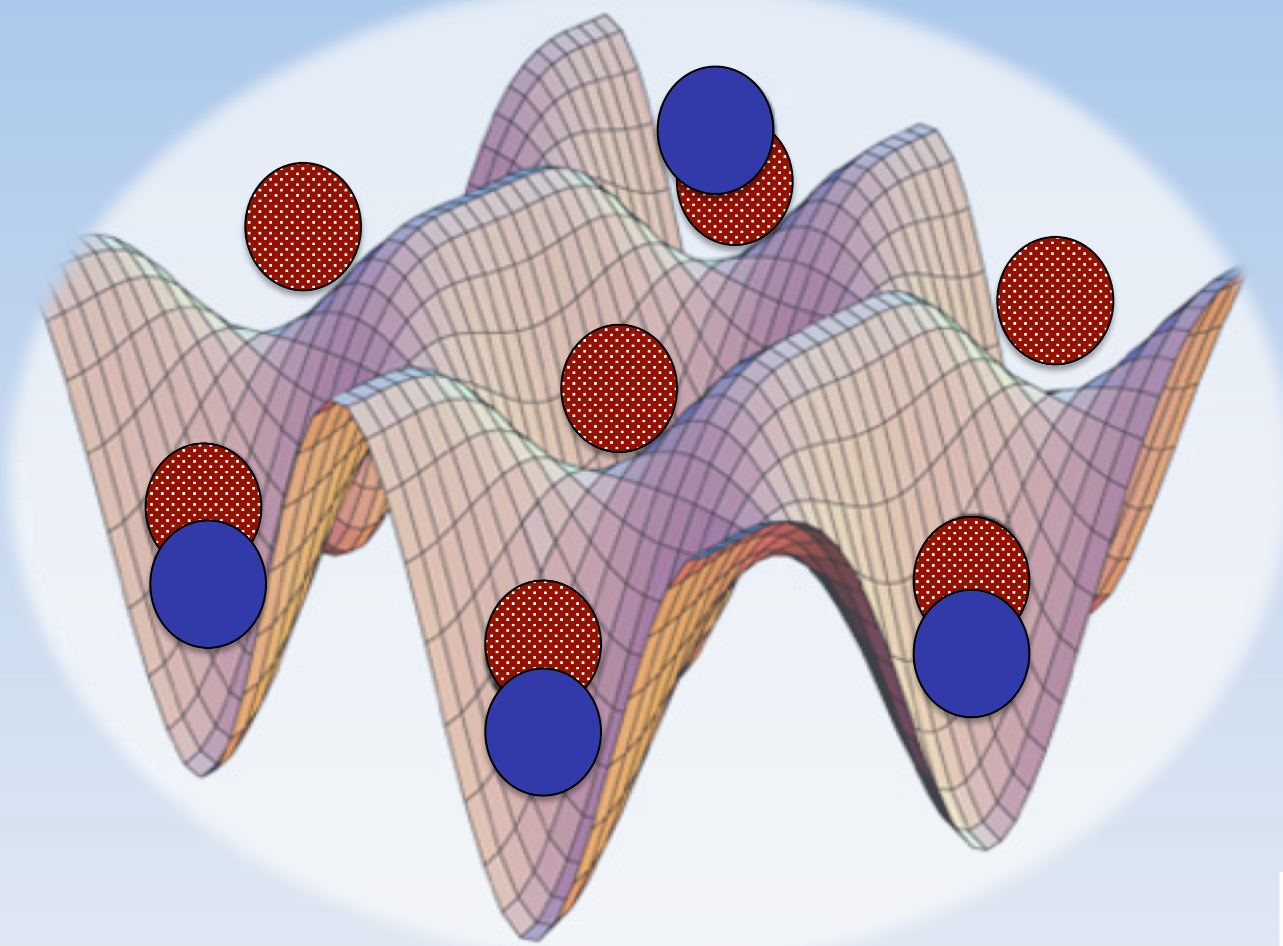
TWO-SPECIES BOSE HUBBARD MODEL

Kalani Hettiarachchi



Collaborators:

Valy Rousseau
Ka-Ming Tam
Juana Moreno
Mark Jarrell

Extreme Science and Engineering Discovery Environment

HIGH PERFORMANCE COMPUTING

LSU Center for Computation & Technology

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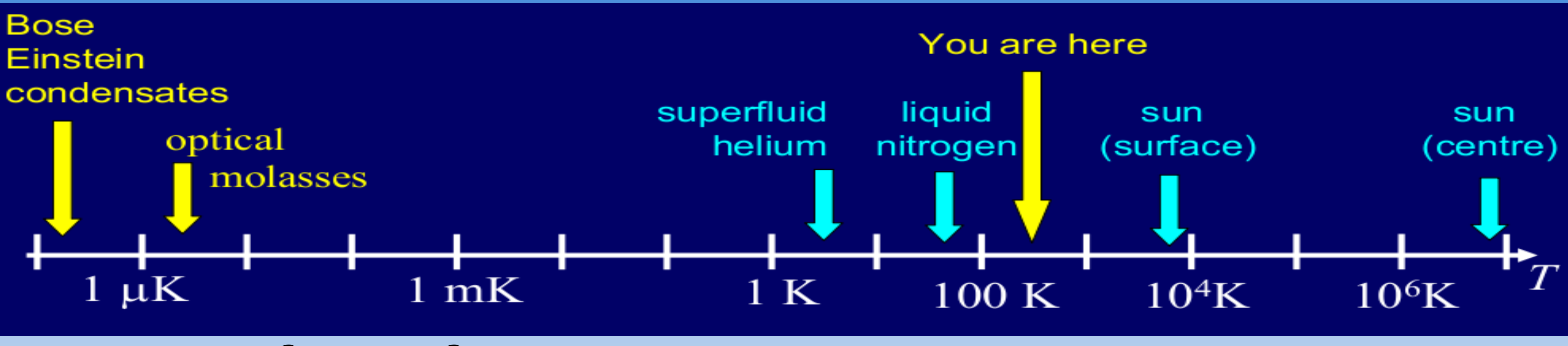
Cold Atoms



- **On Surface of Sun:** Miss many aspects of nature
- **Surface of Earth:** Different states of matter: solid, liquid and gas
- **Further Cooling:** In Kelvin : Superconductivity (1911)

  Superfluidity in Liquid Helium (^4He) (1938)

  In milli-Kelvin: Superfluidity in ^3He (1972)
- **Laser cooling/evaporative cooling(1980):**

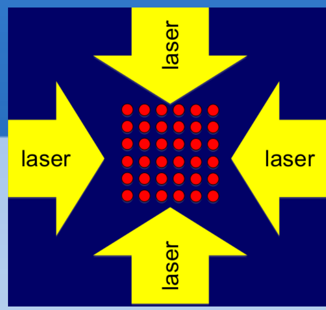
  In nano-Kelvin: Bose-Einstein Condensation (1995)

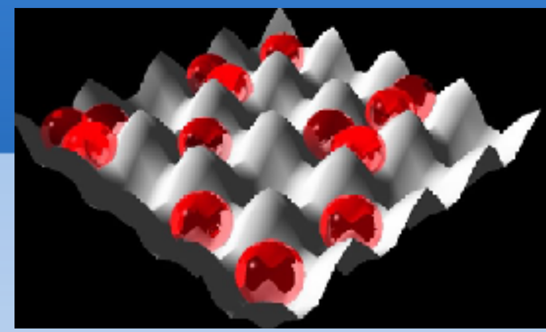
  (This was predicted for photons in 1924 by Bose and Einstein)

These achievements recognized with Nobel prizes!

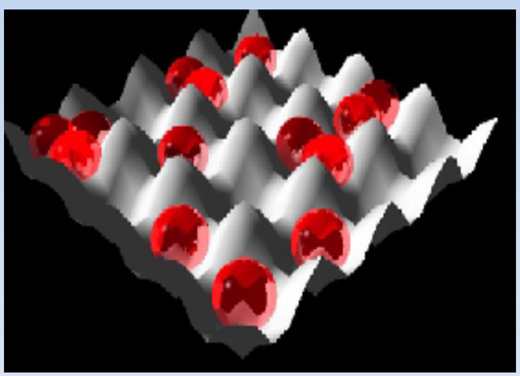
Optical Lattices and Bose Hubbard Model

- **<u>Optical lattices</u>:** Artificial crystal of lights consisting of thousands of optical micro traps: created by interfering of laser beams!



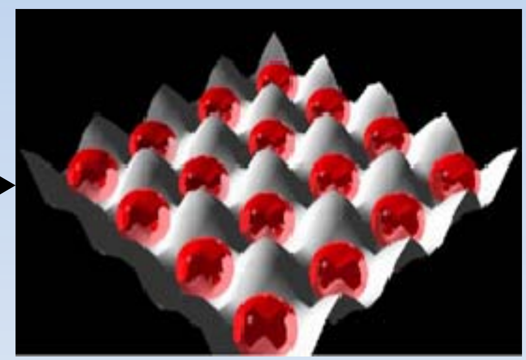


- Bosons loaded in optical lattices undergo a superfluid-Mott insulator transition: Theoretically proposed and verified experimentally!



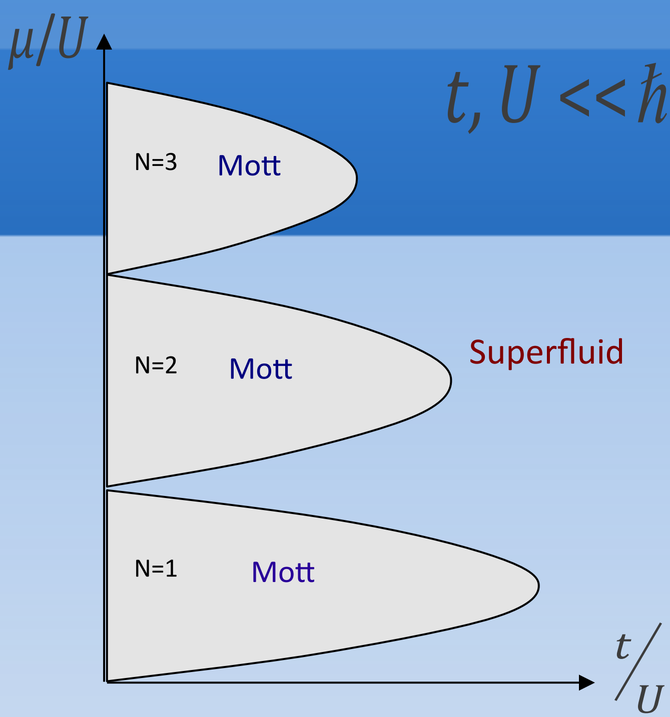
Bose-Hubbard Model

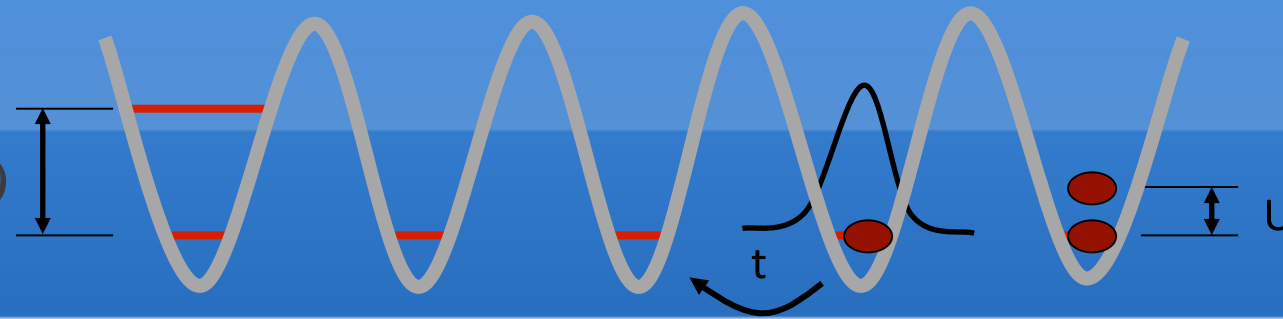
D. Jaksch et al., PRL(1998)
M. P. A. Fisher et al., PRB(1989)
M. Greiner et al., NATURE(2002)



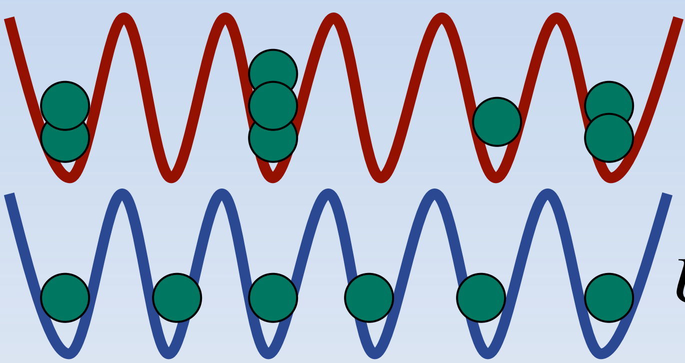
- The advance of optical lattice experiments and the experimental tunability of Hamiltonian parameters using laser and magnetic fields allow the realization of strongly correlated models.

Bose Hubbard model





$$H = -t\sum_{\langle ij\rangle}(a_i^{+}a_j + hc) + \frac{U}{2}\sum_i n_i(n_i - 1) \quad ; \quad n_i = a_i^{+}a_i$$



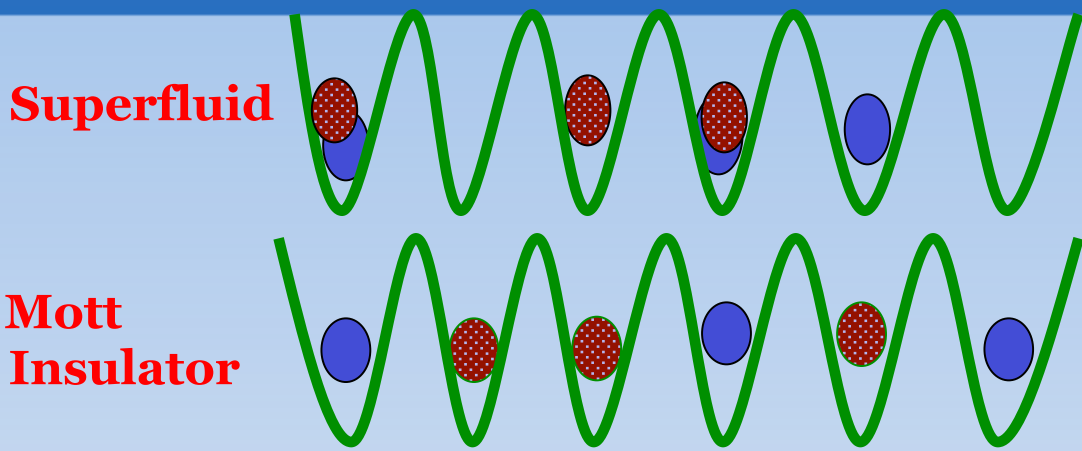
The superfluid phase is characterized by Bose-Einstein condensation, gapless excitations and finite compressibility in the weak coupling regime.

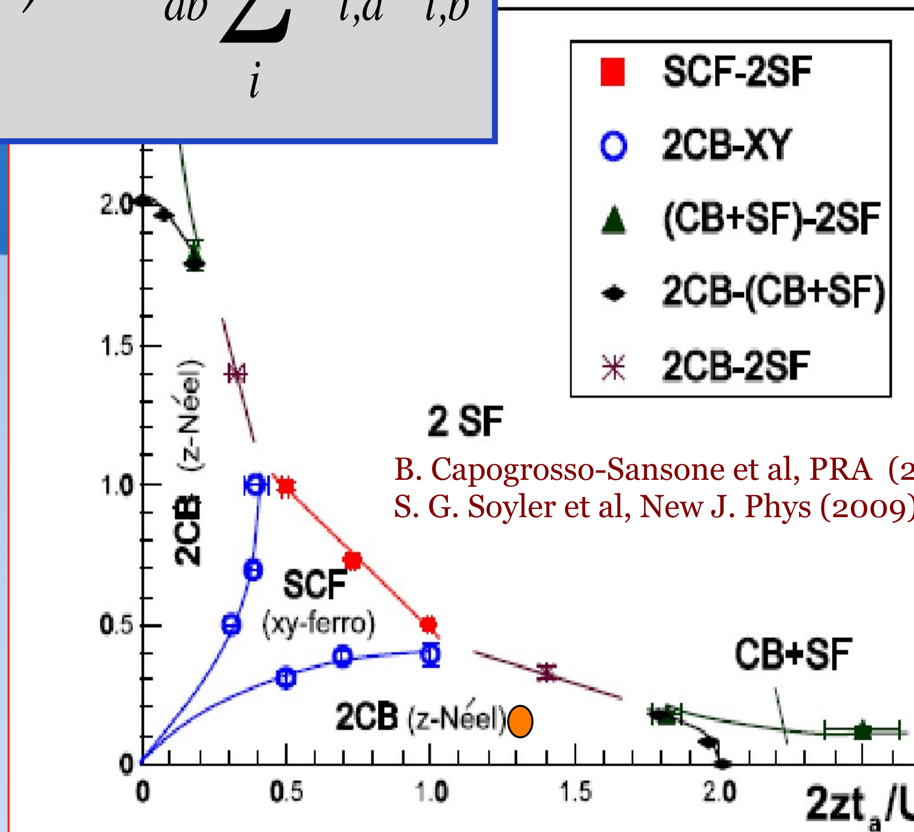
The Mott insulator phase is characterized by commensurate occupations, gapped excitations and incompressibility in the strong coupling regime.

Mixtures of atoms can give rise to even more interesting and complex phases.

Two species hard core bosonic model

$$H = -t_a \sum_{\langle ij \rangle} (a_i^+ a_j + hc) - t_b \sum_{\langle ij \rangle} (b_i^+ b_j + hc) + U_{ab} \sum_i n_{i,a} n_{i,b}$$





B. Capogrosso-Sansone et al, PRA (2010)
S. G. Soyler et al, New J. Phys (2009)

- **Commutation rules on different sites!**
- **Anti-commutation Rules on identical site**

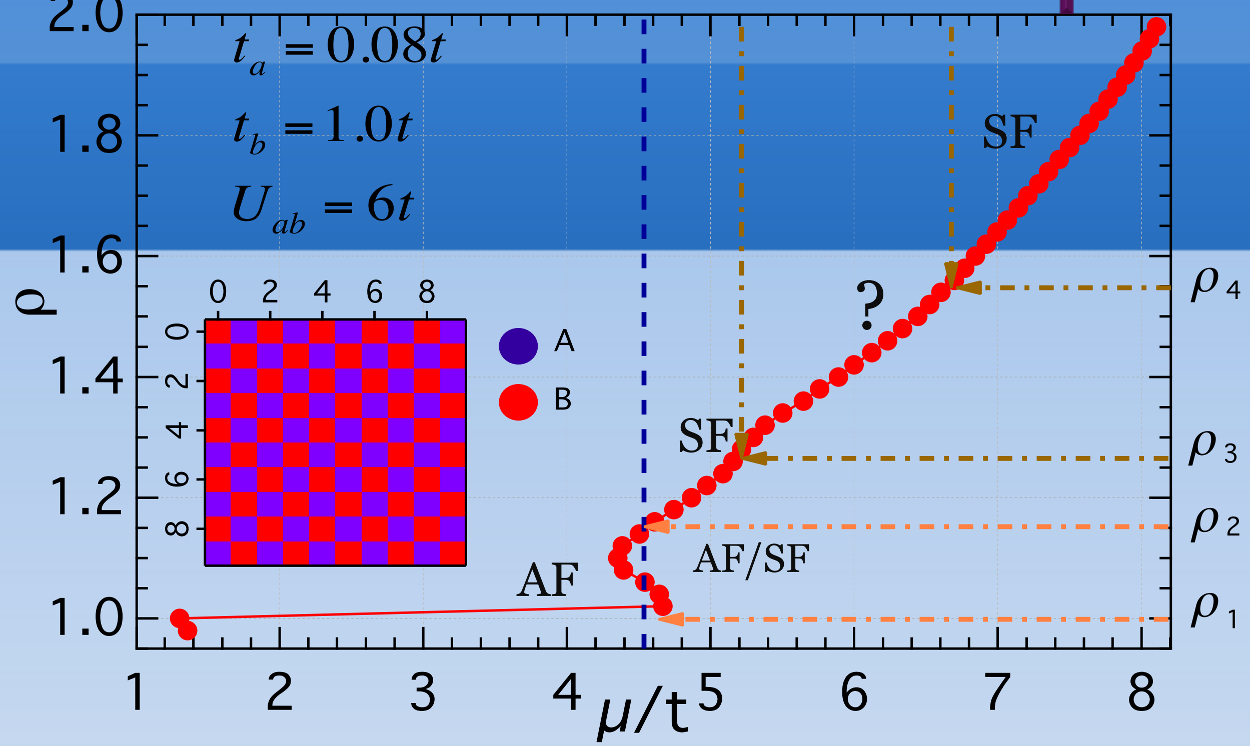
Our focus is to study the model as a function of doping.

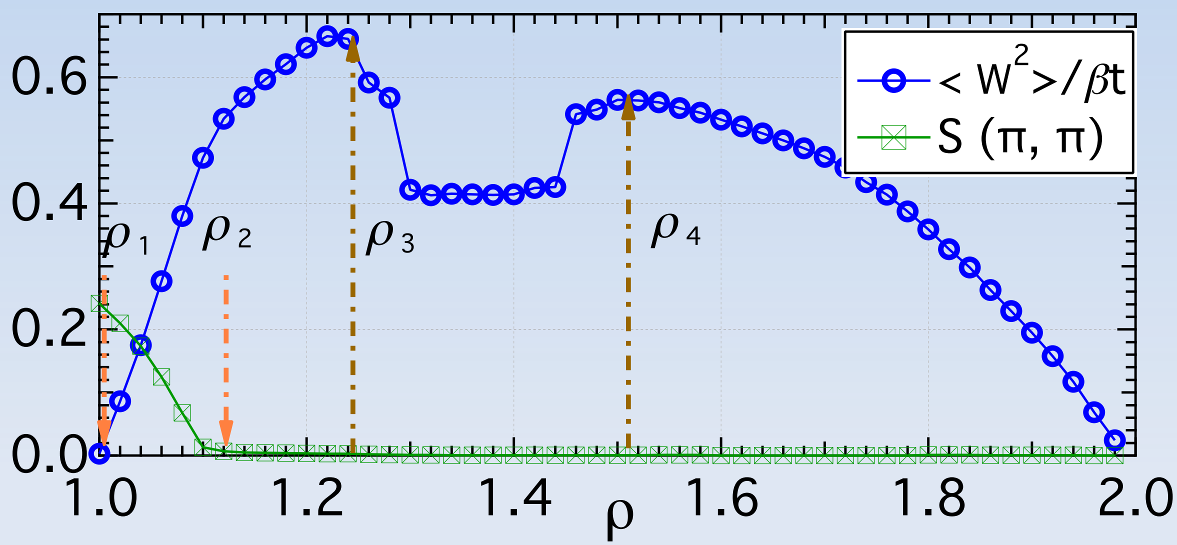
1. Equal populations ($N_a=N_b$) and mass imbalance ($t_a<t_b$).
2. Population imbalance ($N_a \neq N_b$) and mass imbalance ($t_a<t_b$).

Method: QMC simulations using the Stochastic Green function algorithm

V.G. Rousseau, PRE. 78, 056707 (2008), and arXiv:1209.0946

Doping results with mass imbalance between species





$$\rho = \frac{N}{L^2}$$

$$N = N_a + N_b$$

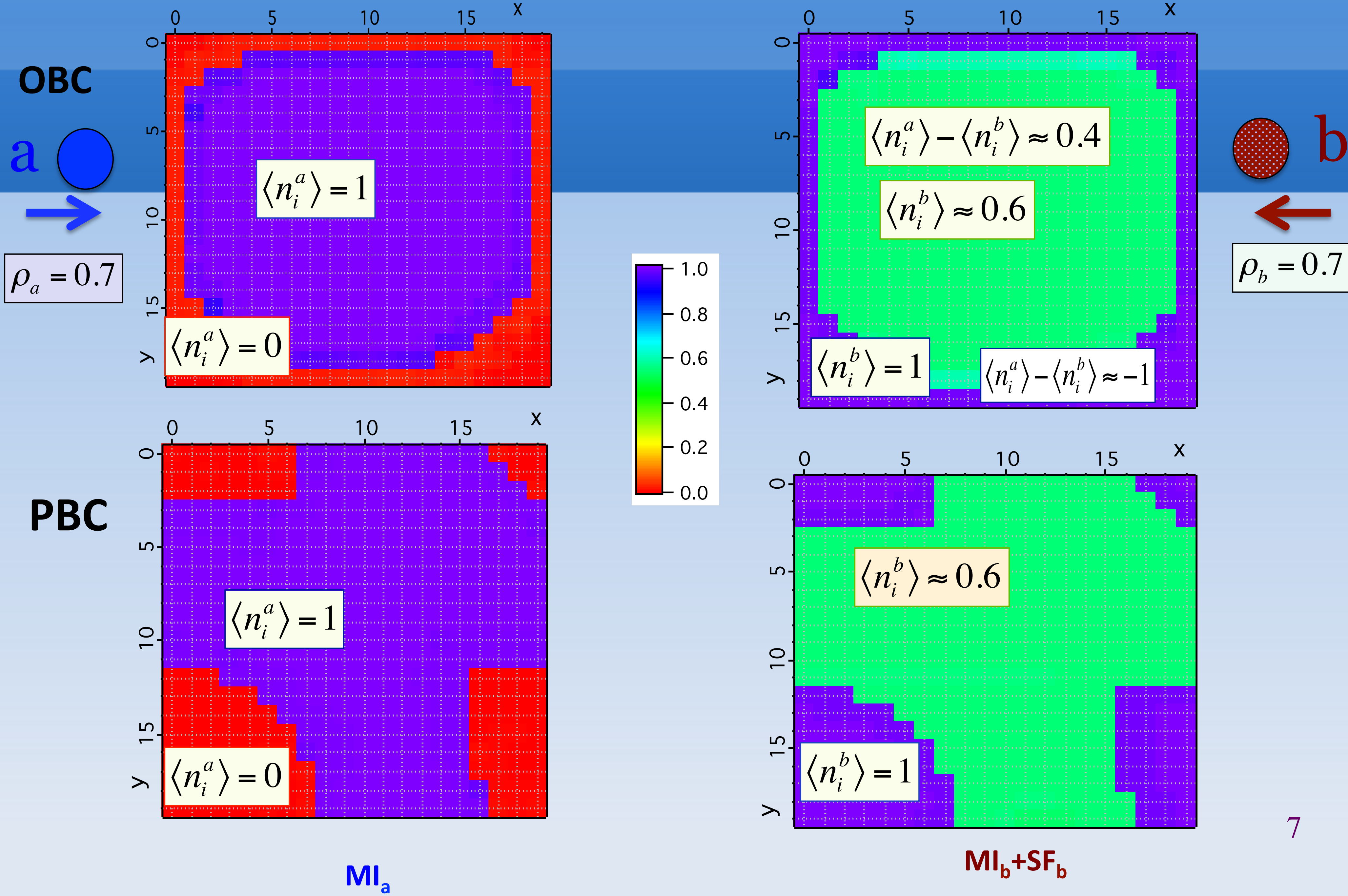
$$N_a = N_b$$

$$\langle W^2 \rangle = \langle (W_a + W_b)^2 \rangle$$

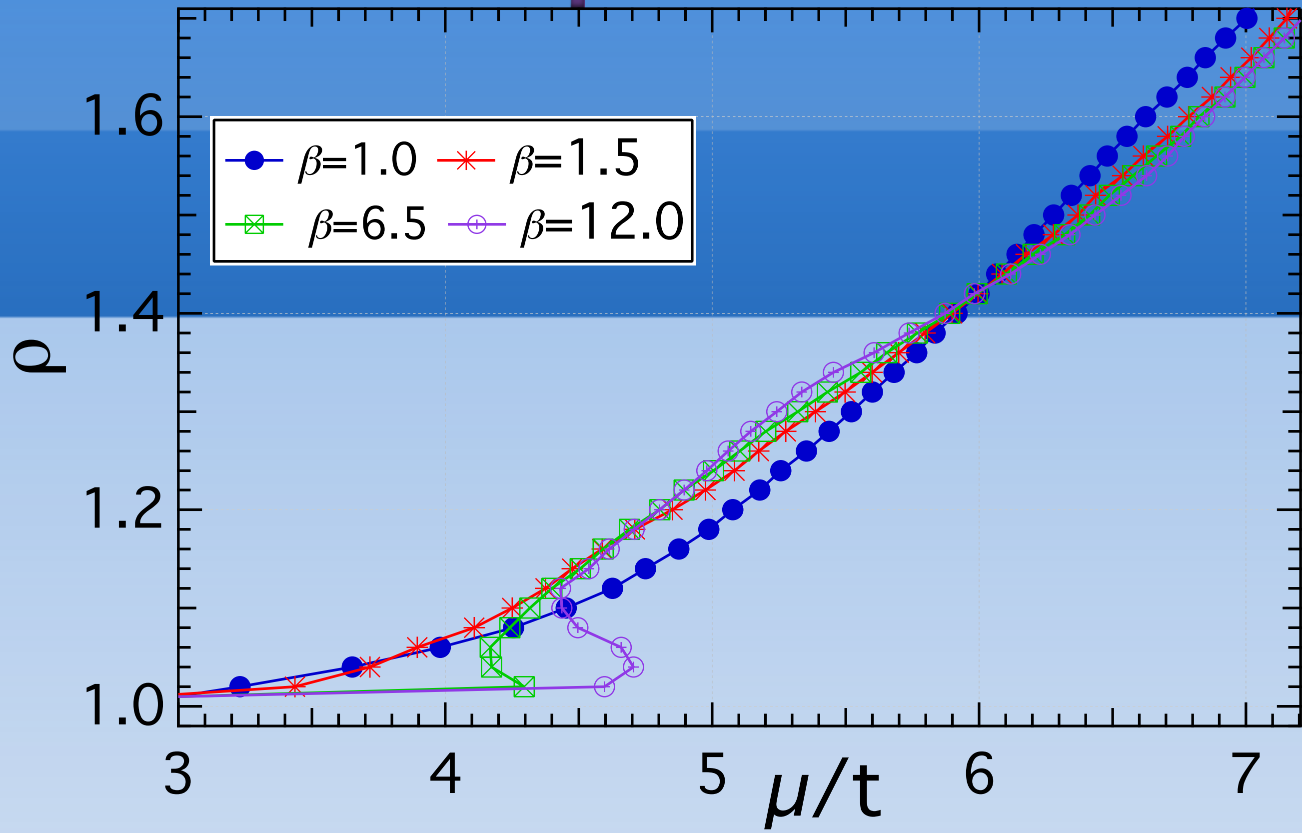
$$\rho_{SF} = \frac{\langle W^2 \rangle}{4t\beta}$$

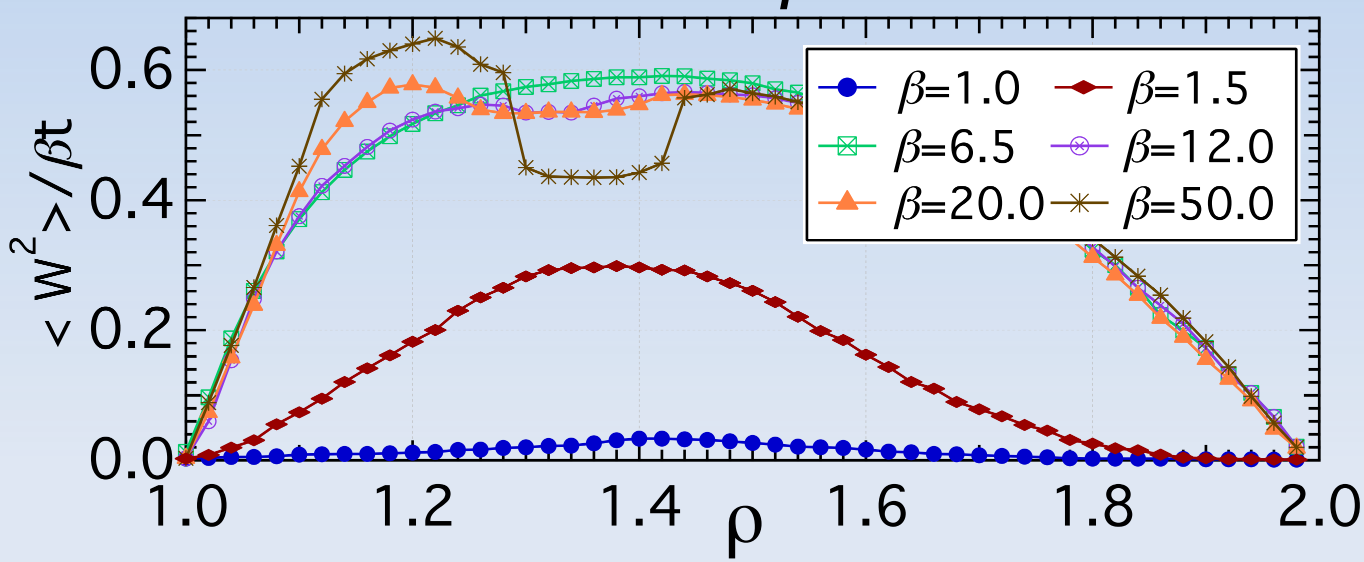
$$S_{a,b}(k) = \sum_{p,q} e^{ik(p-q)} \langle n_p^{a,b} n_q^{a,b} \rangle$$

Ferromagnetic Phase Separation

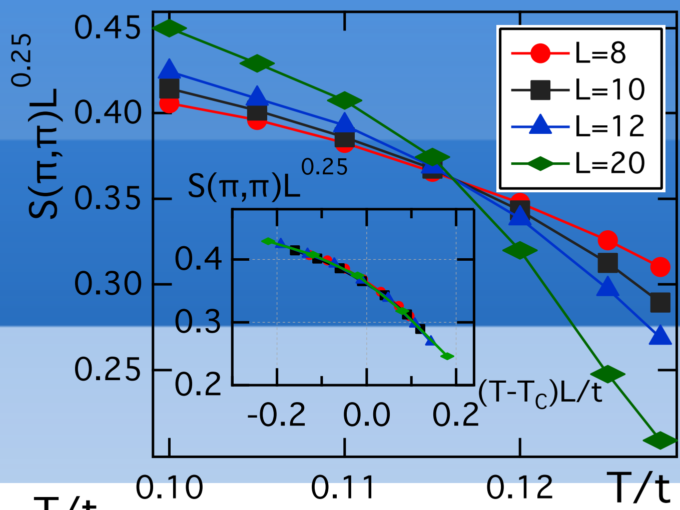


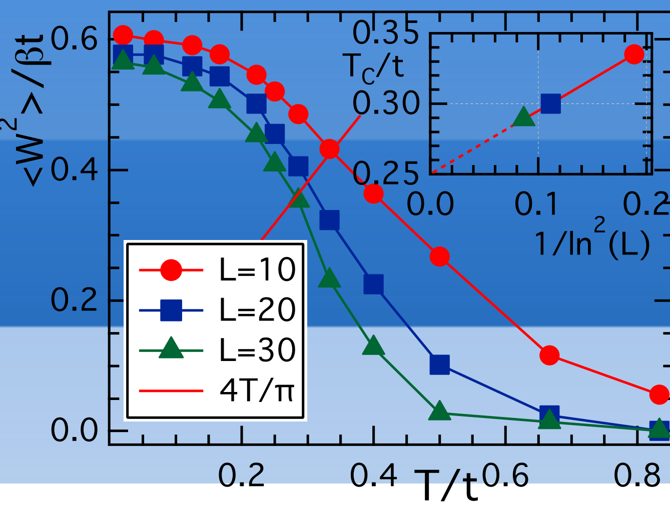
Finite Temperature Results





Phase Diagram of the doped system



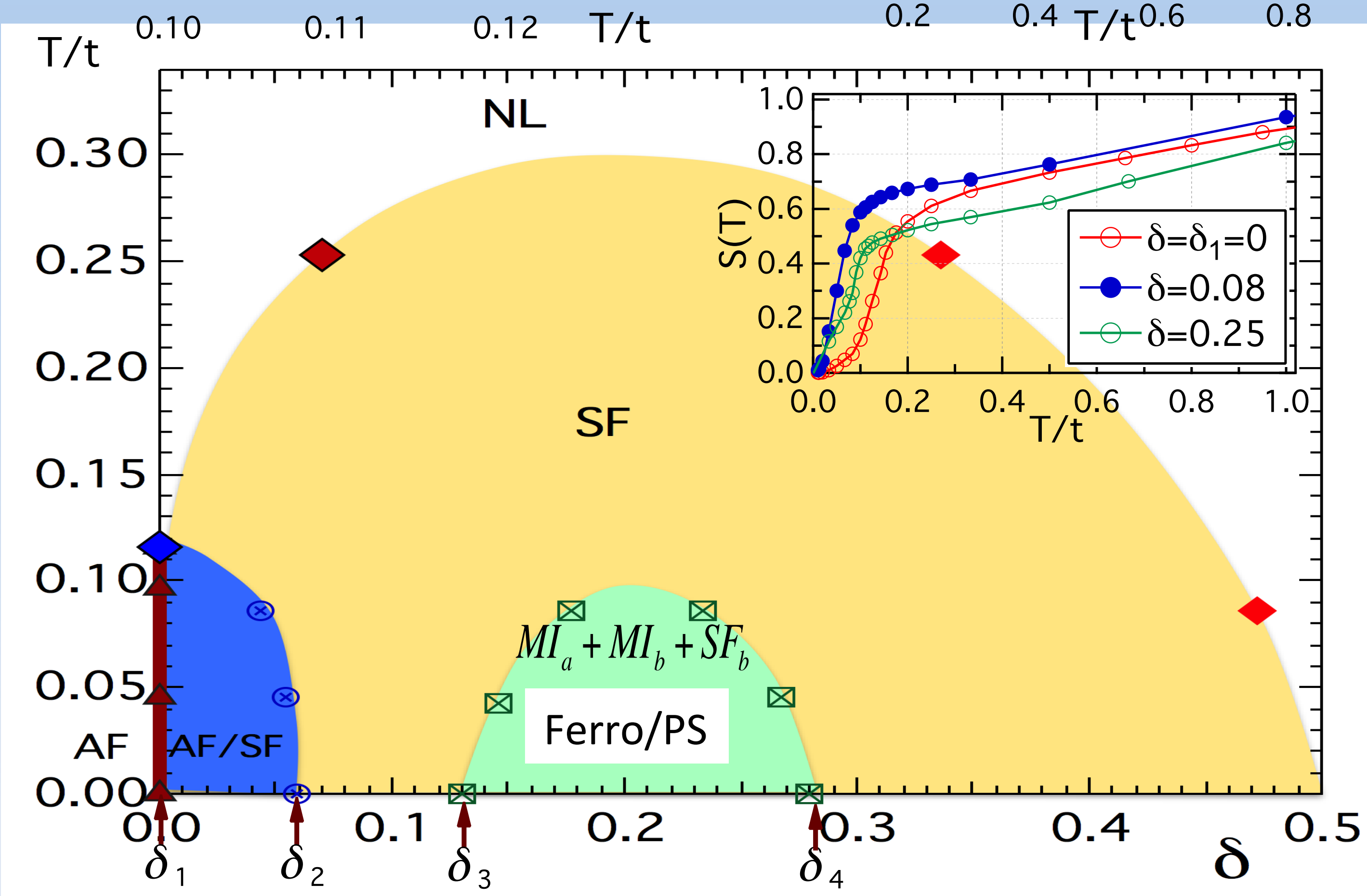


$$S(\pi,\pi) = L^{-(2\beta/\nu)} f((T - T_c^{AF})L^{1/\nu})$$

$$\langle W^2 \rangle = \frac{4}{\pi}$$

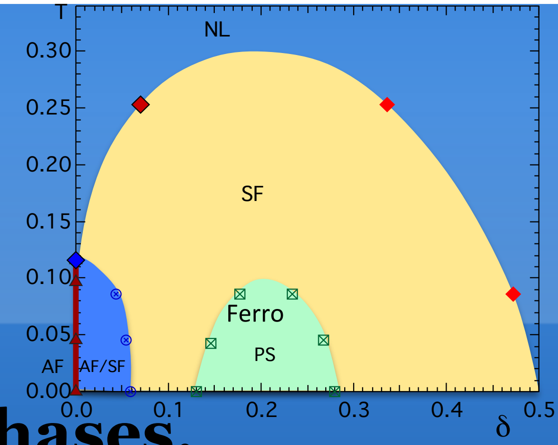
$$T_c(L) - T_c(\infty) \propto \frac{1}{\ln^2(L)}$$

$$S(\beta,n) \;=\; S(0,n) + \beta E(\beta,n) - \int_0^{\beta} E(\beta',n)d\beta'$$



$$\delta = \frac{N_a + N_b}{2 * L^2} - \frac{1}{2}$$

Findings



➢**Model is interesting and it has Competing phases.**

➢**Found five distinct phases!**

- **AF phase** at half filling and low temperature
- **AF to SF phase separation** near half filling
- **NL phase** at finite temperature
- **SF phase** for a broad region of filling
- **Ferro-magnetic PS phase** inside SF phase at low temperature

➢ **PS dome inside SF phase shows greater entropy than AF and similar to the SF phase.**
Experimental realization is possible!

➢Reference: "Complex phases in a two species bosonic Hubbard Model" K. Hettiarachchilage, V. G. Rousseau, Ka-Ming Tam, M. Jarrell, and J. Moreno, Phys. Rev. B 88, 161101(R) (2013).

Ferromagnetism with population imbalance of the species

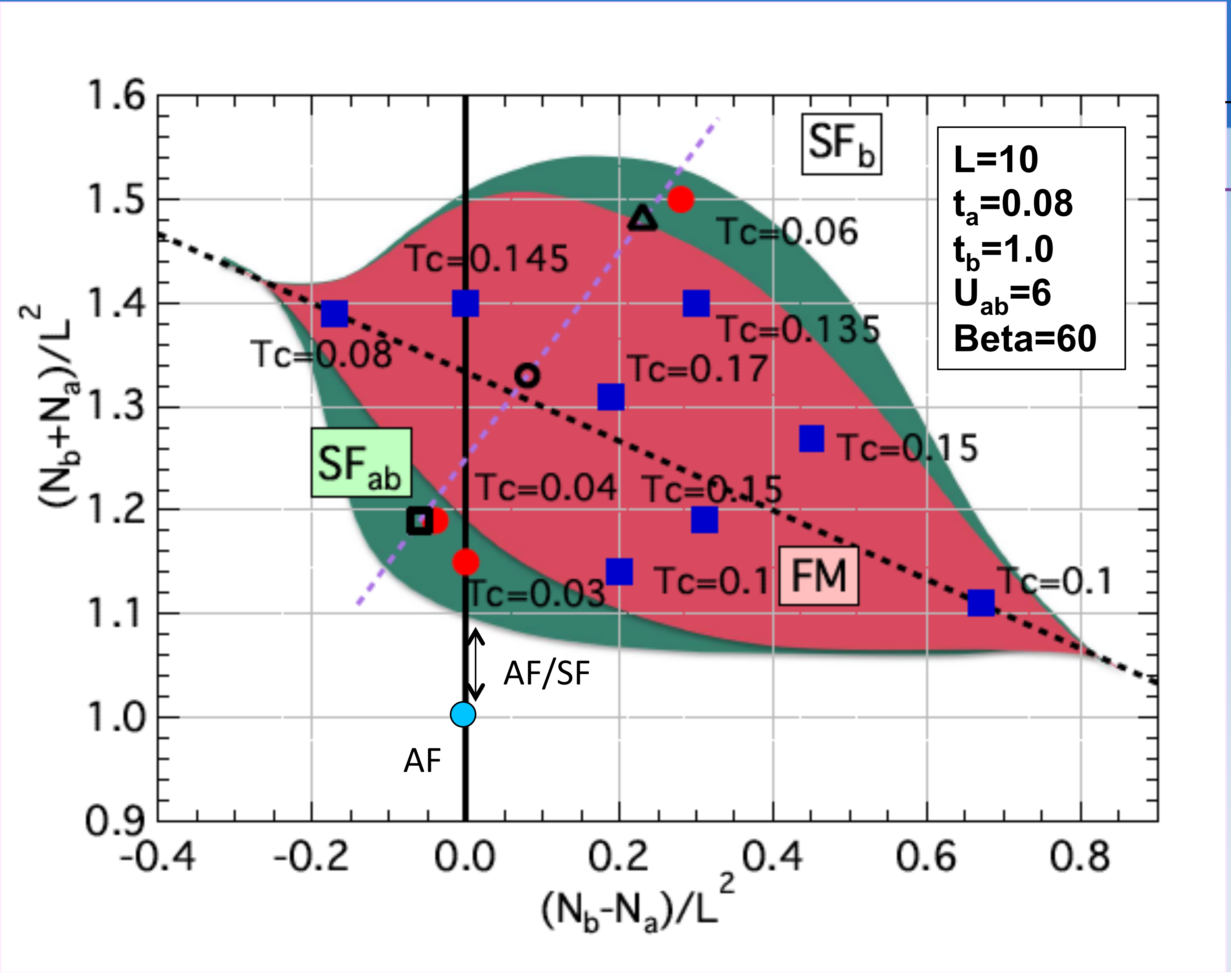
$$H = -t_a \sum_{\langle ij \rangle} (a_i^+ a_j + hc) - t_b \sum_{\langle ij \rangle} (b_i^+ b_j + hc) + U_{ab} \sum_i n_{i,a} n_{i,b}$$

- The prominent experimental challenge of quantum magnetic phases is to reach such low temperatures and entropies needed to observe these phases.

- The relatively high global entropy of the phase-separated ferromagnetic phase suggests that this ferromagnet should be easier to access experimentally.

- Then we thought to explore the extent of the phase-separated ferromagnetic phase as a function of finite polarization.

Extent of ferromagnetic phase with finite polarization



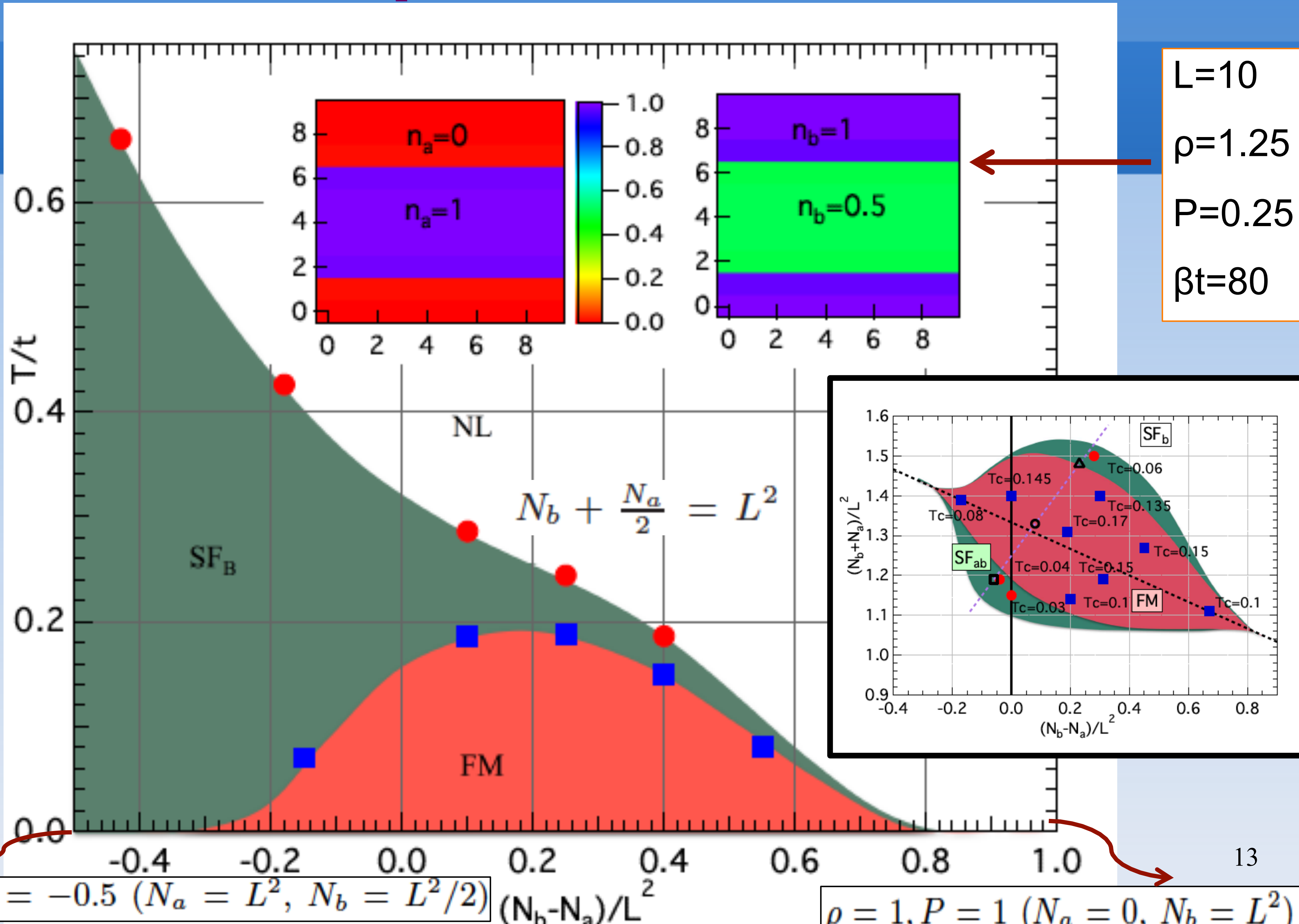
$N_b + \frac{N_a}{2} = L^2$

$N_a = 0.625L^2$

$\rho = \frac{N_b+N_a}{L^2}$

$P = \frac{N_b-N_a}{L^2}$

Phase diagram on the optimal superfluid line



L=10

ρ=1.25

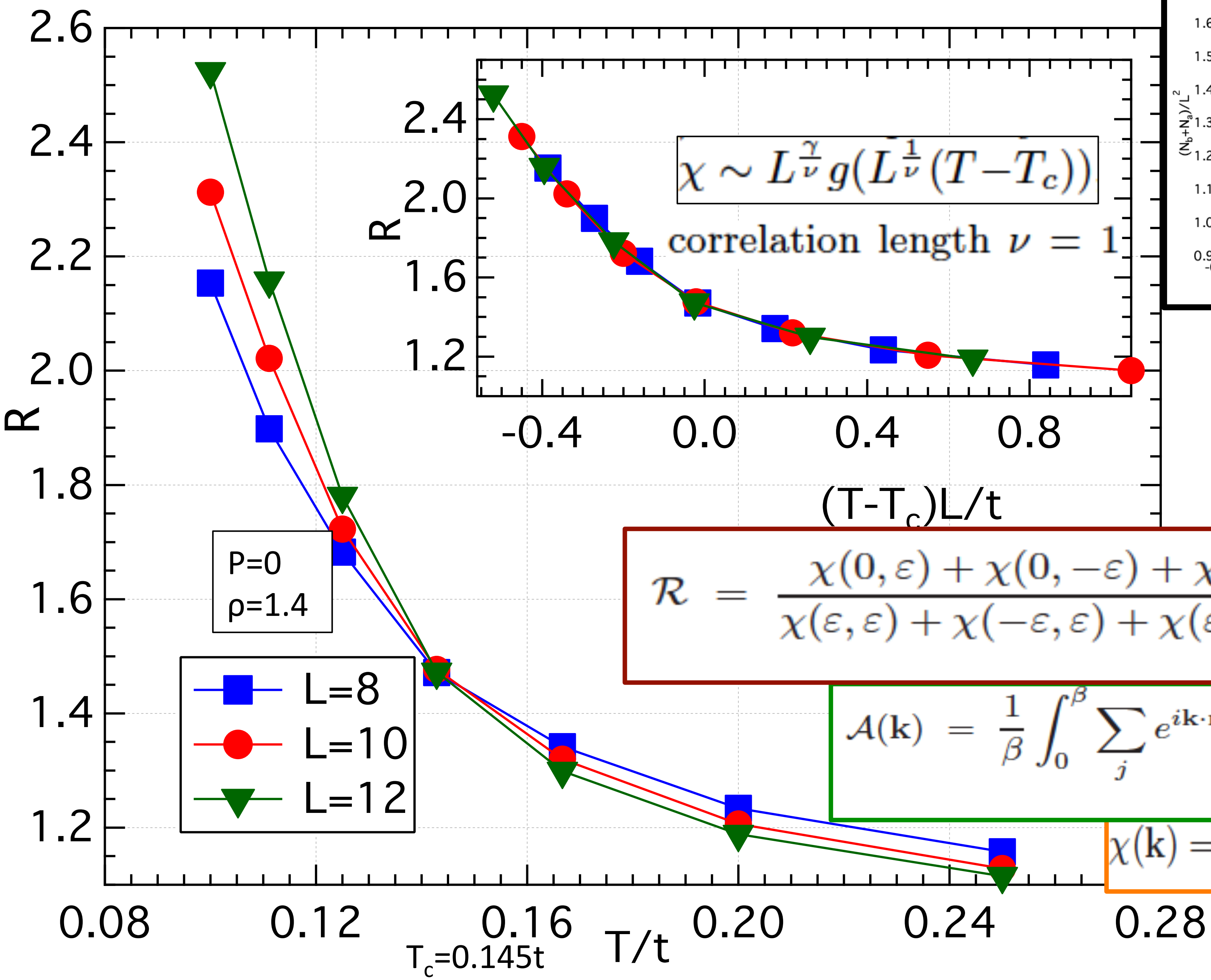
P=0.25

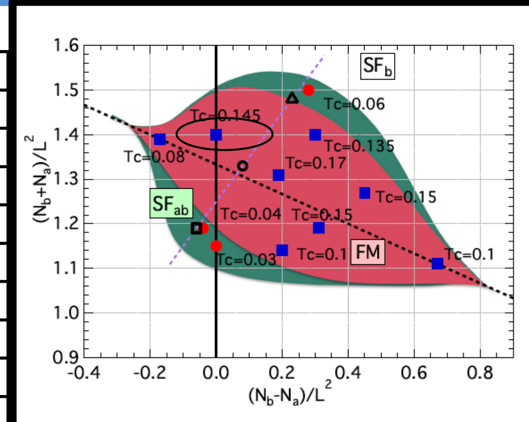
βt=80

$\rho = 1.5, P = -0.5\ (N_a = L^2,\ N_b = L^2/2)$

$\rho = 1, P = 1\ (N_a = 0,\ N_b = L^2)$

Ferromagnetic susceptibility





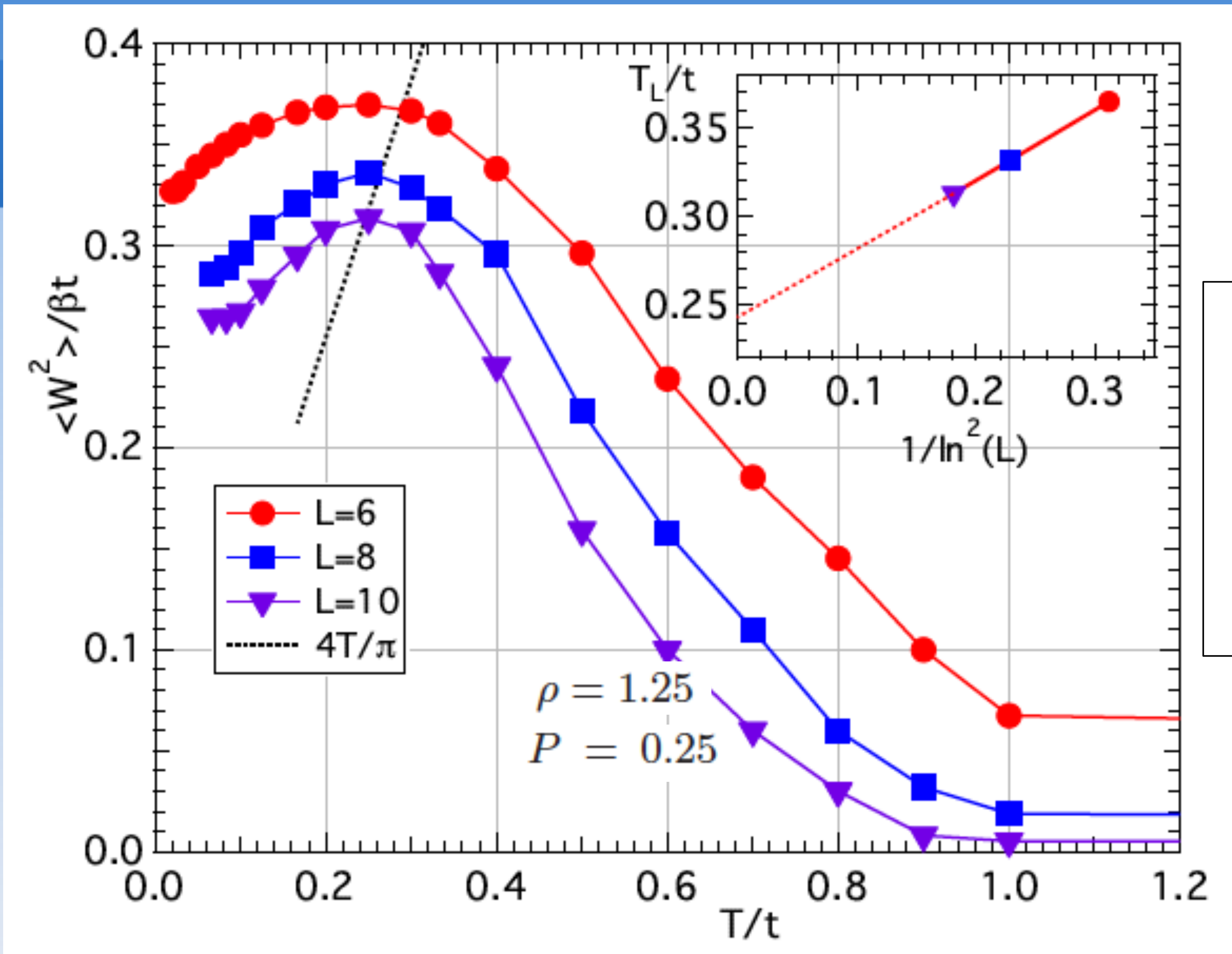
$$\varepsilon = \frac{2\pi}{L}$$

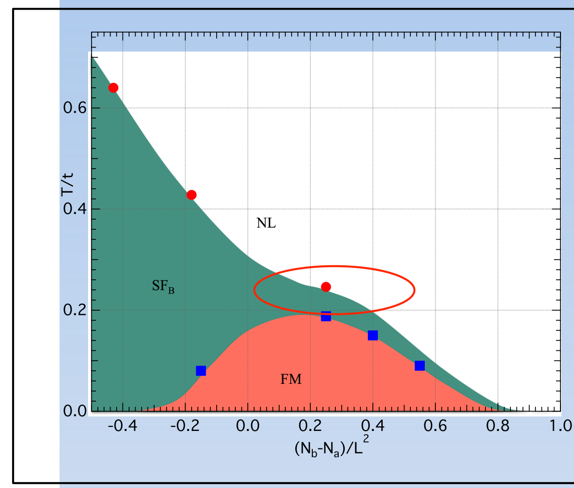
$$\mathcal{R} = \frac{\chi(0,\varepsilon)+\chi(0,-\varepsilon)+\chi(\varepsilon,0)+\chi(-\varepsilon,0)}{\chi(\varepsilon,\varepsilon)+\chi(-\varepsilon,\varepsilon)+\chi(\varepsilon,-\varepsilon)+\chi(-\varepsilon,-\varepsilon)}$$

$$\mathcal{A}(\mathbf{k}) = \frac{1}{\beta}\int_0^\beta \sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j}(n_j^a(\tau)-n_j^b(\tau))\,d\tau.$$

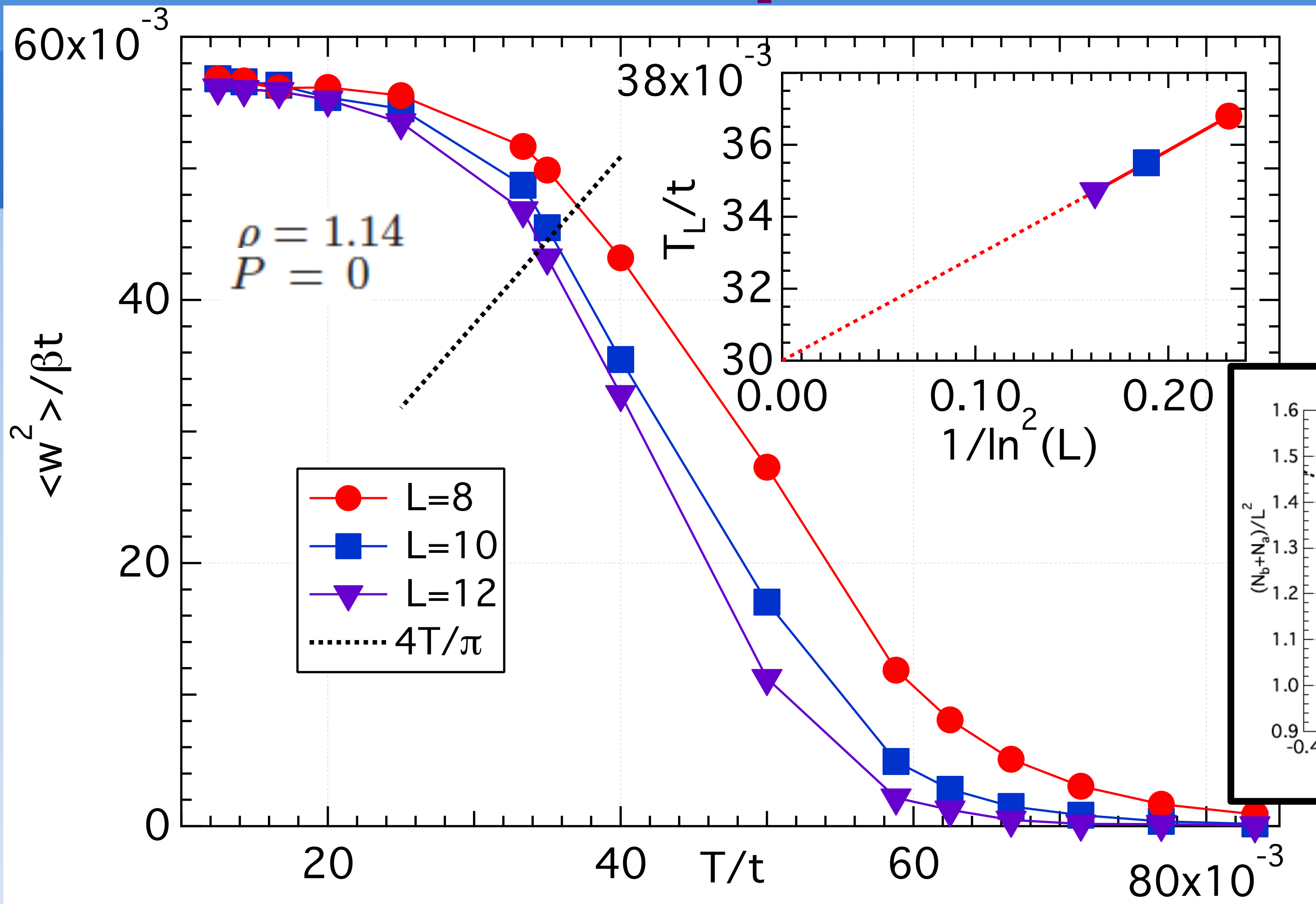
$$\chi(\mathbf{k}) = \langle|\mathcal{A}(\mathbf{k})|^2\rangle - |\langle\mathcal{A}(\mathbf{k})\rangle|^2$$

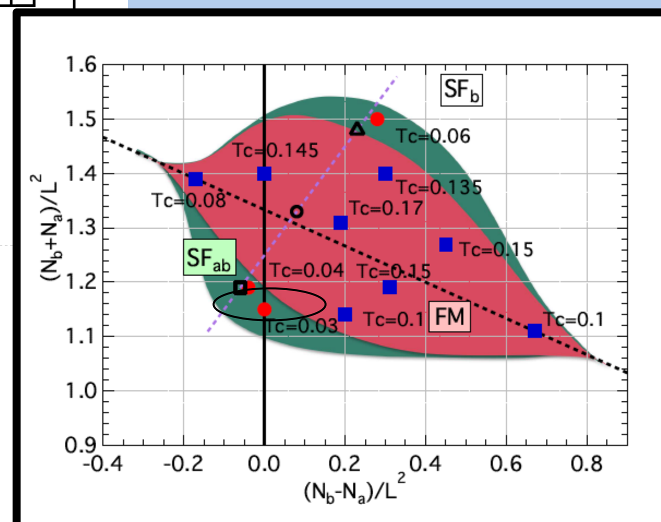
Superfluid density of light species



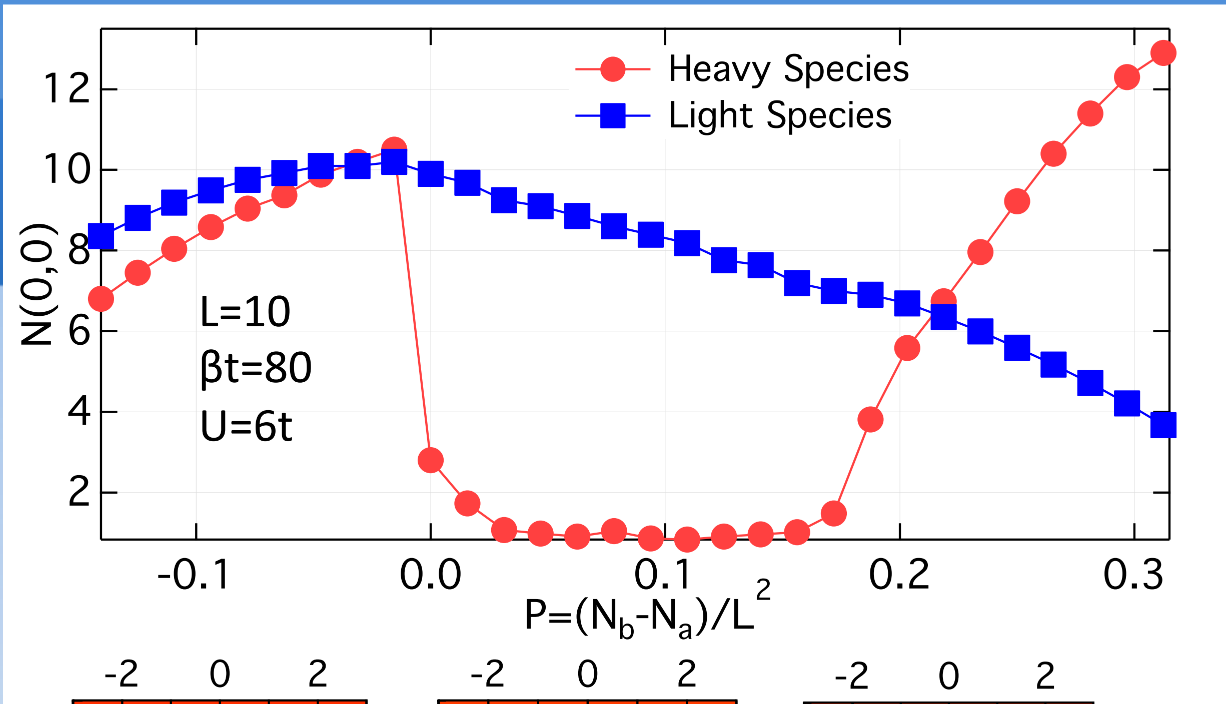


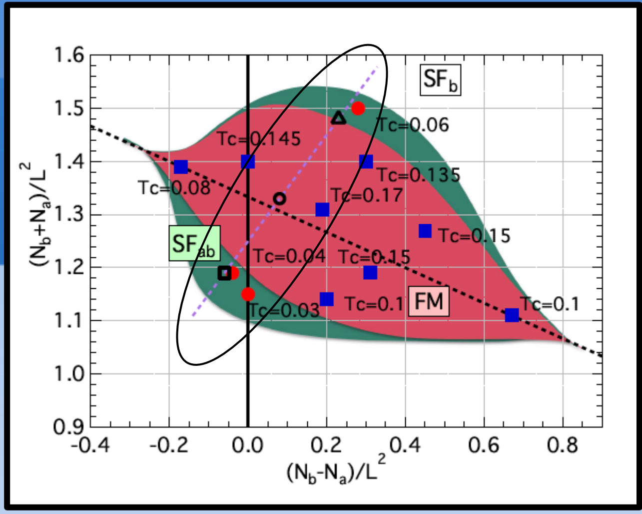
Superfluid density of heavy species

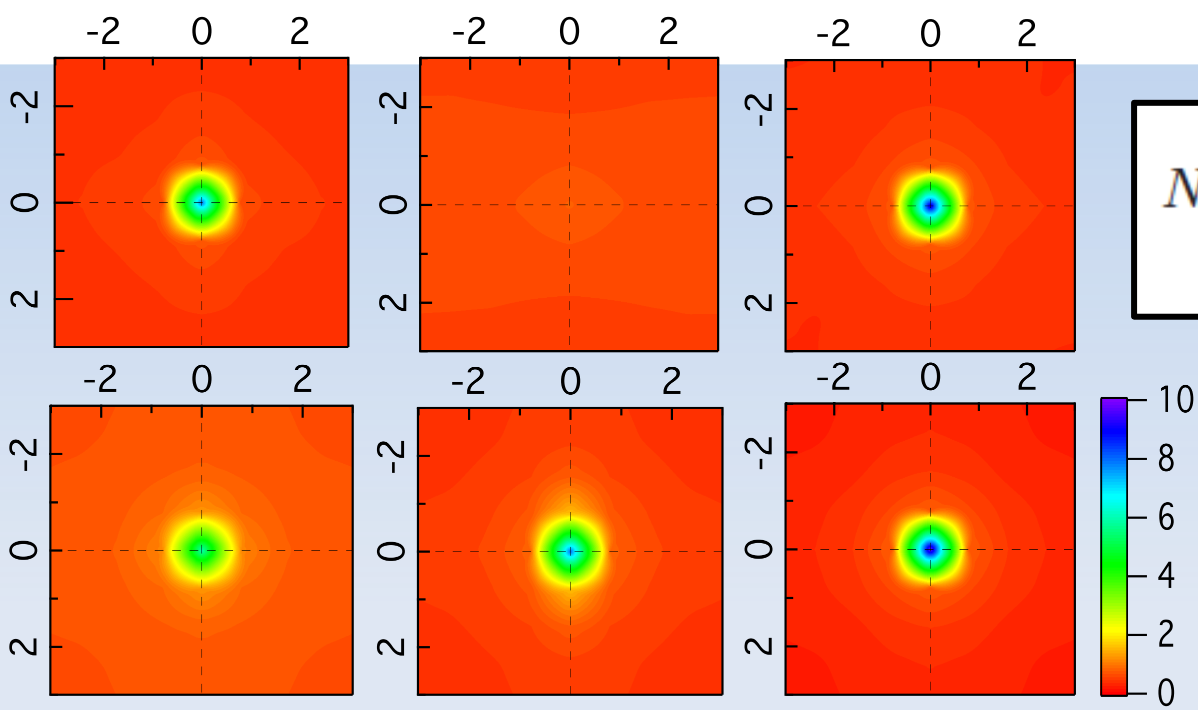




k-space momentum distribution



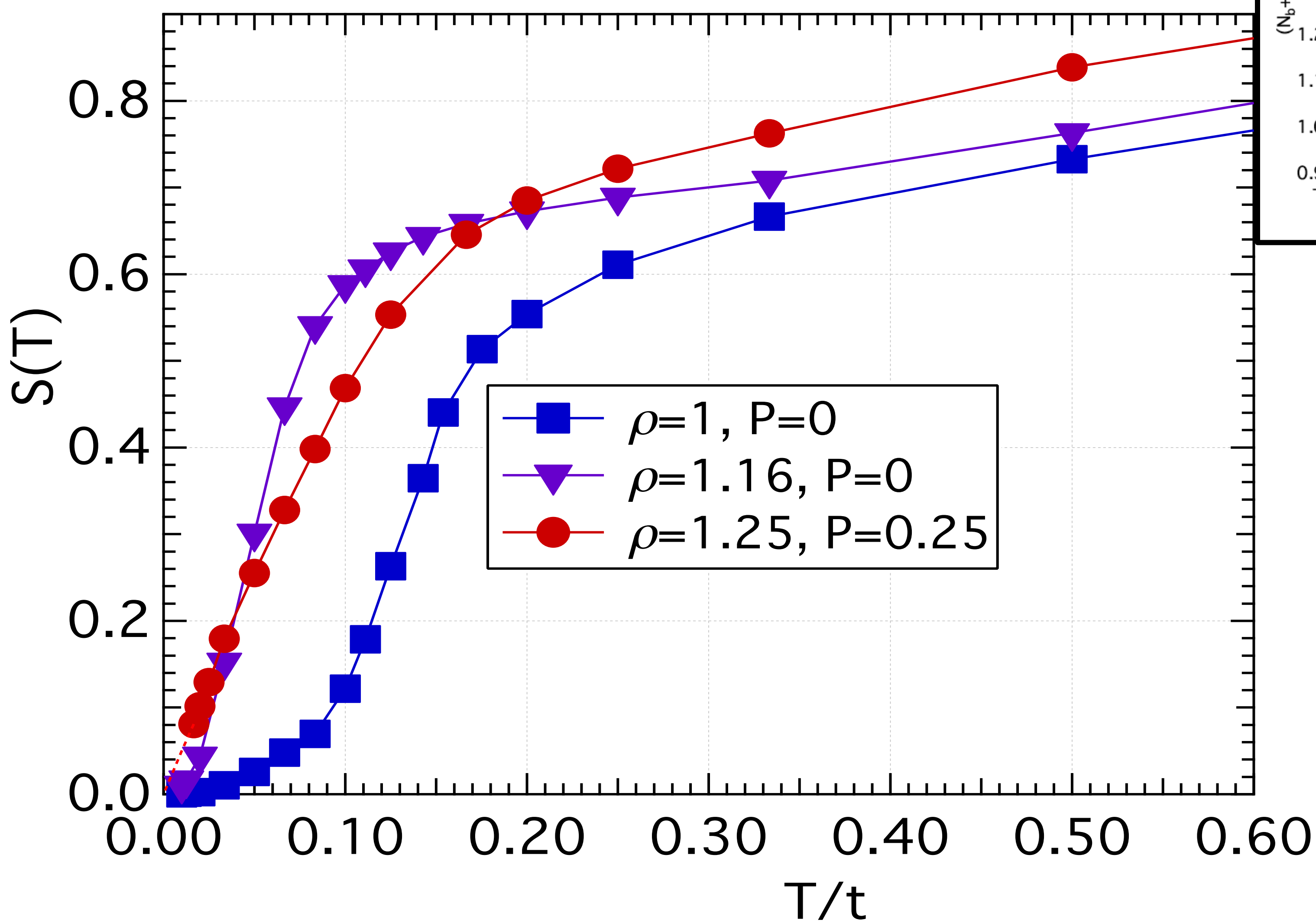


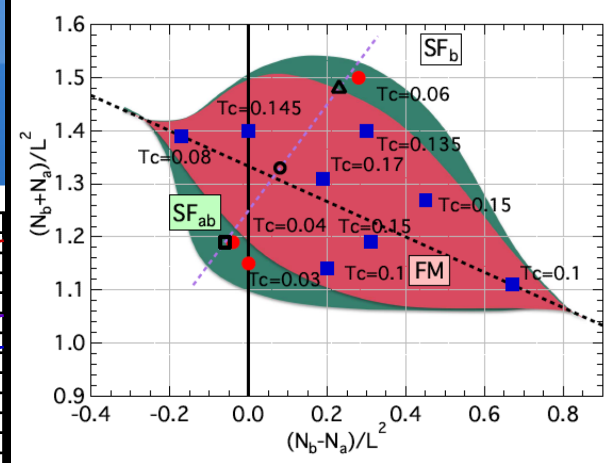


$$N(\mathbf{k}) = \frac{1}{L^2}\sum_{k,l} e^{i\mathbf{k}\cdot(\mathbf{r}_k-\mathbf{r}_l)}\langle a_k^\dagger a_l\rangle$$

High Global Entropy for Ferromagnetic phase

$$\mathcal{S}(\beta, n) \;=\; S(0, n) + \beta E(\beta, n) - \int_0^{\beta} E(\beta', n) d\beta'$$





Findings

- Population imbalance between species extends the region of ferromagnetism.

- We found optimal superfluid line of fully phase separated ferromagnet with average local densities as $n_a \sim 0$ and $n_b \sim 1$ in one region and $n_a \sim 1$ and $n_b \sim 0.5$ on the other.

- **Ferromagnetic phase shows high global entropy**
  Experimental realization is possible!

- Reference: "Ferromagnetic Phase Separated Region in the Polarized Two-species Bose Hubbard Model" K. Hettiarachchilage, V. G. Rousseau, Ka-Ming Tam, M. Jarrell, and J. Moreno, Phys. Rev. B 90, 205104 (2014).

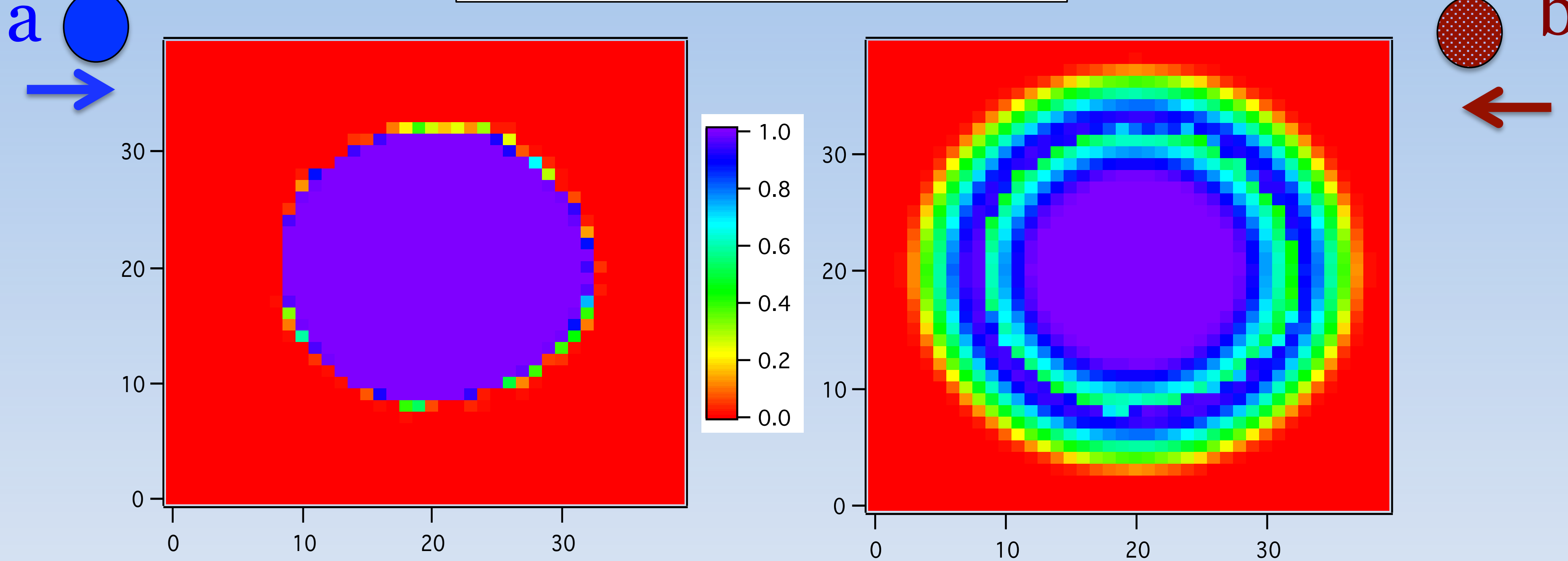
Ferromagnetism with a harmonic trap

- The realization of magnetic phases with the presence of confinement is of interest in experiments involving cold atoms.
- We want to look for the existence of the ferromagnetic phase shown at finite doping and polarization with the presence of a harmonic trapping potential.
- We look for the ferromagnetic phase in both hard-core and soft-core limits.

$$H = -t_a \sum_{\langle ij \rangle} (a_i^{+} a_j + hc) - t_b \sum_{\langle ij \rangle} (b_i^{+} b_j + hc) + U_{ab} \sum_i n_{i,a} n_{i,b} + W \sum_i \left(i - L/2 \right)^2 (n_{i,a} + n_{i,b})$$
$$+ \frac{U_{aa}}{2} \sum_i n_{i,a} \left(n_{i,a} - 1 \right) + \frac{U_{bb}}{2} \sum_i n_{i,b} \left(n_{i,b} - 1 \right)$$

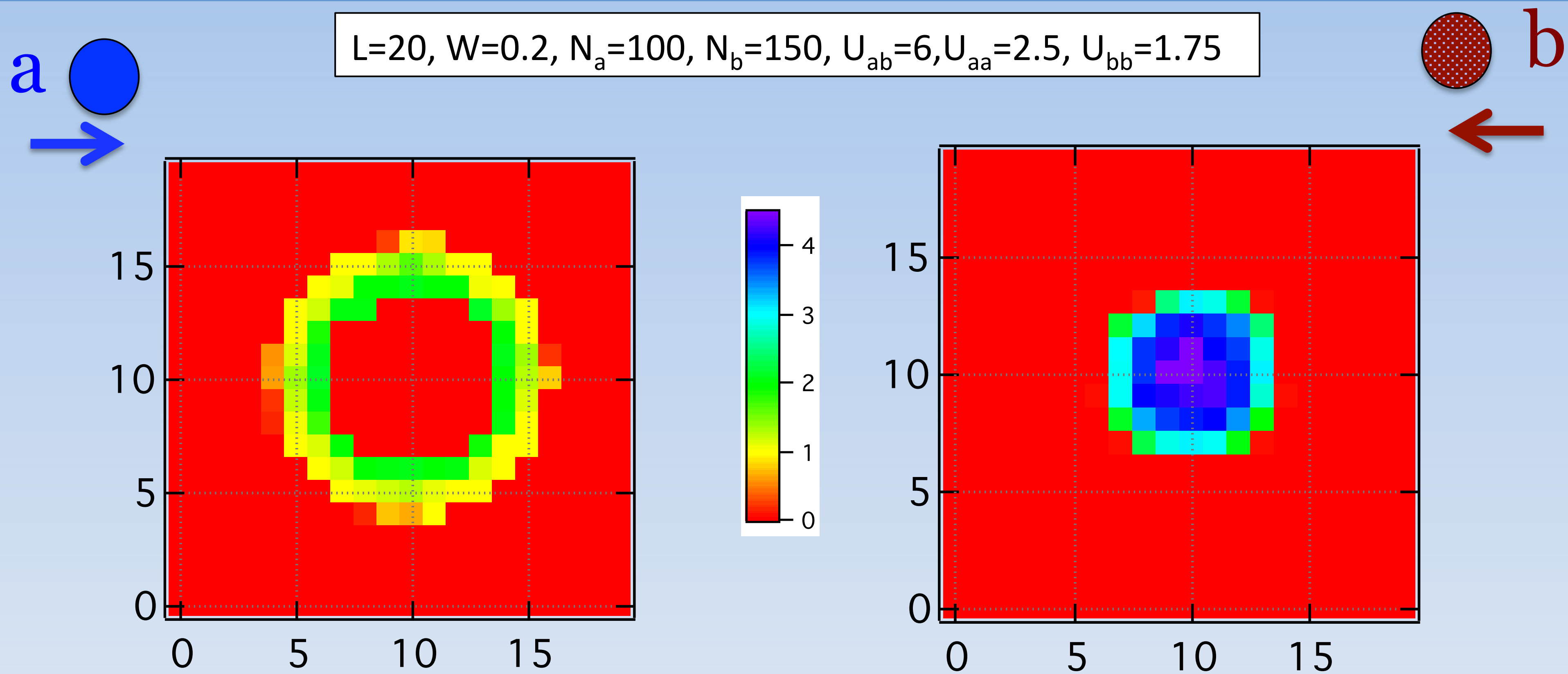
Hard-core limit

L=40, W=0.06, N_a=450, N_b=675, U_{ab}=6t



Soft-core limit

L=20, W=0.2, N_a=100, N_b=150, U_{ab}=6,U_{aa}=2.5, U_{bb}=1.75



Findings

- Such trapping effects can lead to have the ferromagnetic phase in both hard-core and soft-core bosons.
- In hard-core limit, we observe the phase separation where presumably the heavy species is localized in the center of the trap, and surrounded by the light species.
- In soft-core limit, we observe that the light species gets trapped in the center of the lattice, and is surrounded by the heavy species.
- The realization of the model is an open question for experimentalists. In collaborating with an experimental group, we are trying to figure out the precise range of parameters the experiments can reach.

Thank you!