

# Bose Hubbard model

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# Outline

## ① Optical lattices

- ① Laser traps
- ② Standing light waves
- ③ periodic potentials

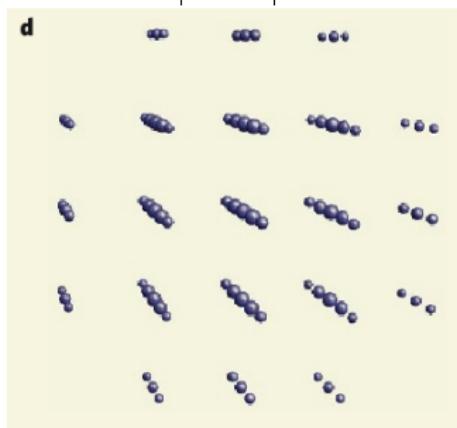
## ② Bose hubbard model

- ① Simple model to describe particles in periodic potentials
- ② Hamiltonian:  $H_B \rightarrow H_{MF}$
- ③ SF - MI phase transition

## ③ SF - MI phase transition

## ④ Summary

From NATURE|Vol 453|5 June 2008 .



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## ① Optical lattices

- ① Laser traps
- ② Standing light waves
- ③ periodic potentials

From <http://plentifulmarketing.com> .

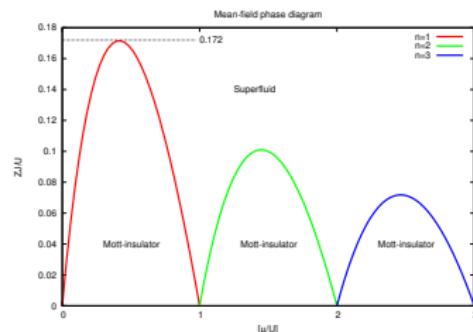


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## ① Optical lattices

- ① **Laser traps**
- ② Standing light waves
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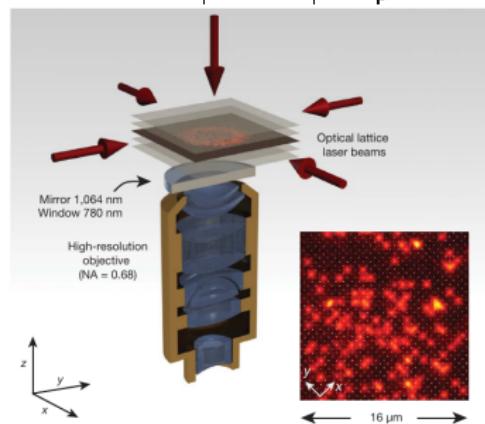
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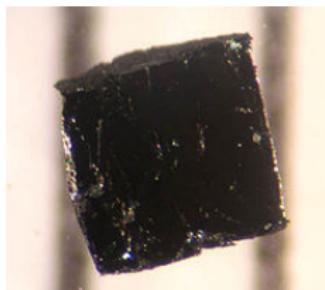
From: NATURE | Vol 467 | 2 September 2010 .



# Motivation

Why are we interested in the Bose Hubbard model?

- High temperature superconductor
- $Bi_2Sr_2Ca_2Cu_3O_{10}$  (BSCCO) (110 K)
- Principle not yet understood



???



From <http://en.wikipedia.org> .  
Adapted from <http://www.profitpath.com> .

# Simplify

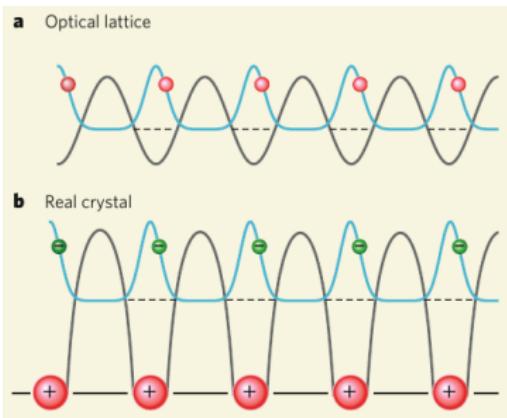
Break the problem down to make it simpler

- ➊ Rebuild the solid state using optical lattices

$$\textcircled{1} \quad d_{lat} \approx \frac{\lambda_{Laser}}{2} \approx 10^{-6} \text{ m}$$

$$\textcircled{2} \quad d_{lat} \approx 10^{-10} \text{ m } (\textcircled{\text{\AA}})$$

- ➋ Investigate superconductivity
- ➌ Explain the superfluid - Mott-Insulator transition



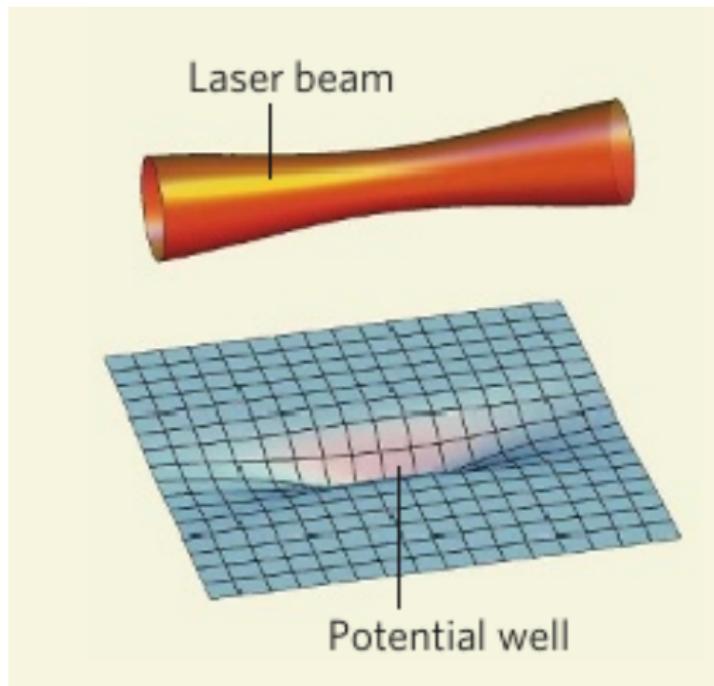
From NATURE|Vol 453|5 June 2008 .

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- 2 Bose Hubbard model
- 3 Phase transition - Experiments
- 4 Summary

# Particle confinement

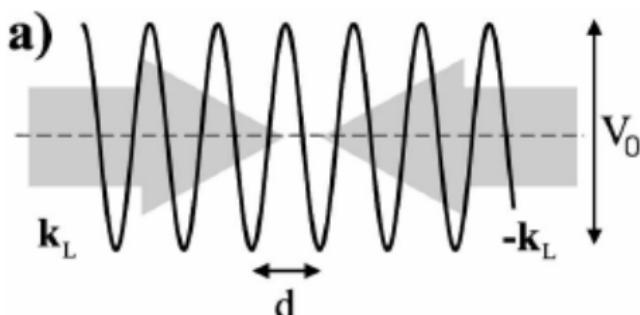
- ① Focused laser beam → potential well
- ② Standing light wave
- ③  $d = \frac{\lambda_{\text{Laser}}}{2}$
- ④ 2D, 1D and 0D confinement
- ⑤  $d_{lat} \approx \frac{\lambda_{\text{Laser}}}{2} \approx 10^{-6} \text{ m}$
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From NATURE|Vol 453|5 June 2008 .

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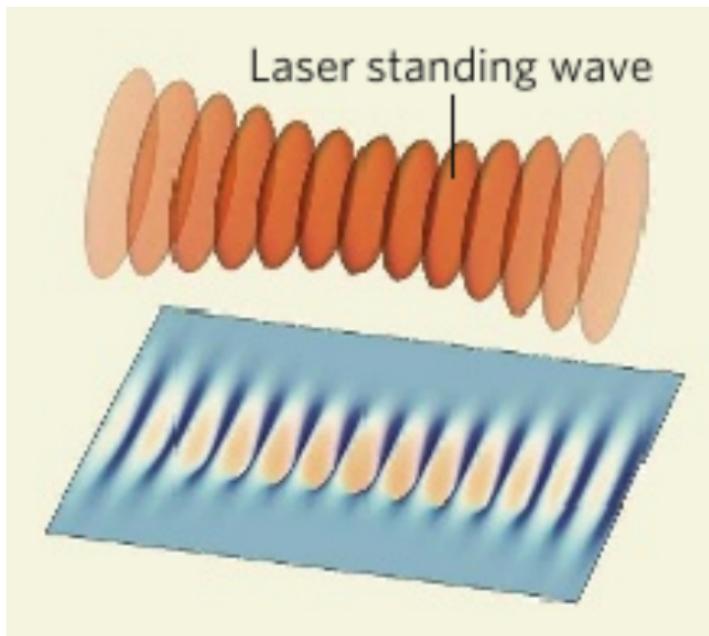
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Adapted from arXiv:physics/9902072v1 .

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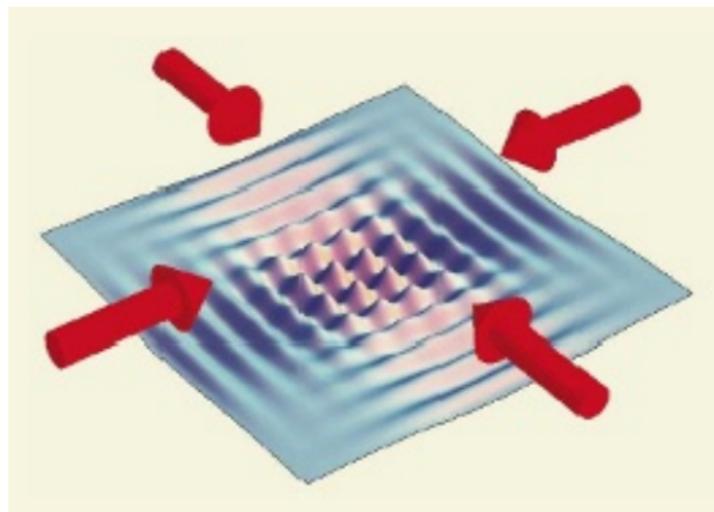
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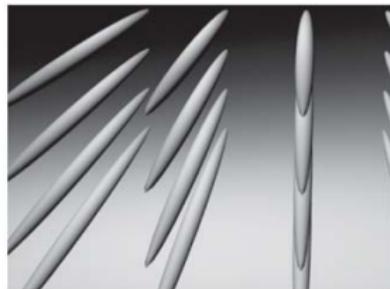
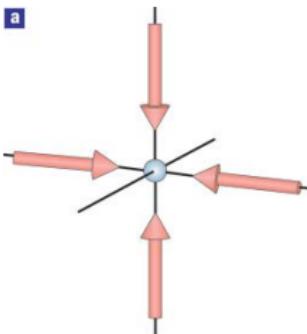
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# Particle confinement

- ① Focused laser beam → potential well



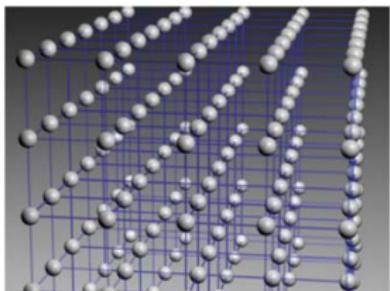
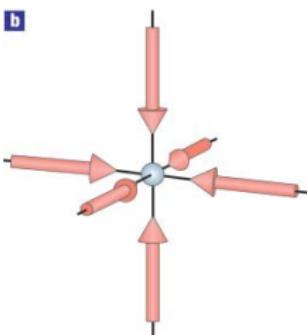
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From Nature Physics 1, 23 - 30 (2005) .

# Light forces

- Use the principle of the AC Stark shift
- Electric dipole moment is induced in the atom
- Energy shift  $\Delta E$

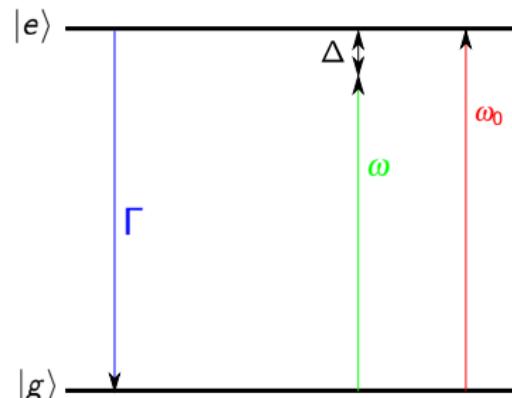
$$\Delta E = U_{dip} = -\frac{1}{2} \langle \mathbf{p} \mathbf{E} \rangle = -\frac{1}{2} \Re(\alpha(\omega)) \langle E^2(t) \rangle$$

$$I = 2\epsilon_0 c \cdot |\tilde{E}|^2$$

$$U_{dip} = -\frac{1}{2\epsilon_0 c} \Re(\alpha(\omega)) \cdot I$$

Dynamic polarization

$$\omega = \omega_0 + \Delta$$



## Potential

$$U_{dip}(r) = \frac{3\pi c^2}{2\omega_0^3} \frac{\Gamma}{\Delta} I(r)$$

# Black Board Calculation I

# Light forces

$$U_{dip} = -\frac{3\pi c^2}{2\omega_0^3} \left( \frac{\Gamma}{\omega_0 - \omega} + \underbrace{\frac{\Gamma}{\omega_0 + \omega}}_{\text{neglect}} \right) I(x)$$

Rotating-wave approximation:

- Resonances at  $\pm\omega_0$
- Tune laser near  $\omega_0 \rightarrow \Delta \equiv \omega - \omega_0 \rightarrow |\Delta| \ll \omega_0$
- $\Delta \ll \omega + \omega_0$

Proof.

$$U_{dip} = \frac{3\pi c^2}{2\omega_0^3} \cdot \frac{\Gamma}{\Delta} \cdot I(x) \propto \frac{\Gamma}{\Delta} \cdot I(x)$$



# Detuning

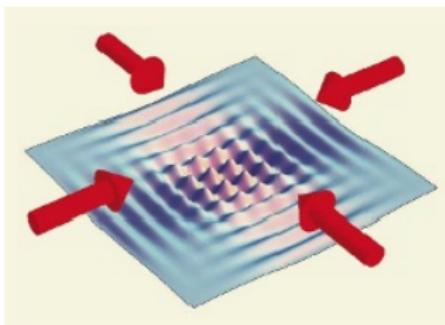
$$U_{dip} = \frac{3\pi c^2}{2\omega_0^3} \cdot \frac{\Gamma}{\Delta} \cdot I(x) \propto \frac{\Gamma}{\Delta} \cdot I(x)$$

$$\Gamma_{sc} = \frac{3\pi c^2}{2\hbar\omega_0^3} \cdot \left(\frac{\Gamma}{\Delta}\right)^2 \cdot I(x) \propto \left(\frac{\Gamma}{\Delta}\right)^2 \cdot I(x)$$

- Below atomic resonance (“red” shifted) ( $\omega < \omega_0$ )
  - $\Delta < 0 \rightarrow U_{dip} < 0$
  - attractive potential

# Experimental issues

- Potential  $\propto \frac{I}{\Delta}$
- Scattering rate  $\propto \frac{I}{\Delta^2}$



From NATURE|Vol 453|5 June 2008 .

## Fact

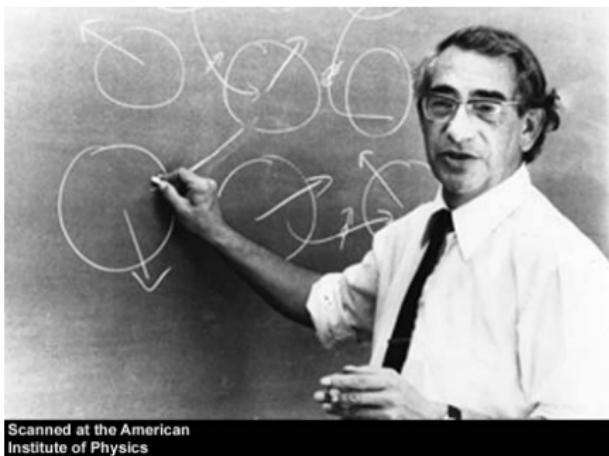
*Use for optical traps (at a certain potential depth)*

- *large detunings*
- *high intensities*

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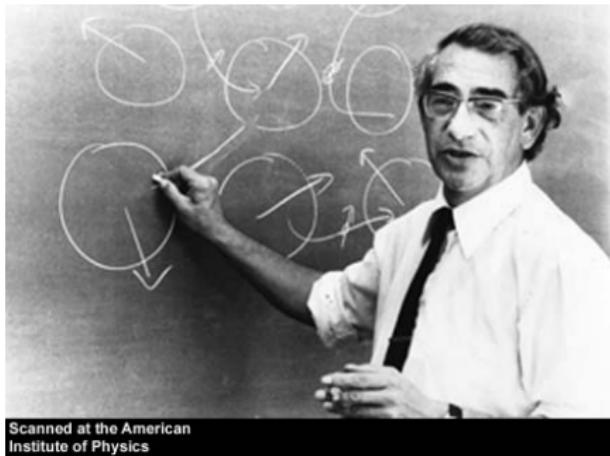
# Fermi Hubbard model (FHM)



- Proposed 1963 by John Hubbard
- Describe  $e^-$  in transition metals
- Investigate magnetic properties

From: theor.jinr.ru .

# Bose Hubbard model (BHM)

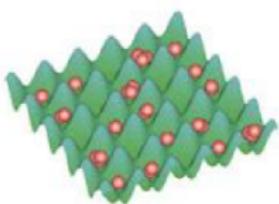


- Cooper pairs (CP) - Josephson tunneling
- He atoms moving on substrates
- Ultracold atoms in optical lattices
- **SF-MI phase transition**
- **CP/ $e^-$  transition is neglected**

From: theor.jinr.ru .

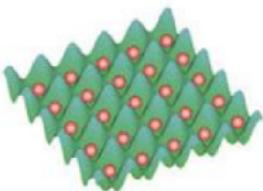
# SF and MI Introduction

(a) Superfluid state



Atoms freely move around in an optical lattice.

(b) Mott-insulator state



Atoms localize at lattice sites because of inter-atomic interactions.

- $U=0$ : Superfluid phase

$$|\Psi_{SF}\rangle_{(U=0)} = \frac{1}{\sqrt{N!}} \left( \frac{1}{\sqrt{N_L}} \sum_{i=1}^{N_L} \hat{b}_i^\dagger \right)^N |0\rangle$$

- phase coherence

- $J=0$ : Mott insulating phase

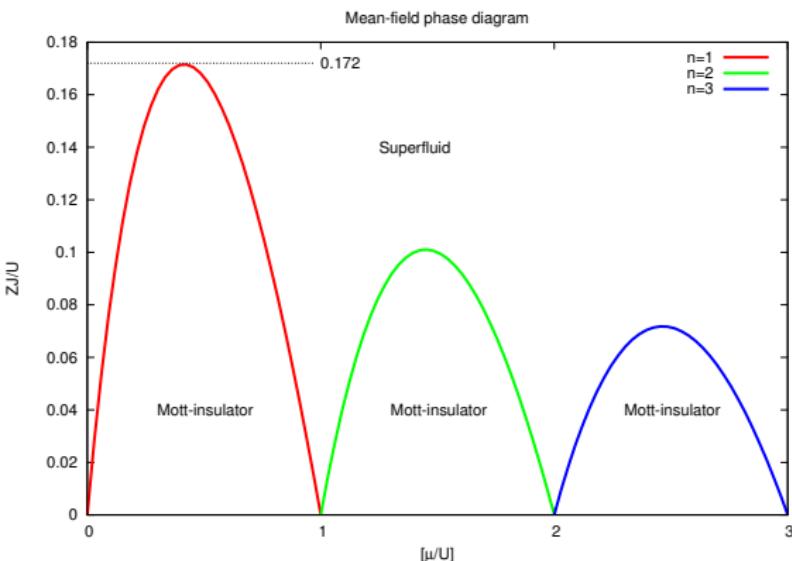
$$|\Psi_{MI}\rangle_{(J=0)} \propto \prod_{i=1}^{N_L} \left( \hat{b}_i^\dagger \right)^n |0\rangle$$

- no phase coherence
- perfect correlation in  $n$

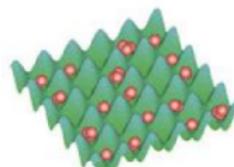
Adapted from: [www.ntt-review.jp](http://www.ntt-review.jp).

# Further plan

What we want to do within this part.

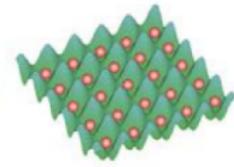


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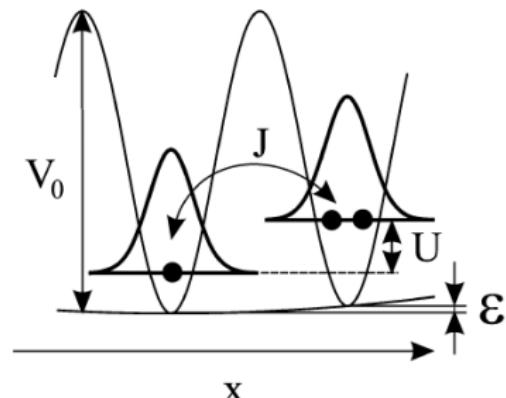
# Bose Hubbard Hamiltonian

According to a tight binding model the Hamiltonian is

$$H_B = -J \sum_{\langle ij \rangle} \left( \hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i \right) - \mu \sum_i \hat{n}_{bi} + \frac{U}{2} \sum_i \hat{n}_{bi} (\hat{n}_{bi} - 1)$$

$$[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij}$$

- $J$ : Allows hopping of bosons / Josephson tunneling
- $\mu$ : Chemical potential  $\equiv$  number of bosons
- $U > 0$ : Repulsive interaction



From D. Jaksch, P. Zoller / Annals of Physics  
315 (2005) 52–79 .

# Mean-field theory

Now: Have a look on a **single** lattice site !

Model the properties of  $H_B$  by the best possible sum of single-site hamiltonians:

$$H_{MF} = \sum_i \left( -\mu \hat{n}_{bi} + \frac{U}{2} \hat{n}_{bi} (\hat{n}_{bi} - 1) - \Psi_B^* \hat{b}_i - \Psi_B \hat{b}_i^\dagger \right)$$

- $\Psi_B$ : variational parameter (complex)
- $\mu$ : Chemical potential
- $U > 0$ : Repulsive interaction

## Black Board Calculation II

# Phase transition

$$H_B = -J \sum_{\langle ij \rangle} \left( \hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i \right) - \mu \sum_i \hat{n}_{bi} + \frac{U}{2} \sum_i \hat{n}_{bi} (\hat{n}_{bi} - 1)$$

Set  $J = 0 \rightarrow$  single-site Hamiltonian becomes

$$H_{B.i} = -\mu \hat{n}_{bi} + \frac{U}{2} \hat{n}_{bi} (\hat{n}_{bi} - 1) = \frac{U}{2} \left[ \hat{n}_{bi} \left( \hat{n}_{bi} - 1 - 2 \frac{\mu}{U} \right) \right]$$

$$E_0 = \langle n | H_{B.i} | n \rangle = \frac{U}{2} \left[ n \left( n - 1 - 2 \frac{\mu}{U} \right) \right]$$

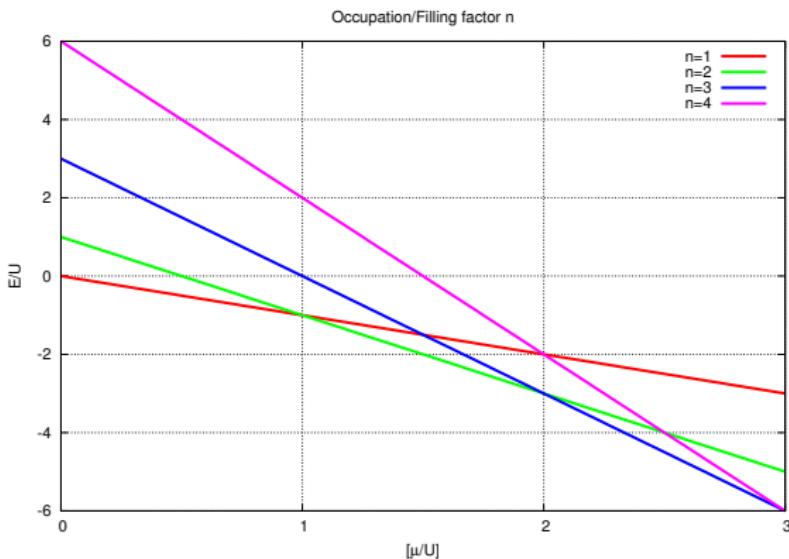
$$n = \text{integer} \left( \frac{\mu}{U} + \frac{1}{2} \right)$$

# Phase transition

$$E = \frac{U}{2} \left[ n \left( n - 1 - 2 \frac{\mu}{U} \right) \right]$$

$$\frac{E}{U} = \frac{1}{2} \left[ n \left( n - 1 - 2 \frac{\mu}{U} \right) \right]$$

$$n = \begin{cases} 0 & \mu/U < 0 \\ 1 & 0 < \mu/U < 1 \\ 2 & 1 < \mu/U < 2 \\ \vdots & \vdots \\ n & n-1 < \mu/U < n \end{cases}$$

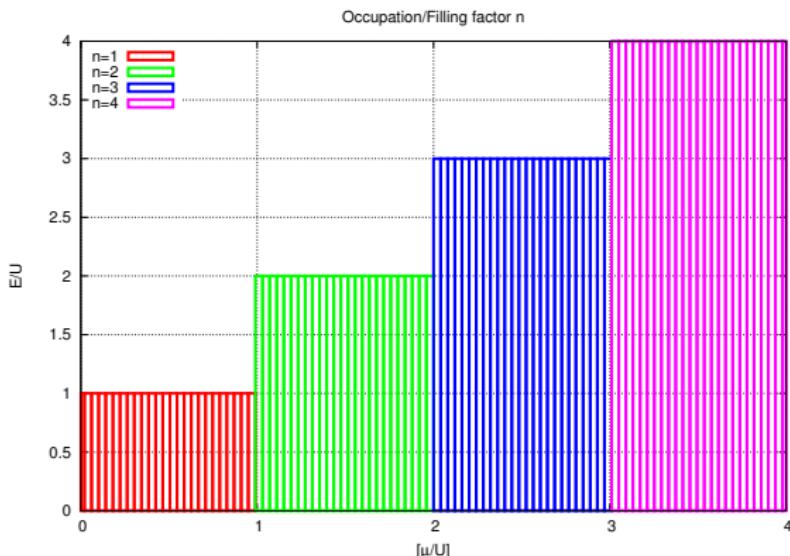


# Phase transition

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$$n = \frac{\partial E}{\partial \mu} = \text{const.}$$

$$\frac{\partial n}{\partial \mu} = 0$$



Corollary

Mott insulating phase is **incompressible** !

# Phase transition

Expand  $E_0$  in powers of  $\Psi_B$

$$E_0 = E_{00} + q |\Psi_B|^1 + r |\Psi_B|^2 + s |\Psi_B|^3 + \mathcal{O}\left(|\Psi_B|^4\right)$$

Landau: Symmetry of phase transition (second order) leads to

$$E_0 = E_{00} + r |\Psi_B|^2 + \mathcal{O}\left(|\Psi_B|^4\right)$$

Use perturbation theory till second order and identify  $r$

$$r = ZJ \cdot (1 - ZJx_0)$$

$$\begin{aligned} x_0(\mu/u) &= \frac{n(\mu/u) + 1}{Un(\mu/u) - \mu} + \frac{n(\mu/u)}{\mu - u(n(\mu/u) - 1)} \\ &= -\frac{\mu + U}{(Un - \mu)(U(n - 1) - \mu)} \end{aligned}$$

# Phase transition

$$H_{MF,i} = -\mu \hat{n} + \frac{U}{2} \hat{n}(\hat{n}-1) - ZJ \left( \Psi_B^* \hat{b} + \Psi_B \hat{b}^\dagger - \Psi_B^2 \right)$$

$$\hat{V} = -JZ \Psi_B \left( \hat{b} + \hat{b}^\dagger \right)$$

$$\begin{aligned} E_n^{(1)} &= \langle n | \hat{V} | n \rangle \\ &= -JZ \Psi_B \langle n | \hat{b} | n \rangle - JZ \Psi_B \langle n | \hat{b}^\dagger | n \rangle \\ &= -JZ \Psi_B \sqrt{n} \langle n | n-1 \rangle - JZ \Psi_B \sqrt{n+1} \langle n | n+1 \rangle \\ &= 0 \end{aligned}$$

$$\begin{aligned} \Psi_n^{(1)} &= -JZ \Psi_B \sum_{m \neq n} |m\rangle \cdot \frac{\langle m | \hat{V} | m \rangle}{E_n - E_m} \\ &= -JZ \Psi_B \left( \frac{\sqrt{n}}{E_n - E_{n-1}} |n-1\rangle + \frac{\sqrt{n+1}}{E_n - E_{n+1}} |n+1\rangle \right) \end{aligned}$$

# Phase transition

$$E_n^{(2)} = \left\langle n | \hat{V} | \Psi_n^{(1)} \right\rangle$$

$$= J^2 Z^2 \Psi_B^2 \left( \frac{n}{E_n - E_{n-1}} + \frac{n+1}{E_n - E_{n+1}} \right)$$

$$E_n^{(0)} = JZ \Psi_B^2 + \frac{U}{2} n(n-1) - \mu n$$

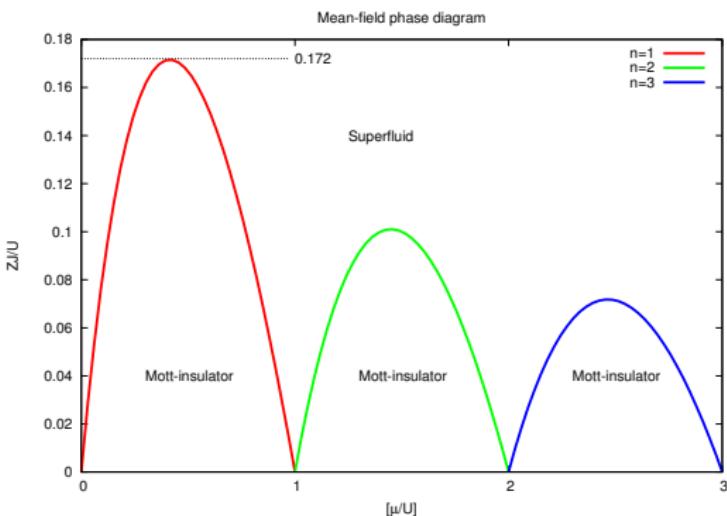
$$E_n - E_{n-1} = U(n-1) - \mu$$

$$E_n - E_{n+1} = \mu - Un$$

$$E_n^{(2)} = - \frac{U + \mu}{(\mu - Un)(U(n-1) - \mu)} J^2 Z^2 \Psi_B^2$$

$$E_0 = \frac{U}{2} n(n-1) - \mu n + \left( JZ - \frac{U + \mu}{(\mu - Un)(U(n-1) - \mu)} J^2 Z^2 \right) \Psi_B^2$$

# Phase transition



$$r = ZJ \cdot \underbrace{\left(1 - ZJx_0\right)}_{=0} = 0$$

Corollary

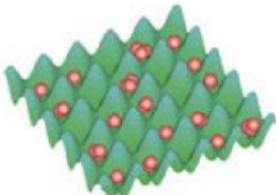
$$\frac{ZJ}{U} = \frac{\left(n - \frac{\mu}{U}\right) \left(1 - n + \frac{\mu}{U}\right)}{1 + \frac{\mu}{U}}$$

Critical point ( $n = 1$ ):

$$\frac{ZJ}{U} \approx 0.172 \dots \leftrightarrow \frac{U}{JZ} \approx 5.8$$

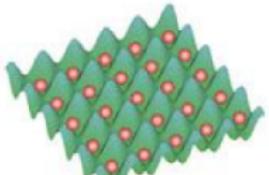
# Phase transition

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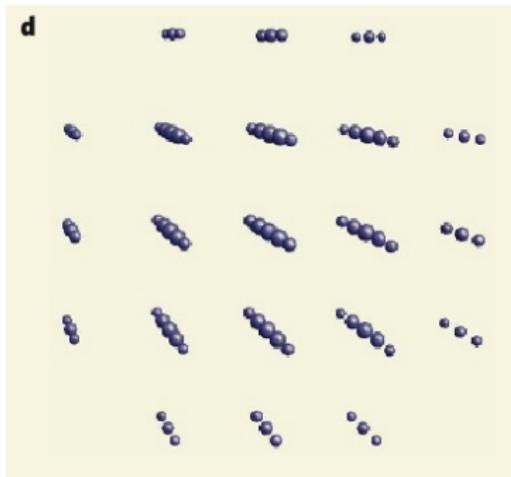
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# Quantum Phase transition

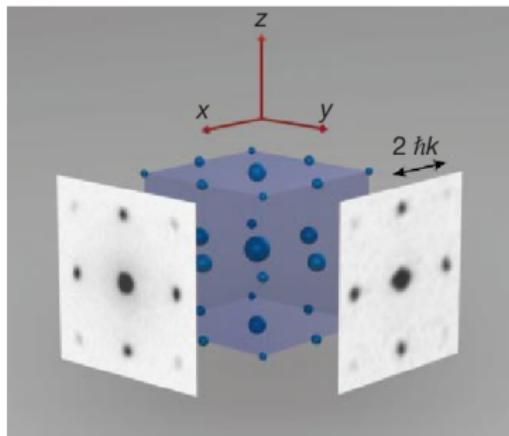
- ➊ Optical lattice with  $d_{lat} = 426 \text{ nm}$
- ➋ Expand 15 ms (ToF)
- ➌ Take image
- ➍ Coherence/Decoherence
- ➎  $|\Psi(x)\rangle \propto \cos\left(\frac{\pi}{d_{lat}} \cdot x\right)$
- ➏  $|\Psi(k)\rangle \propto \delta\left(k \pm \frac{\pi}{d_{lat}}\right)$



From NATURE|Vol 453|5 June 2008 .

# Quantum Phase transition

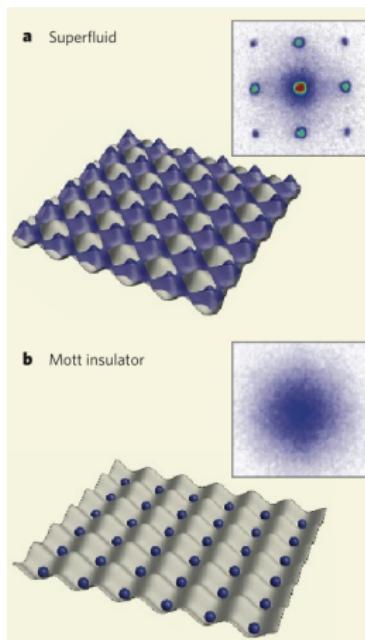
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From: NATURE | VOL 415 | 3 JANUARY 2002

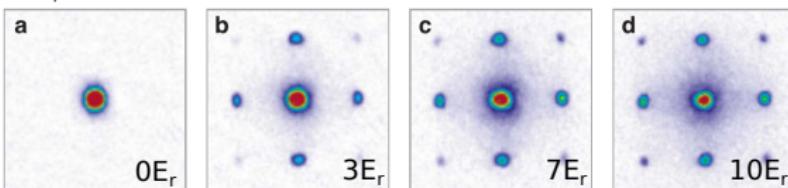
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From NATURE|Vol 453|5 June 2008 .

# Quantum Phase transition - Experiment |

 $U/J = 0$ 

 $U/J = 36$ 
 $U/J = \infty$ 

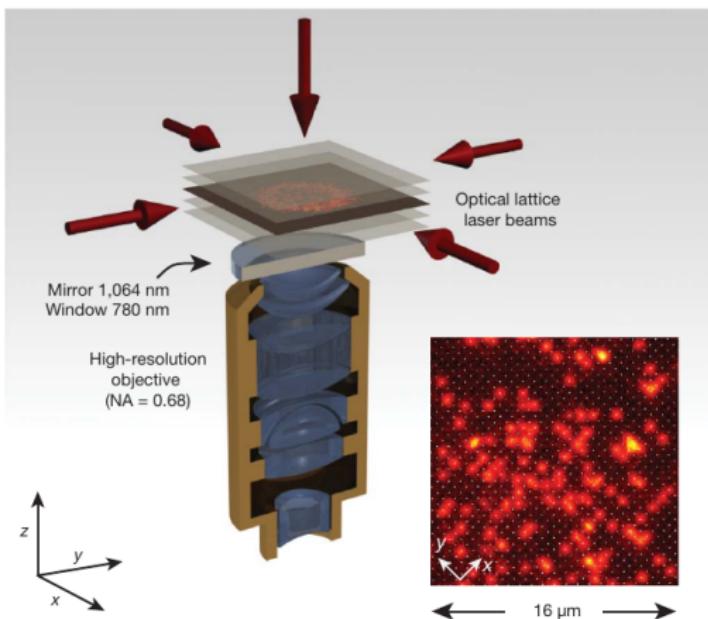
From: NATURE | VOL 415 | 3 JANUARY 2002 .

## Example

SF-MI transition (experiment):  $U/J = 36|_{Z=6} \rightarrow U/JZ = 6$

SF-MI transition (theory):  $U/JZ = 5.8$

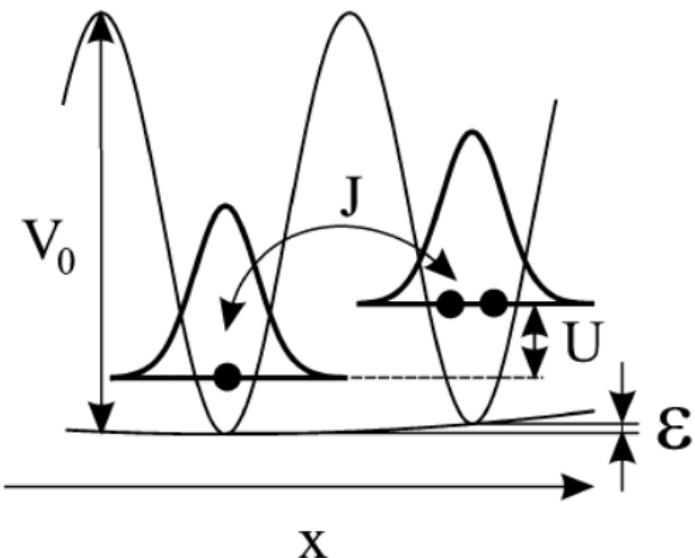
# Quantum Phase transition - Experiment II



- BEC in 2D optical lattice
- high-resolution fluorescence imaging
- very strong optical particle confinement
- only Mott insulating phases visible
- occupation mod2

From: NATURE | Vol 467 | 2 September 2010 .

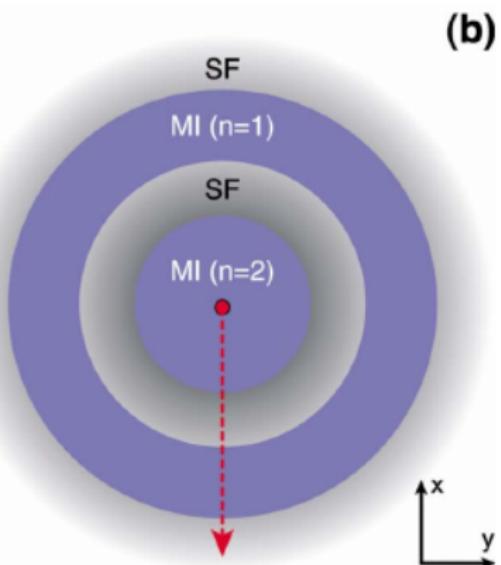
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From D. Jaksch, P. Zoller / Annals of Physics 315

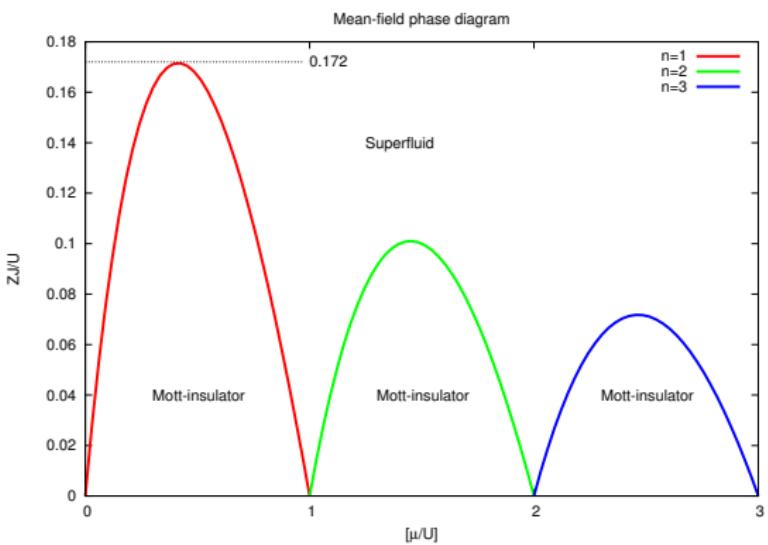
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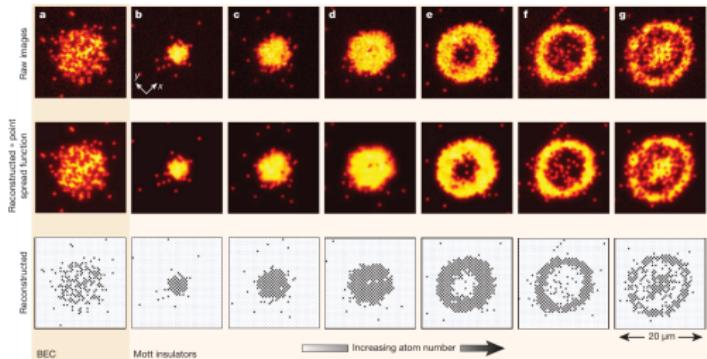
From: Rev.Mod.Phys., Vol.80, No.3, July-Sept 2008 . (2005)  
52-79 .

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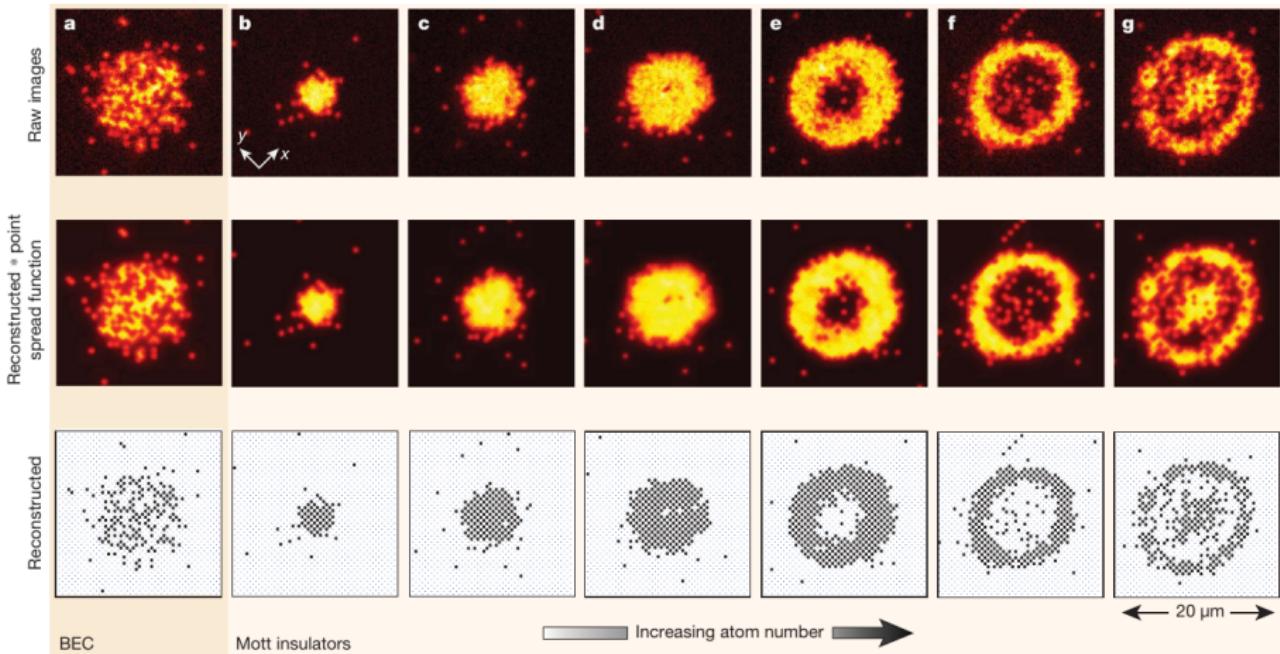
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# Outline

- 1 Optical lattices
- 2 Bose Hubbard model
- 3 Phase transition - Experiments
- 4 Summary

# Summary

What we have learned today

## ① Optical lattice:

$$U_{dip}(\mathbf{r}) = \frac{3\pi c^2}{2\omega_0^3} \frac{\Gamma}{\Delta} I(\mathbf{r})$$

## ② Bose Hubbard Hamiltonian

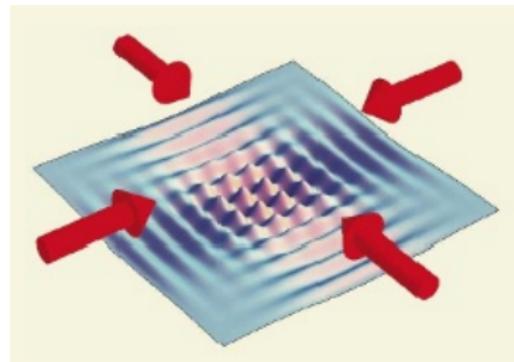
$$H_B = -J \sum_{\langle ij \rangle} (\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i) - \mu \sum_i \hat{n}_{bi} + \frac{U}{2} \sum_i \hat{n}_{bi} (\hat{n}_{bi} - 1)$$

$$H_{MF} = \sum_i \left( -\mu \hat{n}_{bi} + \frac{U}{2} \hat{n}_{bi} (\hat{n}_{bi} - 1) - \Psi_B^* \hat{b}_i - \Psi_B \hat{b}_i^\dagger \right)$$

## ③ Phase diagram given by

$$\frac{ZJ}{U} = \frac{(n - \frac{\mu}{U})(1 - n + \frac{\mu}{U})}{1 + \frac{\mu}{U}}$$

## ④ Today experimentally proven



From NATURE|Vol 453|5 June 2008 .

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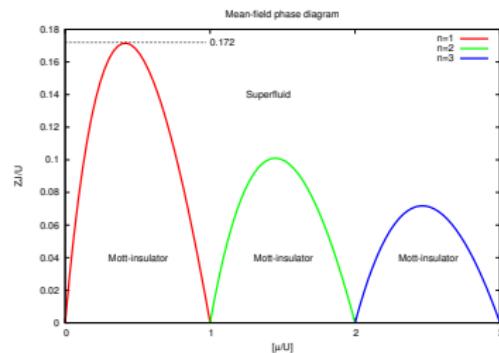
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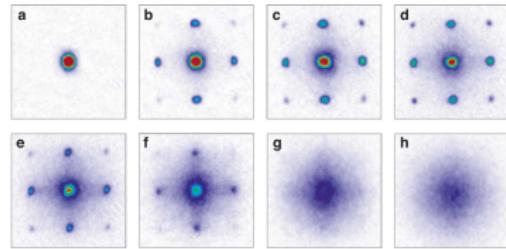
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From: NATURE | VOL 415 | 3 JANUARY 2002

# Thank you!

**Thank you for your attention!**

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# For Further Reading |