), Prokof'ev et al. (1998)

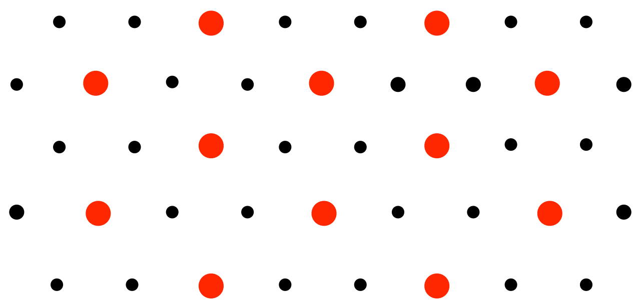
- *This work*: *WA, Pollet et al. (2007) -- grand canonical ensemble*

What is a lattice "supersolid" ?



Externally imposed lattice periodicity
one hard core boson per site and a small concentration of **mobile vacancies**:
Weakly interacting dilute Bose gas
superfluid at T=0, **not supersolid**

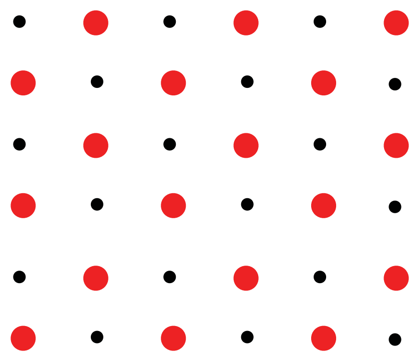
*More generally, supersolid $\neq$ superfluid with **externally imposed** density modulation (e.g., superconductor, or fluid layer of ^{4}He adsorbed over crystalline inert layer)*



Supersolid is defined with respect to a lattice of particles with different lattice constant than the one externally provided

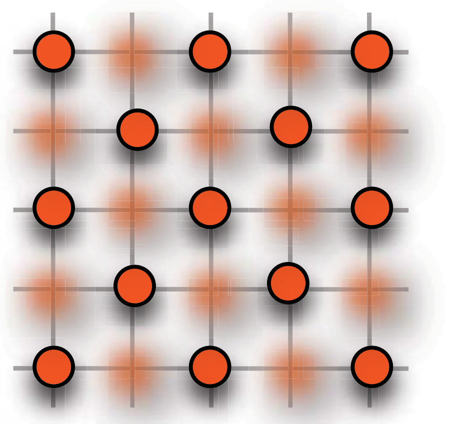
Simplest geometry: square lattice

Search for Supersolid phase near classical crystal



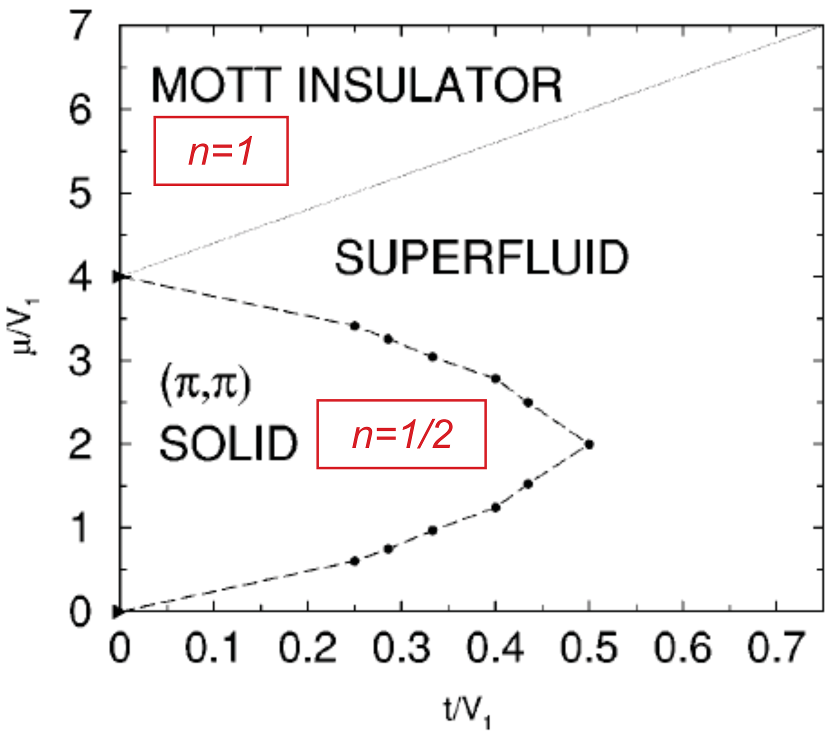
"checkerboard"
[(π,π)]

Classical ground state "checkerboard" crystal at half-filling
Quantum fluctuations destabilize it for $V < 2t$

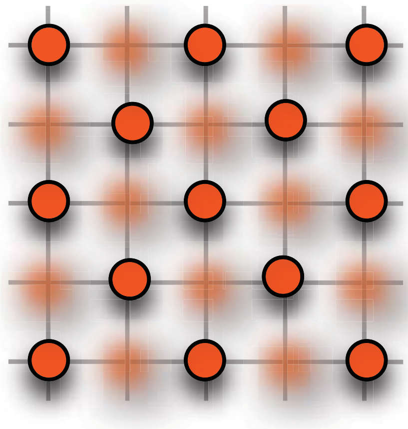


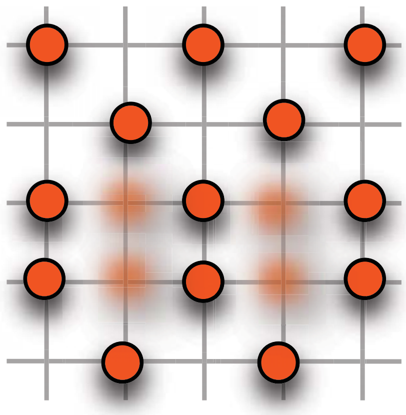
Hypothesis: Supersolid upon doping with vacancies or interstitials ?
(Simplest possible model of supersolid...)

Supersolid phase near half-filling ?



- <u>No SS phase exists near half-filling</u>
  First-order phase transition between "checkerboard" solid and superfluid



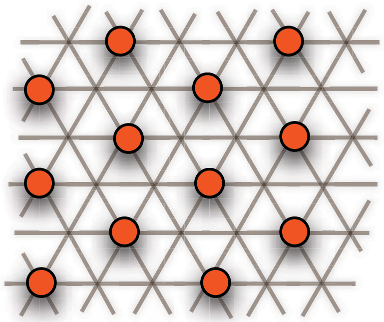


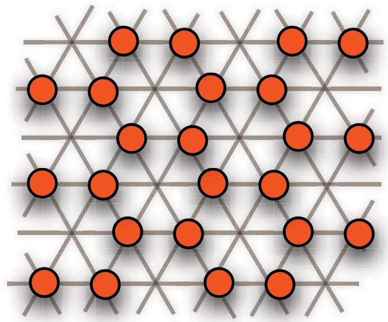
- Phase separation predicted in ^{4}He too (MB *et. al.*, 2007)
- Fairly *ubiquitous* (observed for different lattice geometries)
- It can render experimental identification of supersolid *quite tricky*

A different lattice geometry: triangular

- Classical limit: $t/V=0$

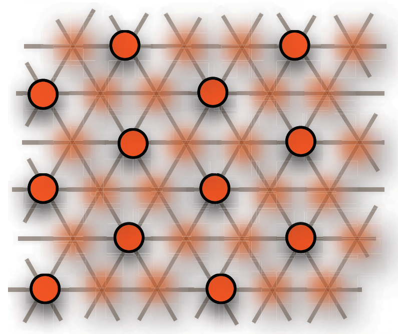
$\rho=1/3$





$\rho=2/3$

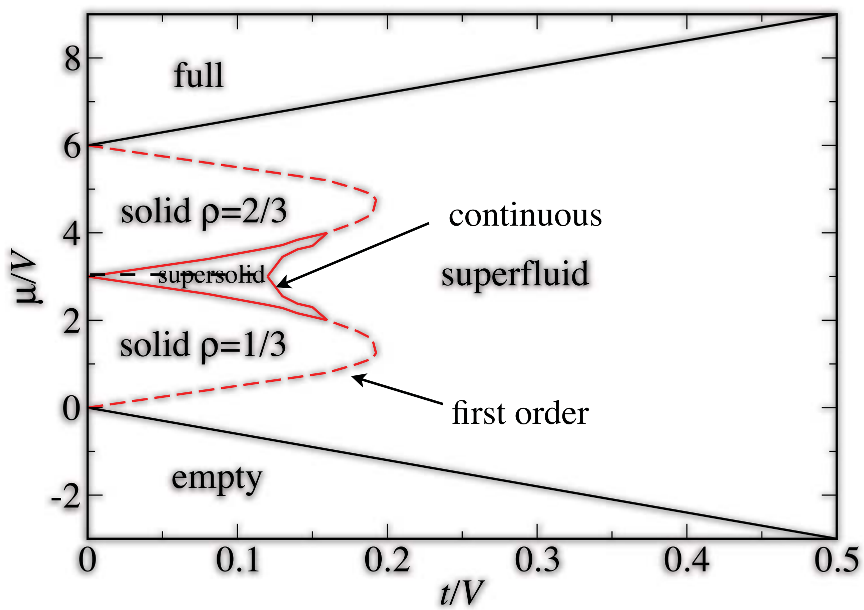
- Quantum system: *interstitial-* and/or *vacancy*-based SS near *commensurate* fillings

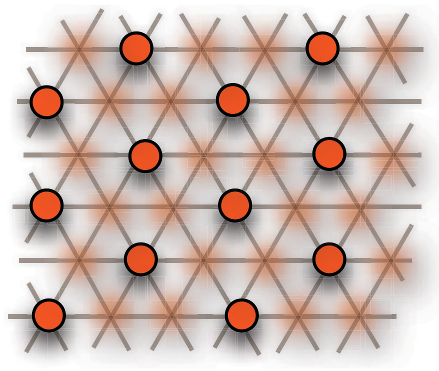


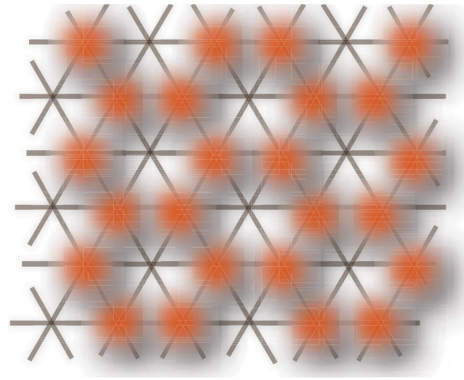
- All other fillings (except 0 and 1): *infinitely degenerate classical ground states*

    Order-by-Disorder scenario: degeneracy may be lifted by either *thermal* or *quantum* fluctuations, and order ensue

T=0 phase diagram







Wessel and Troyer, 2005
Heidarian and Damle, 2005
Melko *et al.*, 2005
MB and Prokof'ev, 2005

First-order phase transition between Superfluid and Commensurate crystal below density 1/3 (above 2/3) (*vacancy side*)

Continuous phase transition between commensurate crystal and **Supersolid** above density 1/3 (below 2/3) **and** between Supersolid and Superfluid

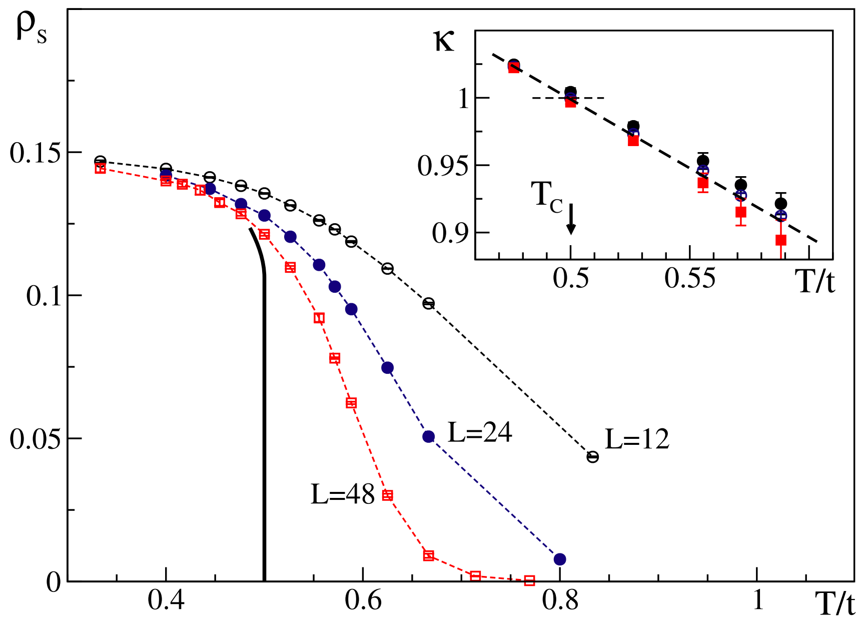
Quantum first-order phase transition at half-filling between two interstitial supersolids

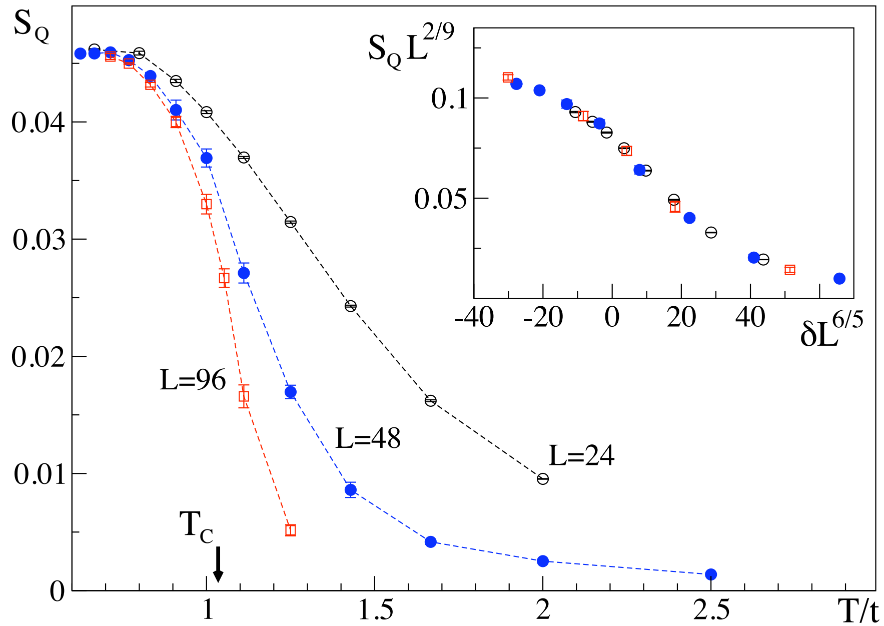
Supersolid phase on **interstitial** side only (*particle-hole symmetry*)

S. Wessel's talk on Thursday

Finite-*T* phase diagram

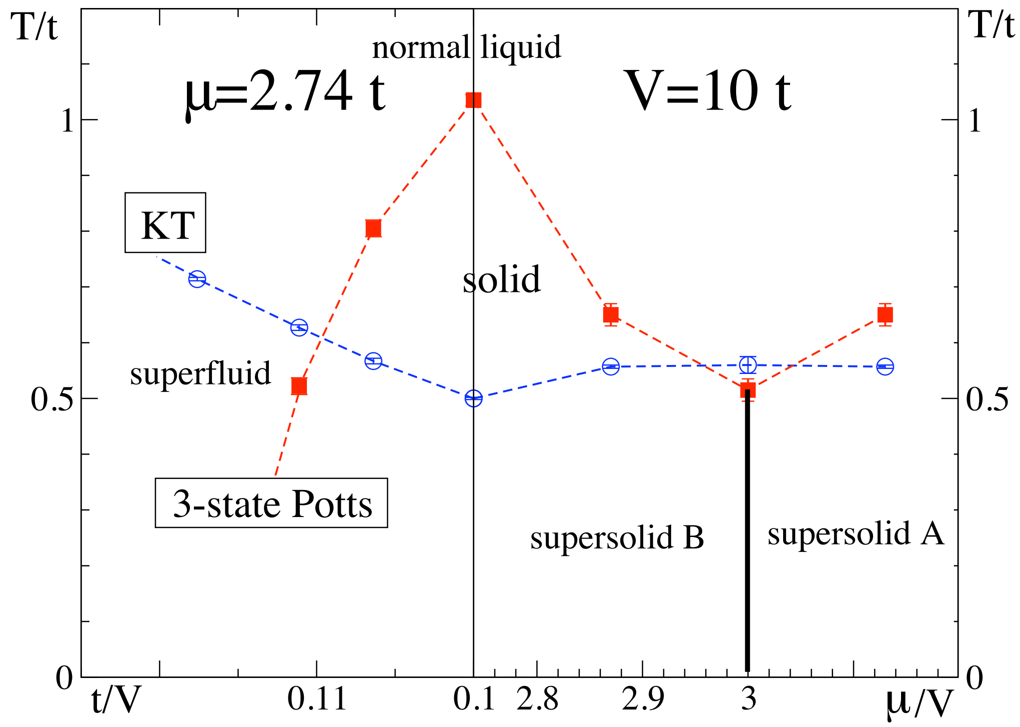
MB and N. Prokof'ev, 2005





- Normal-to-superfluid transition in the solid phase predicted to be of the same character as in the liquid (Toner *et al.*, 2006)
- Scaling of numerical data for ρ_S near respective T_c consistent with **Kosterlitz-Thouless** universality class
- Scaling of data for S_q (for q=(4π/3,0)) near transition consistent with **3-state Potts** (liquid-solid) universality class (three equivalent sublattices)

Finite-*T* phase diagram
(cont'd)

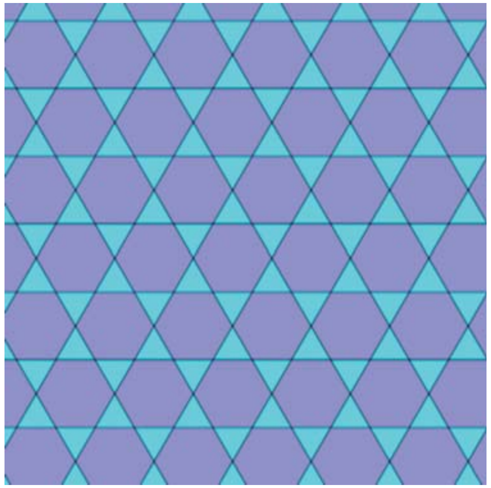


- Intersecting *2nd order* KT and Potts lines away from half-filling
  - *order parameters **not** strongly interacting*
- **No** evidence of algebraic order at half-filling
  - *Transition temperatures for KT and Potts coincide, within statistical errors of calculations*

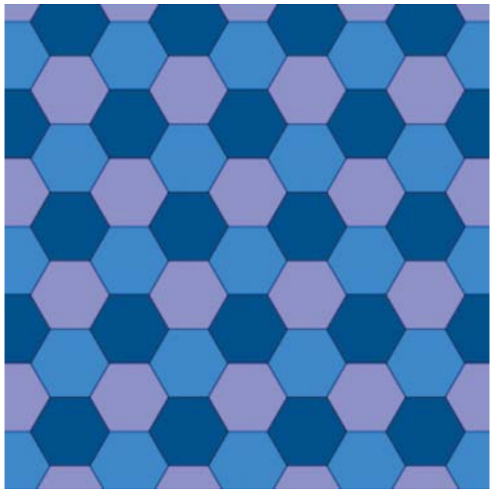
- Supersolid phase can occur both when a superfluid is cooled, as well as through the superfluid transition of a normal solid
  - *Predictions testable experimentally in OLs*

What about other lattice geometries ?

Reminder: hard core bosons and nearest-neighbor hopping ***only***



No Supersolid phase on *Kagome* lattice
Melko *et al*, 2007



No Supersolid phase on *Honeycomb* lattice
Wessel, 2007

General Remarks

- How does one "beat" phase separation on all of these geometries ?

  Soft Core onsite interactions **--** Sengupta *et al.* (2005)

  Next-nearest neighbor hopping -- Melko *et al.* (2008)

  Next-nearest neighbor repulsion ("striped" SS on square lattice) Batrouni and Scalettar (2000)

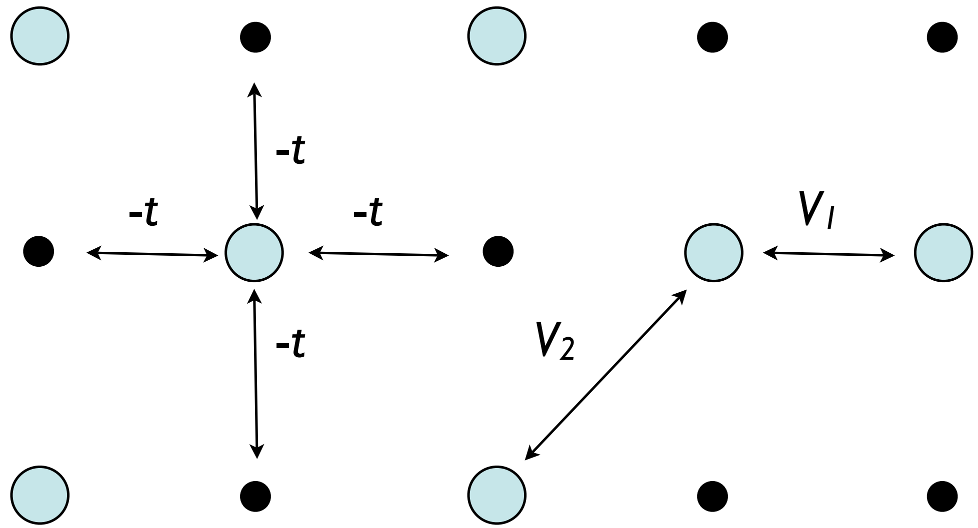
- **Empirical** observations

  Supersolid ***present*** *when connected ("percolating") path exists for interstitials to roam freely (triangular lattice)*

  Supersolid ***not*** *observed at* ***commensurate*** *density (superfluid response vanishes)*

- What about ***vacancy*** supersolidity ? Why ***interstitials*** only ?

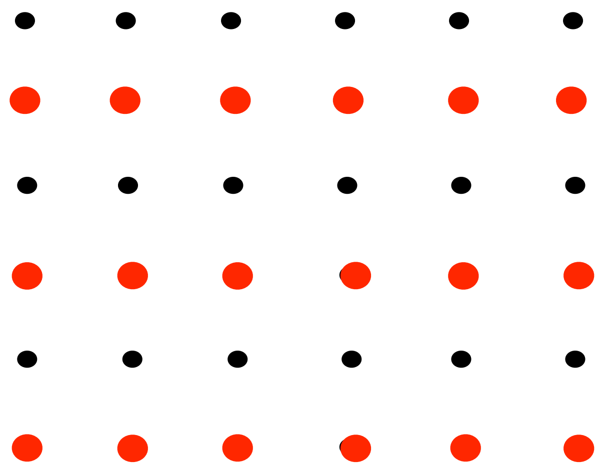
Generalization: hard core and next nearest neighbor interactions



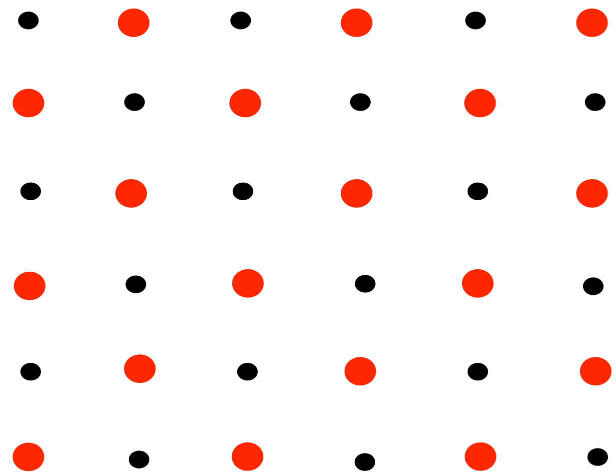
- *Aims of this study*:
  search for supersolid phases
  study evolution from one supersolid phase to another
  assess stability of **vacancy** and **interstitial** supersolid

  Similar study: Cao, Chen, Melko and Wessel (2008) [included next nearest neighbor hopping *t'* as well]

Classical crystals at half filling



stripe [(0,π), (π,0)] $V_1 > 2V_2$

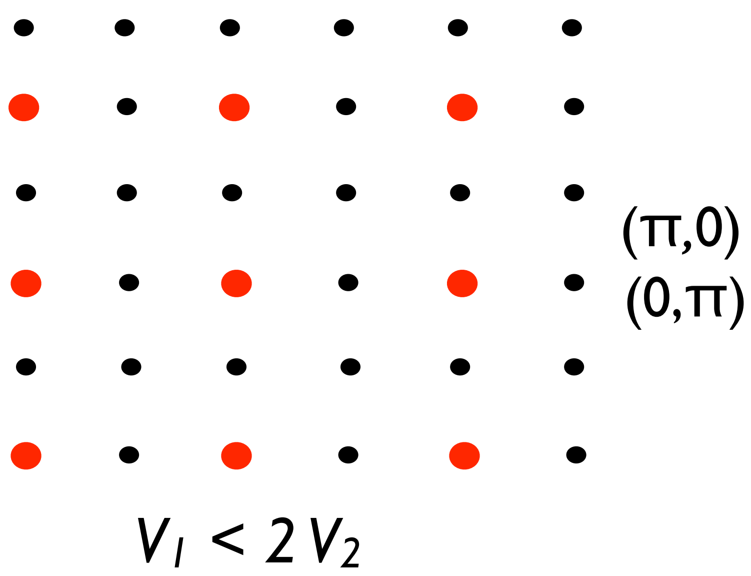


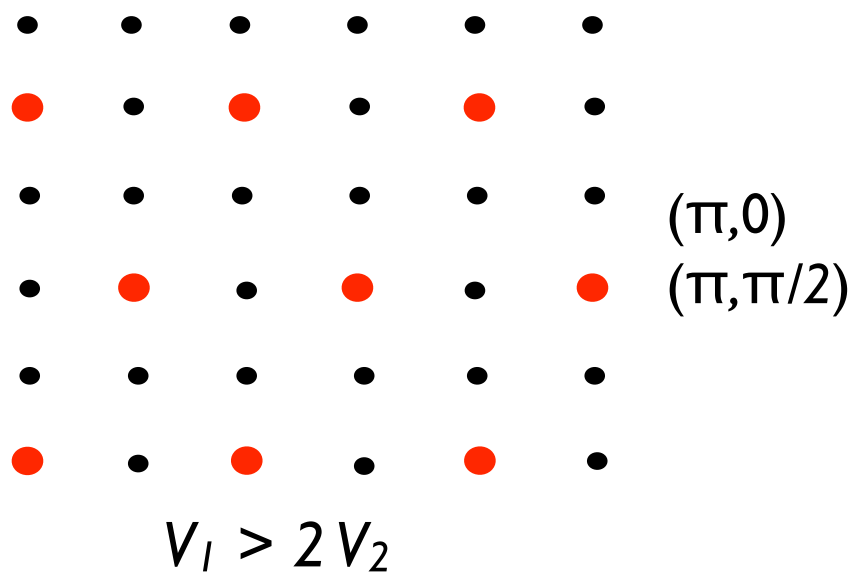
checkerboard [(π, π)] $V_1 > 2V_2$

Striped supersolid phase exists in the quantum system, near half-filling for sufficiently large V_2

No checkerboard supersolid observed (Batrouni and Scalettar, 2000)

Classical crystals at quarter filling



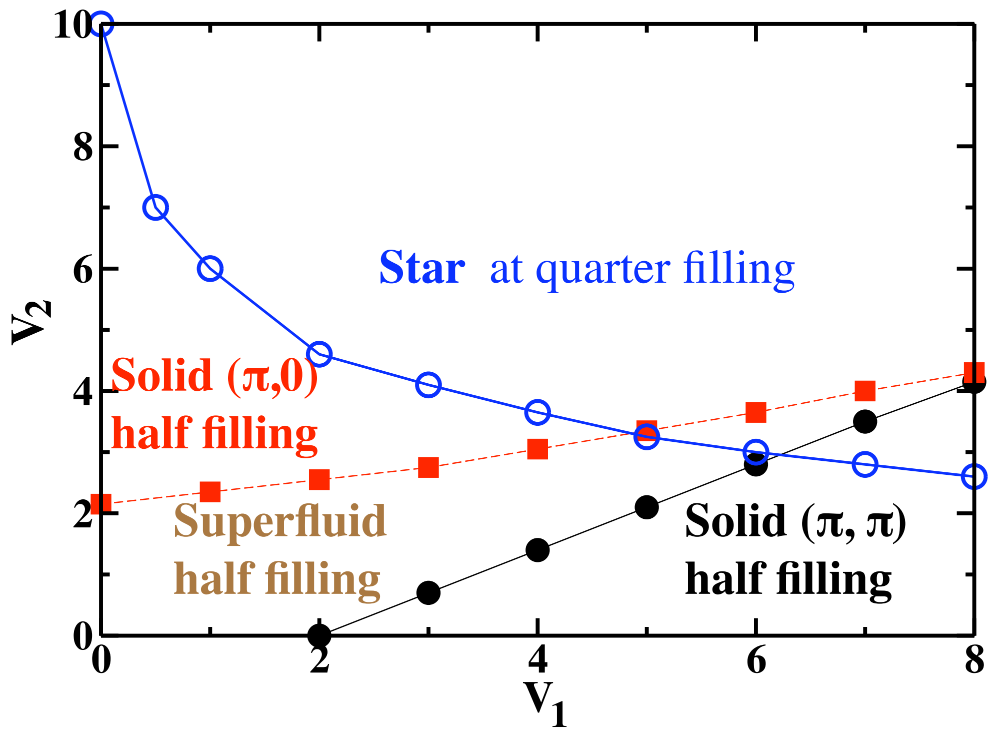


Crystal phase ("star") present at quarter-filling

Lower density possibly more relevant to adsorbed commensurate helium films

Two equivalent classical ground states -- degeneracy **lifted** by quantum fluctuations in favor of either (left) or (right) depending on V_2/V_1

Ground state phase diagram



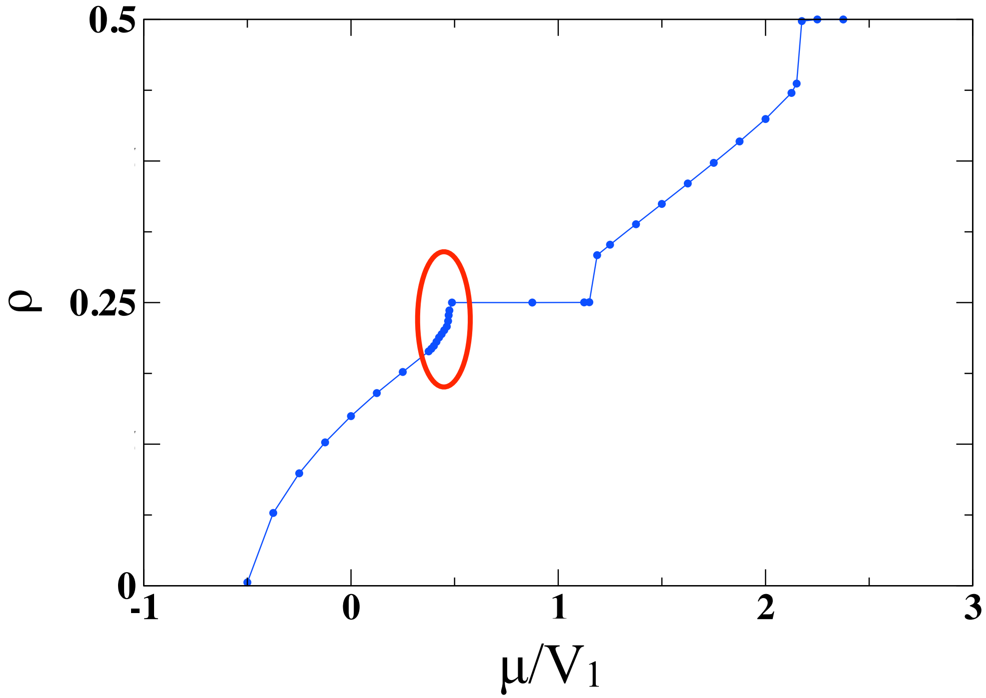
Three different regimes can be identified, in the presence of the "star" crystal at quarter filling, differing by the phase at half filling:

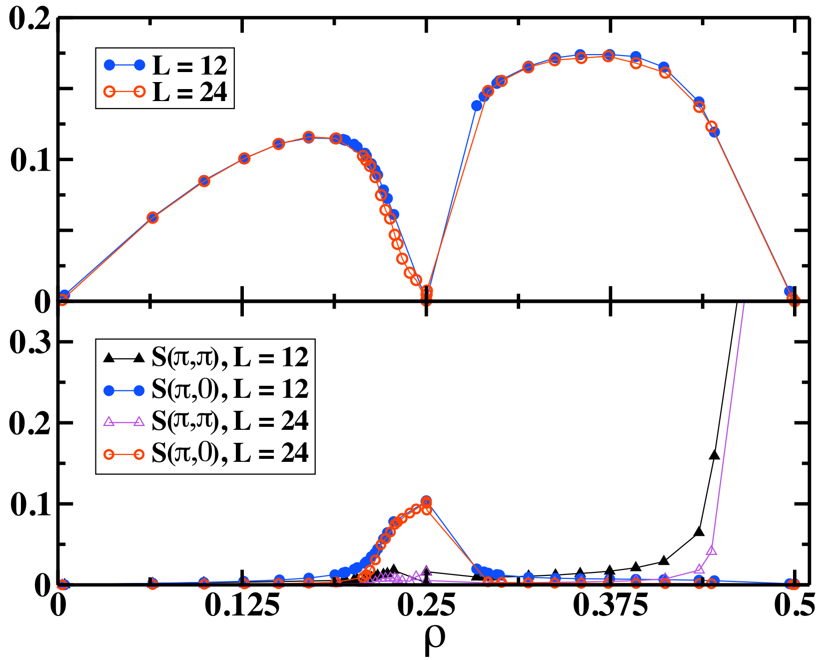
Superfluid

Checkerboard (π,π)

Striped (π,0) *or* (0, π)

Case 1: Checkerboard solid at half filling



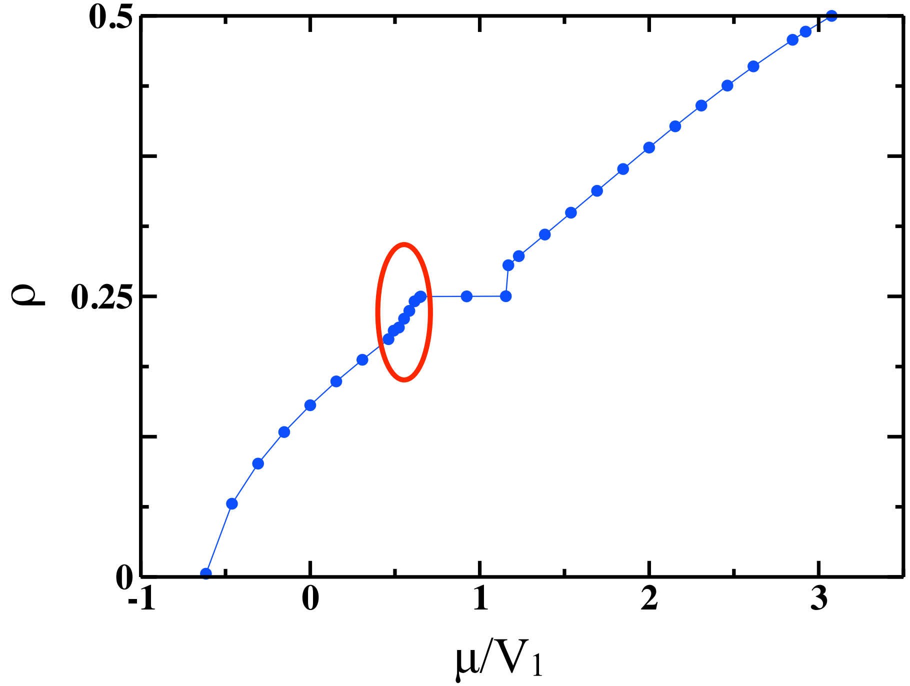


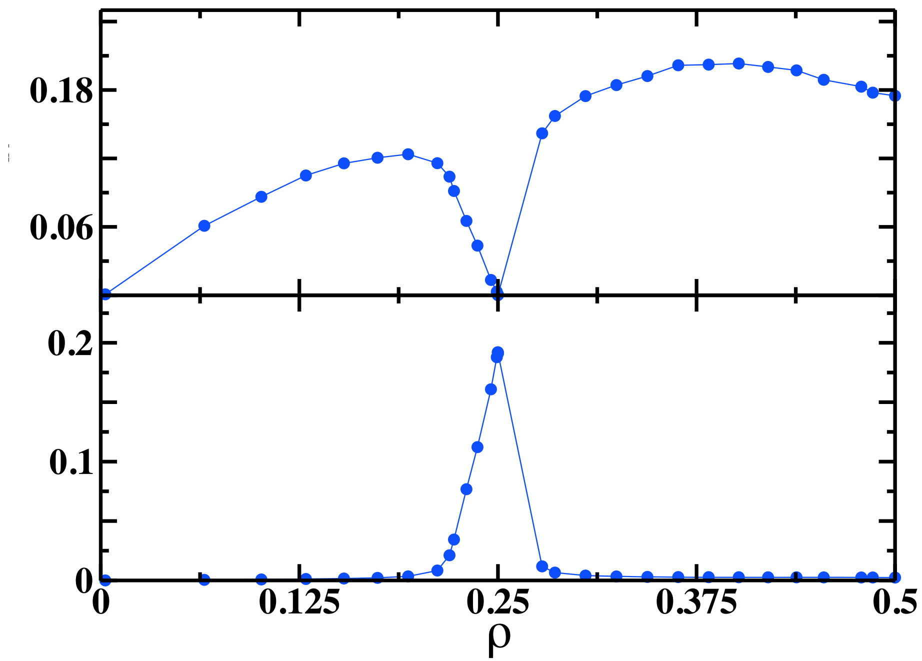
Vacancy Supersolid present below quarter filling

First-order phase transition between star crystal and (reentrant) Superfluid above quarter-filling

First-order phase transition between reentrant Superfluid and checkerboard crystal at half filling

Case II: Superfluid at half filling

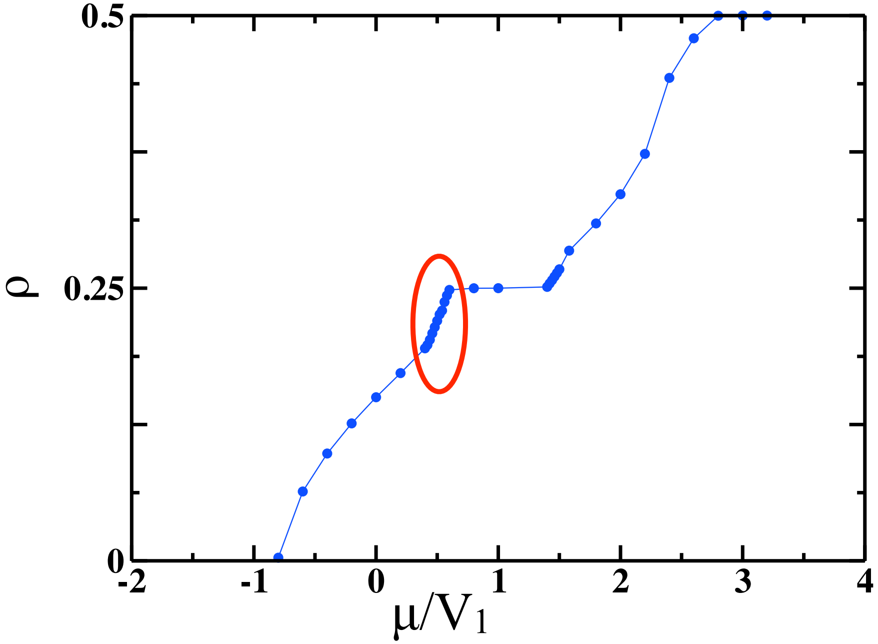


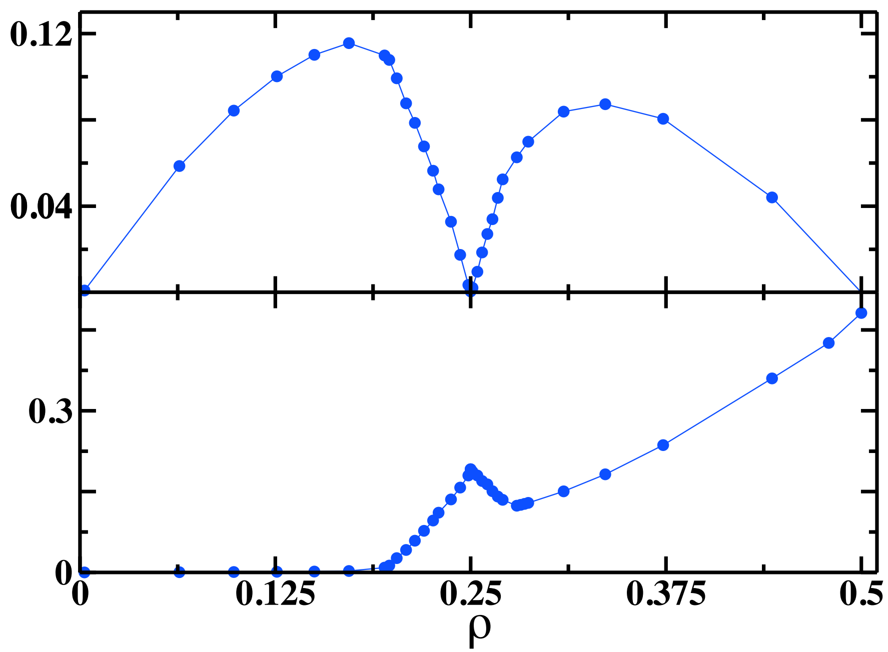


Vacancy Supersolid present below quarter filling

First-order phase transition between star crystal and (reentrant) Superfluid above quarter-filling

Case III: Striped crystal at half filling





Vacancy Supersolid present below quarter filling

Continuous phase transition between star crystal and **Insterstitial Supersolid** above quarter-filling

(First order ? Continuous ?) phase transition between **Star** and **Stripe Supersolid** above quarter filling [Chen, Cao, Melko and Wessel, 2008]

Summary of results

Vacancy Supersolid **always present** below quarter filling

Interstitial Supersolid **only** present if phase at half filling is stripe crystal

Upon doping the star crystal, symmetry is spontaneously broken with the selection of either the (0,π) *or* (π,0) *stripe crystal*

In this case, the ground state of the system is ***supersolid*** *below quarter filling and above quarter filling all the way to half-filling*

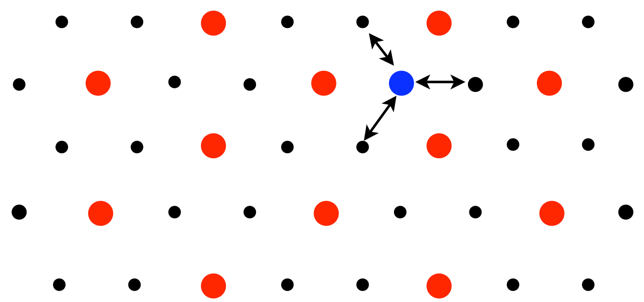
Commensurate supersolid phase **not** observed

Superfluid density vanishes at quarter and half filling

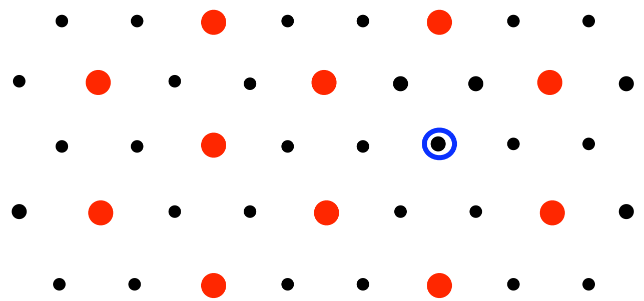
Claim of commensurate supersolid at quarter filling by Ng and Chen (2007) *likely result of incorrect finite-size scaling analysis*

When does one see a defect supersolid ?

In all cases in which vacancy/interstitials form a homogeneous phase (i.e, no phase separation between commensurate crystal and superfluid occurs), defects can move **without frustration** through the lattice, along a *isoenergetic path*



Interstitial particle in 1/3 phase on triangular lattice moves in a constant potential



Vacancy in 1/3 phase can hop to adjacent lattice site going through a configuration of increased potential *V*

Same considerations explain absence of supersolid on honeycomb and kagome lattices, and why it is recovered upon introduction of *t'* term

Conclusions

Vacancy and interstitial Supersolid phases can be predicted based on simple geometrical and energetic considerations -- existence of iso-energetic paths for defects to move around the system

Otherwise, phase separation between non-superfluid commensurate crystal and superfluid ensues

Long-range interactions generally strengthen Supersolid phase, as observed on the square lattice.

Tunability of interaction might be achievable in Optical lattices -- less clear what this says about likelihood of observing Supersolid phases in adsorbed films

Commensurate Supersolid phases **not** observed in any geometry nor for any relative interaction strength

Theorem proved by Prokof'ev and Svistunov in 2005 for continuous-space systems -- need not hold for lattice systems as well

Reference: L. Dang, MB and L. Pollet, ArXiv-0803.1116