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Lattice models of supersolids

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PLAN

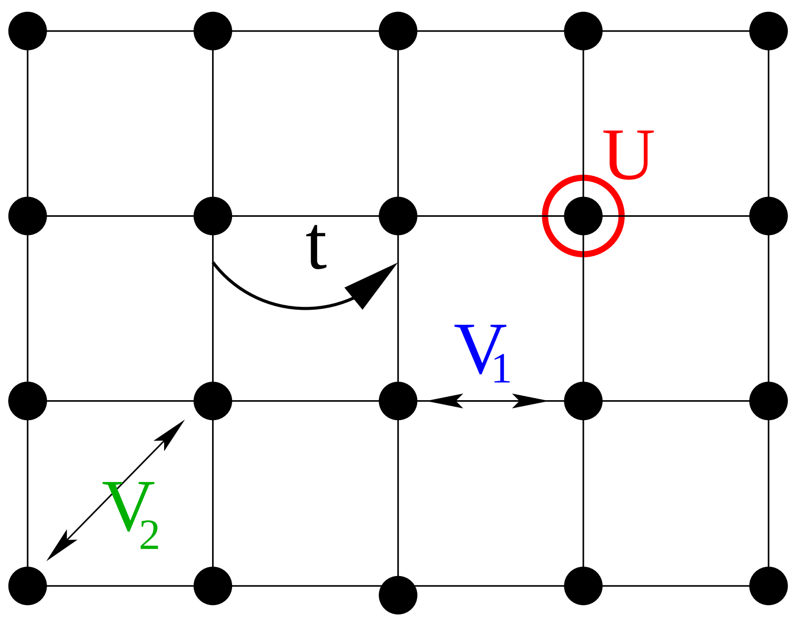
- Models
- Review of QMC results for lattice SS models
  - 2d square lattice
  - 2d triangular lattice
- One dimensional extended Hubbard model
  - QMC results: Phases, dispersion, critical exponents

Lattice models

The Bosonic Hubbard model

$$H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) + V_1 \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j + V_2 \sum_{\langle\langle i,j \rangle\rangle} \hat{n}_i \hat{n}_j$$

where: $[b_i, b_j^\dagger] = \delta_{ij}, \hat{n}_i = b_i^\dagger b_i$



Simulation Algorithms

- World Line algorithm
- PIMC
- Worm algorithm
- Stochastic Series Expansion

Calculated quantities

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

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

A peak at some value, k^*, gives information about the type of order present.

Supersolid: $\rho_s \neq 0$ AND $S(k^*) \neq 0$

Excitation energies: We need dynamic information. Expensive.

f-Sum rule

Use the Feynman result

$$\Omega(k) = \frac{\int \mathrm{d}\omega \;\omega\, S(k,\omega)}{\int \mathrm{d}\omega S(k,\omega)}$$

And where

$$N_b S(k) = \int \mathrm{d}\omega S(k,\omega)$$

Use f-Sum rule:

$$\int \mathrm{d}\omega \;\omega\, S(k,\omega) = N_b E_k$$

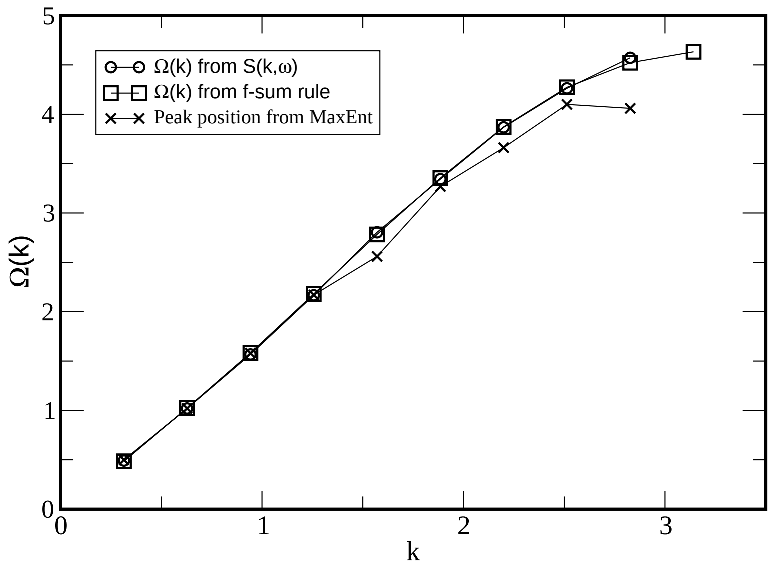
$$E_k = \frac{-t}{L} \left(\cos(2\pi k/L) - 1\right) \langle 0| \sum_{i=1}^{L} \left(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i\right) |0\rangle$$

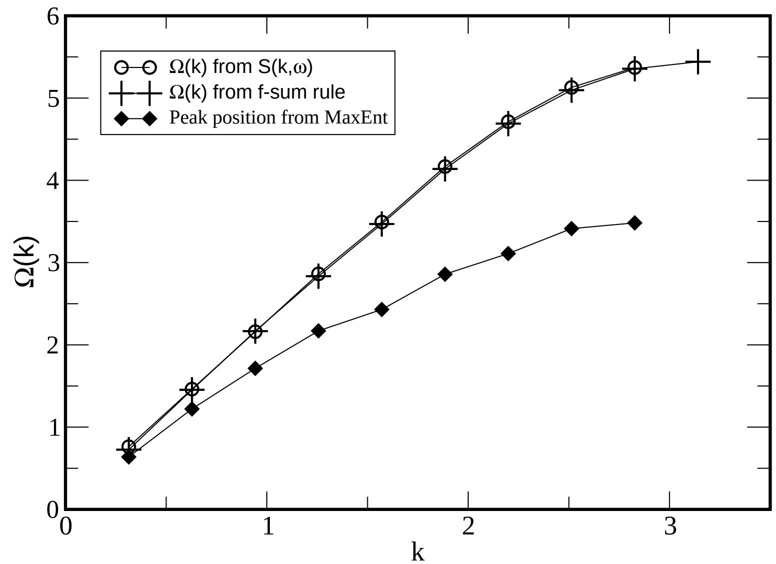
to get

$$\Omega(k) = \frac{E_k}{S(k)}$$

Dispersion relation: Superfluid

Uniform system: $L = 20,\ N_b = 15,\ L_\tau = 200,\ \beta = 10$



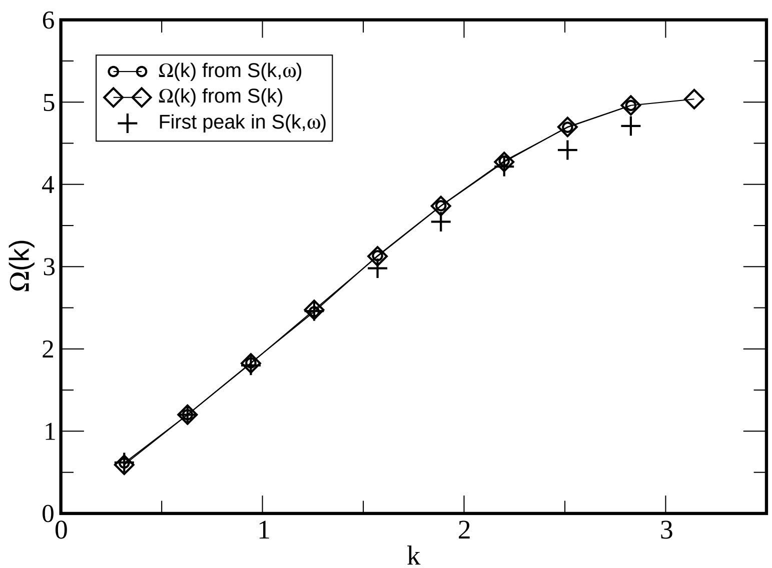


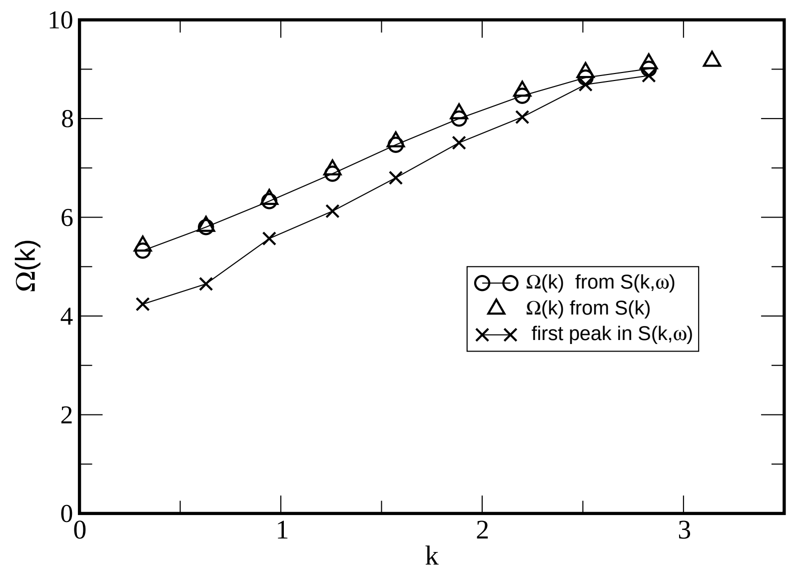
$U = 2t$ $\qquad\qquad$ $U = 8t$

- f-Sum rule and direct evaluations of $\Omega(k)$ agree.
- $\Omega(k) \propto k$ for small k. "Stable" superfluid, phonon excitations.
- $\Omega(k)$ and $\omega(k)$ agree when peaks are very narrow.

Dispersion relation: Superfluid-Mott

Uniform system: $L = 20,\ N_b = 20,\ L_\tau = 200,\ \beta = 10$





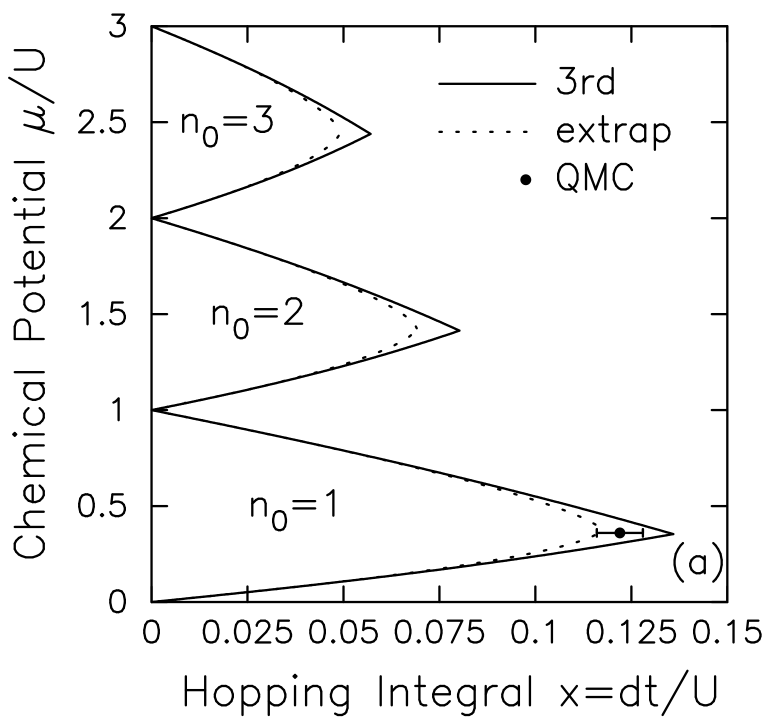
$U = 2t$ $\qquad$ $U = 8t$

- f-Sum rule and direct evaluations of $\Omega(k)$ agree.
- For $U = 2t$, $\Omega(k) \propto k$ for small k. "Stable" superfluid, phonon excitations.
- For $U = 8t$, $\Omega(k \to 0) \approx 5t$: The gap.
- $\Omega(k)$ and $\omega(k)$ agree when peaks are very narrow.

Phase diagram $V_1 = V_2 = 0$

$$H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1)$$

Phases, transitions and exponents first discussed by Fisher *et al* Phys. Rev. **B40**, 546 (1989).
Strong coupling expansion phase diagram, Freericks & Monien, Phys. Rev. **B53** 2691 (1996).

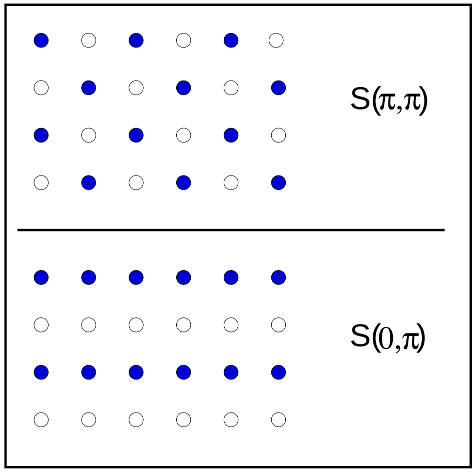


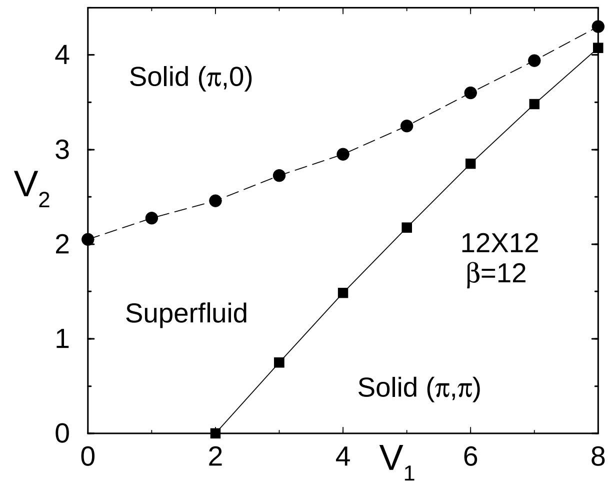
Freericks and Monien, Phys. Rev. B, Figure 2a

Only superfluid and Mott insulator phases.

Phase diagram $V_1, V_2 \neq 0$

$\rho = 1/2$, hardcore (particle-hole symmetry)



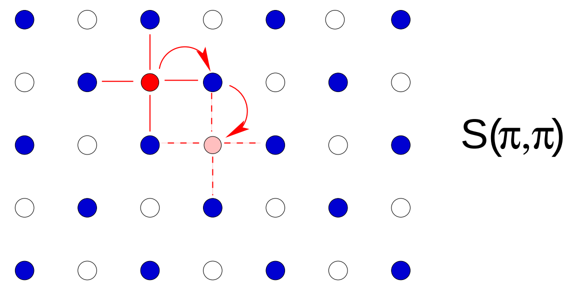


Measure $S(k_x, k_y)$ and ρ_s gives the phase diagram:

- V_1 dominates: No near neighbors.
- V_2 dominates: No next near neighbors.
- In between: Superfluid.

F. Hébert, G. G. Batrouni, R. T. Scalettar, G. Schmidt, M. Troyer and A. Dorneich, *Physical Review* **B65**, 014513 (2002)

Introduce defects: (π, π)



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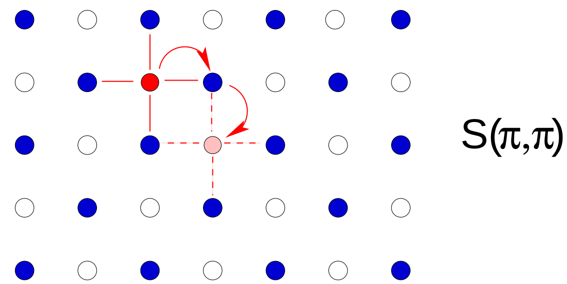

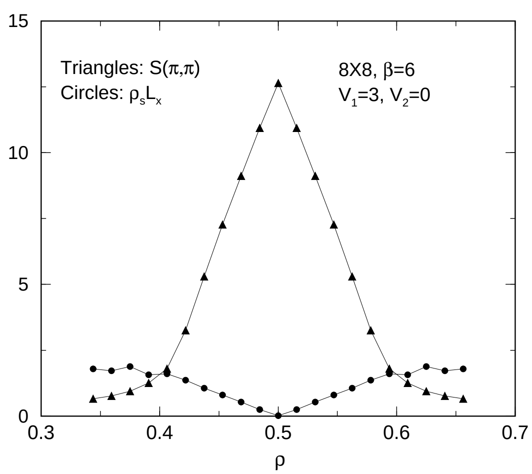

G. G. Batrouni, R. T. Scalettar, *Physical Review Letters* **84** 1599 (2000).

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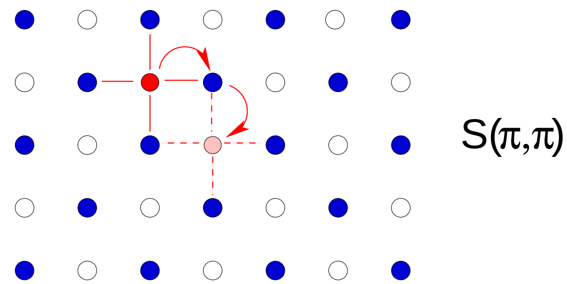

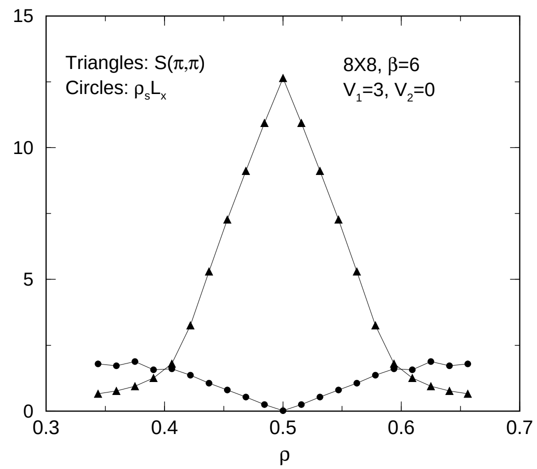

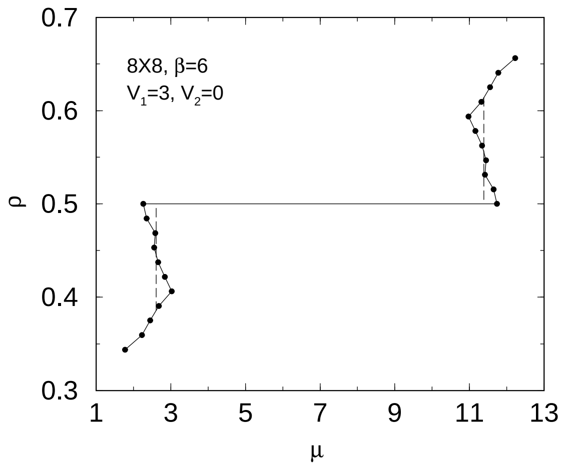

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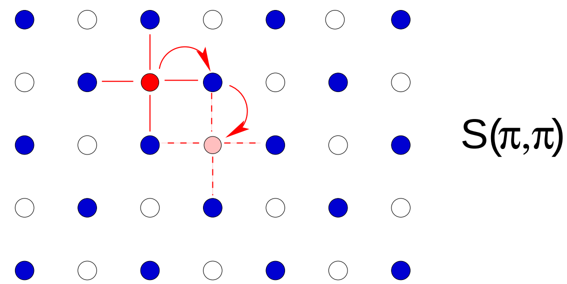
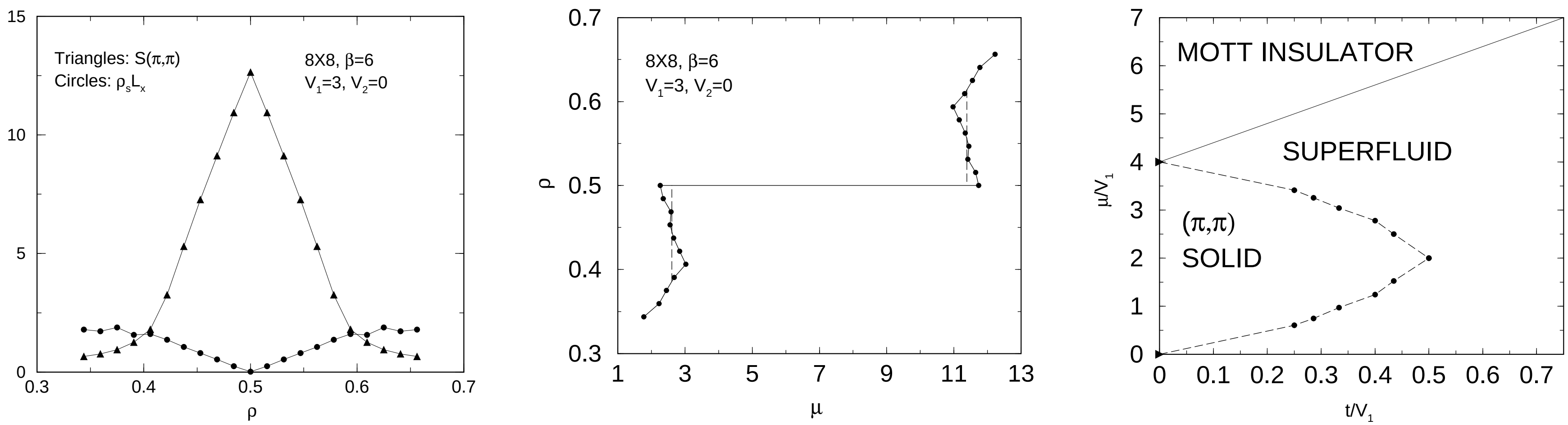
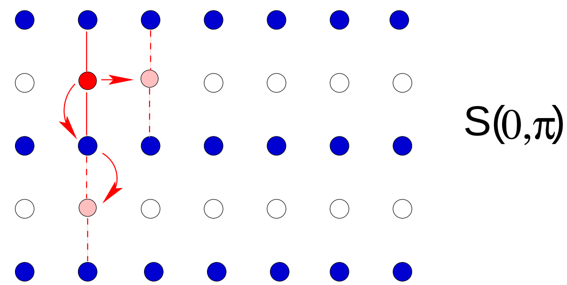




G. G. Batrouni, R. T. Scalettar, *Physical Review Letters* **84** 1599 (2000).

Introduce defects: $(\pi, 0)$



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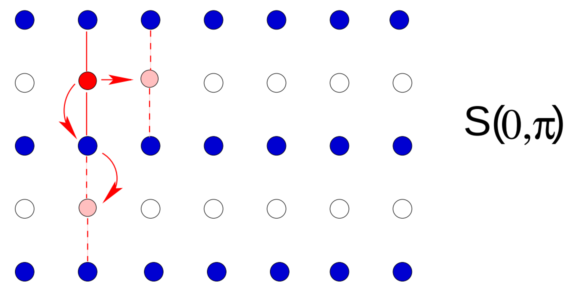
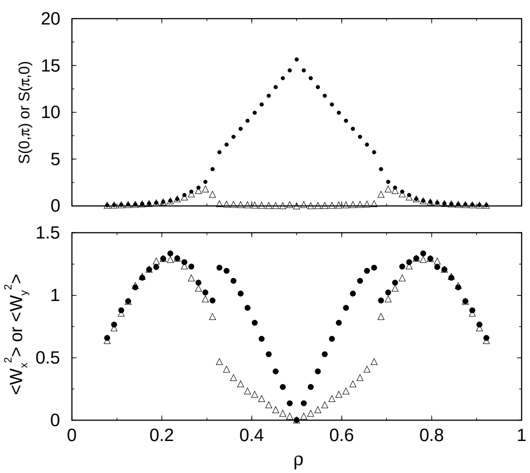


$8X8$, $V_1 = 0$, $V_2 = 5$



G. G. Batrouni, R. T. Scalettar, *Physical Review Letters* **84** 1599 (2000).

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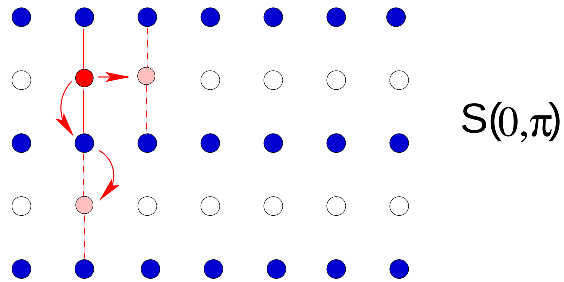

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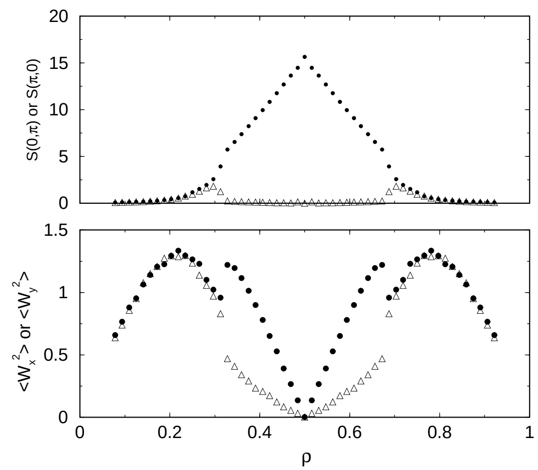

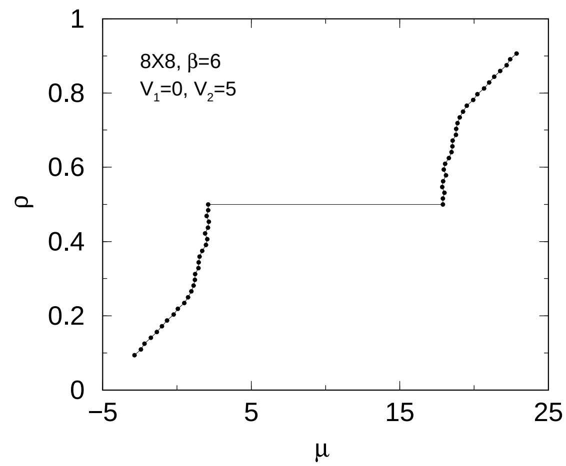

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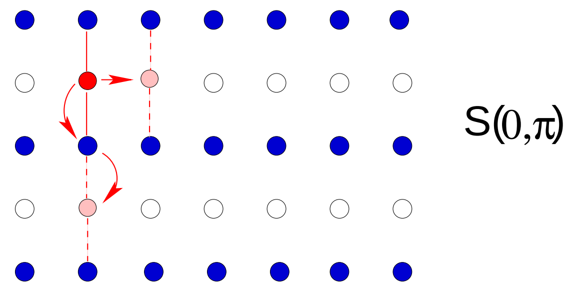

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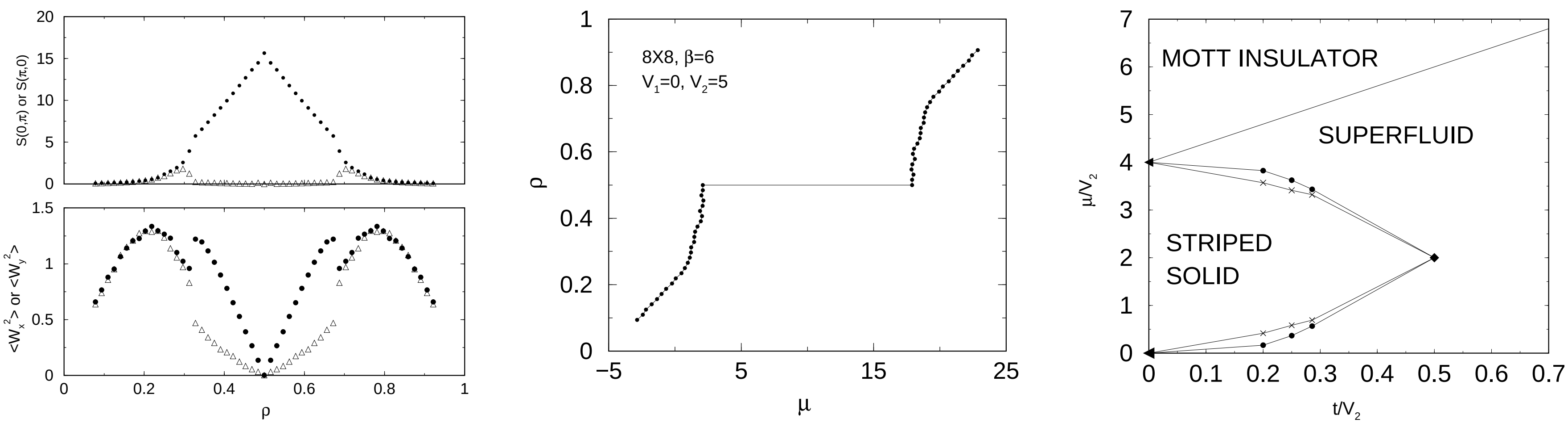
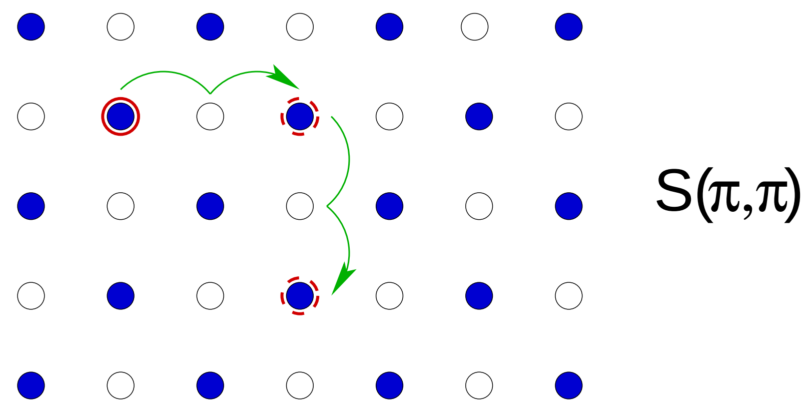


G. G. Batrouni, R. T. Scalettar, *Physical Review Letters* **84** 1599 (2000).

Supersolid phase

$V_1 \neq 0, V_2 = 0$

Soft Core

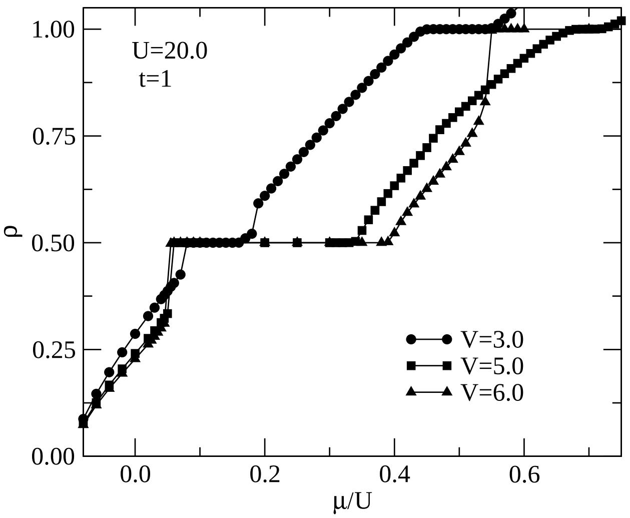


- U and V_1 large: $\rho = 1/2$ is checkerboard solid.
- $U < 4V_1$: less costly to have double occupancy than near neighbor.
- Extra particle can jump, via double hops, from one occupied site to another.
- Effective two-boson defect delocalizing.
- Supersolid?

$V_1 \neq 0, V_2 = 0$

Soft Core

Supersolid versus phase separation: depends on U and V_1



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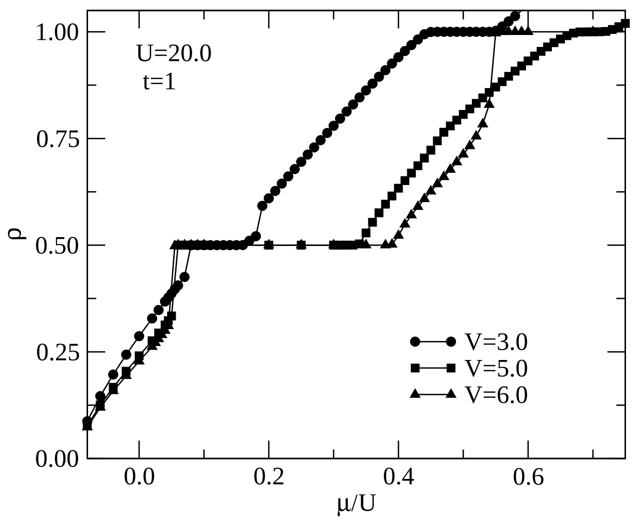

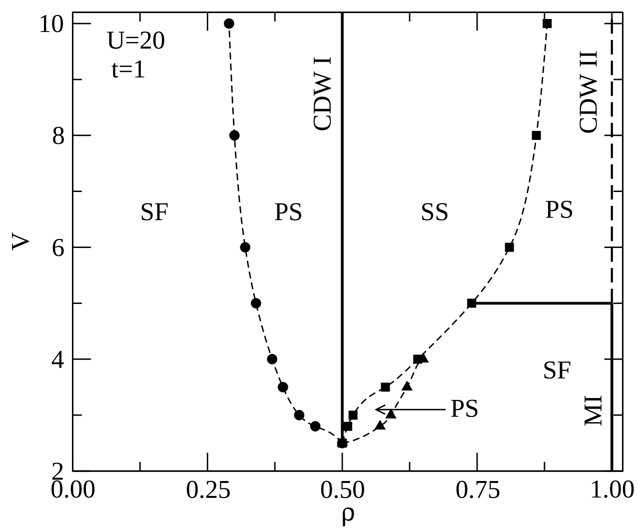

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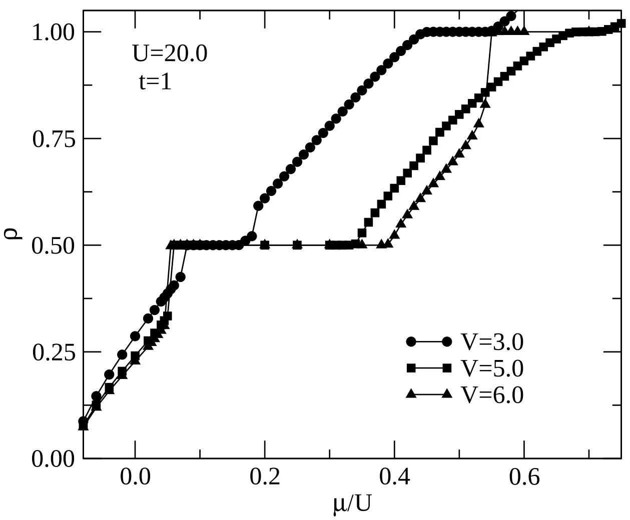
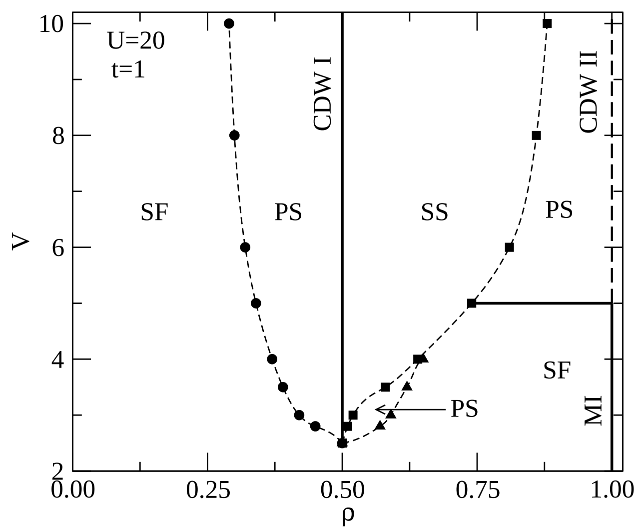
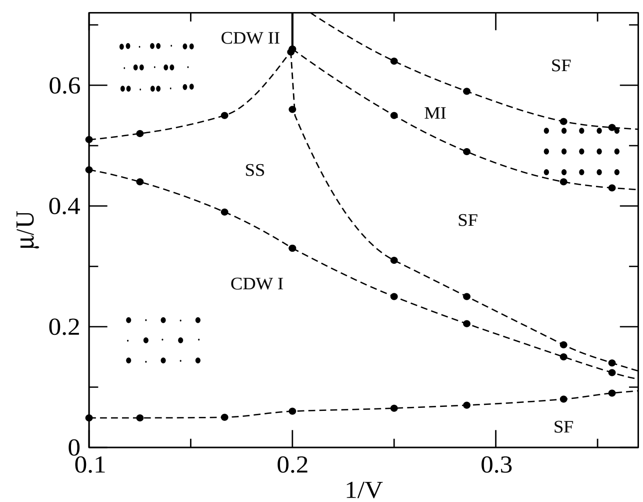






Checkerboard supersolid

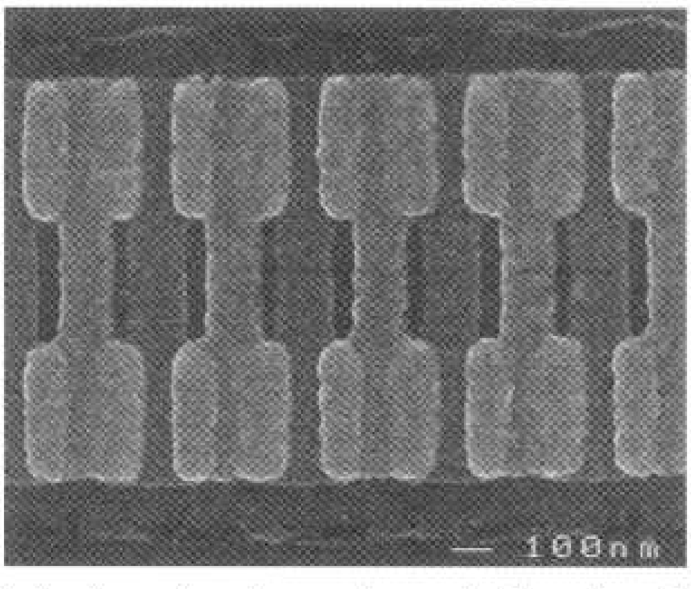
P. Sengupta *et al* Physical Review Letters **94**, 207202 (2005)

Quantum Phase Model

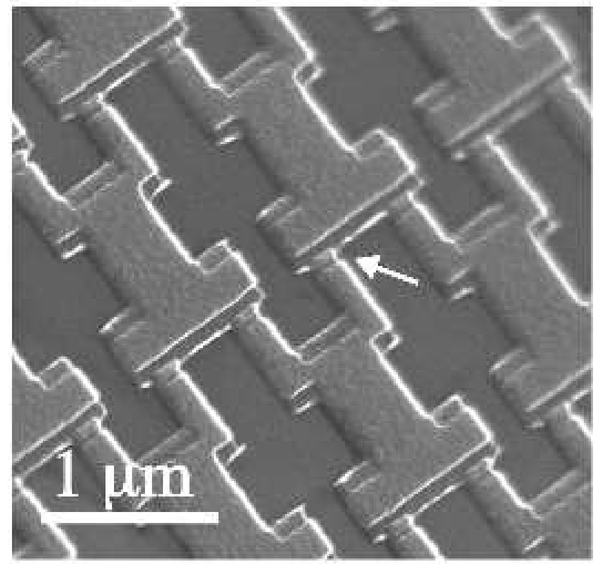
$$H = \frac{1}{2}\sum_{ij} U_{ij}(n_i - \bar{n})(n_j - \bar{n}) + \sum_{\langle ij\rangle} t[1 - \cos(\phi_i - \phi_j)], \qquad [n_i, \phi_j] = -i\delta_{ij}$$

$U_0 \neq 0$ and $U_1 \neq 0$, represent Coulomb interaction between charges on different grains

Second term is Josephson coupling.



Chow *et al* PRL**81** 204 (1998)



van Oudenaarden *et al* PR**B57** 11684 (1998)

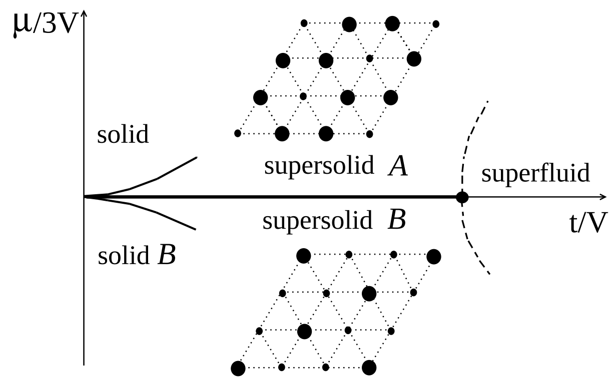
Supersolidity in this model

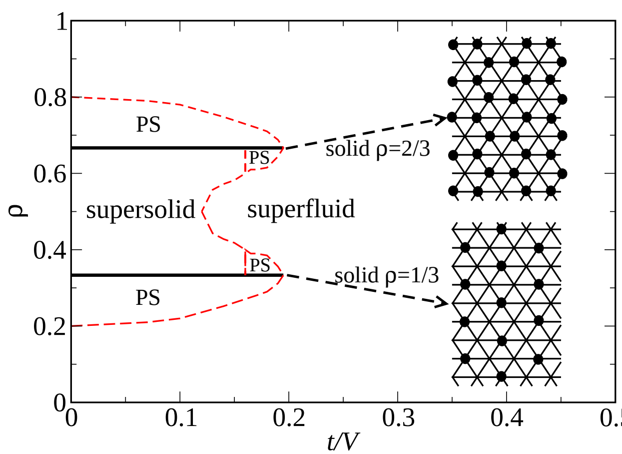
Roddick and Stroud, PR**B51** 8672 (1995)

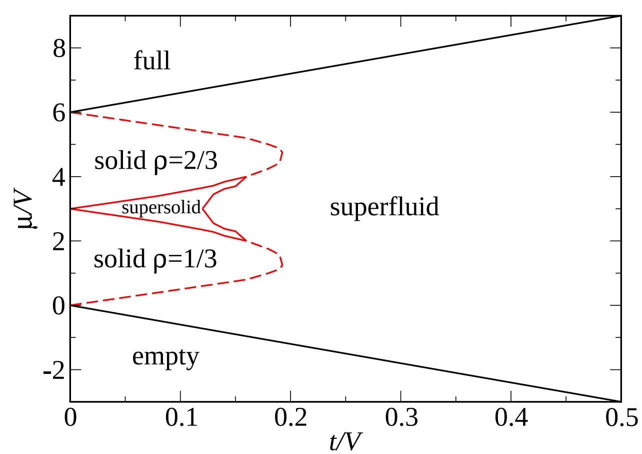
van Otterlo and Wagenblast, PRL**72**, 3598 (1994)

Triangular Lattice

Hard core Hubbard model with near neighbor repulsion



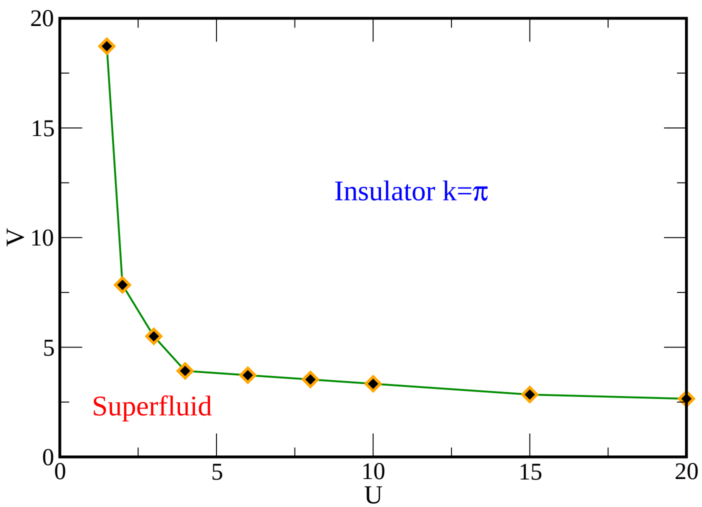


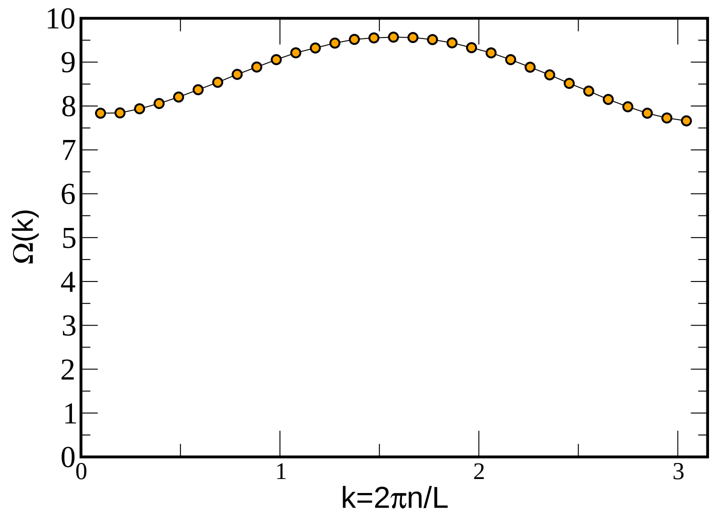


Wessel and Troyer, PRL**95**, 127205 (2005); Boninsegni and Prokofev PRL**95**, 237204 (2005); Melko *et al*, PRL**95**, 127207 (2005); Heidarian and Damle, PRL**95**, 127206 (2005)

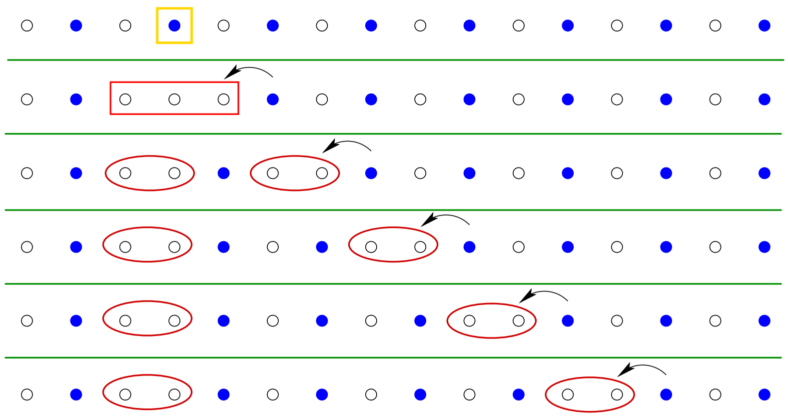
One Dimension

$$H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + U \sum_i \hat{n}_i(\hat{n}_i - 1) + V \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j$$





Dope: Vacancies



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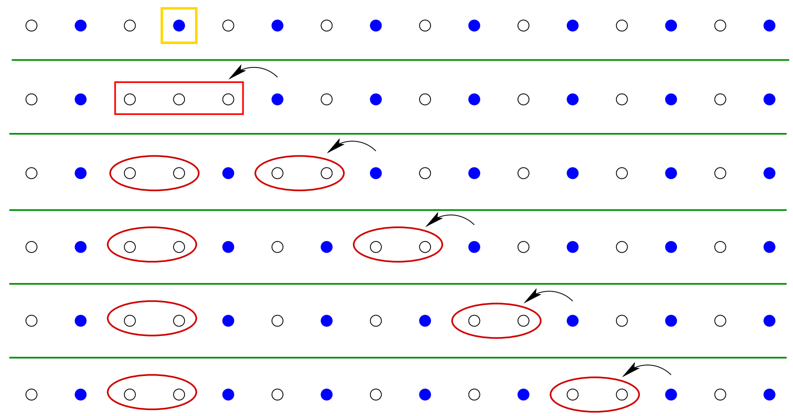
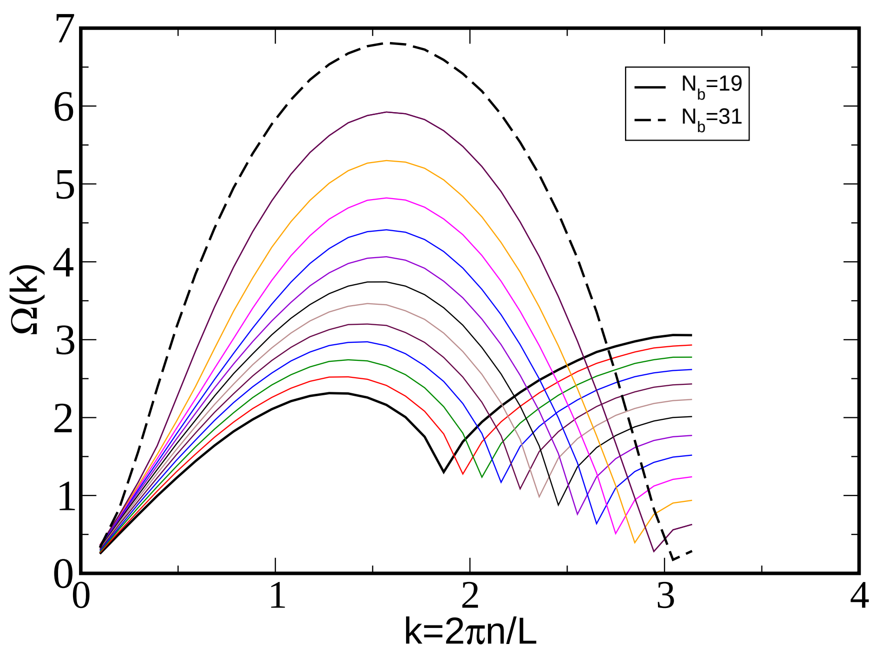
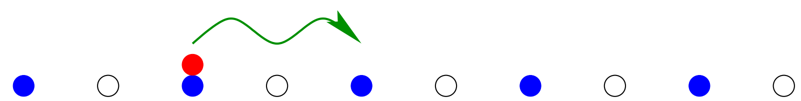




Dope: Add particles



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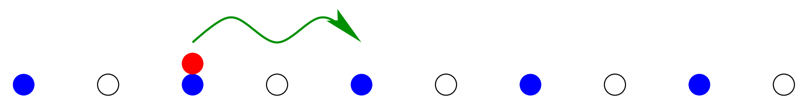
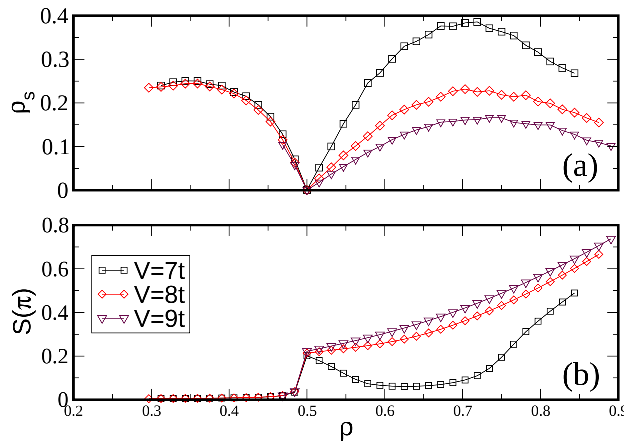
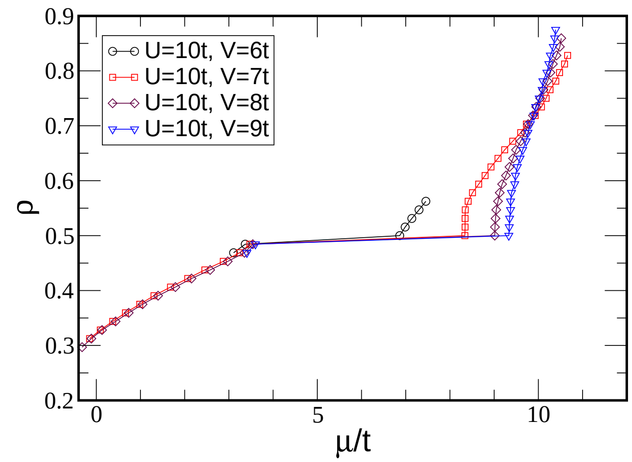
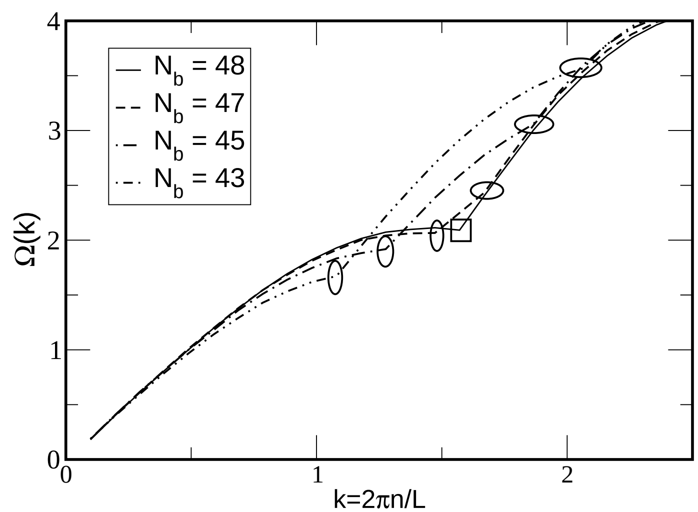
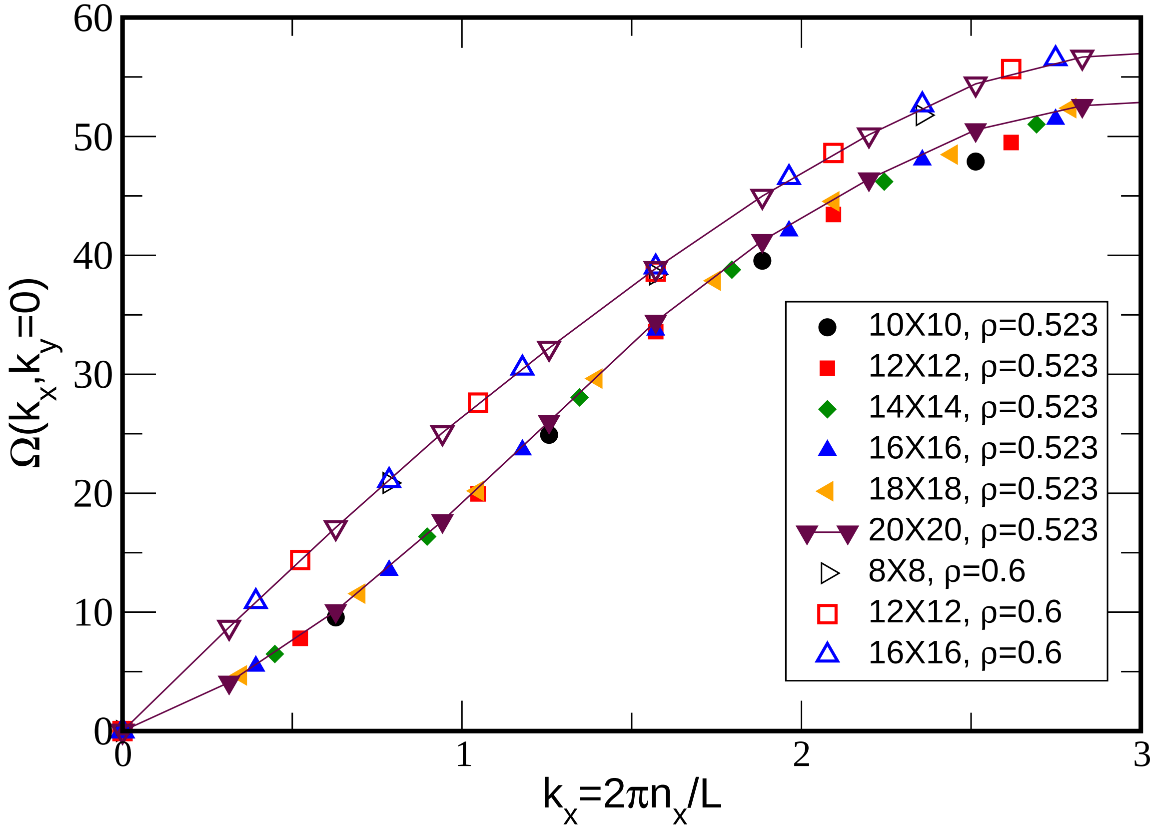








Two dimensions



Conclusions

Lattice models display:

- Solid phase
- Superfluidity
- Supersolidity: Under certain conditions
- Phase separation: Very easy to get