Seminar at ENS

Quantum Monte Carlo Study of Superfluidity and Supersolidity in Bosonic Lattice Systems

The University of Tokyo

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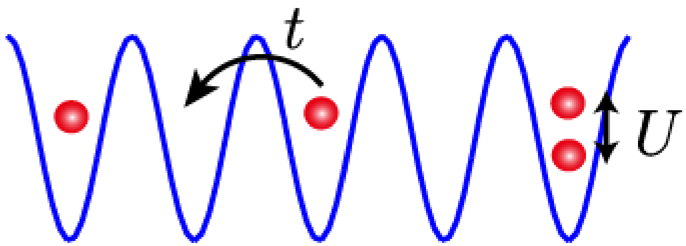
Optical Lattice Systems and Bose-Hubbard Model

【Bose-Hubbard Model】

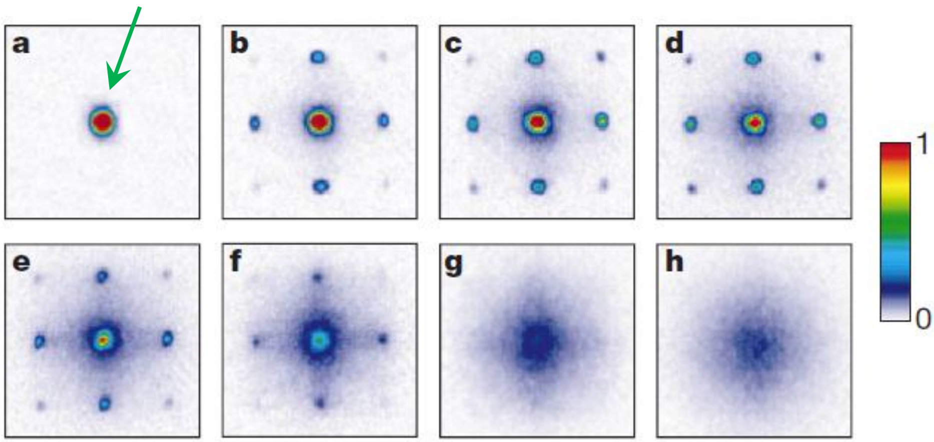
$$H = -t\sum_{\langle i,j\rangle}\left(b_i^{\dagger}b_j + h.c.\right) - \mu\sum_i n_i + \frac{U}{2}\sum_i n_i\left(n_i - 1\right)$$

K. Jaksch *et al.*, Phys. Rev. Lett. **81** 3108 (1998)



【Observation of the SF-MI Transition】

Sharp peak which indicates the SF (BEC)



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

<u>High controllabitiy of system parameters</u>

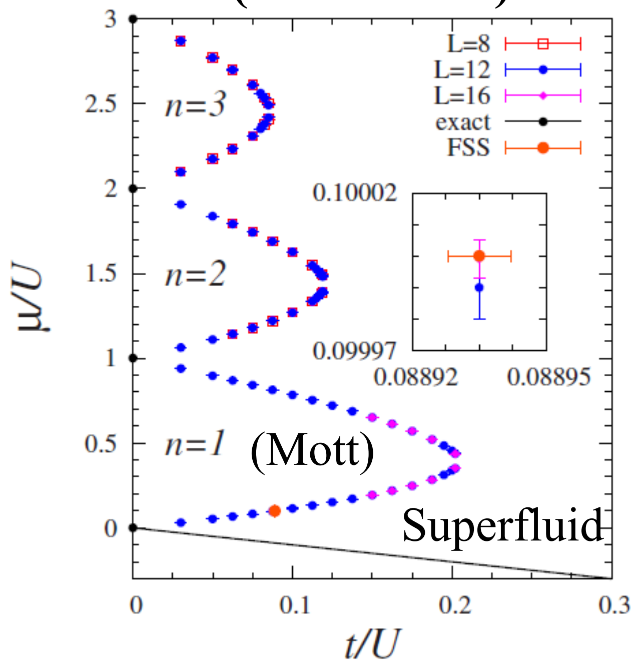
- We can control the ratio t/U by changing the potential depth V_0.
  (In the right figure, t/U is decreased from **a** to **h**.)

- By using the Feshbach resonance, we can also control the short-range interaction U.

A system of bosonic atoms trapped in optical lattices is well described by the Bose-Hubbard model.

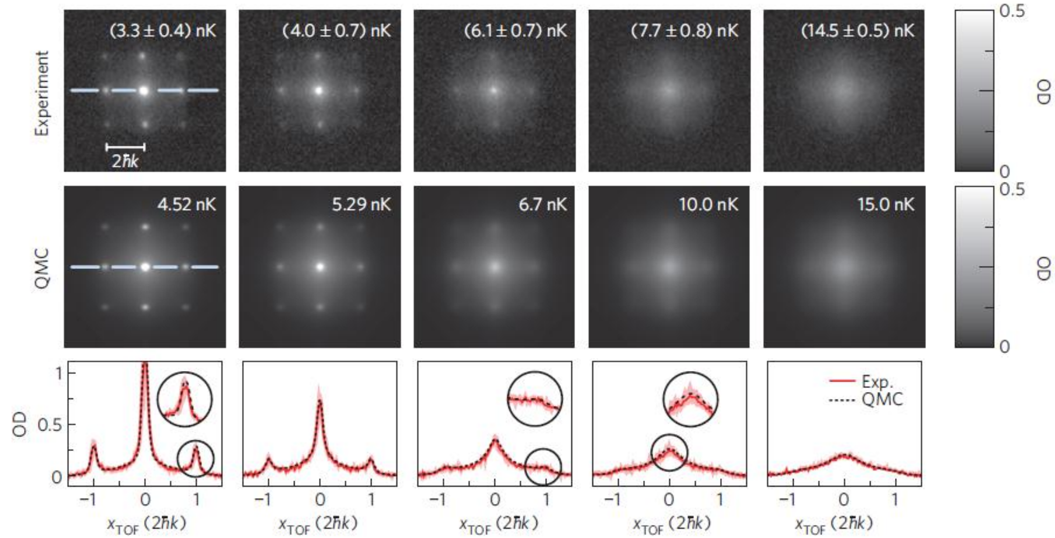
Optical Lattice Systems and Quantum Monte Carlo

【Ground-state phase diagram】
(cubic lattice)



Y. Kato and N. Kawashima, PRE **81** 011123 (2010)

【Comparison with experimental results】



S. Trotzky *et al.*, Nat. Phys. **6** 998 (2010)

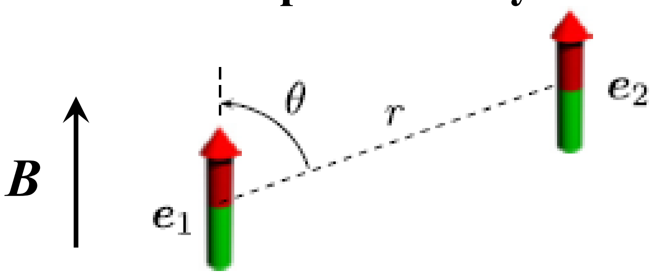
cf. The transition temperature of a uniform system is T_c=5.3nK

<u>Advantages of the quantum Monte Carlo (QMC) method</u>

1. We can obtain the unbiased accurate results within statistical errors.
2. We can perform simulation of large systems (~10^5 particles).

Cold atoms with large dipole moments

【Dipole moments polarized by an external field】



T. Lahaye *et al.*, Rep. Prog. Phys. **72** 126401 (2009)

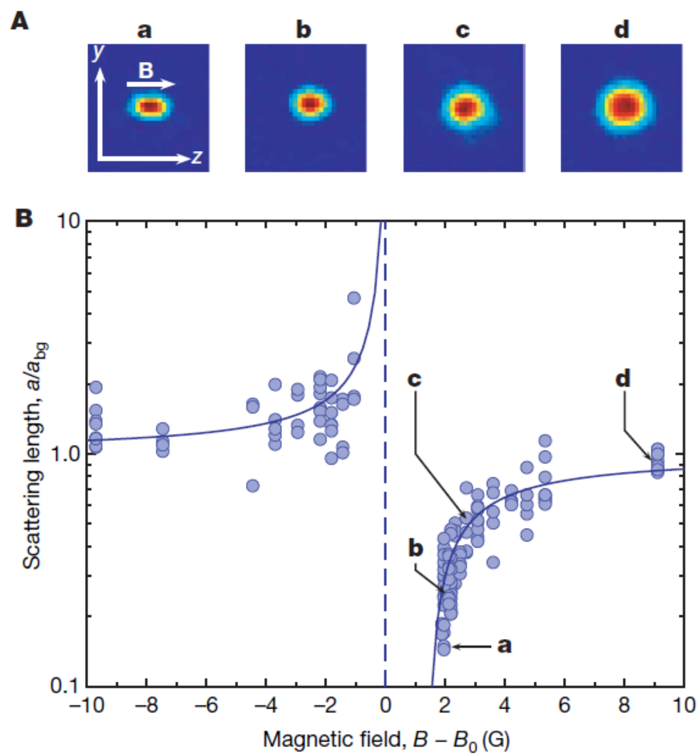
Effective potential in low-energy regimes

$$V_{\mathrm{eff}}(\boldsymbol{r}) = \frac{4\pi\hbar^2 a_s}{m}\delta(\boldsymbol{r}) + \frac{\mu_0 \mu_m^2}{4\pi}\frac{1-3\cos^2\theta}{r^3}$$

S. Yi and L. You, Phys. Rev. A **63** 053607 (2001)

By suppressing the short-range interaction through the Feshbach resonance, we can enhance the dipole-dipole interaction relatively.

【Observation of BEC of ^{52}Cr ($\mu_m=6\mu_B$)】



T. Lahaye *et al.*, Nature **448** 672 (2007)

$B_0 \fallingdotseq 589$G

Owing to the long-range (and anisotropic) nature of the dipole-dipole interaction, new phenomena are expected to be realized.

Motivation of our study

Especially for a system of cold dipolar atoms trapped in an optical lattice, the presence of exotic quantum phases such as checkerboard solid and its supersolid phase are predicted theoretically.

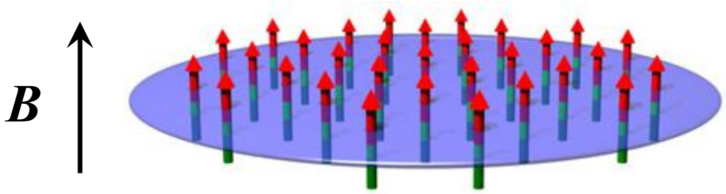
Ex. S. Yi *et al.*, Phys. Rev. Lett. **98** 260405 (2007)

[Our study]
By using the QMC method, we have investigated and explore exotic quantum states such as a supersolid state in the Bose-Hubbard models that include the effect of the long-range interaction.

1. **Bose-Hubbard model with the nearest-neighbor repulsion**

   One of the simplest models that support the presence of the supesolid phase. Furthermore, it may be realized approximately in a cold dipolar atoms trapped in a 2D optical lattice.

【Cold atoms whose dipole moments are polarized perpendicularly to the 2D plane】



T. Lahaye *et al.*, Rep. Prog. Phys. **72** 126401 (2009)

2. **Bose-Hubbard model with the dipole-dipole interaction (without cutoff)**

   We can understand the effect of the long-range interaction precisely.

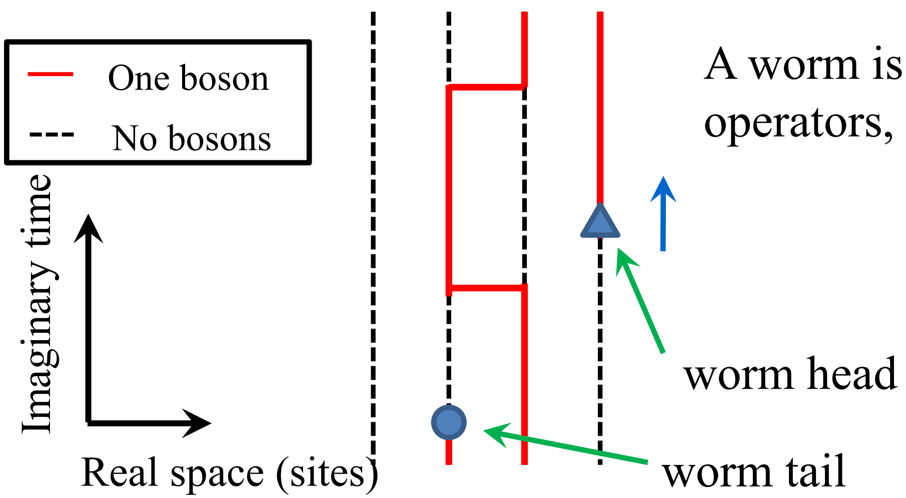
Contents

Worm Algorithm

<u>Worm algorithm</u>…One of the most efficient and generic QMC methods based on the path-integral (world-line) representation.

N. V. Prokof'ev, B. V. Svistunov and I. S. Tupitsyn, Sov. Phys. JETP **87** 310 (1998)
O. F. Syljuasen and A. W. Sandvik, Phys. Rev. E **66** 046701 (2002)

【A world-line configuration with a worm】



A worm is a pair of creation and annihilation operators, i.e. $a^{\dagger}$ and a.

<u>Anvantages</u>

1. Efficient simulations due to the global updates.
2. Calculation of the Green's function. etc.

Contents

Bose-Hubbard model with the nearest-neighbor interaction

【Bose-Hubbard model with the nearest-neighbor repulsion】

(We consider the *d*-dimensional hypercubic lattices)

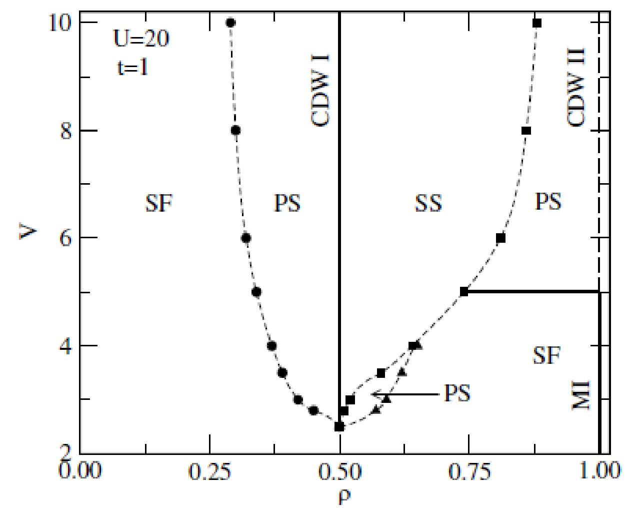
$$H = -t\sum_{\langle i,j\rangle}\left(b_i^{\dagger}b_j + h.c.\right) - \mu\sum_i n_i + \frac{U}{2}\sum_i n_i\left(n_i - 1\right) + \sum_{\langle i,j\rangle} V n_i n_j$$

【Ground-state phase diagram for square lattices (by QMC)】

P. Sengupta *et. al.* Phys. Rev. Lett. **94** 207202 (2005)

Filling factor ρ=1/2
(commensurate)
Checkerboard solid

Filling factor ρ>1/2
(incommensurate)
Supersolid

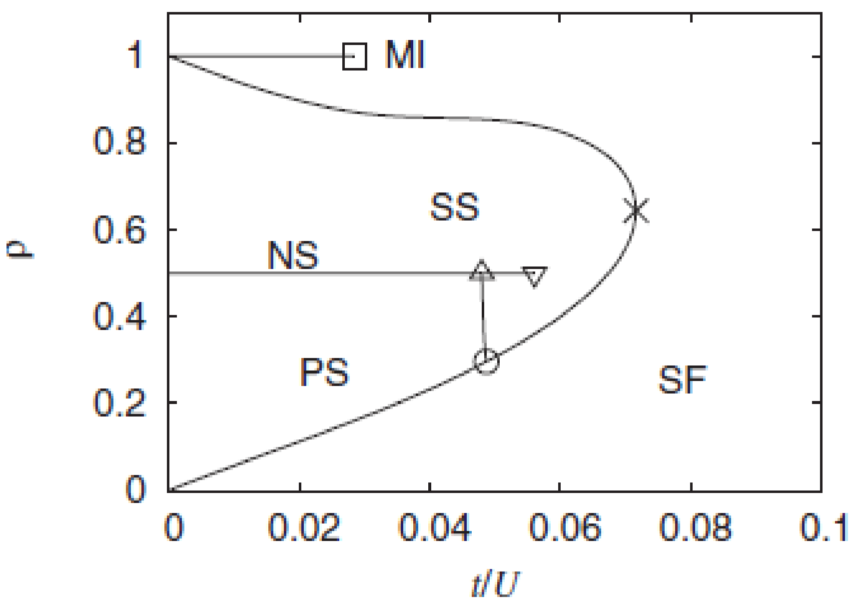


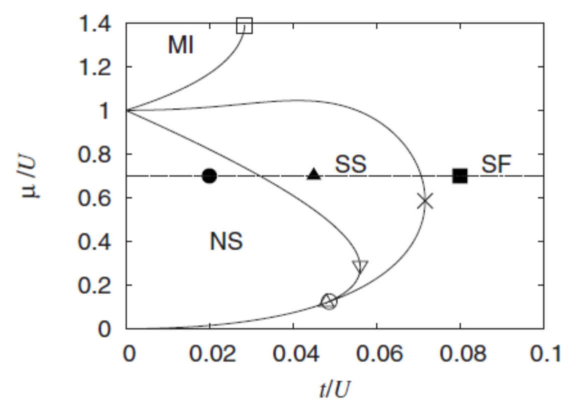
For square lattices, the supersolid (SS) phase has been found for $\rho > 1/2$.

Ground-state phase diagram by the Mean-field analysis

【Mean-field ground-state phase diagram (zV/U=1)】

K. Yamamoto, S. Todo and S. Miyashita, Phys. Rev. B **79** 094503 (2009)





cf. The presence of SS phase below ρ=1/2 has already been confirmed by the QMC simulations in the same work.

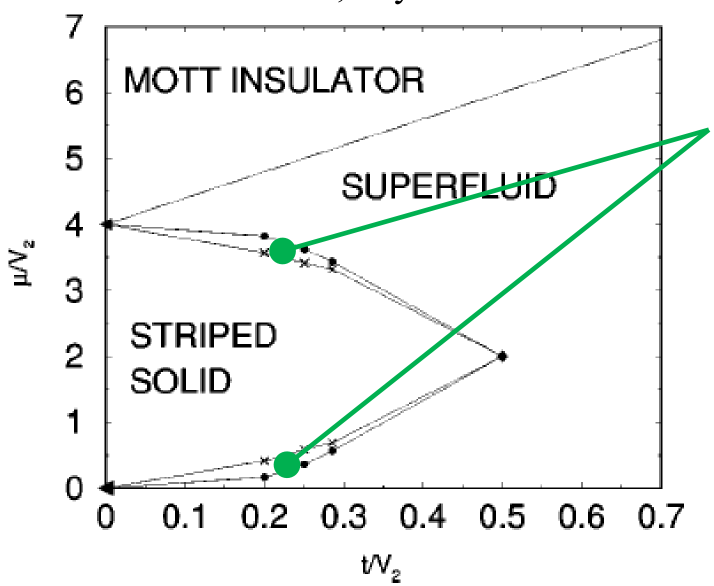
At the mean-field level, the supersolid phase exists below and at ρ=1/2 as well as above ρ=1/2.

Purpose of this study

Most supersolids appear when particles or holes are doped into perfect commensurate solids.

【Ex. The ground-state phase diagram of hard-core bosons on a square lattice with the next-nearest-neighbor repulsion V_2】

G. G. Batrouni and R. T. Scalettar, Phys. Rev. Lett. **84** 1599 (2000)



Supersolid

We need doping of particles or holes to produce a supersolid state.

【Purpose】
We investigate the presence of a supersolid at the commensurate filling 1/2 for a square lattice as well as a cubic lattice.

Ground-state phase diagram for a cubic lattice

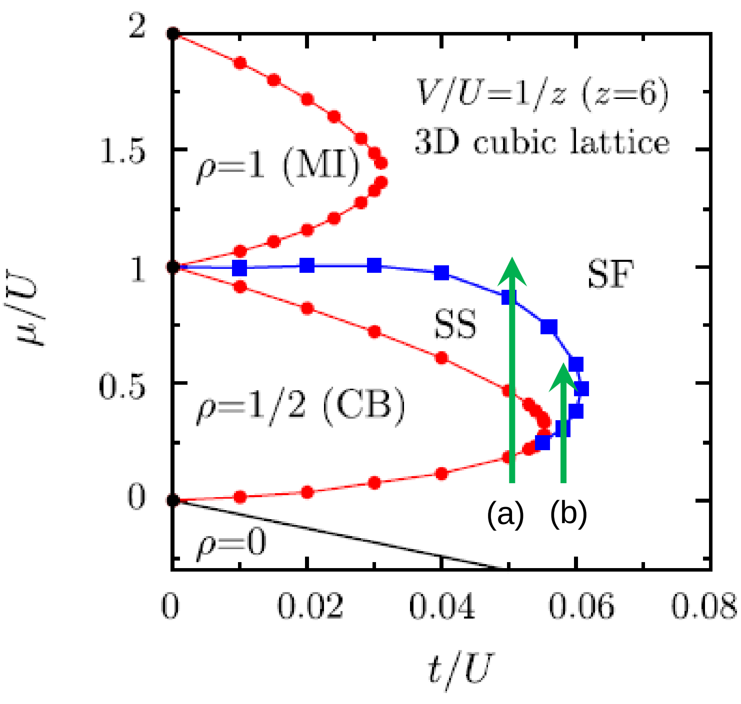
First, we have obtained the ground-state phase diagram for a cubic lattice and confirmed that it agrees qualitatively with the mean-field result.

【Measured quantities】

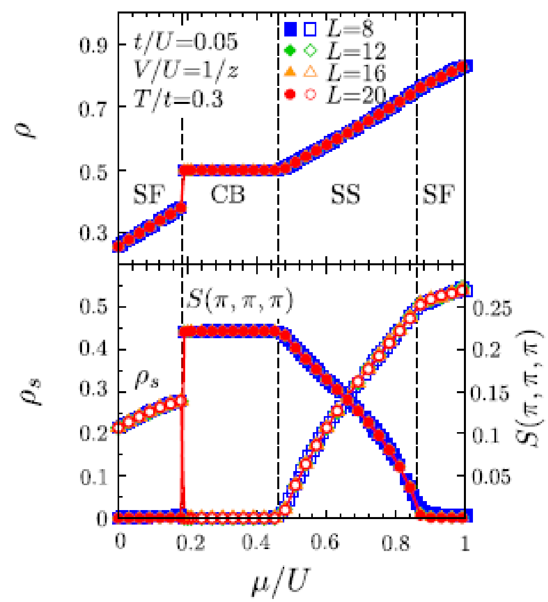
Particle density $\rho = \frac{1}{N}\left\langle \sum_i n_i \right\rangle$, Superfluid density $\rho_s = \frac{\langle W^2 \rangle T}{Lt}$

Structure factor $S(\boldsymbol{k}) = \frac{1}{N^2}\sum_{i,j} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)}\left(\langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle\right)$

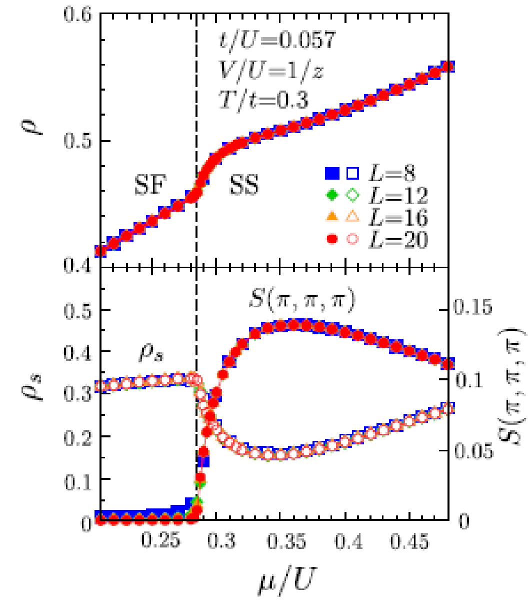
【Ground-state phase diagram (cubic lattice)】



(a) t/U=0.05



(b) t/U=0.057



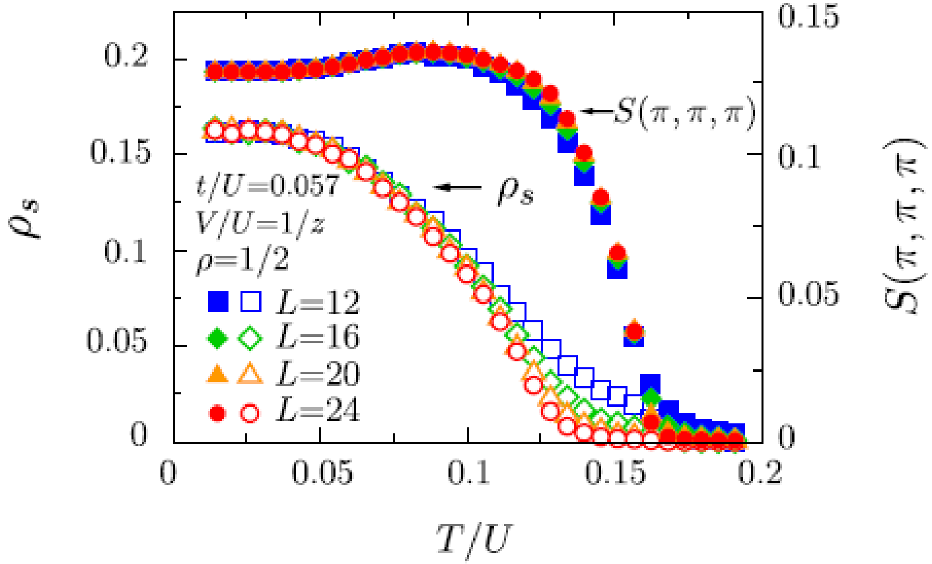
We obtained the ground-state phase diagram.

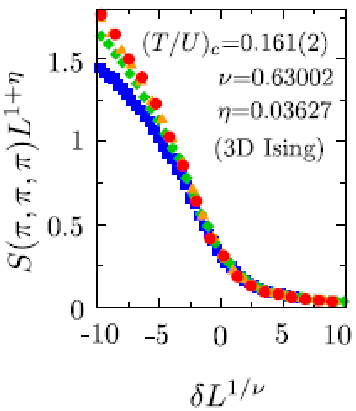
Direct evidence of SS at the commensurate filling 1/2

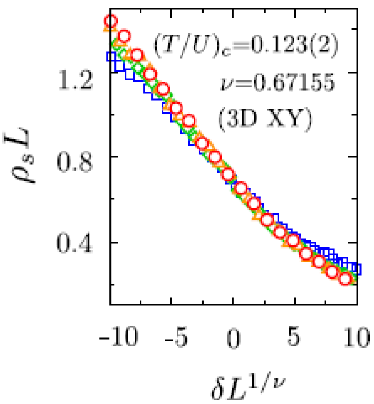
To show direct evidence of SS at ρ=1/2, we obtained the numerical results for the canonical ensemble at ρ=1/2.

【Finite-size scaling analysis】

【Temperature dependence of ρ_s and $S(\pi, \pi)$】







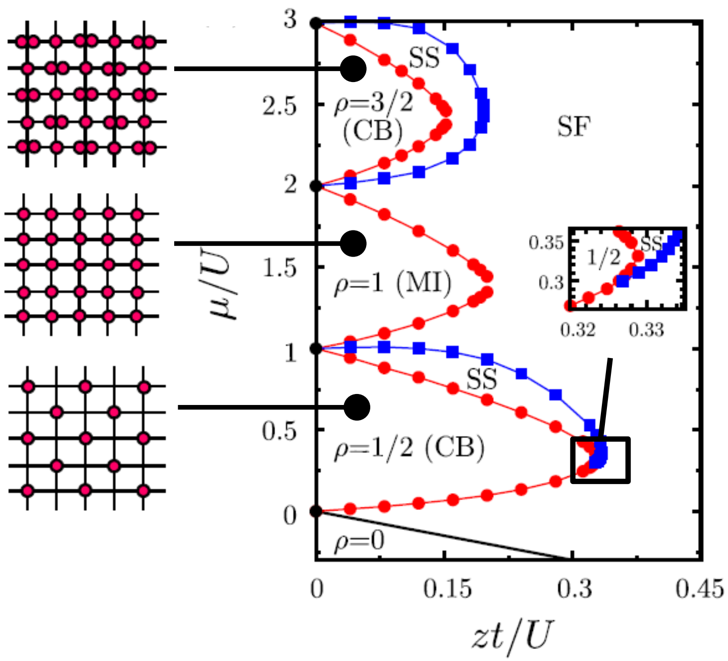
CB transition →3D Ising universality class

SF transition→ 3D XY universality class

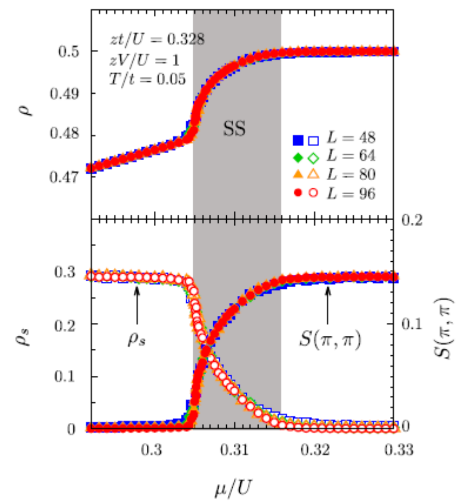
We have showed direct evidence of a supersolid at the commensurate filling factor 1/2.

Ground-state phase diagram for square lattices

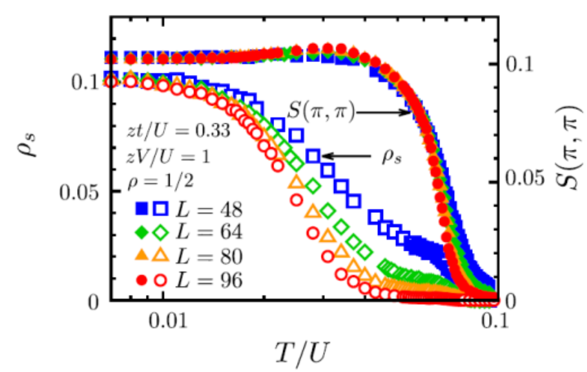
【Ground-state phase diagram (square lattice, zV/U=1)】



【Evidence of SS for ρ<1/2】



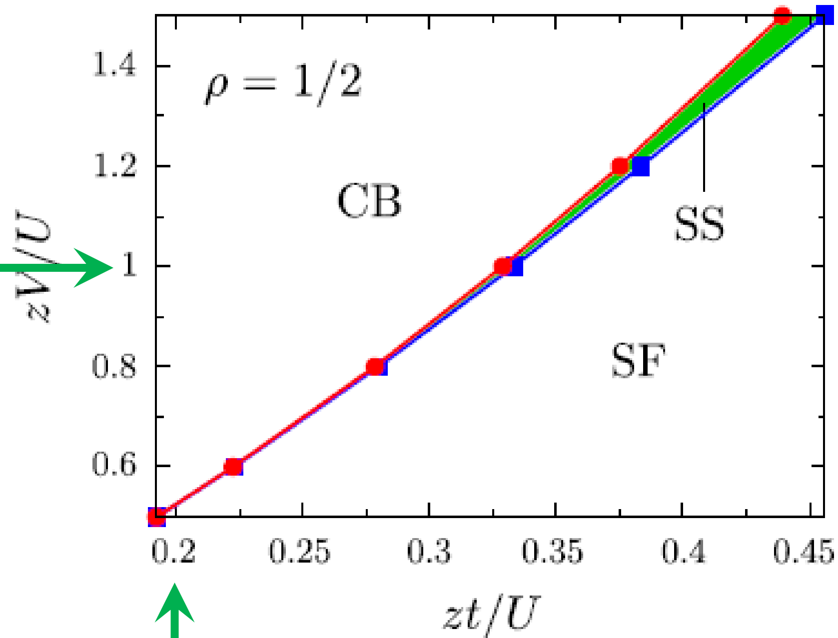
【Evidence of SS at ρ=1/2】



The SS phase below and at ρ=1/2 exists in a square lattice as well as a cubic lattice.

Ground-state phase diagram at ρ=1/2

【Ground-state phase diagram (square lattice)】



The parameter in our work

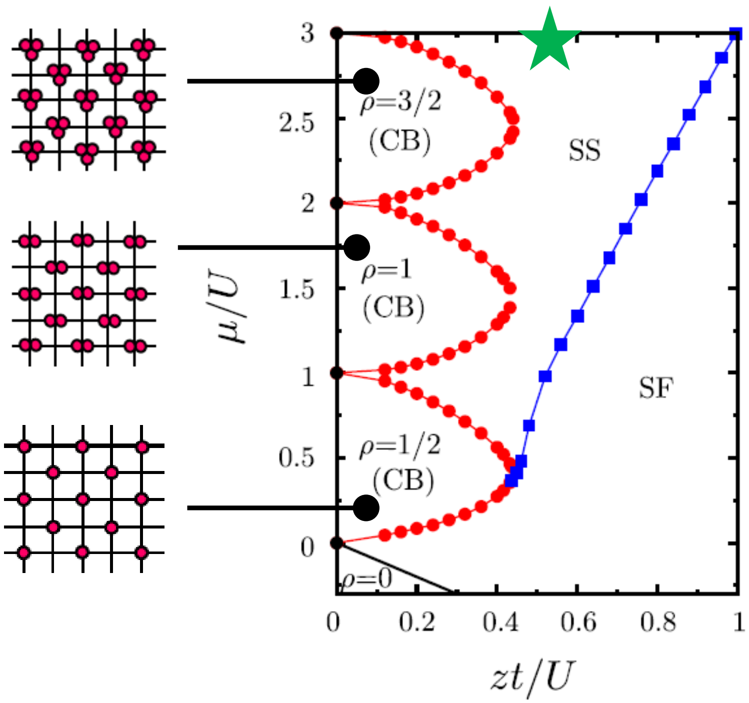
The parameter in the previous work

P. Sengupta *et. al.* Phys. Rev. Lett. **94** 207202 (2005)

The supersolid phase at ρ=1/2 extends for large hopping amplitudes and nearest-neighbor repulsions.

Phase diagram for strong nearest-neighbor repulsions

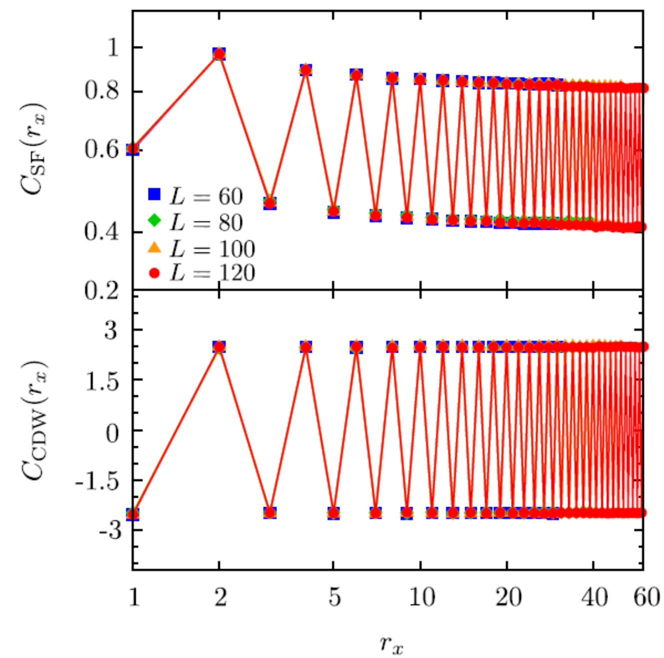
【Ground-state phase diagram (zV/U=1.5)】



【Correlation functions at ★】

$$C_{SF}(r_{ij}) = \langle b_i^{\dagger} b_j \rangle$$

$$C_{CDW}(r_{ij}) = \langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle$$

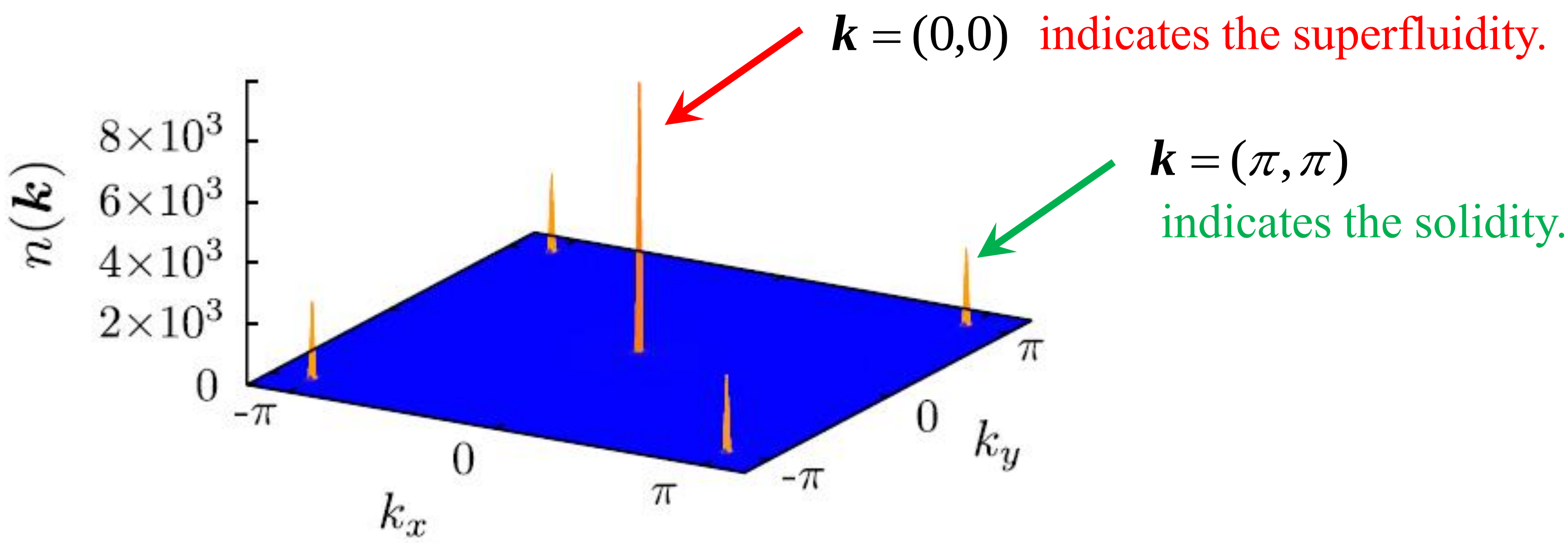


For large hopping amplitudes and nearest-neighbor repulsions,
the supersolid phase occupies the broad region in the phase diagram.

Double-peak structure in the momentum distribution

As a result of oscillation in the off-diagonal correlation function,
the momentum distribution shows a characteristic structure.

【**Momentum distribution** $n(k) = \frac{1}{N}\sum_{i,j}\langle b_i^\dagger b_j \rangle e^{ikr_{ij}}$ **in the supersolid state**】



Observation of the double-peak structure will become clear evidence of supersolid state.

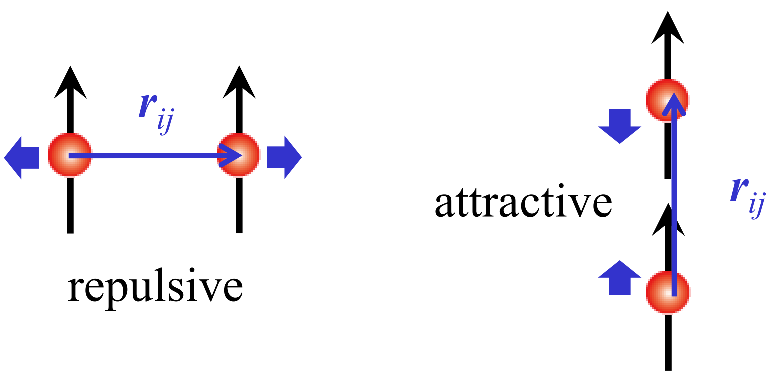
Contents

Model and previous works

【Bose-Hubbard model with the dipole-dipole interaction】

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

The dipole-dipole interaction $V_{ij} = V\dfrac{1-3\cos^2\theta}{r^3_{ij}}$ $\left(V = \dfrac{\mu_0\mu_m^{\;2}}{4\pi}\right)$

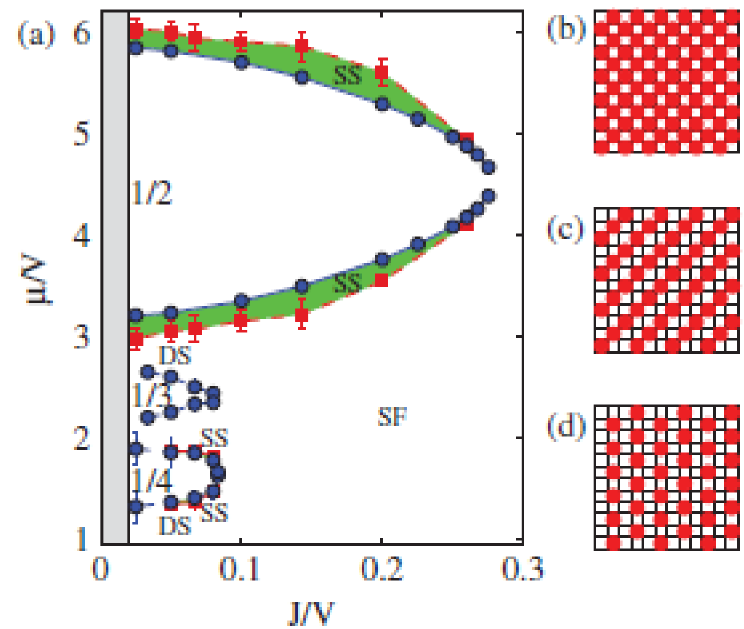


$\theta=\pi$ $\theta=0$

【Ground-state phase diagram of hard-core bosons】

(square lattice, $\theta=\pi$)

B. Capogrosso-Sansone *et. al.* Phys. Rev. Lett. **104** 125301 (2010)



Owing to the long-range interactions, several exotic phases appear.
[several types of solid phases, their supersoild phases, and devil's staircase]

Purpose of this study

In contrast to the case of long-range interaction $1/r^3$, the checkerboard supersolid of *hard-core* bosons cannot be stabilized by the nearest-neighbor repulsion only.

G. G. Batrouni and R. T. Scalettar, Phys. Rev. Lett. **84** 1599 (2000)

【Motivation1】
Why does the long-range interaction stabilize the checkerboard supersolid of hard-core bosons?

The anisotropic nature of interactions or multiple occupations of bosons may also produce novel physics.

【Motivation2】
How does the phase diagram change if the dipole-dipole interactions becomes anisotropic?

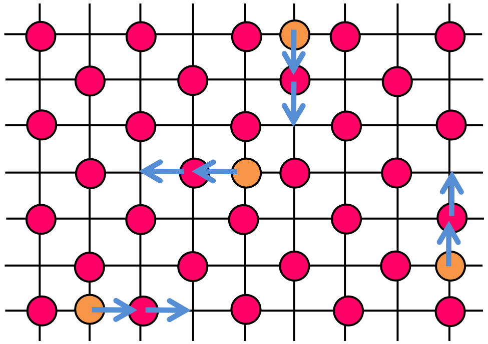
【Motivation3】
How does the phase diagram change if bosons becomes soft-core?

SS vs Domain wall (nearest-neighbor repulsion)

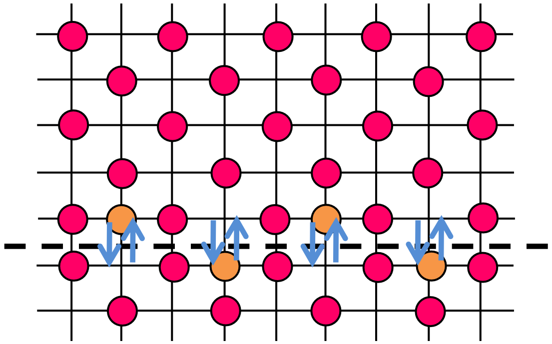
We can understand the absence of the supersolid by strong-coupling argument.

cf. P. Sengupta *et. al.* Phys. Rev. Lett. **94** 207202 (2005)

Supersolid
(Delocalization of doped particles)



Domain wall
(which is formed by doped particles)



Energy cost of doping a particle

<u>t=0</u> $E_0 \equiv zV - \mu$ = E_0 The same energy In the zeroth order

When we consider a small kinetic term,

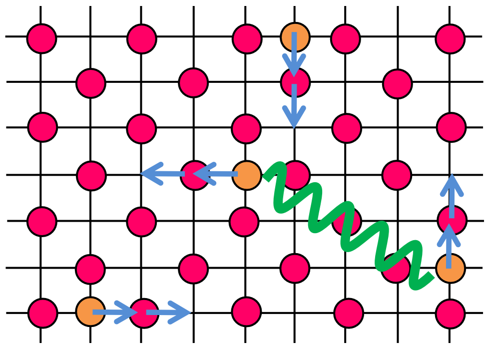
<u>0<t<<V</u> $-O(t^2)$ ✕ $-O(t)$ ○ Not the same order In the kinetic energy gain

The checkerboad SS is unstable against the domain-wall formation.

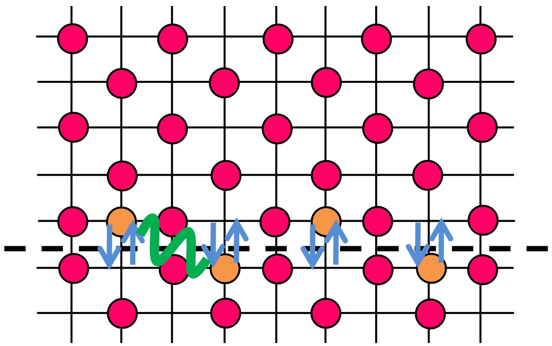
SS vs Domain wall ($1/r^3$ interaction)

How does the situation change for the long-range interacting systems?

Supersolid



Domain wall



$\underline{t=0}$ E_{SS} < E_{DW} Not the same energy In the zeroth order

When we consider a small kinetic term,

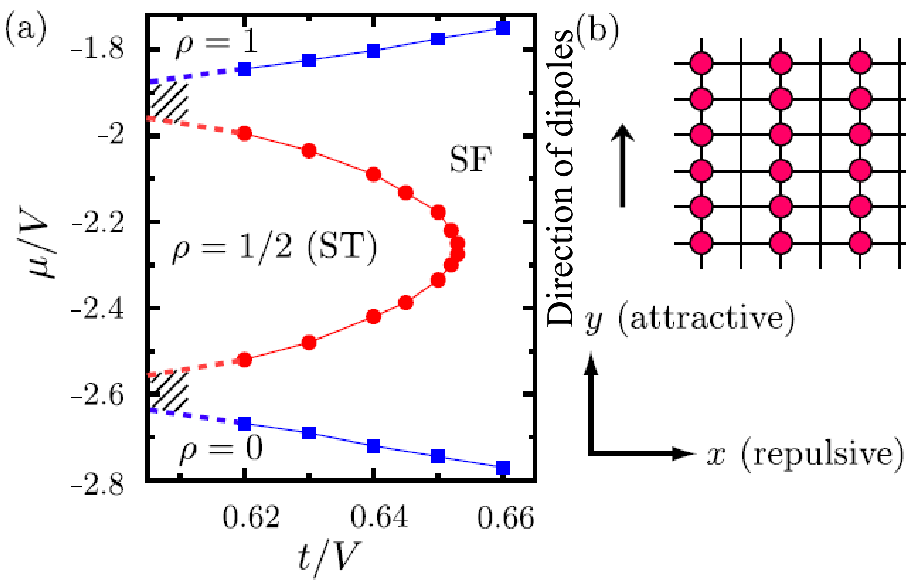
$\underline{0<t<<V}$ $-O(t^2)$ ○ $-O(t^2)$ × The same order In the kinetic energy gain

The repulsions between doped particles increase the energy cost of the domain-wall formation. Therefore, the SS becomes stable against it.

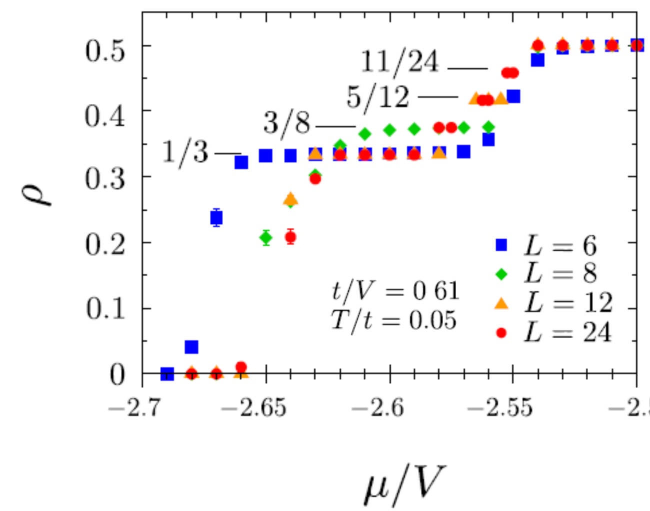
Hard-core bosons with the fully anisotropic dipole-dipole interaction

What happens if the dipole-dipole interactions becomes anisotropic?
→ We studied the case where the dipole moments are polarized parallelly to the 2D plane.

【Ground-state phase diagram】



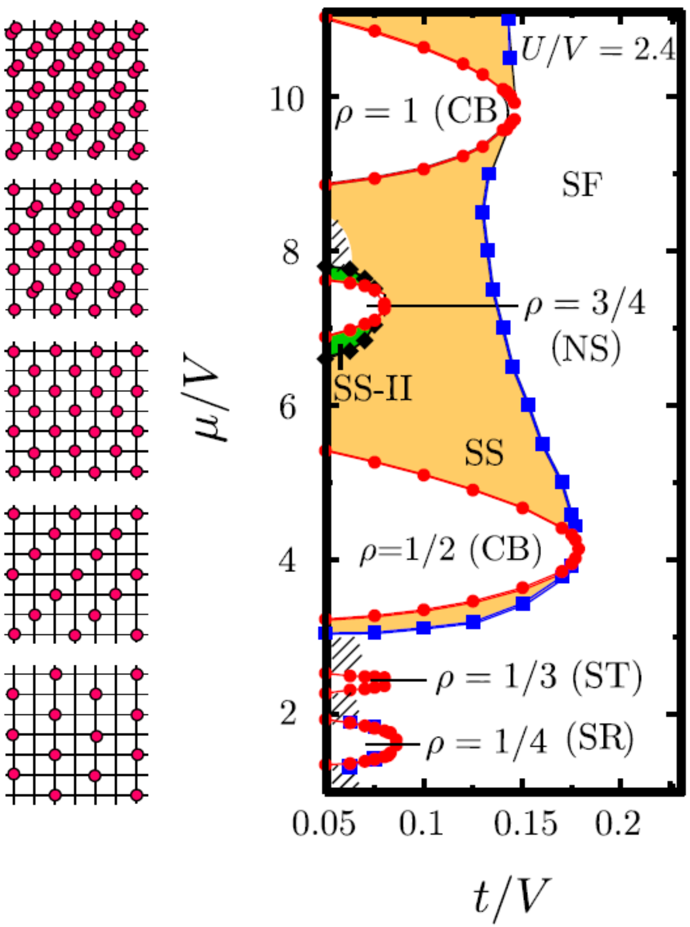
【Multiple plateaus in the shaded regions】



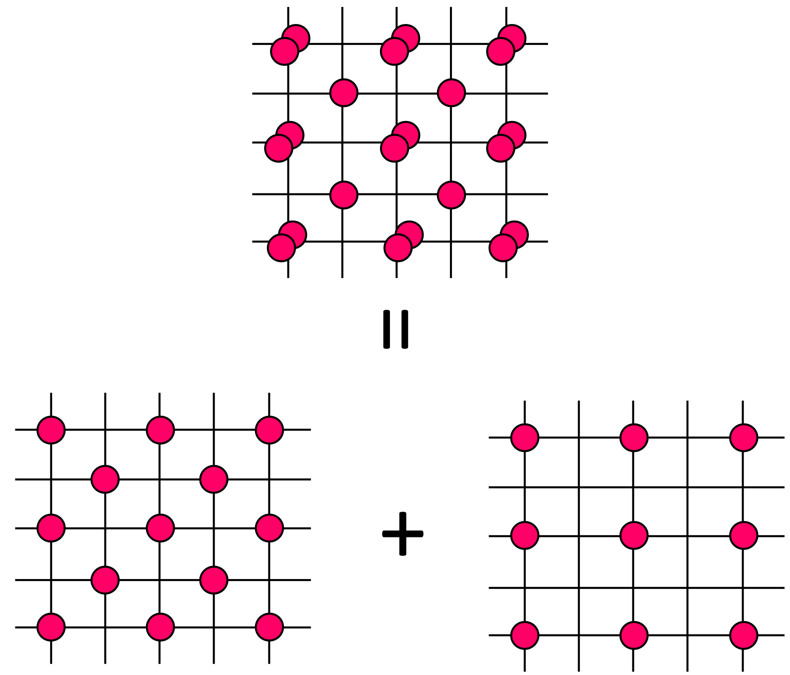
Our phase diagram shows
(i) the presence of the striped solid phase, (ii) the absence of its supersolid phase, and (iii) the presence of regions where multiple plateaus are observed in the particle density.

Ground-state phase diagram of soft-core bosons with the purely repulsive interaction $1/r^3$

【Ground-state phase diagram】



【Nested-solid (NS) structure at ρ=3/4】

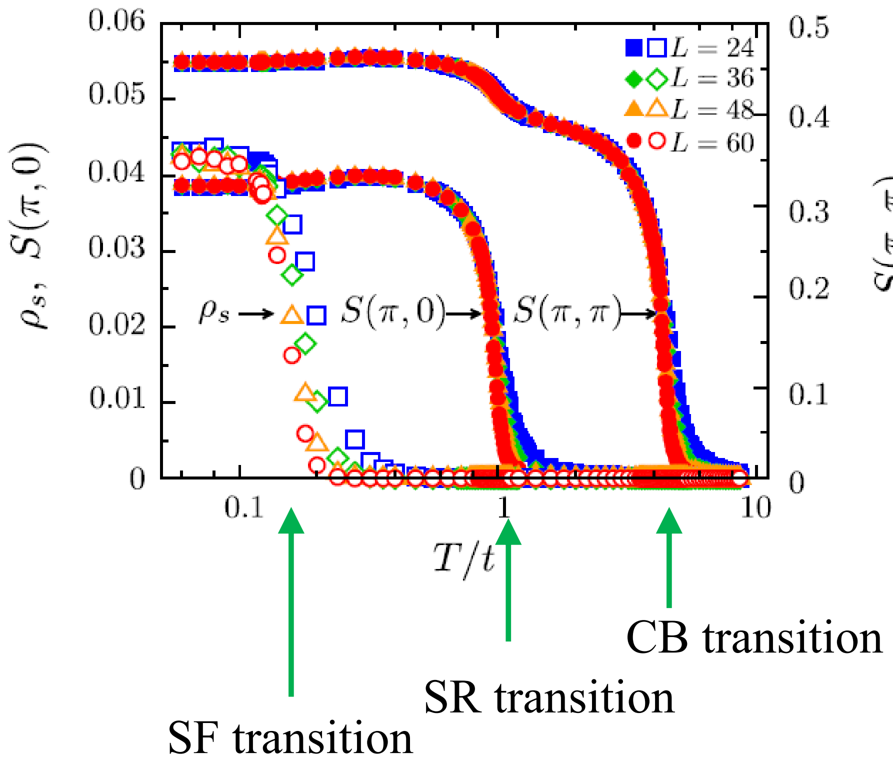


Peaks at the structure factor (π, π) $(\pi, \pi), (\pi, 0)[(0, \pi)]$

Owing to the multiple occupations of bosons and long-range interaction, there appear a nested-solid (NS) phase and its supersolid (SS-II) phase.

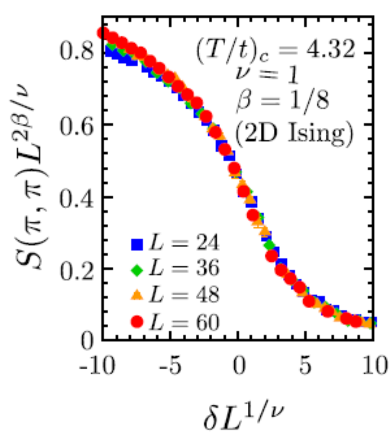
Successive transitions in the SS-II state

【Finite-temperature behaviors in the SS-II phase】
[superfluid density ρ_s
and structure factors $S(\pi, \pi)$, $S(\pi,0)$]

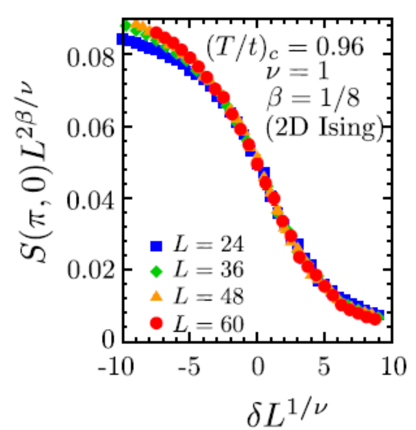


【Finite-size scaling for the two solid-transitions】

1. CB transition



2. SR transition

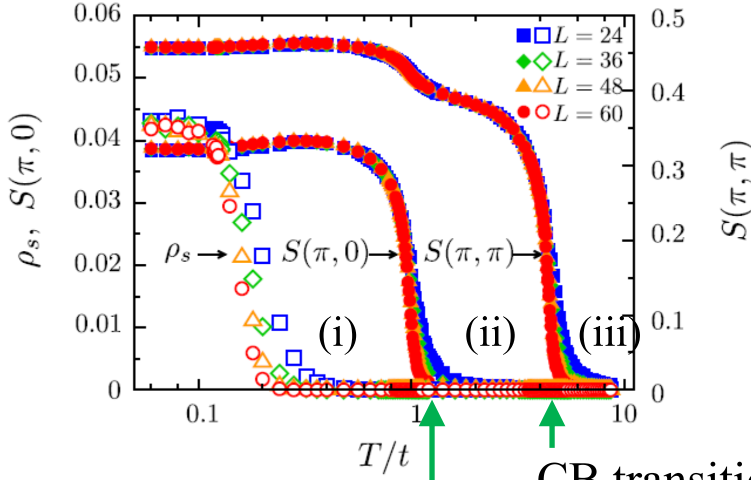


Both transitions belong to the 2D Ising universality class.

The nested-solid structure appears through two successive transitions at finite temperatures.

Why the two Ising-type transitions?

Finally, we give an explain why the two solid-transitions belong to the Ising universality.

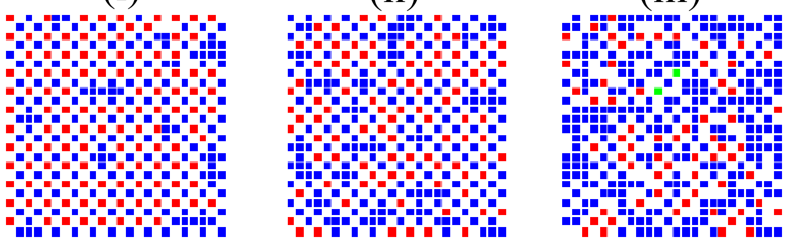


CB transition

SR transition

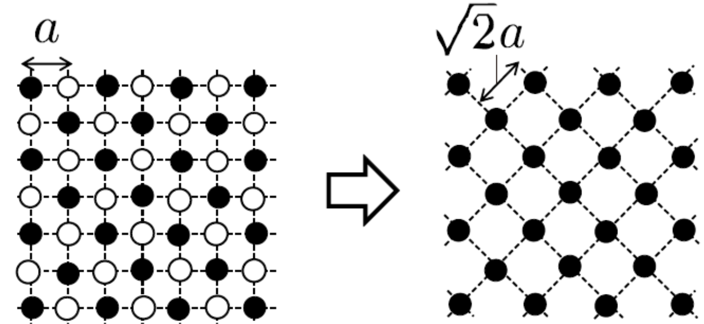
Snapshots

(i) (ii) (iii)

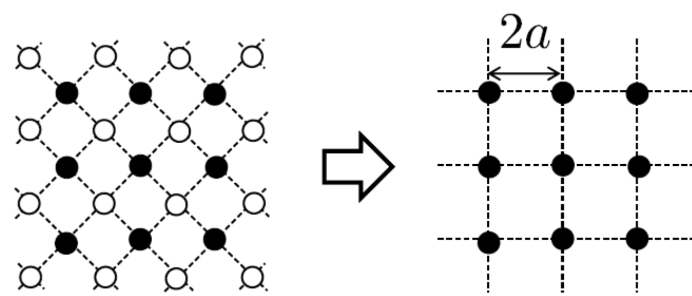


- No bosons
- One boson
- Two bosons
- Three bosons

1. CB transition



2. SR transition



In both two solid-transitions, one of the two sublattices is chosen, and thus they belong to the Ising universality class.

Contents

Summary

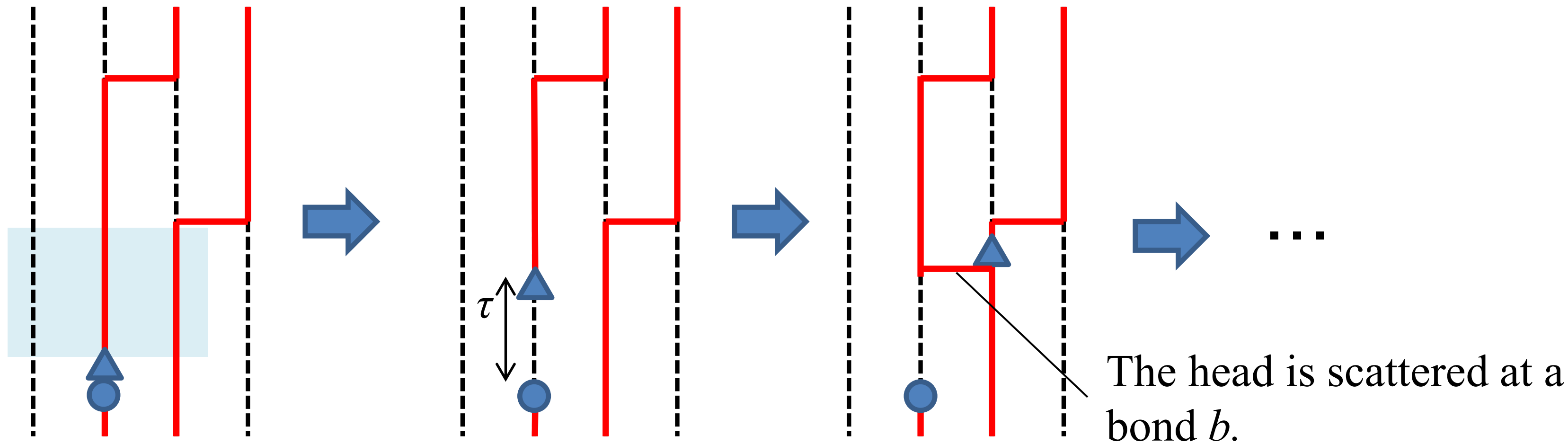
1. For the Bose-Hubbard model with the nearest-neighbor repulsion, we have obtained convincing evidence of a supersolid at the commensurate filling 1/2 for a square lattice as well as a cubic lattice.

2. For the Bose-Hubbard model with the dipole-dipole interaction, we have obtained the ground-state phase diagrams for some cases. As a result, we have found several novel quantum phases such as regions where multiple plateaus are observed in the particle density, a novel nested-solid phase, and its supersoild phase.

Appendices

Previous algorithm

Y. Kato and N. Kawashima, Phys. Rev. E **81** 011123 (2010)



1. Creation of a worm.

2. Generate a distance τ by which the head moves forward.

$$\tau = -\frac{1}{\lambda}\ln R$$

- Averaged number of scattering per unit time $\lambda = \sum_b \lambda_b$ depends on the states in the shaded uniform area.
- $R \in [0, 1)$ is a uniform random number.

3. Scatter the head at stochastically chosen bond *b*.

We update the world-line configuration by repeating vertical movement and scattering of the worm head.

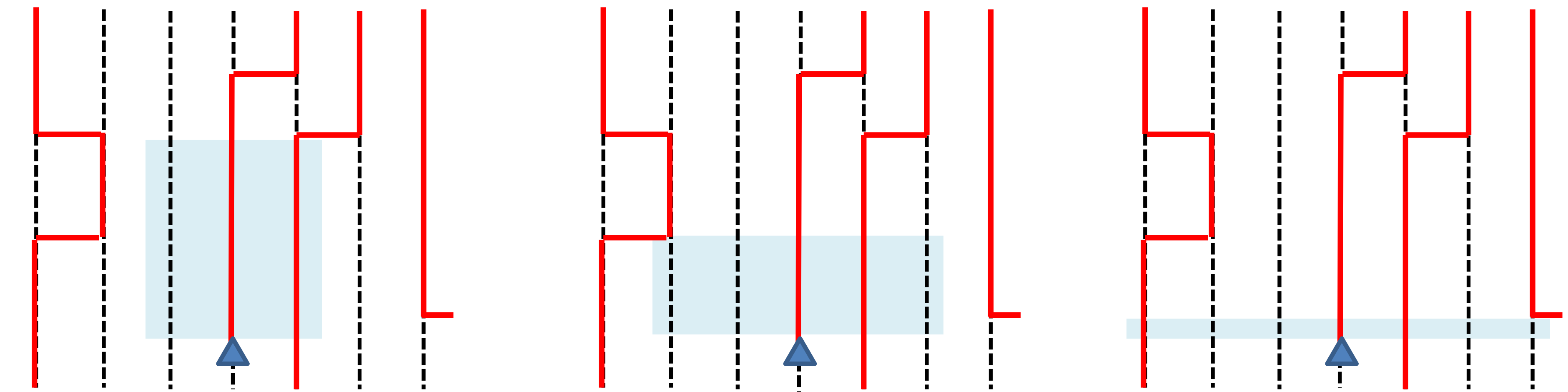
Difficulty in long-range interacting systems

The uniform area becomes global in real space but local in imaginary time, when the longer-range interaction is included.

1. Nearest-neighbor interaction only

2. Up to the next-nearest-neighbor interaction

3. Up to the third-nearest-neighbor interaction



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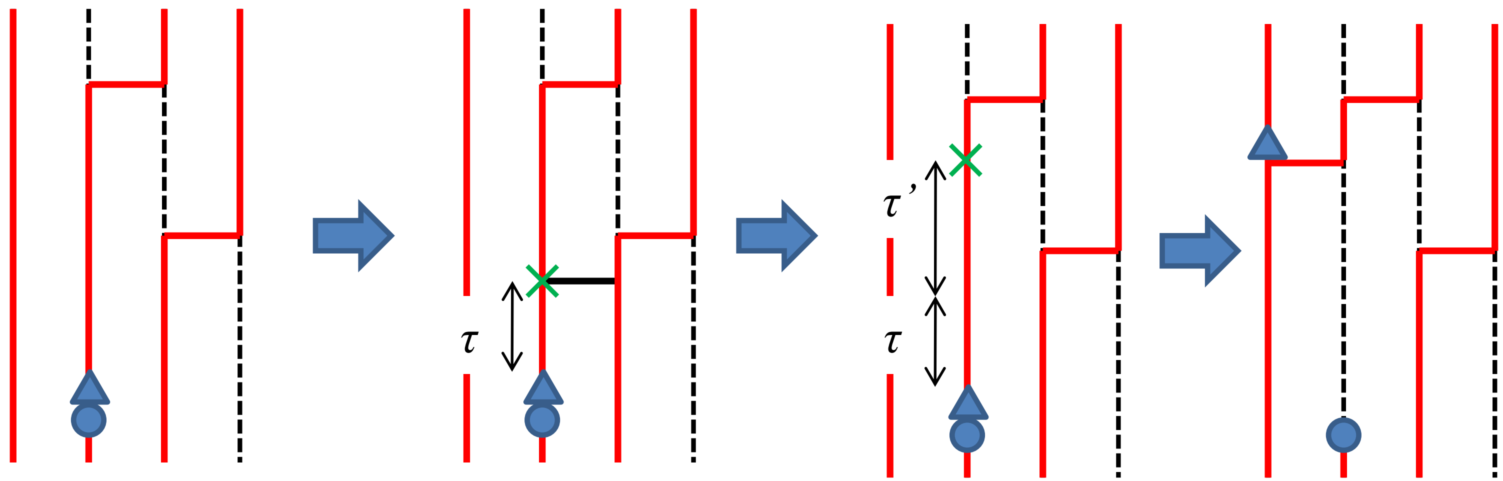
It takes $O(N)$ time to move the worm head forward. (Here, N is the system size.)

Modification of the algorithm



1. Generate a distance τ by which the head moves forward.

$$\tau = -\frac{1}{\lambda'}\ln R$$

- $\lambda' = \sum \lambda'_b$ depends only on the worm head's site and $\lambda'_b \geq \lambda^b_b$ is satisfied.

2. Choose a bond b and accept it by the probability $\Delta_b = \lambda_b' / \lambda_b$.

 (We repeat 1-2 until a bond is accepted.)

cf. K. Fukui and S. Todo, J. Comput. Phys. **228** 2629 (2009)

3. Scatter the worm head at the accepted bond b.

It takes only $O(1)$ time to move the worm head forward.