KITP Program: Moments and Multiplets in Mott Materials

Supersolids in Lattice Boson Models

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arXiv:0708.1807v1

Supersolid

Is it possible to have BEC in a Solid? (Quantum solid: ^{4}He)

ODLRO (Superfluid) DLRO (Crystal Order)

$$\left\langle \widehat{\Psi}(\vec{r}) \right\rangle \neq 0, S_\rho(Q) \neq 0$$

In an ideal commensurate boson crystal at T=0, $N_{atom}=\mathbf{Z}^*N_{lattice}$

$\left\langle \widehat{\Psi}(\vec{r}) \right\rangle \neq 0, S_\rho(Q) \neq 0$ is impossible!

Argue T>0 case is also impossible.

End of Story?

Penrose and Onsager, P.R. 104, 576 (1956).

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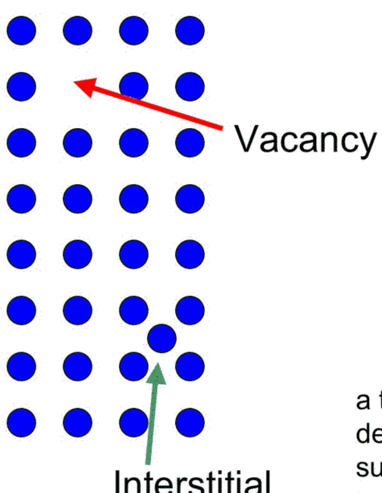
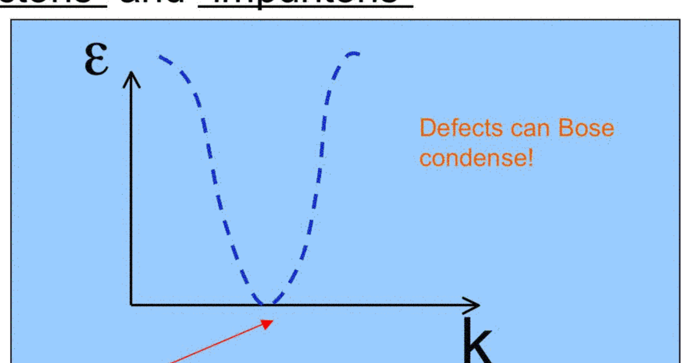
Defect Condensation

- Andreev and Lifshitz, proposed "zero-point vibration". → "defectons" and "impuritons"





a tiny density of quantum defects can give superfluidity while preserving crystalline order

Background crystal
+ Defect superflow
= Supersolid

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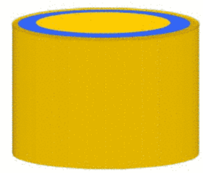
Andreev and Lifshitz, Sov. Phys. JETP **29**, 1107
Chester, PRA, **2**, 250

PRL **25**, 1543 (1970)

Can a Solid Be "Superfluid"?

A. J. Leggett
School of Mathematical and Physical Sciences, University of Sussex, Falmer, Brighton, Sussex, England
(Received 15 September 1970)

It is suggested that the property of nonclassical rotational inertia possessed by superfluid liquid helium may be shared by some solids. In particular, nonclassical rotational inertia very probably occurs if the solid is Bose-condensed as recently proposed by Chester. Anomalous macroscopic effects are then predicted. However, the associated superfluid fraction is shown to be very small (probably $\lesssim 10^{-4}$) even at $T = 0$, so that these effects could well have been missed. Direct tests are proposed.



Leggett proposed to detect supersolid by measuring NCRI (Nonclassical rotational inertia)

$I(T) = I_{classical}[1-f_s(T)]$, $f_s(T)=(\rho_s/\rho)$ is the "superfluid fraction"

Estimate $\rho_s/\rho \approx 10^{-4}$, too small to observe (at that time).

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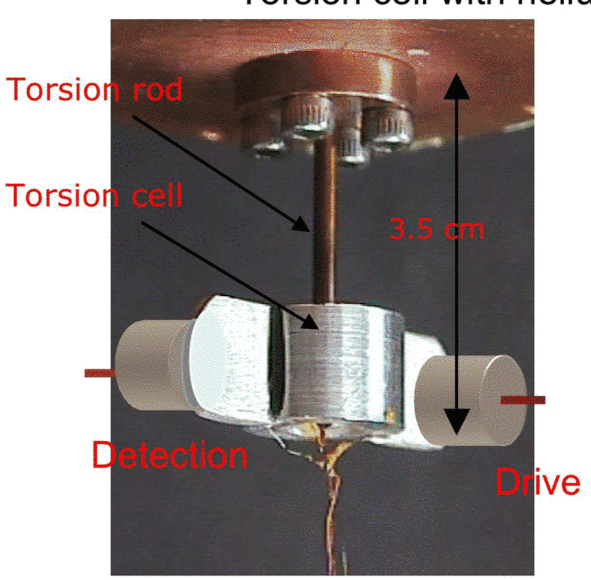
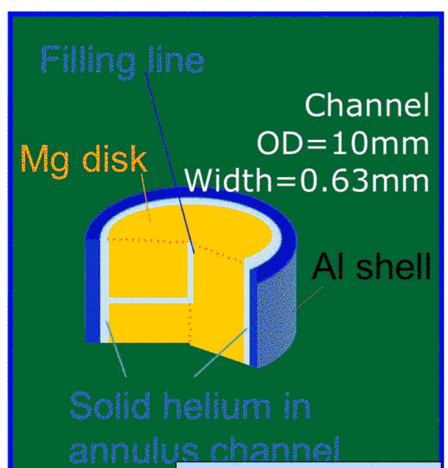
Supersolid in ^{4}He

Torsion cell with helium in annulus





$$\tau_o = 2\pi\sqrt{\frac{I}{K}}$$

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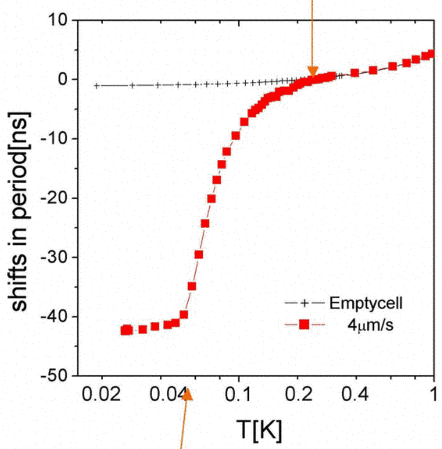
Kim and Chan, Science 305, 1941 (2004);
Nature 427, 225 (2004).

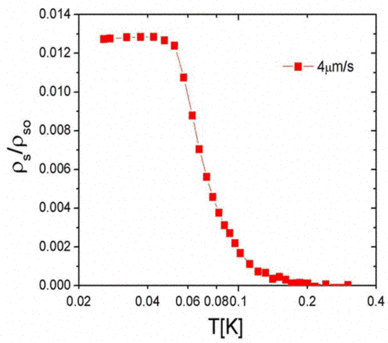
Supersolid in ^4He

T_c=0.175K



Saturate at 0.04K

The supersolid fraction is on the order of 1.3%



$$\tau_o = 2\pi\sqrt{\frac{I}{K}}$$

$I(T) = I_{classical}[1-f_s(T)]$

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Supersolid in ^4He

Existence : Phase separation? Surface phenomenon?

Mechanism : Defect/Impurity condensate? (Annealing, doping with He^3) Grain boundary superfluidity

Does supersolid phase exist in a Perfect Crystal (lattice)?

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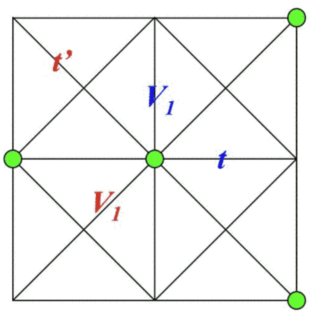
Hard-core Boson Hubbard model

$$\mathcal{H} = \sum_{ij} -t_{ij}(b_i^\dagger b_j + \text{c. c.}) + \sum_{ij} V_{ij} n_i n_j - \mu \sum_i n_i$$

XXZ model

$$\mathcal{H} = J\sum_{i,j}\left[\Delta S_i^z S_j^z + \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)\right] - h\sum_i S_i^z$$



$$S^+ = b^\dagger,\ S^- = b,\ S_z = (b^\dagger b - \frac{1}{2})$$

$$J_x = -2t, J_x' = -2t'$$
$$J_z = V_1, J_z' = V_2$$
$$h = \mu - \frac{1}{2}(zV_1 + z'V_2)$$

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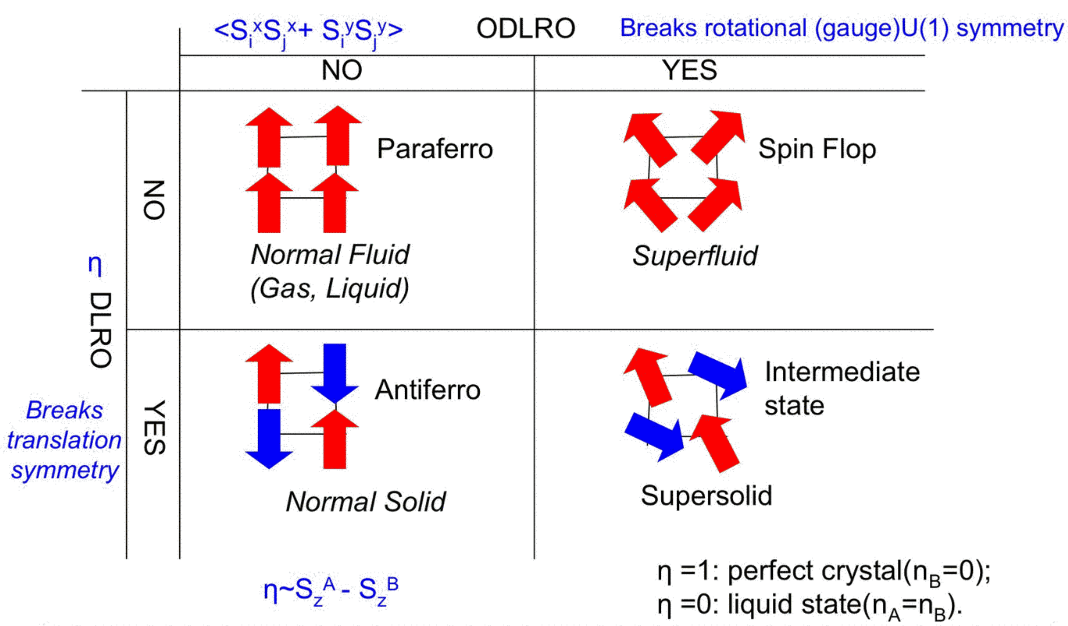
Quantum Lattice Gas



η =1: perfect crystal(n_B=0);
η =0: liquid state(n_A=n_B).

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Matsuda and Tsuento, Supp. Prog. Theo. Phys. 46, 411 (1970)

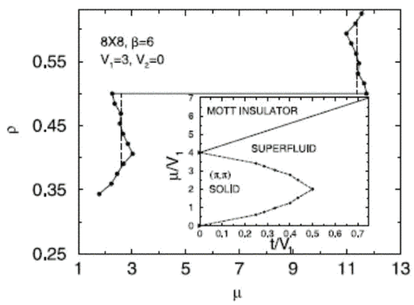
Results of numerical simulations

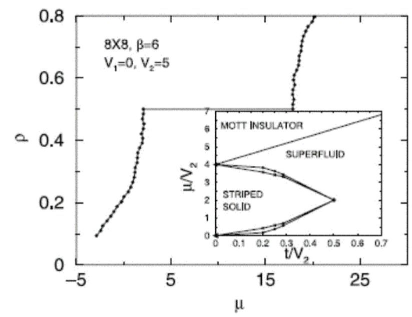
Hard-core Boson model

$$H = -t\sum_{\langle ij\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + V_1\sum_{\langle ij\rangle}\hat{n}_i\hat{n}_j + V_2\sum_{\langle\langle ik\rangle\rangle}\hat{n}_i\hat{n}_k .$$

With N.N. interaction, the SS phase is unstable against phase separation.

With N.N.N. interaction, a stable striped SS is found.





Batrouni *et al.*, PRL 84, 1599 (2000)

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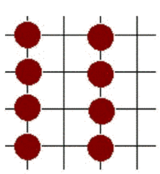
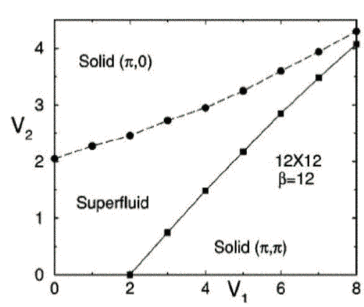
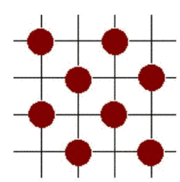
Half-filling

F. Hebert *et al.*, Phys. Rev. B **65**, 014513 (2002)

- V1 dominant, *checkerboard solid* (π,π).
- V2 dominant, *striped solid* (π,0).
- In between, *superfluid*.







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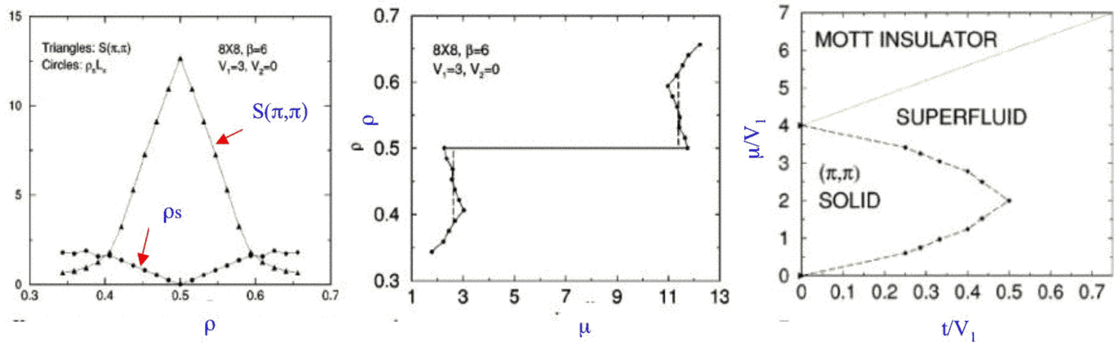
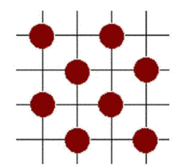
Doped System (V_2=0)



- Coexistence of S(π,π) and superfluidity.
- Negative compressibility $d\rho/d\mu$ indicates the phase is unstable. *Phase separation*.



F. Hebert *et al.*, Phys. Rev. B **65**, 014513 (2002)

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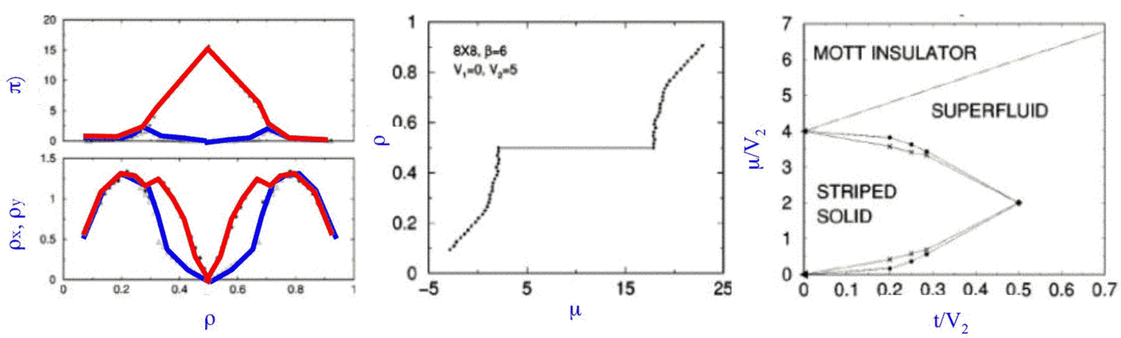
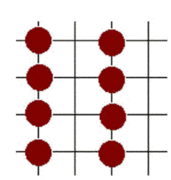
Doped System (V_1=0)



- Superfluidity in x and y direction are both finite, not through one-dimensional channels. However, strong anisotropy.
- Positive compressibility, and the phase is stable.
- A stable supersolid is observed!



F. Hebert *et al.*, Phys. Rev. B **65**, 014513 (2002)

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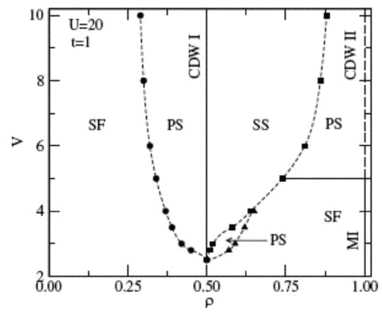
Soft-core Boson model

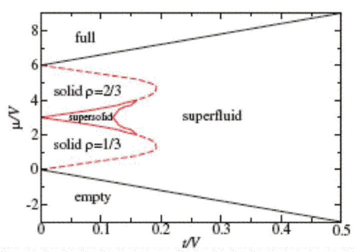
$$H = -t\sum_{\langle i,j\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) - \mu\sum_i n_i + V\sum_{\langle i,j\rangle} n_i n_j + \frac{U}{2}\sum_i n_i(n_i - 1),$$

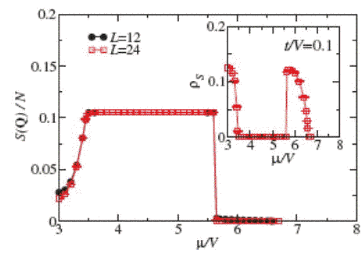
P. Sengupta *et al.*, PRL 94, 207202 (2005)



Supersolid phase of hard-core boson is found to be stabilized in *frustrated triangular lattice* by mechanism of order by disorder

S. Wessel *et al.*, PRL 95, 127205; D. Heidarian *et al.*, PRL 95, 127206; R.G. Melko *et al.*, PRL 95 127207 (2005)





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VMFT, QMC

- Gutzwller variational MF $\quad |\phi_g\rangle = \prod_i f(n_i)|n_i\rangle$
- Quantum Monte Carlo (SSE)

Superfluid density: $\quad \rho_s = \frac{\langle W^2\rangle}{2t\beta L^{d-2}}$

Structure factor: $\quad S(k) = \sum_r e^{ikr}\langle n(r_0)n(r_0+r)\rangle$

M. Gutzwiller, Phys. Rev. Lett. 10, 159 (1963)
A.W. Sandvik and J. Kurkijärvi, PRB 43, 5950 (1991).

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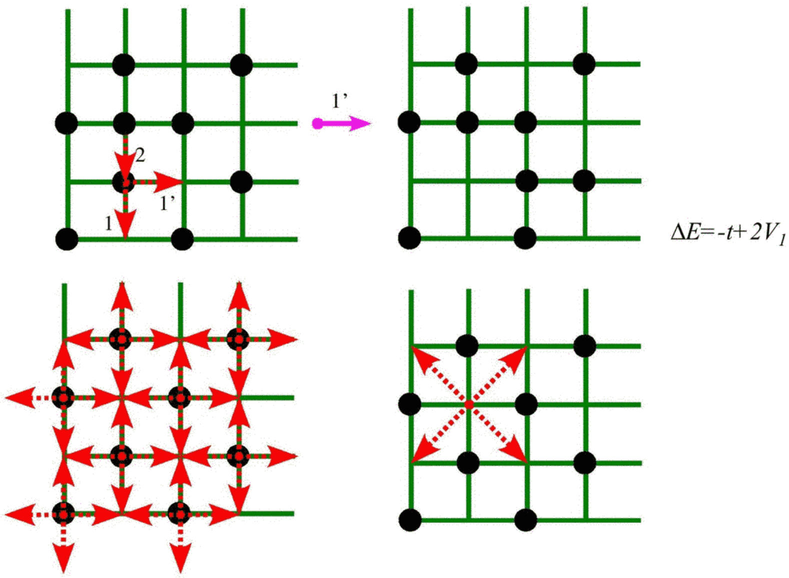
Effects of nnn hopping



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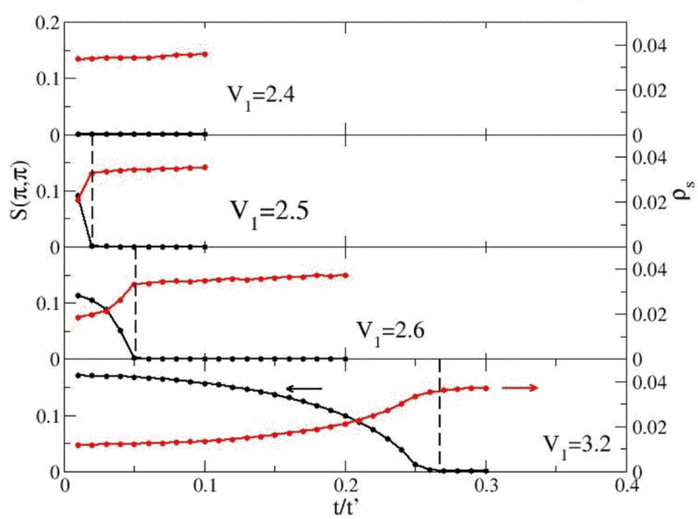
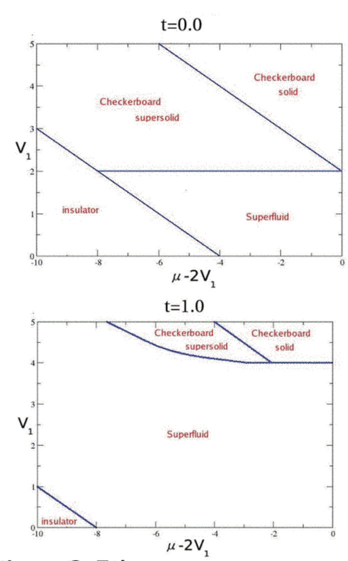
Finite nn hopping t ($V_2=0$)





- Supersolid state emerges when V_1 is larger than 2.5t'.
- When t turns on, supersolid melts into a superfluid.
- What is the effect of nnn repulsion V_2?

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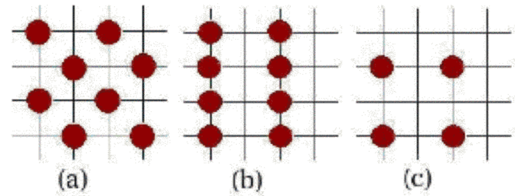
Solid States



Structure factor	checkerboard	striped	quarter-filled
$S(\pi,\pi)$	$\neq 0$	0	$\neq 0$
$O_x + O_y$	0	$\neq 0$	$\neq 0$
$\lvert O_x - O_y \rvert$	0	$\simeq O_x + O_y$	0

$$S(\mathbf{q}) = \frac{1}{N}\sum_{\mathbf{l}} e^{i\mathbf{q}\cdot\mathbf{l}}\langle n_{\mathbf{j}} n_{\mathbf{j+l}}\rangle \qquad S(\pi,\pi),\ \ Ox = S(\pi,0),\ \ Oy = S(0,\pi)$$

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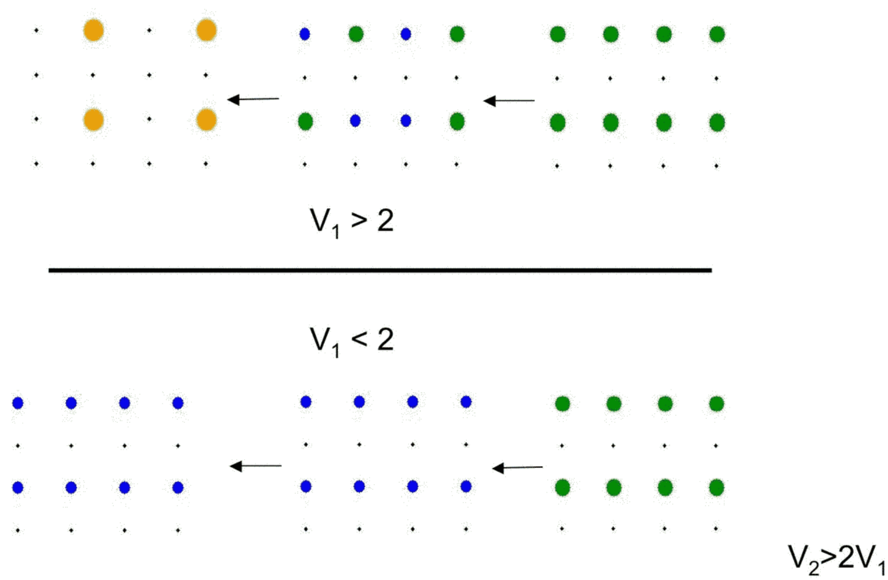
Doping toward ρ=0.25



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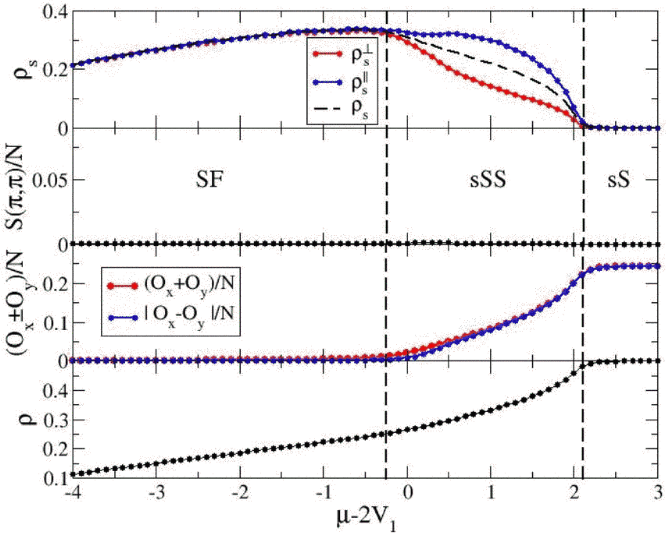
Phases at small V_1



$t=0.9, t'=0.1$
$V_1=1.0, V_2=4.5$
16x16

- Striped solid(sS) becomes supersolid (sSS) upon doping.
- sS melts into superfluid(SF).
- No significant structures at ρ=0.25.
- Strong anisotropy in striped supersolid

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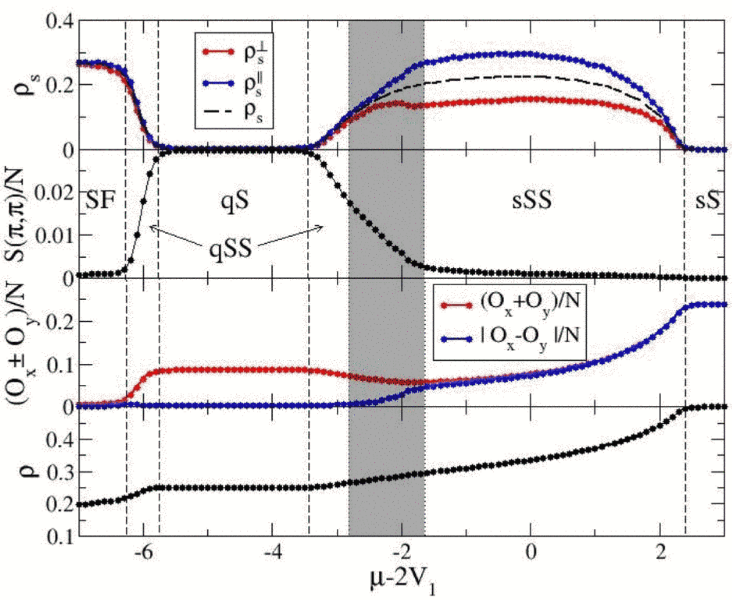
Phases at large V_1



$t=0.9, t'=0.1$
$V_1=4.5, V_2=4.5$
16x16

- A stable quarter-filled solid(qS) is observed at ρ=0.25
- Quarter-filled supersolid(qSS) emerges when system is doped away from ρ=0.25

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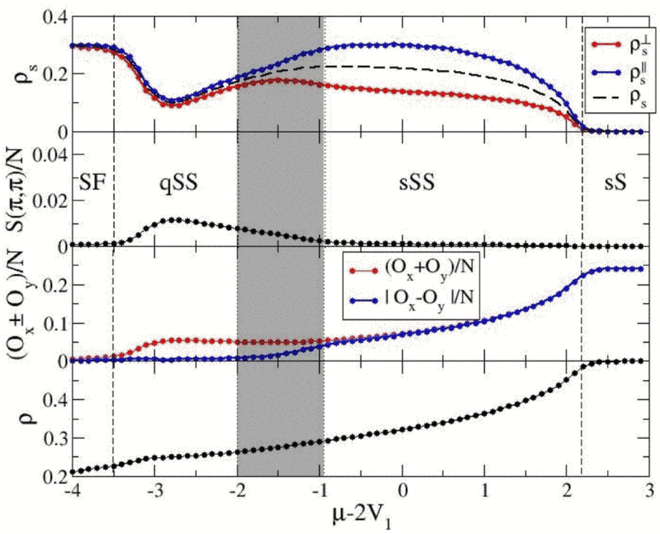
Phases at intermediate V_1



$t=0.9, t'=0.1$
$V_1=3.0, V_2=4.5$
$16x16$

- Finite size scaling shows superfluidity vanishes near ρ=0.25 → solid state
- Grand canonical ensemble simulation, ρ is not fixed
- Canonical ensemble results

- A dip in superfluid density near ρ=0.25, but still finite.
- Is it possible to have supersolid at exactly ρ=0.25?

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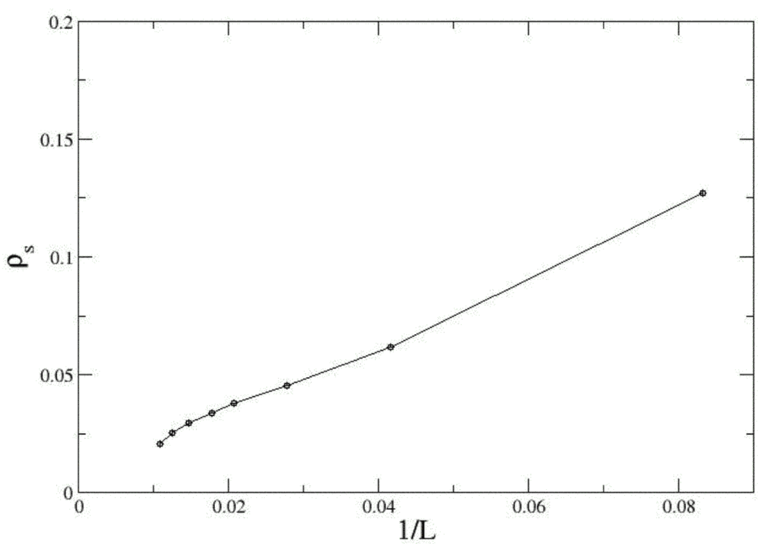
Finite Size Scaling at fixed ρ=1/4



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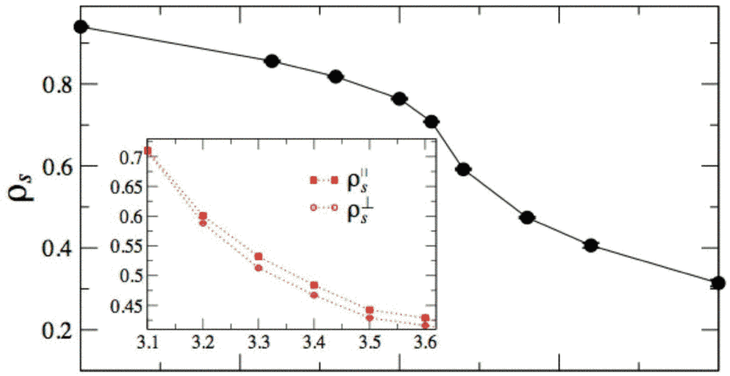
Triangular Lattice t-V_1-V_2 model



Melko et al, PRB 74, 214517 (2006)

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Summary

- At the limit where V_1 is dominant, we observe a *stable checkerboard supersolid* when t' is introduced.
- When V_2 is dominant, but V_1 finite, we observe a *quarter-filled solid* and *corresponding supersolid* phase near ρ=0.25.
- We observe a transition/crossover from quarter-filled solid and striped solid via intermediate supersolid state(s).
- Suggests a Defect Condensation mechanism, but not the simple microscopic phase separation picture.
- Details of the transitions/crossovers? Finite temperature? Long-range dipolar interaction?

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