WAVE FUNCTIONS FOR STRONGLY INTERACTING SYSTEMS

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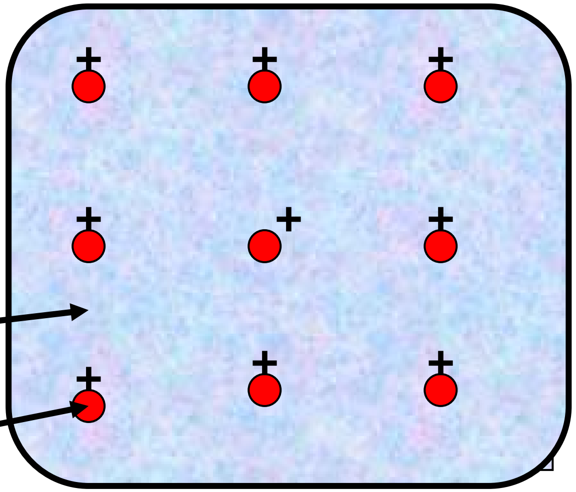
Strongly correlated problems
Many body wave functions
Why variational methods
Why Monte Carlo: many degrees of freedom

Examples of strongly correlated systems

What is a strongly correlated problem?

$$H = \sum_{i} \frac{p_i^2}{2m} + \sum_{i<j} U(r_{ij}) + \sum_{i,\alpha} V(r_i - R_\alpha)$$



MANY DEGREES OF FREEDOM

N-Electron cloud

ion

For PE<<KE

Start with single particle wave functions that diagonalize the KE operator
Treat the effects of PE as a perturbation on the single particle states
If electron-electron interactions can be treated as an effective one body term

$u_{eff}[n]$ ⇒ band structure or electronic structure

Density functional theory
Hohenberg and Kohn
Phys. Rev. 136B, 864 (1964)

For PE>>KE

Start with the classical ground state; highly degenerate;
Perturb with KE

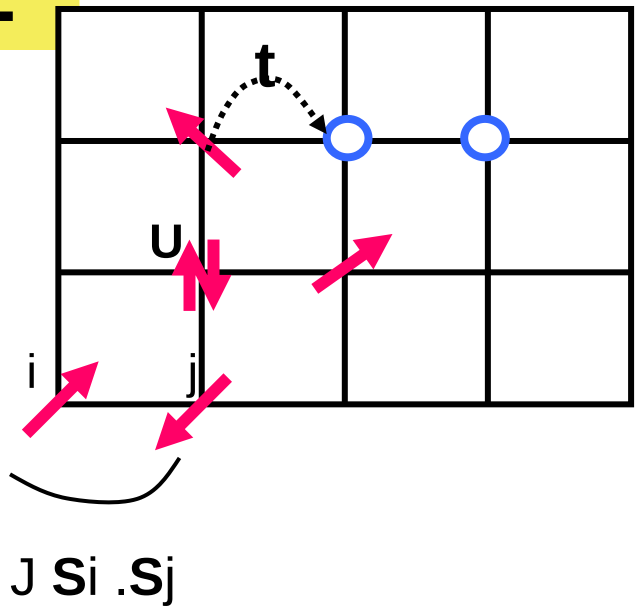
What happens when PE~KE?

HUBBARD MODEL

Kinetic Energy $$= -t \sum_{<i,j>\sigma} c^{+}{}_{i\sigma} c_{j\sigma}$$

$$= \sum_{k} \varepsilon_k c^{+}_{k\sigma} c_{k\sigma}$$

$$\varepsilon_k = -2t(\cos k_x + \cos k_y)$$



Potential Energy $$= U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

U >> t generates AFM exchange

$$J = 4t^2 / U$$

Energy Scales: $$J \le t < U$$

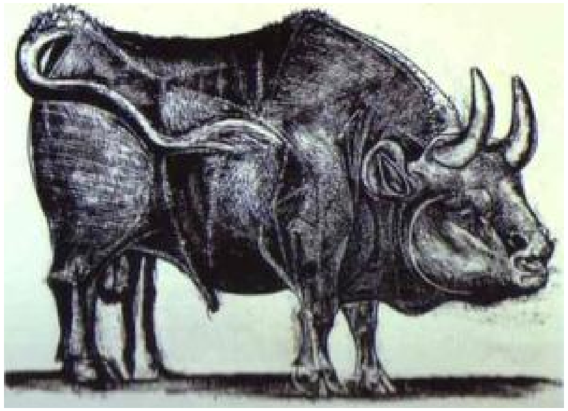
x= Hole doping =fraction of vacancies

Examples: **Lattice models**

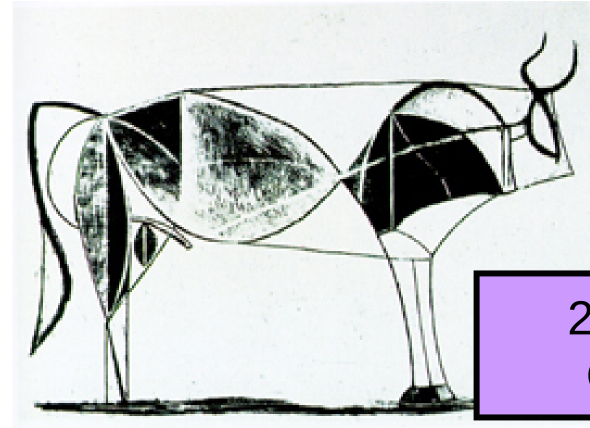
Quantum magnetism:	**Heisenberg antiferromagnet**
Strongly interacting bosons: atoms in traps; optical lattices:	**+U Bose Hubbard model**
Feshbach resonance: BCS-BEC crossover:	**-U Fermion Hubbard Model**
High temperature superconductivity:	**+U Fermion Hubbard model**
Quantum Hall Effect:	

Disorder driven Quantum Phase transitions

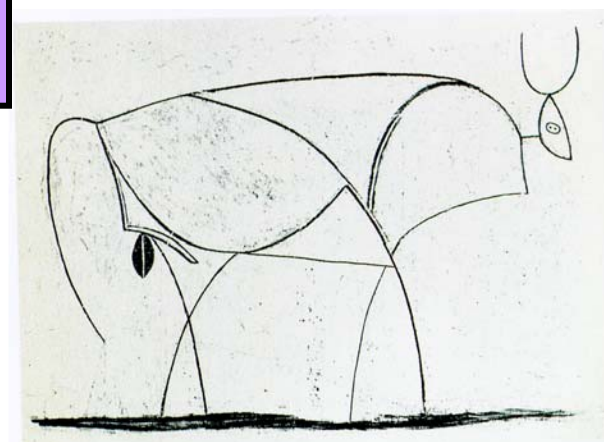
Superfluid—Bose Glass transition: (Josephphson Junction arrays; helium in aerogels)	**+U Bose Hubbard model + disorder**
Superconductor-Insulator Transition: (ultra thin films; high Tc SCs)	**-U Fermion Hubbard model + disorder**
Metal-Insulator transition: (disordered Mott insulators; 2D electron gases)	**+U Fermion model + disorder**



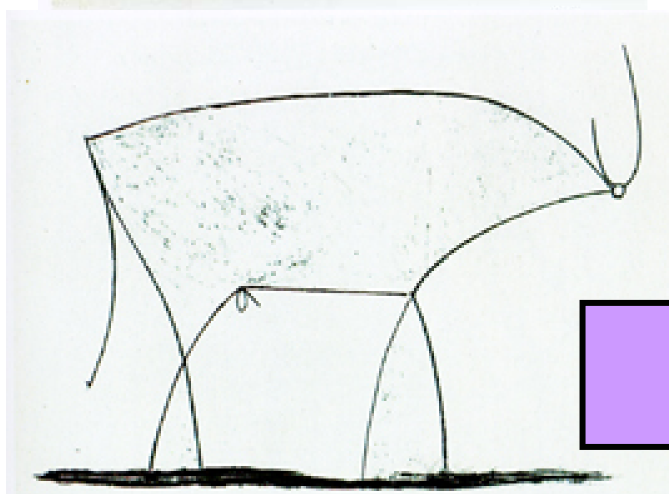
High tc problem



2 dimensions
Cu-O plane



3 band model



1 band model

What theoretical tools do we have to study strongly correlated systems

Feynman diagrams
Series expansion
Functional integrals
Scaling + RG

Need non-perturbative methods
No small parameter

Exact Diagonalization
Variational Methods
Quantum Monte Carlo
Dynamical Mean Field Theory

Id special techniques

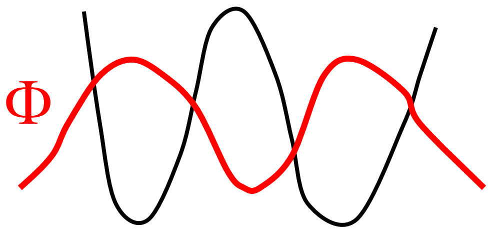
Bose Hubbard Model

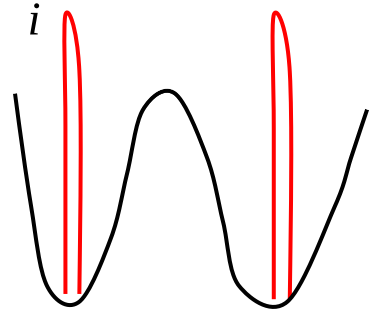
$$H = -t \sum_{<i,j>_{nn}} a_i^+ a_j + \frac{U}{2} \sum_i n_i (n_i - 1)$$

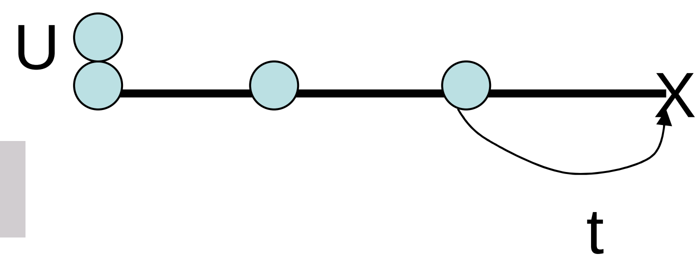
$$\left[a_i , a_i^+ \right] = \delta_{ij}$$

$$n_i = a_i^+ a_i$$

$$Nboson = Nsites$$







Competition between

tunneling

- **delocalization**
- **Number Fluctuations**
- **Fixed phase**

interaction

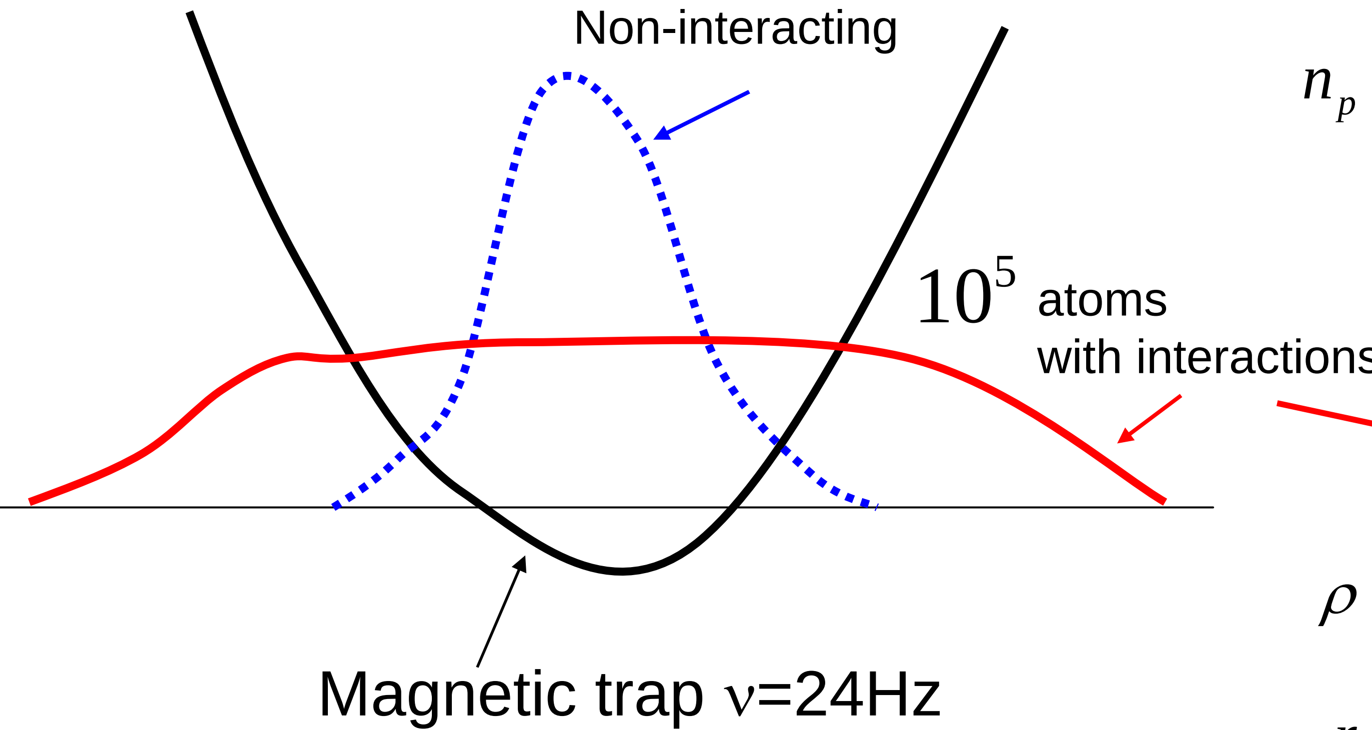
- **Localization**
- **Fixed Number**
- **Phase Fluctuations**

SUPERFLUID

MOTT INSULATOR

QUANTUM PHASE TRANSITION T=0

Bose Einstein Condensation



$$Rb^{87}$$

$$n_p = 37 = n_e \quad n_n = 50$$

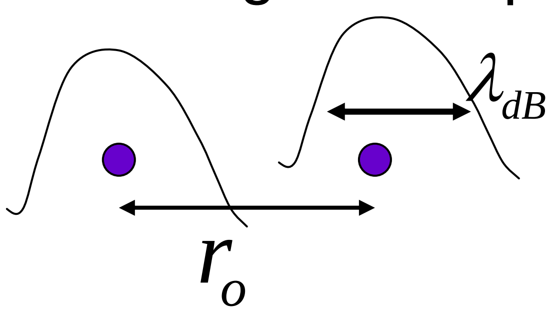
Even ⇨ boson

$$a_{HO} \sim \sqrt{\frac{\hbar}{m\omega}} \sim 1\mu$$

$$\xi \sim 5a_{HO}$$

$$\rho \sim \frac{\#\,atoms}{\xi^3} \sim 10^{15}/cm^3$$

$$r_o \sim 1000\,A^o$$



$$\lambda_{dB} \sim r_o \sim 10^3\,A^o$$

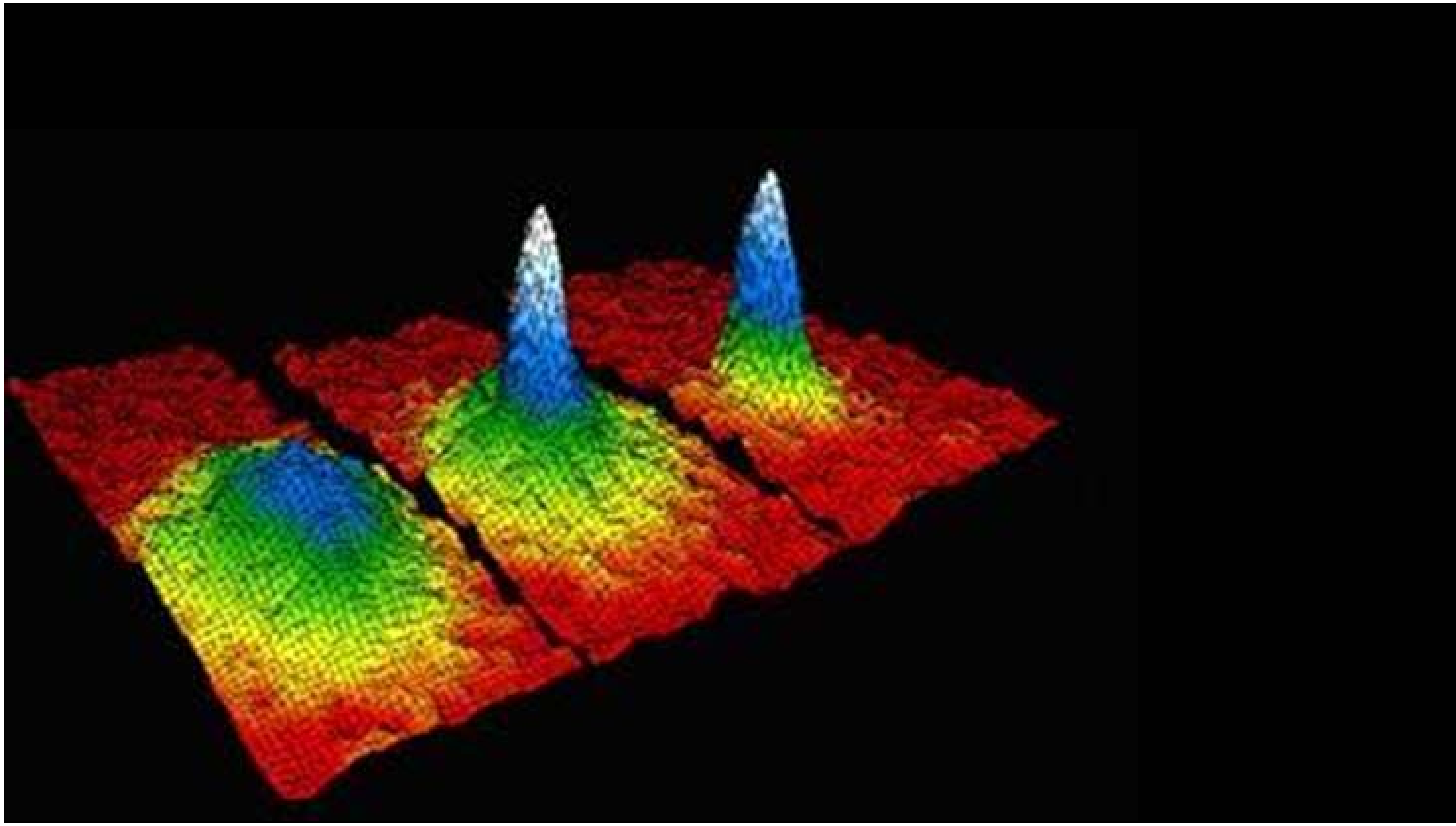
for $k_B T_c \sim 1\mu K$

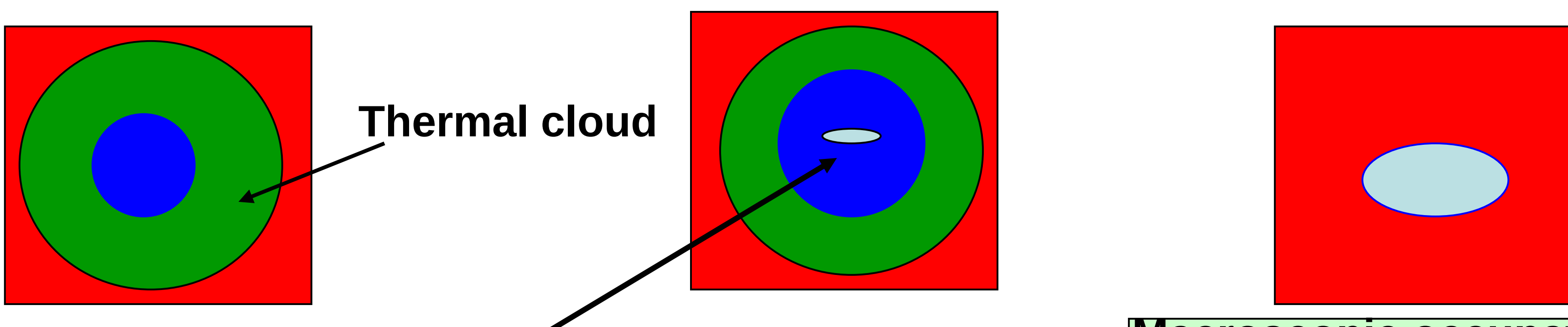
$$\lambda_{dB} = \sqrt{\frac{2\pi\hbar^2}{mk_BT}} \sim \frac{0.02}{\sqrt{k_BT(eV)}}\,A^o$$

Laser cooling; evaporative cooling
All apparatus at room temp!!

Ref: BEC Pethick and Smith (Cambridge)

ABSORPTION IMAGING (BEC in r-space)





Macroscopic occupation of single quantum state

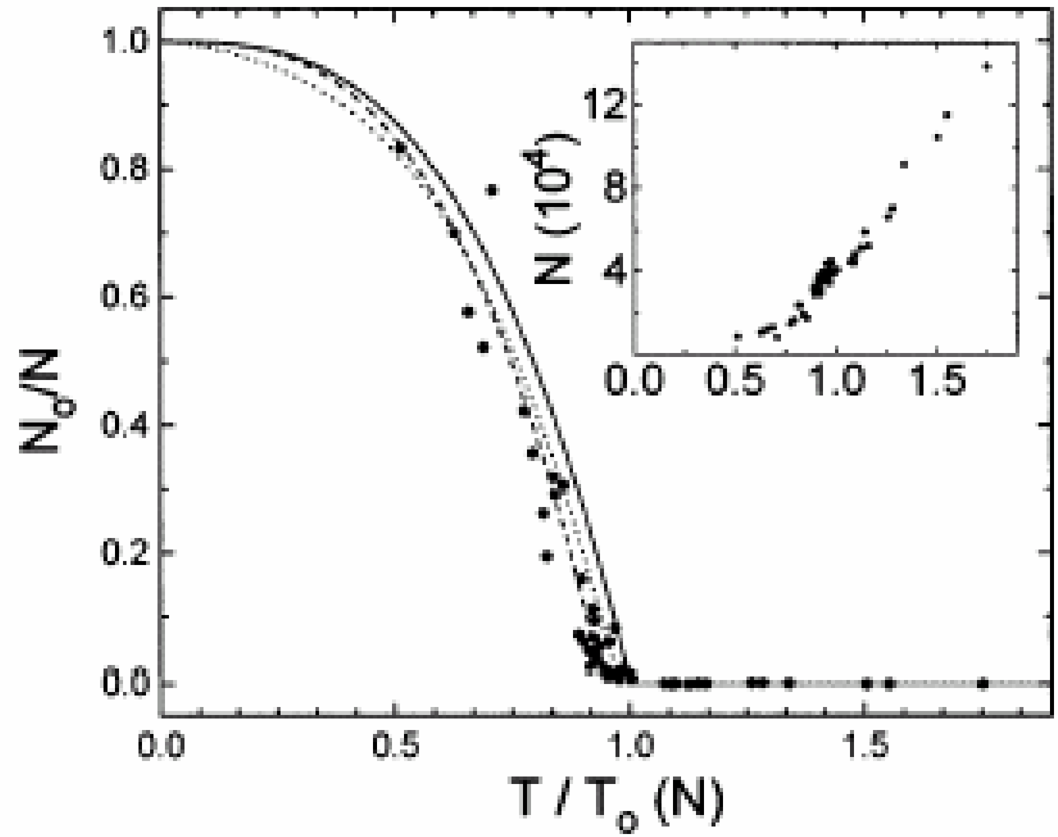
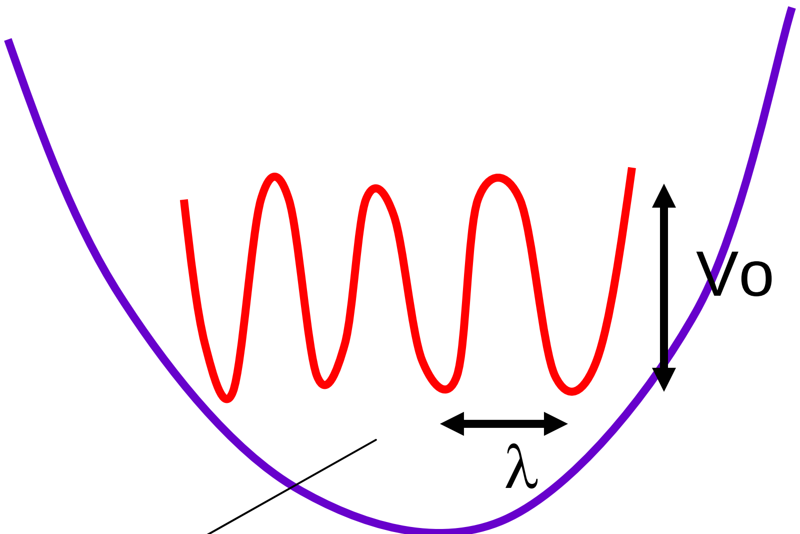


FIG. 1. Total number N (inset) and ground-state fraction N_o/N as a function of scaled temperature T/T_o. The scale temperature $T_o(N)$ is the predicted critical temperature, in the thermodynamic (infinite N) limit, for an ideal gas in a harmonic potential. The solid (dotted) line shows the infinite (finite) N theory curves. At the transition, the cloud consists of 40 000 atoms at 280 nK. The dashed line is a least-squares fit to the form $N_o/N = 1 - (T/T_c)^3$ which gives $T_c = 0.94(5)T_o$. Each point represents the average of three separate images.

OPTICAL LATTICE



$$V(x) = V_o \sin^2(2\pi x / \lambda)$$

Laser intensity

Laser wavelength
852nm

$$E_{laser} = h^2 / 2m\lambda^2$$

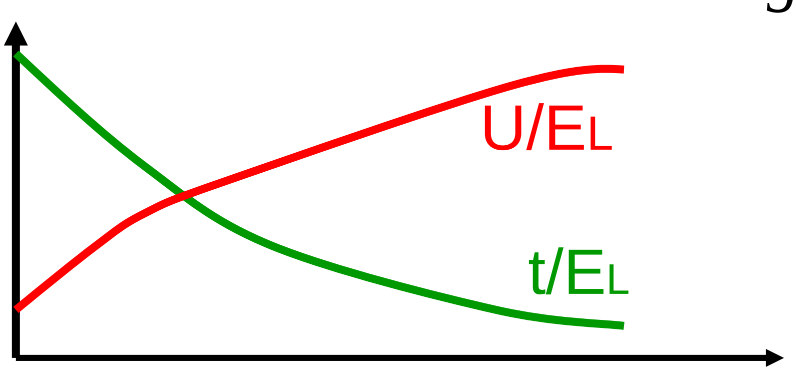
#atoms ~ 2×10^5

#lattice sites~ 15×10^4

~1-2 atoms /site

$$t \sim \int dx \varphi(x - x_i) \left[\frac{-\hbar^2}{2m} \nabla^2 + V(x) \right] \varphi(x - x_j)$$

$$U \sim g \int dx \left| \varphi(x - x_i) \right|^4$$

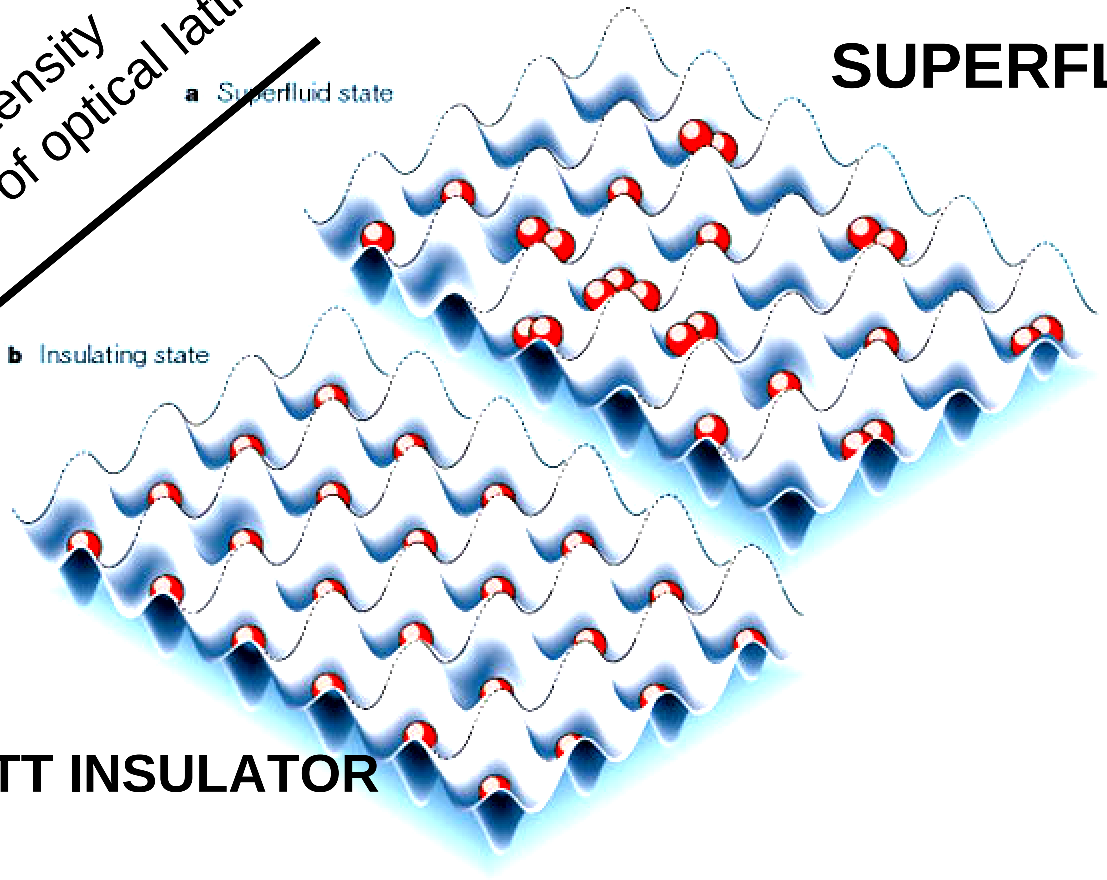


Vo/EL (squeezing)

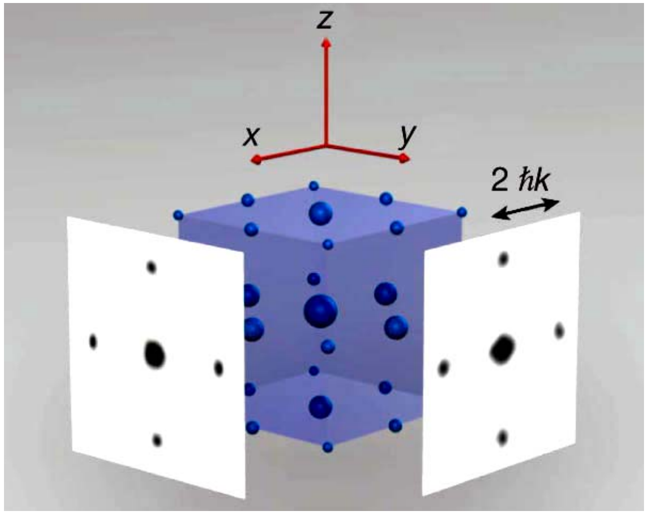
Rb atoms at 10nK

Laser intensity
Depth of optical lattice

SUPERFLUID



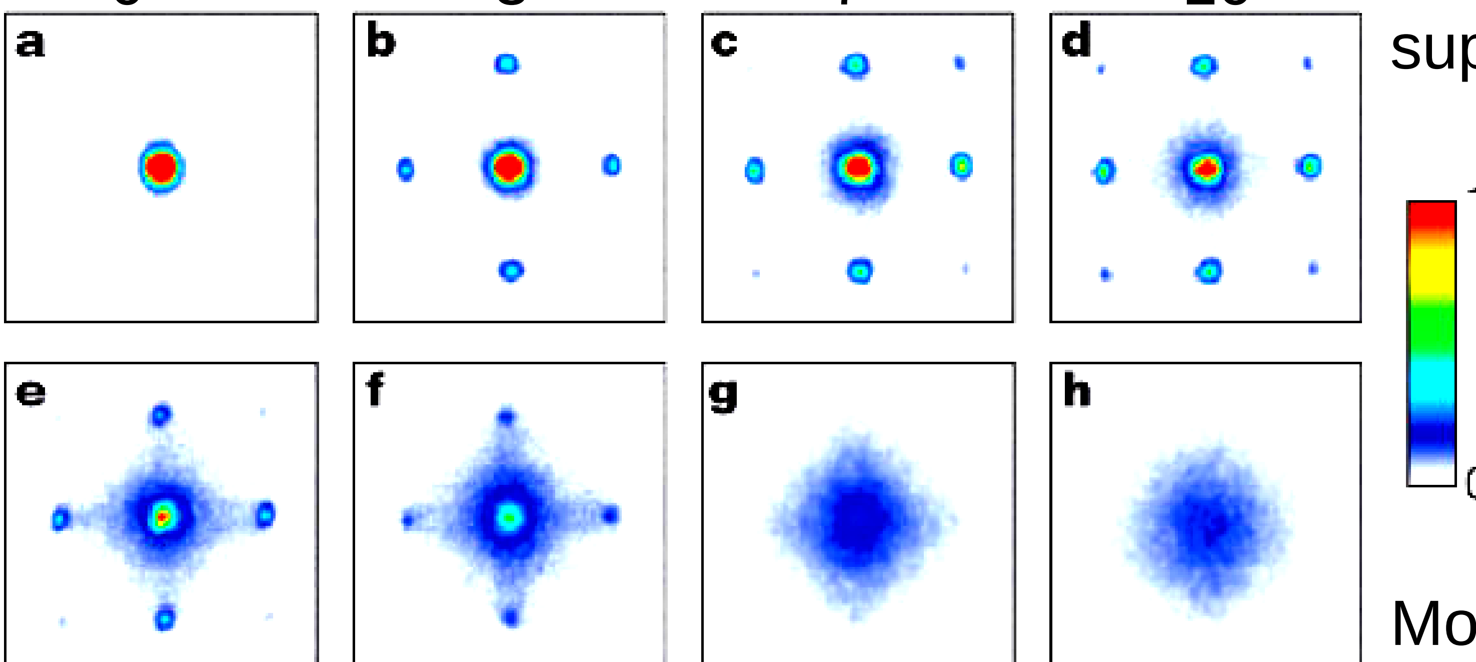
MOTT INSULATOR



tune periodic potential depth Vo/EL

0 3 7 10

superfluid

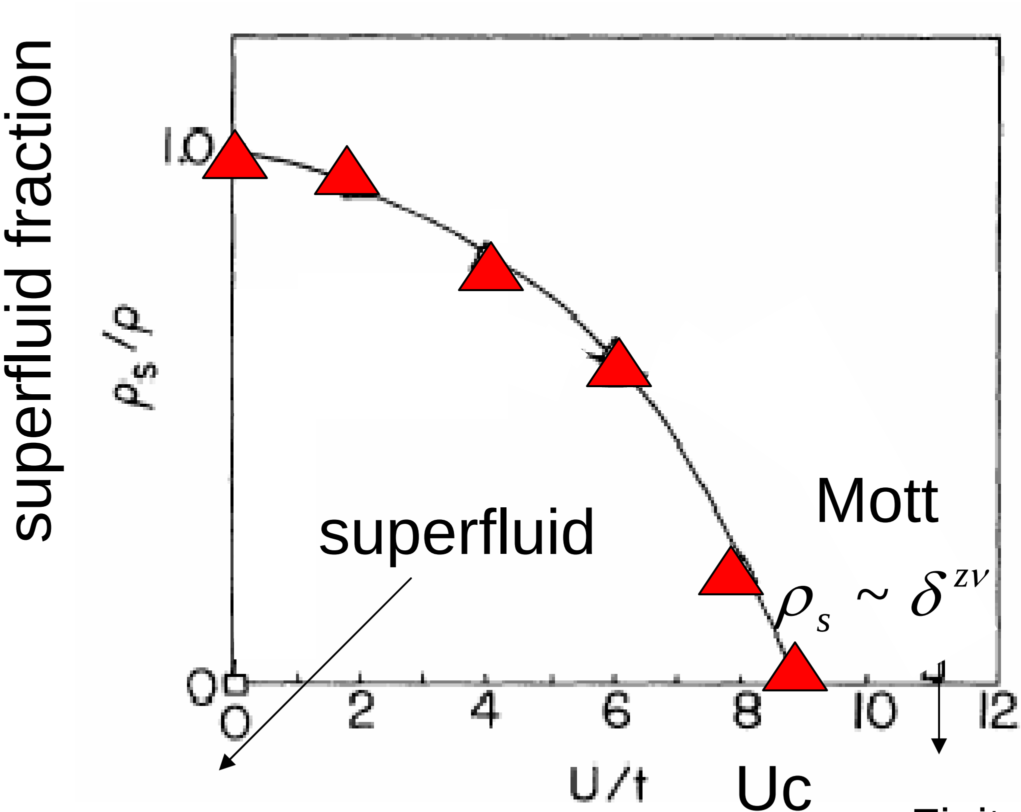


Mott

13 14 16 20

M. Greiner, O. Mandel, T. Esslinger, T.W. Hansch, I. Bloch, Nature 415, 39 (2002)

Bose Hubbard Model



Diverging length scales

$$\xi \sim \delta^{-\nu}$$

Diverging time scales

$$\xi_\tau \sim \xi^z \sim \delta^{-z\nu}$$

Energy $\Omega \sim \delta^{z\nu}$

dynamics and statics linked by H

Gapless excitations: phonons
compressible

Finite gap
incompressible

Universality class: (d+1) XY model
2d: ν=2/3; z=1
Fisher et al PRB 40, 546 (1989)

Krauth and N. Trivedi, Euro Phys. Lett. 14, 627 (1991) QMC 2d

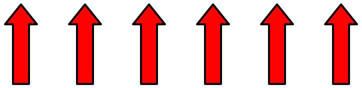
HEISENBERG ANTIFERROMAGNET

S=1/2

$$H = J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j = \frac{J}{2}\sum_{\langle ij\rangle}(S_i^+S_j^- + S_j^-S_i^+) + J\sum_{\langle ij\rangle}S_i^zS_j^z$$

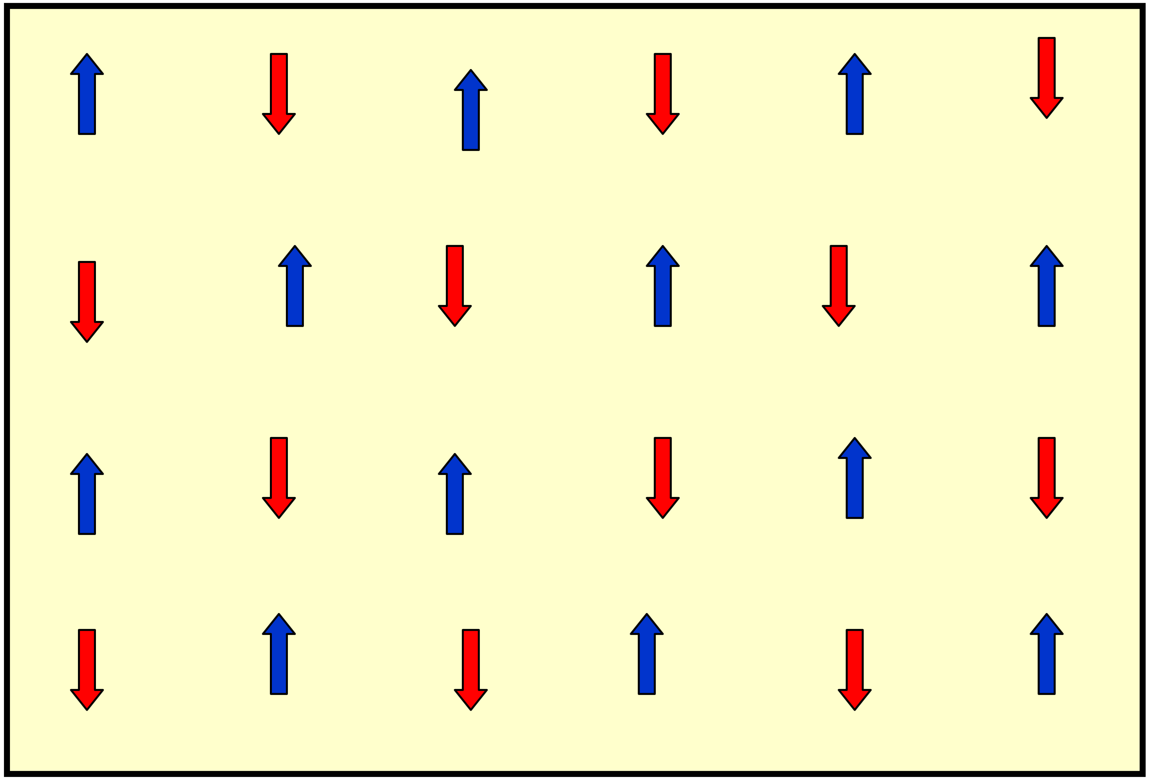
$$S_1^+S_2^-\left|\downarrow\uparrow\right\rangle_{12} = \left|\uparrow\downarrow\right\rangle_{12}$$

For J<0 Ground State:



FERROMAGNET

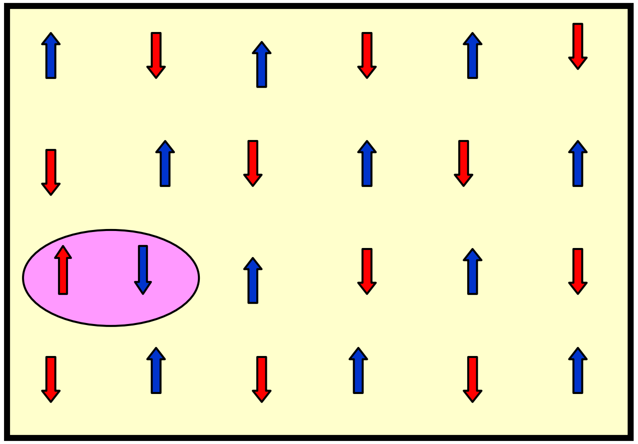
$$J_z > 0; J_{xy} = 0$$



CLASSICAL GROUND STATE: NEEL ANTIFERROMAGNET

$$H = J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j = \frac{J}{2}\sum_{\langle ij\rangle}(S_i^+S_j^- + S_j^-S_i^+) + J\sum_{\langle ij\rangle}S_i^zS_j^z$$

$$J_z > 0; J_{xy} \neq 0$$

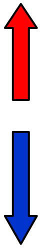


QUANTUM FLUCTUATIONS
INTRODUCED BY SPIN FLIPS

$$S_1^+ S_2^- \left| \downarrow_1 \uparrow_2 \right\rangle = \left| \uparrow_1 \downarrow_2 \right\rangle$$

At finite T thermal fluctuations destroy long range order in $d \leq 2$

What happens at T=0: do quantum fluctuations destroy long range order?



A sublattice

B sublattice

$$\varepsilon_i = \begin{cases} i \in A \\ i \in B \end{cases}$$

$$m^+ = \langle \varepsilon_i S_i^z \rangle$$

1D: Exact results: Bethe and Hulthen, 1930

	Heisenberg QAFM	Neel State
Eo/N	-0.42J	-0.25
m^{+}	0	0.5

Quantum fluctuations completely destroy long range order in 1D

2D: No exact results for Quantum Heisenberg model

XY model: $J_z = 0; J_{xy} \neq 0$ $m^{+} \neq 0$

XXZ model: $J_{xy} / J_z > 1.78$ $m^{+} \neq 0$

Kennedy, Lieb, Shastry
PRL, 61, 2582 (1988);
Kubo and Kishi,
PRL 61, 2585 (1988)

What happens when $J_{xy} = J_z$?

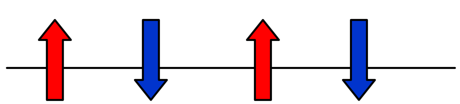
EXACT TRANSFORMATION S=1/2 to hard core bosons

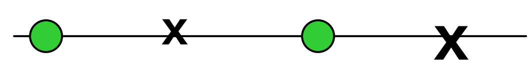
$$H = J\sum_{\langle ij\rangle} S_i \cdot S_j = \frac{J}{2}\sum_{\langle ij\rangle} S_i^+ S_j^- + S_j^- S_i^+ + J\sum_{\langle ij\rangle} S_i^z S_j^z$$

$$S_i^+ \to a_i^+$$

$$S_i^- \to a_i$$

$$S_i^z = S_i^+ S_j^- - \frac{1}{2} \to n_i - \frac{1}{2} = a_i^+ a_i - \frac{1}{2}$$





Matsubara and Matsuda
Prog. Theor. Phys. 16, 569 (1956)

$S_i^{\pm}$ commute on different sites—same as boson operators

$S_i^{\pm}$ anticommute on same site

$$\left(S_i^+\right)^2 |0\rangle = 0 \Rightarrow \left(a_i^+\right)^2 |0\rangle = 0$$

$\Rightarrow n_i = 0,1$ (HARD CORE BOSONS)

Sublattice rotation on B sublattice $S_i^+ \to \varepsilon_i a_i^+$

$$H = -\frac{J}{2}\sum_{<i,j>}(a_i^+ a_j + a_j^+ a_i) + J\sum_{<i,j>} n_i n_j + E_N$$

+ hard core constraint on a given site through commutation relations

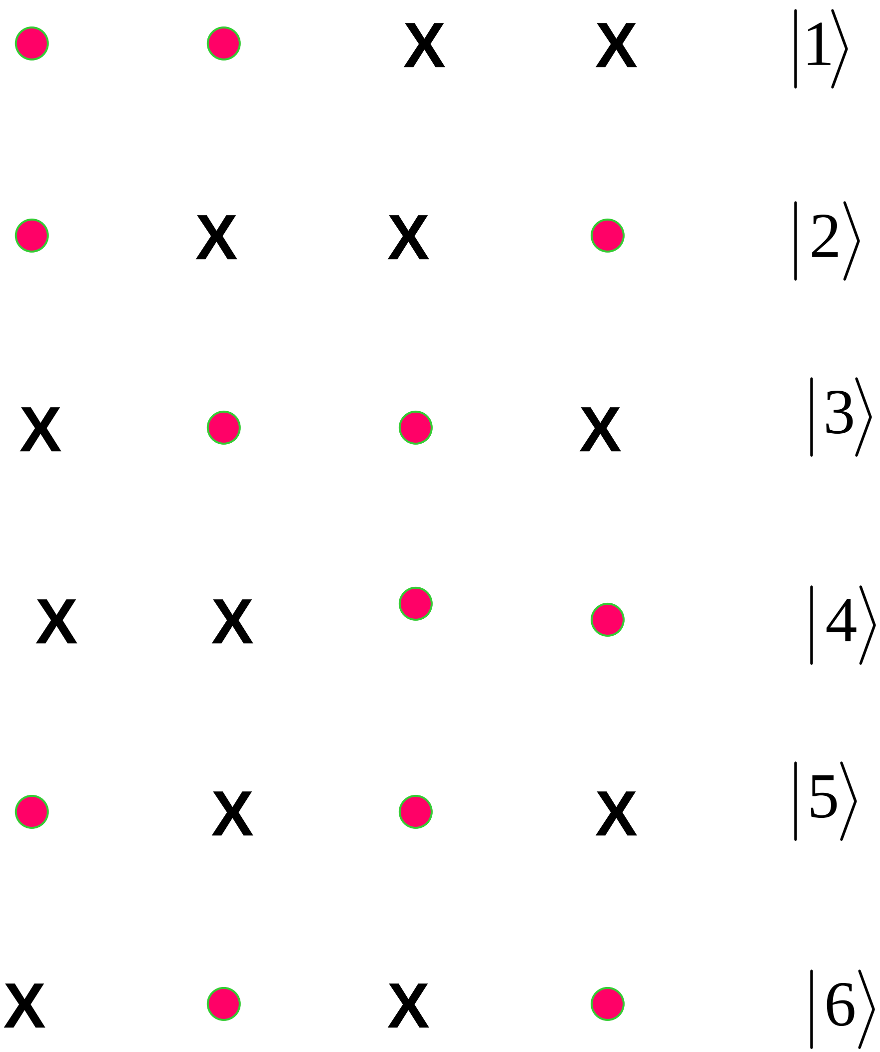
KE of bosons

Repulsion between bosons on nearest neighbor sites

$E_N = -JNz/8$ Classical Neel state energy; z=#neighbors

EXACT DIAGONALIZATION: example: Nsites=4; Nboson=2; Periodic Boundary C

$$H=-\frac{J}{2}\sum_{<i,j>}(a_i^+a_j+a_j^+a_i)+J\sum_{<i,j>}n_in_j$$



$$H=J\begin{pmatrix} 1 & 0 & 0 & 0 & -1/2 & -1/2 \\ 0 & 1 & 0 & 0 & -1/2 & -1/2 \\ 0 & 0 & 1 & 0 & -1/2 & -1/2 \\ 0 & 0 & 0 & 1 & -1/2 & -1/2 \\ -1/2 & -1/2 & -1/2 & -1/2 & 0 & 0 \\ -1/2 & -1/2 & -1/2 & -1/2 & 0 & 0 \end{pmatrix}$$

Eigenvalues: -1, 0, 1,1,1, 2

$$\frac{E_0}{N}=\left(\frac{-1}{4}+\frac{-2}{8}\right)J=-0.5J\xrightarrow[L\to\infty]{}-0.42J$$

Ground State

$$\Psi_0=\frac{1}{\sqrt{12}}\left(1|1\rangle+1|2\rangle+1|3\rangle+1|4\rangle+2|5\rangle+2|6\rangle\right)$$

$$m^+=\left\langle\sum_i\varepsilon_iS_i^z\right\rangle=\left\langle\sum_i\varepsilon_i(n_i-1/2)\right\rangle=\left\langle\sum_i\varepsilon_in_i\right\rangle$$

$$m^+=\frac{\langle 5|\sum_i\varepsilon_in_i|5\rangle}{\langle\Psi_0|\Psi_0\rangle}\times 2=\frac{4}{12}=\frac{1}{3}\xrightarrow[L\to\infty]{}0$$

Limitations of Exact Diagonalization

Suppose we want to study a 4x4 system

Nsites=16 Nboson=8

Number of states $c_8^{\ 16} = \frac{16!}{(8!)^2} = 12870$

Number of elements in H= $12870^2 = 165636900$

Amount of storage 8 bytes per element= $1.33 \times 10^9 \, bytes = 1 GBram$

VARIATIONAL APPROACH

CHOICE OF TRIAL WAVE FUNATION

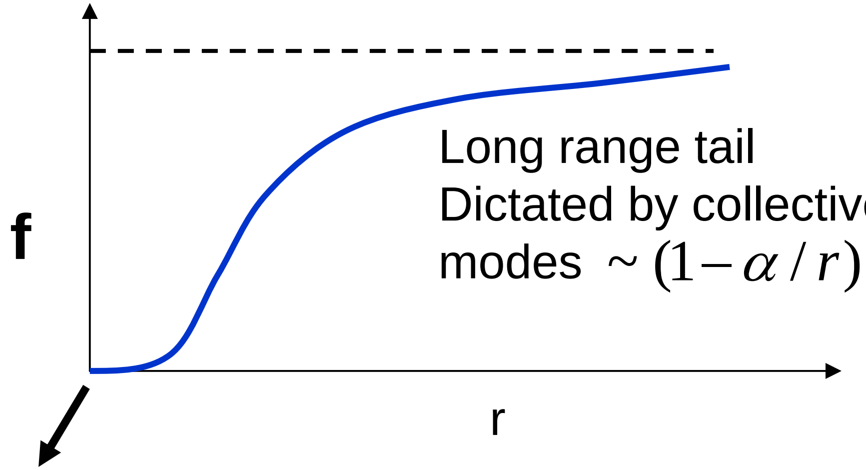
$$\Psi_T(r_1, r_2, \ldots r_N) = e^{-\sum_{i<j} u(r_{ij})} \times 1$$

Analogy with He4
McMillan PR 138 A 442 (1965)

Non-interacting bosons
Perfect condensation in k-space
Uniform in r-space

$$e^{\sum_{i<j} u(r_{ij})} = \prod_{i<j} f(r_{ij})$$

Jastrow correlation factor



Long range tail
Dictated by collective
modes $\sim (1-\alpha/r)$

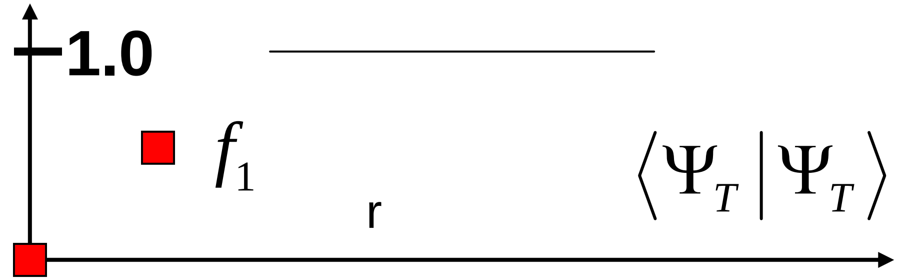
Hard core constraint

Short range suppression
Due to interparticle
repulsion

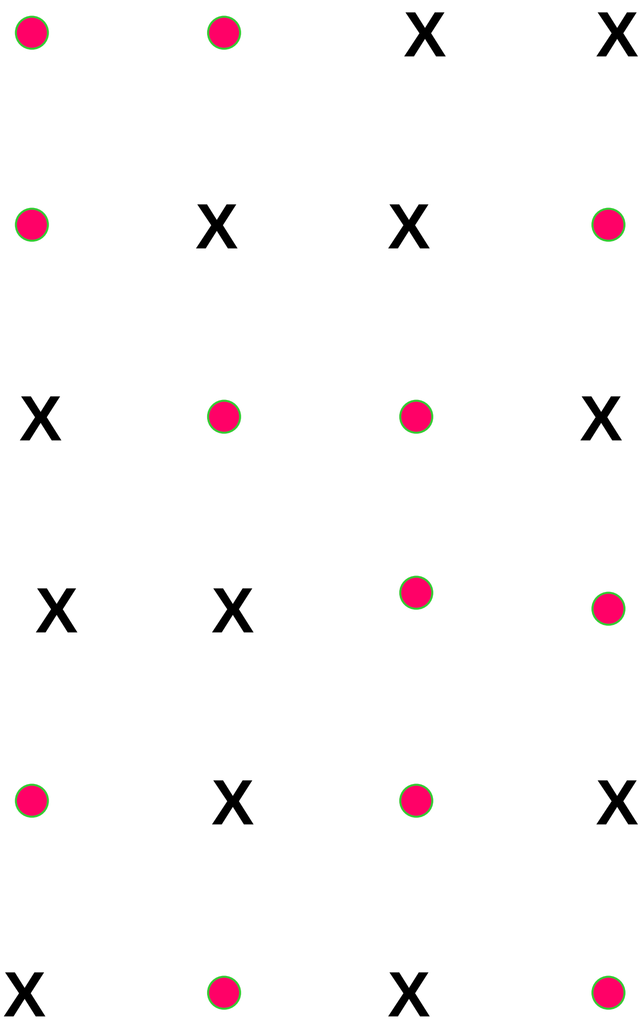
Ground state many body wave function is REAL and NODELESS
Statement of Marshall sign for spin systems

Variational calculation: Example Nsites=4 Nboson=2

$$\Psi_T(R) = \prod_{i<j} f$$



$$\langle \Psi_T | \Psi_T \rangle = 2 + 4 f_1^{\,2}$$



$|1\rangle$ $\langle \Psi_T | 1 \rangle = f_1$

$|2\rangle$ $\langle \Psi_T | 2 \rangle = f_1$

$|3\rangle$ $\langle \Psi_T | 3 \rangle = f_1$

$|4\rangle$ $\langle \Psi_T | 4 \rangle = f_1$

$|5\rangle$ $\langle \Psi_T | 5 \rangle = 1$

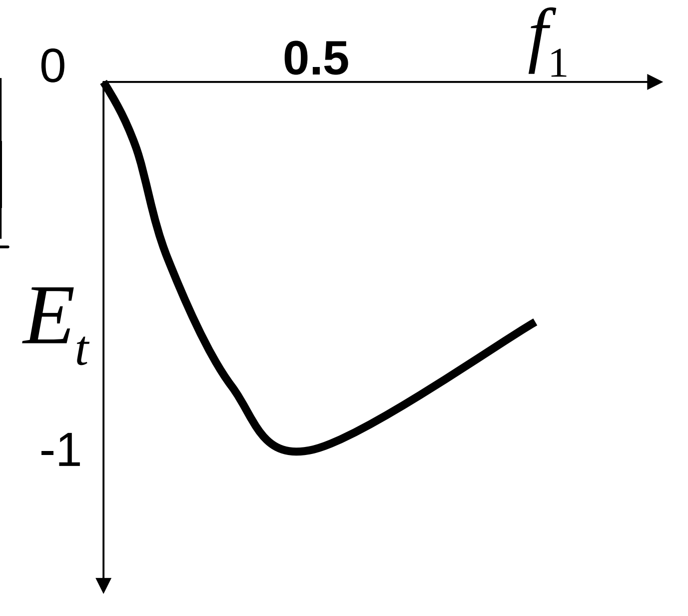
$|6\rangle$ $\langle \Psi_T | 6 \rangle = 1$

$$H = -\frac{J}{2}\sum_{<i,j>}(a_i^+ a_j + a_j^+ a_i) + J\sum_{<i,j>} n_i n_j = -\frac{J}{2}\hat{T} + J\hat{V}$$

$$T\left|\bullet\bullet\times\times\right\rangle = \left|\bullet\times\bullet\times\right\rangle + \left|\times\bullet\times\bullet\right\rangle$$

$$T\left|\times\bullet\times\bullet\right\rangle = \left|\bullet\times\times\bullet\right\rangle + \left|\times\times\bullet\bullet\right\rangle + \left|\times\bullet\bullet\times\right\rangle + \left|\bullet\bullet\times\times\right\rangle$$

$$\langle H\rangle = \frac{\left[-\frac{J}{2}(4f_1\times 2 + 2f_1\times 4) + Jf_1^{\,2}\times 4\right]}{2+4f_1^{\,2}}$$



$$E_t = \frac{-8f_1 + 4f_1^{\,2}}{2+4f_1^{\,2}}$$

$$f_1^* = 1/2$$

$$E_t^* = -1$$

$$E_t/N = -1/4 + E_N/N = -1/4 - 1/4 = -0.5J$$