



**The Abdus Salam  
International Centre for Theoretical Physics**



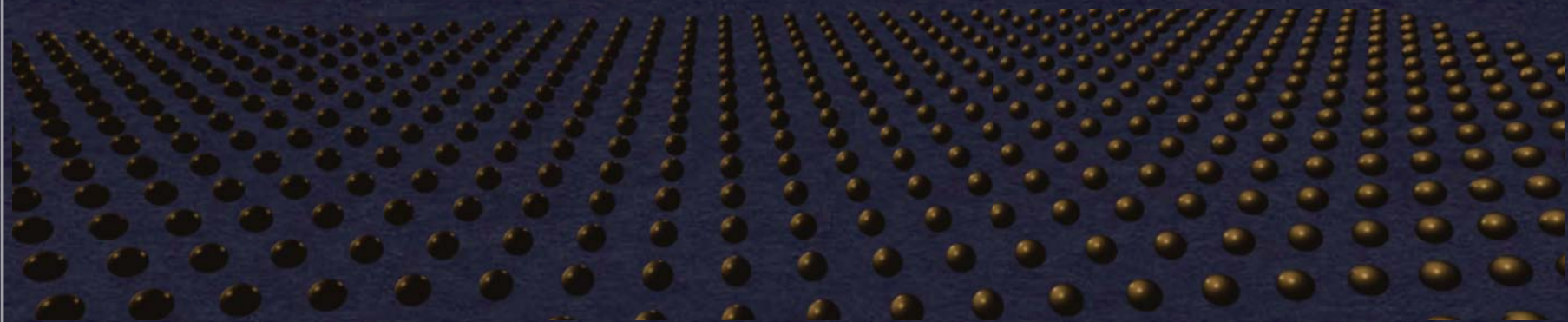
**2030-13**

**Conference on Research Frontiers in Ultra-Cold Atoms**

*4 - 8 May 2009*

**Beyond the Bose-Hubbard model**

MUELLER Erich  
*Cornell University Department of Physics  
109 Clark Hall  
Ithaca NY 14853-2501  
U.S.A.*



# Beyond The Bose Hubbard Model

Erich Mueller: Cornell University

Dan Goldbaum, Kaden Hazzard,

Joern Kuperschmidt

NSF  
DARPA OLE

# Confronting Assumptions

1. Are rubidium atoms in an optical lattice described by the standard Bose-Hubbard model?

Only for  $n < 2$

2. Do interactions play any role in time-of-flight expansion from an optical lattice?

No (for Rb and typical geometries)

3. Is the RF spectrum of bosons in an optical lattice dominated by a single sharp peak?

Yes for Rb, No if interactions are stronger



Are rubidium atoms in an optical lattice described by the standard Bose-Hubbard model?

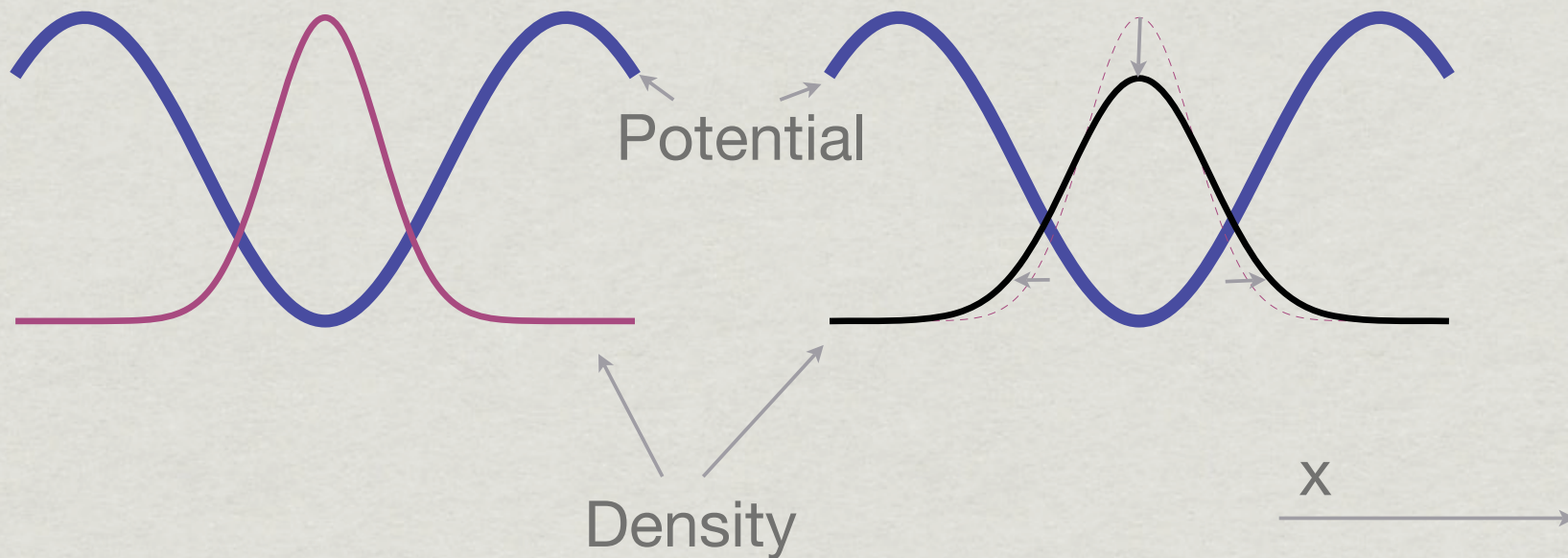
# Including on-site correlations in Bose-Hubbard Model

HAZZARD AND MUELLER, ARXIV:0902.4707

# On-site Correlations

**NON-INTERACTING**

**INTERACTING (REPULSIVE)**



**INTERACTIONS SPREAD  
OUT WAVEFUNCTIONS**

finite  $a$ :  
decrease  $U$   
increase  $t$



# Generalized Hubbard Model

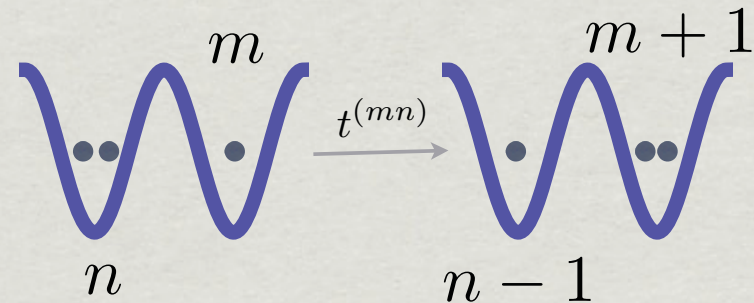
$$H = - \sum_{\langle i,j \rangle; m,n} t_{ij}^{(mn)} |m+1\rangle_i |n-1\rangle_k \langle m|_i \langle n|_j + \sum_{i,n} E_n |n\rangle_i \langle n|_i$$

+ pair hopping +...

## STANDARD HUBBARD MODEL

$$t_{ij}^{(mn)} = t \sqrt{n(m+1)}$$

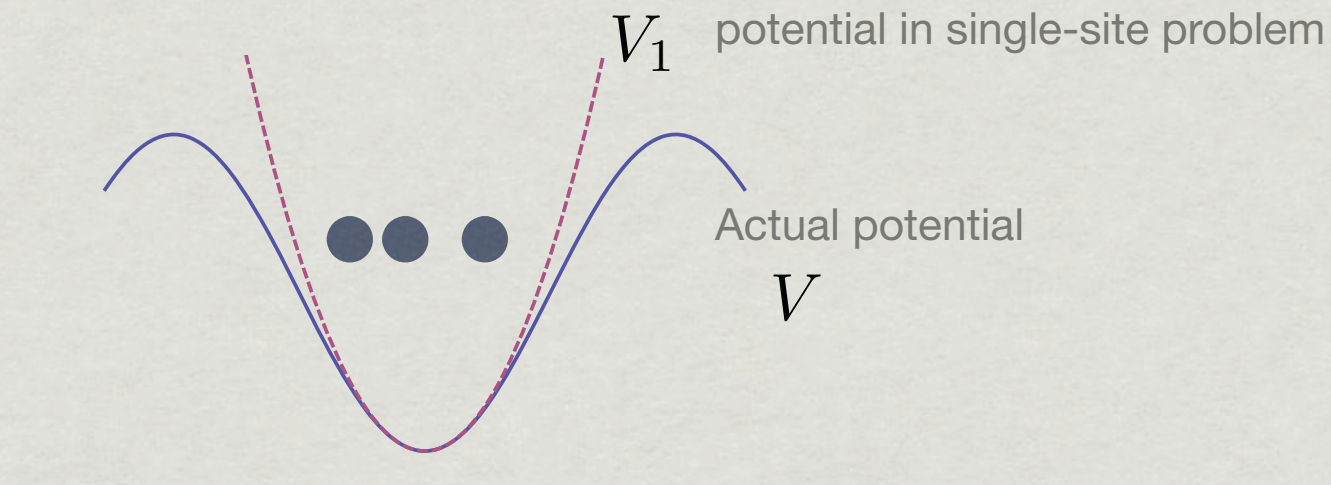
$$E_n = Un(n-1) - \mu n$$



How big are corrections?

# Finding coefficients

## SOLVE n-BODY 1-SITE PROBLEM



Full Hamiltonian

$$E_n \approx \langle n | H | n \rangle$$

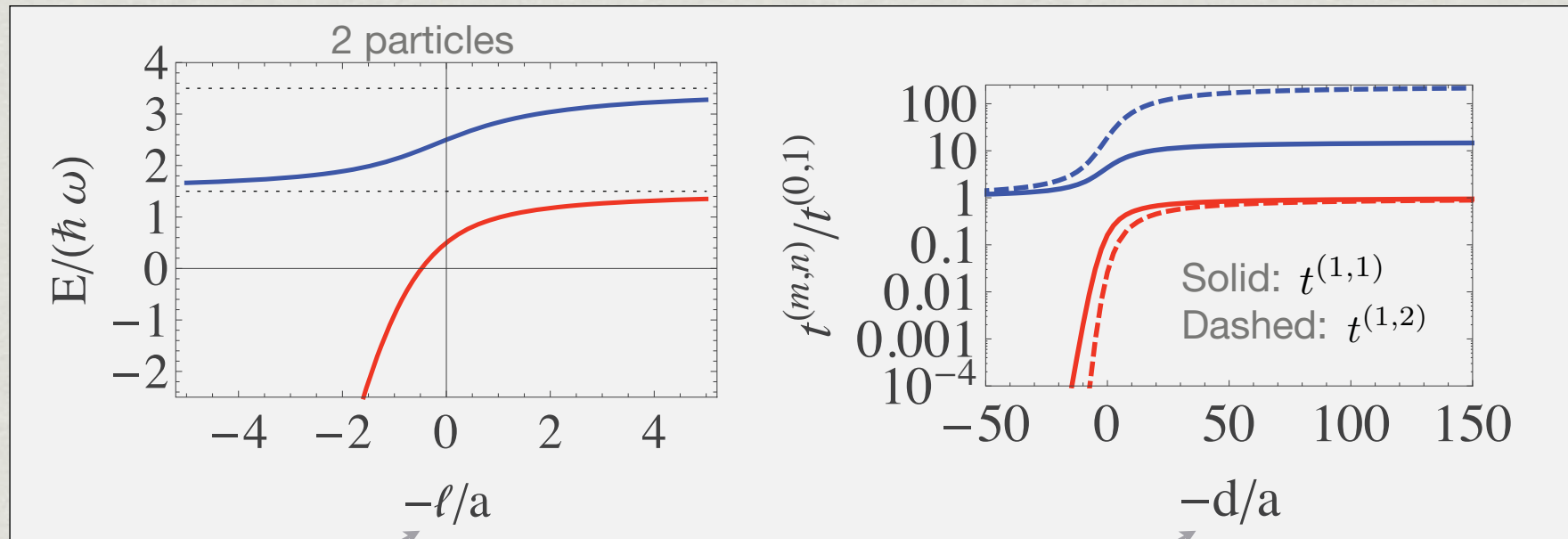
Lowest energy solution to 1-site problem

$$t_{ij}^{(mn)} = - \left[ \langle m+1 |_i \langle n-1 |_j \right] H \left[ |m \rangle_i |n \rangle_j \right] + \frac{E_m + E_n}{2} \left[ \langle m+1 |_i \langle n-1 |_j \right] \left[ |m \rangle_i |n \rangle_j \right]$$

# Results

$$V_{\text{lat}} = 15E_R$$

3D  
CUBIC LATTICE



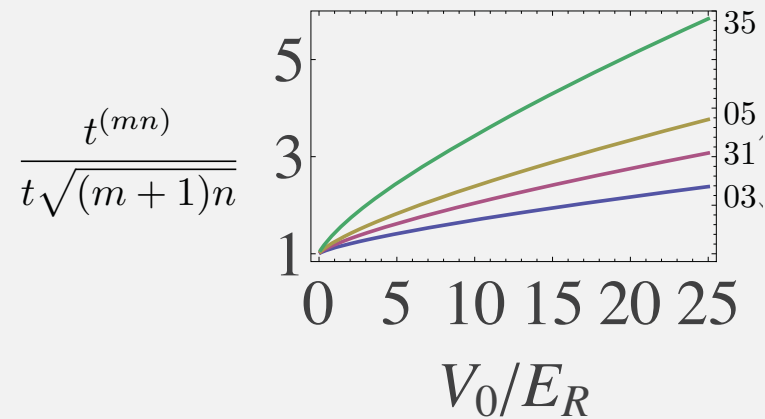
Oscillator Length

Lattice spacing

cf. T. Busch, B.-G. Englert, K. Rzazewski, and M. Wilkens  
Foundations of Physics, 28, 549 (1998)



# Rubidium Parameters

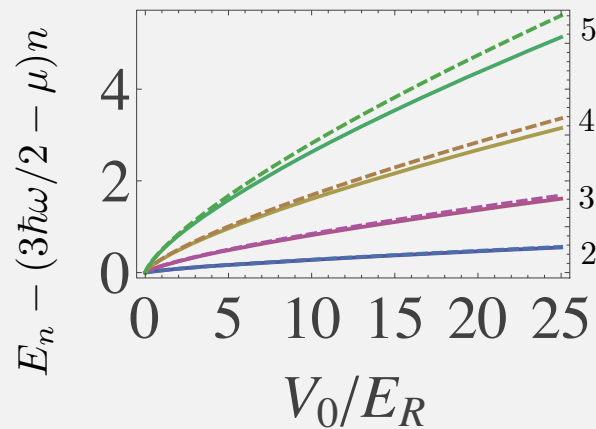


(Gaussian ansatz for single-site wavefunction)

## CONCLUSIONS:

Interactions dramatically modify hopping matrix elements.

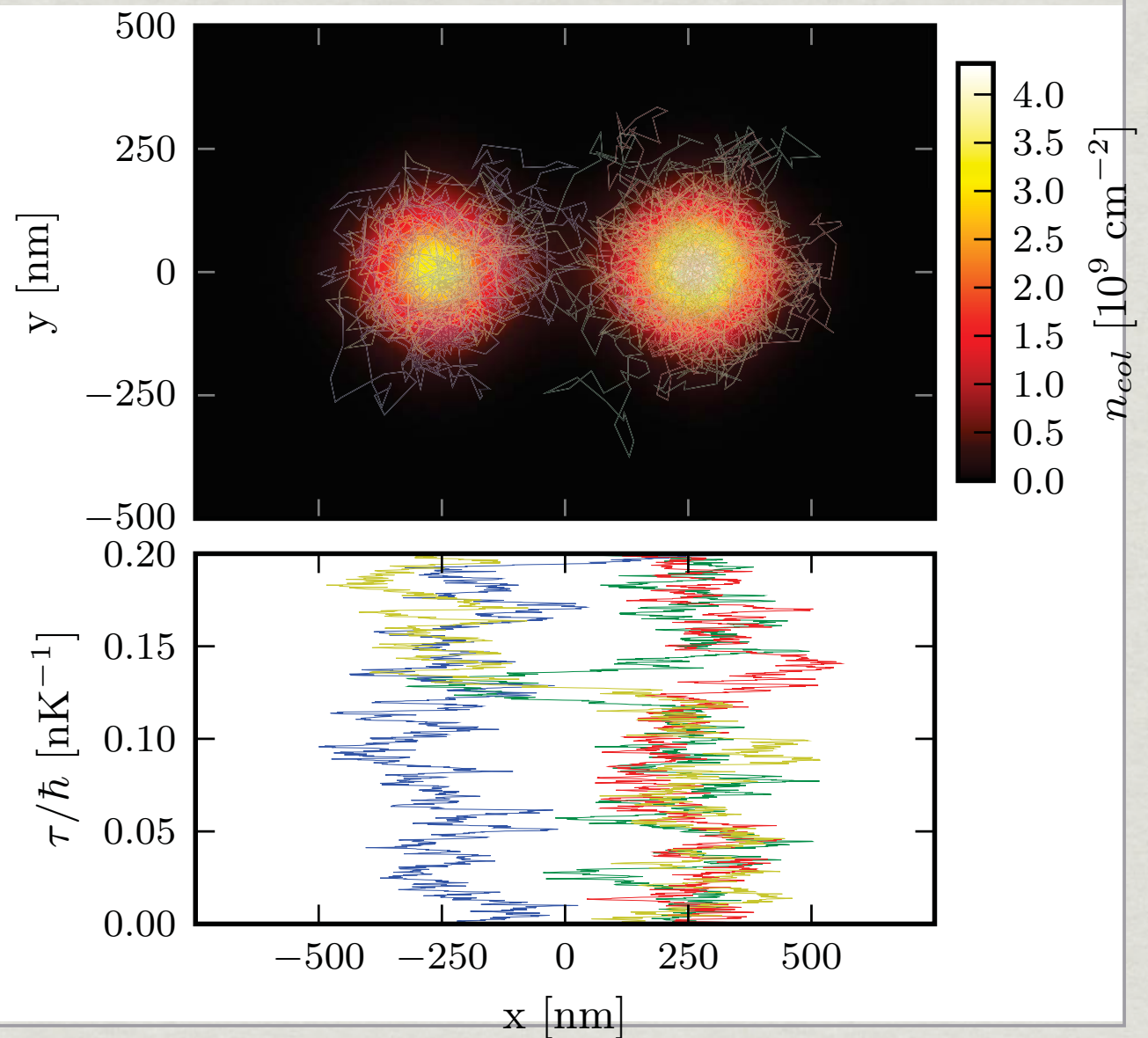
Higher Mott lobes require deeper lattice than thought



Reported in experiments:  
[ex. Campbell et al. Science  
313 (2006)]

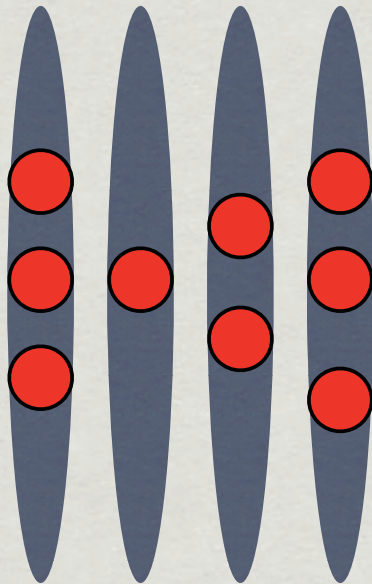
# In progress

- \* Exactly solve 2-site problem -- extract parameters



# More exotic settings

## ARRAYS OF 1D TUBES



Hopping requires rearranging few-body state on each site.

Restrict to lowest energy  $n$ -particle states on each site: **same effective model**

Energy scales below on-site excitation gap:  
topology of phase diagram: same as standard Bose-Hubbard

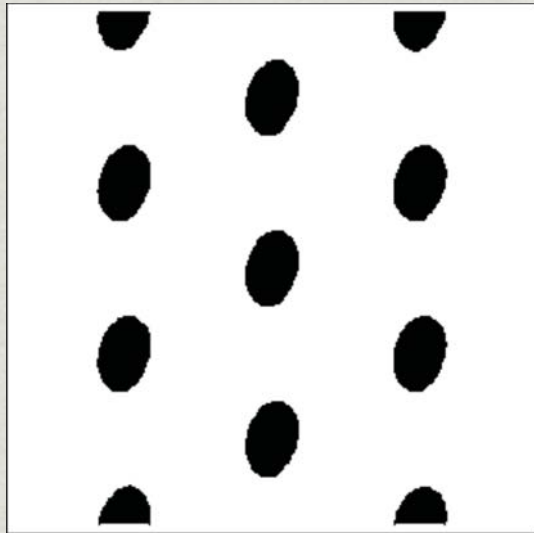
$$H = - \sum_{\langle i,j \rangle; m,n} t_{ij}^{(mn)} |m+1\rangle_i |n-1\rangle_j \langle m|_i \langle n|_j + \sum_{i,n} E_n |n\rangle_i \langle n|_i$$



# More exotic settings

## ARRAYS OF QUANTUM HALL PUDDLES

Experiments (uncoupled puddles):  
Edina Sarajlik, Nate Gemelke, and Steve Chu



rotate near on-site small  
oscillation frequency

---

Theory of spinning up uncoupled puddles:  
Popp, Paredes, and Cirac, PRA 2004  
Baur, Hazzard, and Mueller, PRA 2008

Q: What happens when hopping is allowed?

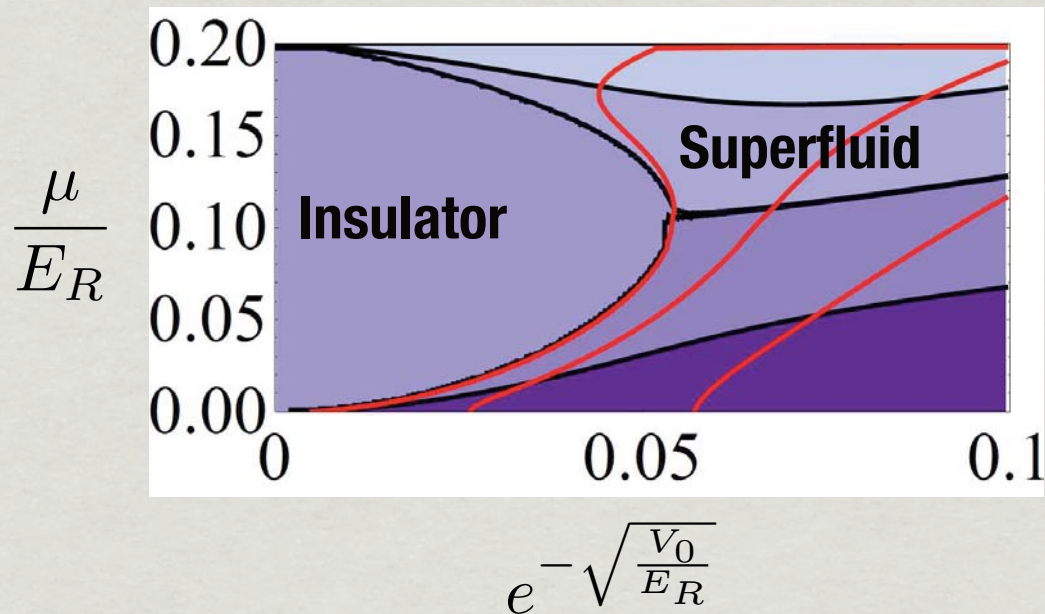
Restrict to lowest energy n-particle states  
on each site: (Laughlin State)

Get same effective model

$$H = - \sum_{\langle i,j \rangle; m,n} t_{ij}^{(mn)} |m+1\rangle_i |n-1\rangle_j \langle m|_i \langle n|_j + \sum_{i,n} E_n |n\rangle_i \langle n|_i$$

# Coupled Quantum Hall Puddles

## PHASE DIAGRAM



## DEEP LATTICE

Integrals -- can do analytically

$$t^{(01)} = t$$

$$t^{(02)} = t \frac{\pi^2}{32} \sqrt{\frac{V_0}{E_R}}$$

$$t^{(12)} = t \frac{\pi^4}{1024} \sqrt{\frac{V_0}{E_R}}$$



# Coupled Quantum Hall Puddles

## SUPERFLUID ORDER PARAMETER

$$\left\langle \sum_i |n\rangle_i \langle n-1|_i \right\rangle = \langle R^\dagger \rangle \neq 0$$

$$R^\dagger \psi(z_1, \dots, z_n) = \phi(z_1, \dots, z_{n+1})$$

$$\propto e^{-|z_{n+1}|^2} \prod_{i=1}^n (z_{n+1} - z_i)^2 \psi(z_1, \dots, z_n)$$

Coupled puddles probes non-local order parameter introduced by Girvin and MacDonald, PRL 58, 1252 (1987)



# Confronting Assumptions

1. Are rubidium atoms in an optical lattice described by the standard Bose-Hubbard model?

Only for  $n < 2$

2. Do interactions play any role in time-of-flight expansion from an optical lattice?

No (for Rb and typical geometries)

3. Is the RF spectrum of bosons in an optical lattice dominated by a single sharp peak?

Yes for Rb, No if interactions are stronger

Do interactions play any role in time-of-flight expansion from an optical lattice?

# Interactions during time-of-flight expansion

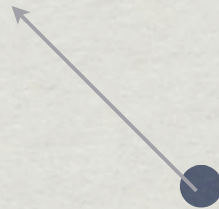
KUPFERSCHMIDT, GOLDBAUM AND MUELLER, UNPUBLISHED  
GOLDBAUM AND MUELLER, PRA (2009)



# Interpreting Time-of-flight expansion

Standard Interpretation: Long-time expansion = Momentum distribution

Any atom that moves distance  $d$  in time  $t$  must have momentum  $p = md/t$



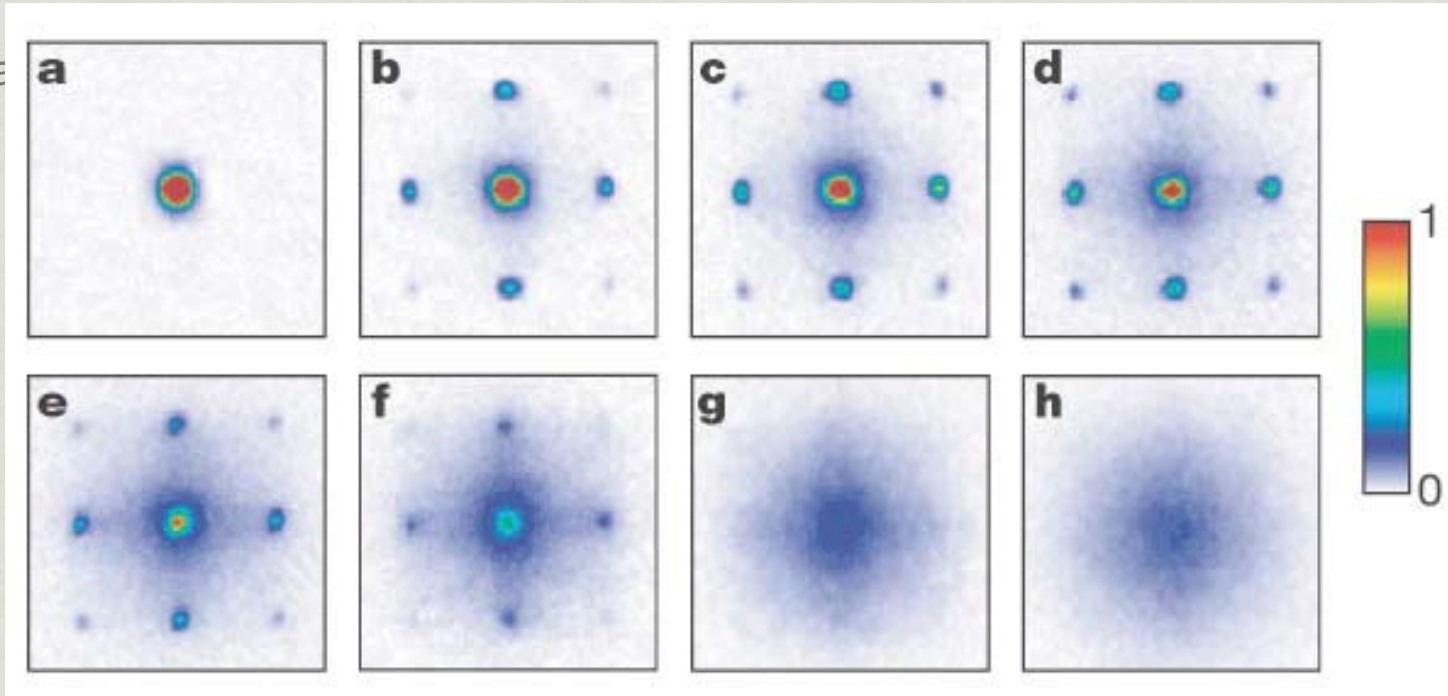
All atoms are initially at  $r=0$

Requires: No interactions during expansion



# Interpreting Time-of-flight expansion

Sta



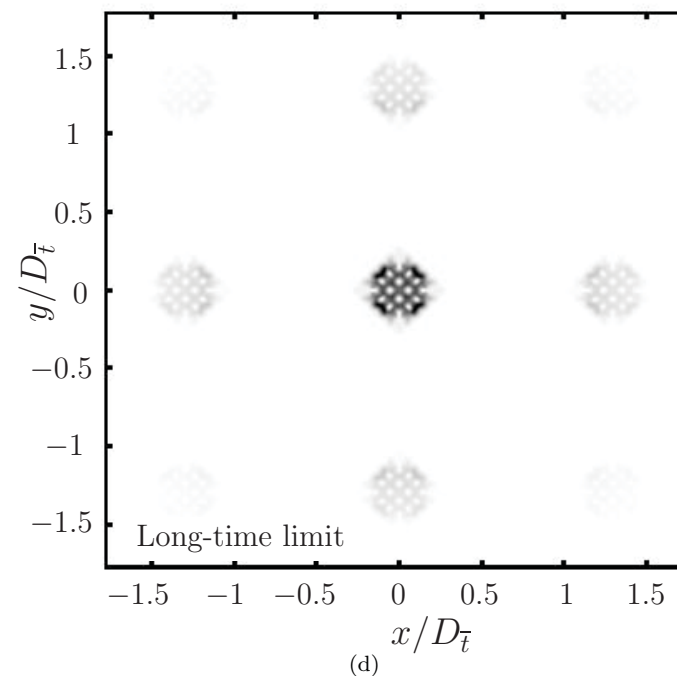
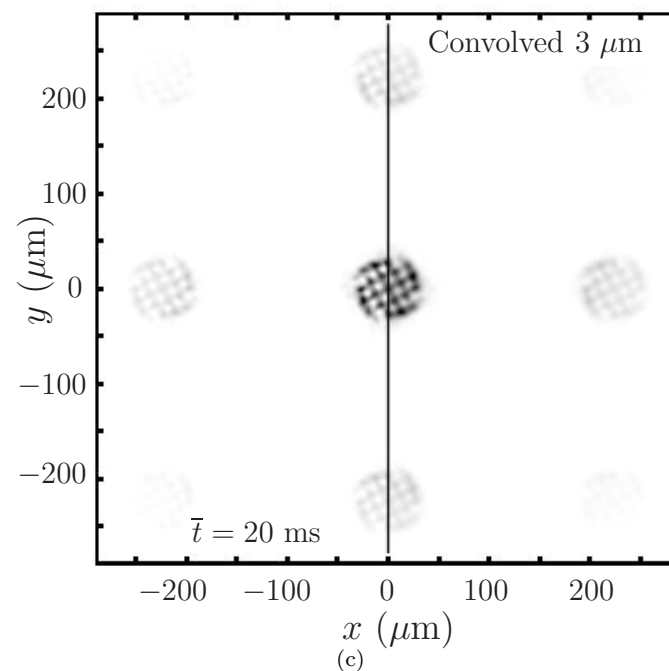
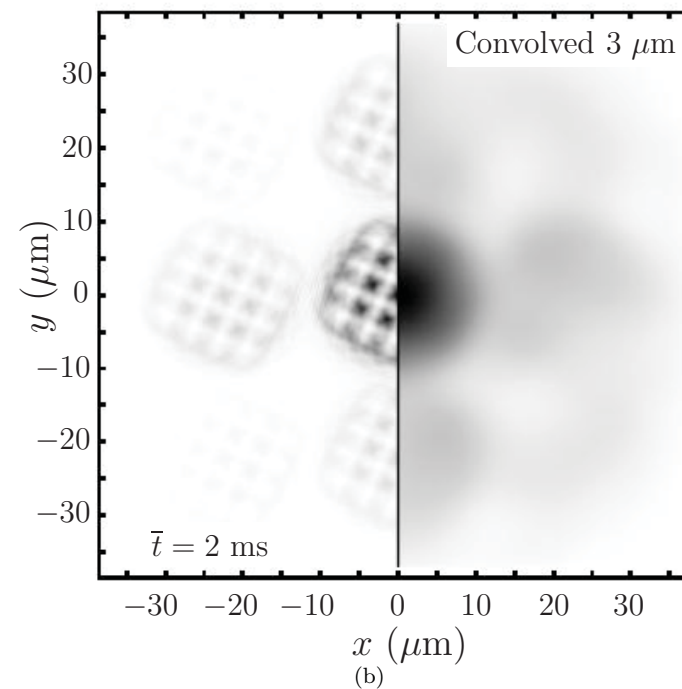
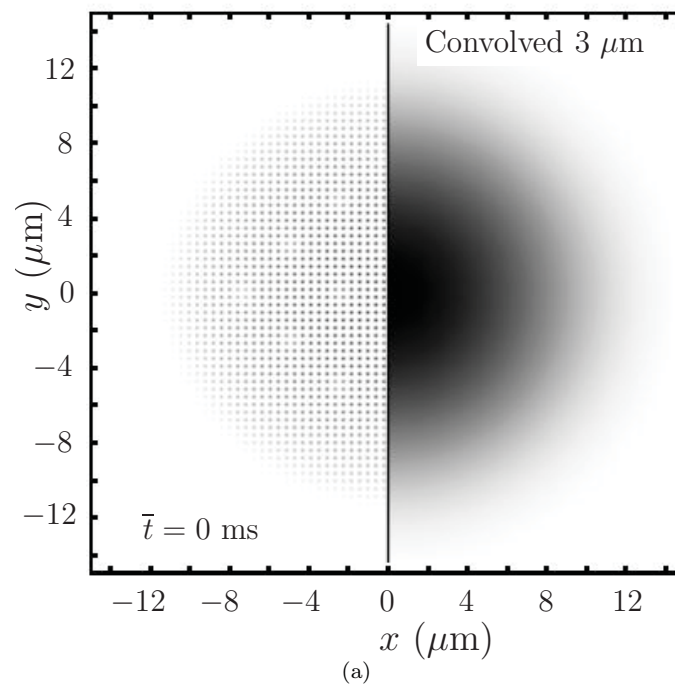
initially at  $r=0$

Requires: No interactions during expansion

# VORTICES IN TIME OF FLIGHT FROM A ROTATING OPTICAL LATTICE

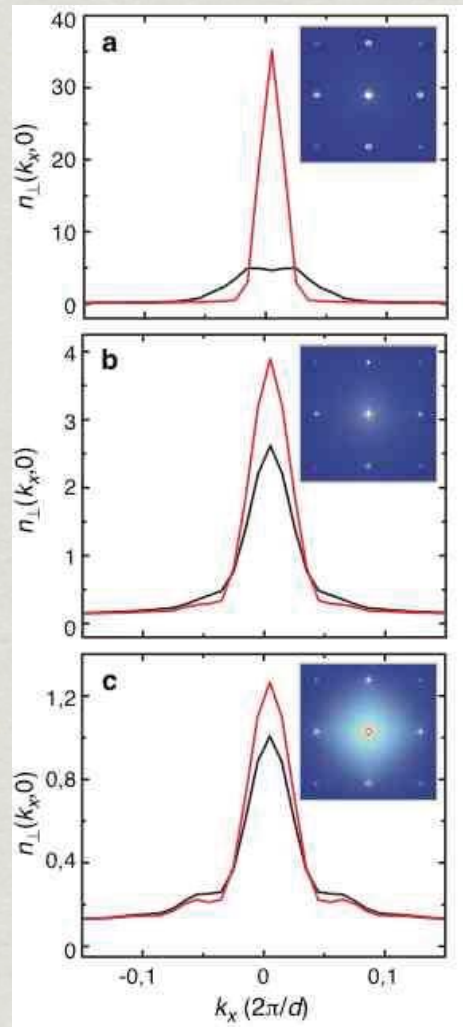
Assumes:  
no interactions  
during expansion

Goldbaum and  
Mueller, PRA 2009





# Quantitative



We now discuss briefly the effect of interactions on the expansion, and show that this is negligible compared to the finite ToF effect. When the cloud has just been released from the lattice potential, each on-site wavefunction  $W_\mu$  expands independently with a characteristic expansion time  $\omega_L^{-1}$ , until  $t \approx t^* = \sqrt{\hbar/(\omega_L E_R)}$  where the wavefunctions expanding from neighboring sites start to overlap. At this time, in the usual situation where  $\omega_L t^* \gg 1$ , the local density has dropped dramatically by a factor  $(\omega_L t)^{-3} \ll 1$ . Hence, the interaction energy converts into kinetic energy on the time scale of a few oscillation periods only, and expansion becomes rapidly ballistic. The parameter controlling the importance of interactions is given by  $\eta = \frac{U}{\hbar\omega_L} \approx \sqrt{8\pi} \frac{a_s n_0}{\lambda_L} \left(\frac{V_0}{E_R}\right)^{1/4}$ , with  $U$  being the on-site interaction energy. For typical parameters,  $\eta$  is small (for instance  $\eta \approx 0.05$  for  $V_0 = 10 E_R$  and the experimental parameters of [3]). Hence, we expect only small corrections to the non-interacting picture of ballistic expansion. This has been confirmed using a variational model of the expanding condensate wavefunction [15]. This model predicts that the "Wannier" envelope expands faster as compared to the non-interacting case, which does not affect the interference pattern, and picks up a site-dependent phase factor formally similar to the Fresnel term discussed previously, but with a very weak prefactor  $\eta \ll 1$  which has negligible influence in practice. We conclude that interactions essentially contribute to the expansion of the on-site wavefunctions, without significant dephasing of the interference pattern.

Gerbier, Trotzky, Foeling, Schnorberger, Thompson, Widera, Bloch, Pollet, Troyer, Capogrosso-Sansone, Prokof'ev, Svistunov, PRL 101, 155303 (2008)



# Method

**INITIAL:**

Gutzwiller Ansatz

$$\psi = \prod_{\text{sites } i} \left[ \sum_{\text{number } n} \phi_i^{(n)} \right]$$

Neglect interactions between atoms on different sites

**AFTER EXPANSION:**

$$\psi = \prod_{\text{sites } i} \left[ \sum_{\text{number } n} \phi_i^{(n)}(t) \right]$$

Just time-evolve the n-body wavefunction on each site.

# Density

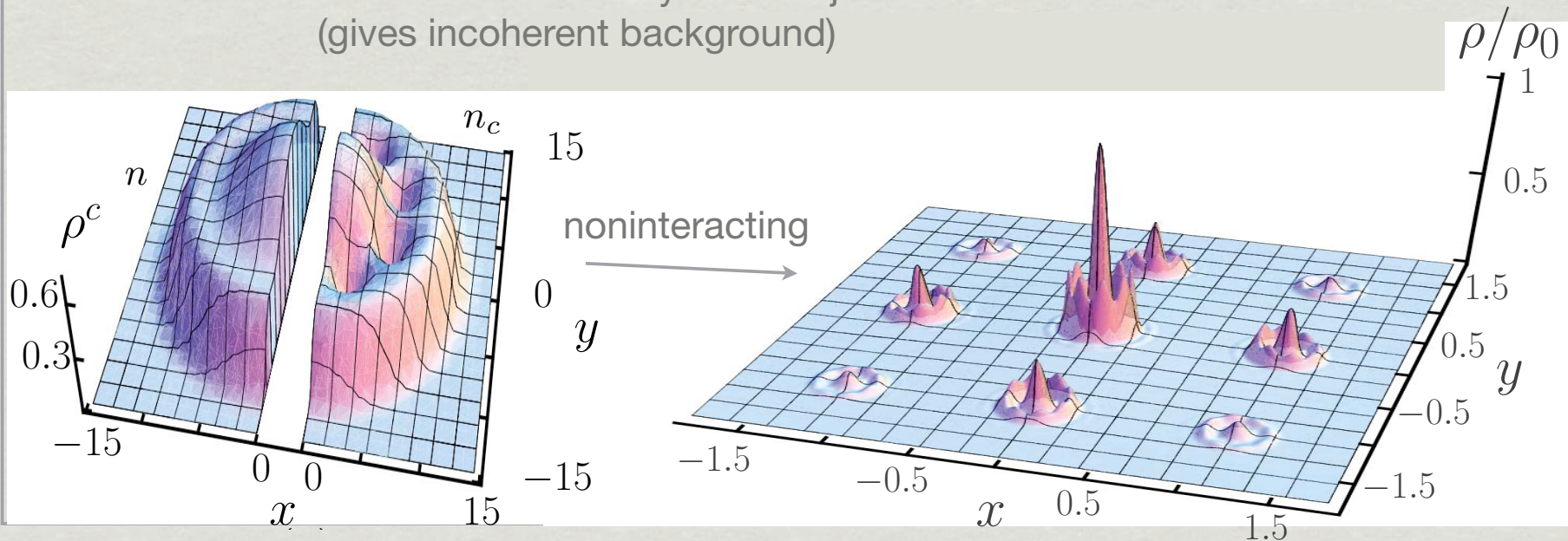
$$n(r, t) = \left| \sum_j \Lambda_j(r, t) \right|^2 + \sum_j \left( \rho_j(r, t) - |\Lambda_j(r, t)|^2 \right)$$

$$\Lambda_j(r, t) = \sum_n \sqrt{n+1} \int dr_1, \dots, dr_n (\phi_j^{(n+1)}(r_1, \dots, r_n, r; t))^* \phi_j^{(n)}(r_1, \dots, r_n; t)$$

= time evolved “superfluid order parameter” on site  $j$   
(gives interference peaks)

$$\rho_j(r, t) = \sum_n n \int dr_1 \dots dr_{n-1} \left| \phi_i^{(n)}(r_1, \dots, r_{n-1}, r; t) \right|^2$$

= time evolved “density” on site  $j$   
(gives incoherent background)





# Density

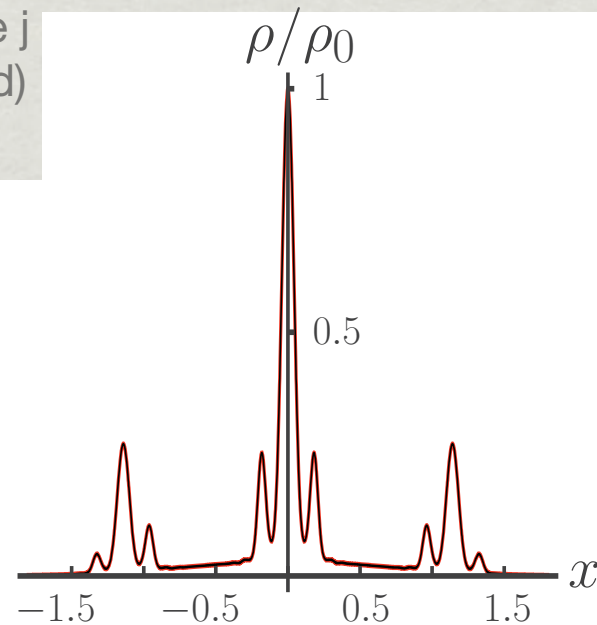
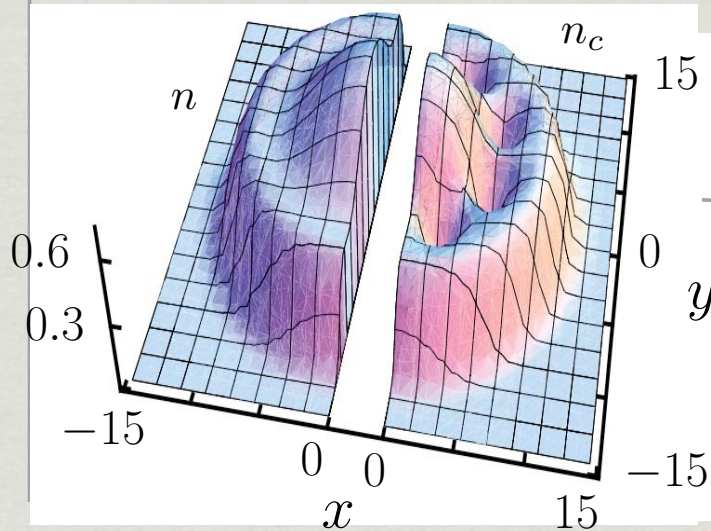
$$n(r, t) = \left| \sum_j \Lambda_j(r, t) \right|^2 + \sum_j \left( \rho_j(r, t) - |\Lambda_j(r, t)|^2 \right)$$

$$\Lambda_j(r, t) = \sum_n \sqrt{n+1} \int dr_1, \dots, dr_n (\phi_j^{(n+1)}(r_1, \dots, r_n, r; t))^* \phi_j^{(n)}(r_1, \dots, r_n; t)$$

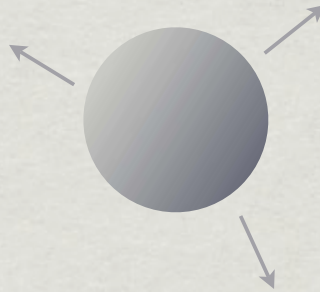
= time evolved “superfluid order parameter” on site  $j$   
(gives interference peaks)

$$\rho_j(r, t) = \sum_n n \int dr_1 \dots dr_{n-1} \left| \phi_i^{(n)}(r_1, \dots, r_{n-1}, r; t) \right|^2$$

= time evolved “density” on site  $j$   
(gives incoherent background)



# Interactions



- \* Sites with more particles spread out more
  - \* Too much spread -- only interfere in overlap region
- \* Sites with more particles gain extra phase
  - \* Dephasing kills interference

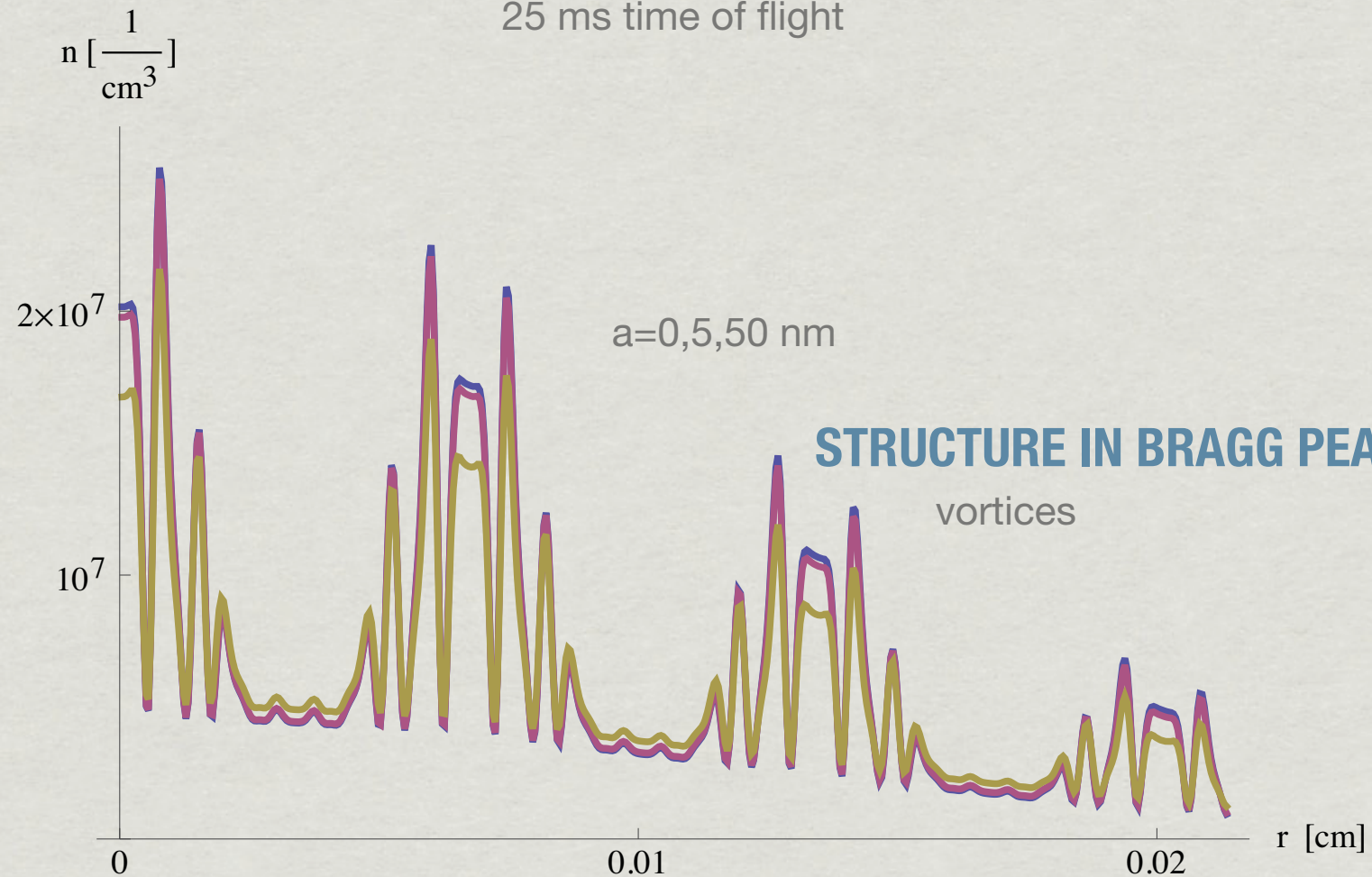


# Result

2D lattice

$$V_0 = 10E_R$$

25 ms time of flight



**SMALL PARAMETER**

$$\frac{\text{scattering length}}{\text{size of Wannier state}} = 0.066$$

# Confronting Assumptions

1. Are rubidium atoms in an optical lattice described by the standard Bose-Hubbard model?

Only for  $n < 2$

2. Do interactions play any role in time-of-flight expansion from an optical lattice?

No (for Rb and typical geometries)

3. Is the RF spectrum of bosons in an optical lattice dominated by a single sharp peak?

Yes for Rb, No if interactions are stronger



Is the RF spectrum of bosons in an optical lattice dominated by a single sharp peak?

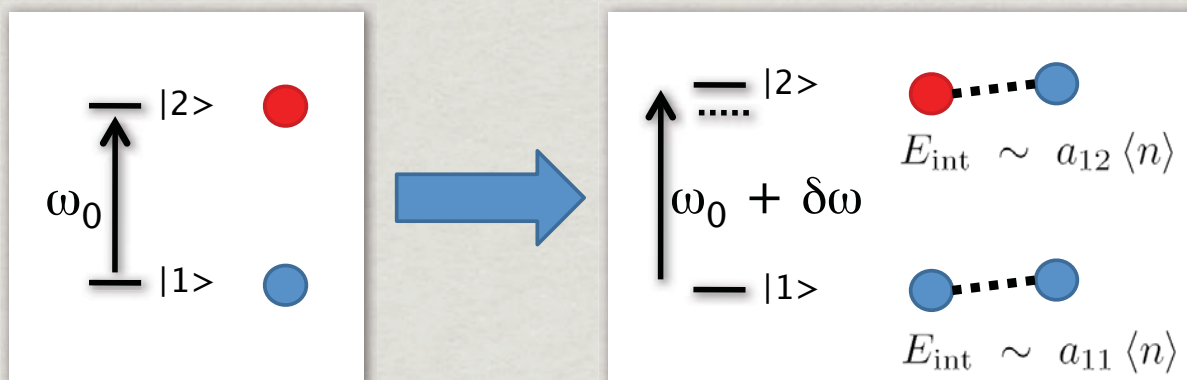
# RF Spectra of Lattice Bosons

HAZZARD AND MUELLER, UNPUBLISHED

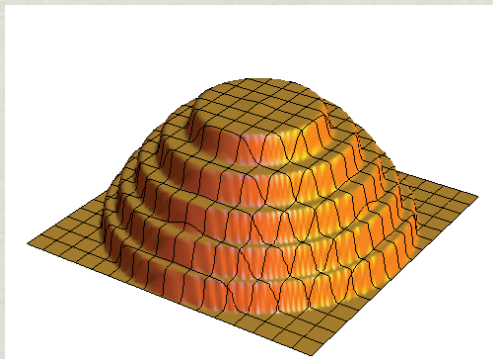
# RF Spectroscopy

## COLD COLLISION SHIFT

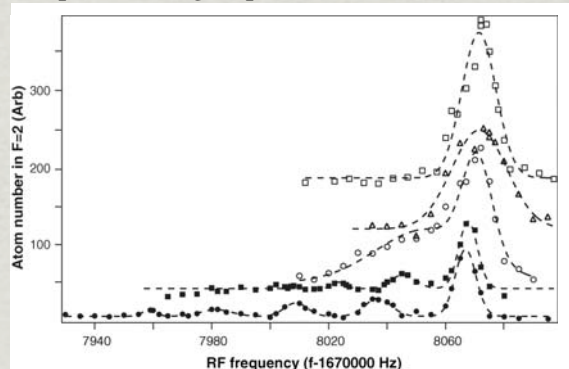
Sum Rule: Oktel and Levitov, PRL 83, 6 (1999)



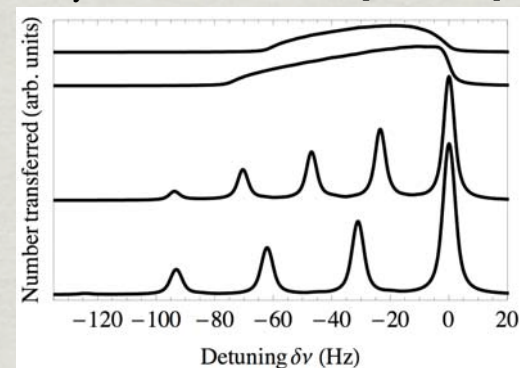
## BOSONS IN OPTICAL LATTICE



Exp: Ketterle group [Science, 313, 649 (2006)]



Thy: Hazzard and Mueller [PRA 2007]



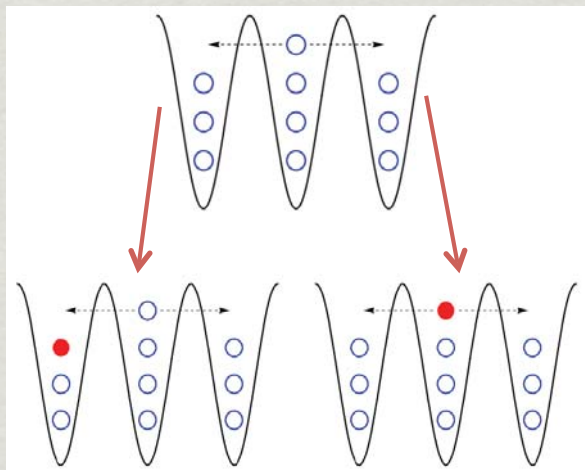


# Beyond the sum rule

Previous assumption: Homogeneous spectrum is sharp  
Line Shape in trap -- solely from inhomogeneities

Question assumption: Sun, Lannert, Vishveshwara, Phys. Rev. A 79, 043422 (2009)  
(simple case -- violated sum rule)

## PHYSICAL PICTURE



RF photon generates one of two  
types of excitations

Homogeneous spectrum:  
bimodal

Our new calculation: Random Phase Approximation

# EOM approach to RPA

$$H = - \sum_{\sigma=\{a,b\},\langle i,j \rangle} t_{\sigma} c_{i,\sigma}^{\dagger} c_{j,\sigma} + \sum_{\sigma,j} (V_{j,\sigma} - \mu) c_{j,\sigma}^{\dagger} c_{j,\sigma} + \sum_j \left( \sum_{\alpha,\beta} \frac{U_{\alpha\beta}}{2} c_{j,\alpha}^{\dagger} c_{j,\beta}^{\dagger} c_{j,\beta} c_{j,\alpha} \right)$$

$$H_{\text{rf}} = \sum_j \gamma(t) c_b^{\dagger} c_a + \text{H.c.}$$

Make time dependent variational ansatz

$$|\psi(t)\rangle = \bigotimes_i \left[ \sum_n (f_n(t) |n, 0\rangle_i + g_n(t) |n-1, 1\rangle_i) \right]$$

Minimize

$$S = \int dt \left[ \frac{1}{i} \langle \psi(t) | \partial_t | \psi(t) \rangle - \langle \psi(t) | H + H_{\text{rf}} | \psi(t) \rangle \right]$$

Solve EOM to linear order in  $H_{\text{rf}}$

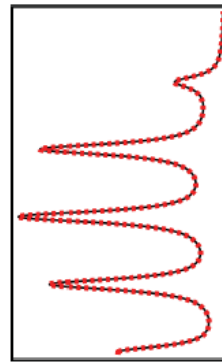
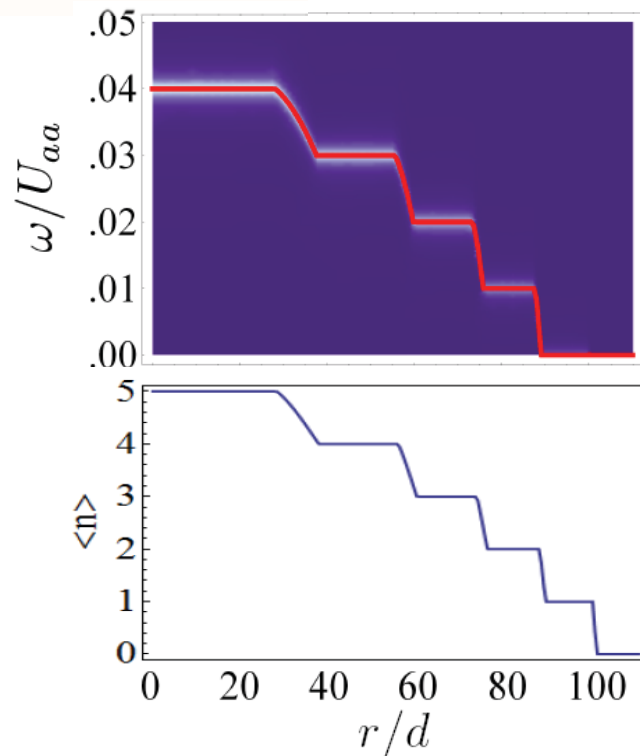
plot rate of transfer vs frequency

**SATISFIES SUM RULES, WARD IDENTITIES,...**



# Result -- Rb parameters

$$U_{ab} = 1.025U_{aa}$$



**Rb**

Final state int almost same as initial

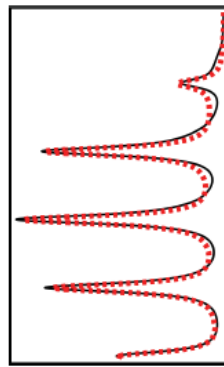
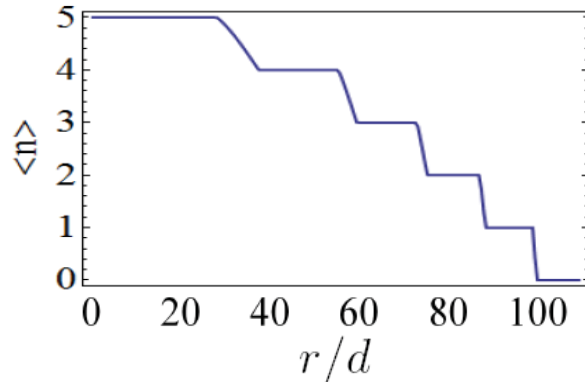
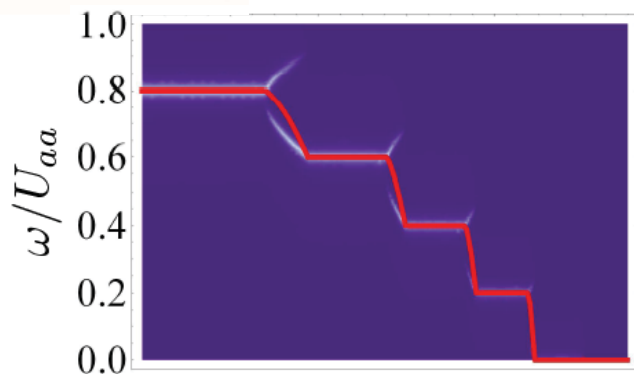
**RESULT**

Homogeneous spectrum is unimodal

Red line: Sum Rule Calculation

# Result -- Stronger int

$$U_{ba} = 1.2U_{aa}$$



$\chi^{(R)}$

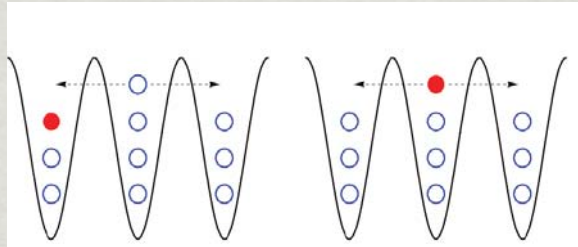
Bimodality observable:

Spatially resolved spectrum shows two shells

Trap averaged spectrum  
(no signature)



# Hybridization

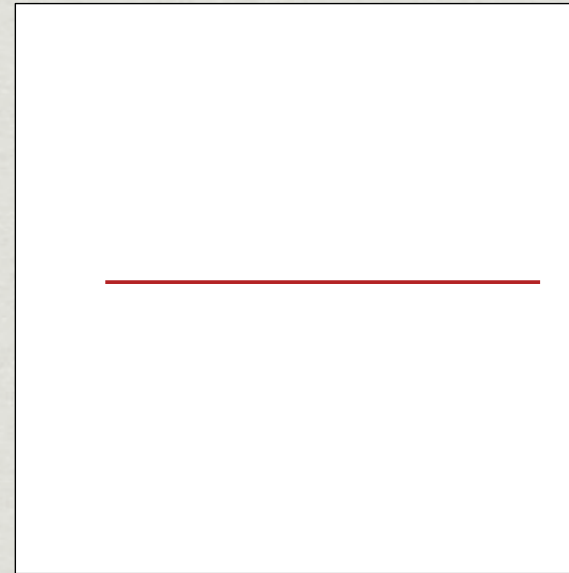


KE cost:

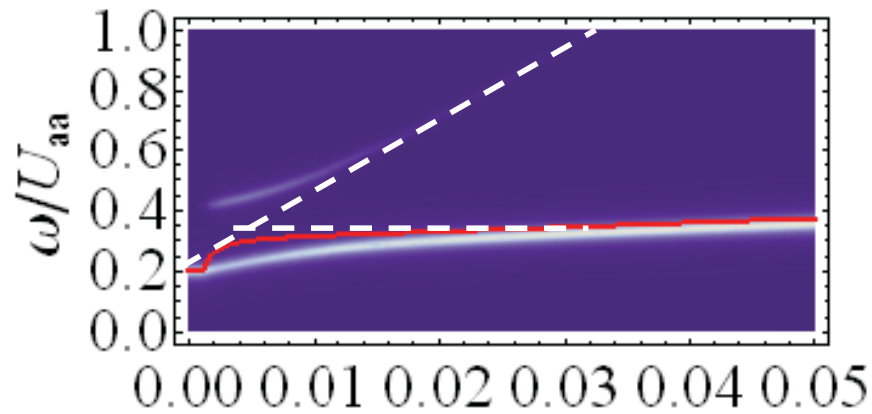
Blocks hopping of  
excess particles

KE cost:

loss of Bose enhancement

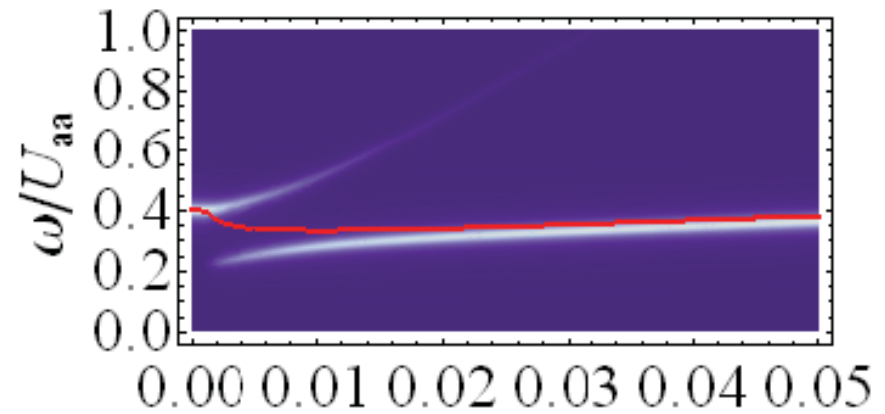


$\mu = 1.98$



$$U_{ba} = 1.2U_{aa} \quad t_a/U_{aa}$$

$\mu = 2.02$



$$t_a/U_{aa}$$

# Summary

1. Are rubidium atoms in an optical lattice described by the standard Bose-Hubbard model?

Only for  $n < 2$

2. Do interactions play any role in time-of-flight expansion from an optical lattice?

No (for Rb and typical geometries)

3. Is the RF spectrum of bosons in an optical lattice dominated by a single sharp peak?

Yes for Rb, No if interactions are stronger