Quantum condensation on bilayer Bose Hubbard model

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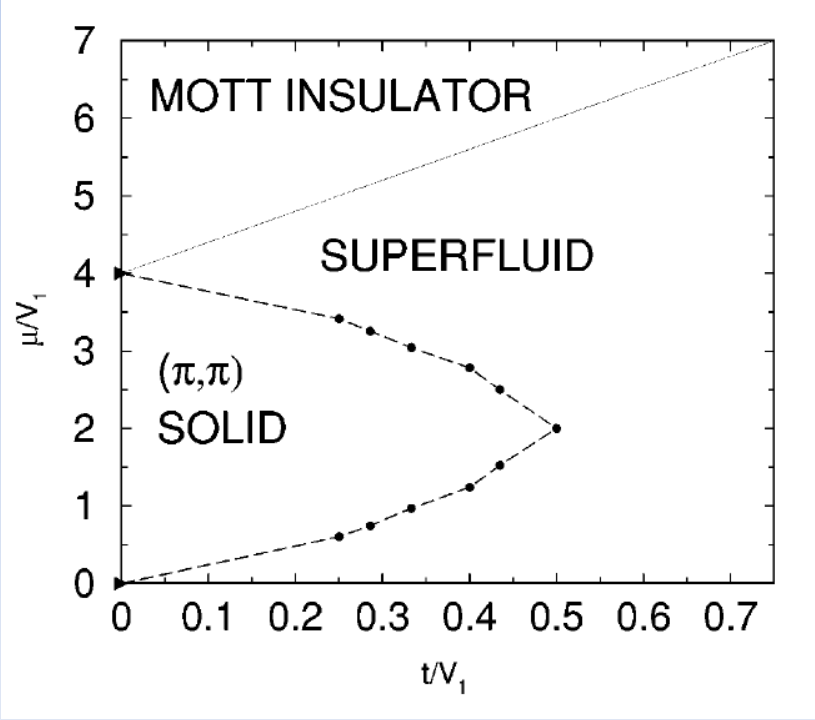
Review of hardcore Bose-Hubbard model

$$H = -t\sum_{\langle ij\rangle}(b_i^+ b_j + h.c.) + V_1\sum_{\langle ij\rangle} n_i n_j - \mu\sum_i n_i$$

2D square lattice

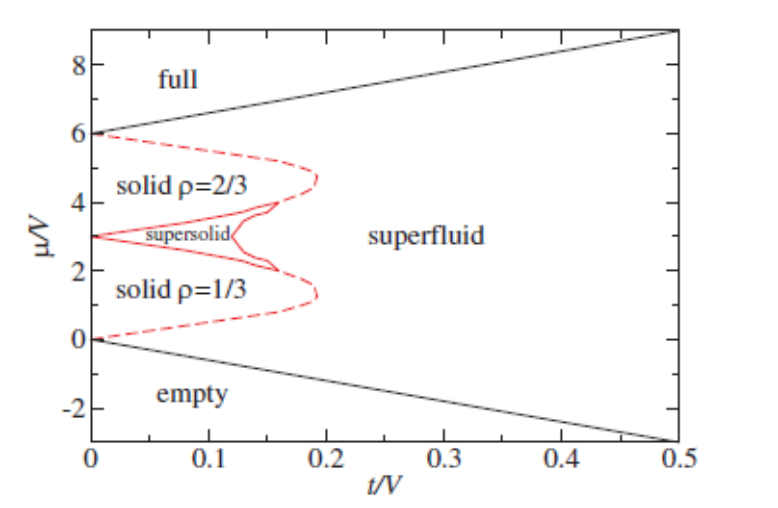


- repulsive interaction V_1
- Checkerboard quantum solid arises at small hoppings
- Supersolid phases is not stable against phase separation, unless next-nearest neighbor repulsion is included.

Hebert *et al.*, PRB 65, 014513 (2001)

Review of hardcore Bose-Hubbard model

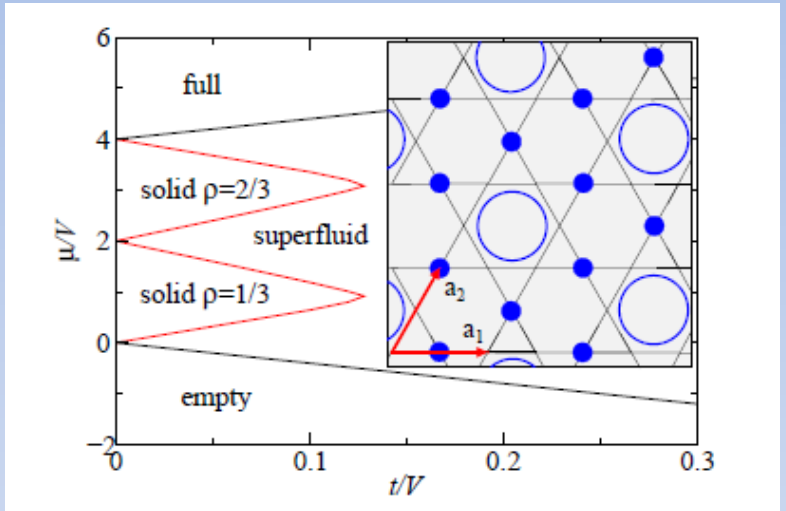
2D triangular lattice



Wessel *et al.,* PRL 95, 127205 (2005)

- Two solid phases with different densities
- A supersolid phase is stabilized via order by disorder mechanism

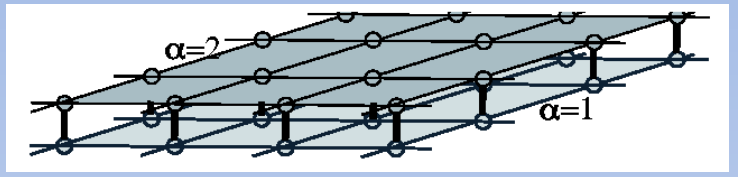
2D Kagome lattice



Isakov *et al.,* PRL 97, 147202 (2006)

Review of hardcore Bose-Hubbard model

Bilayer square lattice



Antiferromagnetic Heisenberg spin-1/2 model

$$H_s = J\sum_i \mathbf{S}_{1,i}\cdot\mathbf{S}_{2,i} + J'\sum_{l,\langle ij\rangle}\mathbf{S}_{l,i}\cdot\mathbf{S}_{l,j} - g\mu_B H\sum_{l,i}\mathbf{S}^z_{l,i}$$

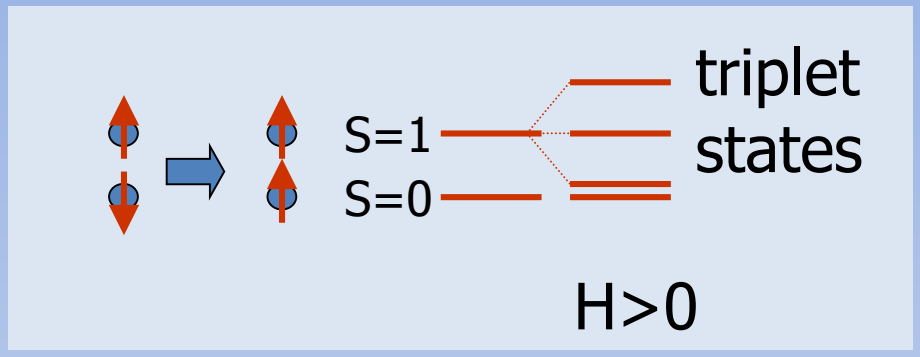
$$J > J'$$

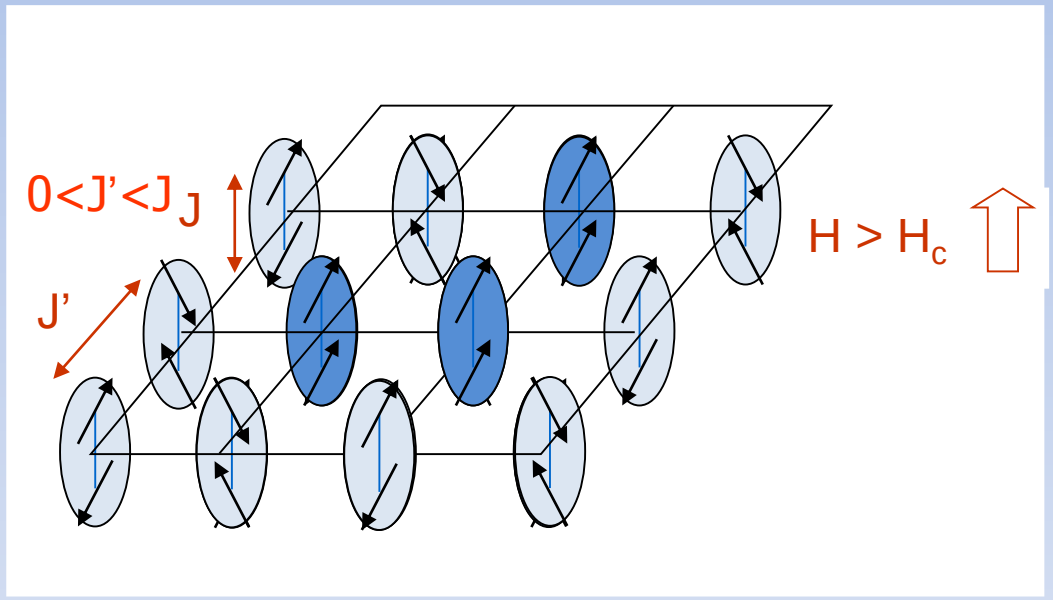
Equivalent to Bose-Hubbard model (*V=2t*)*:*

$$S^+ \to b^+ \quad S^- \to b^- \quad S^z \to n - \frac{1}{2}$$

mag. field *H* plays the role of μ.

Bose-Einstein condensation of triplets (triplons) has been observed in many dimer materials: $BaCuSi_2O_6$, $TlCuCl_3$, $KCuCl_3$ and S=1 compound $NiCl_2$-4SC$(NH_2)_2$ (where the single ion anisotropy *D* plays the role of *J*.)





If we ignore t_- and t_0 states, it becomes a hard-core boson model:

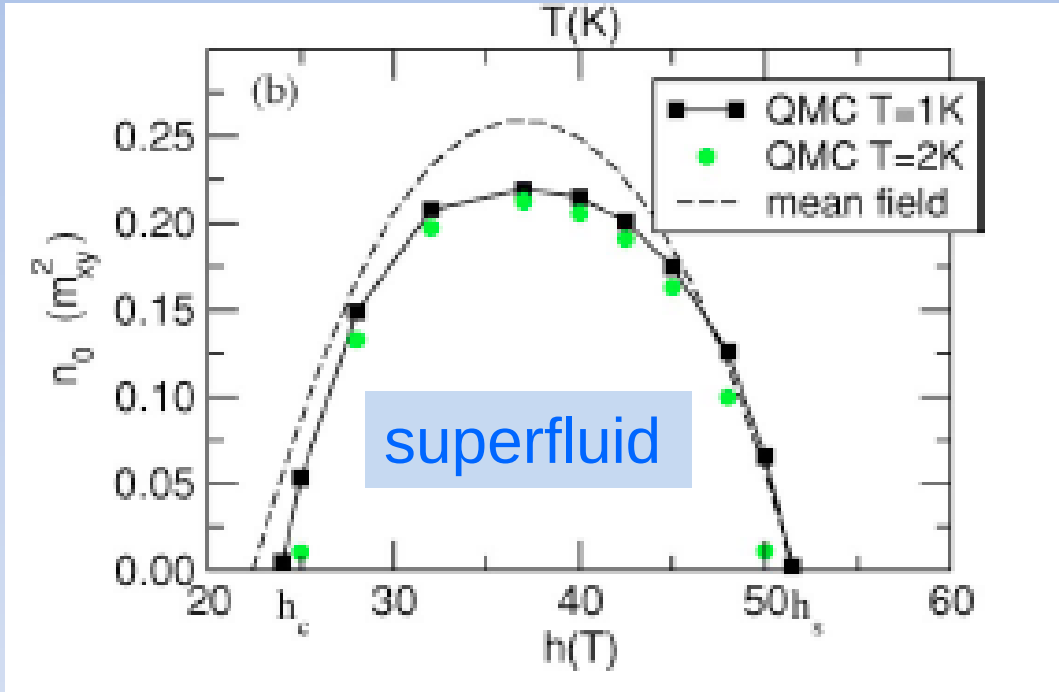
$$H_b = t\sum_{\langle ij\rangle}\left(d_i^+ d_j + d_j^+ d_i\right) + V\sum_{\langle ij\rangle} n_i n_j - \mu\sum_i n_i$$

$$t = V = J'/2; \quad \mu = g\mu_B H - J$$

$$d_i^+ = \frac{(-1)^i}{\sqrt{2}}\left(S_{1i}^+ - S_{2i}^+\right)$$

Review of hardcore Bose-Hubbard model

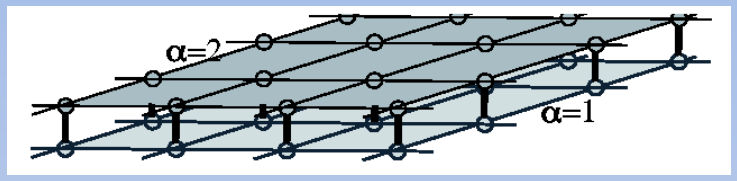
Bilayer square lattice



K.K. Ng and T.K. Lee, PRB **73**, 014433 (2006).

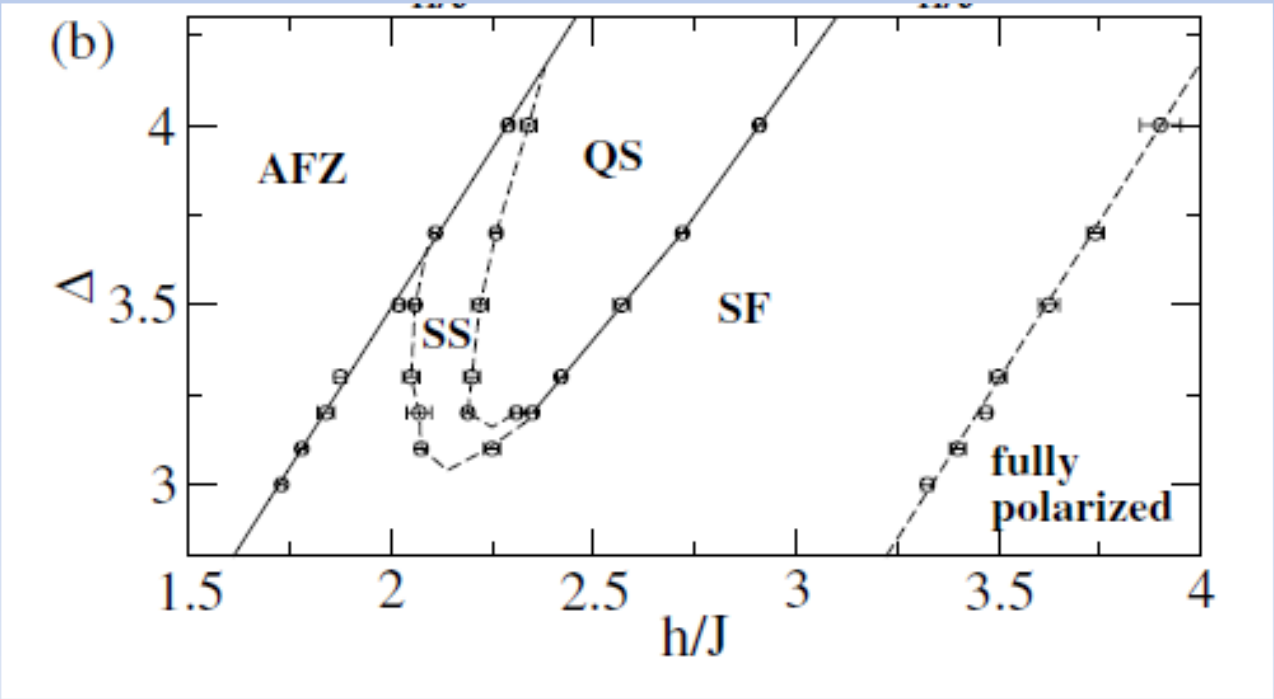
Review of hardcore Bose-Hubbard model

Bilayer square lattice



In-plane XXZ

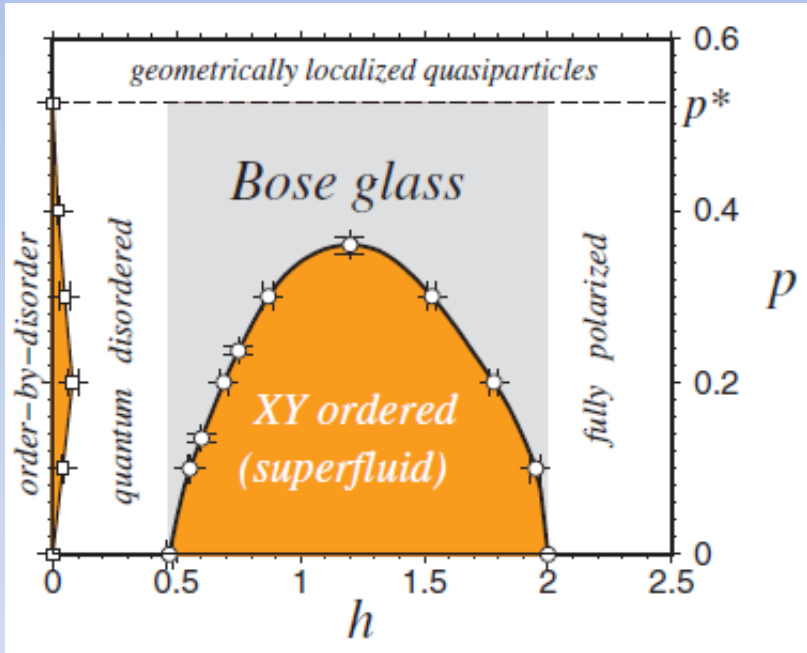
$$H_{XXZ} = J\sum_i \mathbf{S}_{1,i}\cdot\mathbf{S}_{2,i} + J'\sum_{l,\langle ij\rangle}\left(S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z\right) - g\mu_B H\sum_{l,i}\mathbf{S}_{l,i}^z$$



Ng *et al.,* PRL 97, 127204 (2006)

Review of hardcore Bose-Hubbard model

Bilayer square lattice

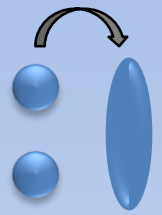


- Bose glass due to site dilution

T. Roscilde and S. Hass, PRL 95, 207206 (2005)

Review of hardcore Bose-Hubbard model

Remark:



- There is only condensation of bosons, but not dimers. (the hopping of triplons in the singlet background involve only one boson)
- Also in the QMC calculations, either the boson condensate density $n_o = \langle b_i^+ b_j \rangle = \langle b \rangle^2$

  or superfluidity (via winding number) $\rho_s = \frac{1}{\beta}\langle W^2 \rangle$

  is measured.
- However, it has been shown that special two loops (worms) algorithm is necessary to simulate pair (dimer) superfluids.

K.K. Ng and M.F. Yang, PRB 83, 100511(R) (2011)

L. Bonnes and S. Wessel, PRL 106, 185302 (2011)

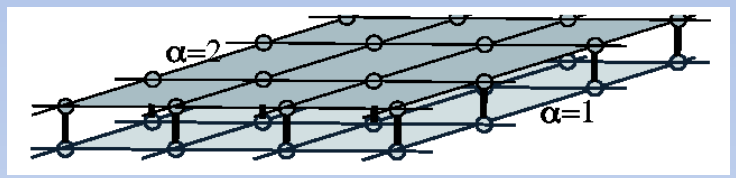
Our model

Bilayer hardcore Bose-Hubbard model

$$H = \sum_i \left[-t(b_{i1}^+ b_{i2} + h.c.) + V n_{i1} n_{i2} \right] + \sum_{\alpha \langle ij \rangle} \left[-t'(b_{i\alpha}^+ b_{j\alpha} + h.c.) + V n_{i\alpha} n_{j\alpha} \right] - \mu \sum_{i\alpha} n_{i\alpha}$$

Inter-layer attraction: $V < 0$

Intra-layer repulsion: $V' > 0$



- When *V* is strong, dimers will be dominate.

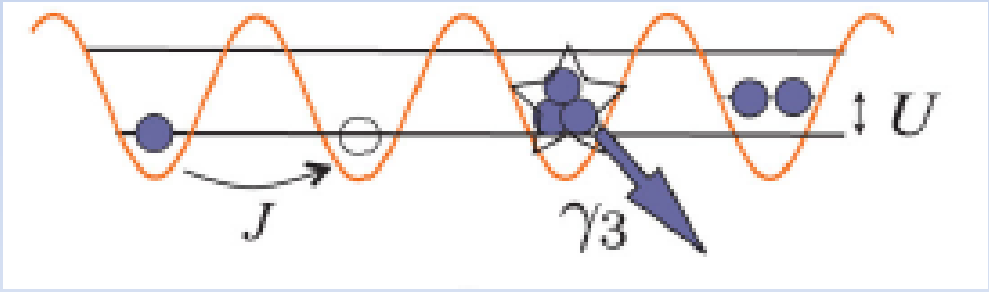
Questions:

- Could dimers condense and form pair superfluids or even pair supersolids?
- What is the ground state phase diagram?
- How does it differ from that of three-body constraint system or two-species model?

Similar systems:
Attractive Bose-Hubbard model with three-body constraint

Daley *et al.* (PRL **102**, 040402 (2009)) proposed that the large three-body combination loss process (via triatomic Efimov resonance [Kraemer *et al.* Nature 440, 315 (2006)]) can leads to an effective three-body interactions – a three-body hard-core constraint.

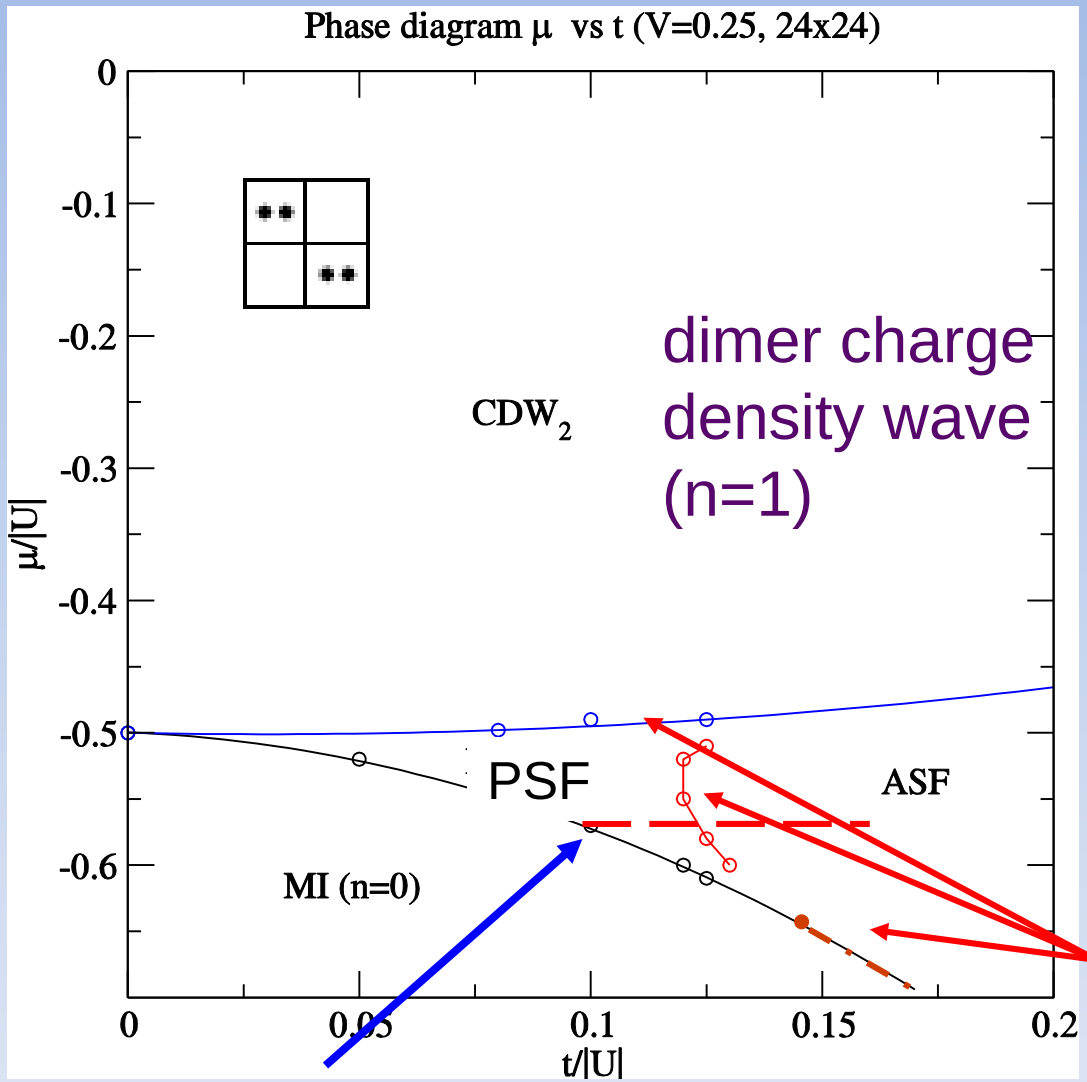
$$a_i^{+3} \equiv 0$$



Ground state phase diagrams:

T/|U|=0.001

n <= 1



ASF

$\langle b \rangle \neq 0$ $\langle b^2 \rangle \neq 0$

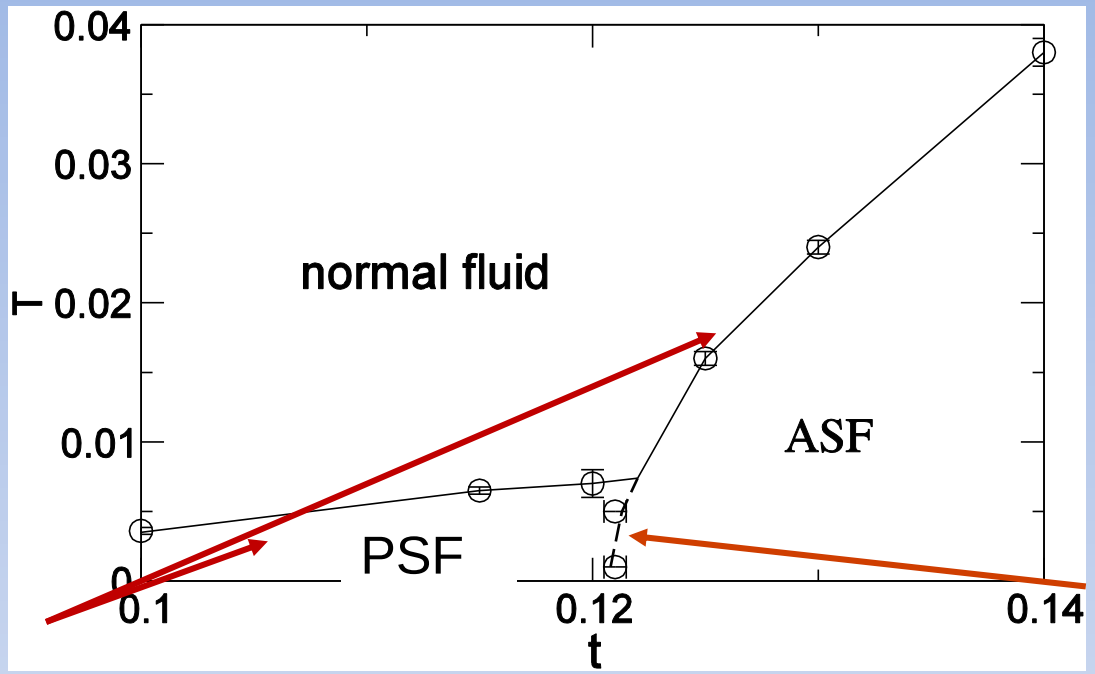
PSF

$\langle b \rangle = 0$ $\langle b^2 \rangle \neq 0$

1st order

2nd order

Finite temperature phase diagram.

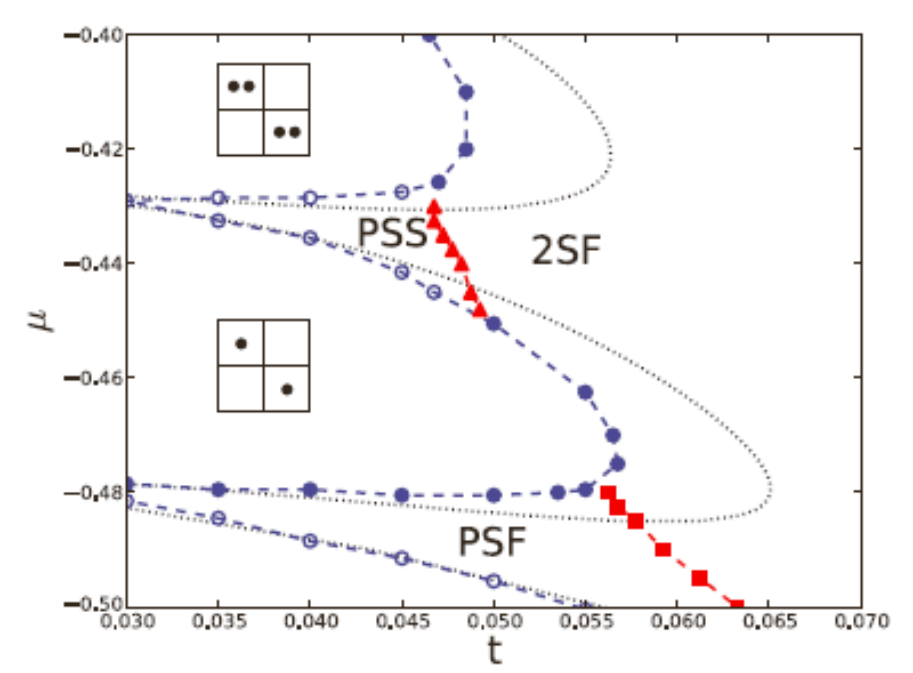


KT type

1st order

- Both of continuous KT (Kosterlitz-Thouless) type, but with distinct characters.
- universal stiffness jump of PSF is 4 times larger than that of ASF
- PSF-N transition is driven by the unbinding of half-vortices.
- the underlying Coleman-Weinberg mechanism is not spoiled by the thermal fluctuations.

Similar systems:
Two-species bonons



C.M. Chung *et al.,* PRB **85**, 214513 (2012)

Pair supersolid is stabilized and the bosons are softcore.

Numerical Methods

We try to study numerically the PSF phase using SSE (stochastic series expansion) method.

Order parameters:

Superfluidity (spin stiffness) ρ is related to the winding number (W) fluctuations in the simulation.

$$\rho_{even(odd)} = mT\left\langle W^2_{even(odd)} \right\rangle$$

$$m \equiv 1/2t$$

m is the effective mass in square lattice

1. To identify the ASF and PSF, we measure the odd and even winding number separately.
2. In the ASF phase, both ρ_{odd} and ρ_{even} are finite.
3. While the PSF phase, ρ_{even} is finite but ρ_{odd}=0 (two bosons move together) .

Numerical Methods

Basic idea of Stochastic Series Expansion (SSE)

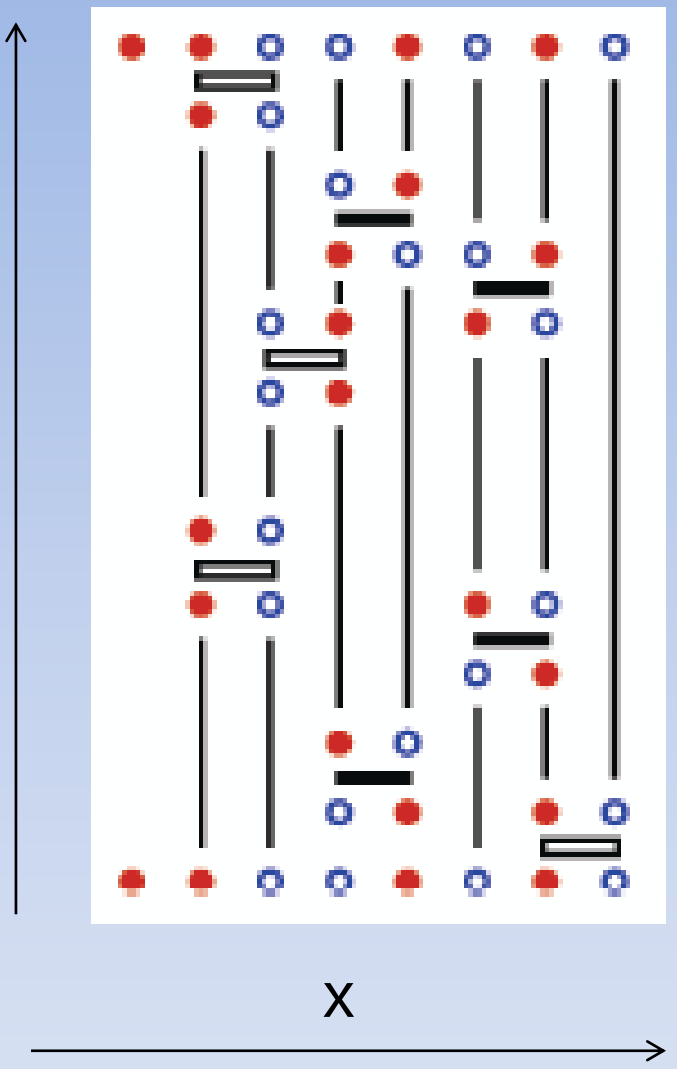
Thermal expectation value

$$\langle A \rangle = \frac{1}{Z} Tr\left[A e^{-\beta H} \right], \quad Z = Tr\{ e^{-\beta H} \}$$

$$Z = \sum_{\alpha} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle \alpha | (-H)^n | \alpha \rangle$$

$$H = -\sum_{a,b} H_{a,b}$$

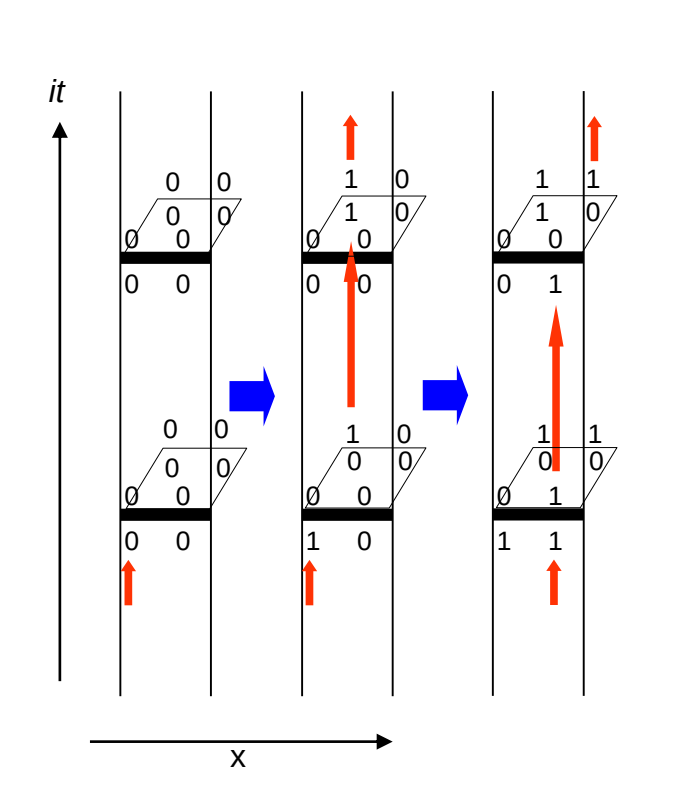
$$Z = \sum_{\alpha} \sum_{\{H_{ab}\}} \frac{\beta^n (M-N)!}{M!} \langle \alpha | \prod_{i=1}^{M} H_{a(i),b(i)} | \alpha \rangle$$



Numerical Methods

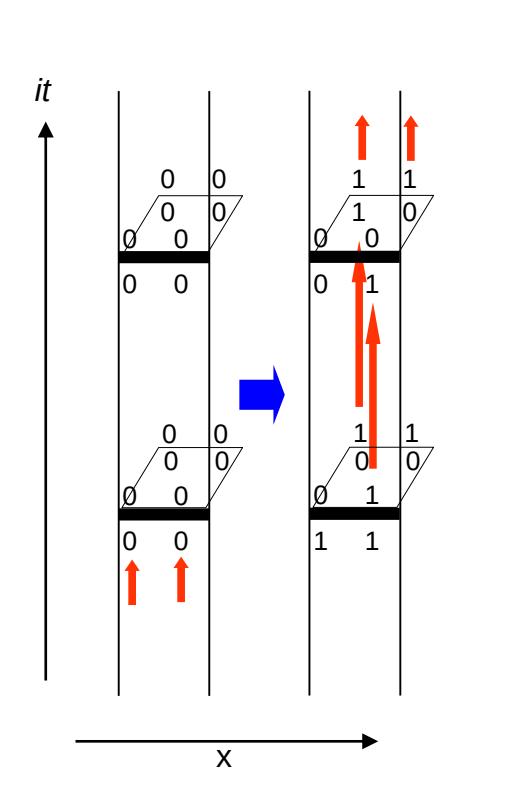
Examples of dimer hopping

Conventional bond-based one loop algorithm



This two steps hopping is very ineffective, especially in large lattice size.

Cluster-based two loops algorithm



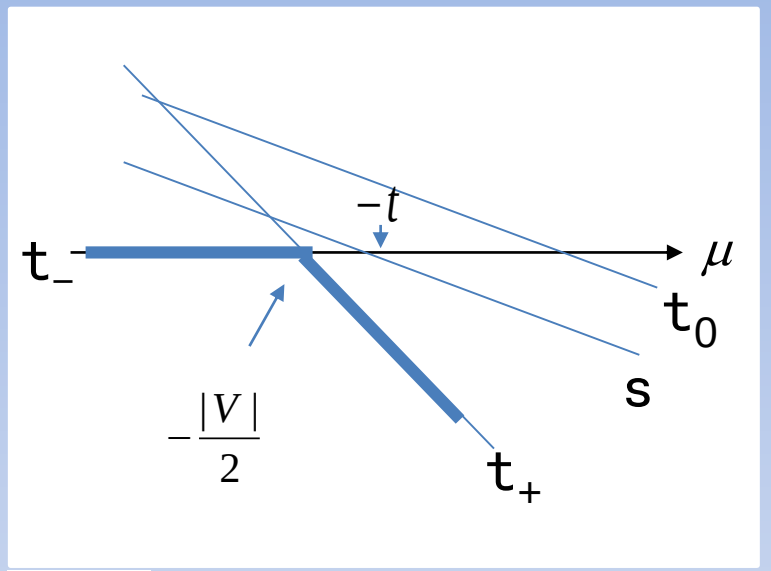
The dimer hopping always lead to even winding number.

Analysis of localized dimers (t'=0)

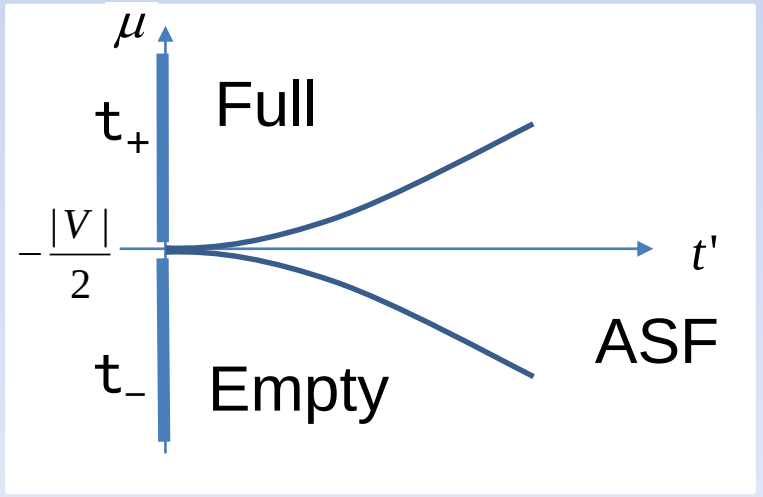
$$V'=0$$

Independent dimer:

		Energy
t_+	$\left\|\begin{matrix}1\\1\end{matrix}\right\rangle$	$-\|V\|-2\mu$
s	$\frac{1}{\sqrt{2}}\left(\left\|\begin{matrix}1\\0\end{matrix}\right\rangle-\left\|\begin{matrix}0\\1\end{matrix}\right\rangle\right)$	$-t-\mu$
t_0	$\frac{1}{\sqrt{2}}\left(\left\|\begin{matrix}1\\0\end{matrix}\right\rangle+\left\|\begin{matrix}0\\1\end{matrix}\right\rangle\right)$	$t-\mu$
t_-	$\left\|\begin{matrix}0\\0\end{matrix}\right\rangle$	0



$t<\frac{|V|}{2}$ Strong interlayer attraction (hardcore dimer)

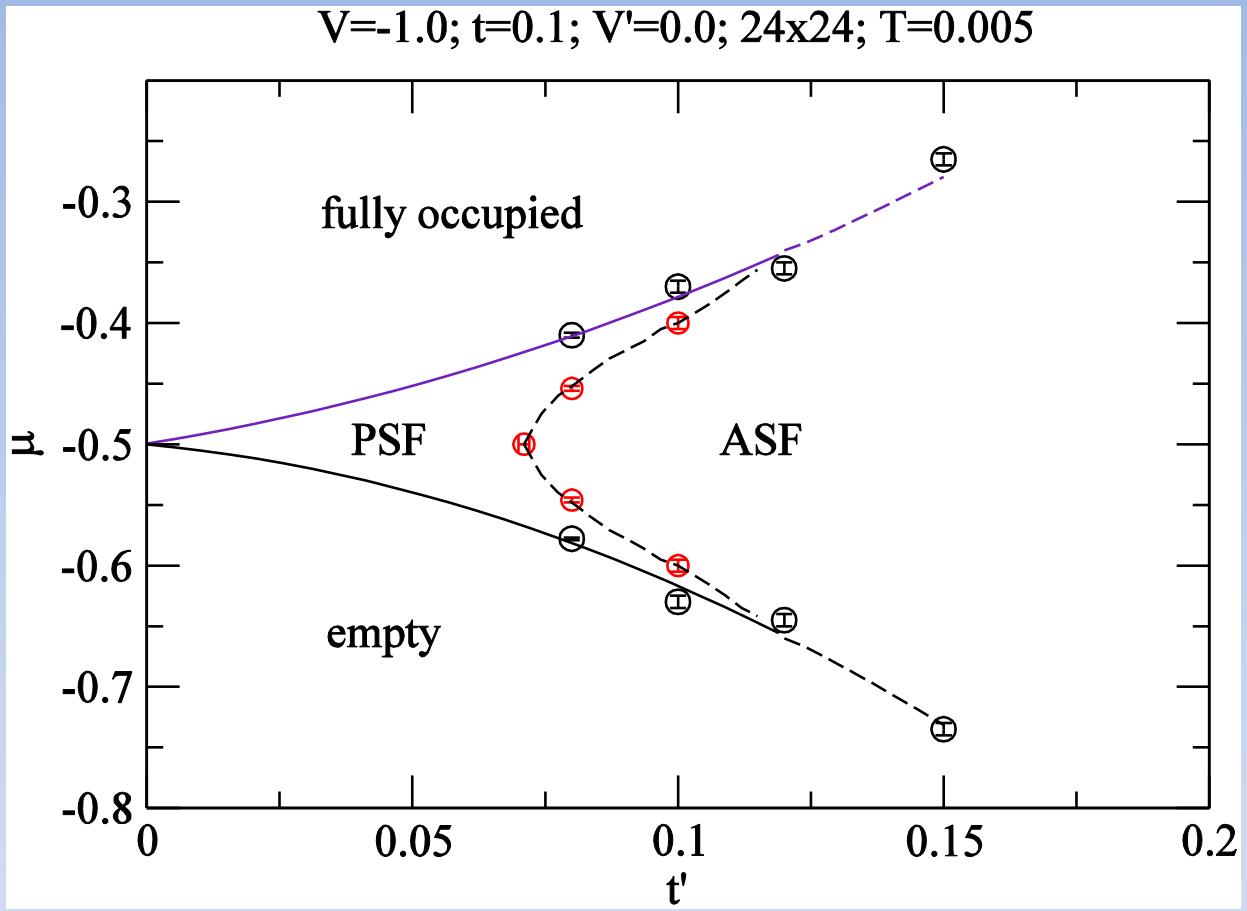


Numerical Results

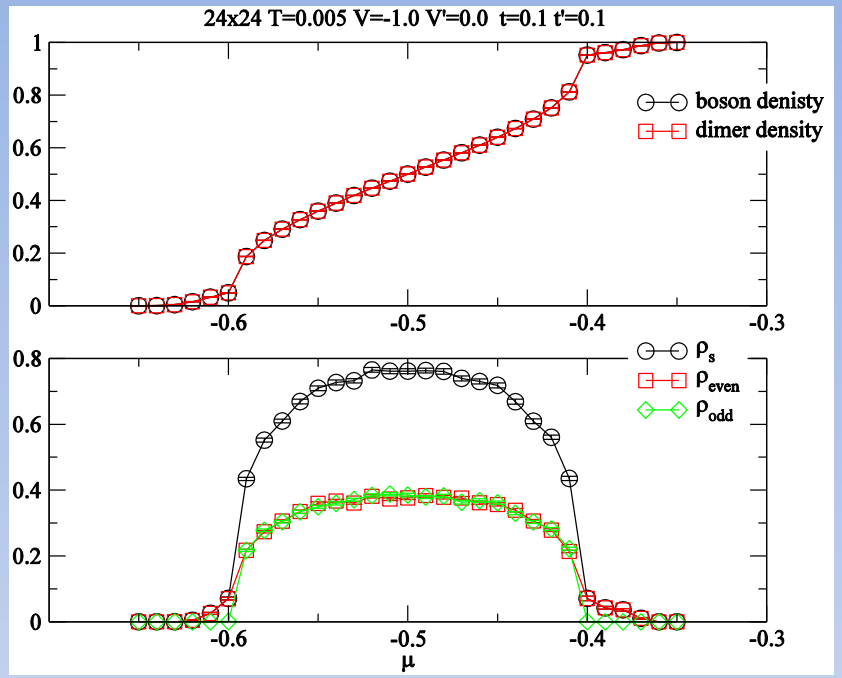
hardcore dimer regime

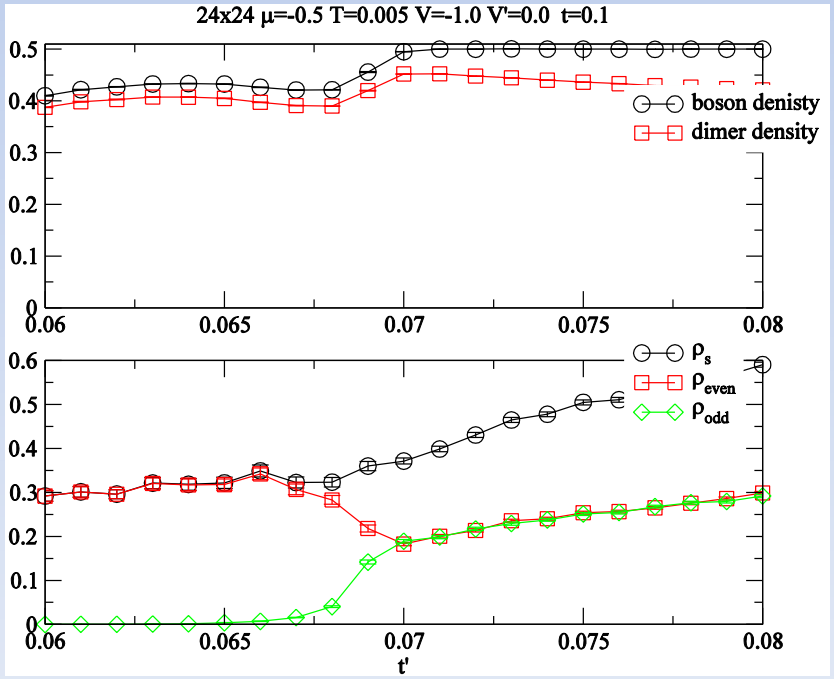
V=-1; t=0.1
V'=0

No intra-layer repulsion, therefore no checkerboard soild phase.

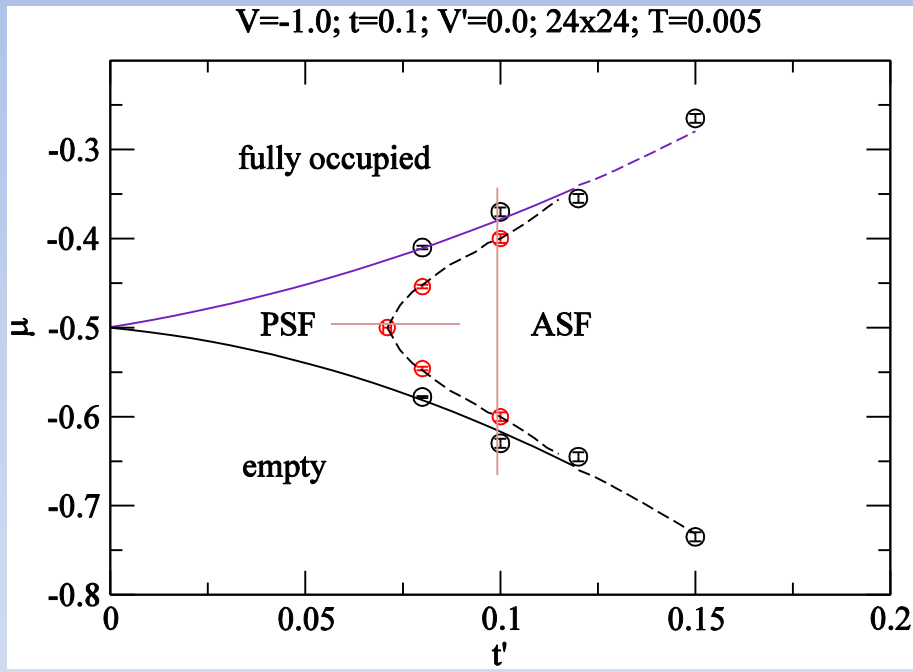


- Inter-layer attractive *V* is set to be -1 for all calculations.
- Temperature is fixed to 0.005 (probe the ground state properties)
- System size 24x24x2


24x24 T=0.005 V=-1.0 V'=0.0 t=0.1 t'=0.1
boson denisty
dimer density
ρs
ρeven
ρodd
μ


24x24 μ=-0.5 T=0.005 V=-1.0 V'=0.0 t=0.1
boson denisty
dimer density
ρs
ρeven
ρodd
t'

t'=0.1

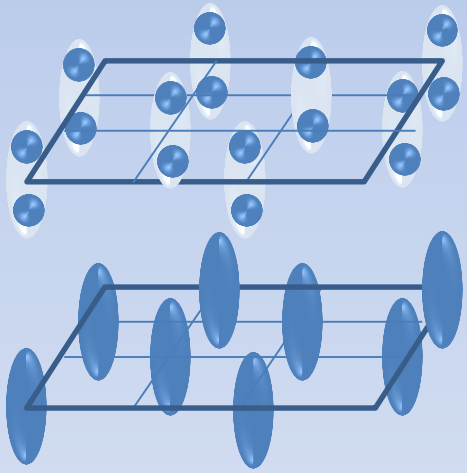

V=-1.0; t=0.1; V'=0.0; 24x24; T=0.005
fully occupied
PSF
ASF
empty
μ
t'

μ=-0.5

Analysis of localized dimers (t'=0)

$V'>0$ interacting dimer:

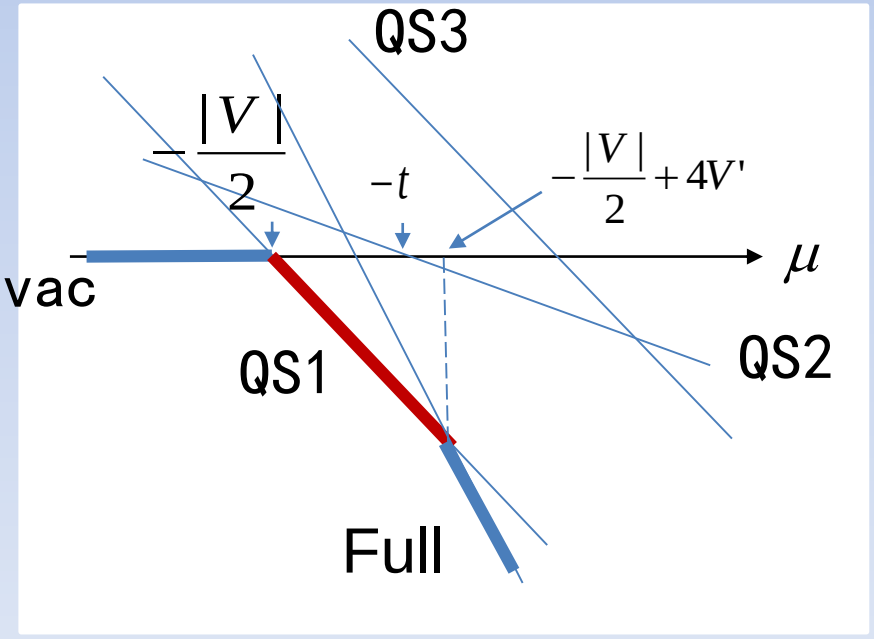
		Energy/dimer
full	$\left\|\begin{matrix}1\\1\end{matrix}\right\rangle\left\|\begin{matrix}1\\1\end{matrix}\right\rangle\left\|\begin{matrix}1\\1\end{matrix}\right\rangle\left\|\begin{matrix}1\\1\end{matrix}\right\rangle\cdots$	$-\lvert V\rvert-2\mu+4V'$
QS1	$\left\|\begin{matrix}1\\1\end{matrix}\right\rangle\left\|\begin{matrix}0\\0\end{matrix}\right\rangle\left\|\begin{matrix}1\\1\end{matrix}\right\rangle\left\|\begin{matrix}0\\0\end{matrix}\right\rangle\cdots$	$-\frac{\lvert V\rvert}{2}-\mu$
QS2	$\lvert s\rangle\left\|\begin{matrix}0\\0\end{matrix}\right\rangle\lvert s\rangle\left\|\begin{matrix}0\\0\end{matrix}\right\rangle\cdots$	$-\frac{t}{2}-\frac{\mu}{2}$
QS3	$\lvert s\rangle\lvert s\rangle\lvert s\rangle\lvert s\rangle\cdots$	$-t-\mu+V'$
QS4	$\lvert s\rangle\left\|\begin{matrix}1\\1\end{matrix}\right\rangle\lvert s\rangle\left\|\begin{matrix}1\\1\end{matrix}\right\rangle\cdots$	$-\frac{t}{2}-\frac{\lvert V\rvert}{2}-\frac{3\mu}{2}+2V'$

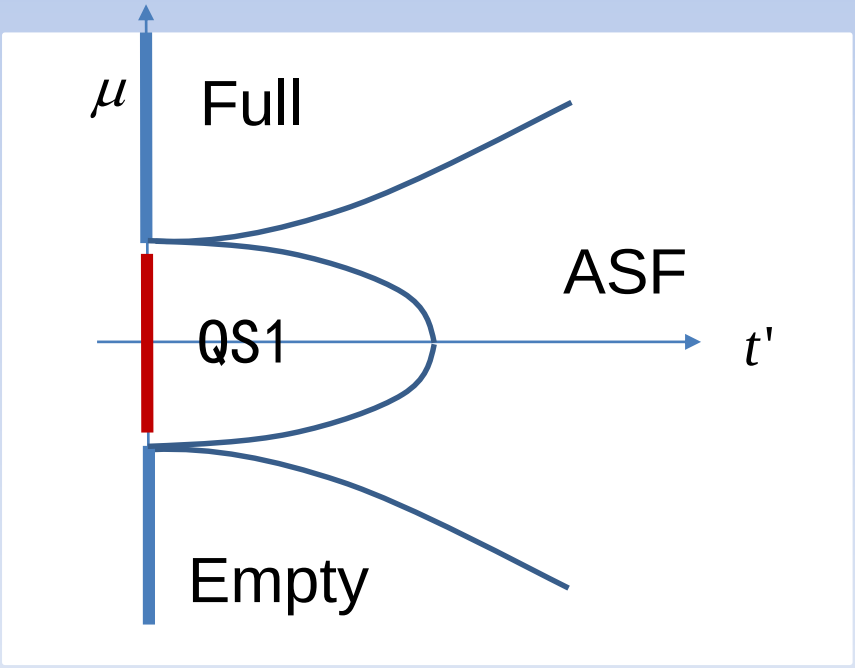


Analysis of localized dimers (t'=0)

$V' > 0$ interacting dimer:

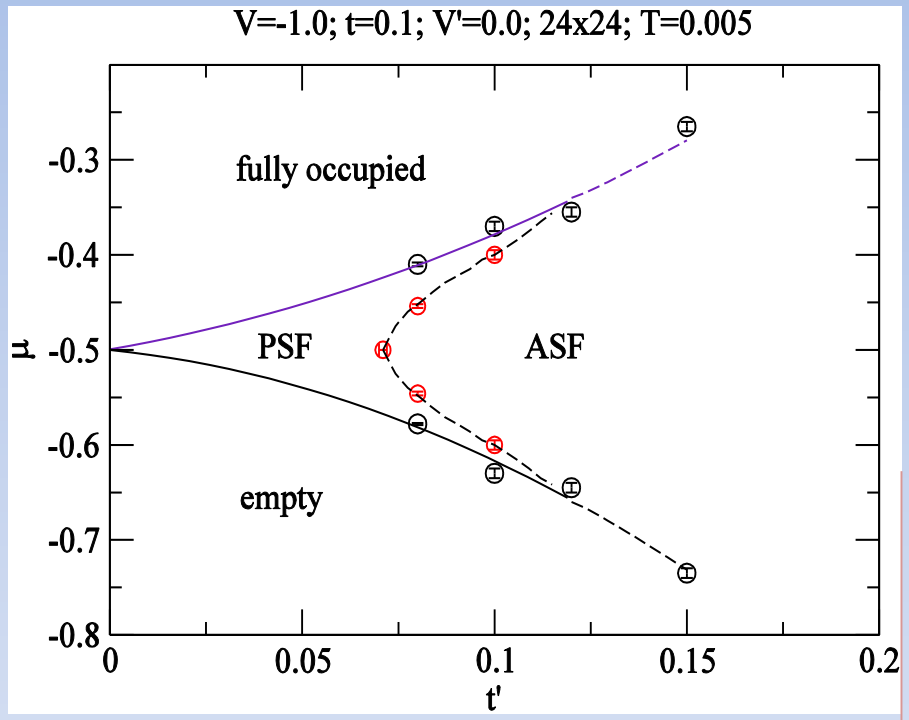
$t < \frac{|V|}{2}$ hardcore dimer regime



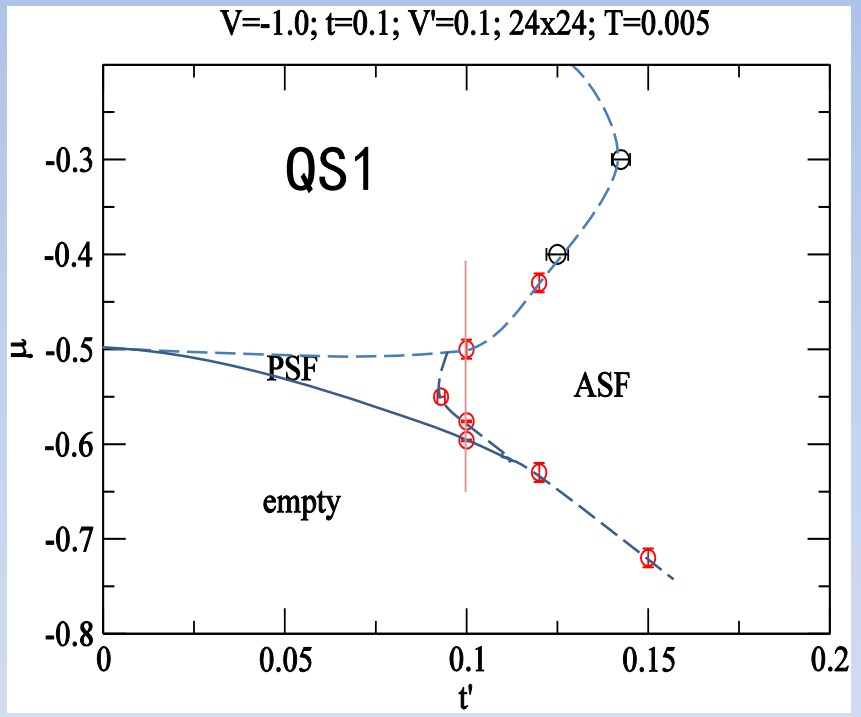


Numerical Results

V'=0

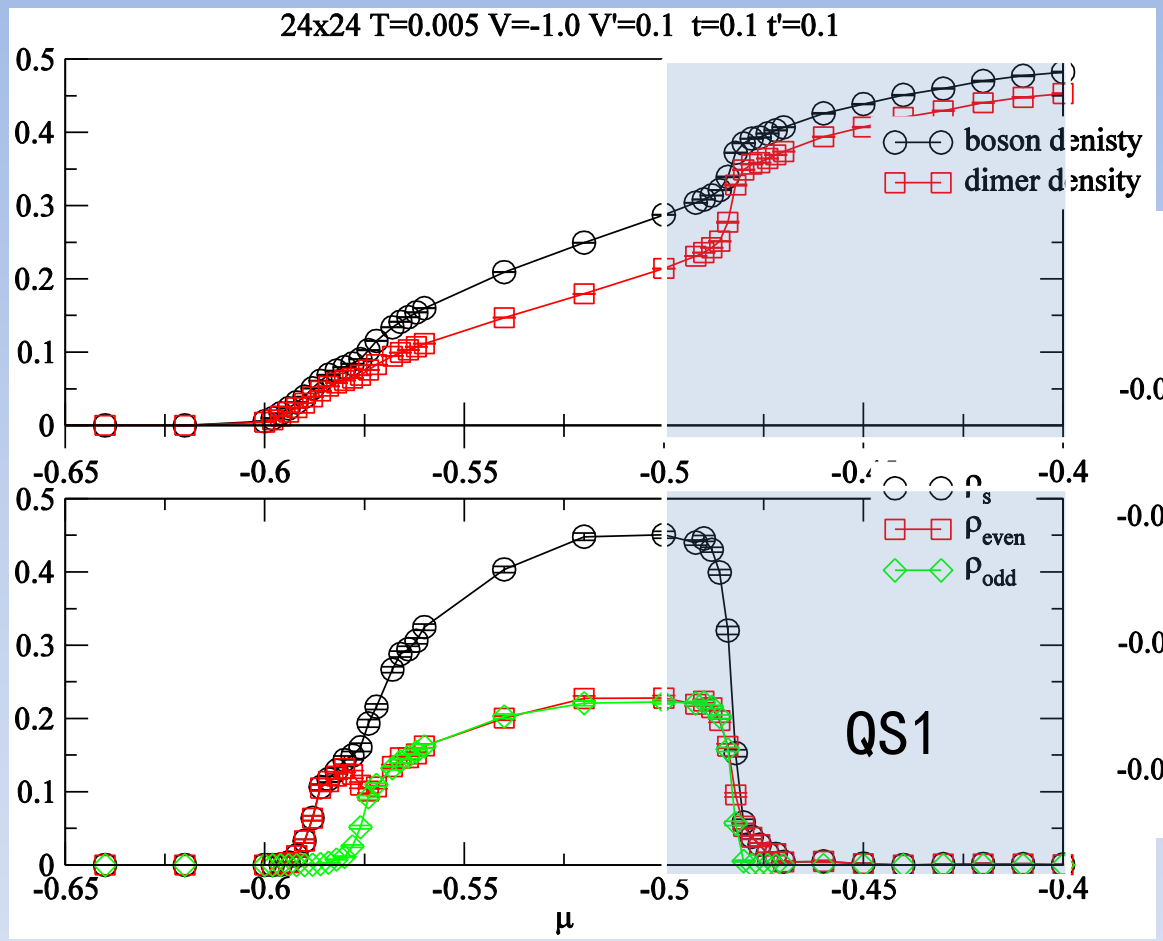


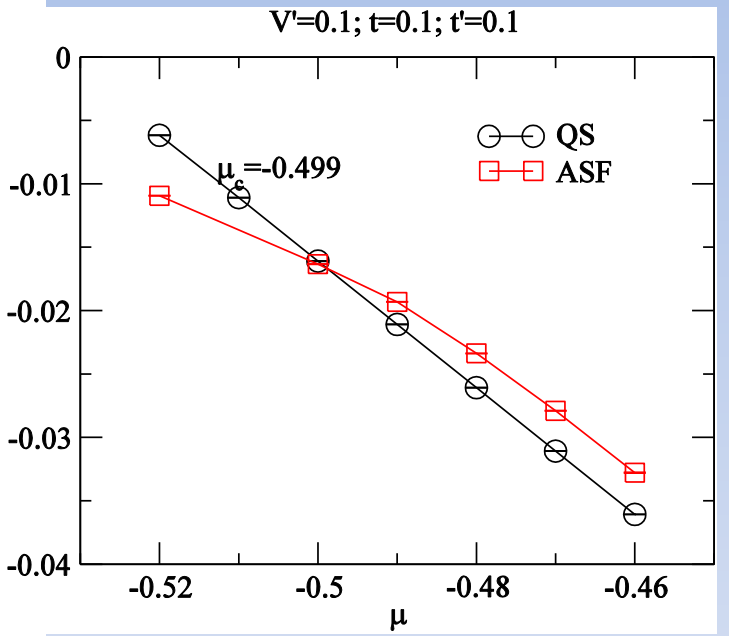
V'=0.1



- QS1 is stabilized.
- PSF is favored against ASF (dimer formation is enhanced).

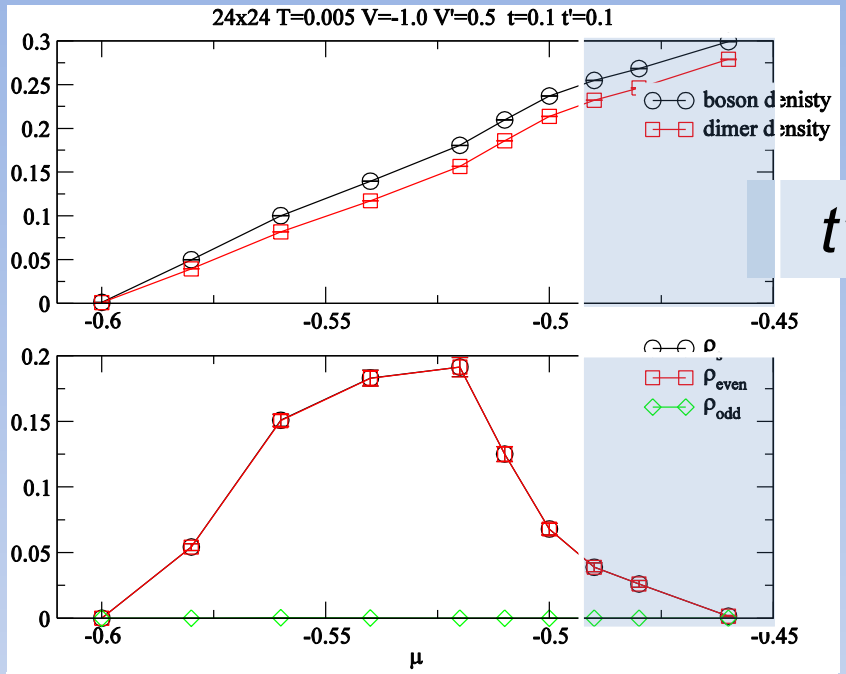
V'=0.1 t'=0.1



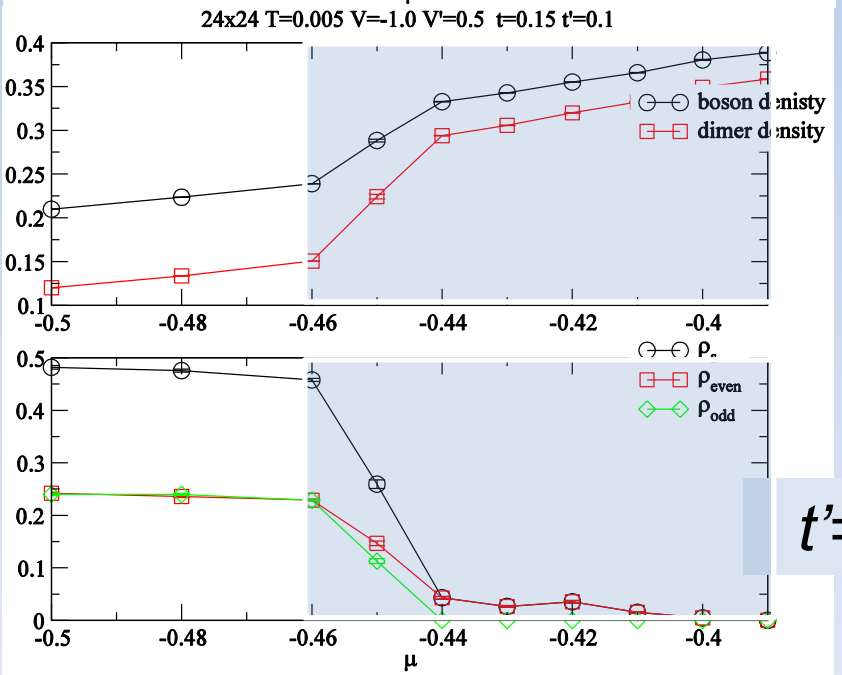


- Convergence is slow near the solid phase
- Energy comparison with the solid phase confirms the 1st order phase transition.

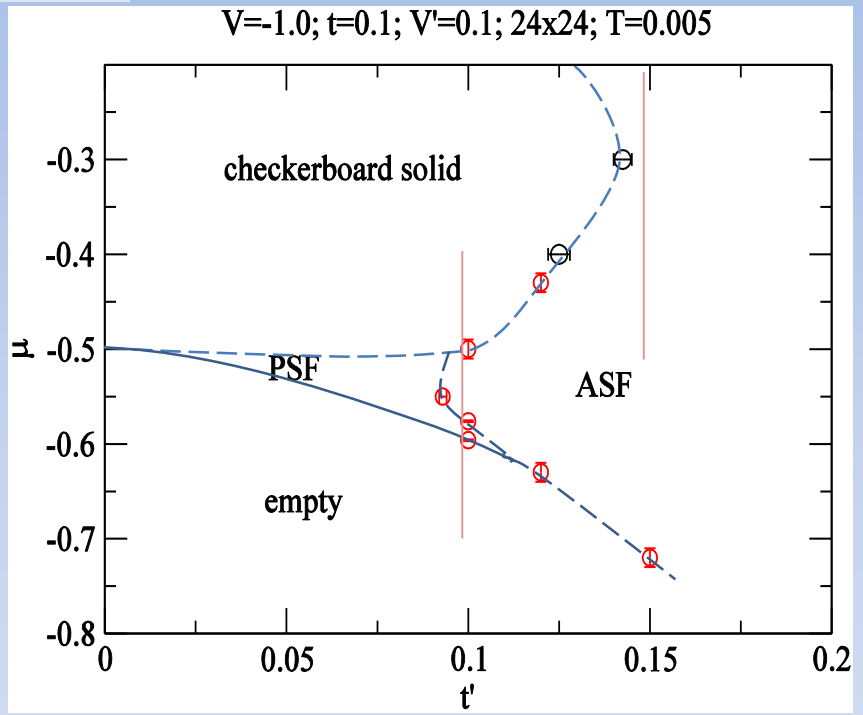
Increase V' to 0.5



t'=0.1



t'=0.15



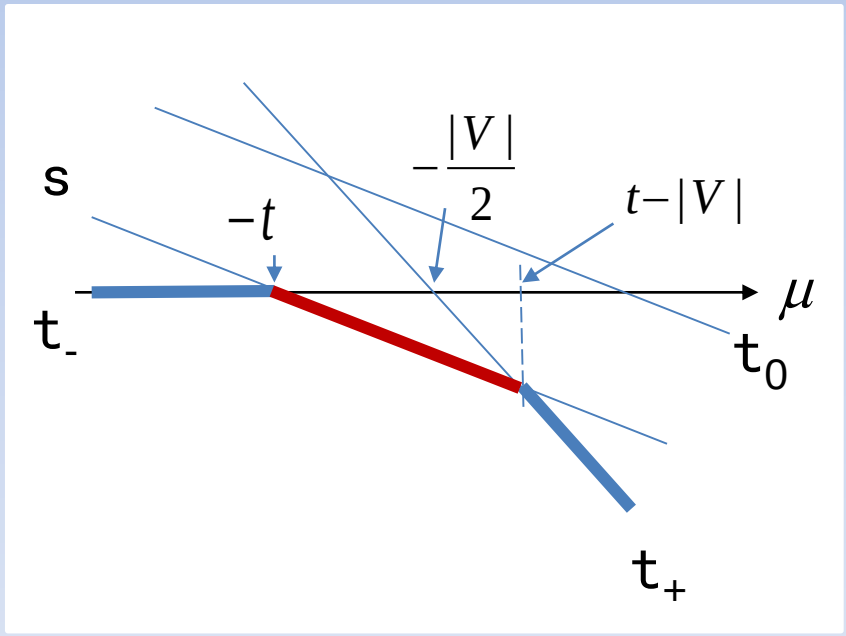
- Increasing *V'* would enlarge QS1 regime
- also favor PSF over ASF.

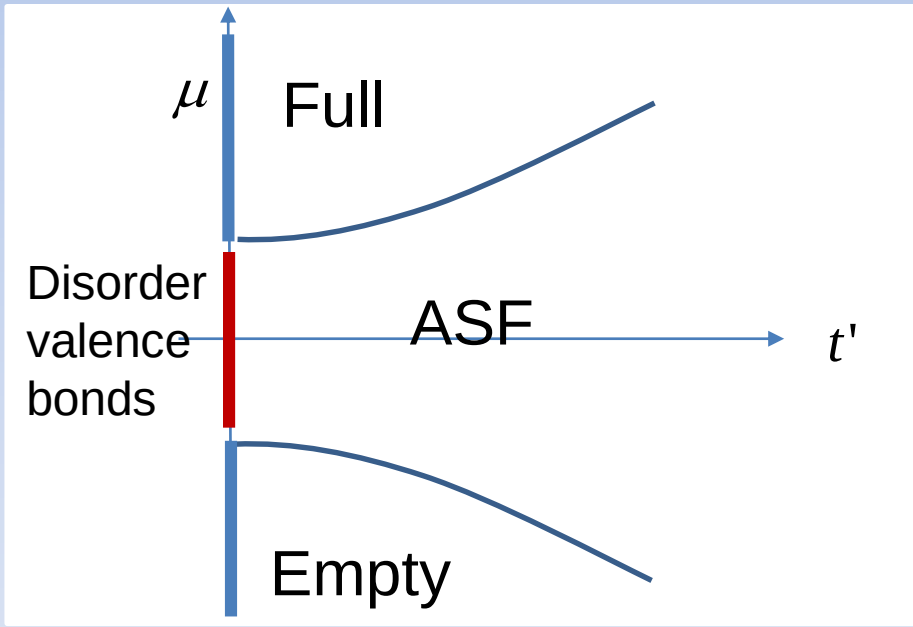
Analysis of localized dimers (t'=0)

$t > \frac{|V|}{2}$

Soft dimer regime

Independent dimer: $V' = 0$



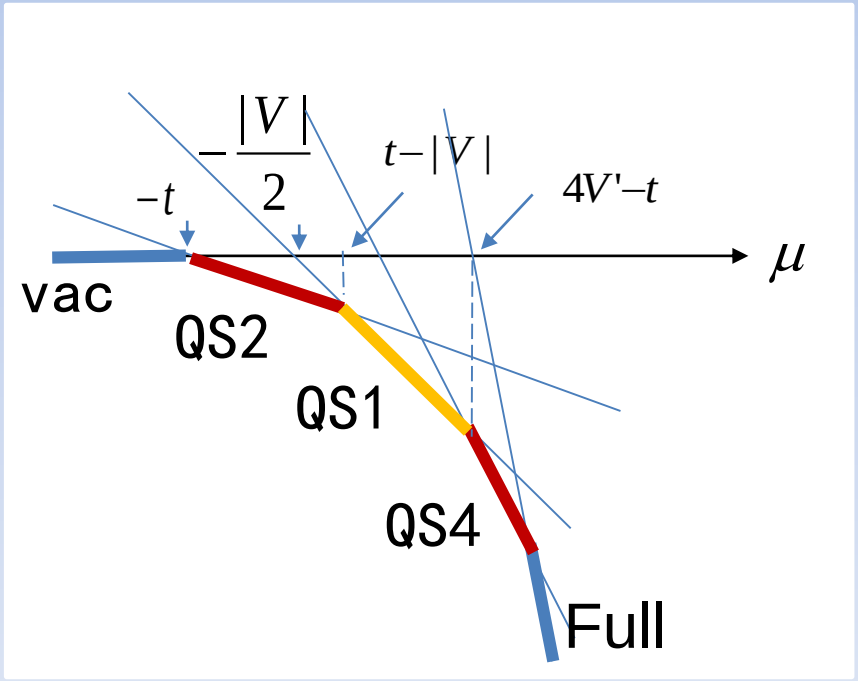


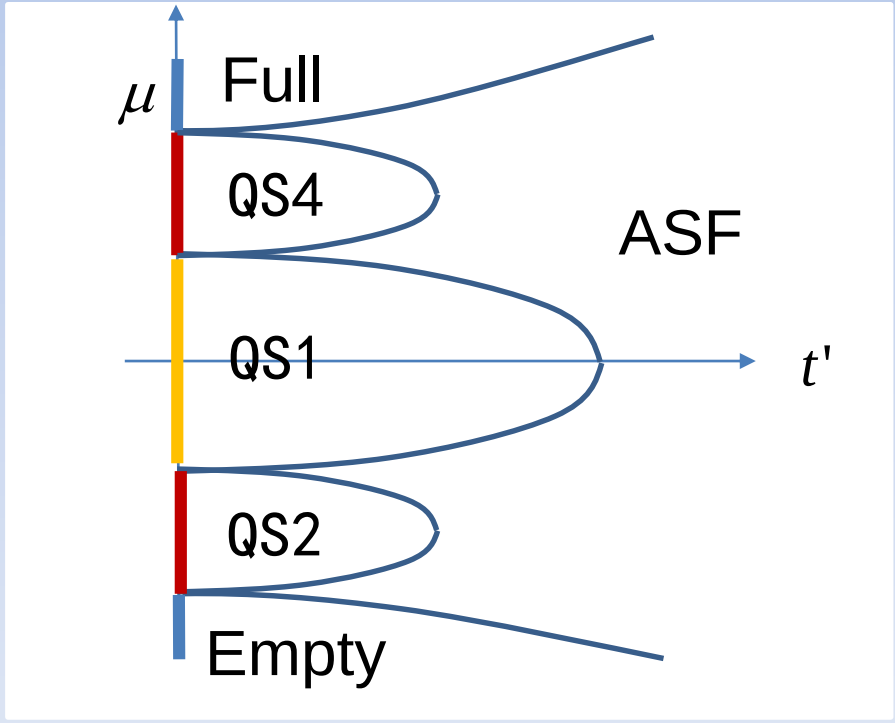
Analysis of localized dimers (t'=0)

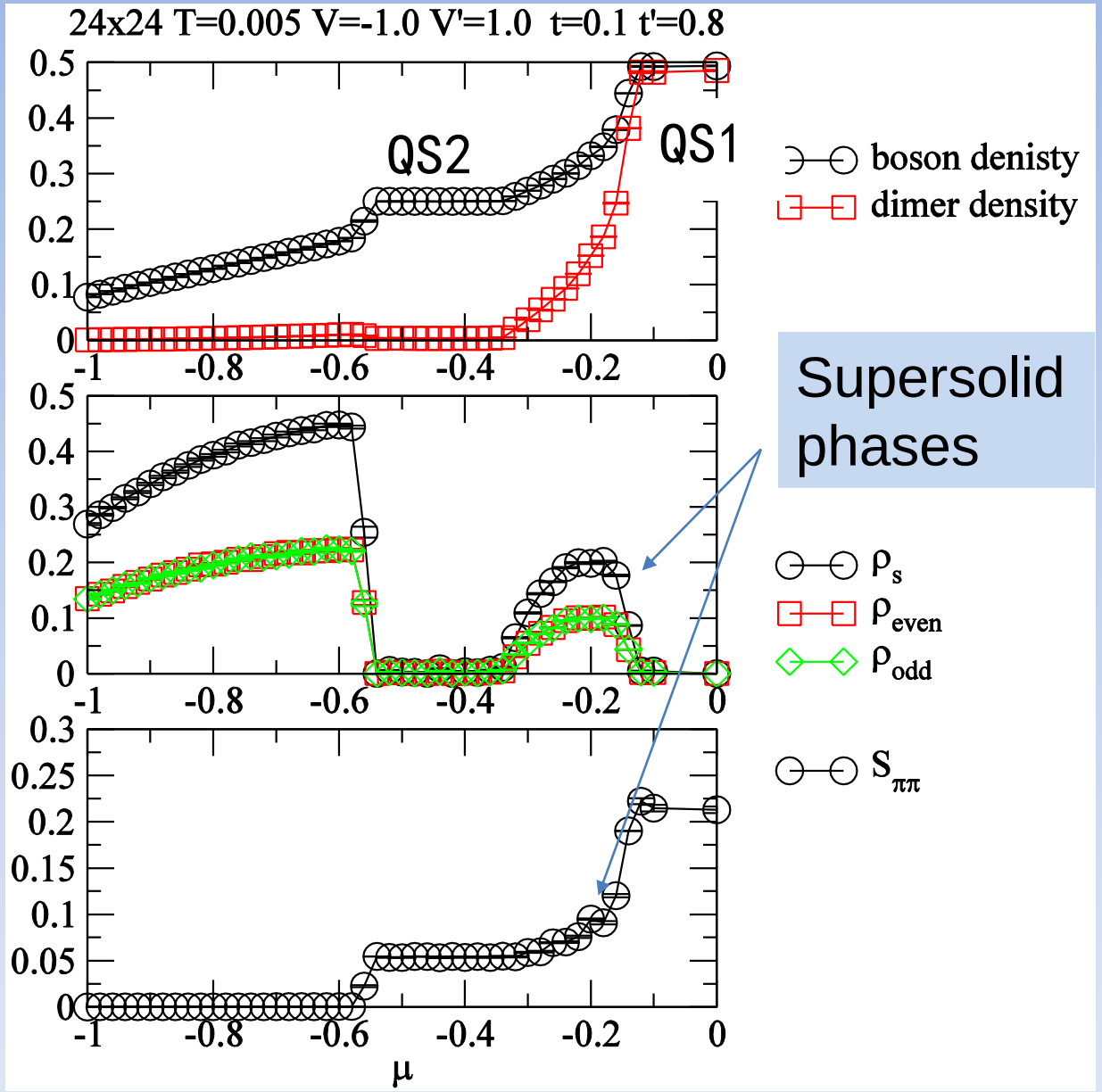
$t > \frac{|V|}{2}$ Soft dimer regime

Interacting dimer: $V' > 0$

QS3 is stabilized if $V' < t - |V|/2$, otherwise QS1 is favored.







Supersolid phases

- Both superfluidity and structure factor are finite.

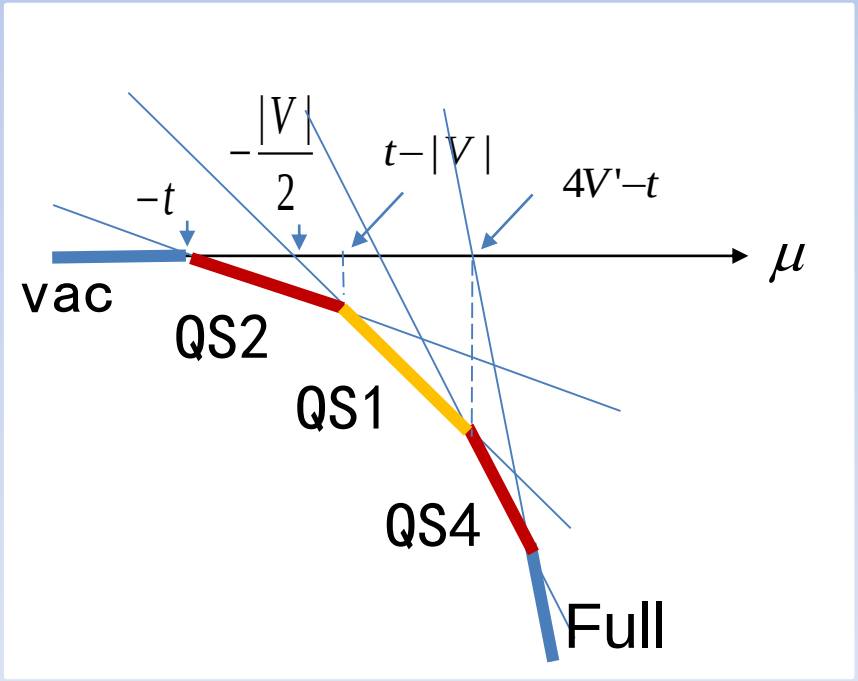
- Are there two SS?
- What is the nature of the transition?

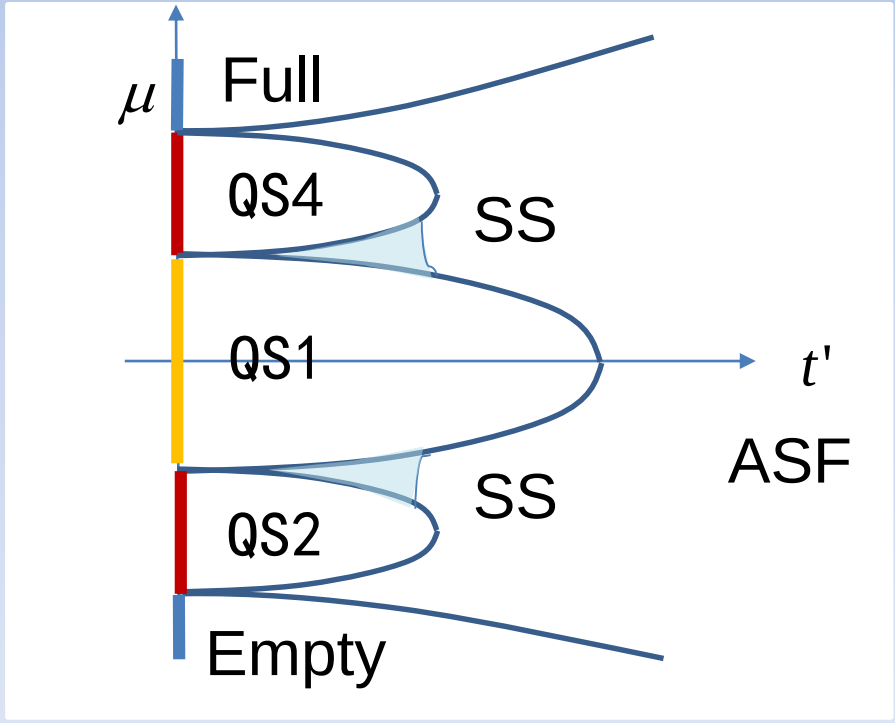
Analysis of localized dimers (t'=0)

$t > \frac{|V|}{2}$ Soft dimer regime

Strong interacting dimer: $V' > t - |V|/2 > 0$

QS3 is stabilized if $V' < t - |V|/2$, otherwise QS1 is favored.





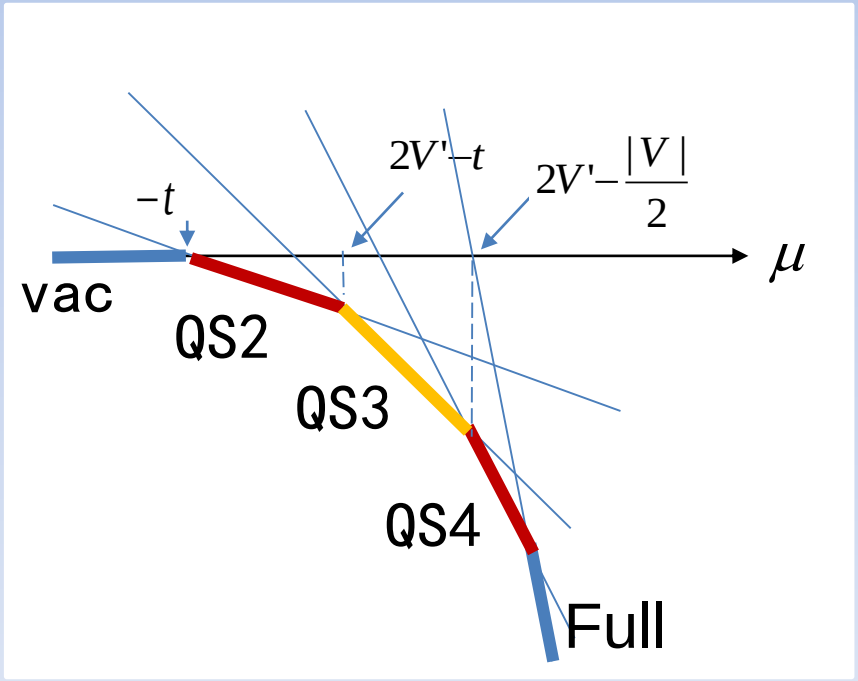
Analysis of localized dimers (t'=0)

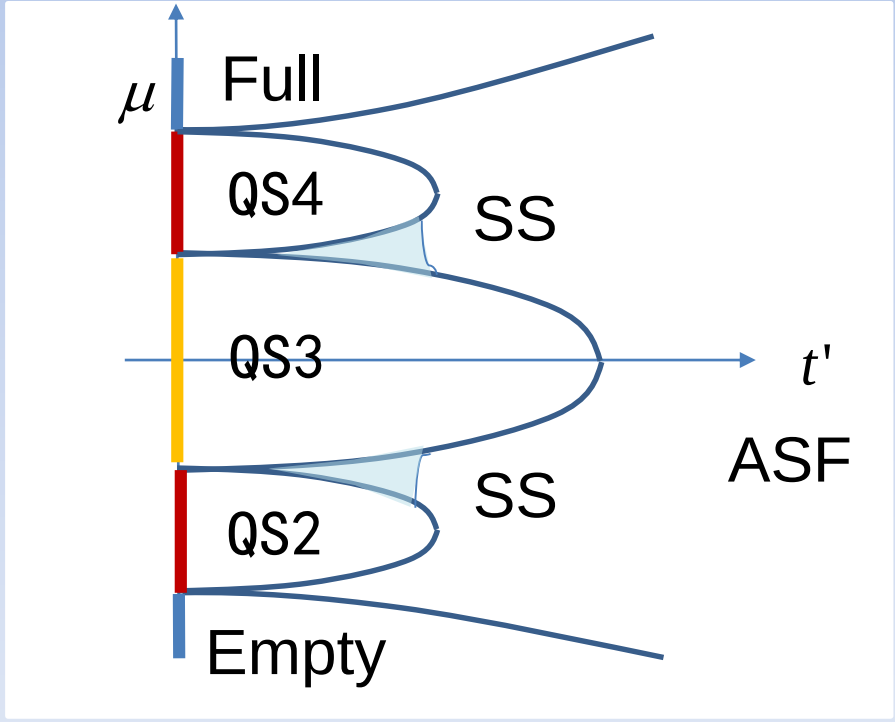
$$t > \frac{|V|}{2}$$

Soft dimer regime

Weak interacting dimer:

$$t - |V|/2 > V' > 0$$





Summary

1. **Bilayer Bose-Hubbard model shows very rich ground state phase diagrams.**
2. **Hard-core dimer regime: ASF, PSF and CB quantum solid.**
3. **Soft-core dimer regime: valence bond soilds, CB quantum solids, (VB and CB) supersolids.**
4. **Strong intra-layer repulsion V' will in general enhance solid phases, and also favor PSF over ASF phase.**
5. **Strong intra-layer hopping, on the other hand, favor ASF phase.**
6. **Complete picture of ground state phase diagram is still missing, as well as the nature of phase transitions is not well understood.**
7. **Thermal phase transitions is worthy to study in the future.**