Stability of 4/7 phase of He absorbed on graphite

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Outline of talk

1. Model
2. 4/7 phase of He adsorbed on graphite
3. Doping of particle and vacancy into the 4/7 phase
4. Promotion to the 3rd layer on 4/7 phase
5. Summary and future plans

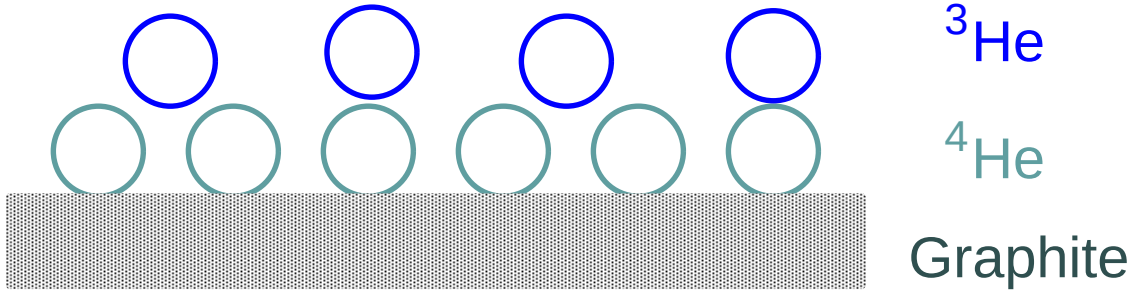
Model

Structure of the system

Substrate	**Graphite**
1st layer	**^{4}He triangular lattice**
2nd layer	**^{3}He 4/7($\sqrt{7} \times \sqrt{7}$) lattice for 1st layer**

1st layer density 12.0 nm^{-2} (saturated density)

D.S. Greywall et al. Phys. Rev. Letts. 67 1535 (1991)

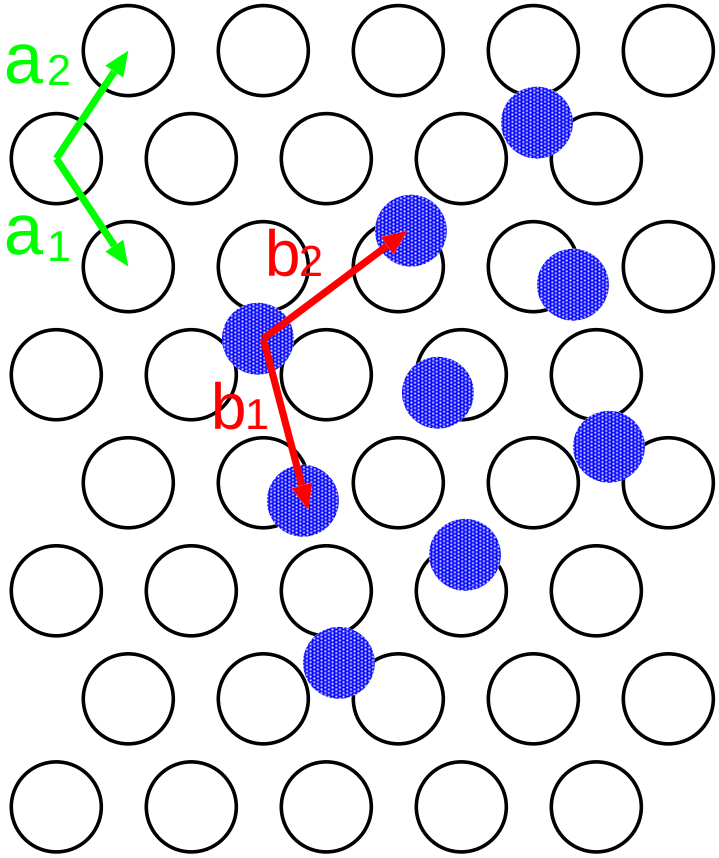


Why is the $4/7$ phase important?

It is a stable commensurate phase.

Various properties change around this density.

$\sqrt{7} \times \sqrt{7}$ (4/7) structure



Primitive vectors

1st layer ^{4}He

$$\boldsymbol{a}_1 = a\left(\frac{1}{2}\boldsymbol{e}_x - \frac{\sqrt{3}}{2}\boldsymbol{e}_y\right)$$

$$\boldsymbol{a}_2 = a\left(\frac{1}{2}\boldsymbol{e}_x + \frac{\sqrt{3}}{2}\boldsymbol{e}_y\right)$$

$$a = 1.045\tilde{\sigma} = 0.310\text{nm}$$

2nd layer ^{3}He

$$\boldsymbol{b}_1 = \boldsymbol{a}_1 - \frac{1}{2}\boldsymbol{a}_2$$

$$\boldsymbol{b}_2 = \frac{1}{2}\boldsymbol{a}_1 + \frac{\sqrt{3}}{2}\boldsymbol{a}_2$$

Our problems **We dope vacancies and particles into this phase.**

- **How do the doped vacancies behave? → Hole-like? Does it melt the lattice?**
- **How do the excess particles behave? → Going into the 2nd layer or 3rd layer?**

Binder Parameter

We use Binder parameter to check stability of the 4/7 phase.

Definition **Binder parameter** $\mathcal{G}_L(T)$, L**: lattice size**

$$\mathcal{G}_L(T) = 1 - \frac{1}{3}\frac{\langle\, |\hat{\rho}(\boldsymbol{G}_1)|^4 \,\rangle_L}{\langle\, |\hat{\rho}(\boldsymbol{G}_1)|^2 \,\rangle_L}$$

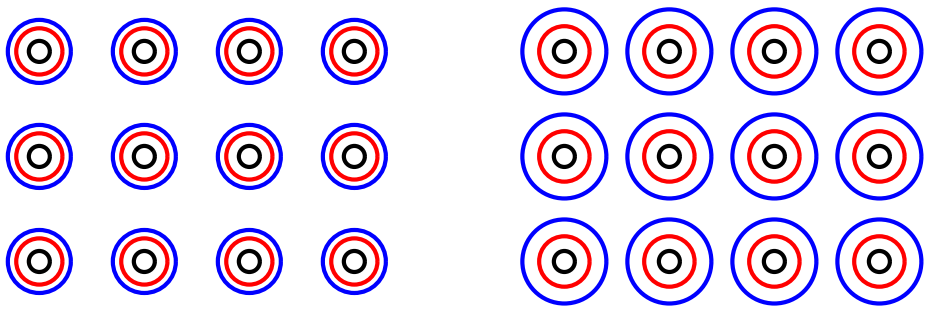
$\boldsymbol{G}_1$ **: one of the reciprocal lattice in 2nd layer.**

$$\boldsymbol{G}_1 = \frac{2\pi}{a^2}\frac{4}{21}(5\boldsymbol{a}_1 + \boldsymbol{a}_2),$$

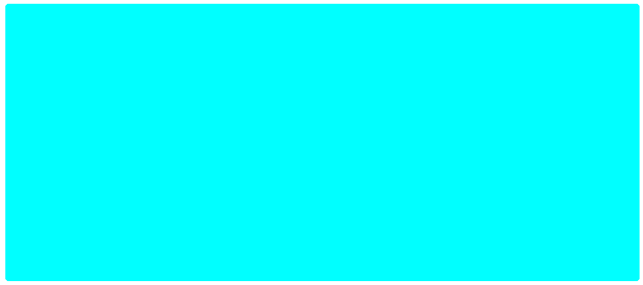
$\hat{\rho}(\boldsymbol{G}_1)$**: Fourier amplitude of particle density.**

$$\hat{\rho}\,(\boldsymbol{G}_1) = \frac{1}{\Omega}\int \mathrm{d}\boldsymbol{r}\, \exp(-\mathrm{i}\,\boldsymbol{G}_1 \cdot \boldsymbol{r})\,\rho(\boldsymbol{r}\,)$$

Binder Parameter takes value,



$\mathcal{G}_L = 2/3$ **for perfect lattice**



$\mathcal{G}_L = 1/3$ **for liquid phase**

We use path integral Monte Carlo method to study the system.

Hamiltonian

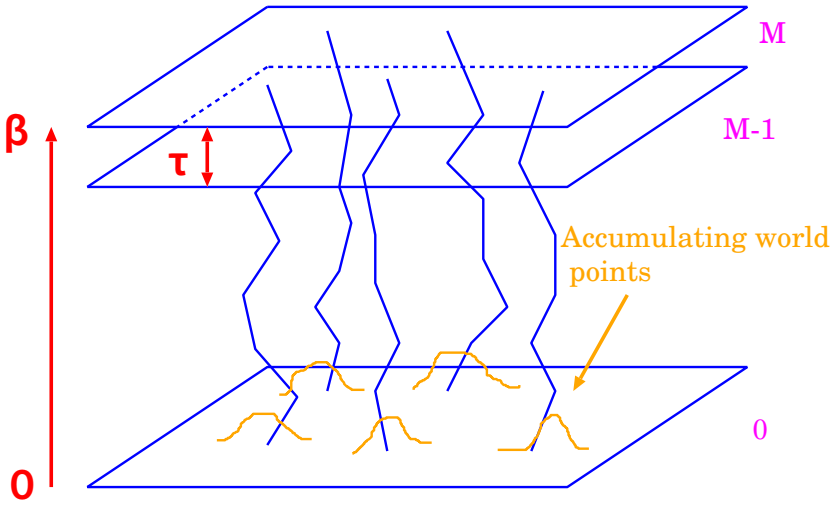
$$H = \sum_{i=1}^{N_3} \frac{\boldsymbol{p}_i^2}{2m_3} + \sum_{i=1}^{N_4} \frac{\boldsymbol{p}_i^2}{2m_4} + \sum_{<i,j>} V_{\mathrm{He-He}}(r_{ij}) + \sum_{i=1}^{N_3+N_4} U_{\mathrm{C-He}}(z_i)$$

N_3, N_4: **number of ^{3}He, ^{4}He,** m_3, m_4: **mass of ^{3}He, ^{4}He.**

Partition function in the path integral form are given,

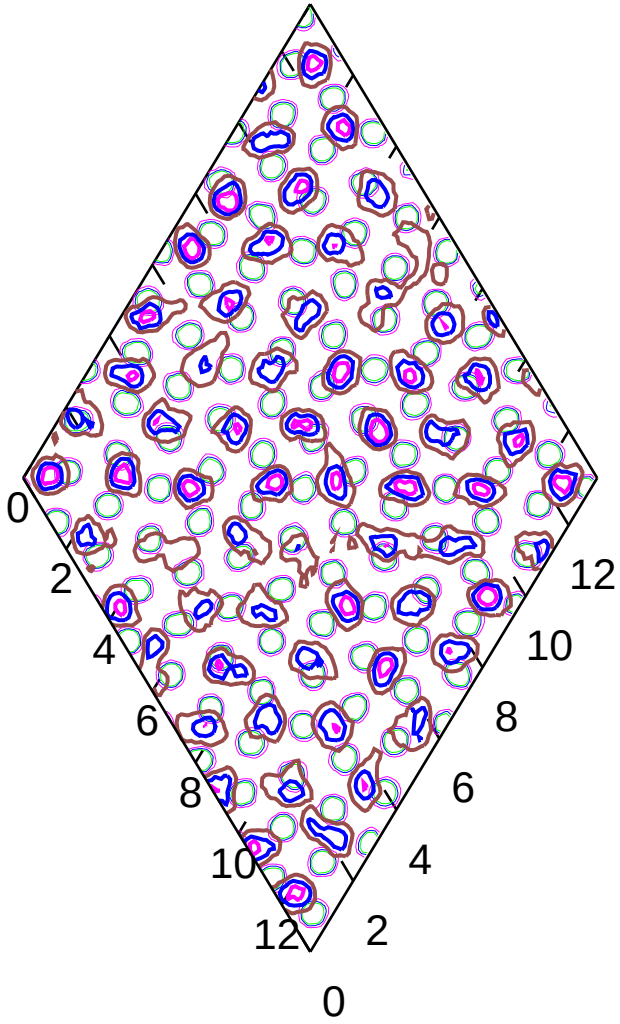
$$\langle R \mid \exp(-\beta H) \mid R \rangle$$
$$= \int \mathrm{d}R(0) \int \mathrm{d}R(1) \cdots \int \mathrm{d}R(M-1) \langle R(M-1) \mid \exp(-\tau H) \mid R(M-2) \rangle \times$$
$$\langle R(M-2) \mid \exp(-\tau H) \mid R(M-3) \rangle \cdots \langle R(1) \mid \exp(-\tau H) \mid R(0) \rangle$$

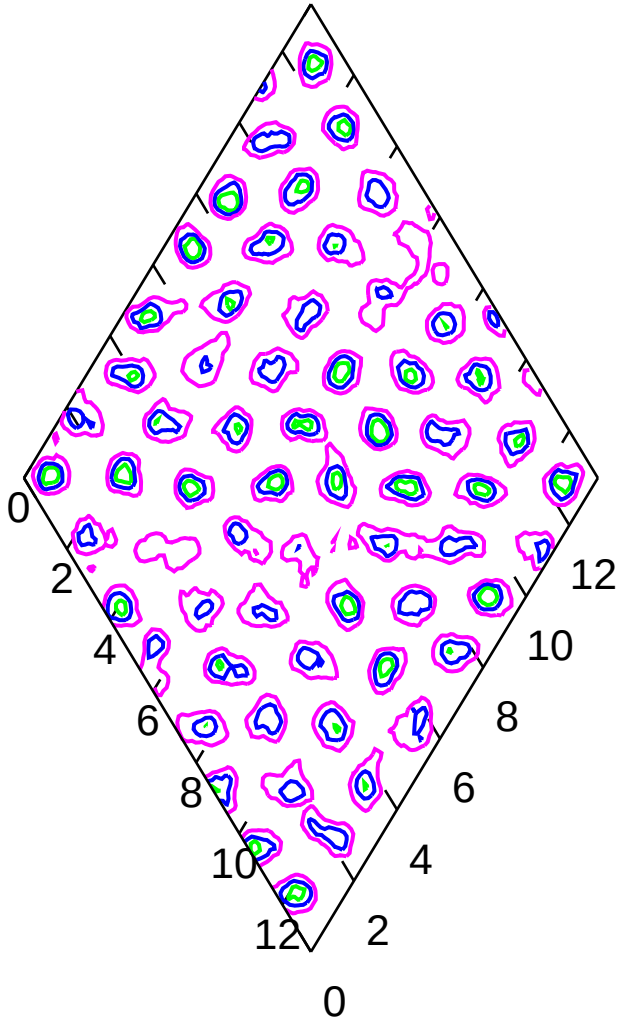
World line



- **We move all pathes.**
- **All particles are distinguishable (classical statistics) because system is in solid state around 4/7 phase.**

Density profile of the 4/7 phase



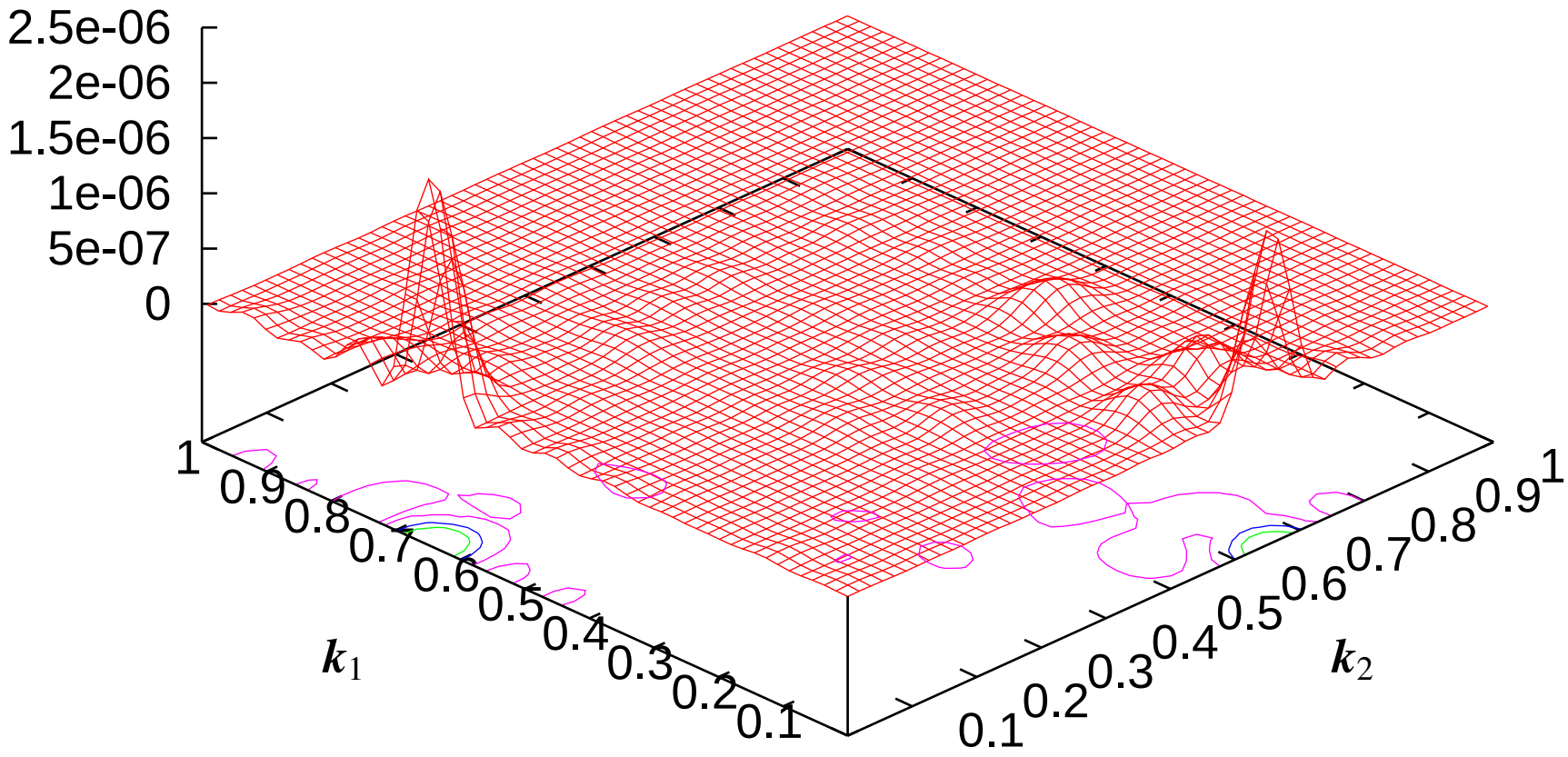


Solid phase: $N_1 = 64, N_2 = 112$ **no vacancy at** $T = 0.539$**K. Sampling term: 1000mcs.**

Particle density profile strongly fluctuates.

The 2nd layer structure is modulated by the 1st layer periodicity.

Fourier spectrum of the 4/7 phase



The $k-$vector is scaled by the norm of the reciprocal vector of the 1st layer.

Some satellites due to fluctuation are observed.

We dope particles and vacancies into the 2nd layer, and check stability of the lattice.

Computed configulations

2nd layer	ΔN	**density**	**1st layer**
$N_2 = 36$	$\Delta N = -1$,	**3.60%**	$N_1 = 49$
$N_2 = 64$	$\Delta N = \pm 1$,	**1.56%**	$N_1 = 112$
	$\Delta N = \pm 2$,	**3.12%**	$N_1 = 112$
$N_2 = 100$	$\Delta N = -1$,	**1.00%**	$N_1 = 175$
	$\Delta N = -2$,	**2.00%**	$N_1 = 175$

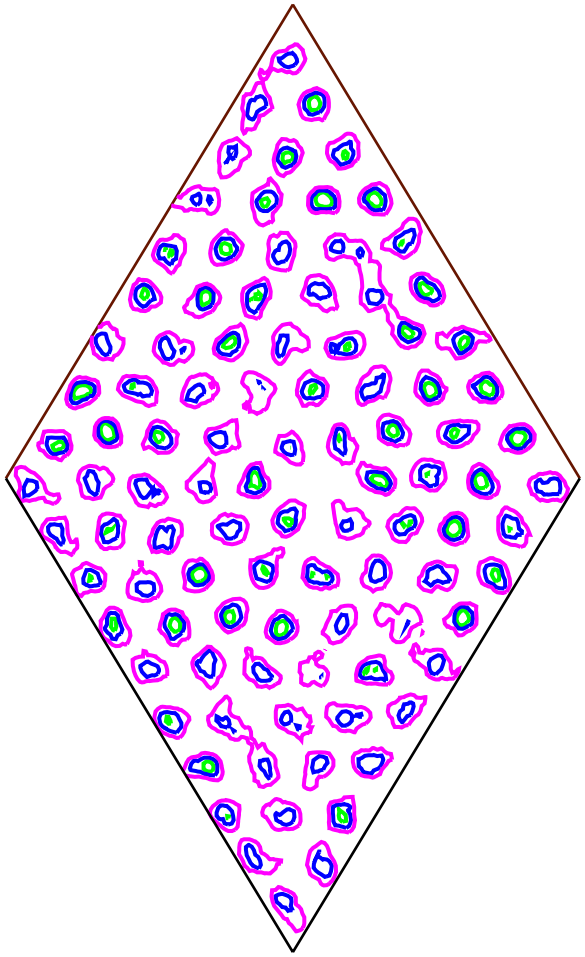
Particle statistics	**distinguishable (no path exchange)**
Temperature	**0.539K**
Data processing	**every 20000MCS**

Estimation of lattice stability

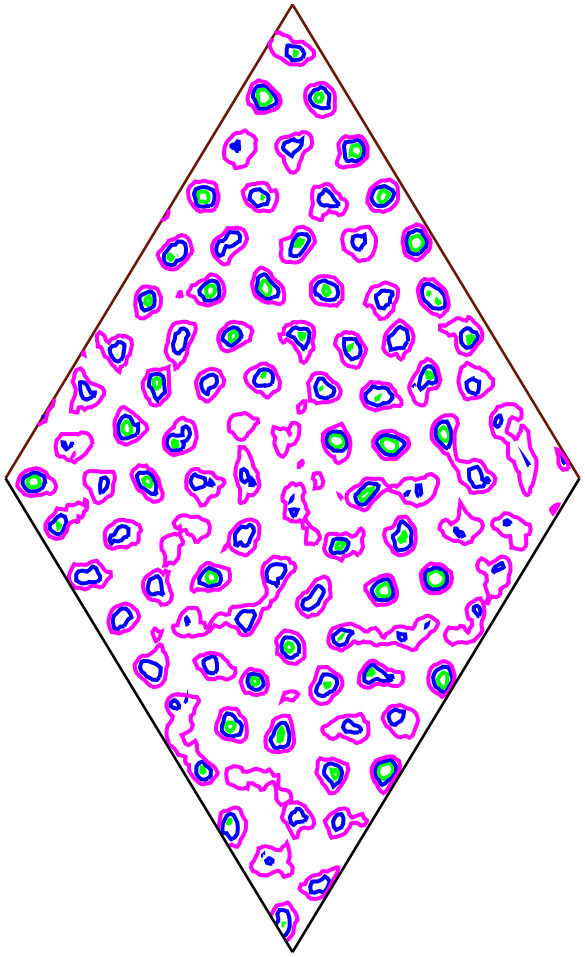
- **Liquid and Solid phases are determined by Binder parameter.**

Initial and equilibrium density profiles of 1.00% vacancy doped case.

$N = 274(N_1 = 99, N_{\text{hole}} = 1, N_2 = 175)$



Initial configuration

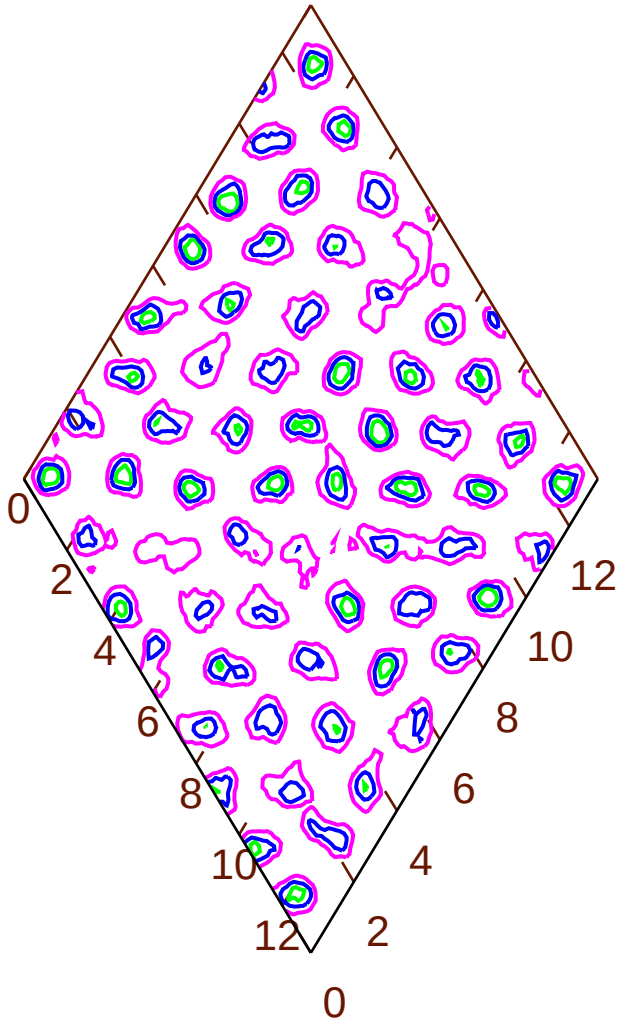


Equilibrium configuration

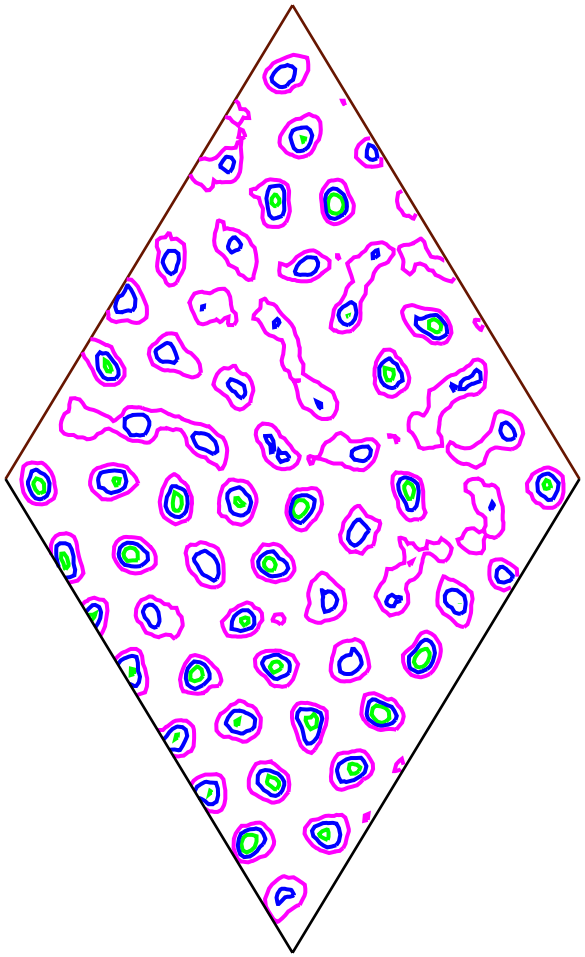
The vacancy can not clearly observed in real space. Vacancy has a wide band width.

Pure 4/7 phase and 1.56% vacancy doped system.

$N = 175(N_1 = 63, N_{\text{hole}} = 1, N_2 = 112)$



Pure 4/7.

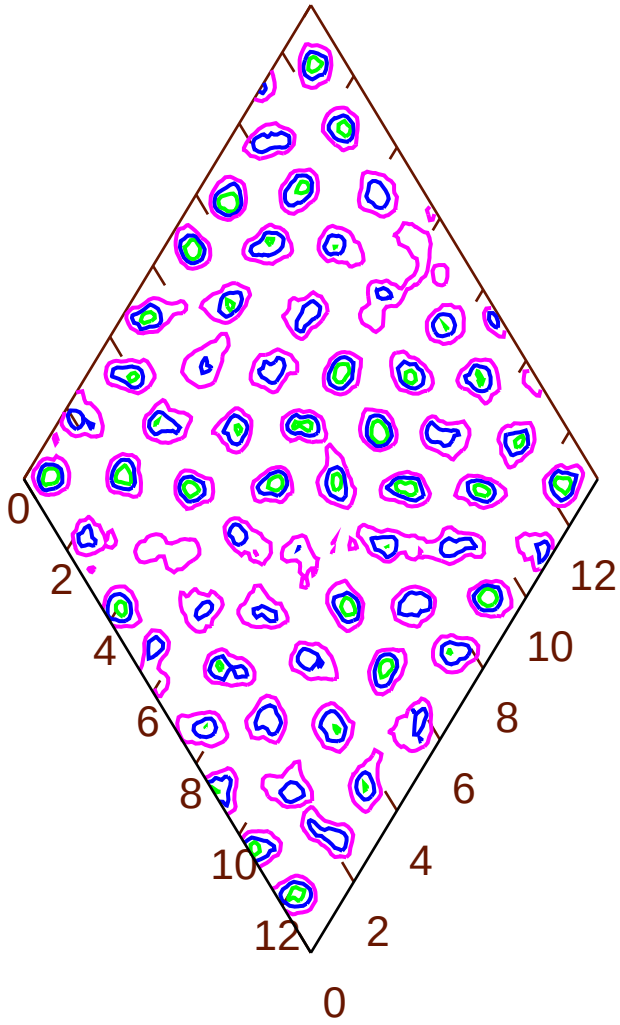


$N_{\text{vacancy}} = 1$ (1.56%)

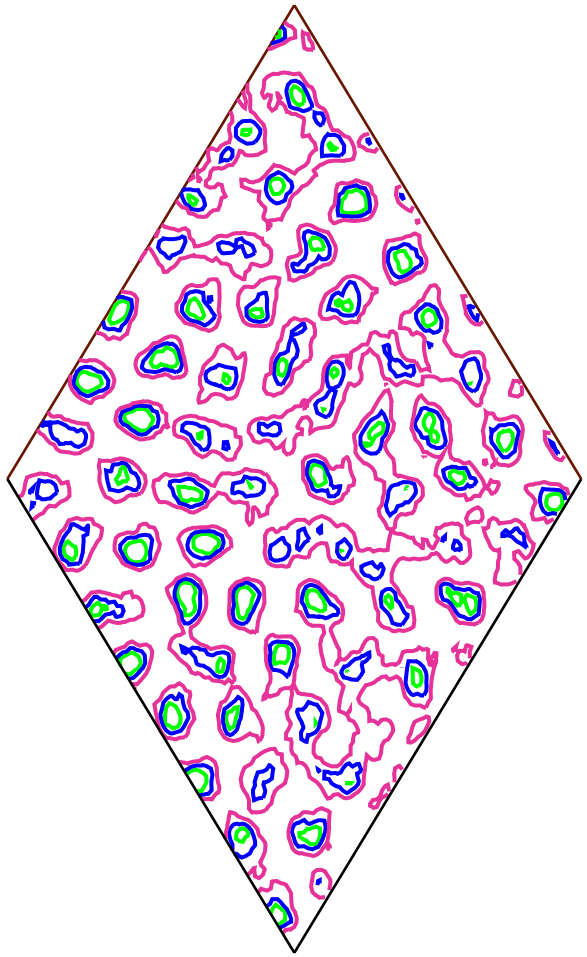
Doped vacancy enhances fluctuation of the system.

Pure 4/7 phase and excess 1.56% particle added system.

$N = 175(N_1 = 63, N_{\text{hole}} = 1, N_2 = 112)$



Pure 4/7

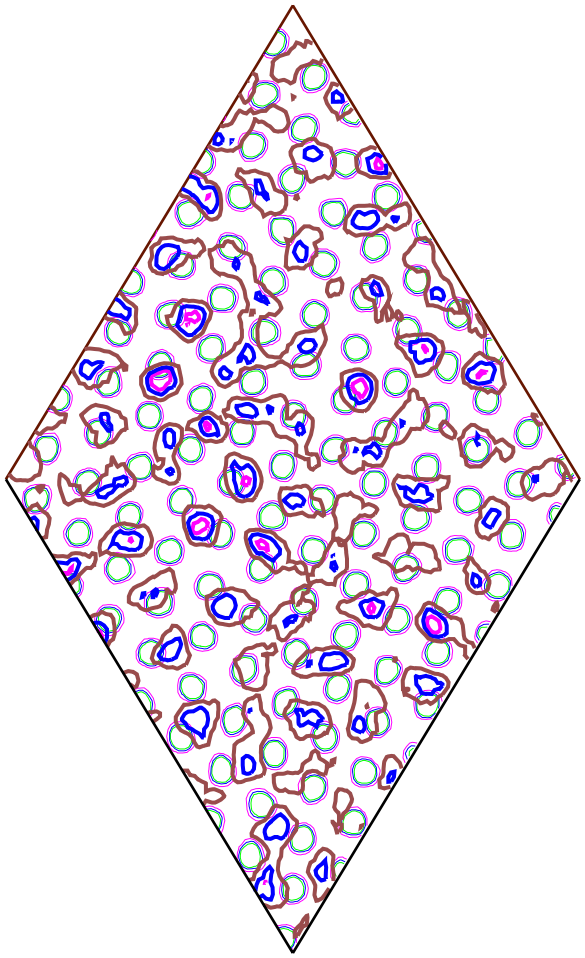


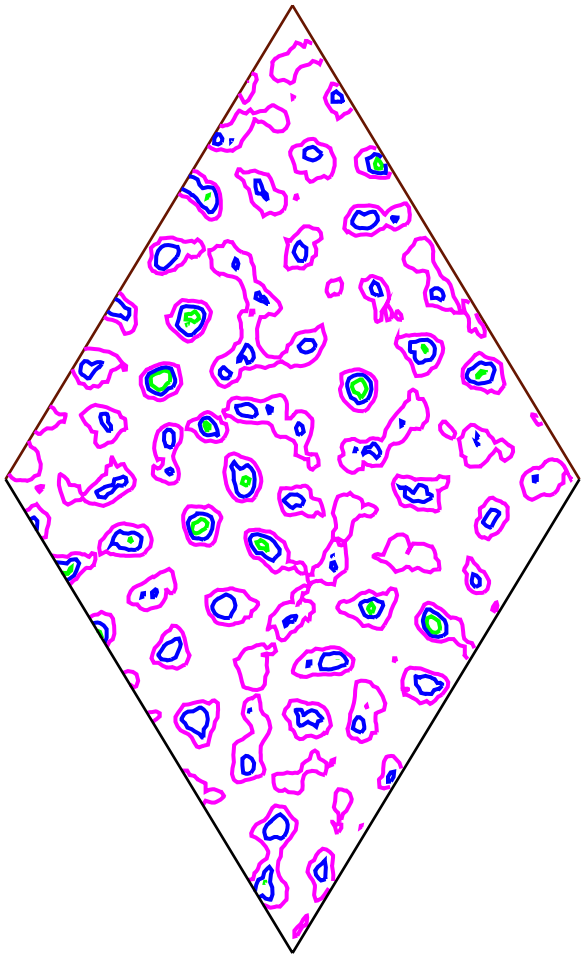
$N_{\text{excess}} = 1$ (1.56%)

Periodicity of the lattice is destroyed by the interstitially placed particle.

3.12% of vacancies doped system

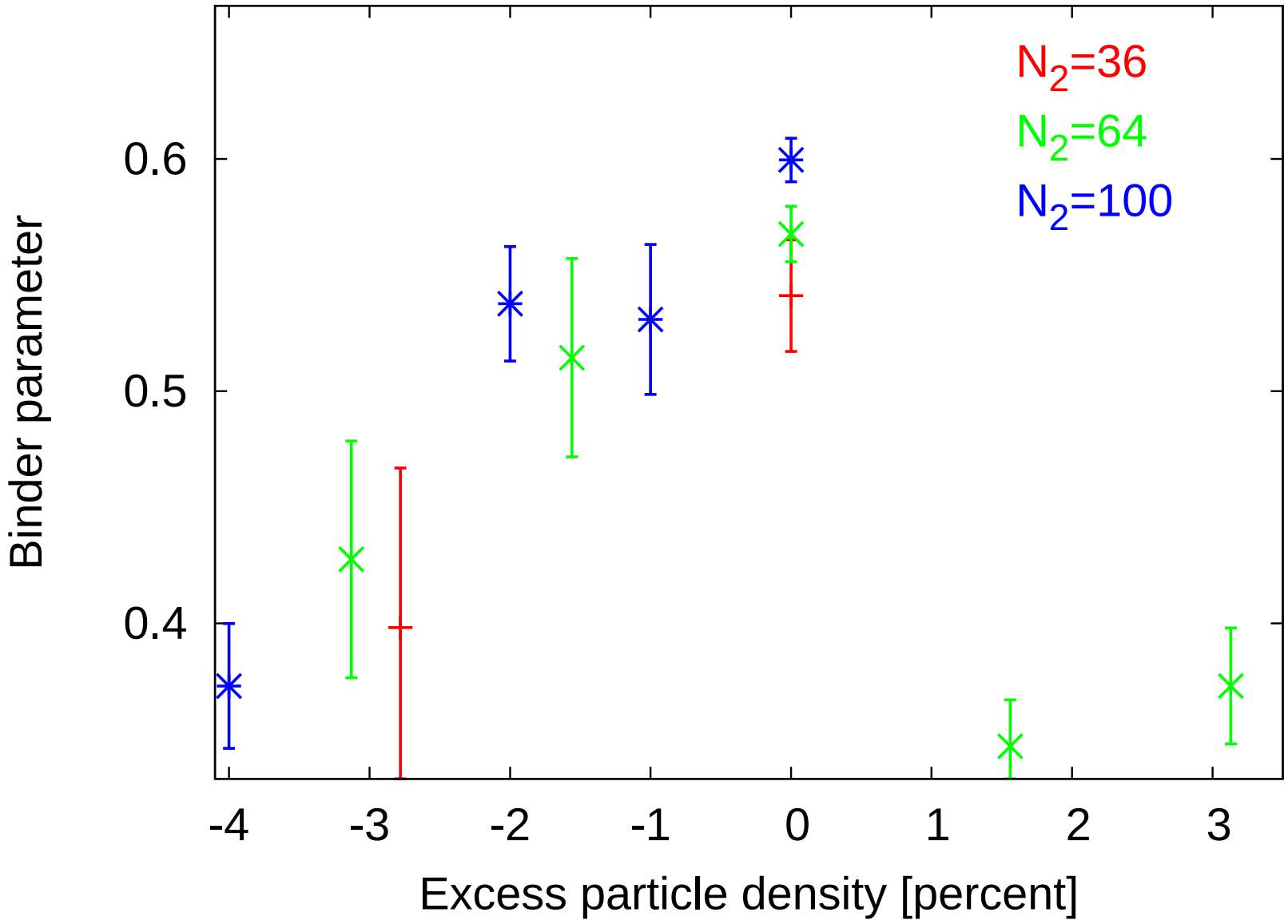
$N = 174(N_1 = 62, N_{\text{hole}} = 2, N_2 = 112)$,





The lattice is melted. The configuration of 2nd layer is affected by that of 1st layer periodicity.

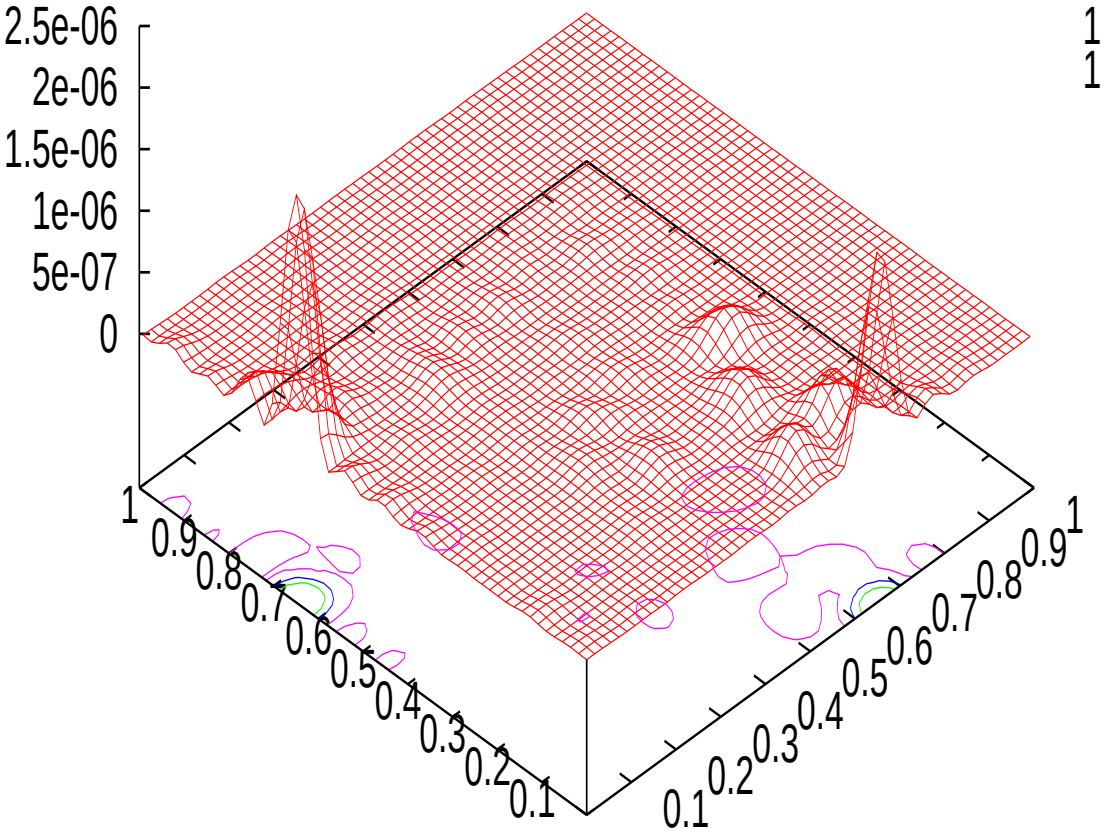
Excess particle density dependent Binder parameter



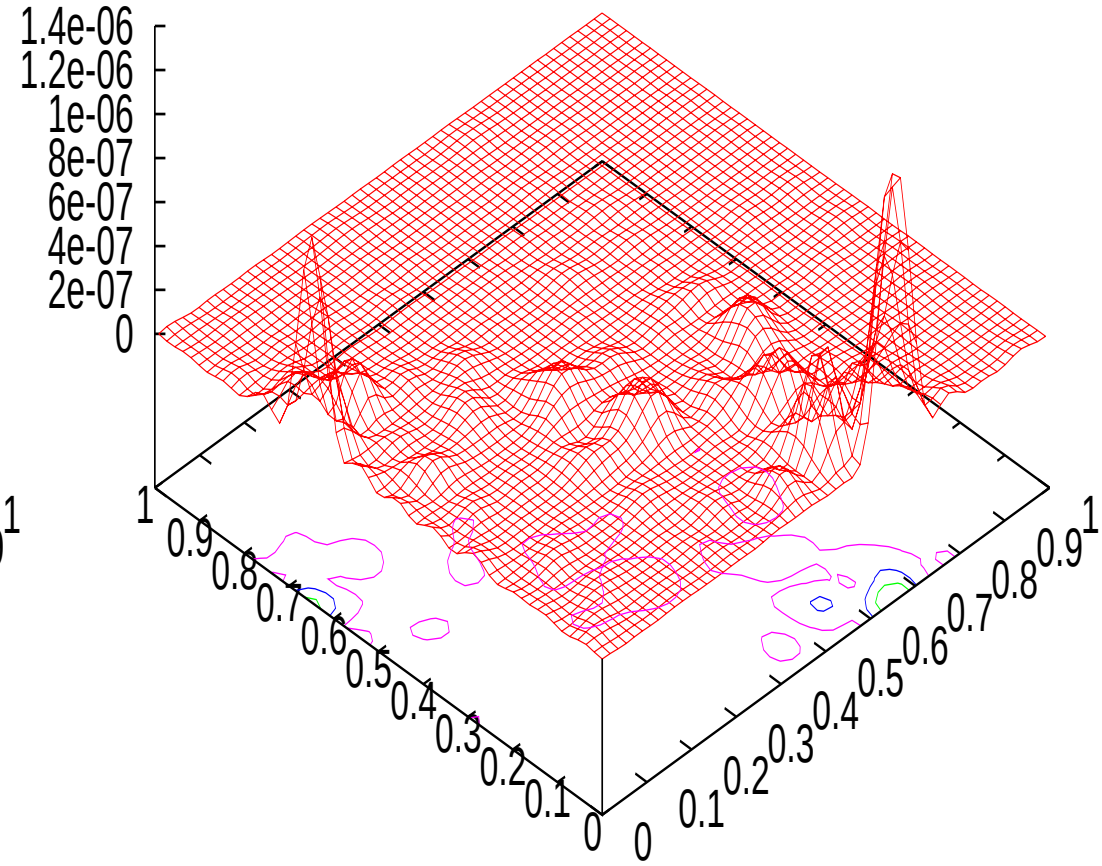
4/7 structure is stable against up to 2% of vacancies doping. A excess interstitial particle destroys the lattice.

Fourier spectrum of pure 4/7 phase and 1.56% vacancy doped system.

$N = 175 (N_1 = 64, N_2 = 112)$



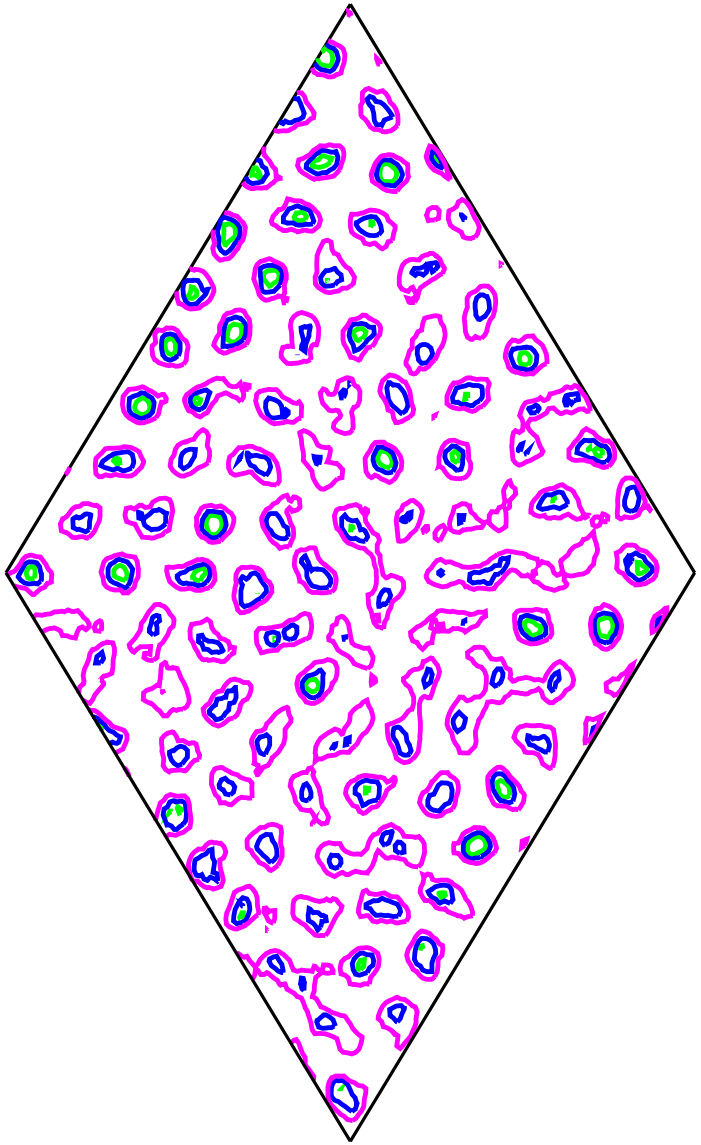
Pure 4/7

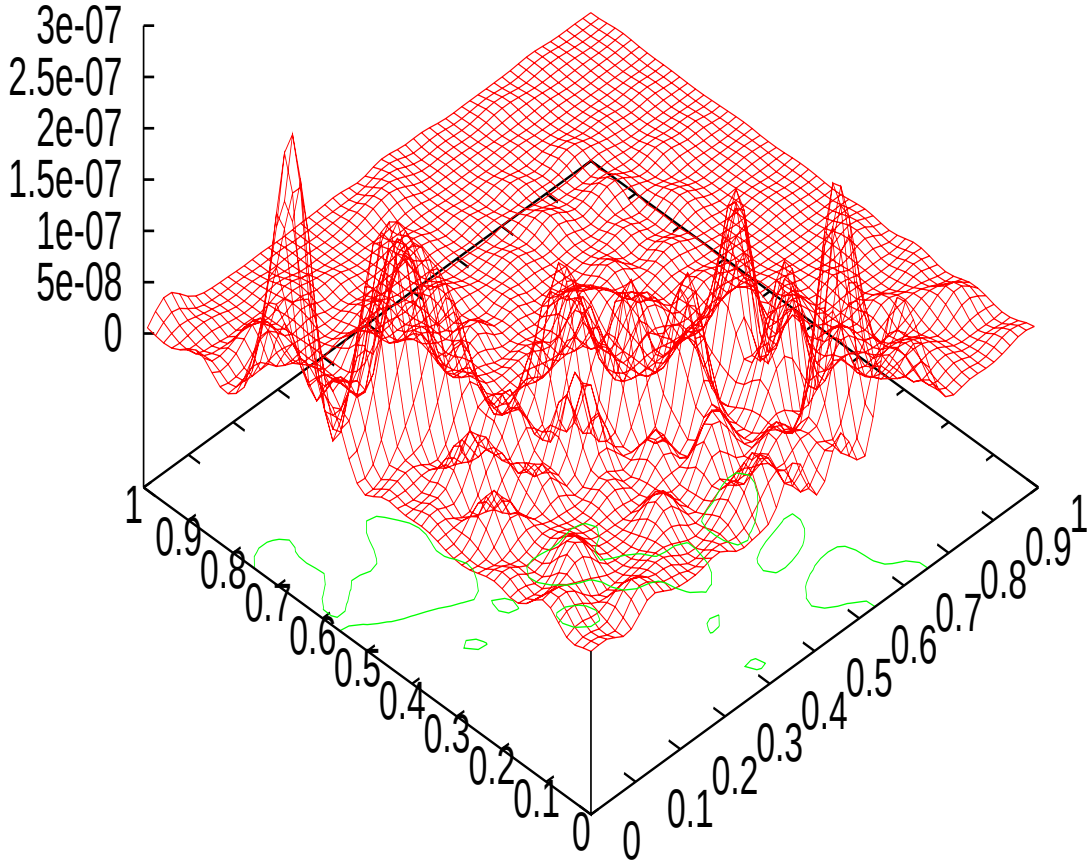


$N_{\text{vacancy}} = 1$ (1.56%)

In the doped system, satellite peaks grow, but main peaks are still pronounced.

2% of vacancy doped system, $N = 273(N_1 = 98, N_{\text{hole}} = 2, N_2 = 173)$

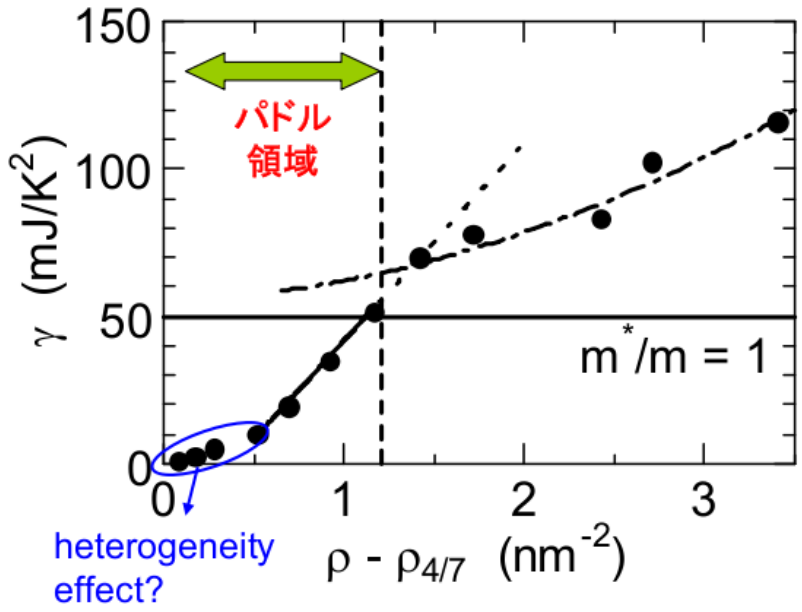




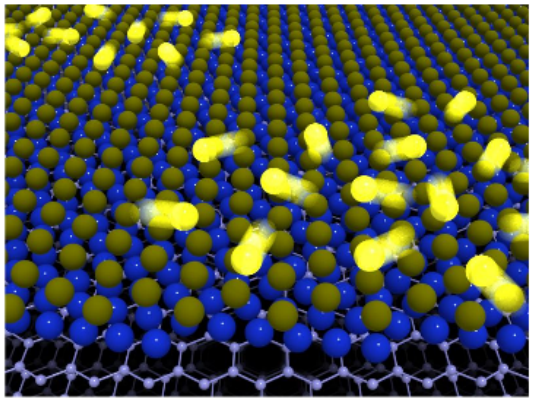
Lattice structure is barely kept and no particle-hole separation is observed.

We consider the case in which excess particles form the 3rd layer.

Degenerate Fermi-liquid puddles in the 3rd layer



パドル：低密度自己凝縮フェルミ液体 (1 nm^{-2})が存在



D. Sato, T. Matui, and H. Fukuyama, PSJ meeting (2009 fall)

In this conjecture, excess particles form the 3rd layer, and show specific heat of degenerate Fermi-liquid.

Problem: **Can excess particles form the 3rd layer?**

Negative reasons:

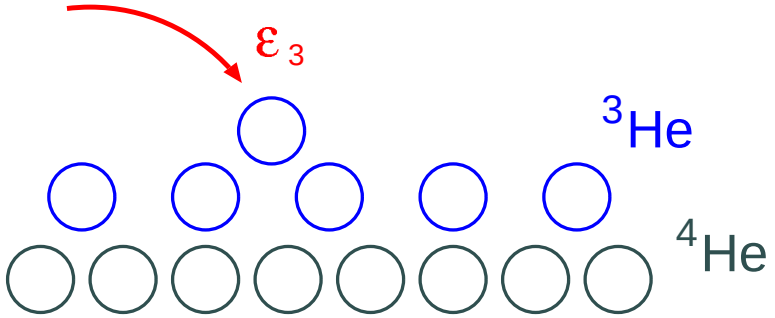
- **The 4/7 phase exists, but it is easily broken by the hole and particle doping.**
- **Particle energy of the 2nd layer is** $\varepsilon_2 = -23.4$**K, and that of the 3rd layer is** $\varepsilon_2 = -10.3$**K. Two energies are much different.**

In order to confirm promotion to the 3rd layer, we have to compute chemical potential of both layers.

We estimate critical density σ_c of the promotion to 3rd layer

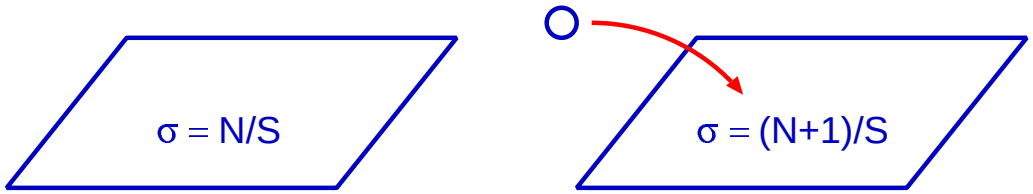
Let us compute chemical potential $\mu_2(\sigma_2)$ and μ_3, and estimate σ_c.

Add to the 3rd layer **Putting single particle in the 3rd layer**



$\varepsilon_3 = \mu_3$ **is the chemical potential of 3rd layer.**

Add to the 2rd layer **Increase of particle density of 2nd layer.**



$\varepsilon_2(\sigma_2)$: **Energy per particle in the 2nd layer at the density σ_2.**

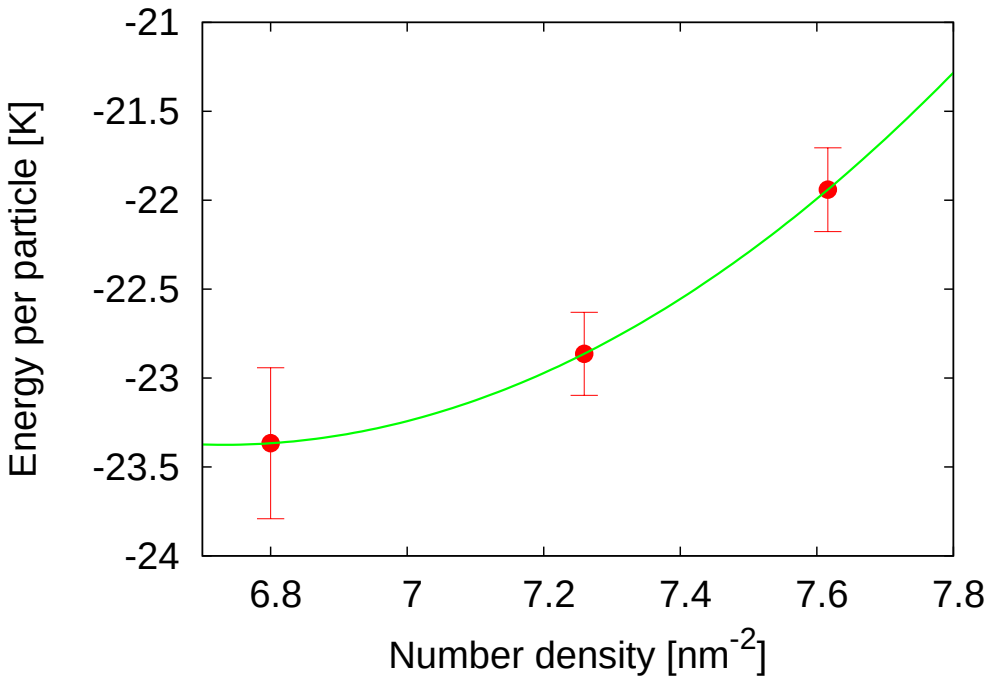
Increased energy by adding one particle,

$$\Delta E = (S\sigma_2 + 1)\cdot\varepsilon_2\left(\frac{S\sigma_2 + 1}{S}\right) - S\sigma_2\cdot\varepsilon_2(\sigma_2)$$

Taking a limit, $S \to \infty$

$$\mu_2(\sigma_2) = \sigma_2\frac{d\varepsilon_2}{d\sigma_2} + \varepsilon_2(\sigma_2)$$

Computing chemical potential of the 2nd layer, μ_2.



Single particle energy on the 3nd layer

$$\mu_3 = \varepsilon_3 = -10.3 \pm 1.8[\mathrm{K}]$$

ε_2 **Energy par particle of the 2nd layer**

σ_2 **number density of the 2nd layer**

$$\mu_2(\sigma_2) = \sigma_2 \frac{\mathrm{d}\varepsilon_2(\sigma_2)}{\mathrm{d}\sigma_2} + \varepsilon_2(\sigma_2)$$

Density dependent particle energy of the 2nd layer,

for 28/49(6.80nm^{-2}), 16/25(7.26mn^{-2}), 49/81(7.61nm^{-2})

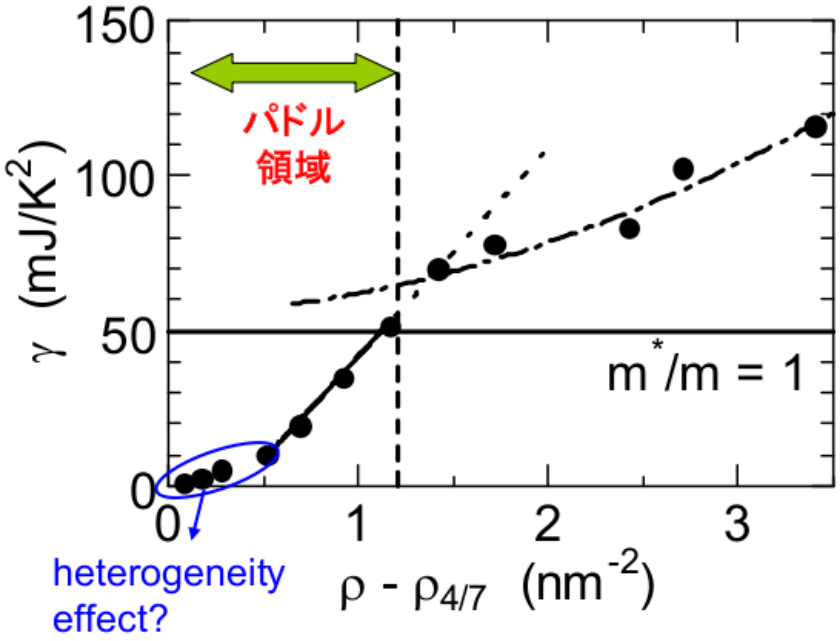
Fitting to a quadratic polynomial form, and we get,

$$\mu_2(\sigma_2) = 5.484\sigma_2^2 - 49.21\sigma_2 + 59.42[\mathrm{K}]$$

Critical density of promotion to the 3rd layer

Critical density σ_{2c} is estimated from the condition,

$$\mu_2(\sigma_{2c}) = \mu_3. \quad \rightarrow \quad \sigma_{2c} = 7.1 \pm 0.1 \mathrm{nm}^{-2}$$



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Our computation result,

$\rho_{2c} - \rho_{4/7} = 0.3 \pm 0.1$ **nm**$^{-2}$

Not the heterogeneity effect?

It should come from intrinsic origin.

Summary

- **4/7 structure is stable against upto 2% of vacancies doping.**
- **4/7 structure is unstable for the interstitial particle addition.**
- **Promotion to the 3rd layer occurs at the $\sigma_2 = 7.1\text{nm}^{-2}$.**
  It agrees with the empirical result.

Future Plans

- **Computing growth of the 3rd layer, and observing demotion to the 2nd layer.**
- **Determining characters of the 3rd layer.**