Polarized atomic Fermi gases in optical lattices with elongated traps : DMFT study

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Overview

Attractively interacting +

Polarized atomic Fermi gases in optical lattices
with elongated traps :
DMFT study

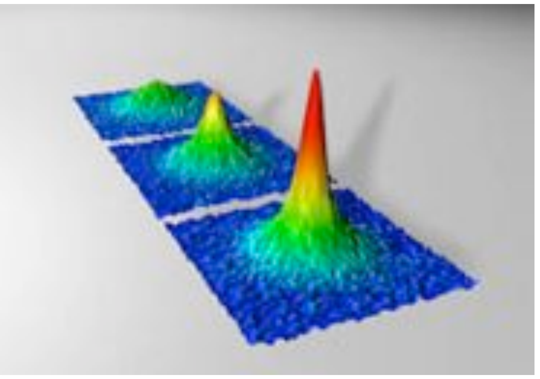
1. What is a dynamical mean-field theory?

2. What do we have using DMFT?

Ultracold Fermi Atomic Gases

Fermion atoms are cooled down in magneto-optical traps.

^{6}Li ^{40}K ... to 10-100 nK
to quantum degeneracy



Fermi condensates, JILA

New playground for condensed matter physics!

1. Spins <= hyperfine states

   RF pulse to control populations

   population-imbalance
   (analog of magnetic field)

2. Interactions <= atom-atom scattering

   Feshbach resonance to control attractive/repulsive

   Cooper pairs

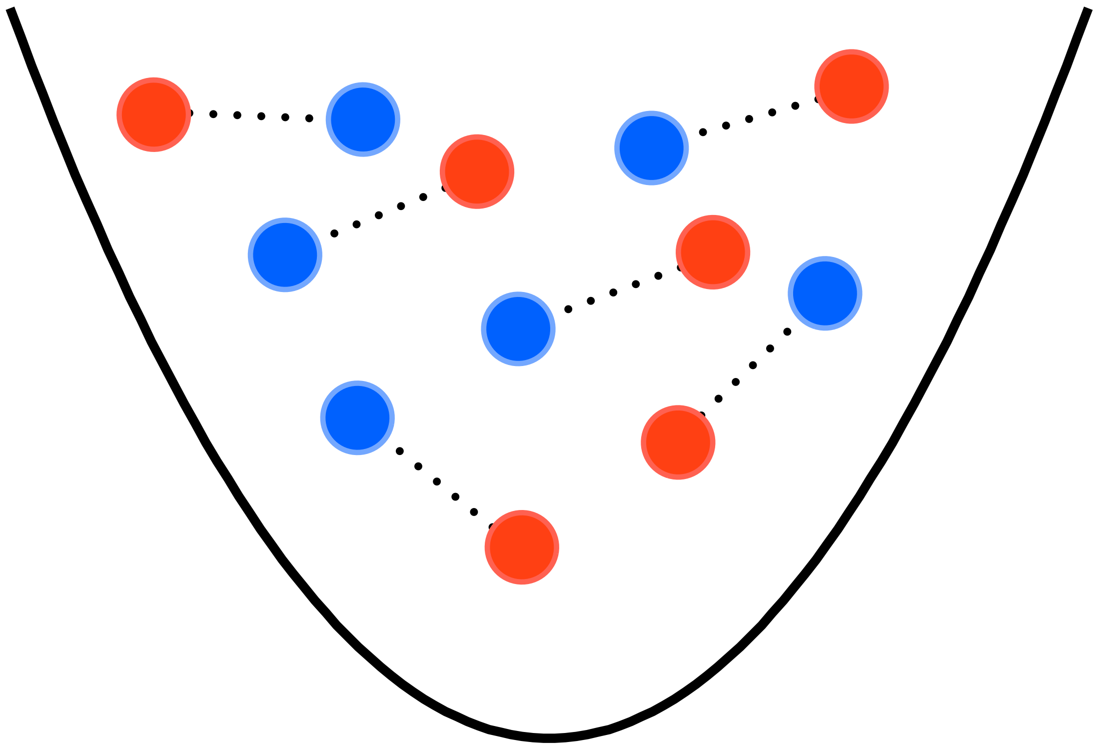
3. Loaded on Optical Lattices

   Laser directions/intensity to control dimensions, hopping ...

   Hubbard Hamiltonian

"New Quantum Simulator" -- Science 320, 312 (2008).

Harmonic trapping potential



$$V(\mathbf{r}) = \frac{1}{2}(w_x^2 x^2 + w_y^2 y^2 + w_z^2 z^2)$$

essential to ultracold atomic gases!

≠ conventional solid states

1. Local density approximation (LDA)

   locally homogeneous system with $\mu'_\sigma(r) = \mu_\sigma - V(r)$

2. Explicit consideration from the beginning

Fermi gases with population imbalance

$$N_\uparrow \neq N_\downarrow$$

$$\mu_\uparrow \neq \mu_\downarrow$$

1. Magnetism versus Superconductivity

Chandrasekhar-Clogston limit

Chandrasekhar, APL **1**, 7 (1962).

Clogston, PRL **9**, 266 (1962).

critical magnetic field to break superconductivity

Naive argument: $\delta\mu_c \sim \Delta/\sqrt{2}$ (BCS)

No CC limit (BEC)

Very hard to be tested in conventional solid state systems.

2. Exotic superconducting phase?

Fulde-Ferrell-Larkin-Ovchinnikov state

FF, PR 135, A550 (1964)

LO, JETP 20, 762 (1965)

Oscillating order parameter

$$\Delta \equiv \Delta_0 \exp(iqx) \quad \text{(FF)}$$

$$\Delta \equiv \Delta_0 \cos(qx) \quad \text{(LO)}$$

Experiments with ^6Li at unitarity

	MIT[1]	RICE[2]	LKB[3]
Trap Aspect Ratio $\alpha = w_{xy} / w_z$	5.65	45.1	14.5 - 22.6
Number of atoms	10^7	10^4 - 10^5	10^5
T/T_F	≤ 0.06	≤ 0.05	≤ 0.09
P_c	**0.77**	**> 0.9**	**0.76**

[1]Shin et. al., PRL **97**, 030401 (2006)

[2]Partridge et. al., Science **311**, 5760 (2006)

[2]Partridge et. al., PRL **97**, 190407 (2006)

[3]Nascimbene et. al., PRL **103**, 170402 (2009)

[4]Lobo et. al., PRL **97**, 200403 (2006)

Local Density Approximation (LDA)

$$\mu'_\sigma(r) = \mu_\sigma - V(r)$$

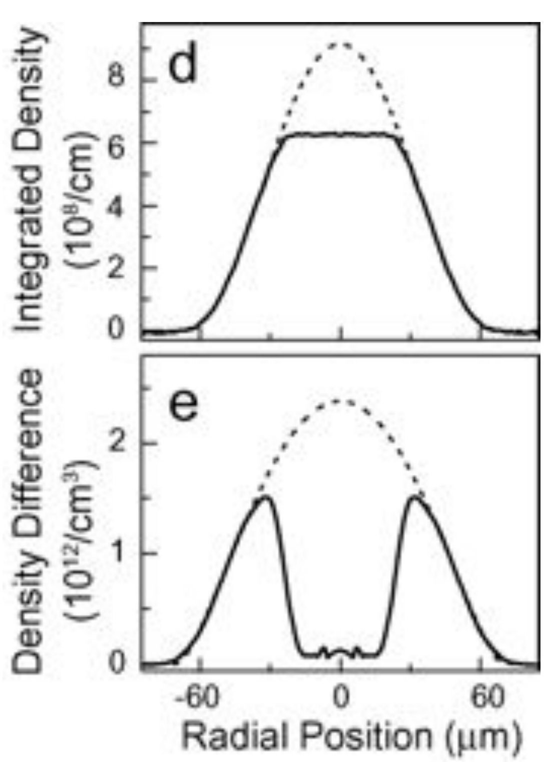
$$P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$

QMC+LDA[4]

P_c=0.77

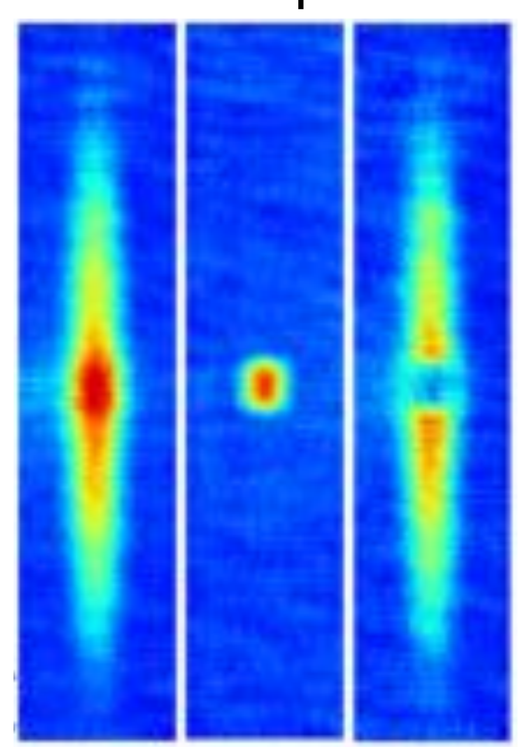
MIT (P=0.58)

"flat top" agrees with LDA (SF+N+FP)



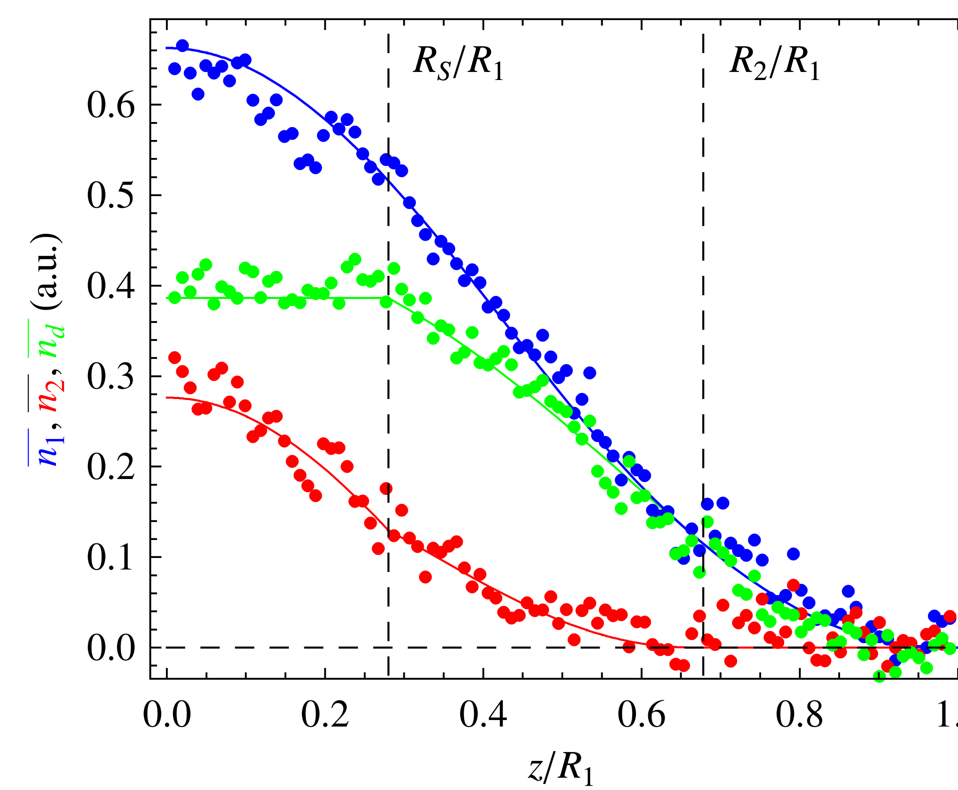
RICE (P=0.79)

Phase Separation



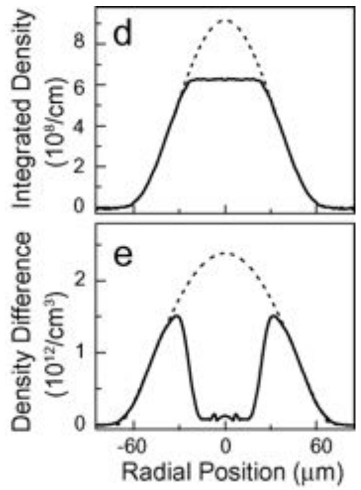
LKB (P=0.54)

SF + N + FP

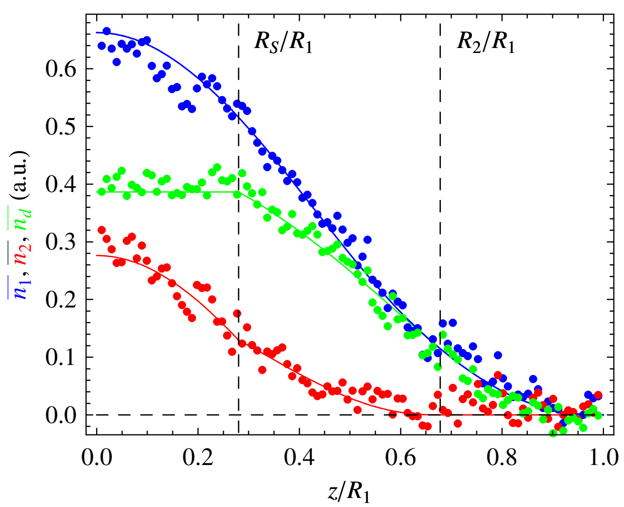


Our DMFT approach beyond LDA

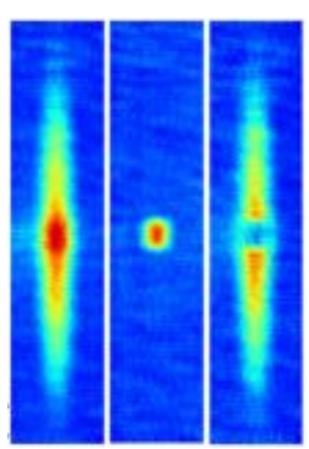
MIT $\alpha = 5.65$



LKB $\alpha = 22.6$



RICE $\alpha = 45.1$



agrees with LDA

LDA breaks down

What would happen in optical lattices?

We want to go beyond just mean-field theory.

We want to see things in strongly interacting regime.

We want to go beyond local density approximation.

Local Density Approximation (LDA)

$$\mu'_\sigma(r) = \mu_\sigma - V(r)$$

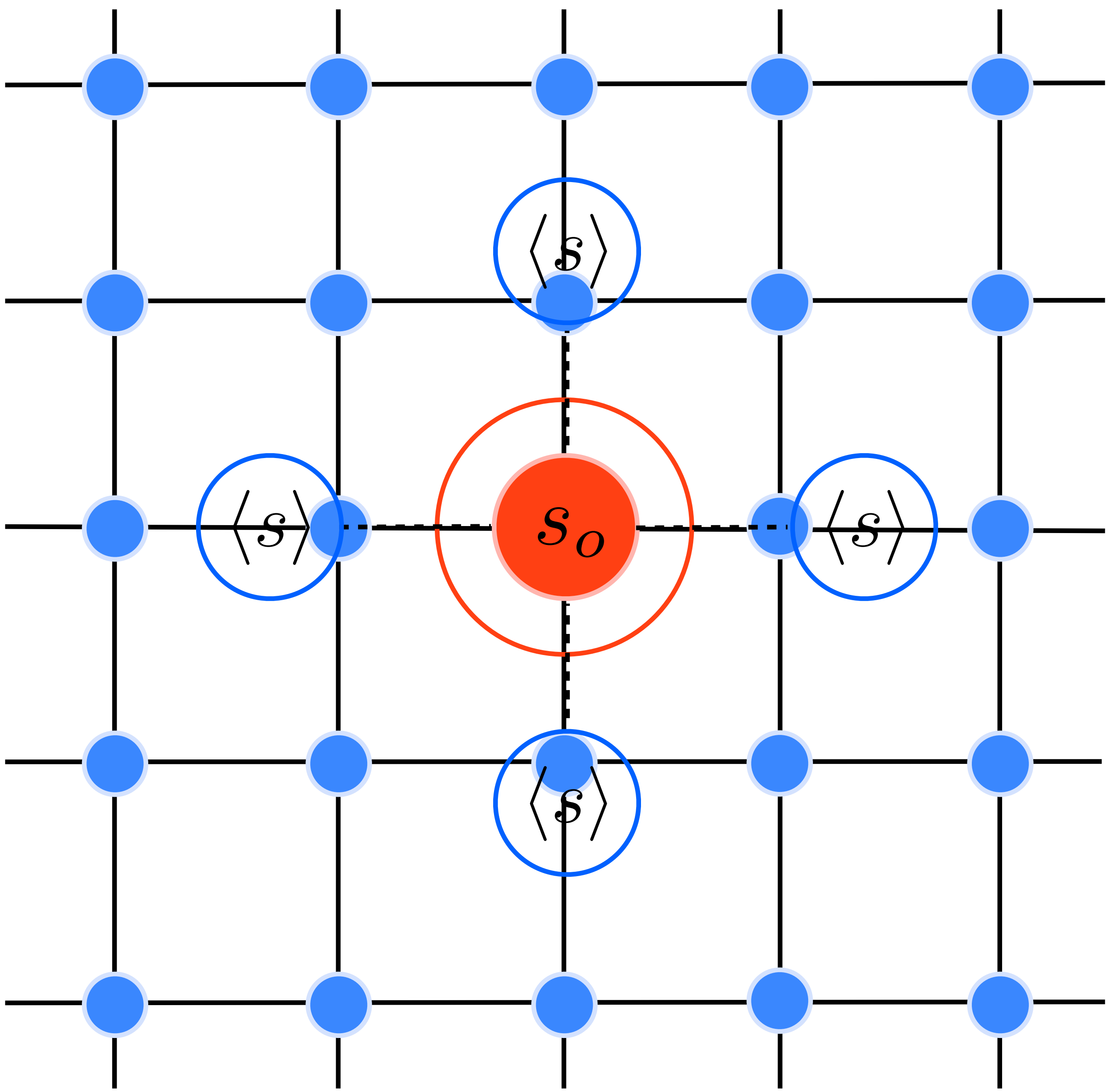
We need to deal with anisotropic traps explicitly.

Dynamical mean-field theory

Dynamical mean field theory: the basic idea

Quantum analog of Weiss Mean Field Theory

Ising model



$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j + h \sum_i s_i$$

$$\mathcal{H}_{\text{eff}} \equiv h_{\text{eff}} s_o = (zJ\langle s \rangle + h) s_o$$

$$E_{\text{eff}} = \pm(zJ\langle s \rangle + h)$$

$$\langle s \rangle = \tanh(\beta z J \langle s \rangle + \beta h)$$

self-consistency condition

Dynamical mean field theory: the basic idea

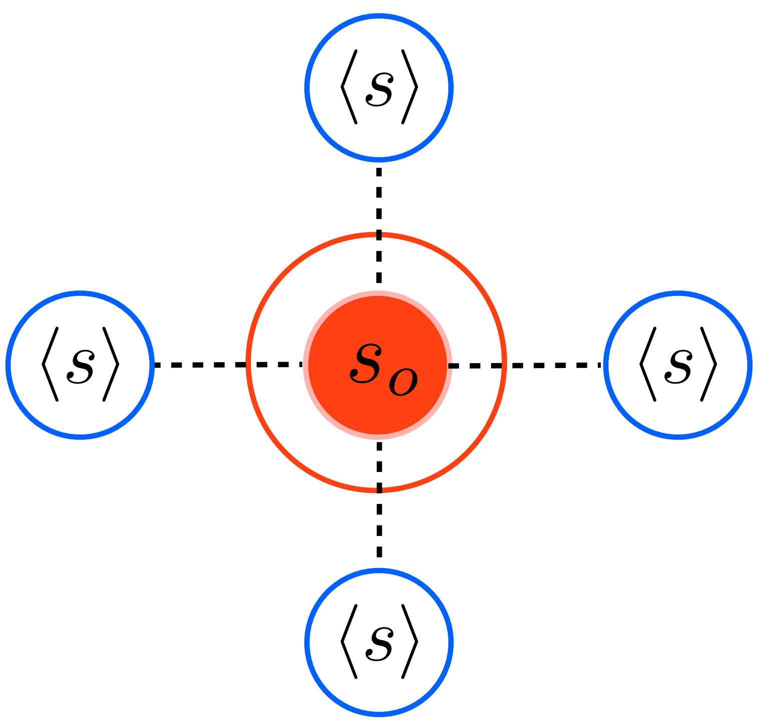
Review: RMP **68**, 13 (1996).

Quantum analog of Weiss Mean Field Theory

Ising model

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j + h \sum_i s_i$$

$$\mathcal{H}_{\text{eff}} \equiv h_{\text{eff}} s_o = (zJ\langle s \rangle + h) s_o$$



$$\langle s \rangle = \tanh(\beta z J \langle s \rangle + \beta h)$$

self-consistency condition

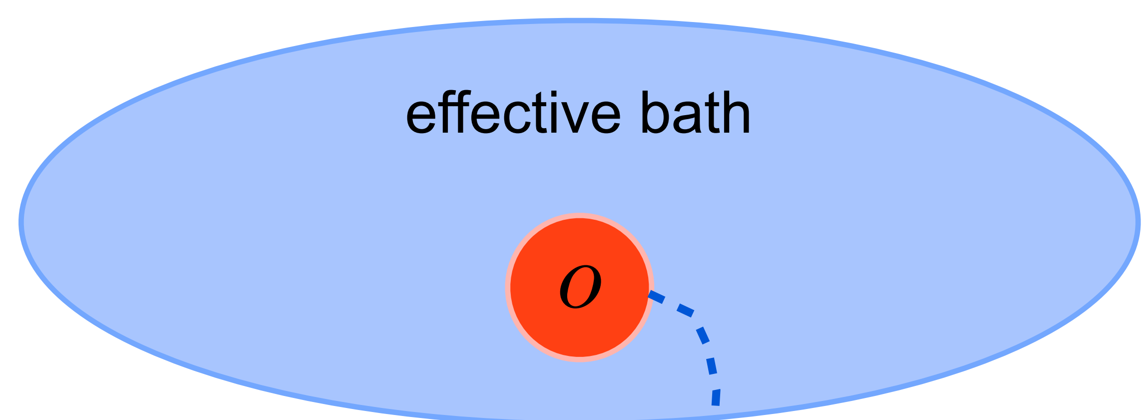
Hubbard model

$$\mathcal{H} = -\sum_{\langle ij \rangle \sigma} t_{ij} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$\mathcal{S}_{\text{eff}} = -\int_0^\beta \mathrm{d}\tau \int_0^\beta \mathrm{d}\tau' \sum_\sigma c^\dagger_{o\sigma}(\tau) \mathscr{G}_0^{-1}(\tau - \tau') c_{o\sigma}(\tau') + U \int_0^\beta \mathrm{d}\tau \, n_{o\uparrow}(\tau) n_{o\downarrow}(\tau)$$

Weiss MF

-> Anderson impurity model



$$\mathscr{G}_0(i\omega_n)^{-1} = i\omega_n + \mu + G(i\omega_n)^{-1} - R[G(i\omega_n)]$$

Dynamical mean field theory: the basic idea

Quantum analog of Weiss Mean Field Theory

But, there are similarities and differences.

(Unfortunate) Similarities

Basic idea: It neglects (some) fluctuations.

Limitation: It is exact only in the infinite dimension.

Differences

The impurity model is still a nontrivial quantum problem.

DMFT still has full local quantum fluctuations.

→ where "dynamic" in DMFT comes from.

DMFT in practice

It works as an approximation in D<∞.

homogeneous lattice system

No k-dependence in SELF ENERGY!

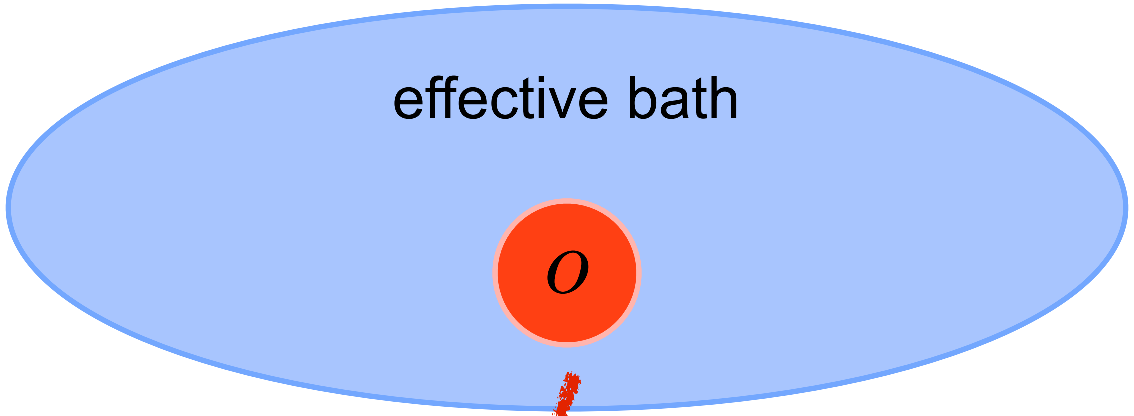
$$G(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma(\not{\mathbf{k}}, i\omega_n)}$$

non-interacting

local

$$G(i\omega_n) = \sum_{\mathbf{k}} G(\mathbf{k}, i\omega_n)$$

Solve an impurity problem !



$\mathcal{S}_{\text{eff}}$

Dyson equation

$$\Sigma(i\omega_n) = \mathscr{G}_0^{-1}(i\omega_n) - G^{-1}(i\omega_n)$$

Weiss mean-field

Quantum Monte Carlo

Numerical Renormalization Group

Exact Diagonalization

...

Our problem setup with DMFT

Broken symmetry phase:
anomalous Green's function

Spin-dependent formulation

Superfluidity of polarized Fermi gases in optical lattices

with harmonic trapping potentials.

Go beyond LDA: "Real-space" DMFT

Self-energy is local but site-dependent.

Real-space DMFT for polarized superfluid phase

Attractive Hubbard Model with trapping potentials

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} c^\dagger_{i\sigma} c_{j\sigma} - \sum_{i\sigma} [\mu_\sigma - V(\mathbf{r}_i)] \, n_i + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Nambu formalism $\Psi^\dagger \equiv (c^\dagger_\uparrow, c_\downarrow)$

Lattice Green's Function

$$G \to \tilde{G} = \begin{pmatrix} G_\uparrow & F \\ F & G_\downarrow \end{pmatrix} \qquad \mathscr{G}_0 \to \tilde{\mathscr{G}}_0 \qquad \Sigma \to \tilde{\Sigma}$$

$$\tilde{G}^{-1}_{ij}(i\omega_n) = i\omega_n \mathbf{I} + \begin{pmatrix} \mu_\uparrow - V(\mathbf{r}_i) & 0 \\ 0 & -\mu_\downarrow + V(\mathbf{r}_i) \end{pmatrix} \delta_{ij} - \begin{pmatrix} -t_{ij} & 0 \\ 0 & t_{ij} \end{pmatrix} - \tilde{\Sigma}_i(i\omega_n)\delta_{ij}$$

site-dependent self-energy : approx.

Dyson Equation (local)

Weiss mean-field:
(matrix propagator)

$$\widetilde{\mathscr{G}}_0^{-1} = [\widetilde{G}_{ii}]^{-1} - \widetilde{\Sigma}_i$$

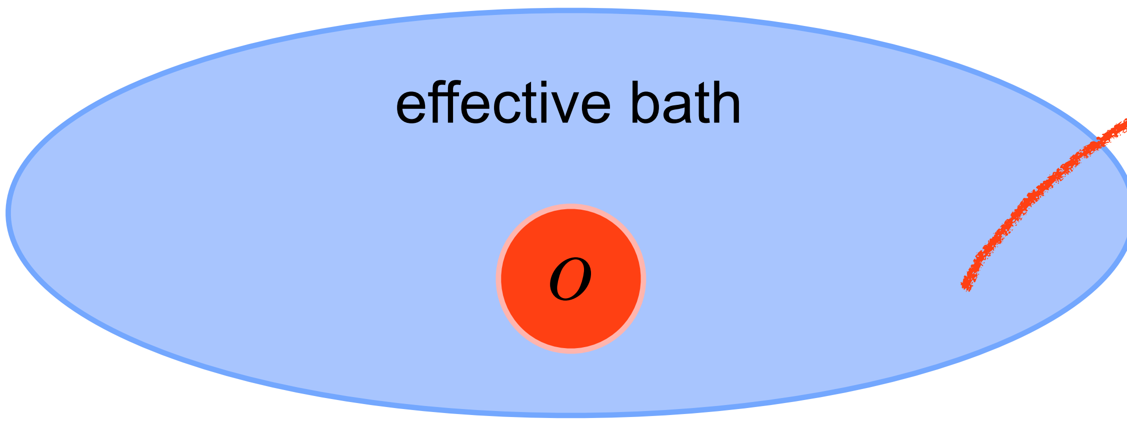
Real-space DMFT for polarized superfluid phase

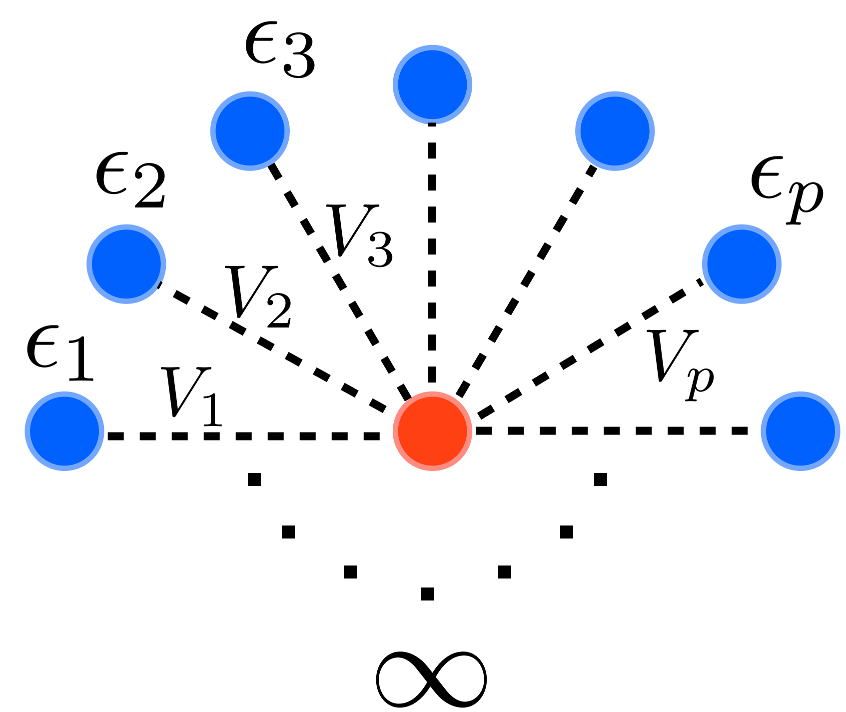
Converting into the impurity problem

matrix propagator

$$\mathcal{S}_{\text{eff}} = -\int_0^\beta d\tau \int_0^\beta d\tau' \Psi^\dagger(\tau) \widetilde{\mathscr{G}}_0^{-1}(\tau - \tau') \Psi(\tau') + U \int_0^\beta d\tau n_\uparrow(\tau) n_\downarrow(\tau)$$

superconducting bath





Generalized Anderson Impurity Model

$$\mathcal{H}_{\text{AIM}} = \sum_{p\sigma} \epsilon_{p\sigma} c_{p\sigma}^\dagger c_{p\sigma} + \sum_{p\sigma} V_{p\sigma} (d_\sigma^\dagger c_{p\sigma} + h.c.)$$

$$+ \sum_p \Delta_p (c_{p\uparrow}^\dagger c_{p\downarrow}^\dagger + h.c.)$$

$$- \sum_\sigma [\mu_\sigma - V_{trap}(\vec{r})] n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}$$

Flow chart

0. Initial guess for self-energy

1. Lattice Green's Function : matrix inversion [1]

$$\tilde{G}_{ij}^{-1}(i\omega_n) = i\omega_n \mathbf{I} + \begin{pmatrix} \mu_\uparrow - V(\mathbf{r}_i) & 0 \\ 0 & -\mu_\downarrow + V(\mathbf{r}_i) \end{pmatrix} \delta_{ij} - \begin{pmatrix} -t_{ij} & 0 \\ 0 & t_{ij} \end{pmatrix} - \tilde{\Sigma}_i(i\omega_n)\delta_{ij}$$

2. Weiss Mean-Field (local Dyson eq.)

$$\widetilde{\mathscr{G}}_0^{-1} = [\widetilde{G}_{ii}]^{-1} - \widetilde{\Sigma}_i$$

: looks trivial

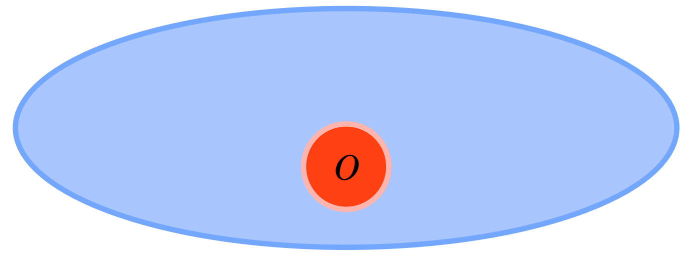
3. Solve the impurity problem

: but how to parametrize?
, and how to solve it? [2]

$$\mathcal{H}_{\mathrm{AIM}} = \sum_{p\sigma} \epsilon_{p\sigma} c_{p\sigma}^\dagger c_{p\sigma} + \sum_{p\sigma} V_{p\sigma}(d_\sigma^\dagger c_{p\sigma} + h.c.) + \sum_p \Delta_p (c_{p\uparrow}^\dagger c_{p\downarrow}^\dagger + h.c.) - \sum_\sigma [\mu_\sigma - V_{trap}(\vec{r})] n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}$$

4. Iterate [3] $\tilde{\Sigma}_{ii}$

Impurity problem



$\mathscr{G}_0(iw)$ $\longrightarrow$

$$\mathcal{H}_{\text{AIM}} = \sum_{p\sigma} \epsilon_{p\sigma} c^\dagger_{p\sigma} c_{p\sigma} + \sum_{p\sigma} V_{p\sigma}(d^\dagger_\sigma c_{p\sigma} + h.c.) + \sum_{p} \Delta_p (c^\dagger_{p\uparrow} c^\dagger_{p\downarrow} + h.c.) - \sum_{\sigma} [\mu_\sigma - V_{trap}(\vec{r})] n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}$$

depends on the method details.

Choose a tool to solve it with first.

Quantum Monte Carlo — sampling a real-time Green's function directly.

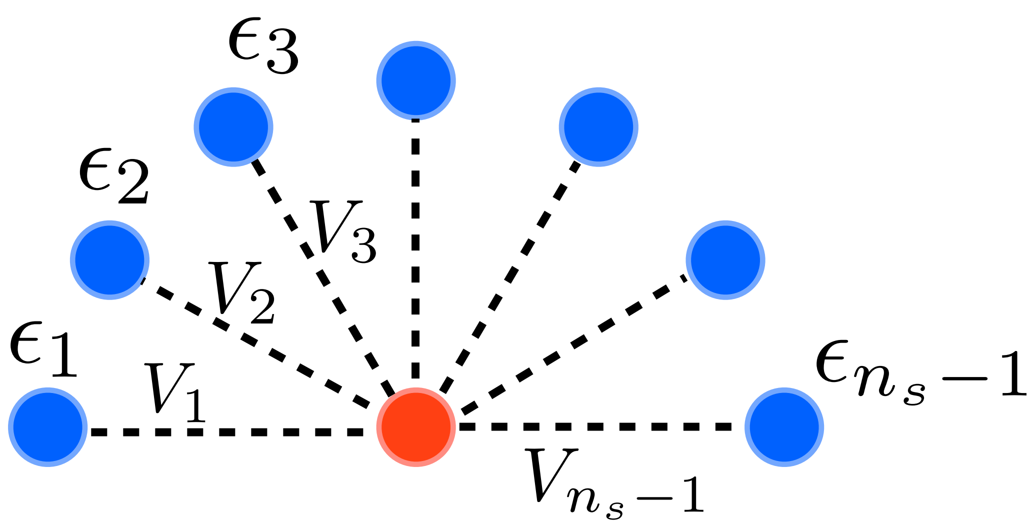
Numerical Renormalization Group — logarithmic discretization of spectrum

Exact Diagonalization — considering a finite number of bath orbitals: p=1, … ,n_s

etc,.

But, all has pros and cons.

Exact Diagonalization : parametrization



$$\mathcal{H}_{\text{AIM}}^{(n_s)} = \sum_{p=1,\sigma}^{n_s-1} \epsilon_{p\sigma} c_{p\sigma}^\dagger c_{p\sigma} + \sum_{p=1,\sigma}^{n_s-1} V_{p\sigma}(d_\sigma^\dagger c_{p\sigma} + h.c.)$$
$$+ \sum_{p=1}^{n_s-1} \Delta_p (c_{p\uparrow}^\dagger c_{p\downarrow}^\dagger + h.c.)$$
$$- \sum_\sigma [\mu_\sigma - V_{trap}(\vec{r})] n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}$$

Weiss mean-field from G_{latt}

$\{\epsilon, V, \Delta\}$: $5(n_s-1)$ variables

$$\widetilde{\mathscr{G}}_0(iw_n) \longrightarrow \widetilde{\mathscr{G}}_{0,n_s}(iw_n)$$

Minimize

$$\sum_n |\widetilde{\mathscr{G}}_0^{-1}(iw_n) - \widetilde{\mathscr{G}}_{0,n_s}^{-1}(iw_n)|^2$$

Main source of an error.

multidimensional minimization: BFGS or CG.
- uncontrollable, depends on many factors.

initial starting point
input Weiss mean-field
range of matsubara frequencies and spacing

Flow-chart: DMFT+ED

$$\tilde{G}_{ij}^{-1}(i\omega_n) = i\omega_n \mathbf{I} + \begin{pmatrix} \mu_\uparrow - V(\mathbf{r}_i) & 0 \\ 0 & -\mu_\downarrow + V(\mathbf{r}_i) \end{pmatrix} \delta_{ij} - \begin{pmatrix} -t_{ij} & 0 \\ 0 & t_{ij} \end{pmatrix} - \tilde{\Sigma}_i(i\omega_n)\delta_{ij}$$

3.

Initial guess: $\{\epsilon, V, \Delta\}$

$$\tilde{\Sigma}_{ii}$$

1.

$$\mathcal{H}_{\mathrm{AIM}}^{(n_s)} = \sum_{p=1,\sigma}^{n_s-1} \epsilon_{p\sigma} c_{p\sigma}^\dagger c_{p\sigma} + \sum_{p=1,\sigma}^{n_s-1} V_{p\sigma}(d_\sigma^\dagger c_{p\sigma} + h.c.) + \sum_{p=1}^{n_s-1} \Delta_p (c_{p\uparrow}^\dagger c_{p\downarrow}^\dagger + h.c.) - \sum_\sigma [\mu_\sigma - V_{trap}(\vec{r})] n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}$$

$$\widetilde{\mathscr{G}}_0(iw_n)$$

2.

Exact Diagonalization

4.

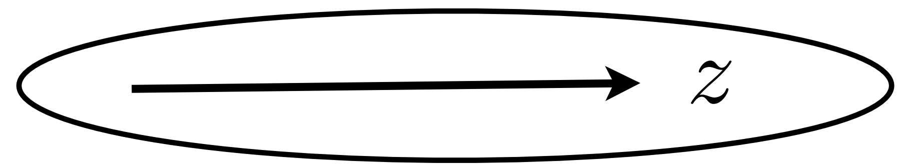
$$\widetilde{\mathscr{G}}_{0,n_s}(iw_n)$$

Minimize $\sum_n |\widetilde{\mathscr{G}}_0^{-1}(iw_n) - \widetilde{\mathscr{G}}_{0,n_s}^{-1}(iw_n)|^2$

System setup

Trapping potential $V_{trap}(x,y,z) = \frac{1}{2} w_0^2 (x^2 + y^2 + \alpha^{-2} z^2)$

Trap aspect ratio: $\alpha = \frac{w_0}{w_z}$



We have $\alpha = 1.0, 2.5, 5.0, 7.5, 10.0$

Interaction

$U = -7.91576$ (unitarity)

# of matsubara frequencies = 1000

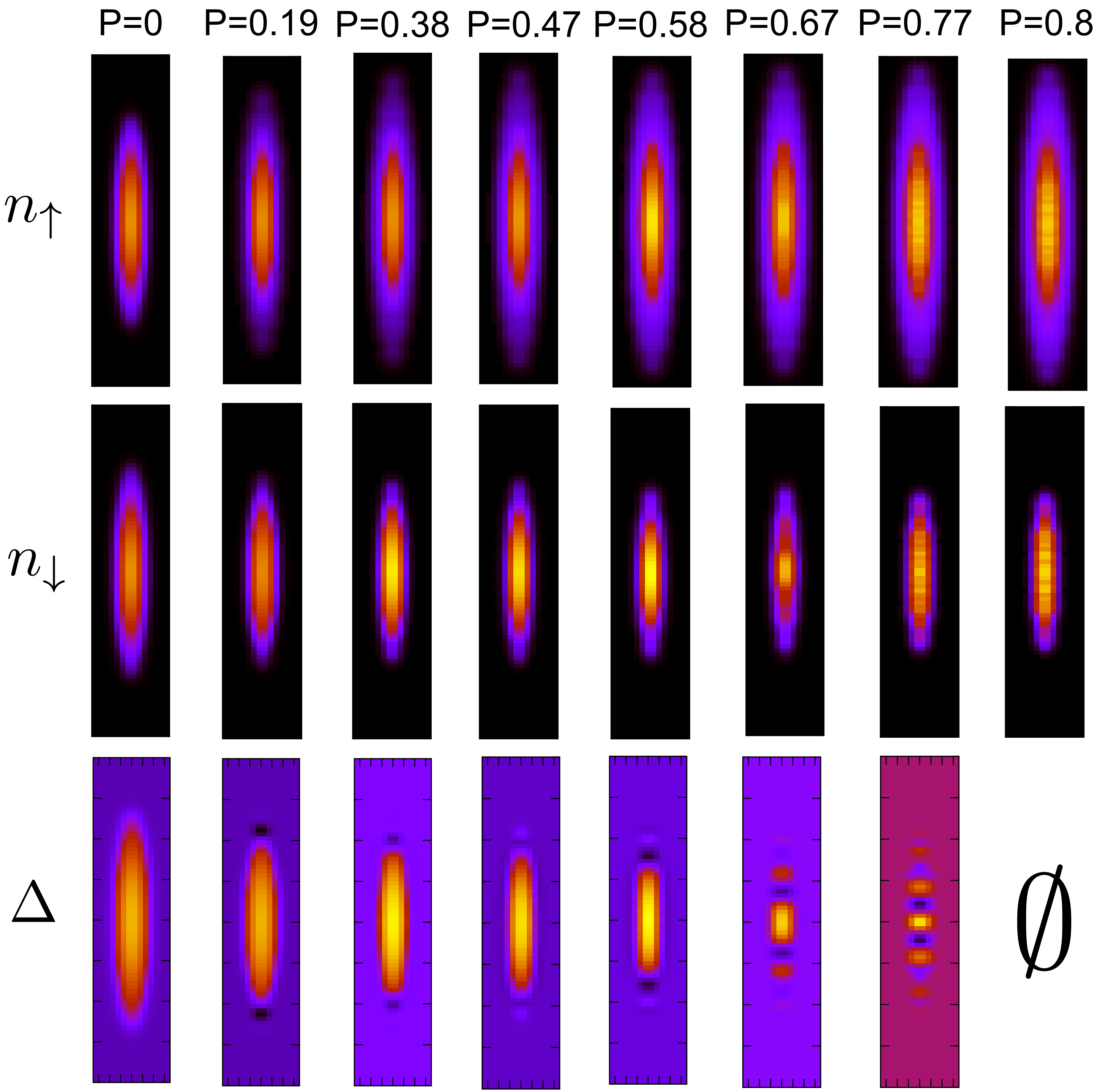
System size:

α=1.0	α=2.5	α=5.0	α=7.5	α=10.0
24x24x24	16x16x40	14x14x70	14x14x80	14x14x100
364 ineqv.	720	980	1120	1400

Total particle number : 210 (roughly) - chemical potentials are controlled.

# of cpu cores used: 128 (takes ~100 iterations to get converged.)

3-Dimensional optical lattices with traps



14x14x80 Lattices

Aspect ratio:

$$w_{xy}/w_z = 7.5$$

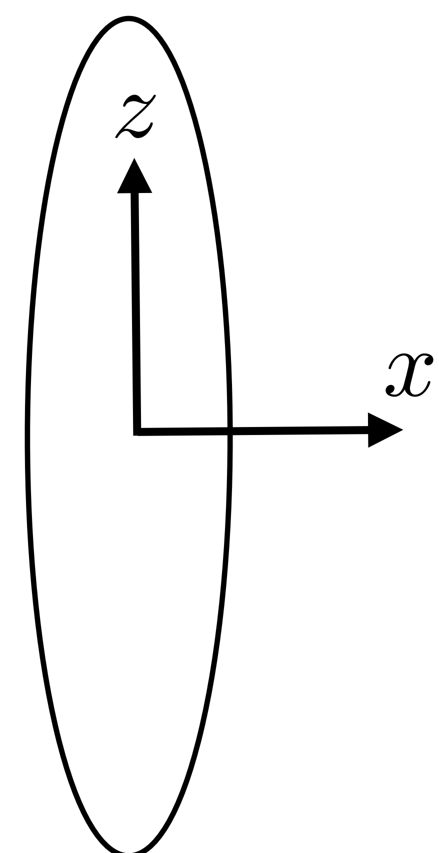
# of atoms:

$$N \sim 210$$

Interaction:

$$U = -7.91576$$

(unitarity)



$$P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$

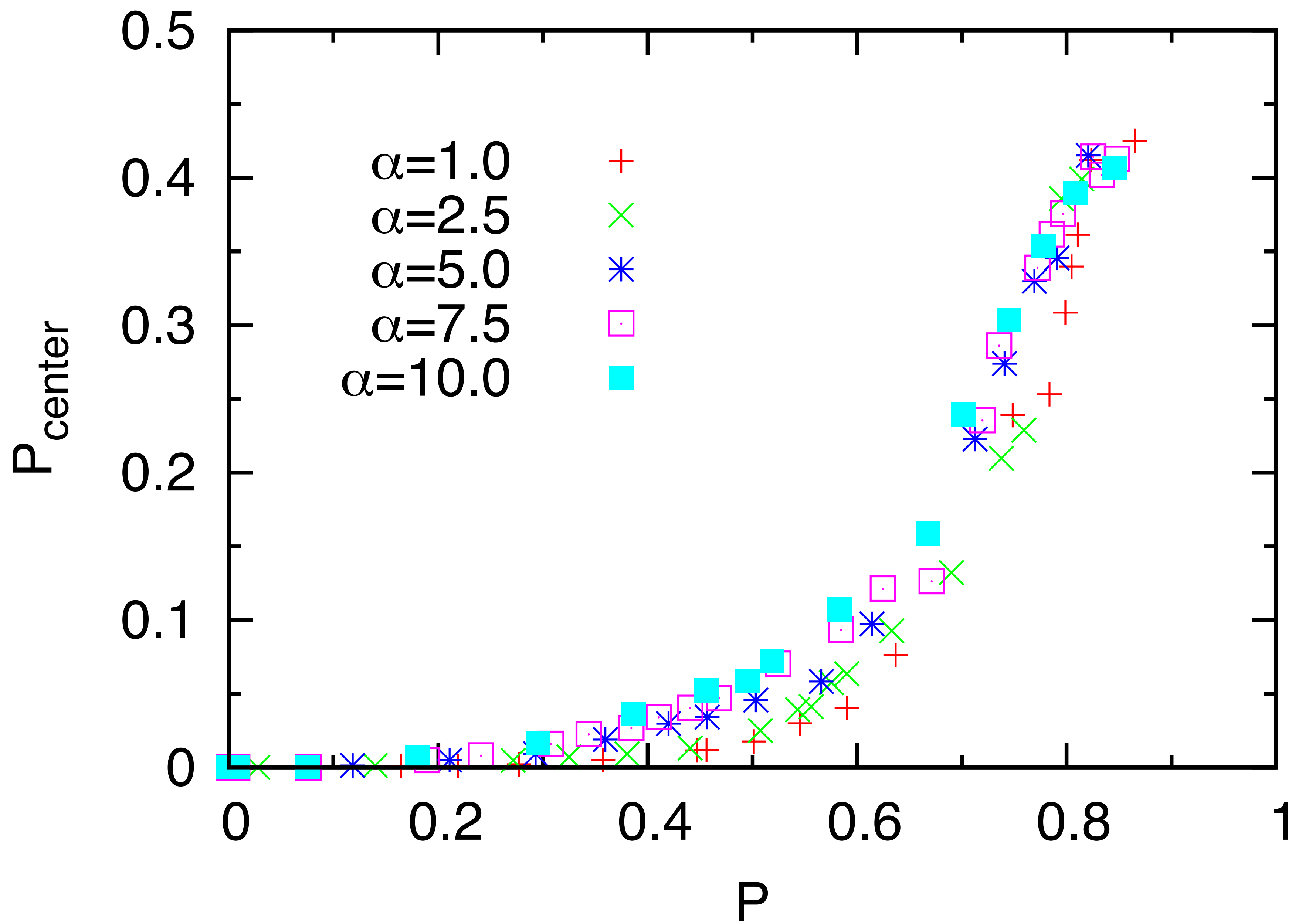
Transition behavior : polarization at center

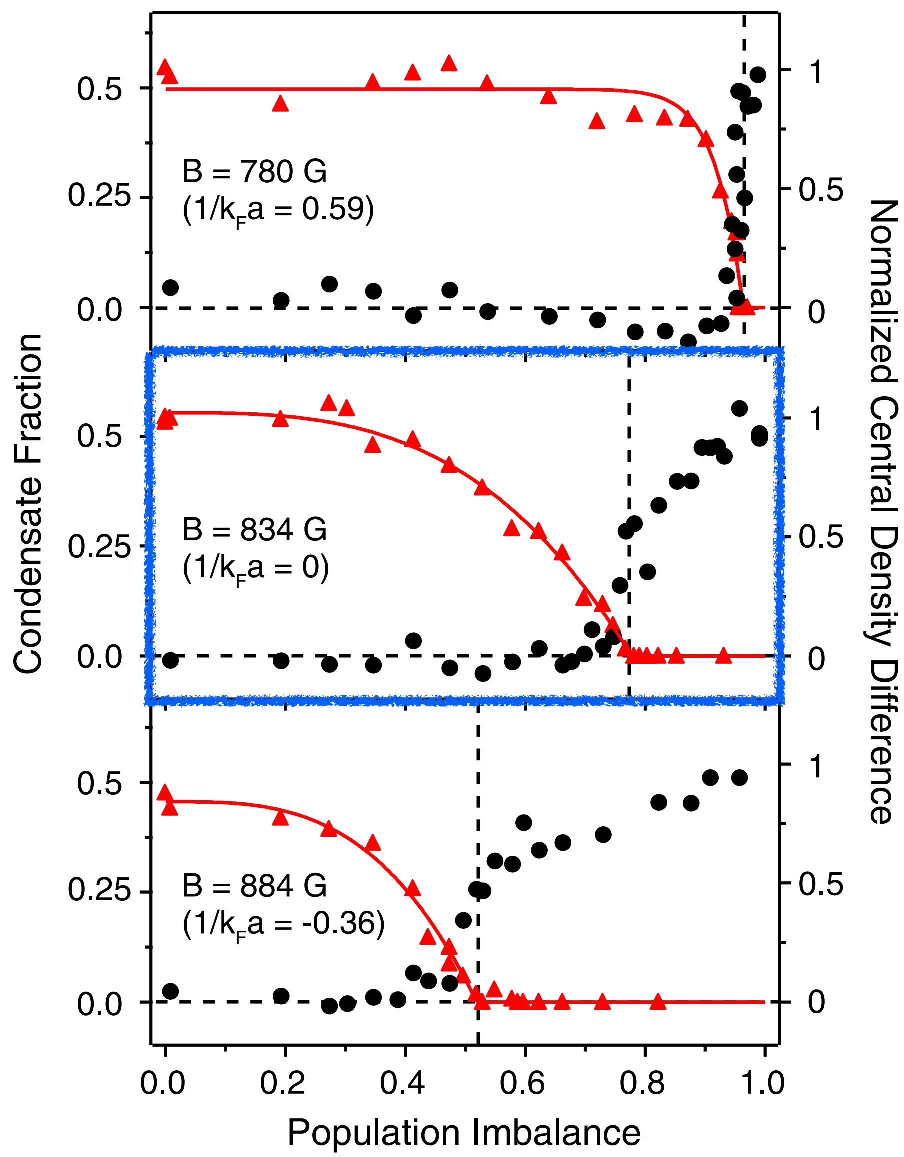
Center polarization increases continuously.
No qualitative difference between different aspect ratios.

$$P_{center} = \frac{n_{\uparrow,center} - n_{\downarrow,center}}{n_{\uparrow,center} + n_{\downarrow,center}}$$

MIT Experiments:
Shin et. al., PRL 97, 030401 (2006)

Our DMFT results

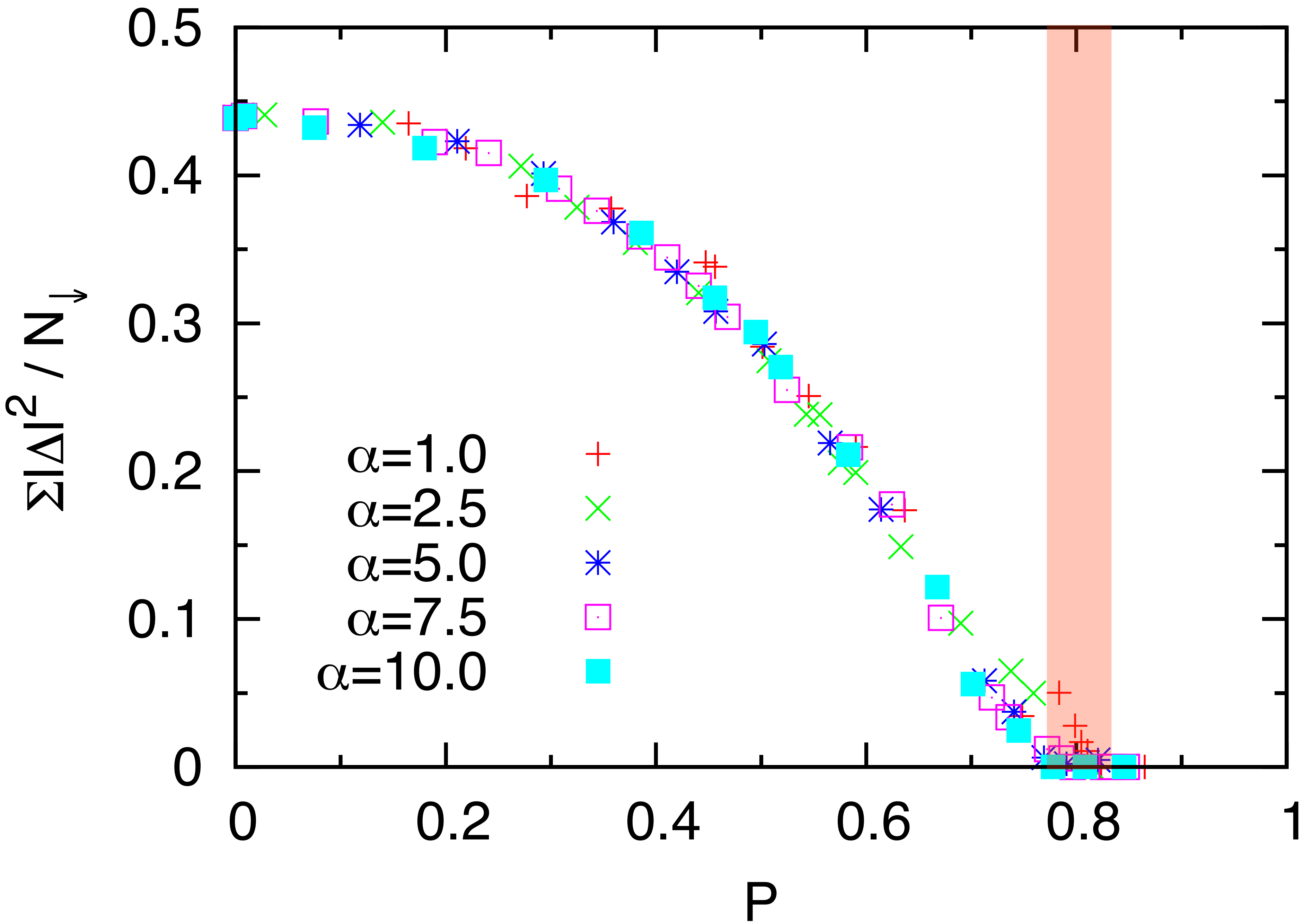




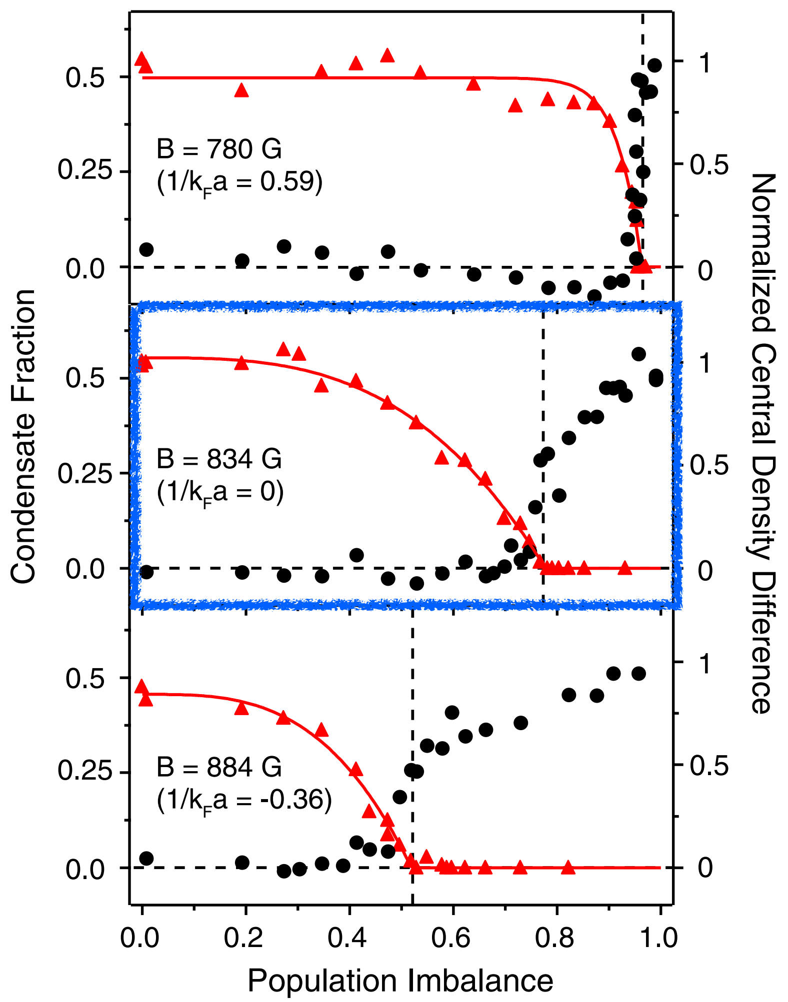
Transition behavior : order parameters

Transition near 0.8!

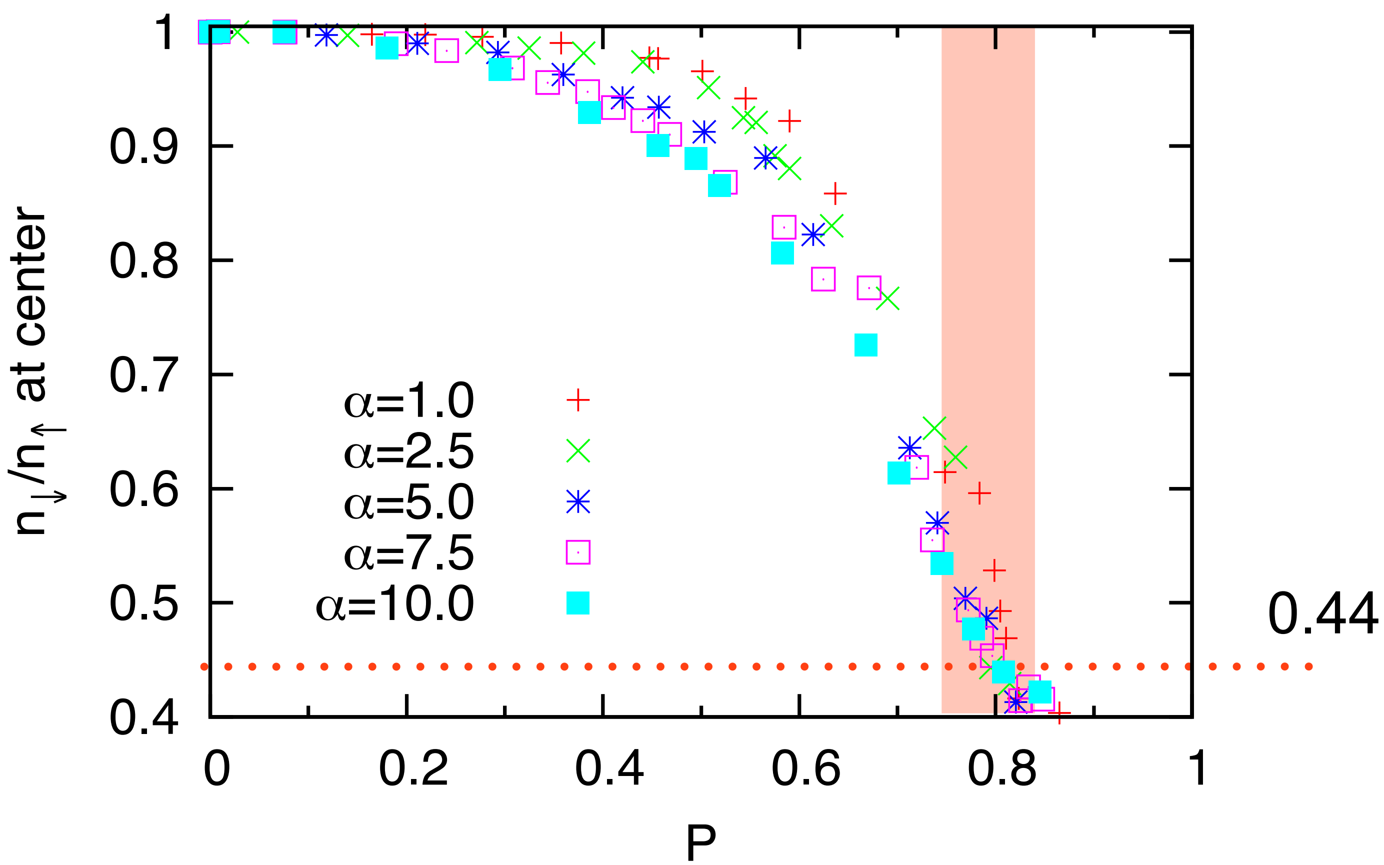
cf. Theory (gas, LDA) : P_C=0.77

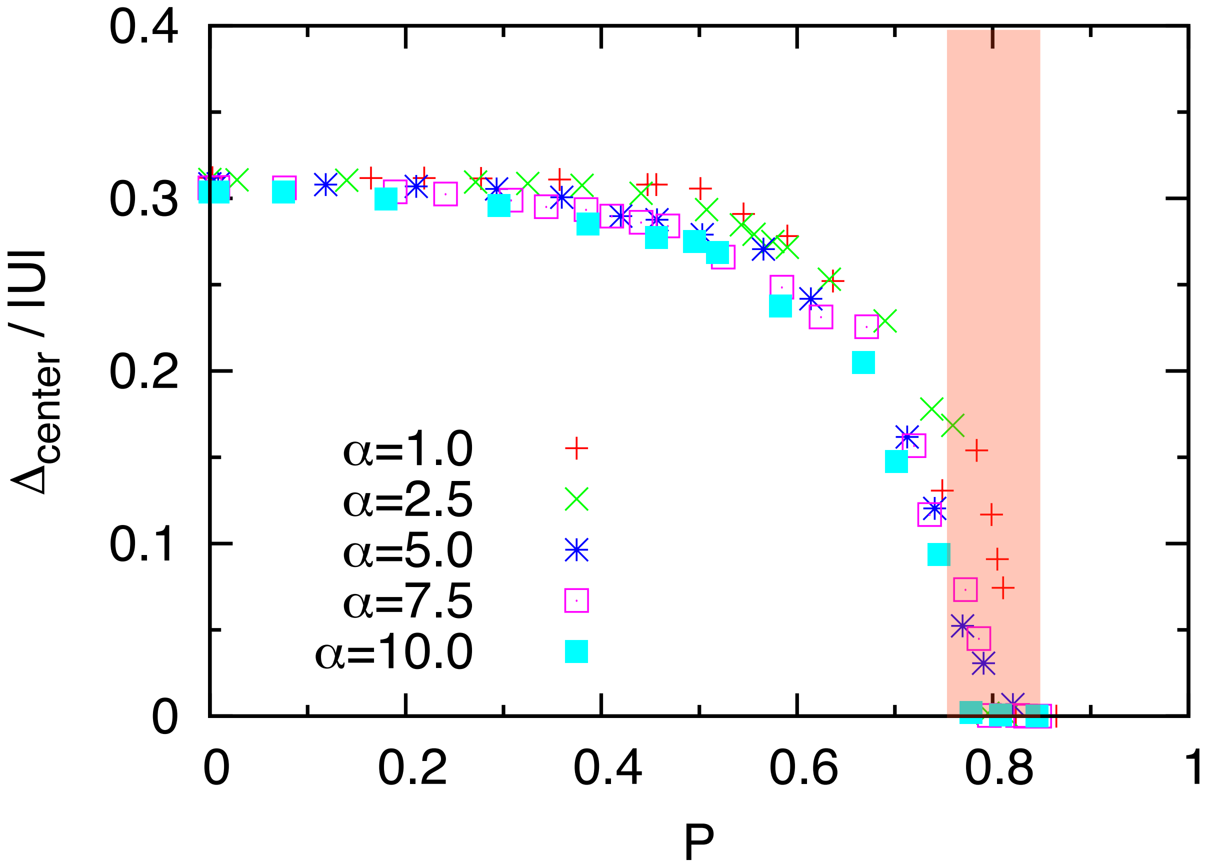


MIT Experiments



Transition : critical density ratio?





Density Ratio:

$$x = \frac{n_\downarrow}{n_\uparrow}$$

QMC with homogenous gases

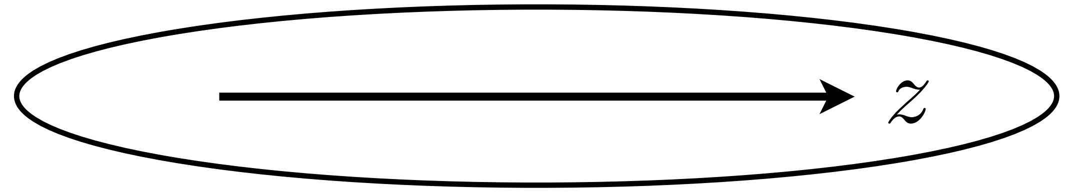
$$x_c = 0.44$$

Lobo, et. al., PRL 97, 200403 (2006).

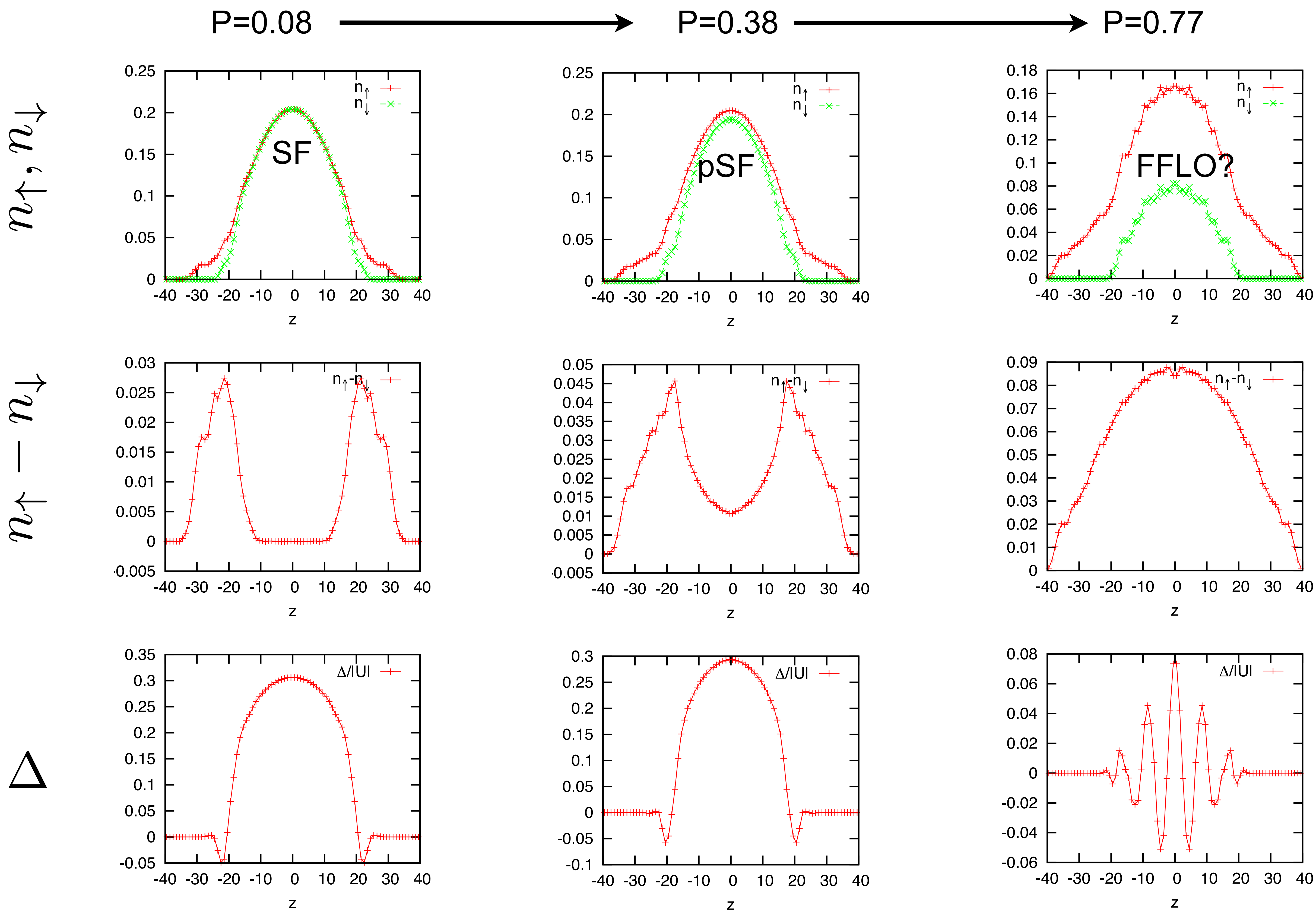
:normal state is unstable above x_c.

Our DMFT: around 0.4 (at trap center)

Axial density profiles



*aspect ratio = 5

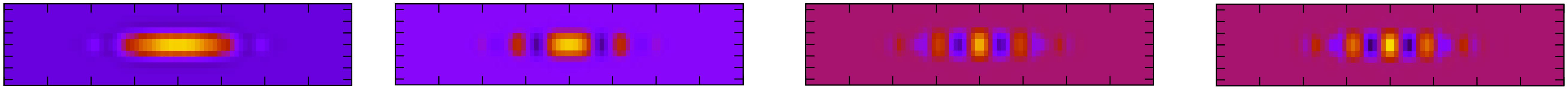


FFLO-like order parameter oscillations vs. polarization

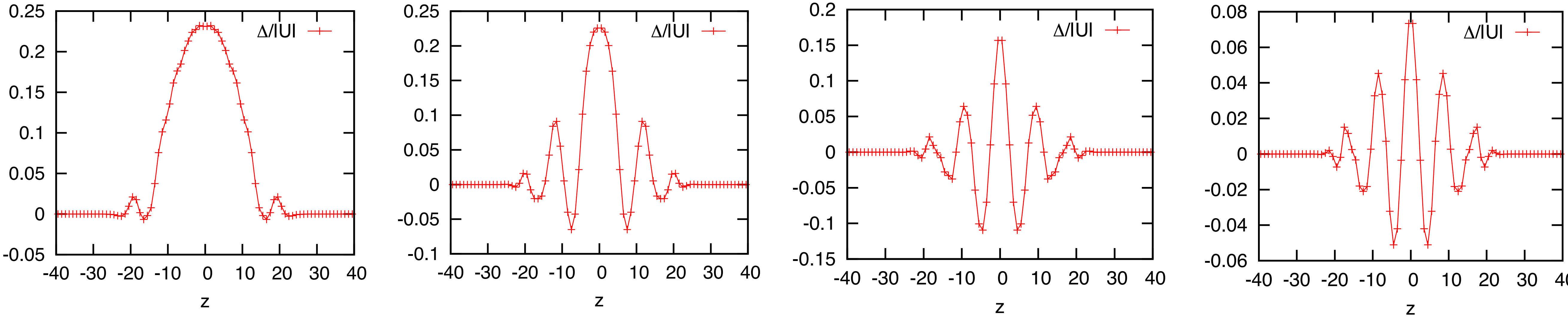
*aspect ratio = 5

P=0.62 P=0.67 P=0.72 P=0.78

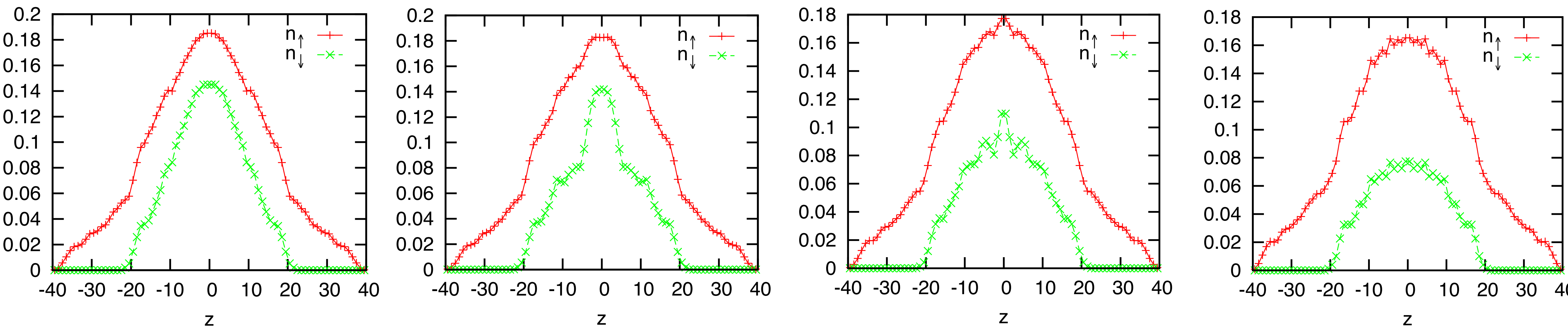
order parameter 2D-cut profiles



order parameter axial profiles



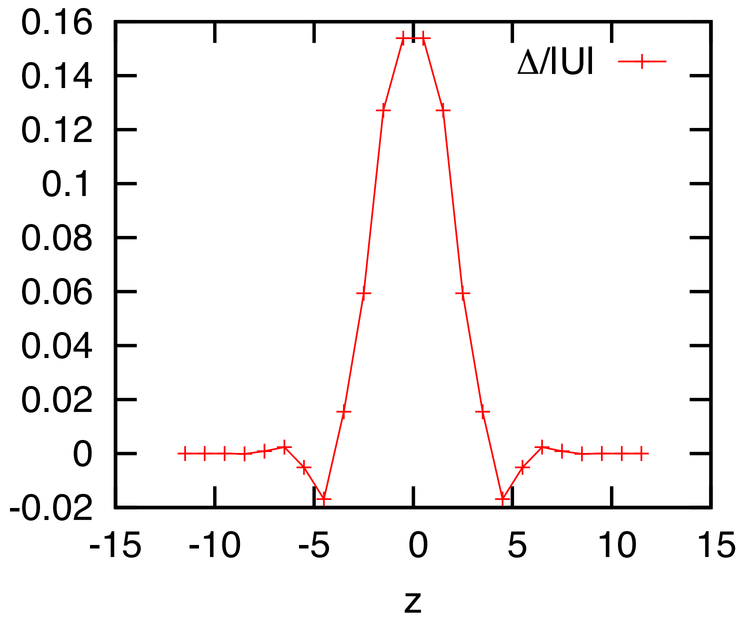
axial density profiles



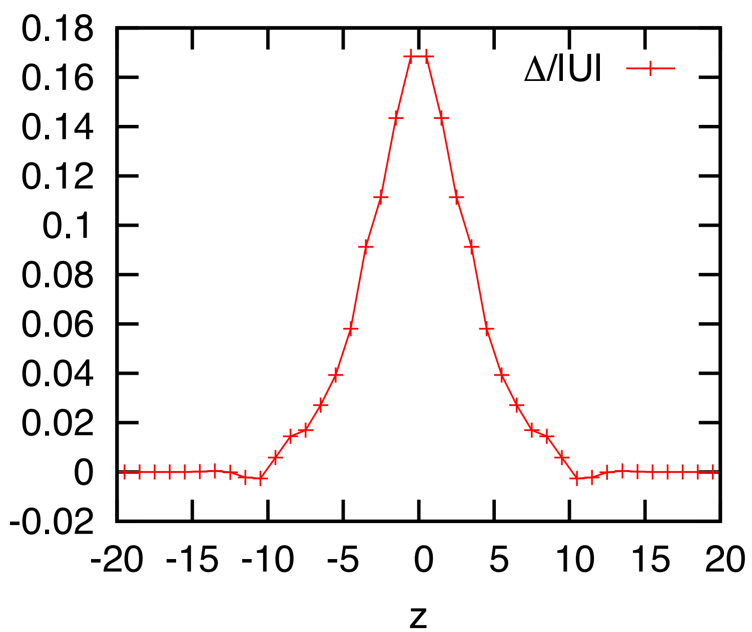
FFLO-like order parameter oscillations vs. trap anisotropy

Heavy oscillations are found only at large aspect ratios.

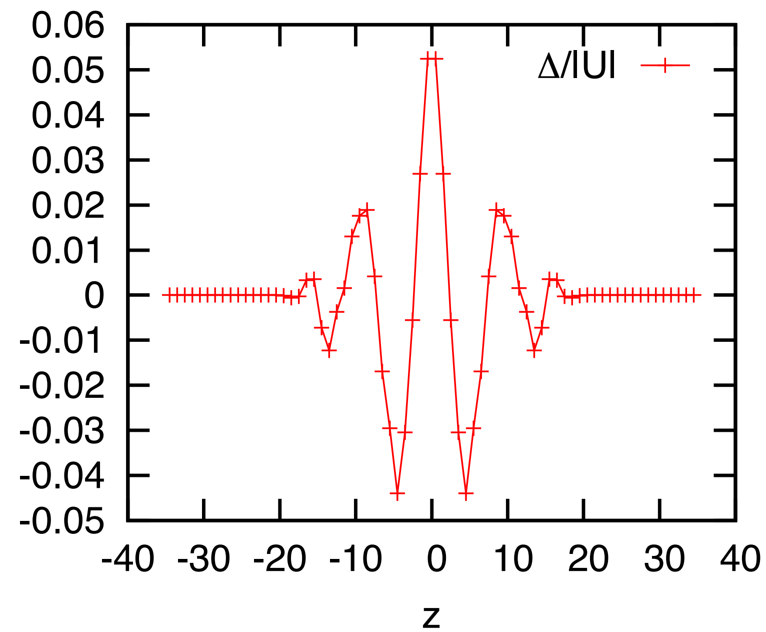
α=1.0, P=0.78



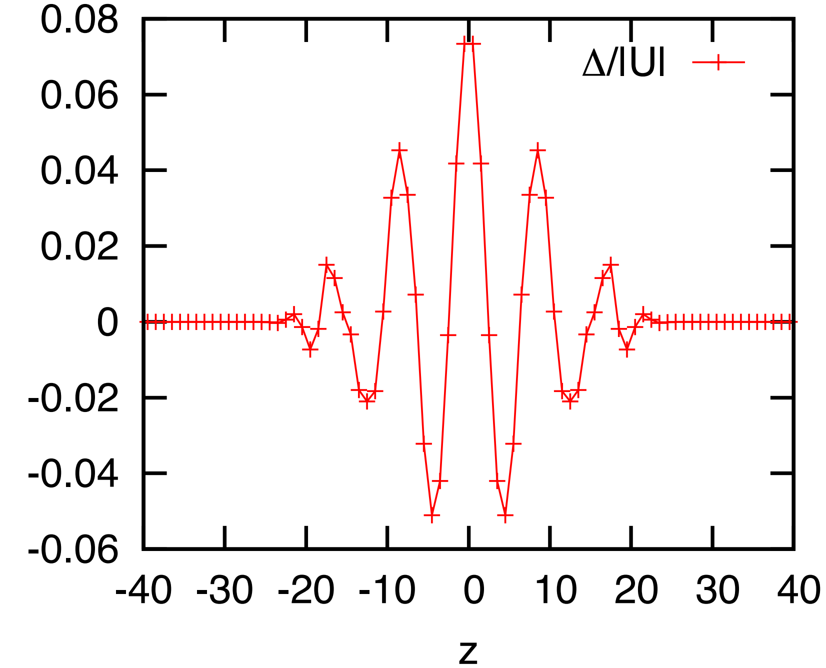
α=2.5, P=0.76



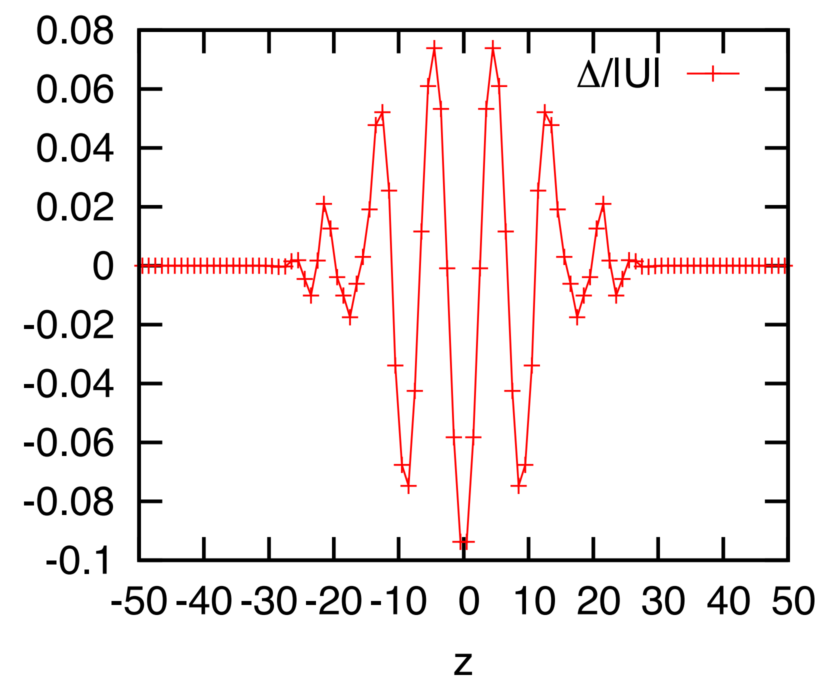
α=5.0, P=0.77



α=7.5, P=0.78



α=10.0, P=0.75



Summary

We have implemented a real-space dynamic mean-field theory with the exact diagonalization technique.

We have studied polarized fermi gases on optical lattices with anisotropic traps using this DMFT+ED.

We have found -

$P_c \sim 0.8$ in all trap aspect ratios tested.

Partially polarized SF core at intermediate polarizations.

FFLO-type order parameter oscillations near transition point in larger aspect ratios.