Workshop on Supersolid 2008

18 - 22 August 2008

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*
  

- **Atomic dynamics** in OL studied experimentally
  

- **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


$U/t$ 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...)

Adsorbed $^4$He films

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

• Phase diagram of $^3$He adsorbed 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 capture *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

- 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”

“Extended” Hubbard Model

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

\[
\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i
\]
Hard Core limit

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

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

**boson language**

$$\hat{H} = -J_\perp \sum_{\langle ij \rangle} \left( \hat{S}^x_i \hat{S}^x_j + \hat{S}^y_i \hat{S}^y_j \right) + J_z \sum_{\langle ij \rangle} \hat{S}^z_i \hat{S}^z_j$$

**spin language**

Crystal: $S_Z \leftrightarrow n$ order
breaks lattice symmetry

Superfluid: $S_x \leftrightarrow \langle \hat{a} \rangle$ 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

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

“checkerboard”
$[(\pi,\pi)]$

Hypothesis: Supersolid upon doping with vacancies or interstitials?
(Simplest possible model of supersolid...)
Supersolid phase near half-filling?

- No SS phase exists near half-filling
  - 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: $t/V = 0$

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

- 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
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
• 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 $\rho_s$ near respective $T_c$ consistent with Kosterlitz-Thouless universality class
• Scaling of data for $S_q$ (for $q=(4\pi/3,0)$) 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

\[ \text{stripe } [(0, \pi), (\pi, 0)] \quad V_1 > 2 V_2 \quad \text{checkerboard } [(\pi, \pi)] \quad V_1 > 2 V_2 \]

**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

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

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 $V_2/V_1$. 

Crystal phase (“star”) present at quarter-filling

Lower density possibly more relevant to adsorbed commensurate helium films
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** ($\pi,\pi$)
- **Striped** ($\pi,0$) or $(0,\pi)$
**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 **Interststitial 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 $(0,\pi)$ or $(\pi,0)$ 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 an 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