Small clusters modeled by continuous Hamiltonians

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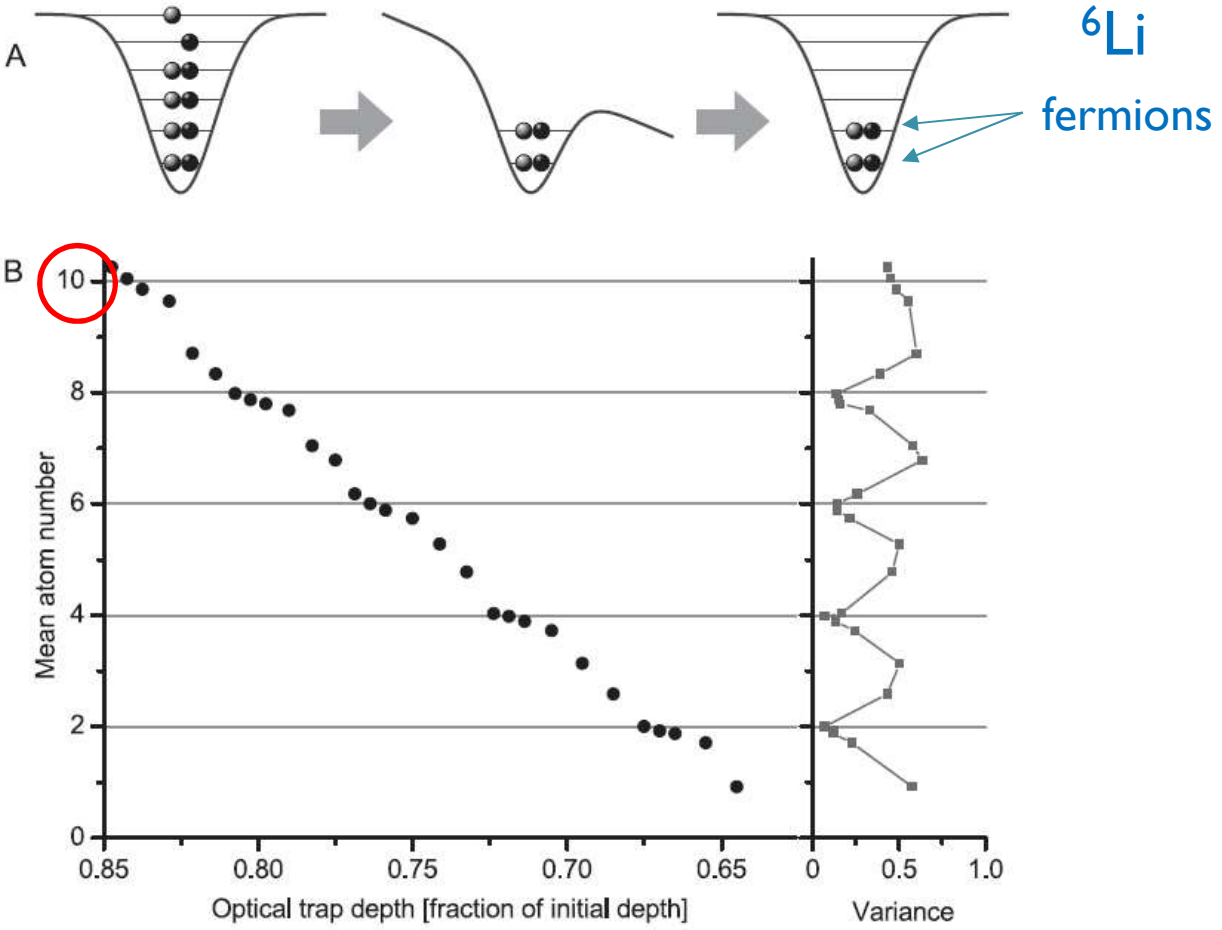
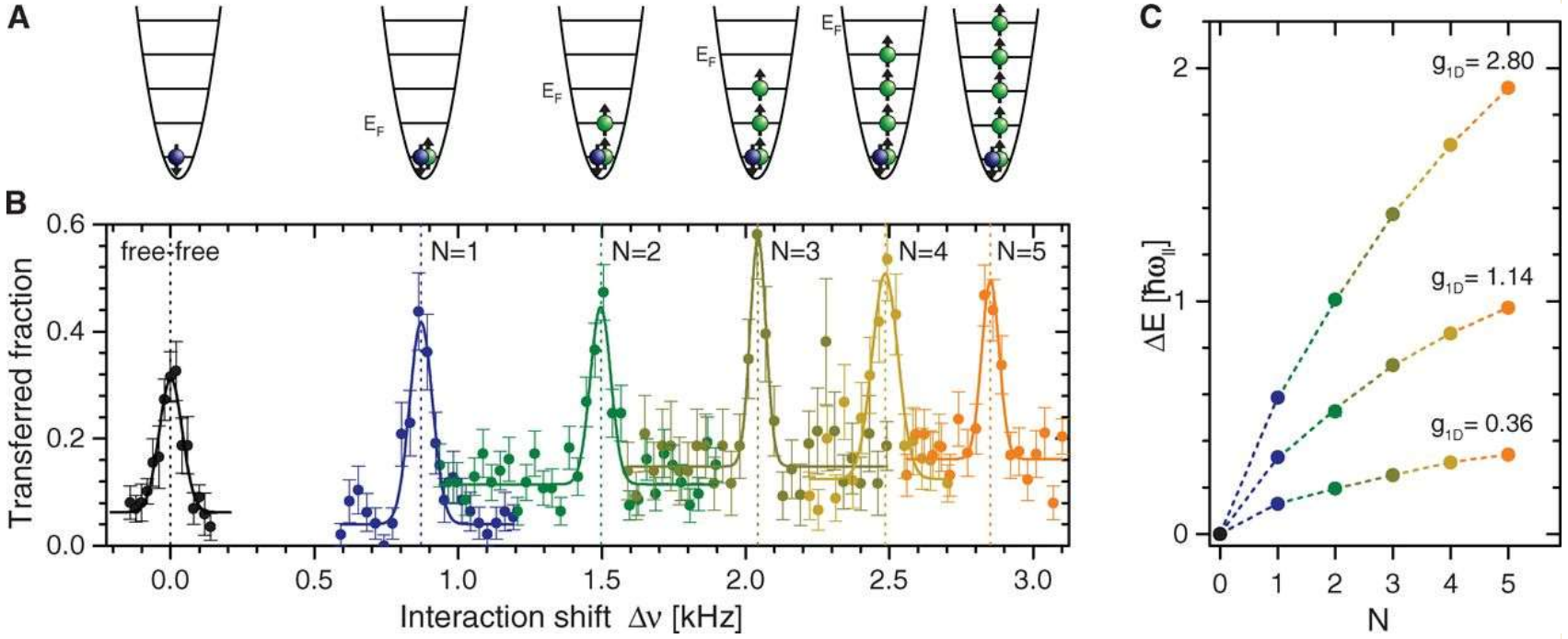
The number of atoms in an optical trap can be controled



1D

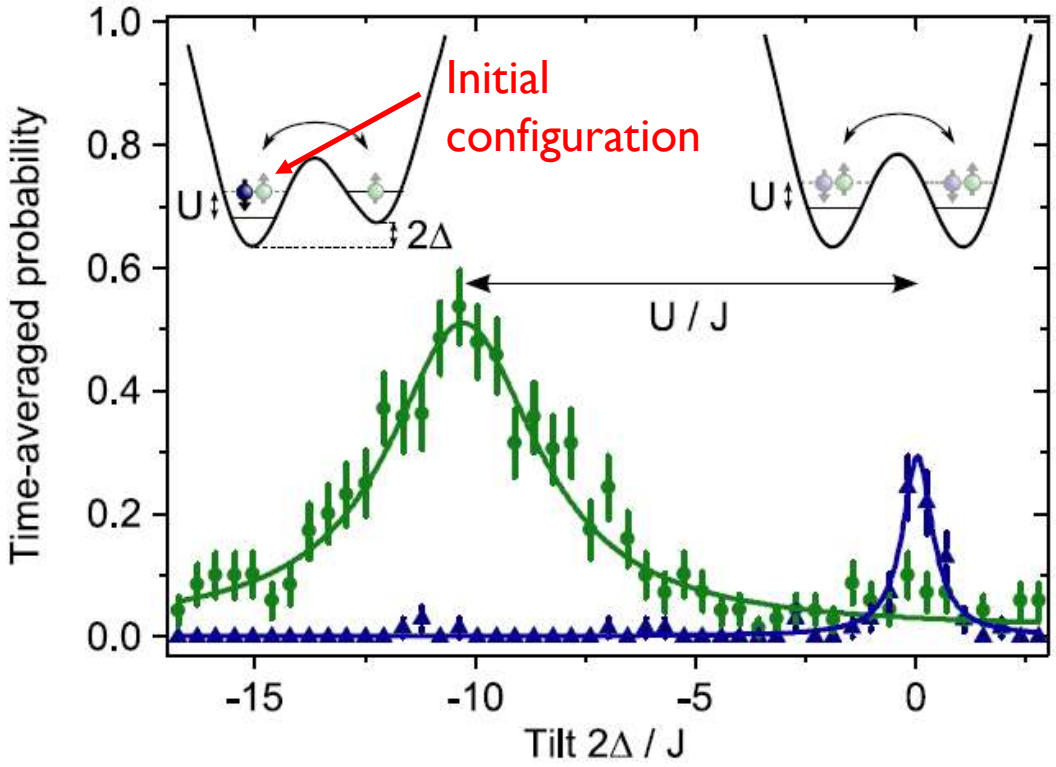
F. Serwane et al. Science 332 336 (2011)

N+1



A. N. Wenz et al. Science 342 457 (2013)

The potential does not have to be harmonic

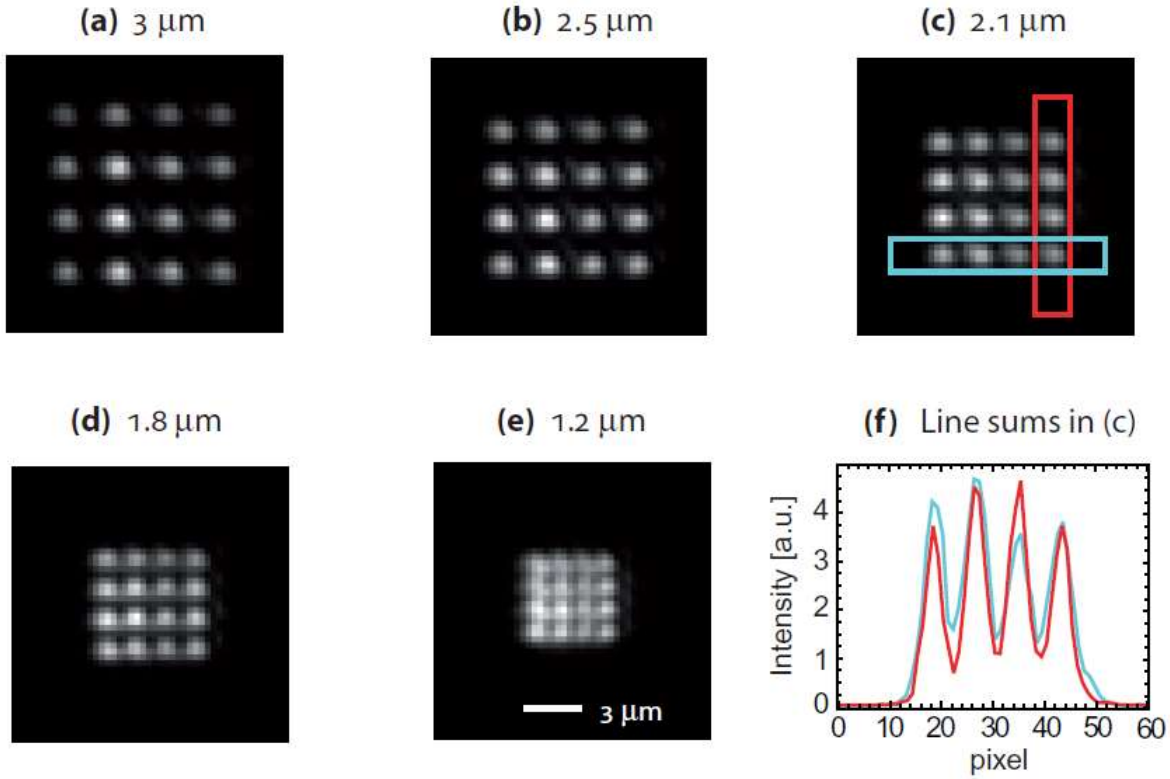


Probability of finding a single particle in the right well

Probability of finding two particles in the right well

S. Murman et al. PRL, 114 080402 (2015)

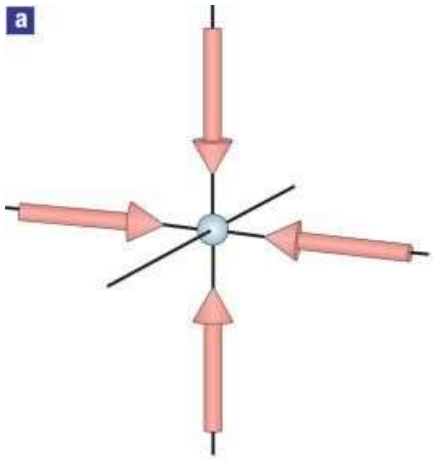
You can have also optical lattice microtraps



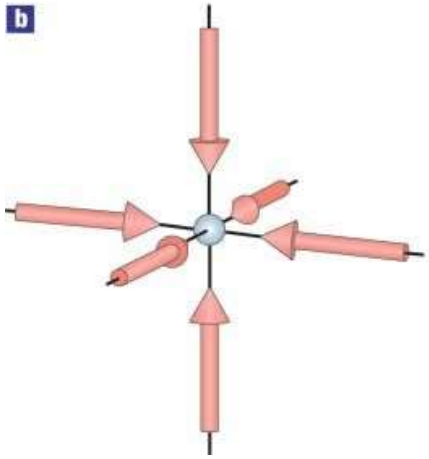
4 x 4 2D optical lattices

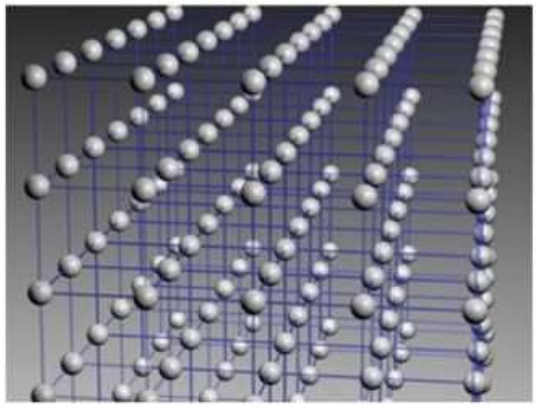
B. Zimmerman et al NJP 13 043007 (2011)

An optical lattice is created by the superposition of standing waves



Quasi-1D



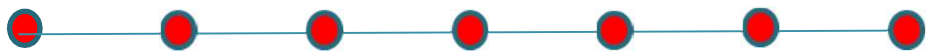


3D

Set of potential minima

I. Bloch Nat. Phys. 1 23 (2005)

A set of atoms loaded in an optical lattice is usually described by the Hubbard model



i i + l

Potential minima

sites

Number of atoms at site i

$$H = -J \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1) + \sum_i \epsilon_i n_i ,$$

Creation and anhililation operators

Bosons or fermions

However, the Hubbard model is only a simplification ⇒

Sometimes it works, sometimes it does not

Full 3D continuous Hamiltonian

Interparticle potential

$$H = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(x_i, y_i, z_i) \right] + \sum_{i<j} V(r_{ij}),$$

Optical lattice potential

$$V_{\text{ext}}(x, y, z) = V_x \sin^2(k_x x) + V_y \sin^2(k_y y) + V_z \sin^2(k_z z),$$

$$k_{x,y,z} = \frac{2\pi}{\lambda_{x,y,z}}$$

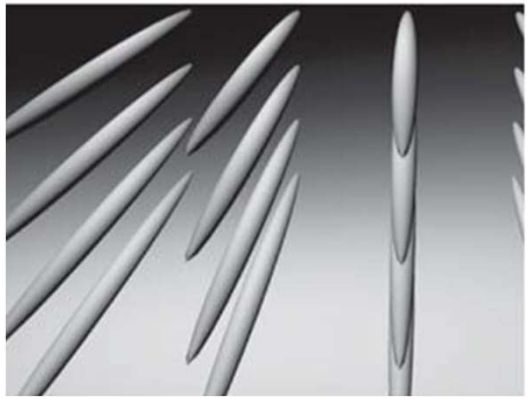
laser wavelength

$$V_{\text{ext}}(x,y,z) = V_x \sin^2(k_x x) + V_y \sin^2(k_y y) + V_z \sin^2(k_z z),$$

When $V_x = V_y >> V_z = V_0 \Rightarrow k_x = k_y \neq k_z = k$

Quasi-1D system confined in the z direction

$$V_{\text{ext}}(x,y,z) = V_0 \sin^2(kz) + \tfrac{1}{2} m\omega_\perp^2 (x^2 + y^2),$$



Harmonic confinement
in the perpendicular direction
$\Rightarrow$ we have a tube

It can be dropped in a pure 1D system

Real wavefunction of the atoms

$$\Phi(z_1, z_2, \ldots, z_N) = \prod_{i=1}^{N} \psi(z_i),$$

In 1D

Functions that depend
on the position of the sites i

$$\psi(z) = \sum_i w_i(z - z_i) b_i,$$

Anihilation operator
for site i

Wannier funcions

$$J_{ij} = -\int dz \; w_i^*(z) \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + V_{\text{ext}}(z) \right] w_j(z).$$

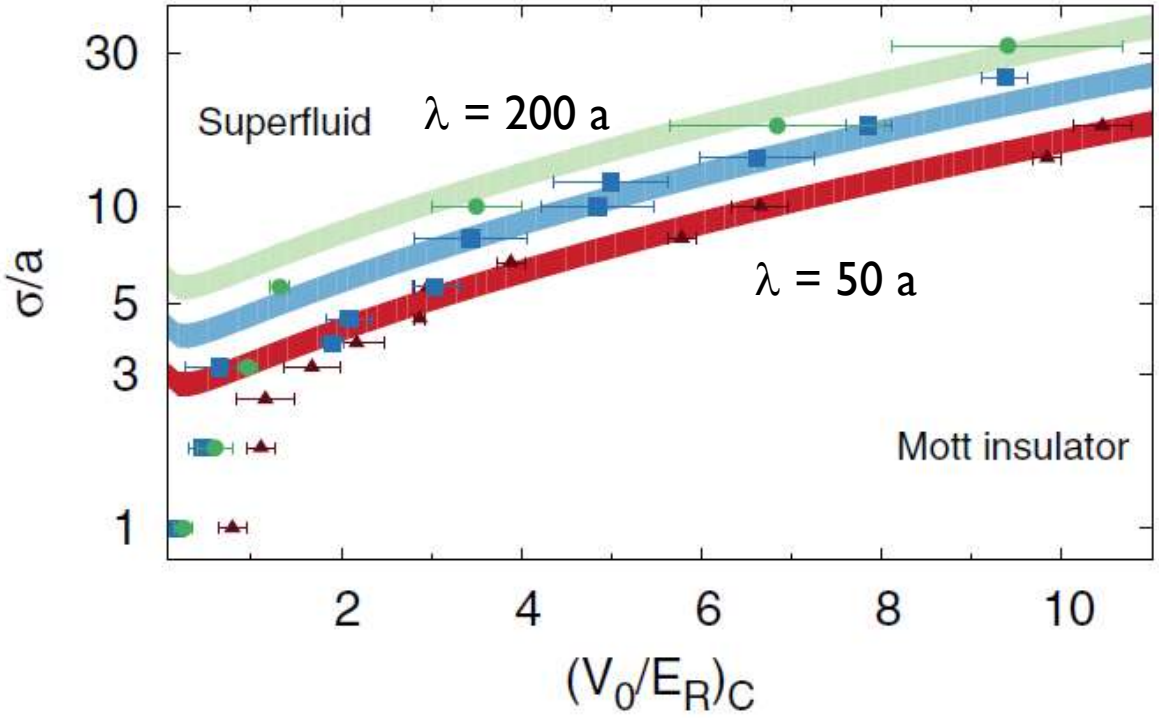
$$U = -\int dz dz' \; w_i^*(z) w_j^*(z') V_{\text{ext}}(z - z') w_k(z) w_l(z)$$

$$\frac{J}{E_R} = \frac{4}{\sqrt{\pi}} E_R \left(\frac{V_0}{E_R}\right)^{3/4} \exp\left[-2\left(\frac{V_0}{E_R}\right)^{1/2}\right]$$

$$E_R = \frac{h^2}{2m\lambda^2}$$

$$U_{1D} = \sqrt{\frac{2}{\pi}}\hbar\omega_\perp \left(\frac{V_0}{E_R}\right)^{1/4} \frac{2\pi}{(\lambda/a)}$$

$$a_\perp = \sqrt{\hbar/\mu\omega_\perp} = \sigma$$



λ = 100 a

Bosons

PRA 87, 063631 (2013) Hard spheres

PRA 93, 021605(R) (2016) 1D

Stripes ⇒ 1D Bose-Hubbard model, good for $V_0/E_R > 3$

Symbols ⇒ continuous quasi-one dimensional model

For 1D clusters

Harmonic potential

$$H = \sum_{i=1}^{N_\uparrow+N_\downarrow} \left[\frac{-\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 x_i^2 + V_{\text{ext}}(x_i) \right]$$

$$+ g_{1D} \sum_{i=1}^{N_\uparrow} \sum_{j=1}^{N_\downarrow} \delta(x_i - x_j),$$

Optical lattice potential (It can be zero)

Contact potential

$$g = \frac{2\hbar^2 a_{3D}}{\mu a_\perp^2} \frac{1}{1 - C a_{3D}/a_\perp}$$

$$a_\perp = \sqrt{\hbar/\mu\omega_\perp} = \sigma$$

μ, reduced mass

C = 1.46

a, scattering length

M. Olshanii. PRL 81 938 (1998)

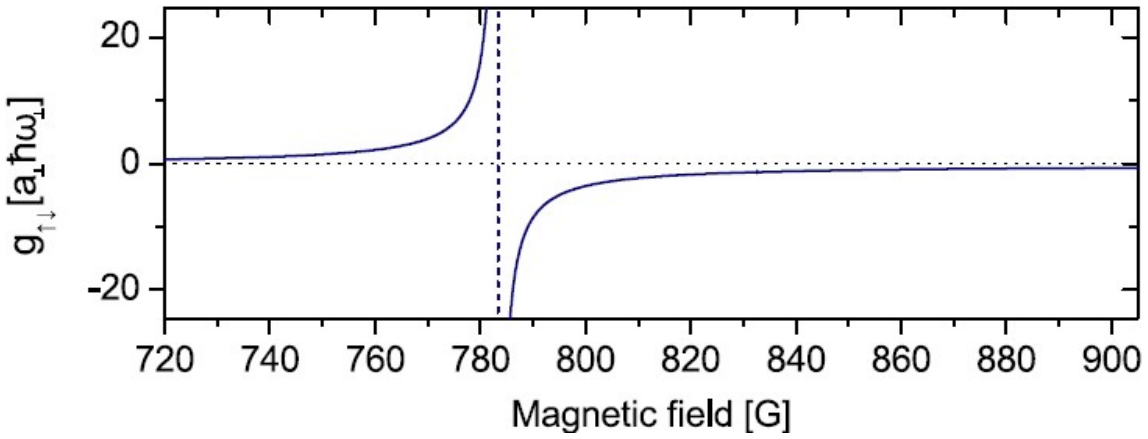
Magnetic field

$$g = \frac{2\hbar^2 a_{3D}}{\mu a_\perp^2} \frac{1}{1 - C a_{3D}/a_\perp}$$

CIR

g can change sign

^{6}Li



G. Zürm et al PRL 108, 075303 (2012)

1D clusters of few fermions $\Rightarrow$ FN-DMC

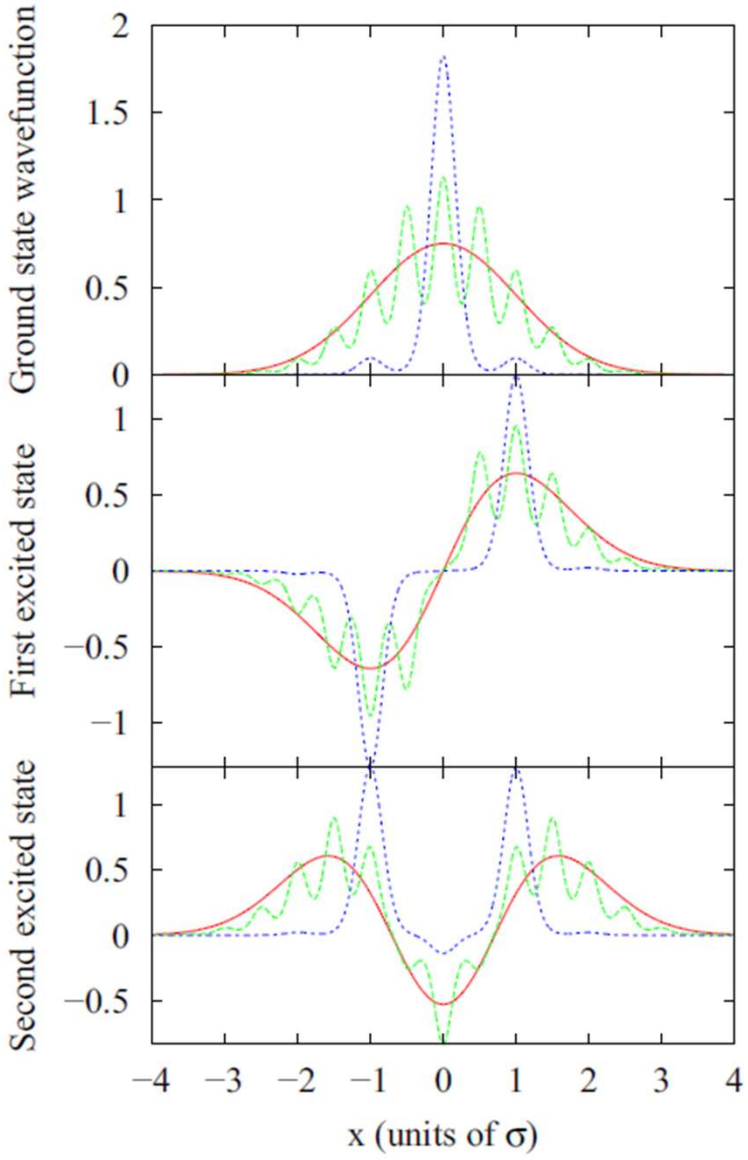
Approximate solution to the many-body Schrodinger equation

It needs an initial approximation $\Rightarrow$ *trial function*

$$\Phi(x_1, \ldots, x_N) = \underbrace{D^{\uparrow} D^{\downarrow}} \prod_{i}^{N_{\uparrow}} \prod_{j}^{N_{\downarrow}} \psi(x_{ij}),$$

Slater determinants containing the solutions to the one-body Schrödinger equation defined by

$$H = \sum_{i=1}^{N_{\uparrow}+N_{\downarrow}} \left[\frac{-\hbar^2}{2m} \nabla^2 + \frac{1}{2} m\omega^2 x_i^2 + V_{\text{ext}}(x_i) \right]$$



Numerical solutions to the non-interacting Schrödinger equation

Slater determinant

$V_0 = 0$ (Harmonic oscillator)

$V_0 = 4\ E_R \quad \lambda = \sigma$

$V_0 = 4\ E_R \quad \lambda = 2\sigma$

Interparticle part of the trial function

distance between two particles of different spin

$$\psi(x_{ij}) = \begin{cases} \cos(k(x_{ij} - R_m)), & x_{ij} < R_m, \\ 1, & x_{ij} \geqslant R_m, \end{cases}$$

$$k a_{1D} \tan(k R_m) = 1 \qquad g_{1D} = -2\hbar^2 / m a_{1D}$$

Variational parameter
R_m = 6-10 σ

In 1D systems the nodes are located only at $x_{ij} = 0$

$\Rightarrow$ No backflow corrections $\Rightarrow$ FN-DMC gives us exact energies

Posible states (not phases) of few-fermion clusters

- Metal (superfluid)
- Mott insulator

} Bosons

- Band insulator
- Antiferromagnetic
- Ferromagnetic

Number of particles : 3-20

Balanced ($N_\uparrow = N_\downarrow$) and imbalanced ($N_\uparrow \neq N_\downarrow$)

$g > 0 \Rightarrow$ Repulsive interactions

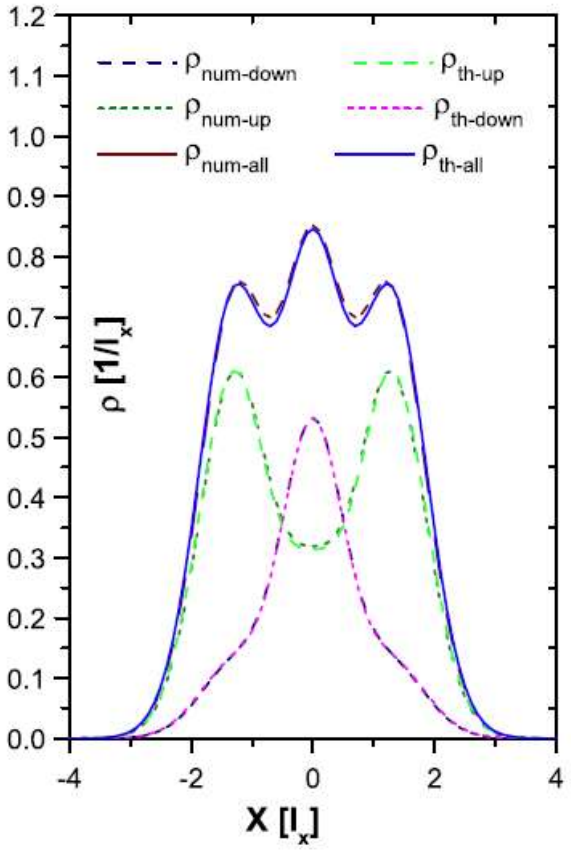
Antiferromagnetism

$N_\uparrow = 2\ N_\downarrow = 1 \Rightarrow 2+1$

The probability of finding the minority particle increases at the center of the cluster

BUT that does not exclude the presence of the mayority particles at the center

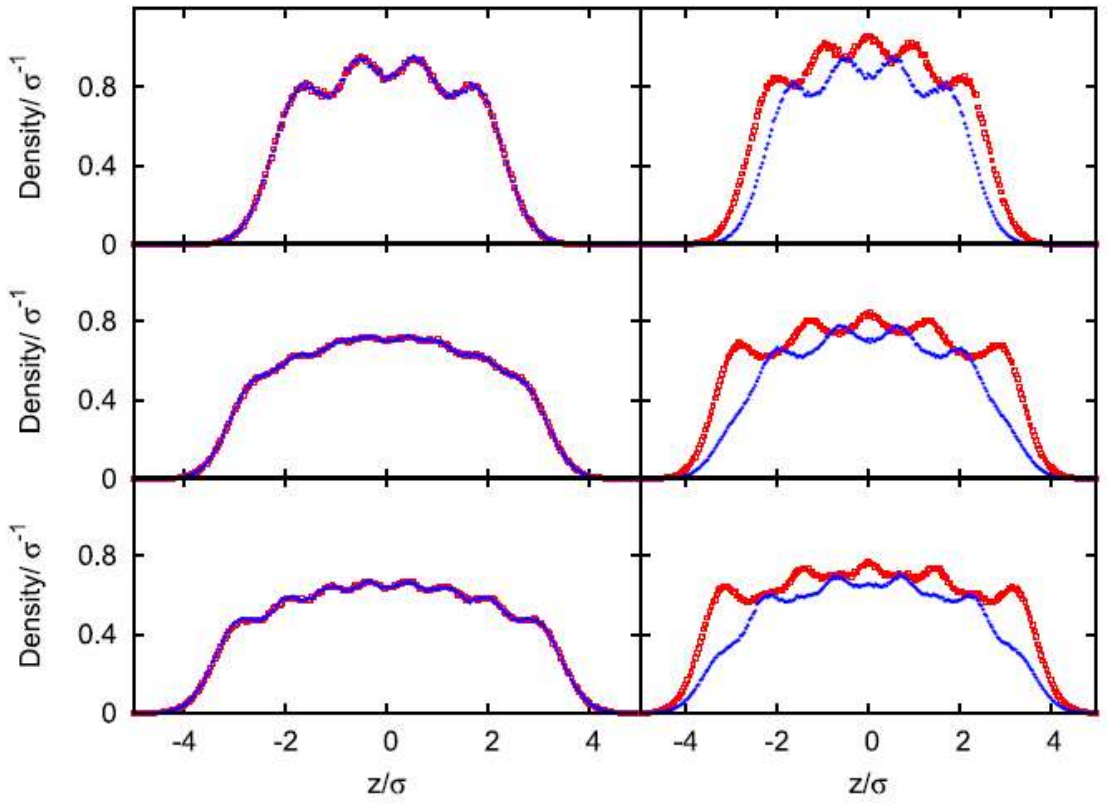
The ferromagnet is not "perfect"



$g = 15 \hbar\ \omega\ \sigma$

L. Guan et al. PRL 102, 160402 (2009)

When the number of atoms increases the separation is less clear



g = 0

g =10 hωσ /2π

g =50 hωσ/2π

4+4 5+4

C. Carbonell-Coronado et al. NJP 18 025015 (2016)

Calculate the probability of different spin orderings

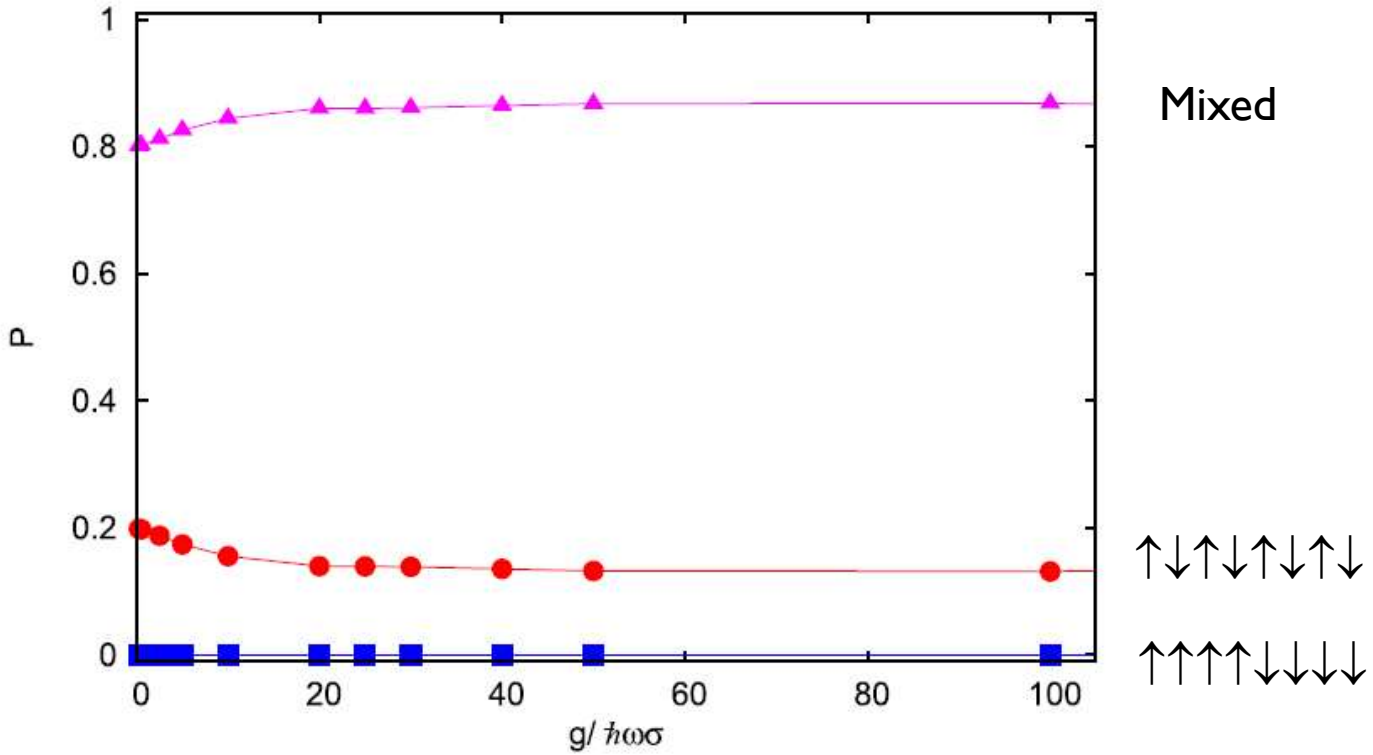


Figure 4. Probability of different spin orderings for a 4 + 4 cluster. Squares, ferromagnetic (F) state; circles, antiferromagnetic (AF) ordering; triangles, mixed (M) configurations.

There is no "pure" antiferromagnet

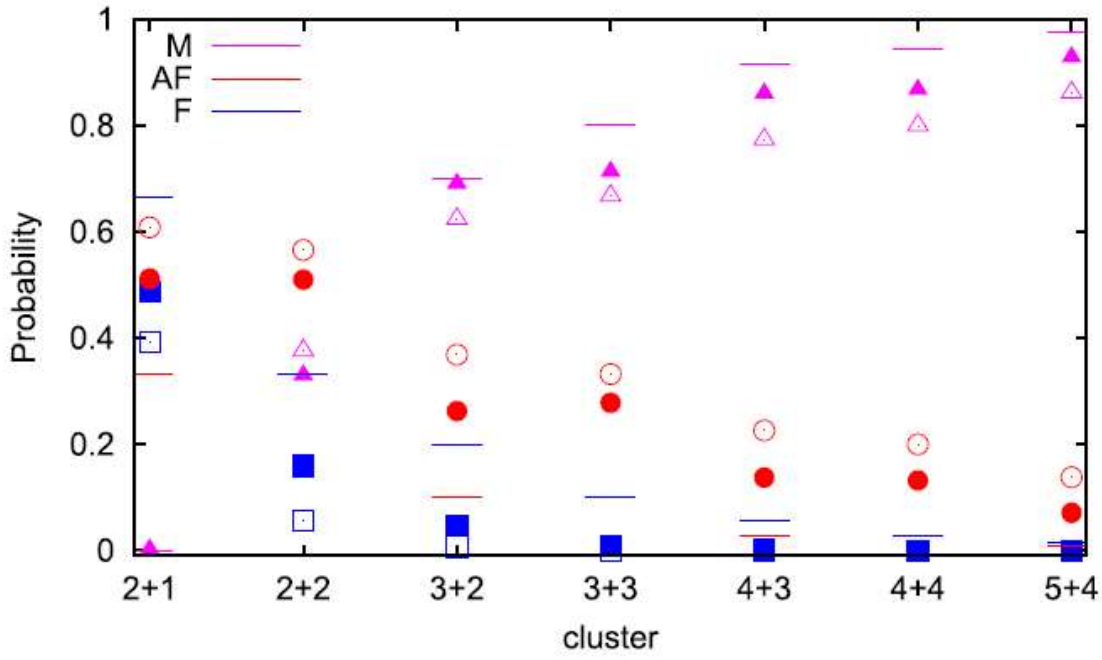


Figure 5. Probability of different spin orderings for different clusters and g's obtained from our simulations: open symbols, $g = 0$; full ones, $g = 50$. Lines indicate the probabilities of each phase if the orderings were purely random. For the $2 + 2$ cluster in the random limit all orderings have the same probability.

Number of configurations

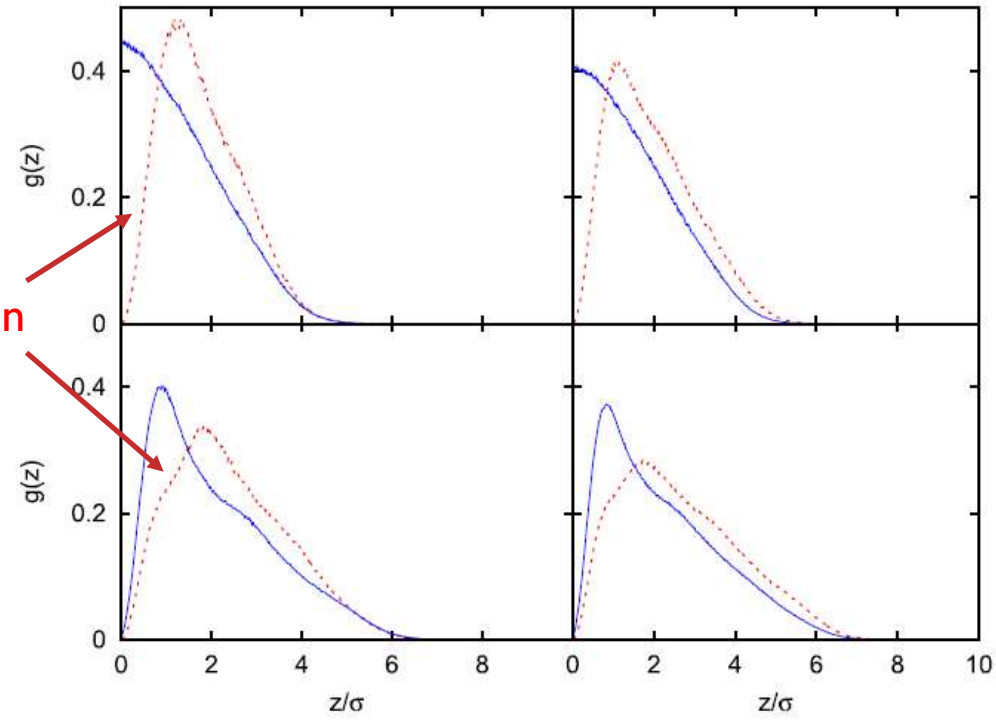
$$C = \frac{(N_\uparrow + N_\downarrow)!}{N_\uparrow!\, N_\downarrow!}$$

$N_\uparrow = N_\downarrow$ C(AF) = 2

$N_\uparrow = N_\downarrow + 1$ C(AF) = 1

C(F) = 2

Local antiferromagnetic correlations



Pauli's exclusion

g = 0

g =50 hωσ/2π

Figure 6. Radial distribution functions for 3 + 3 (left) and 4 + 3 (right) clusters. Dots, same-spin distributions; full lines, different-spin probabilities. Upper panel, $g = 0$; lower panel, $g = 50$. The integral under those curves was set to 1.

Optical lattice clusters

$$H = -J \sum_{\langle ij \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1) + \sum_i \epsilon_i n_i ,$$

External potential
different for each i site

Mott phase in homogeneous system $\Rightarrow \kappa = 0$

$$\kappa = \partial n / \partial \mu = 0$$

In a cluster, μ and κ depend on the site

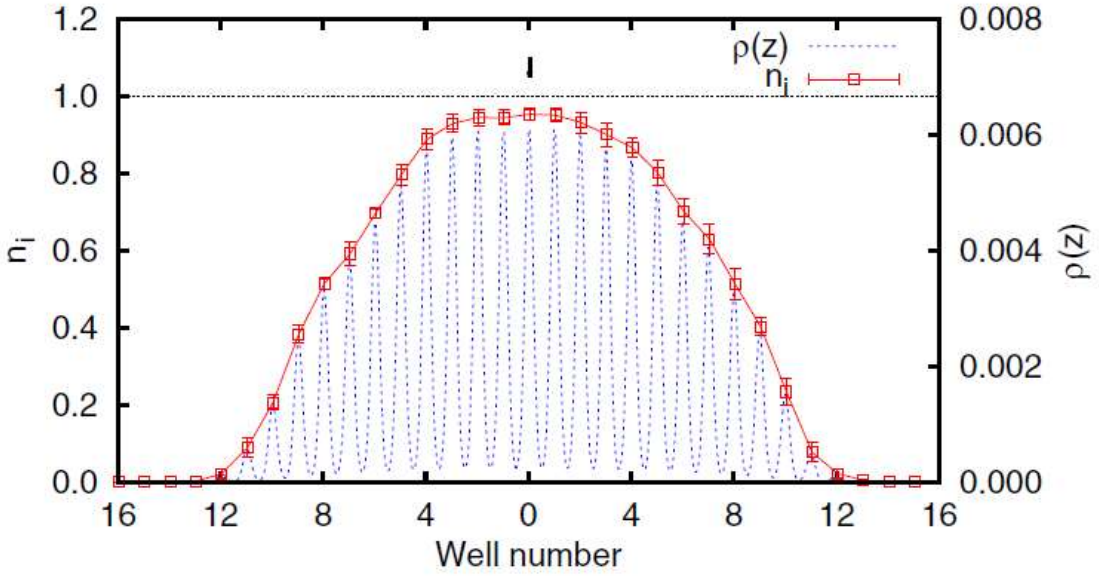
$$\kappa_i = \frac{\partial n_i}{\partial \mu_i}, \quad \mu_i = \mu - V_c r_i^2 = \mu - \tfrac{1}{2} m \omega_z^2 z_i^2, \quad \kappa_i = -\frac{1}{m \omega_z^2 z} \frac{\partial n}{\partial z}$$

$$\kappa_i = -\frac{1}{m\omega_z^2 z}\frac{\partial n}{\partial z}, \qquad n_i = \int_{z_i-\lambda/4}^{z_i+\lambda/4} \rho(z)dz,$$

$\kappa_i = 0 \Rightarrow \quad \Delta_i = \langle n_i^2 \rangle - \langle n_i \rangle^2 = 0,$

at several consecutive sites with $n_i = 1 \Rightarrow$ Mott domain

Bosons



N = 15

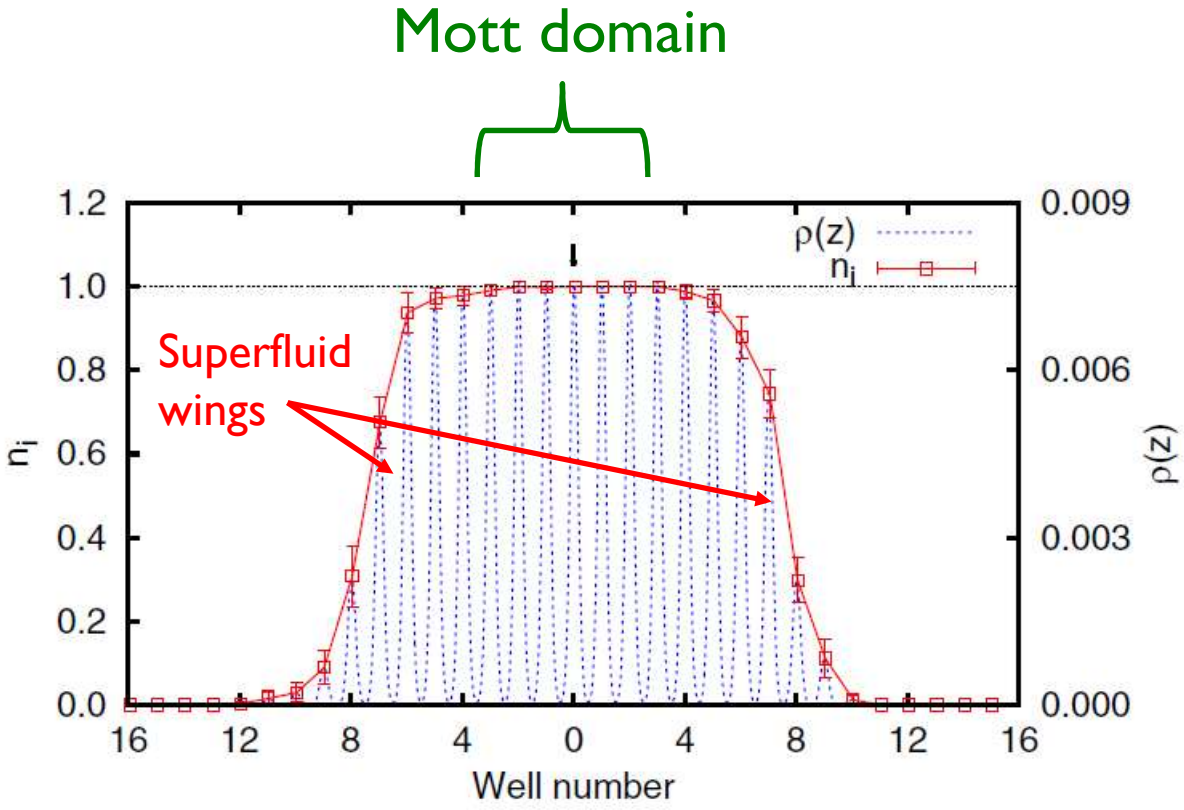
$\omega_z = 2\pi \times 415$ Hz

$V_0 = 7.6\ E_R$

No Mott domain

$\Rightarrow$ superfluid

C. Carbonell-Coronado et al. PRA 90, 013630 (2014)

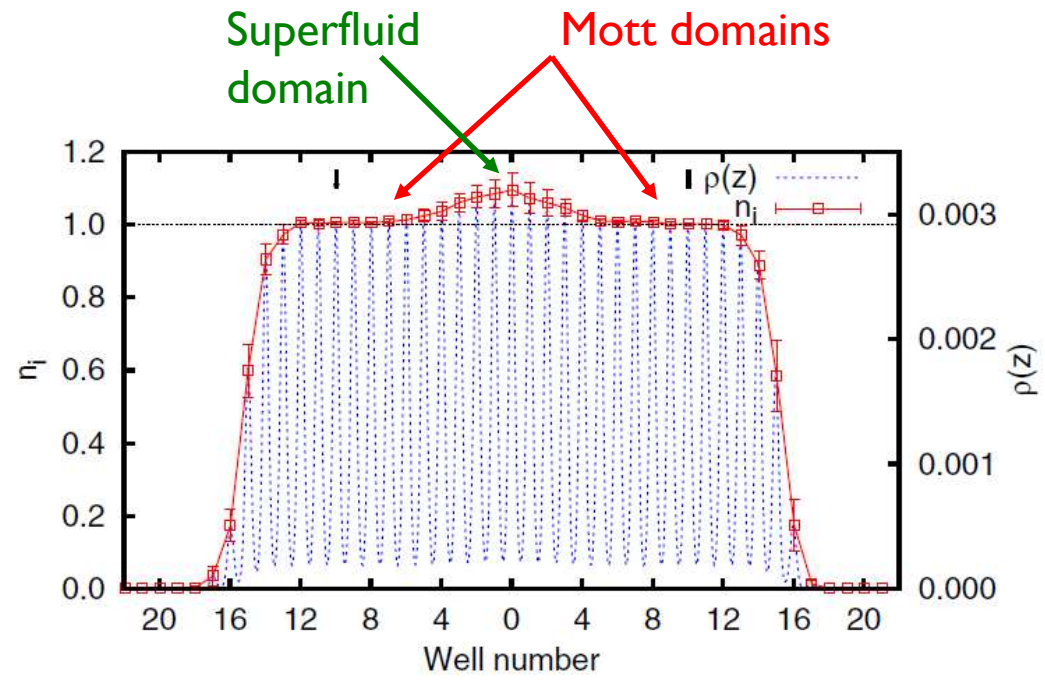


N = 15

$\omega_z = 2\pi \times 415$ Hz

$V_0 = 15.2\ E_R$

We go from a superfluid to a Mott insulator by increasing V_0

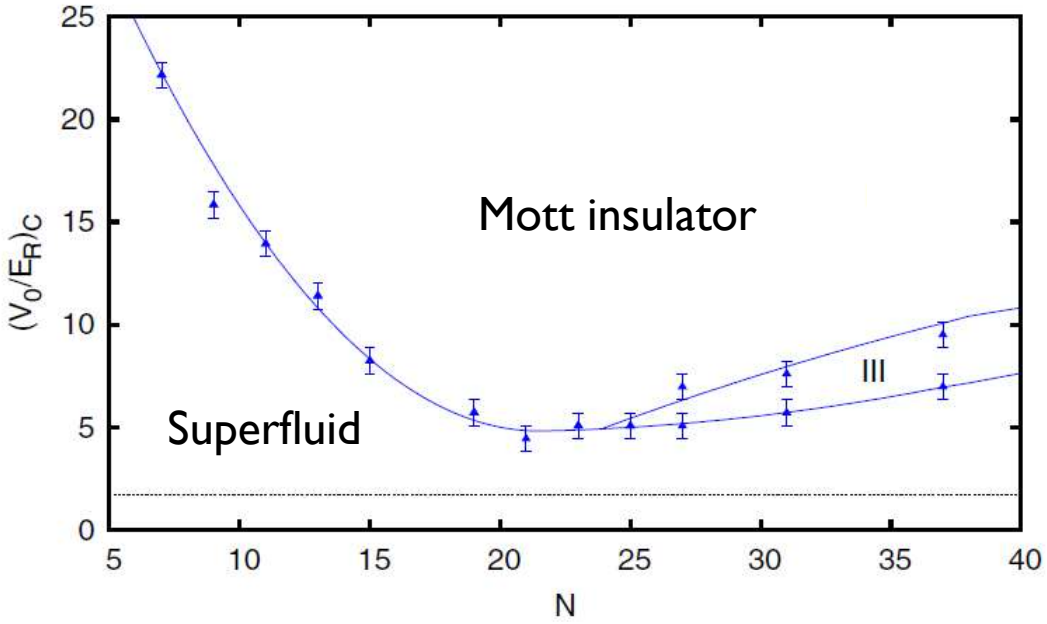


N = 31

$\omega_z = 2\pi \times 415$ Hz

$V_0 = 6.3\ E_R$

State III



State diagram

homogeneous system

Fermionization

When $g \to \infty$ $M_\uparrow$ + $N_\downarrow$ fermions behave as $(M+N)_\uparrow$

Same energy

Same density profile

Girardeau's mapping

M. D. Girardeau, PRA 82, 011607(R) (2010).

$$H = \sum_{i=1}^{N_\uparrow+N_\downarrow} \left[\frac{-\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 x_i^2 + V_{\text{ext}}(x_i) \right]$$

$$+ g_{1D} \sum_{i=1}^{N_\uparrow} \sum_{j=1}^{N_\downarrow} \delta(x_i - x_j), \qquad N_\downarrow = 0$$

Non-interacting Hamiltonian

The energies and the density profiles can be calculated exactly

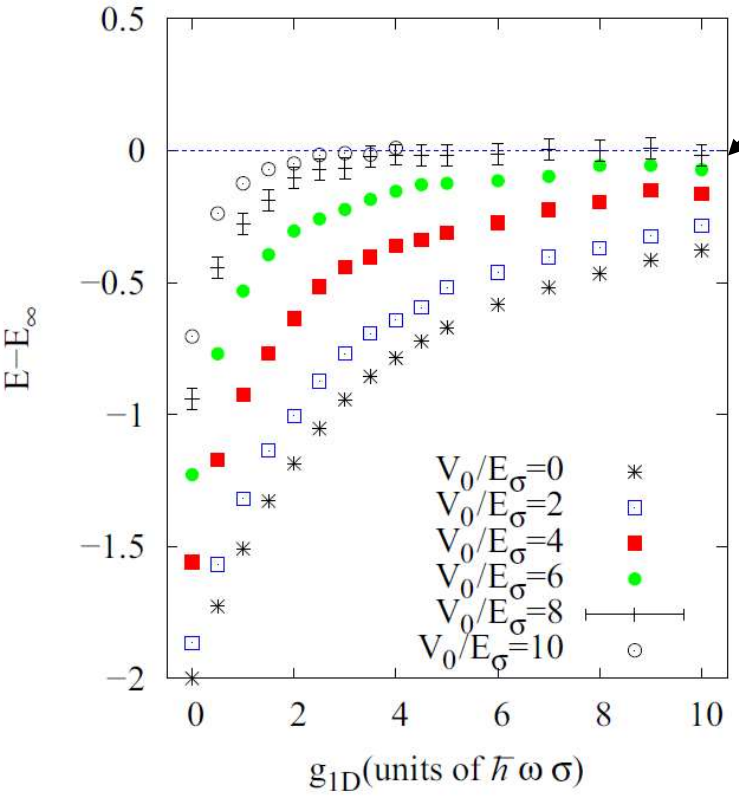
$$\Phi(x_1, \ldots, x_N) = D^{\uparrow}$$

Slater determinant containing the solutions to the non-interacting Hamiltonian

E_∞ is reached for smaller values of g than for the harmonic oscillator

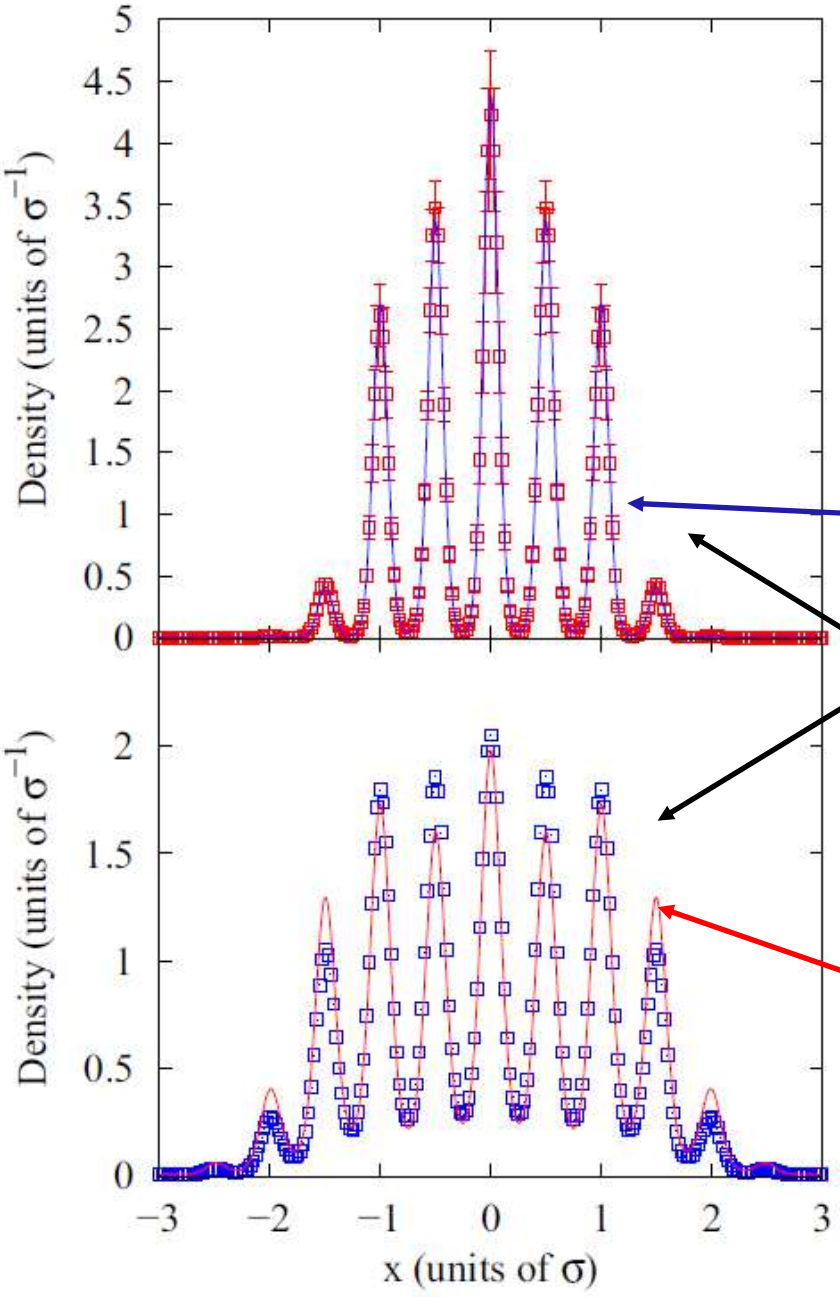
PRA 96, 013614 (2017)

2+1 cluster



$$E_\sigma = \frac{h^2}{2m\sigma^2}$$

$\lambda = \sigma$



$g = 4\ h\omega\sigma/2\pi$

$\lambda = \sigma$

$V_0 = 10\ E_\sigma$

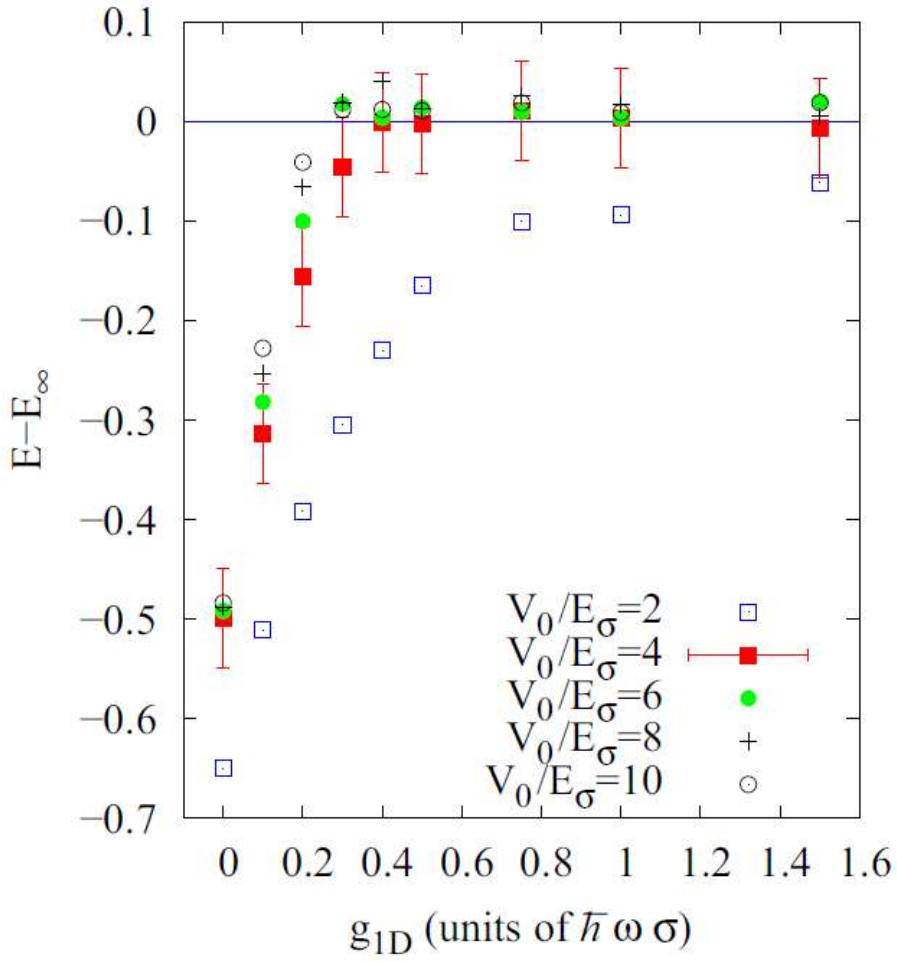
Fermionization limit

The populations in the potential minima are different ⇒ metals

$V_0 = 4\ E_\sigma$

Fermionization limit

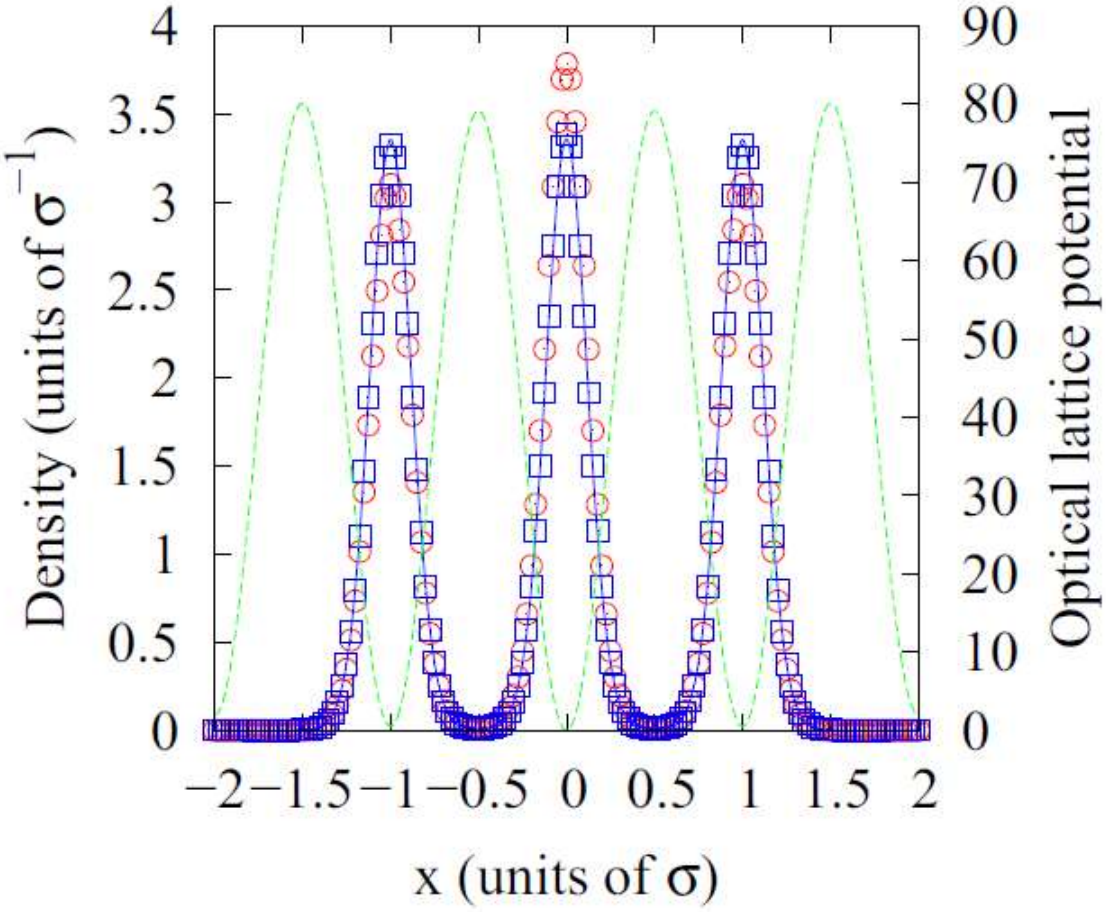
$\lambda = 2\sigma$



E_∞ is reached for smaller values of g than for $\lambda = \sigma$

The system behaves effectively as if g were much larger

$V_0 = 4\,E_\sigma$ $\lambda = 2\sigma$ $g = h\omega\sigma/2\pi$



$g = 5\,h\omega\sigma/2\pi \Rightarrow$ Fermionization limit $\Rightarrow$ Mott insulator

Density profile
at the fermionization
limit ($g \to \infty$)

Profile for non-interacting
cluster of $(M+N)_{\uparrow}$

Calculated from the
non-interacting Hamiltonian

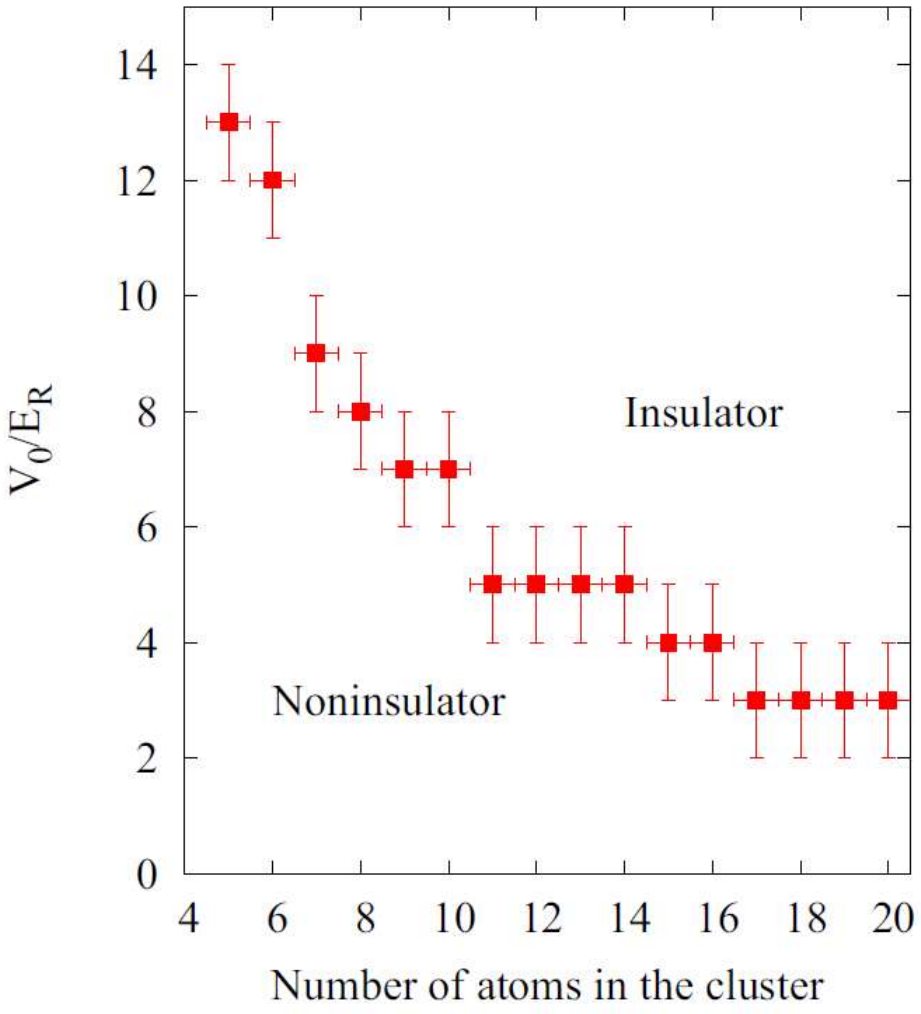
Metal (unequal populations)

(Mott) insulator
(equal populations, $n_i = 1$)

We can predict if a cluster is going to be a Mott insulator
or not from the solutions of the non-interacting Hamiltonian

$\lambda = \sigma$

Clusters with $N_{\uparrow}$

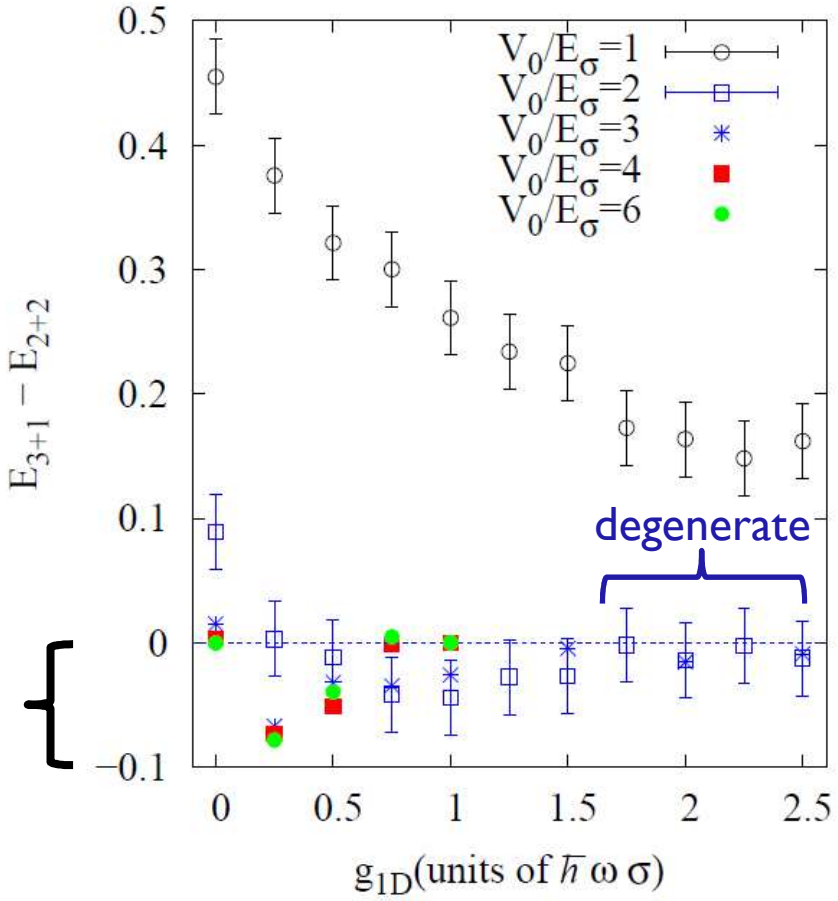


There is no way
a cluster of 20 atoms
is a Mott insulator
for $V_0 < 3\ E_R$
irrespectively of its
internal composition

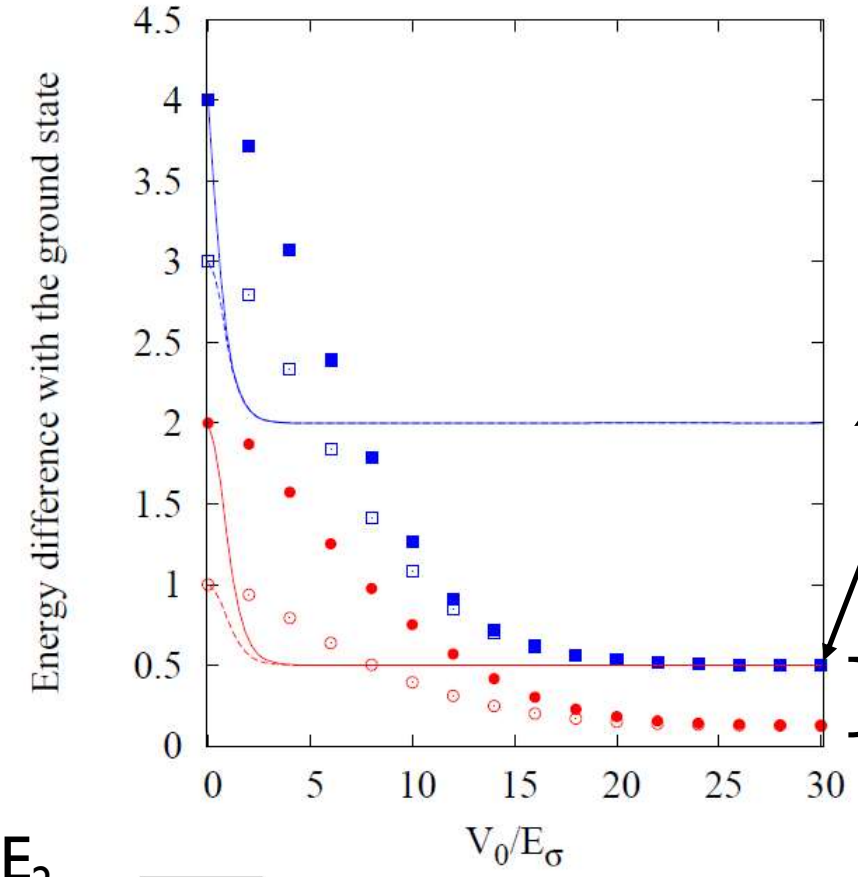
Paramagnetism in N = 4 clusters

$\lambda = 2\sigma$

The 3+1 cluster has smaller energy than the 2+2 cluster



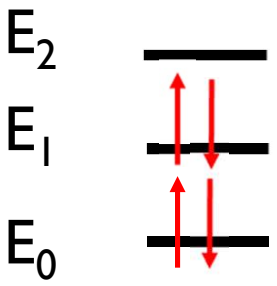
Non-interacting energies

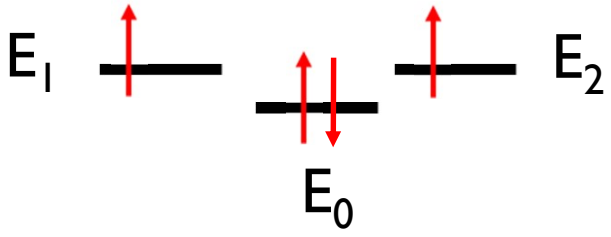


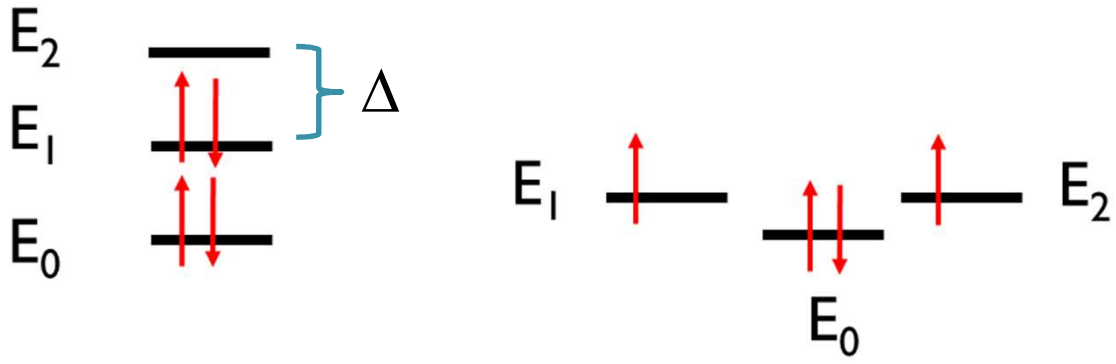
The n and n+1 (n≥1) states become degenerate for deep enough V_0

$\lambda = 2\sigma$

$\lambda = \sigma$







The relative stability of the clusters depends on Δ and g

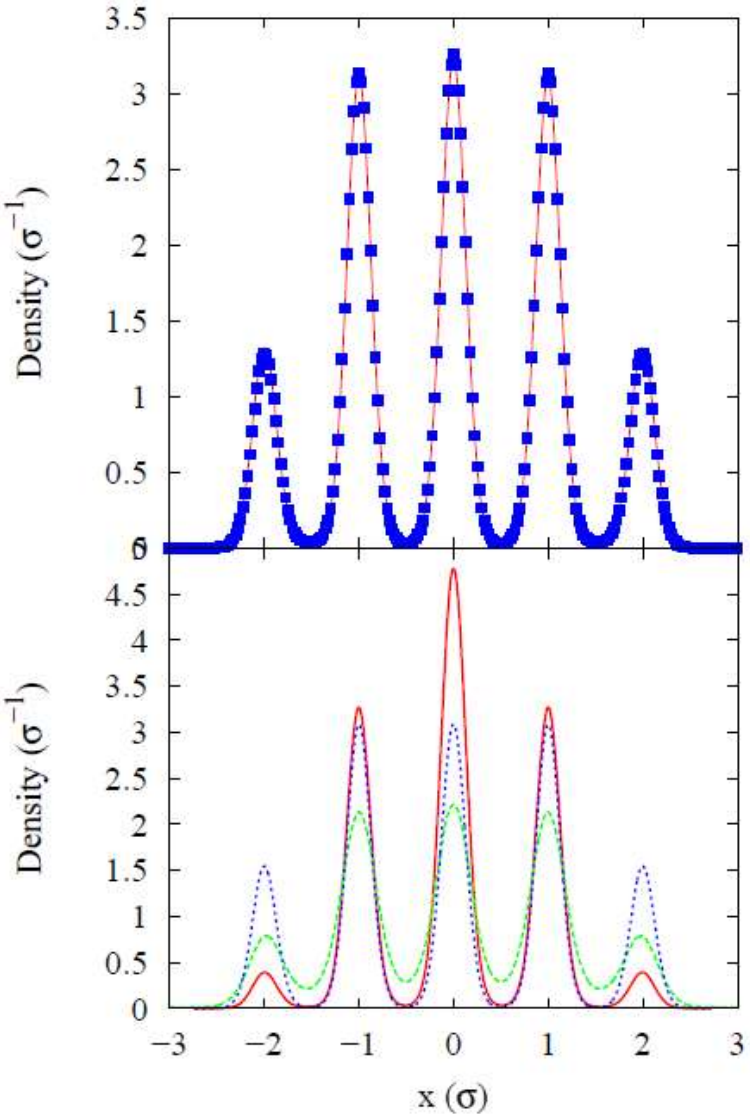
$\Delta \approx 0$ $g > 0$ $\Rightarrow$ cluster 3+1 more stable $\Rightarrow$ paramagnetic

$\Delta > 0$ $\Rightarrow$ cluster 2+2 more stable $\Rightarrow$ diamagnetic

Dia- and paramagnetic degenerate → Metal (mixed)

Dia- and paramagnetic degenerate → Mott insulator

$\lambda = 2\sigma$



$V_0 = 3\ E_\sigma$

$g = 2.5\ h\omega\sigma/2\pi$

3+1 2+2

Metal

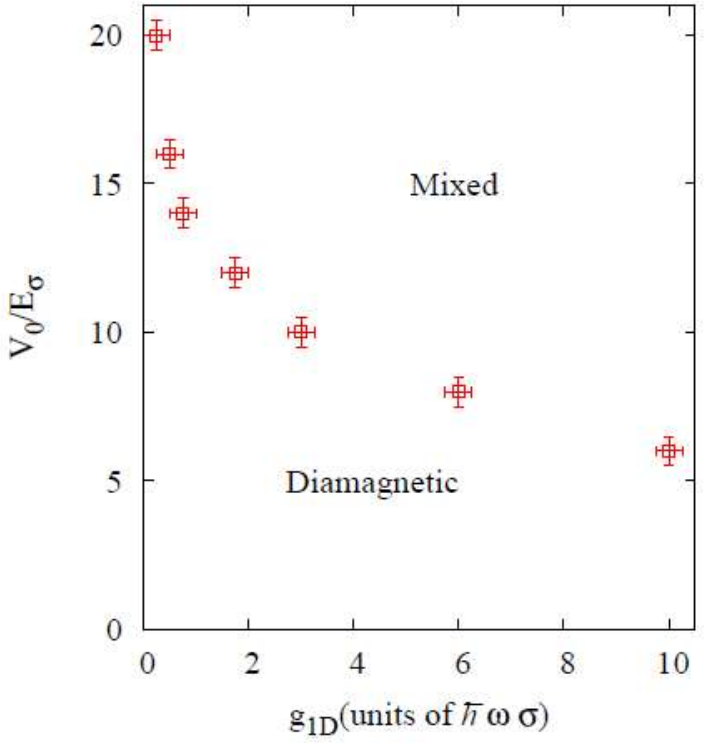
(3+1) $V_0 = 3\ E_\sigma$ $g = h\omega\sigma/2\pi$

(2+2) $V_0 = E_\sigma$ $g = 2.5\ h\omega\sigma/2\pi$

(3+1) $V_0 = 3E_\sigma$ $g = 8\ h\omega\sigma/2\pi$

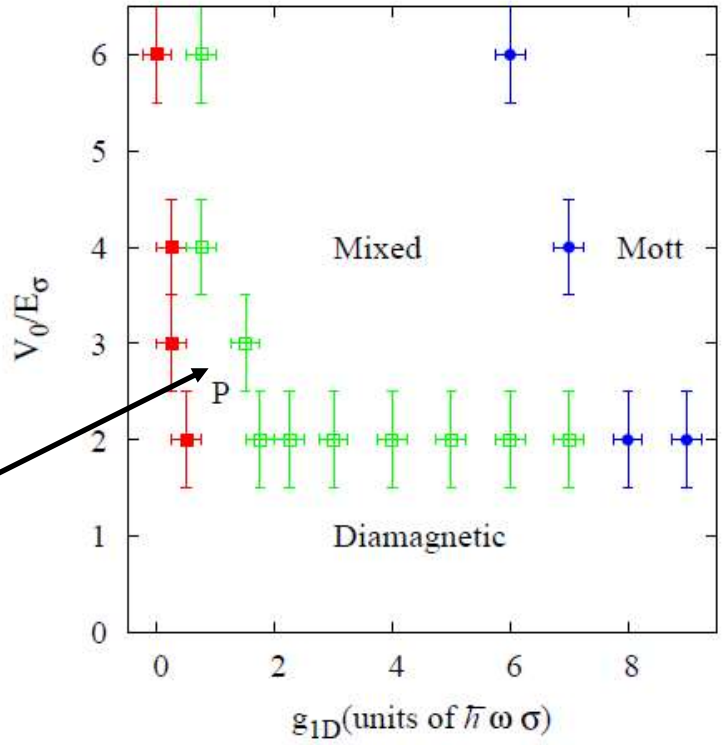
Mott insulator

Phase diagrams for a N = 4 cluster



$\lambda = \sigma$

$\lambda = 2\sigma$



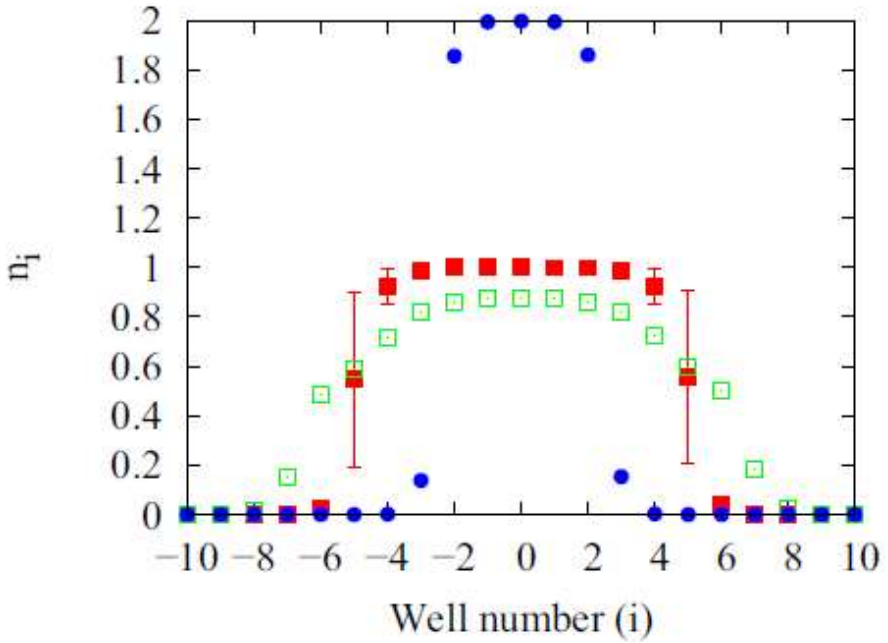
Paramagnetic

Band insulators

$\kappa_i = 0 \Rightarrow \quad \Delta_i = \langle n_i^2 \rangle - \langle n_i \rangle^2 = 0,$

at several consecutive sites with $n_i = 2 \Rightarrow$ band insulator

5+5 $\quad \lambda = \sigma$



$$n_i = \int_{z_i-\lambda/4}^{z_i+\lambda/4} \rho(z)dz,$$

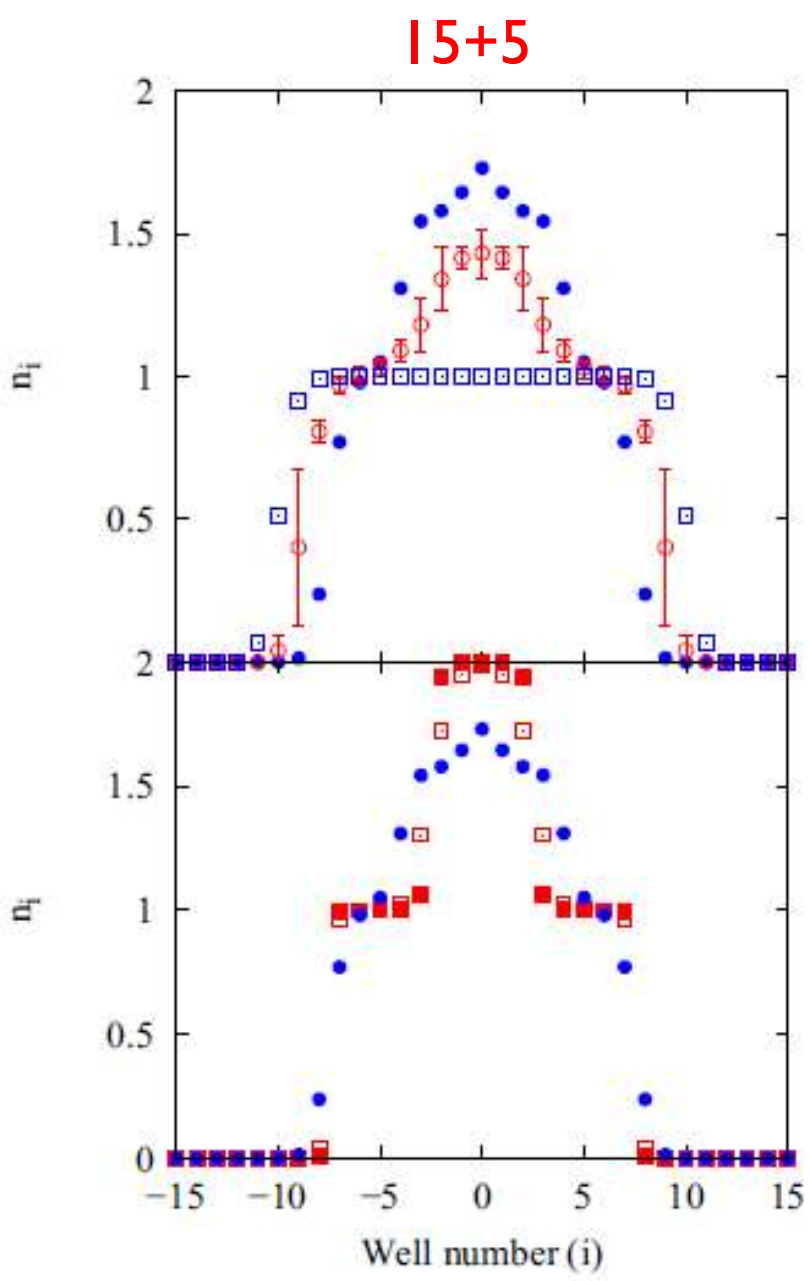
$V_0 = 10\ E_\sigma$ $g = 10\ h\omega\sigma/2\pi$

$V_0 = 4\ E_\sigma$ $g = 4\ h\omega\sigma/2\pi$

$V_0 = 14\ E_\sigma$ $g = 0$

Band insulator

M.C. Gordillo PRA 96, 033630 (2017)



Filled circles (metal)

$V_0 = 6\ E_\sigma\ g = 0$

Open circles (metal)

$V_0 = 6\ E_\sigma\ g = 4h\omega\sigma/2\pi$

Open squares (Mott)

$V_0 = 6\ E_\sigma\ g = 20h\omega\sigma/2\pi$

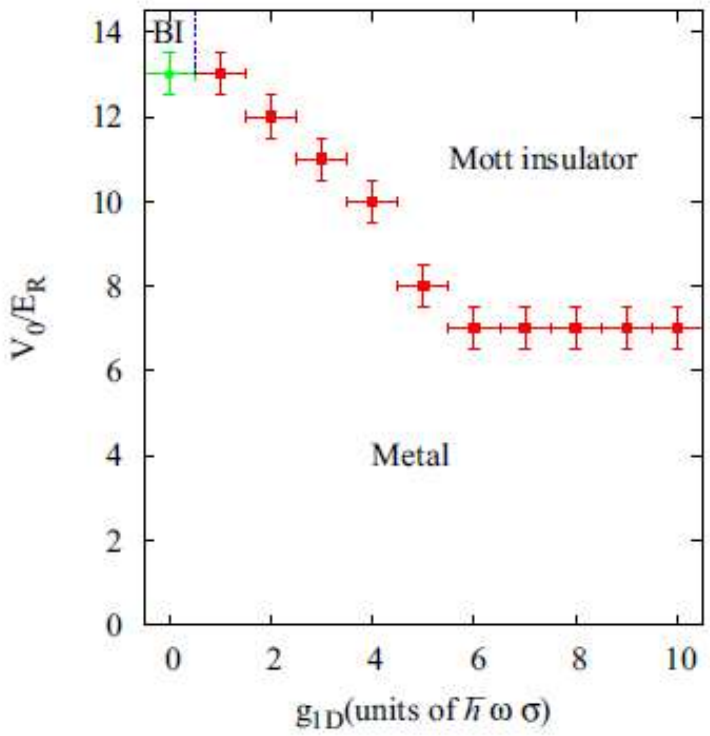
Filled squares (state II)

$V_0 = 14\ E_\sigma\ g = 0$

Open squares (state I)

$V_0 = 10\ E_\sigma\ g = 0$

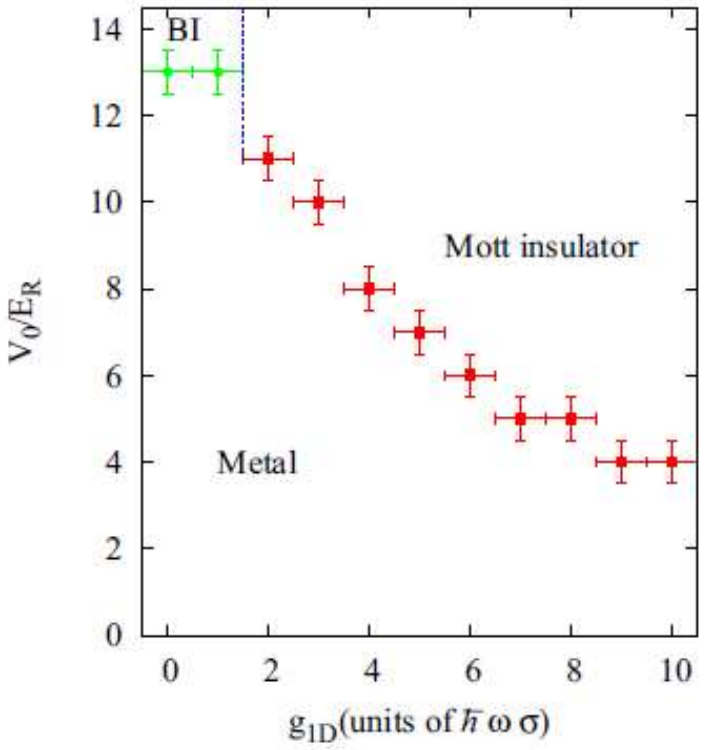
State diagrams



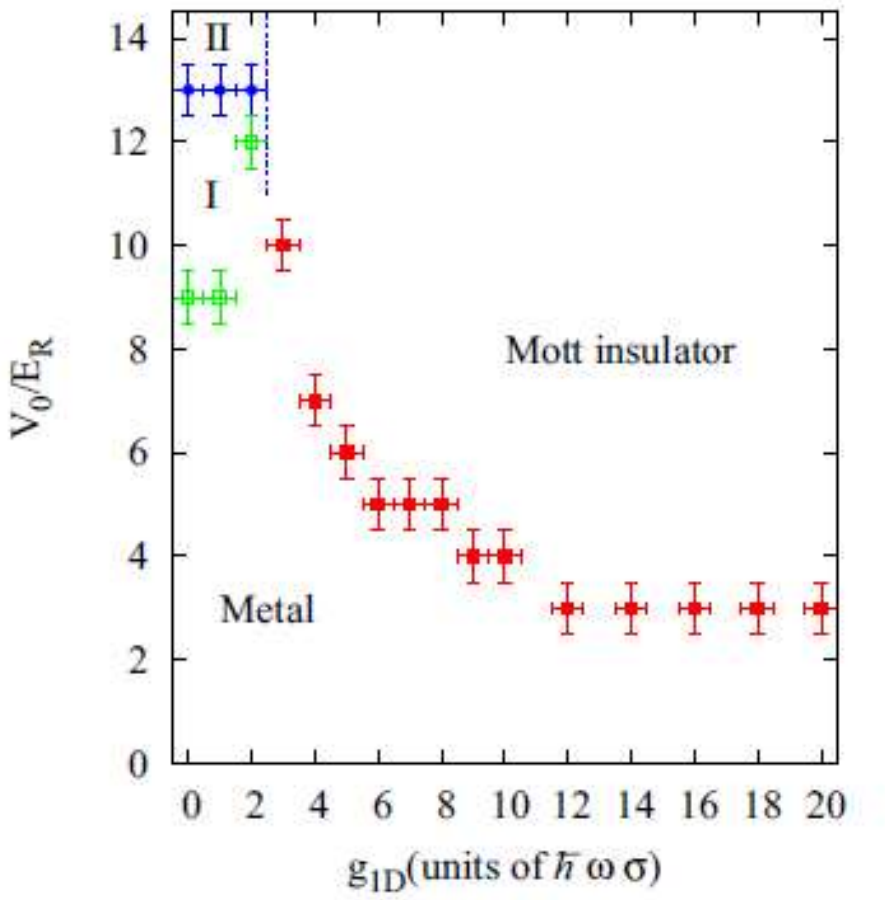
5+5

Only three states

10+5

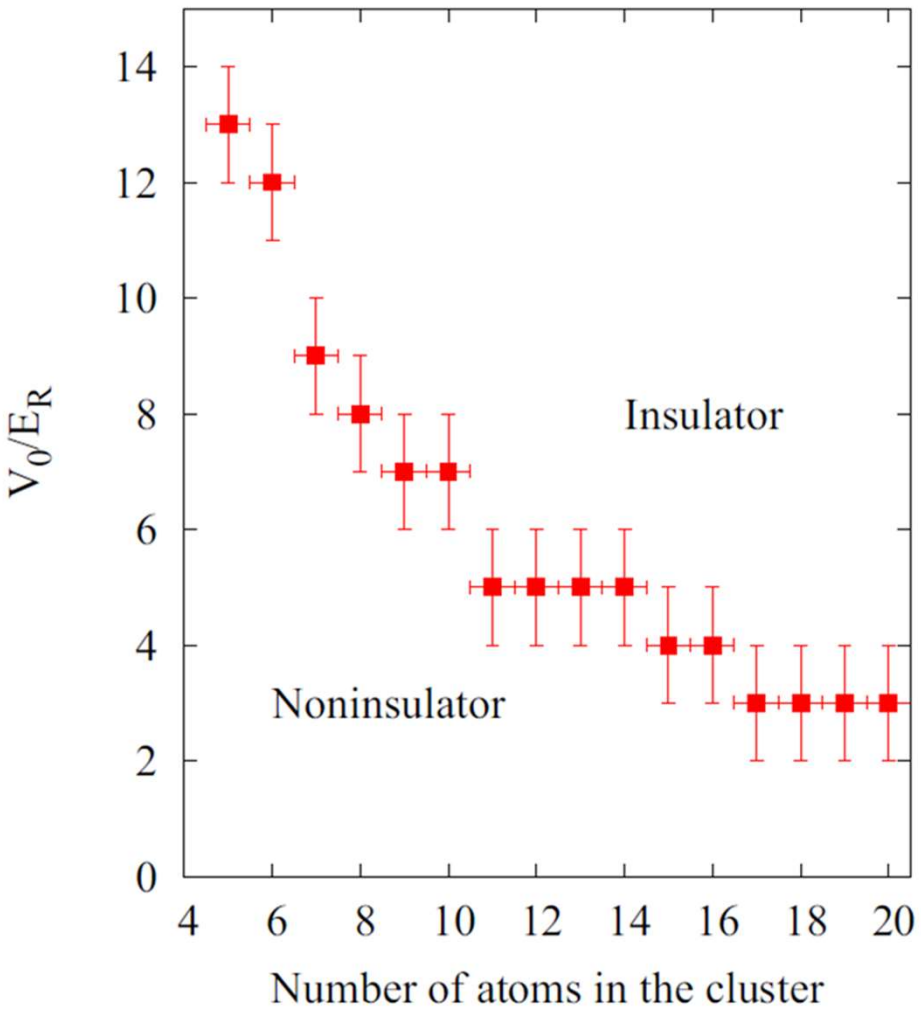


15+5



State I
Mott insulator + metal

State II
Mott insulator +
Band insulator



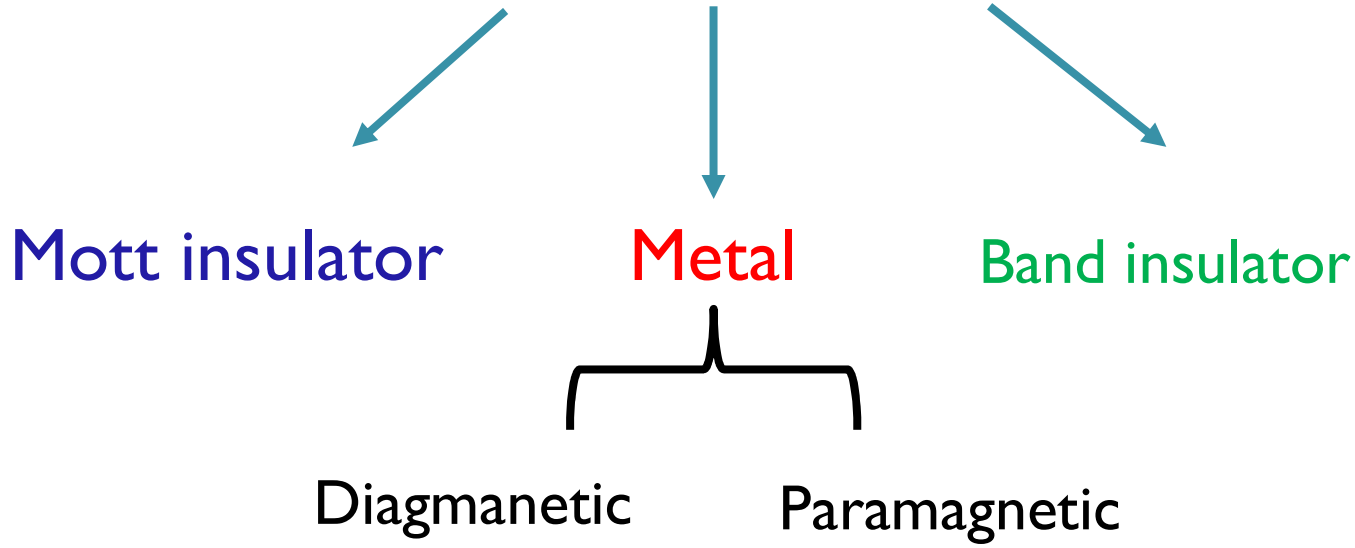
For a n+m cluster (n≥m) to be a band insulator for g→ 0 both m and n clusters have to be insulators

Predicted by the non-interacting solutions of the Hamiltonian

Conclusions

- For harmonic clusters there is no pure antiferromagnetic state

- Small fermion clusters loaded in optical lattices have a wide variety of behaviours



- Some of those behaviours can be predicted from the non-interacting solutions of the Hamiltonian

In the $g \to \infty$ limit
a $M_\uparrow + N_\downarrow$ cluster is a
Mott insulator only
if a $(M+N)_\uparrow$ cluster is
a Mott insulator

The potential depth
needed to have a Mott
insulator decreases with
the size of the cluster

- Some of those behaviours can be predicted from the non-interacting solutions of the Hamiltonian

In the $g \rightarrow 0$ limit
a $M_{\uparrow}$ + $N_{\downarrow}$ cluster is a band insulator only if the $M_{\uparrow}$ and $N_{\uparrow}$ clusters are band insulators

When $M \neq N$ we can have additional states that are mixtures of metals, Mott insulators and band insulators