An overview on Quantum Gases (III)

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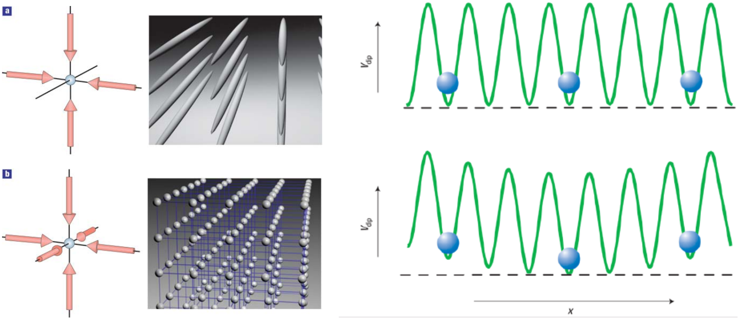
outline

- 1D optical lattices
- DFT as a many-body theory
- 1D Hubbard model
- Spin-DFT formalism for 1D Hubbard model
- Bogoliubov-de Gennes approach (mean-field)
- (T-BdG)

opticall lattices: artificial crystal with light and atoms!



$$V(\mathbf{r}) \propto \sin^2(kx)$$

I. Bloch, Nature Physics, **1**, 203 (2005)
Paredes et.al, Nature **429**, 277 (2004)
Moritz et.al, PRL 91, 250402 (2005)

DFT: the Hohenberg-Kohn theorem

"for his development of the density-functional theory"

Walter Kohn

Inhomogeneous many-body Interacting system.

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \int d^D\mathbf{r}\, V_{\text{ext}}(\mathbf{r})\hat{n}(\mathbf{r})$$

$$\hat{\mathcal{H}}_0 = \hat{T} + \hat{\mathcal{H}}_{\text{int}}$$

Quantum mechanics

$$v(\mathbf{r}) \overset{SE}{\Longrightarrow} \Psi(\mathbf{r}_1, \mathbf{r}_2 \ldots, \mathbf{r}_N) \overset{\langle\Psi|\ldots|\Psi\rangle}{\Longrightarrow} \text{observables}$$

$$\Psi = \Psi[n]$$

DFT

$$n(\mathbf{r}) \overset{HK}{\Longrightarrow} \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \Longrightarrow v(\mathbf{r})$$

Kohn-Sham scheme

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\rm KS}(\mathbf{r}) \right] \varphi_i(\mathbf{r}) = \varepsilon_i \, \varphi_i(\mathbf{r})$$

$$n(\mathbf{r}) = \sum_{i=1}^{N} |\varphi_i(\mathbf{r})|^2$$

$$V_{\rm KS}(\mathbf{r}) = V_{\rm ext}(\mathbf{r}) + V_{\rm H}(\mathbf{r}) + V_{\rm xc}([n_0]; \mathbf{r})$$

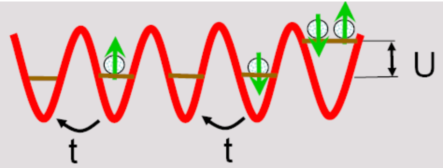
For any **interacting** system there exists a **local single-particle potential** such that the **exact** GS density of the interacting system equals the GS density of the auxiliary system.

How to calculate V_{xc}?

$$V_{\mathrm{xc}}[n_{\mathrm{GS}}](\mathbf{r}) \approx V_{\mathrm{xc}}^{\mathrm{hom}}(n)\Big|_{n \to n_{\mathrm{GS}}(\mathbf{r})}$$

for homogenous system, V_{xc} can be calculated by exact or QMC data.

1D Hubbard model



$$\hat{\mathcal{H}} = -t \sum_{i,\sigma} \left[\hat{c}^\dagger_\sigma(z_i)\, \hat{c}_\sigma(z_{i+1}) + \text{H.c.} \right] + U \sum_i \hat{n}_\uparrow(z_i)\hat{n}_\downarrow(z_i) + \sum_{i,\sigma} V^\sigma_{\text{ext}}(z_i)\, \hat{n}_\sigma(z_i)$$

The homogenous part has been solved exactly: Lieb-Wu solution based on Bethe-Ansatz.

Site-occupation functional theory

$$\sum_j \Big[-t_{ij} + V^\sigma_{\rm ks}[n_\uparrow, n_\downarrow](z_i)\,\delta_{ij} \Big] \varphi_\sigma(z_j) = \varepsilon_\sigma\,\varphi_\sigma(z_i)$$

$$V^\sigma_{\rm KS}[n_\uparrow, n_\downarrow](z_i) = V^\sigma_{\rm ext}(z_i) + V^\sigma_{\rm H}(z_i) + V^\sigma_{\rm xc}(z_i)$$

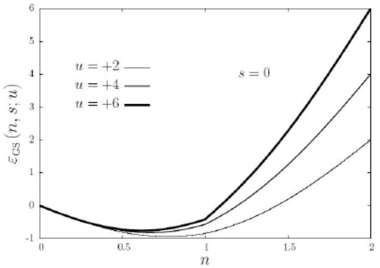
$$n_\sigma(z_i) = \sum_{\rm occ.} |\varphi_\sigma(z_i)|^2$$

$$V^\sigma_{\rm ext}(z_i) = V^\sigma_2\,(z_i - L/2)^2$$

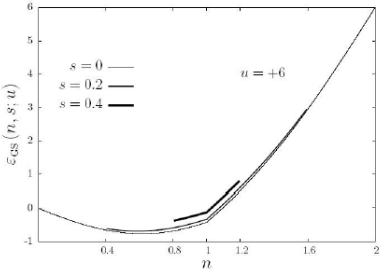
$$V^{\rm BALSDA}_{\rm xc} = V^{\rm hom}_{\rm xc}(n, s; u)\Big|_{\substack{n\to n(z_i)\\ s\to s(z_i)}}$$

$$V^{\rm hom}_{{\rm xc}\,\sigma}(n, s; u) = \mu(n, s; u) \pm \frac{1}{2} h(n, s; u) + 2t\cos\Big[\pi(\frac{n}{2} - s)\Big] - \frac{1}{2}\,u\,n_{\bar\sigma}$$

ground state energy from LW equations



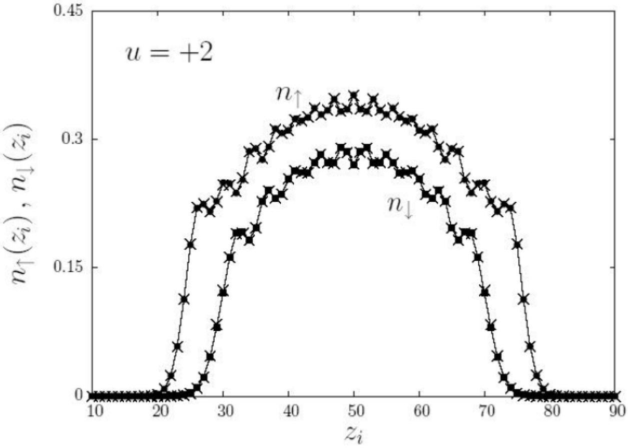
Note the cusp at n=1, signal of Mott-insulator transition !



DFT vs DMRG

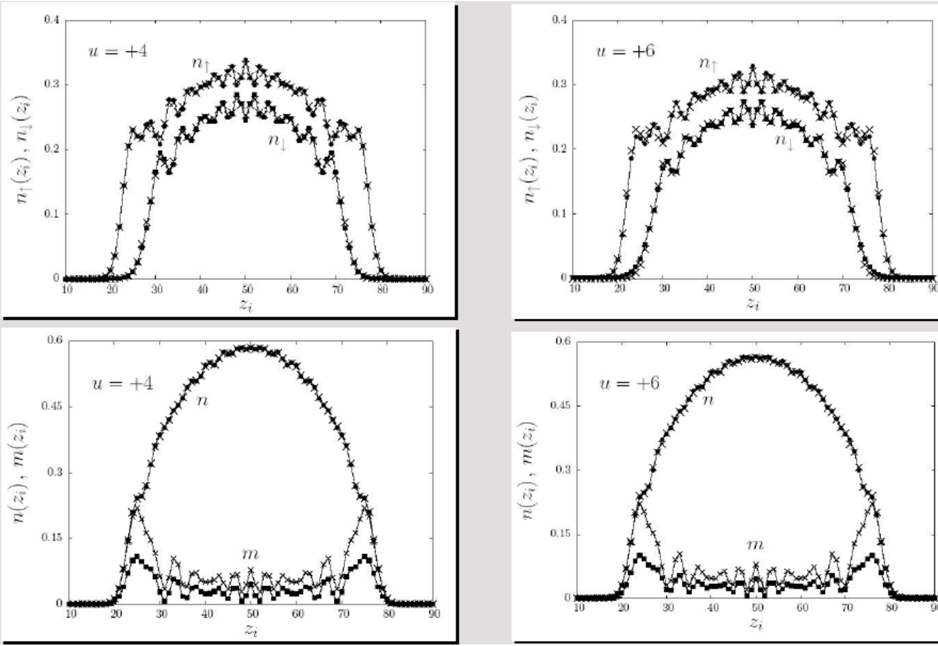
Spin-independent traps

$$V_2^{\uparrow} = V_2^{\downarrow} = V_2$$



$N_\uparrow = 15$ $\quad L = 100$

$N_\downarrow = 10$ $\quad V_2/t = 0.002$

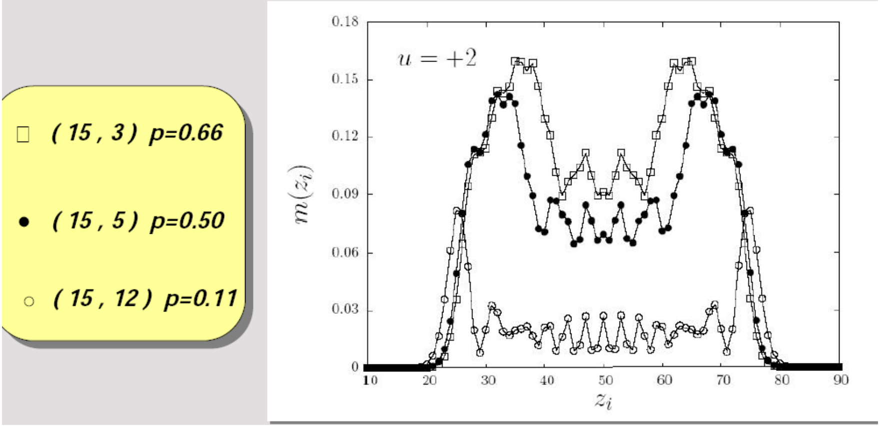


$u = +4$
$n_\uparrow$
$n_\downarrow$
$n_\uparrow(z_i)\,,\,n_\downarrow(z_i)$
z_i
0 0.1 0.2 0.3 0.4
10 20 30 40 50 60 70 80 90
$u = +6$
$n_\uparrow$
$n_\downarrow$
$n_\uparrow(z_i)\,,\,n_\downarrow(z_i)$
z_i
$u = +4$
n
m
$n(z_i)\,,\,m(z_i)$
z_i
0 0.15 0.3 0.45 0.6
$u = +6$
n
m
$n(z_i)\,,\,m(z_i)$
z_i

features

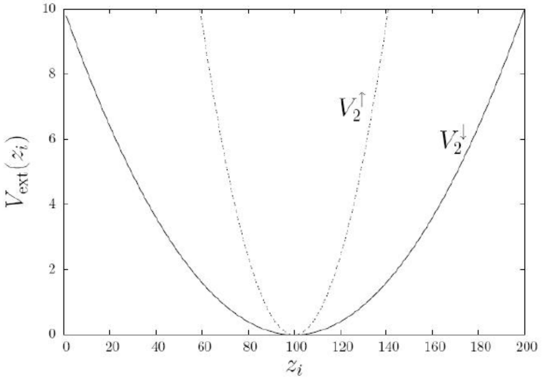
- on-site repulsion $\Longrightarrow$ out-of-phase oscillation
- Oscillations cancel each other in n and are enhanced in m: Spin-density waves (SDW) in the bulk of the trap.
- $U \gg \quad \Longrightarrow$ broaden the spin-resolved density profiles and increasing the amplitude of the SDW .

effect of polarization



With the spin imbalanced populations in the spin-independent trap, both species are always in the bulk of the trap: no phase separation occurs !

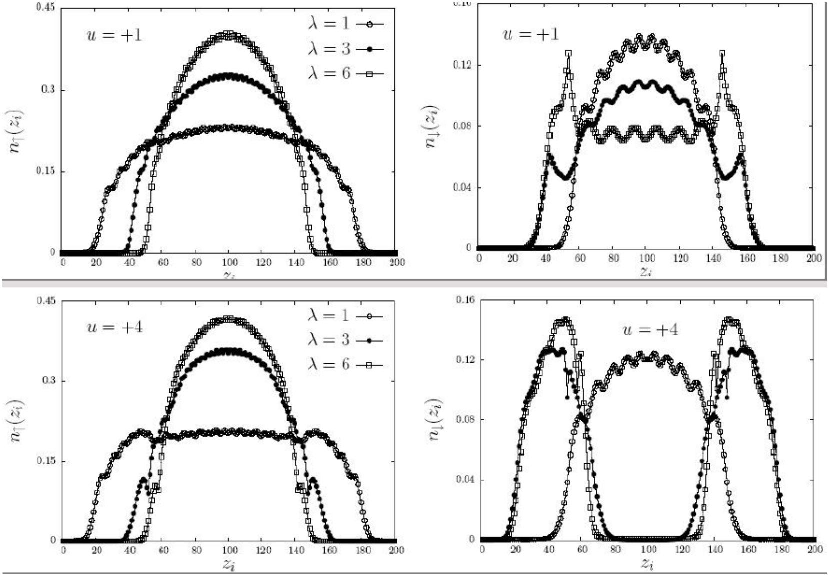
spin-dependent trap



$$\lambda = \frac{V_2^{\uparrow}}{V_2^{\downarrow}}$$

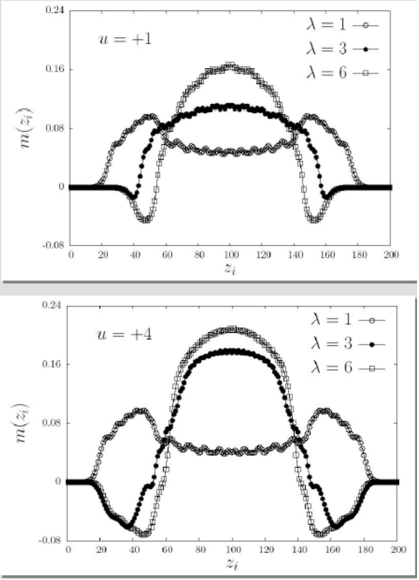
Spin-up atoms are more confined.

$$V_{ext}^{\sigma}(z_i) = V_2^{\sigma}\,(z_i - L/2)^2$$



$u = +1$
$\lambda = 1$
$\lambda = 3$
$\lambda = 6$
$n_\uparrow(z_i)$
z_i
$u = +1$
$n_\downarrow(z_i)$
z_i
$u = +4$
$\lambda = 1$
$\lambda = 3$
$\lambda = 6$
$n_\uparrow(z_i)$
z_i
$u = +4$
$n_\downarrow(z_i)$
z_i

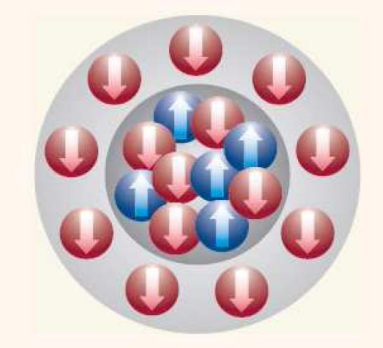
The strong repulsive interaction prohibits the existence of spin-down atoms in the bulk and they have to move to the periphery of the trap: complete phase-separation between two components in the bulk of the trap !



non-BCS pairing

FFLO (Fulde-Ferrel-Larkin-Ovchinikov) state: non-uniform order parameter

$$\Delta(\mathbf{r}) = \Delta_0 e^{i\,2\mathbf{q}.\mathbf{r}}$$



Mean-field Hamiltonian for 1D interacting trapped Fermi gas

$$
\begin{aligned}
\mathcal{H}_{mf} &= -t \sum_{i,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \, \hat{c}_{i+1,\sigma} + h.c \right) + \sum_{i} \left(\Delta_i \hat{c}^{\dagger}_{i,\uparrow} \, \hat{c}^{\dagger}_{i,\downarrow} + h.c \right) \\
&+ \sum_{i,\sigma} \left\{ \left(V_i^{ext} - \mu_\sigma \right) - U \bar{n}_{i,\bar{\sigma}} \right\} \hat{c}^{\dagger}_{i,\sigma} \, \hat{c}_{i,\sigma} \\
\Delta_i &\equiv -U < \hat{c}_{i,\downarrow} \, \hat{c}_{i,\uparrow} > \\
V_i^{ext} &= V_0 \left(i - \frac{L}{2} \right)^2
\end{aligned}
$$

discrete Bogoliubov-deGennes formalism

- Bogoliubov transformation

$$\hat{c}_{i,\sigma} = \sum_{\alpha} \left(u_{\alpha i \sigma} \hat{\gamma}_{\alpha\sigma} - \sigma v^{\star}_{\alpha i \sigma} \hat{\gamma}^{\dagger}_{\alpha\bar{\sigma}} \right)$$

- diagonalized H

$$\mathcal{H}_{mf} = E_0 + \sum_{\alpha\sigma} E_{\alpha\sigma} \, \hat{\gamma}^{\dagger}_{\alpha\sigma} \, \hat{\gamma}_{\alpha\sigma}$$

- BdG equations

$$\sum_{j=1}^{L} \begin{pmatrix} \mathcal{H}^{\sigma}_{i\,j} & \Delta_{i\,j} \\ \Delta_{i\,j} & -\mathcal{H}^{\bar{\sigma}}_{i\,j} \end{pmatrix} \begin{pmatrix} u_{\alpha j \sigma} \\ v_{\alpha j \bar{\sigma}} \end{pmatrix} = E_{\alpha\sigma} \begin{pmatrix} u_{\alpha j \sigma} \\ v_{\alpha j \bar{\sigma}} \end{pmatrix}$$

$$\begin{aligned} \mathcal{H}^{\sigma}_{i\,j} &= -t\,\delta_{i,i\pm 1} + \left(V^{ext}_{i} - \mu_{\sigma} \right) \delta_{i\,j} \\ \Delta_{i\,j} &= \Delta_{i}\,\delta_{i\,j} \end{aligned}$$

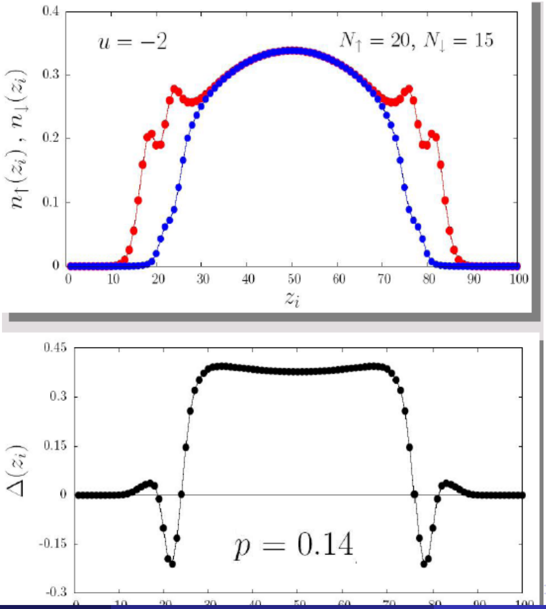
Self-consistent equations

$$n_i^\sigma = \sum_{\alpha=1}^{L} \left[|u_{\alpha i \sigma}|^2 f(E_{\alpha\,\sigma}) + |v_{\alpha i \sigma}|^2 f(-E_{\alpha\,\bar{\sigma}}) \right]$$

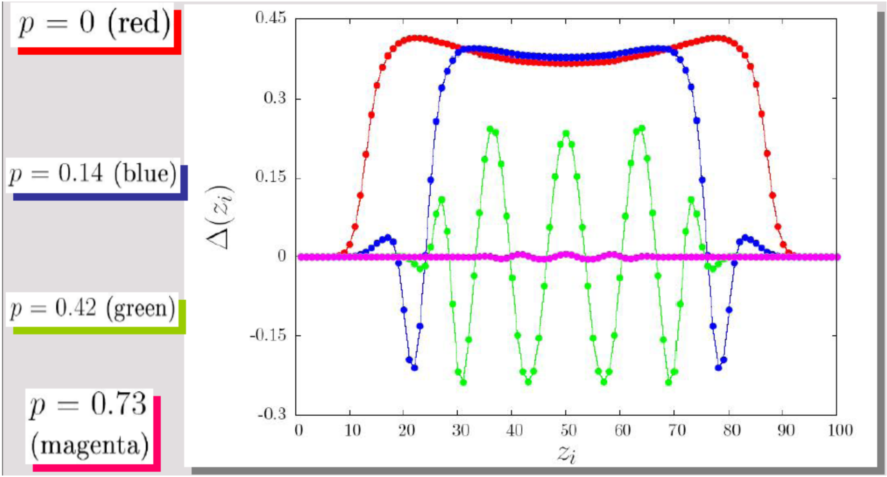
$$\Delta_i = -U \sum_{\alpha=1}^{L} \left[u_{\alpha i \uparrow}\, v_{\alpha i \downarrow} f(E_{\alpha\,\uparrow}) - u_{\alpha i \downarrow}\, v_{\alpha i \uparrow} f(-E_{\alpha\,\downarrow}) \right]$$

$$\sum_i n_i^\sigma = N_\sigma$$

densities at mean-field level



FFLO feature



Time to say goodbye...