UCDAVIS

Phase Diagram and Visibility of Optically Trapped Bosons

- Optically Trapped Atoms and Boson Hubbard Model
- Matter Wave Interference Experiment
- Equilibrium Phase Diagram: Uniform System
- Equilibrium Phase Diagram: Confined System
- Visibility
- "Pause" in Evolution with U
- Conclusions

Collaborators

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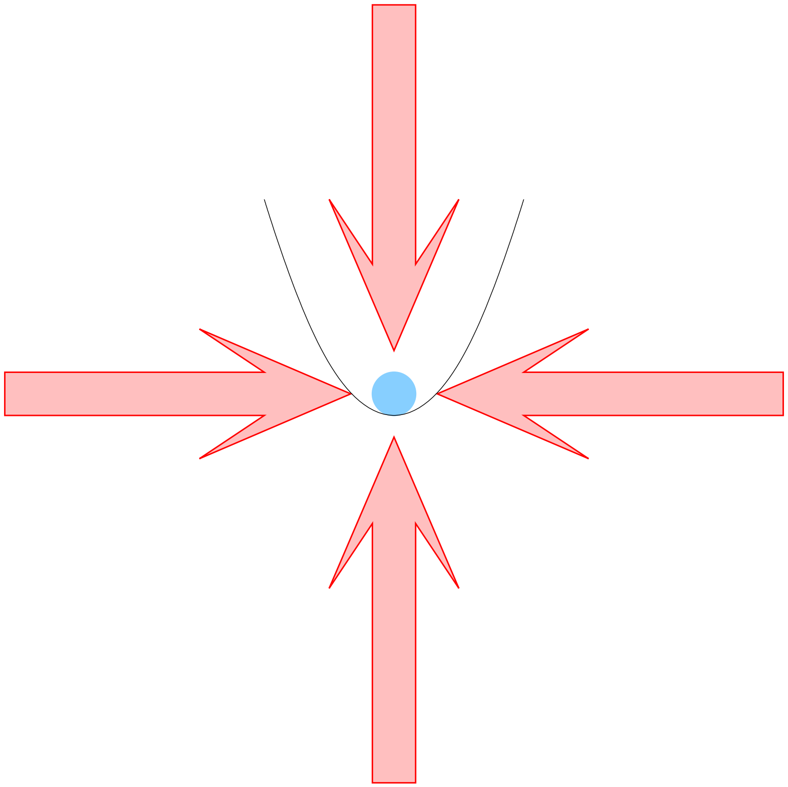
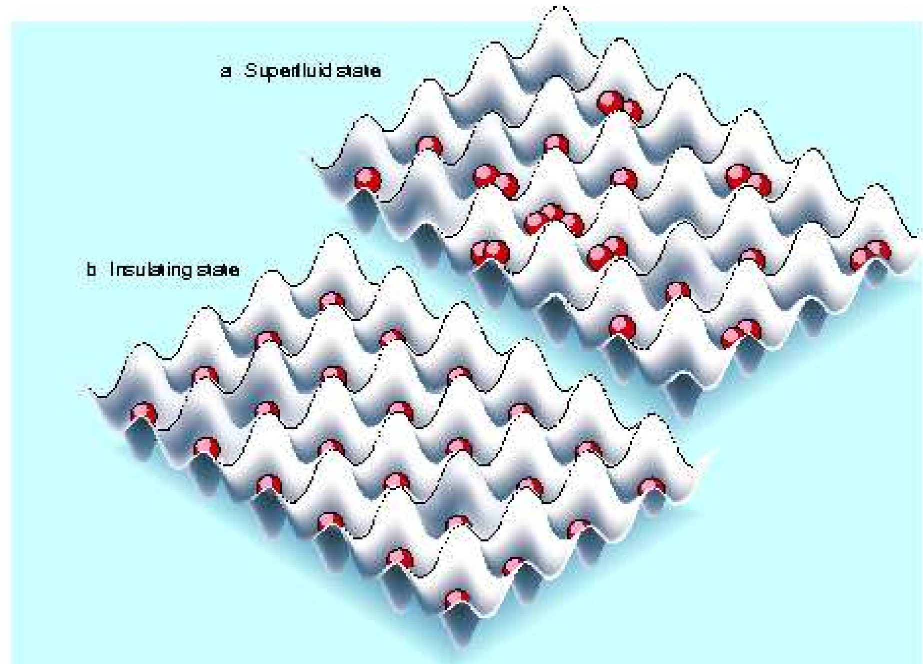
Optical lattice in a trap





The lattice sites are the nodes of the standing wave

Lattice spacing $a = \lambda/2$

The model

The Hamiltonian for bosonic atoms in external trap:

$$
\begin{aligned}
H &= \int \mathrm{d}^3x\ \psi^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m} \nabla^2 + V_0(\mathbf{x}) + V_T(\mathbf{x}) \right) \psi(\mathbf{x}) \\
&\quad + \frac{1}{2} \frac{4\pi a_s \hbar^2}{m} \int \mathrm{d}^3x\ \psi^\dagger(\mathbf{x}) \psi^\dagger(\mathbf{x}) \psi(\mathbf{x}) \psi(\mathbf{x})
\end{aligned}
$$

$\psi(\mathbf{x})$: boson field operator, $V_T(\mathbf{x})$: confining potential

a_s : scattering length $V_0(\mathbf{x})$: optical lattice potential

Simplest case:

$$
\begin{aligned}
V_0(\mathbf{x}) &= \sum_{j=1}^{d} V_{j0} \sin^2(k x_j) \\
k &= \frac{2\pi}{\lambda} \\
a &= \frac{\lambda}{2}
\end{aligned}
$$

The bosonic Hubbard model

Well described by the tight-binding bosonic Hubbard model,[1]

$$H = -J \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + \sum_i V_T(\mathbf{x_i}) \hat{n}_i + U \sum_i \hat{n}_i (\hat{n}_i - 1)$$

where

$$[b_i, b_j^\dagger] = \delta_{ij}, \quad \hat{n}_i = b_i^\dagger b_i$$

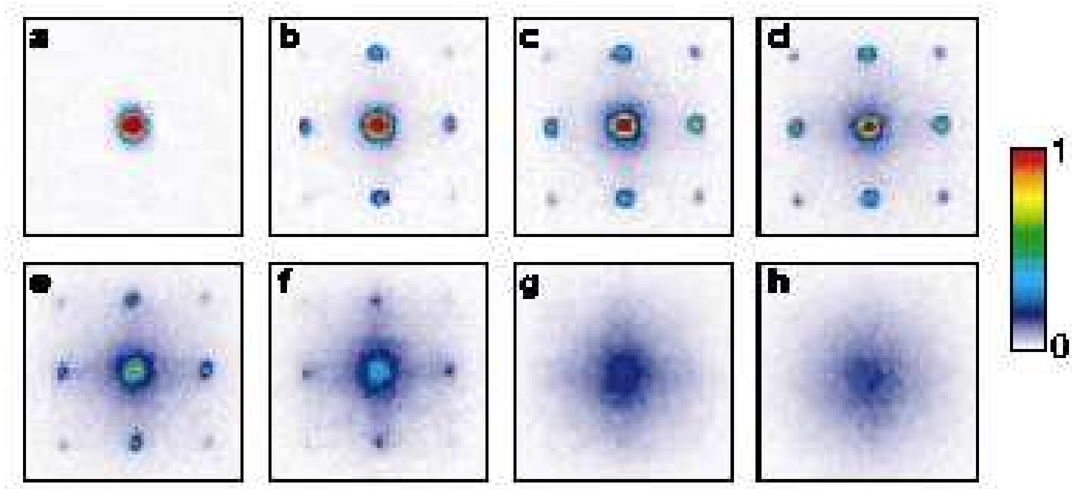
Model parameters can be tuned.

A great deal is known about this model without trap including its phase diagram

[1] D. Jaksch *et al*, Phys. Rev. Lett. **81**, 3108 (1998).

Experiment

Greiner *et al*, Nature **415** (2002) 39.



Absorption images (in 3D) of multiple matter wave interference patterns. (a) $U = 0E_r$, (b) $U = 3E_r$, (c) $U = 7E_r$, (d) $U = 10E_r$, (e) $U = 13E_r$, (f) $U = 14E_r$, (g) $U = 16E_r$, (h) $U = 20E_r$ ($E_r = \frac{\hbar^2 k^2}{2m}$)

The claim: Quantum phase transition SF$\rightarrow$ Mott Insulator for $U \approx 12E_r$

Several recent experiments produced MI on 1D optical lattices in traps

Review 1D uniform ($V_T(x) = 0$) model

One dimensional uniform Hubbard model in the ground state[2]

$$H = -J\sum_{\langle i,j\rangle}(b_i^\dagger b_j + b_j^\dagger b_i) + U\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu\sum_i n_i$$

No hopping limit: $J/U = 0$

$$H = U\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu\sum_i \hat{n}_i$$

Ground state is obtained by minimizing the energy,

$$\epsilon(n) = Un(n-1) - \mu n$$

where $n \geq 0$ is the occupation of the site. For

$$2(n-1) < \frac{\mu}{U} < 2n$$

The energy is minimized by having n bosons on each site.
μ can be changed in this interval and n does not change:
Excitation energy gap, incompressible Mott Insulator.
Perturbation shows that this Mott Insulator extends into the finite J/U region.

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[2] G. Batrouni *et al.* Phys. Rev. Lett. **65** 1765 (1990).

World-Line Quantum Monte Carlo Simulations

Inverse Temperature discretized: $\beta = L\Delta\tau$

$$Z = \text{Tr}e^{-\beta H} = \text{Tr}[e^{-\Delta\tau H}]^L$$

Checkerboard Decomposition:
Divide Hamiltonian into two mutually commuting pieces

$$\begin{aligned} H_a &= -J\sum_{i\,\text{odd}}(b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i) + U/2\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu/2\sum_i \hat{n}_i \\ H_b &= -J\sum_{i\,\text{even}}(b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i) + U/2\sum_i \hat{n}_i(\hat{n}_i - 1) - \mu/2\sum_i \hat{n}_i \end{aligned}$$

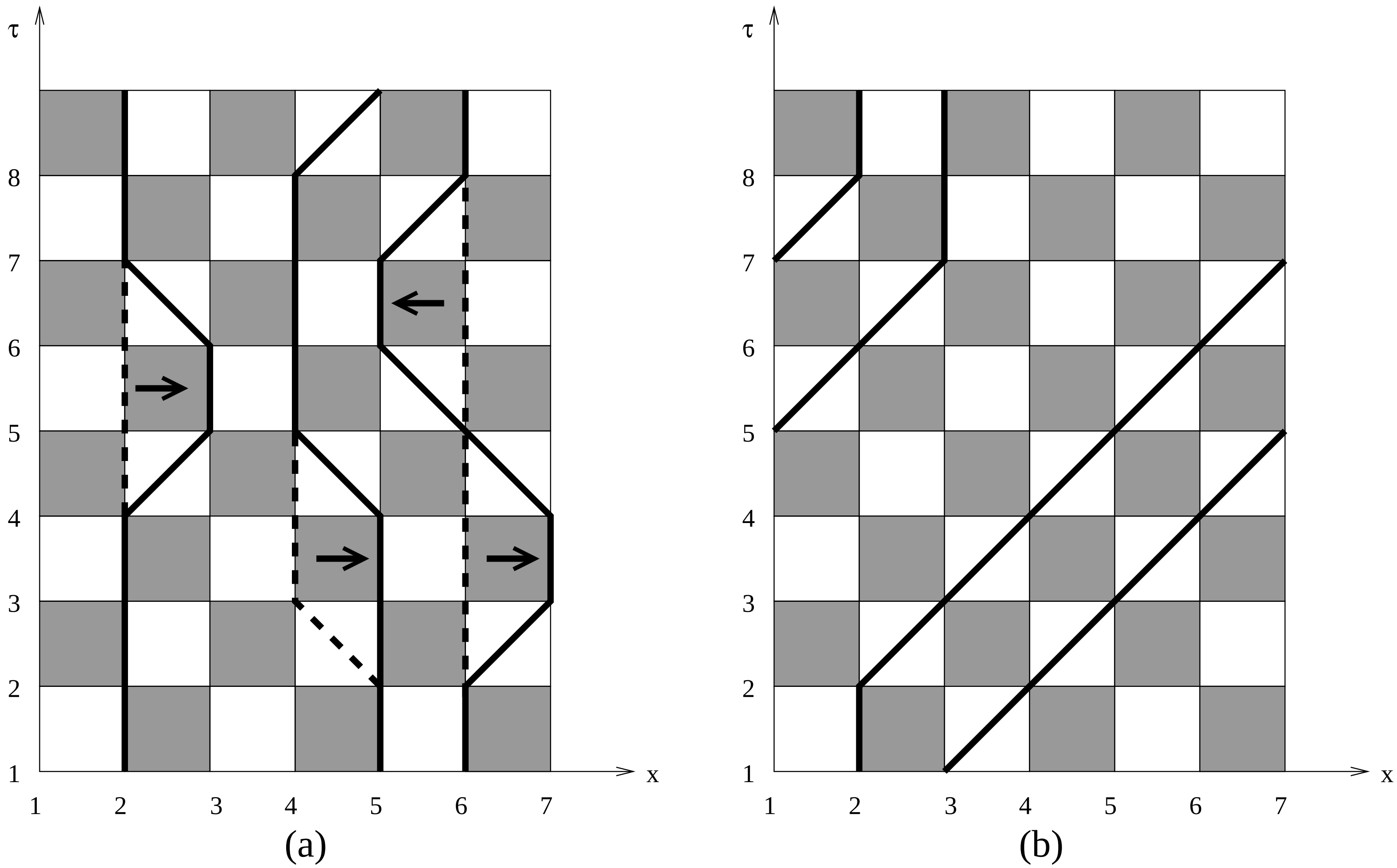
Insert complete sets of occupation number states

$$Z = \sum_{n_l} \langle n_0|e^{-\Delta\tau H_a}|n_1\rangle\langle n_1|e^{-\Delta\tau H_b}|n_2\rangle\langle n_2|e^{-\Delta\tau H_a}|n_3\rangle\langle n_3|e^{-\Delta\tau H_b}|n_4\rangle$$

$$\ldots\langle n_{2L-2}|e^{-\Delta\tau H_a}|n_{2L-1}\rangle\langle n_{2L-1}|e^{-\Delta\tau H_b}|n_0\rangle$$

State of system represented by occupation number paths $n_{\mathbf{i}}(\tau)$

Paths sampled stochastically



Zero Winding

Non-Zero winding

Measurable quantities

$$\rho_s = \frac{\langle W^2 \rangle}{2dt\beta} \qquad \mu(N) = E(N+1) - E(N)$$

$$j(\tau) = \sum_{i=1}^{N_b} [x(i,\tau+1) - x(i,\tau)] \qquad \mathcal{J}(\tau) = \langle j(\tau) j(0) \rangle$$

$$\mathcal{J}(\omega) = \sum_{\tau} e^{i\omega\tau} \mathcal{J}(\tau) \qquad \mathcal{J}(\omega \to 0) = \frac{1}{\beta} \langle W^2 \rangle$$

$$S(k) = \sum_r e^{ikr} \langle n(r_0) n(r_0 + r) \rangle$$

Stochastic Series Expansion[3]

Express Hamiltonian as sum of diagonal and non-diagonal operators on bonds of lattice

$$
\begin{aligned}
H &= \sum_i (H_{Ui} + H_{Ji}) \\
H_{Ui} &= U n_i(n_i - 1) - \mu n_i \\
H_{Ji} &= -J(b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i)
\end{aligned}
$$

Expand partition function in powers of H

$$
Z = \mathrm{Tr}\ e^{-\beta H} = \sum_\alpha \sum_n \frac{(-\beta)^n}{n!} \langle \alpha | H^n | \alpha \rangle .
$$

Insert/remove operators stochastically, satisfying detailed balance.

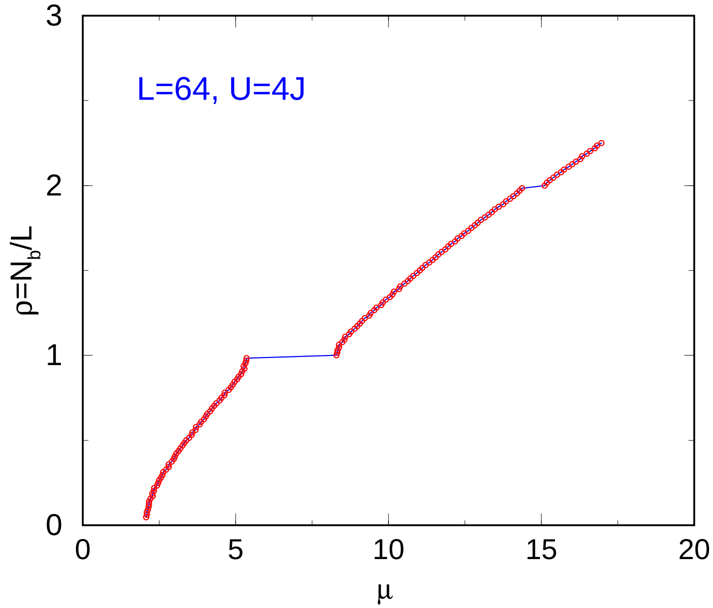
Considerable similarities with (advanced) world-line algorithms.

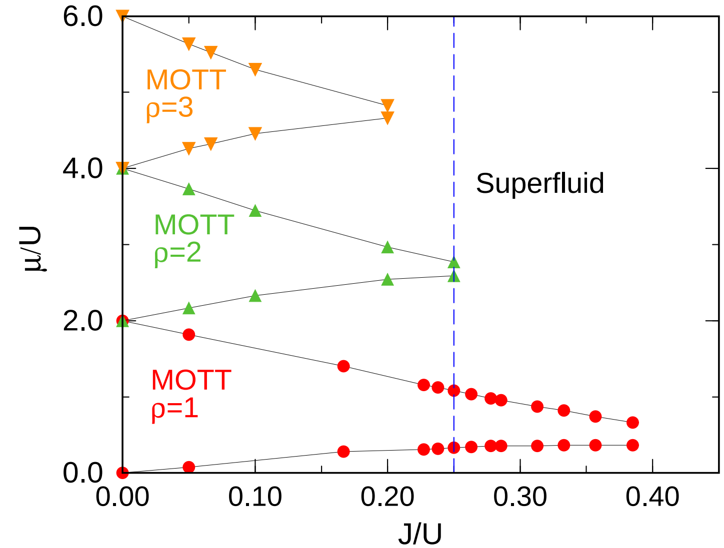
Advantages over our (older) world-line implementation:

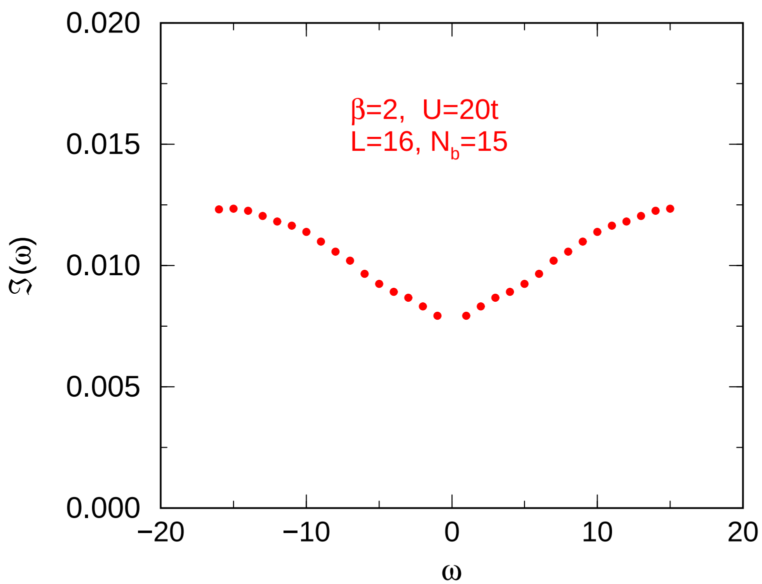
- Loop updates (reduce autocorrelation times).
- Greens function measurements possible.

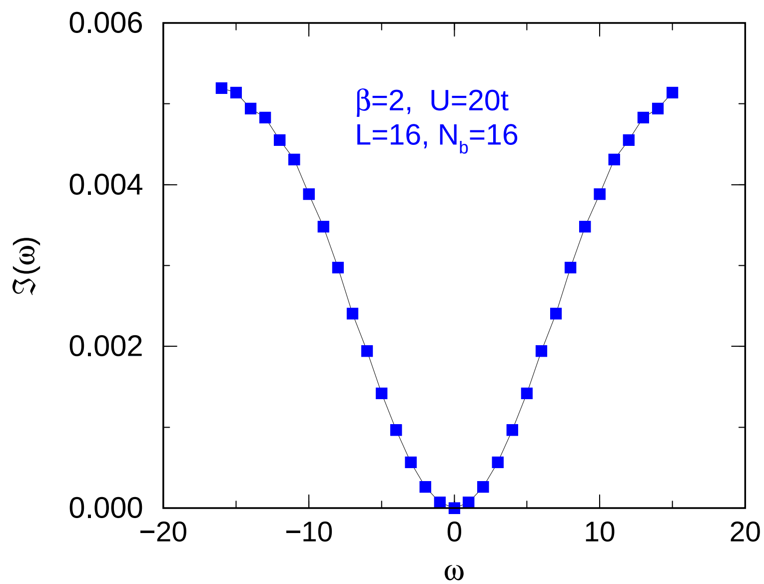
[3] A. W. Sandvik and J. Kurkijarvi, Phys. Rev. B **43**, 5950 (1991).

Phase diagram









Quantum Phase Transition

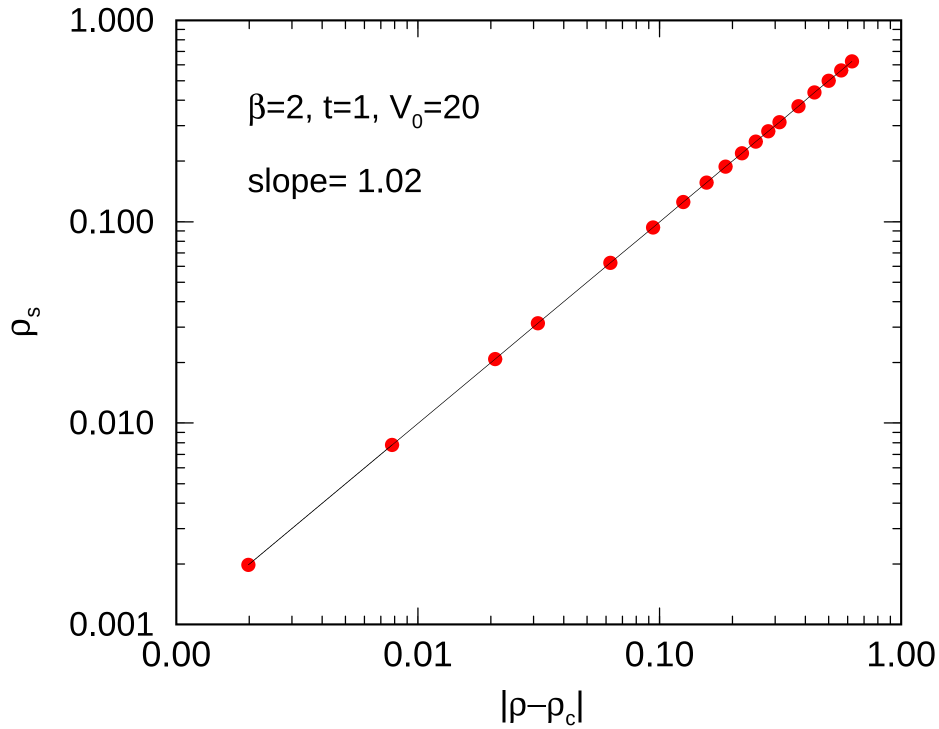
$$\kappa = \frac{\partial \rho}{\partial \mu} \rightarrow |\mu - \mu_c|^{-\nu/2} \text{ as } \mu \rightarrow \mu_c \qquad \rho_s \sim |\rho - \rho_{Mott}|^{z-d}$$

System sizes ranging from

$L = 16$ to $L = 256$

Quantum phase transition!

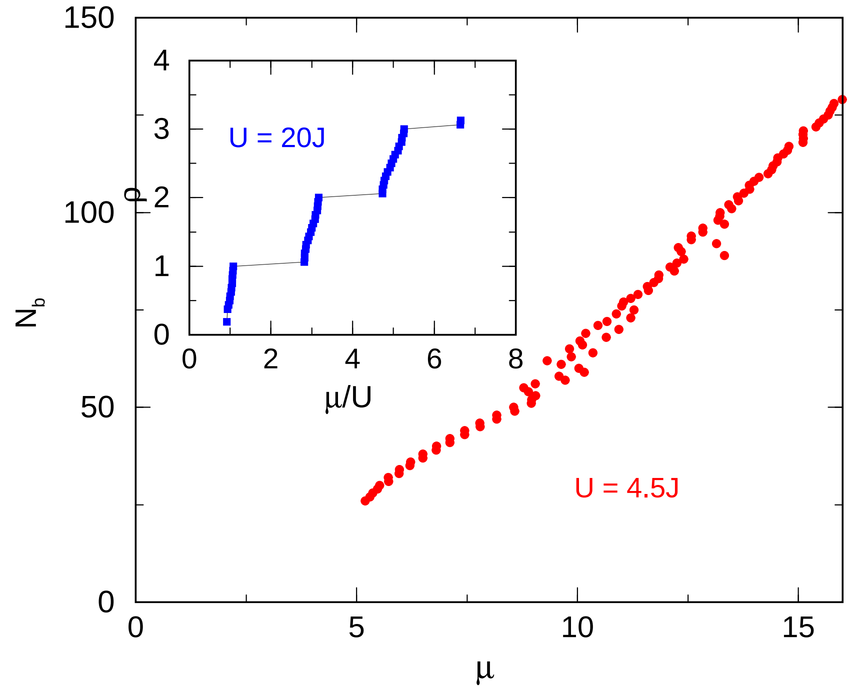
$z = 2, \quad \nu = 1$

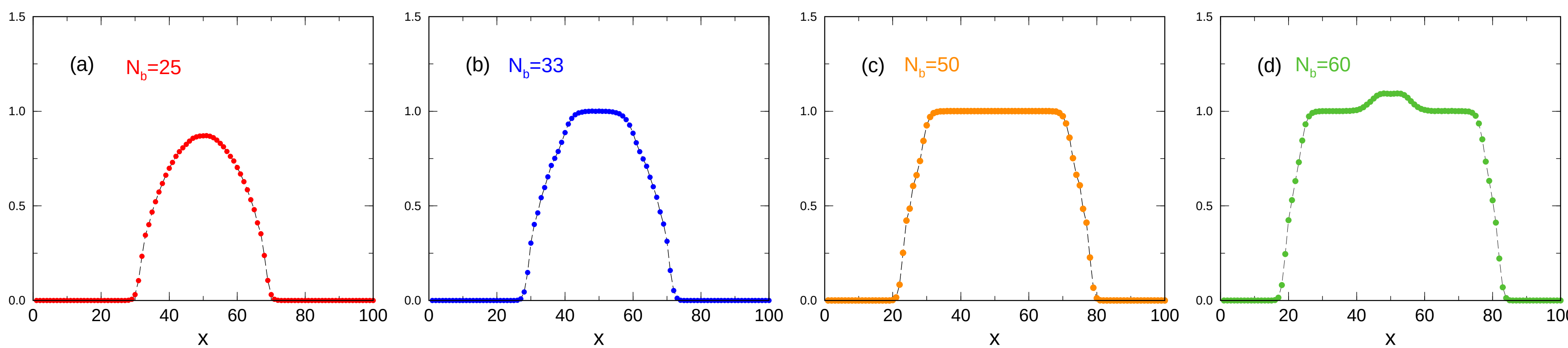


(1)

One dimensional trapped Boson Hubbard model

No globally incompressible Mott plateau in the trapped system!
As a whole, the system is always compressible.



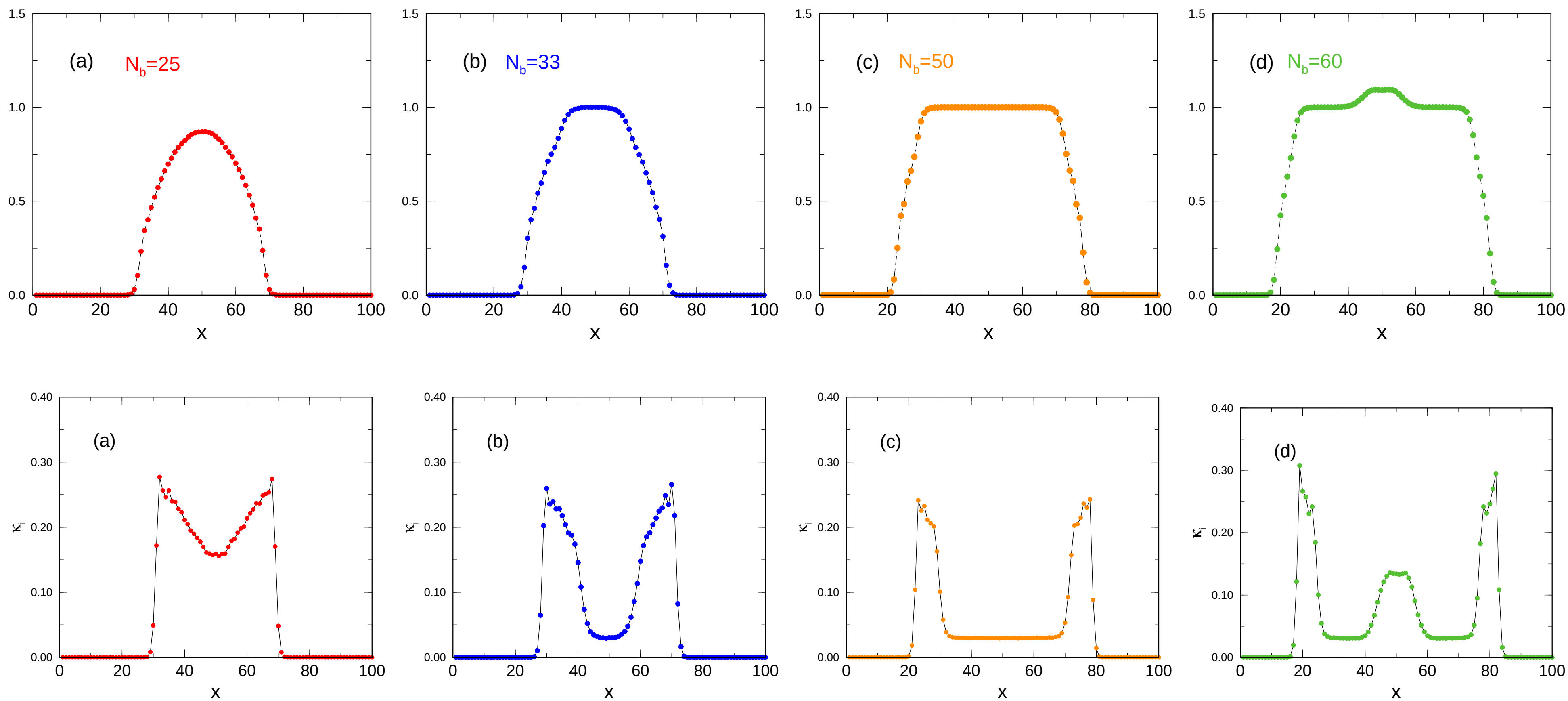


G. G. Batrouni *et al*, Phys. Rev. Lett. **89** 117203 (2002).

Local compressibility

Several possible definitions of local compressibility. Simplest:

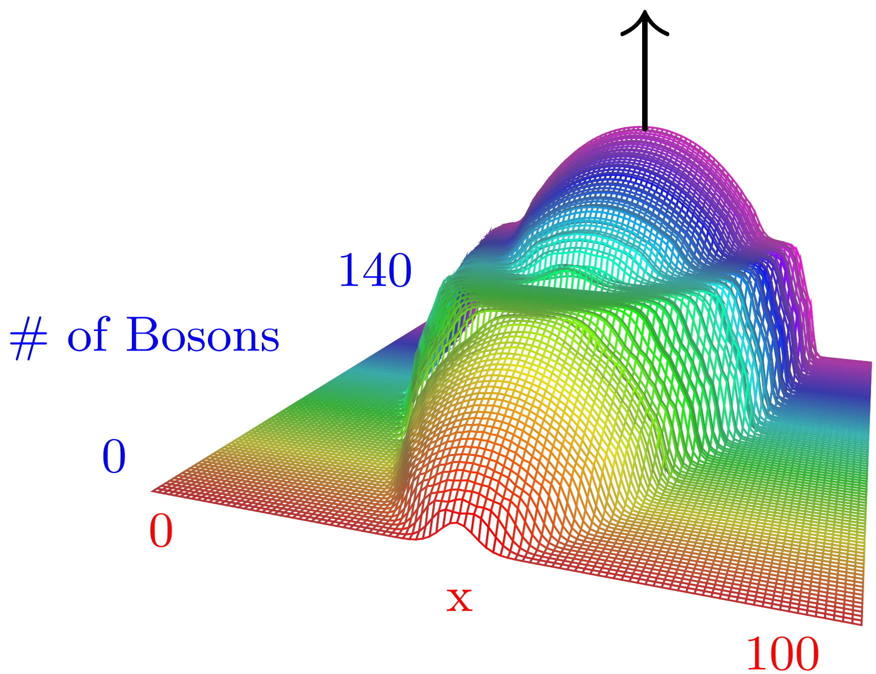
$$\kappa_i = \frac{\partial n_i}{\partial \mu_i}$$



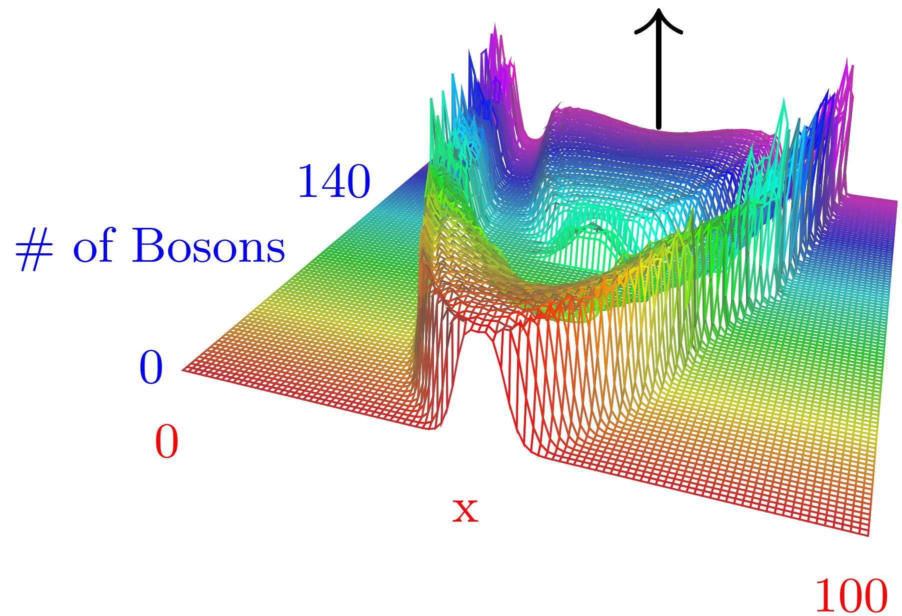
No evidence of κ diverging: No quantum phase transition

ρ and κ profiles: Fixed U=4.5

Local Density $\rho(x)$

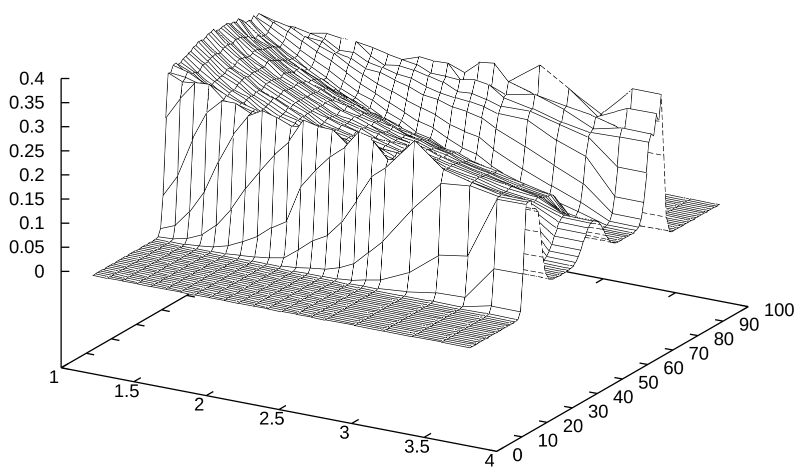


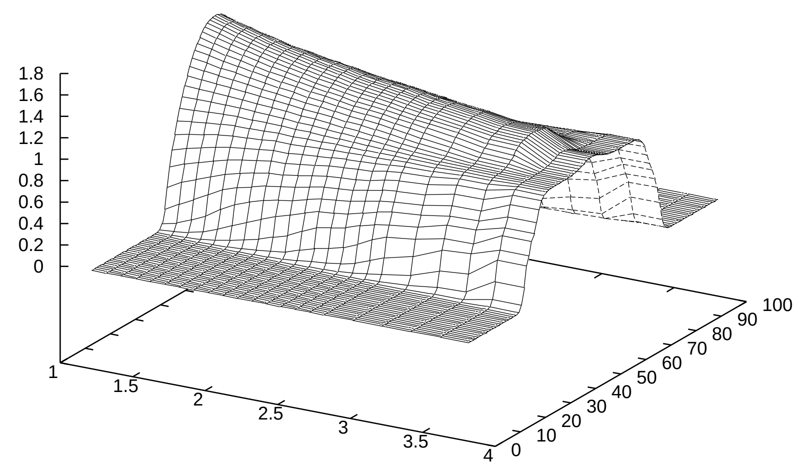
Local Compressibility $\kappa(x) = \frac{\partial \rho(x)}{\partial \mu(x)}$



Mott regions always co-exist with SF

ρ and κ profiles: Fixed $N_b = 50$

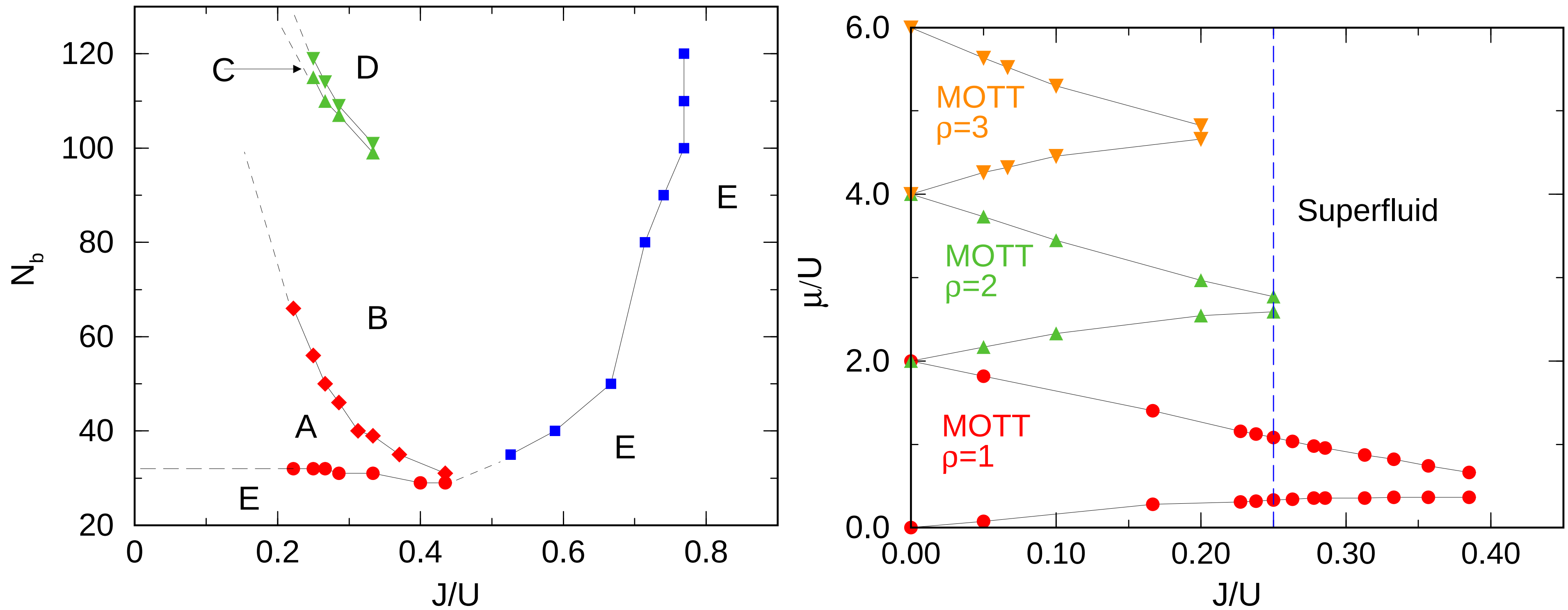




As U is increased, the system **gradually** crosses over to Mott:

No quantum phase transition.

State diagram



A: $\rho = 1$ Mott

B: SF in center + $\rho = 1$ Mott

C: $\rho = 2$ Mott + SF + $\rho = 1$ Mott

D: SF in center + $\rho = 2$ Mott + SF + $\rho = 1$ Mott

E: SF

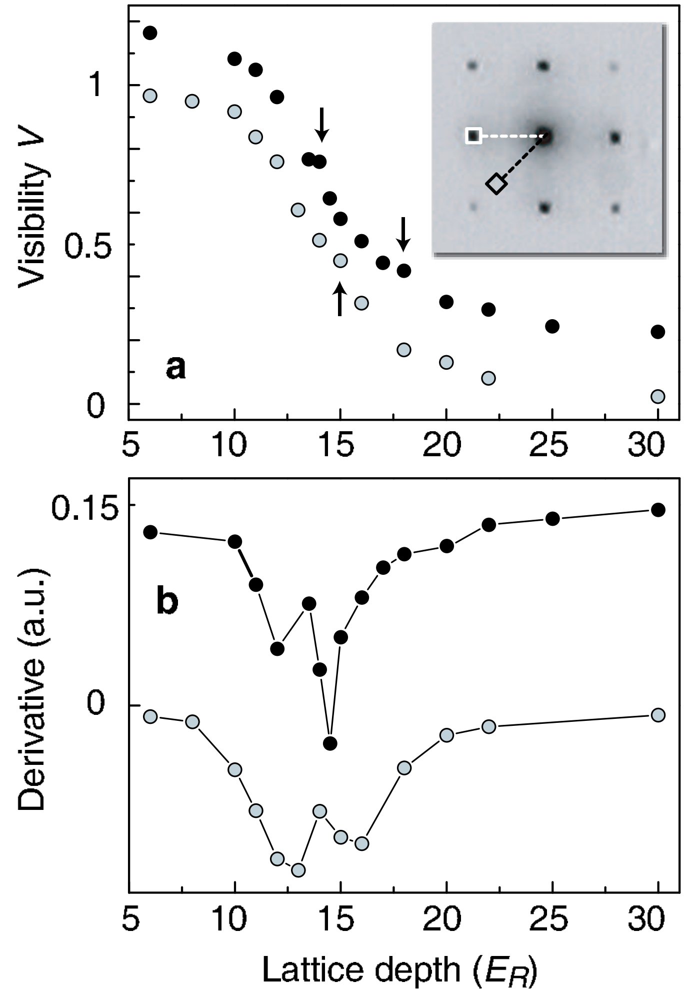
The trapped one dimensional bosonic Hubbard model does not exhibit quantum critical behavior like the uniform system.

Visibility Experiments

$$\mathcal{V} = \frac{S_{\max} - S_{\min}}{S_{\max} + S_{\min}}.$$

$S_{\max}(S_{\min})$ are max(min) of momentum distribution,

$$S(\mathbf{k}) = \frac{1}{L}\sum_{j,l} \mathrm{e}^{i\mathbf{k}.(\mathbf{r_j}-\mathbf{r_l})}\langle a_j^\dagger a_l\rangle.$$



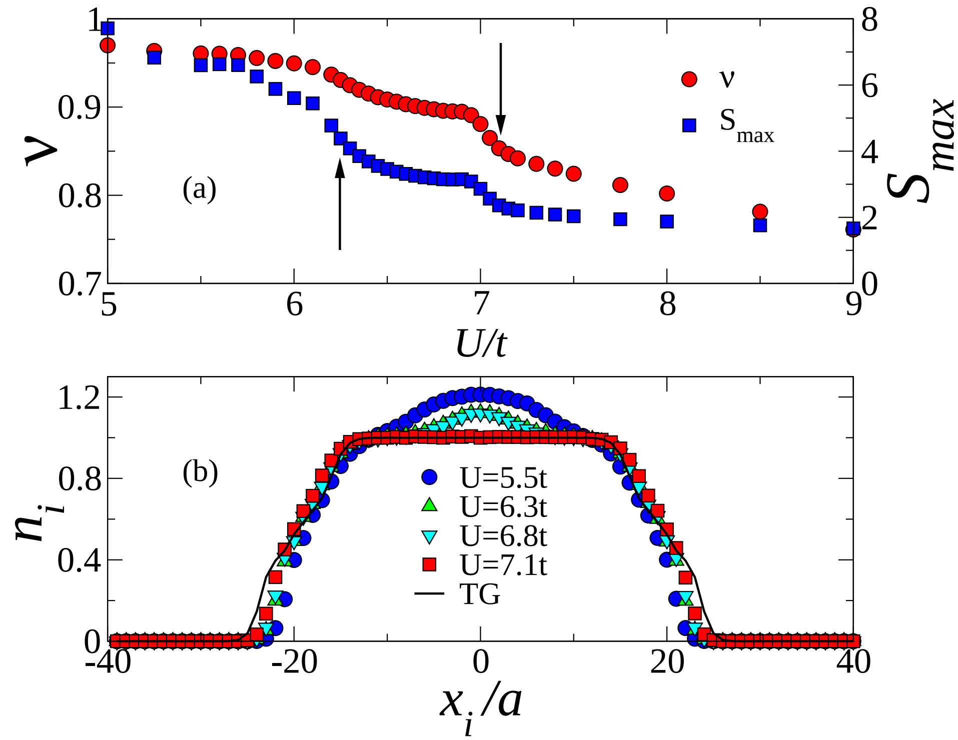
- Optical lattice depth (U) increases: visibility decreases.
- Special values of U: $\mathcal{V}$ displays "kinks" then decreases again.
- Reflects density redistribution: SF shells transform to MI regions.[4]

[4] F. Gerbier *et al.*, Phys. Rev. Lett. **95**, 050404 (2005).

QMC Simulations in d=1

Density Profiles and Visibility

Simplest case: density $n < 2$. Only Mott domains with $n = 1$.



First kink: MI plateau emerge at sides of central SF, $U = 6.3t$.

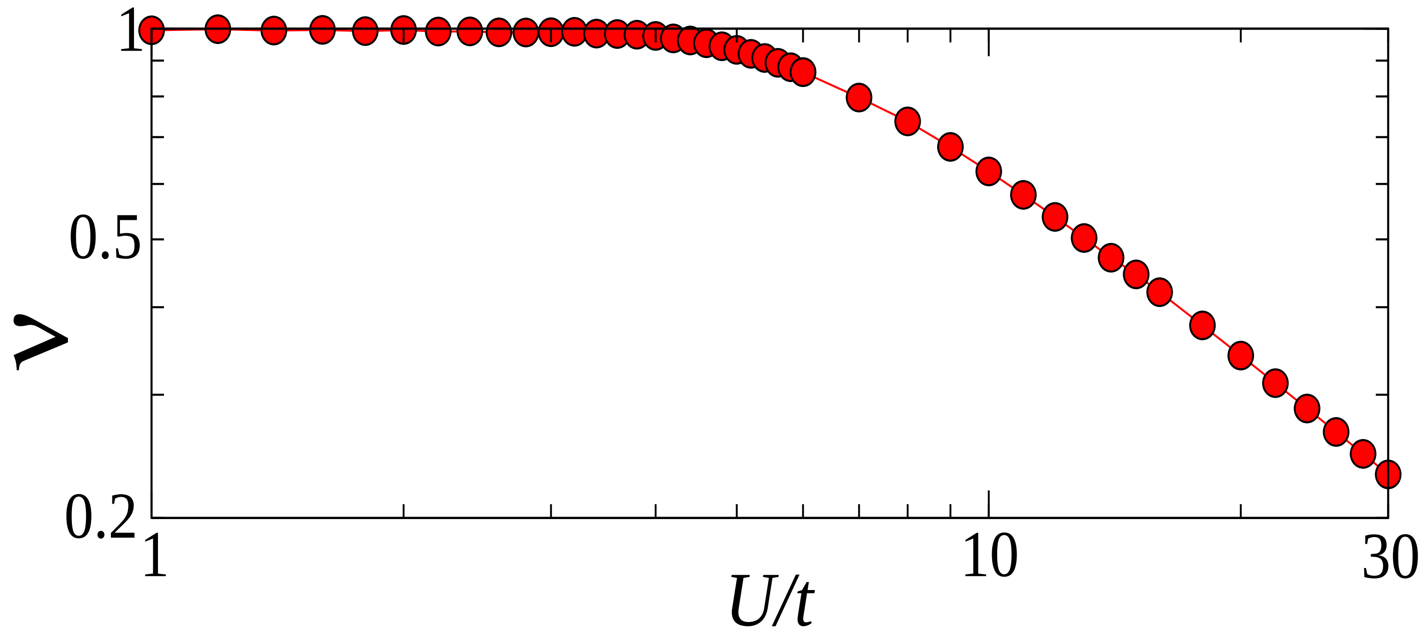
Second kink: full MI domain in middle of trap, $U = 7.1t$.

Experimental control parameter: (lattice depth)/(recoil energy).

U/t depends exponentially on this quantity.

Unexpected feature: freezing of the density profiles.

Visibility For Unconfined System

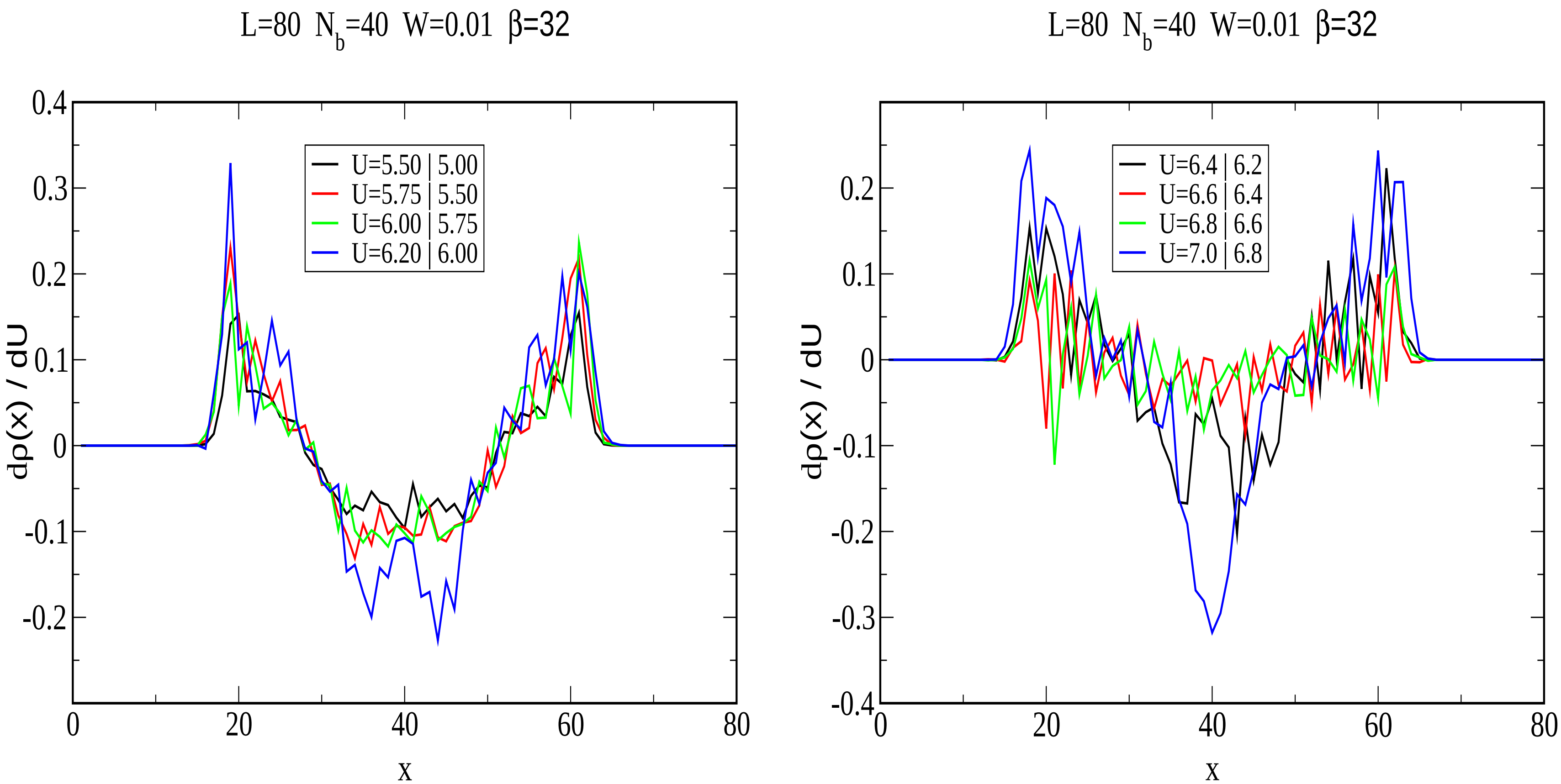


Comparatively Featureless.

Does Exhibit signature of Mott Transition at $U \approx 4.5t$.

Visibility begins to decrease from $\nu = 1$.

Further Signatures of Pause in Density



Difference in densities between U and $U + \delta U$

$6.40 \gtrsim U$: $d\rho(x)/dx < 0$ center; $d\rho(x)/dx > 0$ shoulders.

$6.80 \gtrsim U \gtrsim 6.40$: $d\rho(x)/dx \sim 0$ everywhere.

$U \gtrsim 6.80$: $d\rho(x)/dx < 0$ center; $d\rho(x)/dx > 0$ shoulders.

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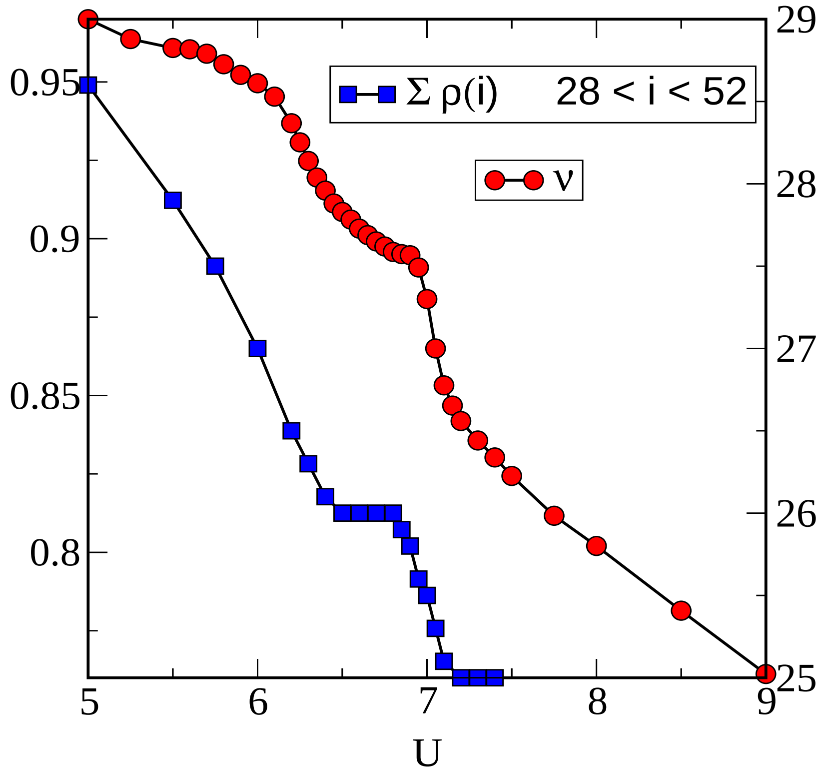
“Central Density” and Visibility



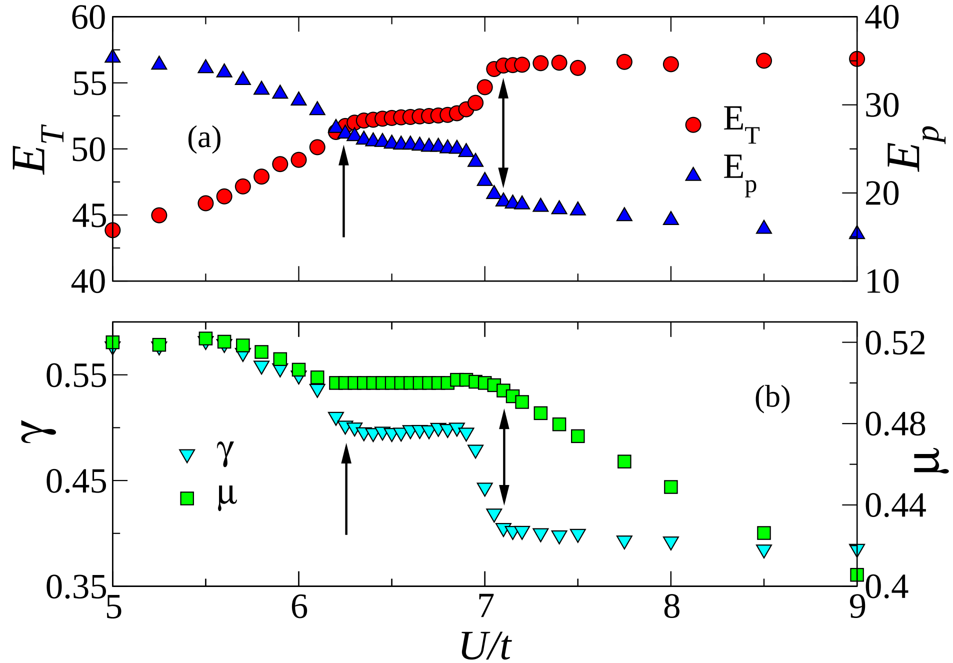
Pause in the “central density” $\sum_{i=28}^{52} \rho(i)$.

Coincides with the plateau-like behavior of $\mathcal{V}$.

$6.3 < U < 6.8$: bosons no longer pushed out of central regions
even though center is compressible SF!

Explanation: Emerging MI domains at the sides trap SF.
U/t must increase finite amount before particle transfer.

Signatures of Pause in Energetics

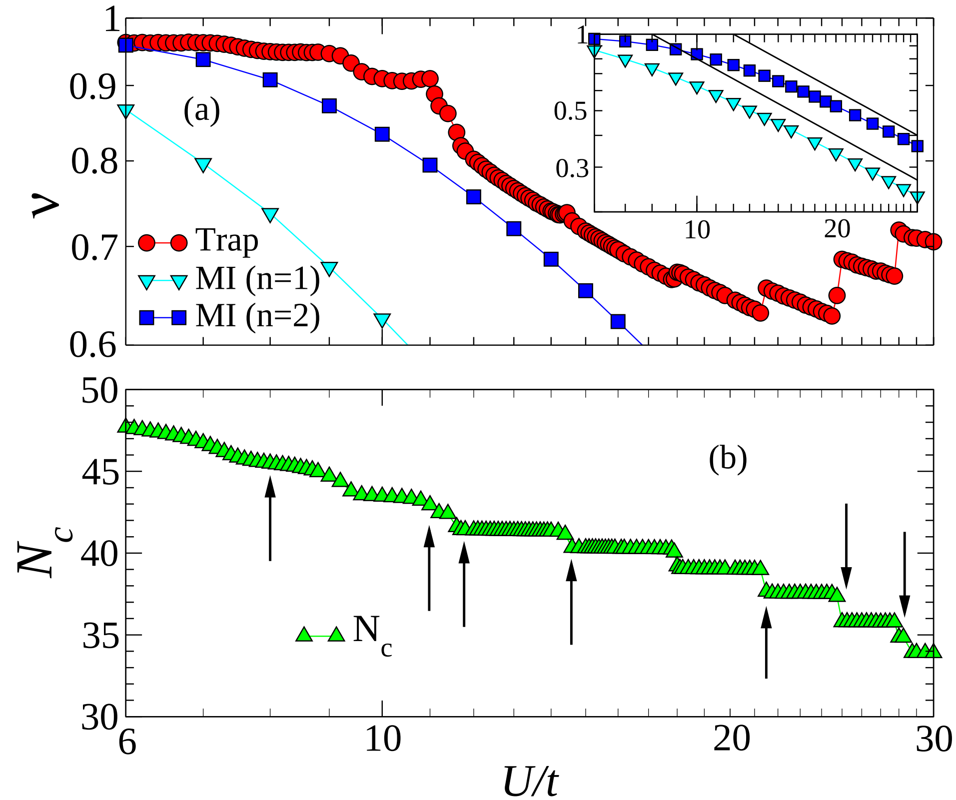


In interval $U/t = 6.3$–6.8 different pieces of energy pause:

- Total trapping energy E_T .
- Interaction energy E_P .
- Chemical potential μ.
- Ratio of potential to kinetic energy, $\gamma = |E_P/E_K|$.

Total energy (not shown) increases continuously.
Decrease in magnitude of the (negative) kinetic energy.

Visibility for System with $\rho = 2$ Mott Lobe



Up to $U/t \sim 13$, ν is similar to lower density

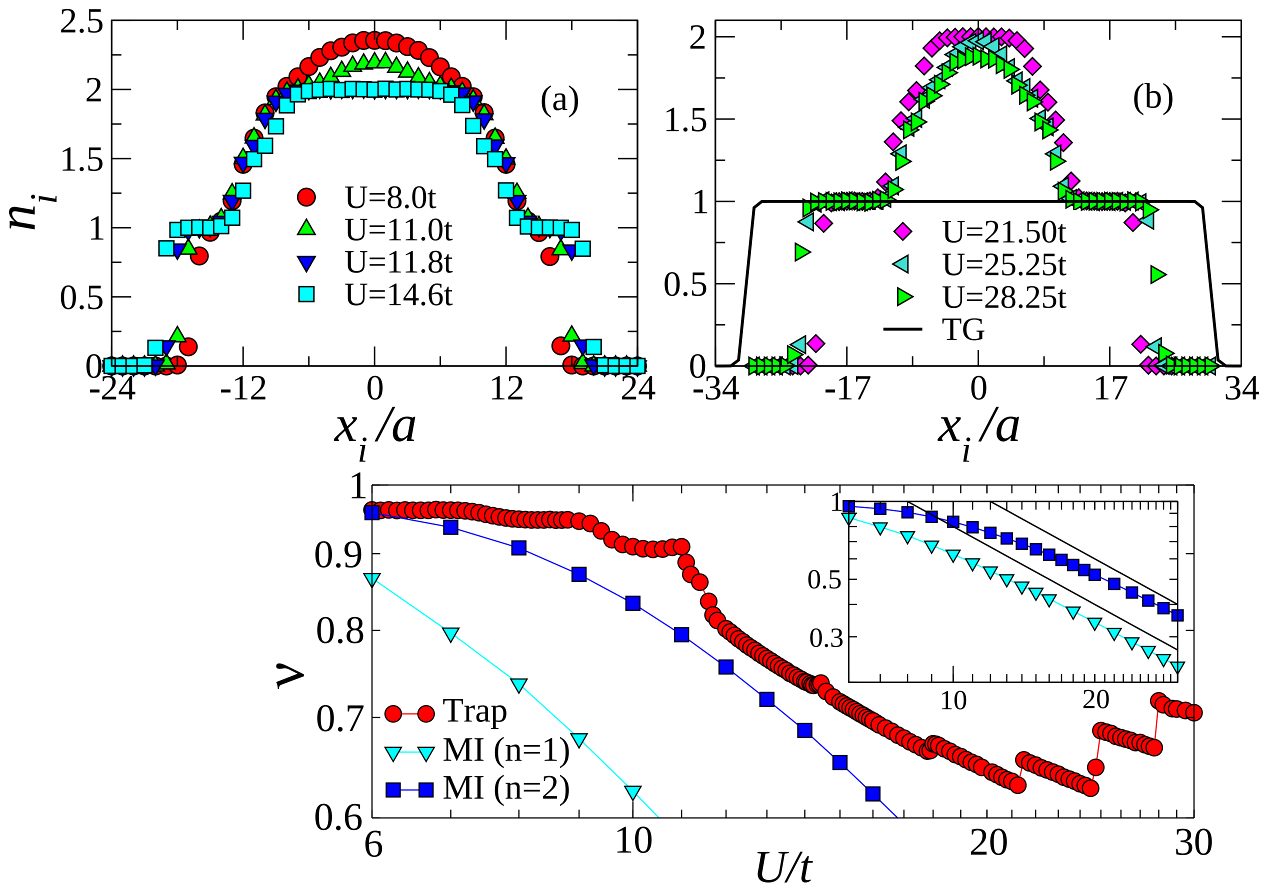
Above $U/t = 13$, additional structure.

Visibility kinks from redistribution between $n = 2$ and $n = 1$ MI

(Not from the formation of new SF or MI regions.)

Redistribution occurs discontinuously in U.

Density Profiles for System with $\rho = 2$ Mott Lobe



Visibility structures at $U = (11 - 12)t$ associated with
$\rho = 1$ MI shoulder development, and
appearance of $\rho = 2$ MI at trap center.
Further features in ν for $U \gtrsim 20$ upon breakup of $\rho = 2$ MI.

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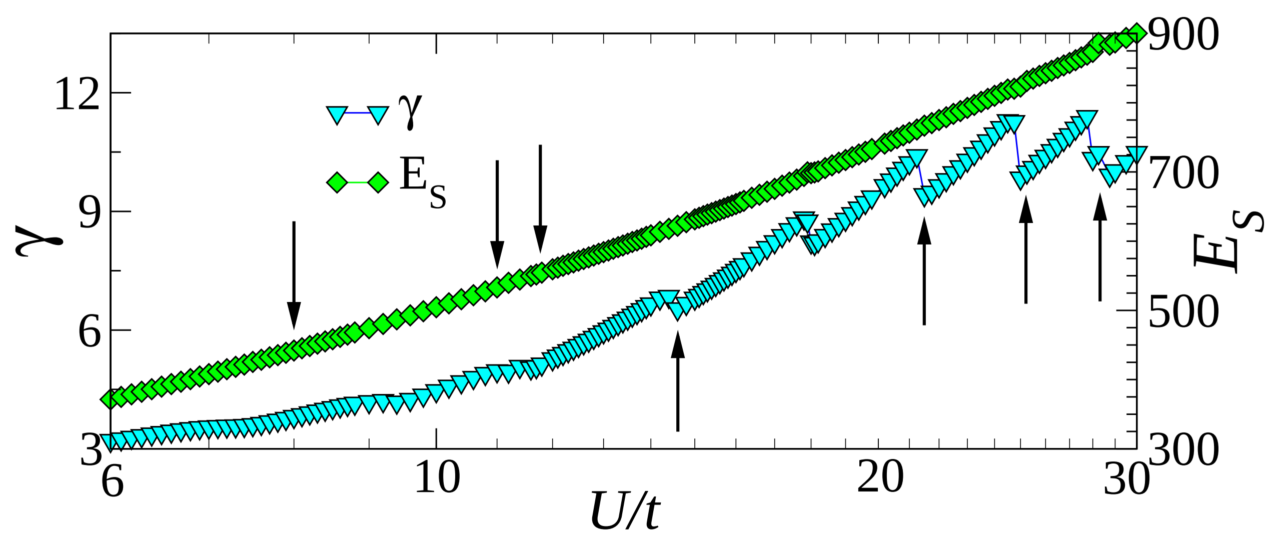
Energetics for System with $\rho = 2$ Mott Lobe



Trap center density larger than one (large double occupancy):

- γ and E_P increase with U/t.
- γ reflects the jumps produced by particle redistribution.
- Total energy of the system (E_S) increases continuously.

CONCLUSIONS

Equilibrium Phase Diagram of Confined Bosons

- Mott regions always coexist with SF.
- No quantum phase transition, in contrast to uniform case.

"Pause" in Evolution with On-Site Repulsion U

- Density distribution constant even when U increases by $t/2$.
- Emergence of static behavior caused by formation of MI "shoulders"
  Transfer of bosons to outer parts of system blocked.

Visibility

- Visibility behaves similar to experiment.
- Kinks: Redistribution of density between MI and SF regions.