### **Quantum phase transitions in cold gases**

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### Atomic and molecular gases

#### Bose-Einstein condensation

- Gross-Pitaevskii equation
- non-linear dynamics

#### Rotating condensates

- vortices
- fractional quantum Hall

# Quantum degenerate *dilute* atomic gases of fermions and bosons Barry tunability

#### Molecules

- Feshbach resonances
- BCS-BEC crossover
- polar molecules

#### Optical lattices

- Hubbard models
- strong correlations
- exotic phases

### Quantum gases in optical lattices

#### Experimental groups

- I. Bloch, Mainz
- T. Porto, NIST
- T. Esslinger, ETH Zürich
- D. Weiss, Penn State
- R. Grimm, Innsbruck
- W. Ketterle, MIT
- M. Inguscio, Florence
- J. Dalibard, Paris
- K. Sengstock, Hamburg
- M. Oberthaler
- M. Greiner, Harvard
- K. Zimmermann, Tübingen



### Theory groups

- ...

### Quantum gases in optical lattices

#### Optical lattices

- properties of an optical lattice
- Bose-Hubbard model



#### Many-body theory

- Phase diagram
- Mean-field theory and effective theory
- 1D Bose-Hubbard model





### Interaction between light and atoms

- Hamiltonian between atoms and light: dipole approximation

$$
H = -\mathbf{d}\mathbf{E}(t, \mathbf{r})
$$

- external laser field:
- $\Omega = |\langle e| \mathbf{d} \mathbf{E}_{\omega} |g\rangle|/\hbar$ - rabi frequency:
- detuning:



 $\mathbf{E}(t) = \mathbf{E}_{\omega} e^{-i\omega t} + \mathbf{E}_{\omega}^* e^{i\omega t}$ 

- AC Stark shift (change in the grounds state energy due to coupling to excited state)





### Interaction between light and atoms

- spontaneous emission:  $\Gamma_e$ excited state has a finite life time due to spontaneous emission - AC Stark shift  $\Delta E_g = \frac{\hbar\Omega^2\Delta}{\Delta^2+\Gamma_c^2/4}$ 

- loss of atoms from the ground state

$$
\Gamma_g = \frac{\Omega^2 \Gamma_e}{\Delta^2 + \Gamma_e^2/4}
$$



- limits life-time of a BEC in an optical lattice
- requires large detuning

 $\Delta \gg \Gamma_e$ 

- high laser power

- a far-detuned standing laser wave provides a periodic potential for the particles

$$
V(\mathbf{x})=V_0\cos(\mathbf{k}\mathbf{x})^2
$$



- recoil energy: 
$$
E_r
$$
 =

- structure in 3D

$$
\mathbf{E}(t,\mathbf{r})=\sum_i \mathbf{E}^i_{\omega_i} \cos(\mathbf{k}_i \mathbf{r}) e^{-i\omega_i t}+c.c.
$$

 $\hbar^2 k^2$ 

 $2m$ 

- : wave length fixed by the atomic transition
- $\omega_i$ : slightly different frequencies to cancel cross terms
- : polarization as additional degree of freedom

$$
V(\mathbf{x}) = \sum_i V_i \cos(\mathbf{k}_i \mathbf{r})^2
$$











#### Tricks with 2D optical lattice

J. Sebby-Strabley, M. Anderlini, P.S. Jessen, and J.V. Porto, Phys Rev. A 73, 033605 (2006)



$$
V(\mathbf{x}) = V_0 \left[ \cos(kx)^2 + \cos(ky)^2 \right]
$$

- in plane polarization - cross terms disappear



$$
V(\mathbf{x}) = V_0 \left[\cos(kx) + \cos(ky)\right]^2
$$

- polarization along z-axes
- lattice with cross terms



- combined lattice - lattice of double wells



## **Many body Hamiltonian**



### Microscopic Hamiltonian

Many-body Hamiltonian

- pseudo-potential approximation
- $\psi(x),\psi^\dagger(x)$ - field operator

$$
H = \int dx \, \psi^+(x) \left( -\frac{\hbar^2}{2m} \Delta + V(x) \right) \psi(x) + \frac{g}{2} \int dx \, \psi^+(x) \psi^+(x) \psi(x) \psi(x)
$$
  
optical  
lattice  

$$
g = \frac{4\pi \hbar^2 a_s}{m}
$$
: interaction strength of the Pseudo potential

Derivation of effective low energy theory:

D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Rev. Lett. 81, 3108 (1998)

> (i) Solve the single particle problem in an optical lattice

(ii) Add the interaction as perturbation



Hubbard model for Fermions and bosons

### Magnetic Feshbach resonance



#### Feshbach resonances

- two interal states of the atoms:
	- open channel
	- closed channel (only virtually excited)
- bound state close to the continuum of the open channel
- tuning of the energy of the molecular state via magnetic field or Raman transition

$$
a_{\textrm{\tiny eff}} = a_s (1 + \frac{\Delta \nu}{E-E_{\textrm{\tiny res}}})
$$

: width of the resonance  $\Delta \nu$  $\nu = E - E_{res}$ : detuning

### Single particle problem

lattice vector

 $V(\mathbf{r}+\mathbf{R}_i)=V(\mathbf{r})$ 

Hamiltonian

- particle in a periodic potential

$$
H=\frac{{\bf p}^2}{2m}+V({\bf r})
$$

- Bloch wave functions
	- $\phi_{n,\mathbf{k}}(\mathbf{r})=e^{i\mathbf{kr}}u_{n,\mathbf{k}}(\mathbf{r})$

 $E_n(\mathbf{k})$ : energy dispersion : quasi momentum within  $\bf k$ first Brillouine zone

- Bloch theorem

$$
\phi({\bf r}+{\bf R}_i)=e^{i{\bf k}{\bf r}}\phi({\bf r})
$$



### Wannier functions



### Microscopic Hamiltonian

#### Hubbard model

- express the bosonic field operator in terms of Wannier functions

$$
\psi(\mathbf{r})=\sum_{i,n}w_n(\mathbf{r}-\mathbf{R}_i)b_{n,i}
$$

creation/annihilation operator for particles at site *i* in band *n*

L

$$
H = \int dx \, \psi^+(x) \left( -\frac{\hbar^2}{2m} \Delta + V(x) \right) \psi(x) + \frac{g}{2} \int dx \, \psi^+(x) \psi^+(x) \psi(x) \psi(x)
$$

- restriction to lowest bloch bands

- only largest terms

$$
H_{\text{BH}} = -J \sum_{\langle ij \rangle} b_i^{\dagger} b_j + \frac{U}{2} \sum_i b_i^{\dagger} b_i^{\dagger} b_i b_i
$$
\nhopping energy interaction energy

### Bose-Hubbard Model

Bose-Hubbard model (Fisher et al PRB '81)

$$
H_{\text{BH}} = -J \sum_{\langle ij \rangle} b_i^{\dagger} b_j + \frac{U}{2} \sum_i b_i^{\dagger} b_i^{\dagger} b_i b_i - \sum_i \mu_i b_i^{\dagger} b_i
$$
\n
$$
\text{hopping energy} \qquad \text{interaction energy} \qquad \text{chemical potential and trapping}
$$
\n
$$
\text{Coupling parameters in 1D}
$$
\n
$$
U = \sqrt{2/\pi} \hbar \omega_{\perp} \frac{a_s}{a_0}
$$
\n
$$
J = \frac{4}{\sqrt{\pi}} \sqrt{VE_r} \left(\frac{V}{E_r}\right)^{1/4} e^{-2\sqrt{V/E_r}} \qquad \qquad \cdots
$$
\n
$$
U/2
$$

 $\overline{15}$ 

 $\overline{10}$ 

 $\overline{\mathbf{s}}$ 

 $20$ 

 $\sqrt{\frac{25}{6}}E_r$ 

- validity

### Bose-Hubbard Model

Weak interactions

- the mixing of different Bloch-bands is suppressed for weak interactions

> $U\ll\hbar\omega_0$  $a_s < a_0$

- Next-nearest-neighbor hopping
- small in the tight binding limit, but have to be included fore weak opitcal lattices

 $V_0 \lesssim E_r$ 

#### Nearest-neighbor interaction

- nearest-neighbor interactions are present, but are suppressed due to the decay of the wannier functions

$$
U_1 \sim \int d\mathbf{r} |w(\mathbf{r})|^2 |w(\mathbf{r}-\mathbf{R}_i)|^2
$$







Characteristic parameters

- wave length

 $\lambda \sim 1000 \text{nm}$ 

- lattice spacing

 $a \sim 500$ nm



 $E_r = \frac{2\pi^2\hbar^2}{m\lambda^2} \approx 9\textbf{kHz}$  $\approx 430$ nK

 $U \approx 0.5E_r$  $J \approx 0-0.5E_r$ 

- temperatures<br> $T_{\text{\tiny BEC}} \approx 1 \mu \mathbf{K}$  $T_{\rm min} \sim 1 \text{nK}$  $(1Hz \equiv 50pK)$ Exchange coupling
	- anti-ferromagnetic coupling in a fermionic Hubbard model





- effective interaction can become extremely small
- extremely challenging for temperature and stability

#### **Superfluid**  $J \gg U$

- weakly interacting Bose-Einstein condensate

$$
\phi_{\text{\tiny BEC}}\sim \left(\sum_i b_i^\dagger\right)^N\left|0\right\rangle
$$

- linear excitation spectrum
- off-diagonal long-range

$$
\langle \psi({\bf r}) \psi^{\dagger}(0) \rangle \to n_0
$$

#### Mott insulator  $U \gg J$

- commensurate filling
- zero temperature phase
- fixed particle number per lattice site

$$
\phi_{\text{\tiny Mott}}=\prod_i b_i^\dagger|0\rangle\\ \Delta\sim U
$$

- excitation gap



- delocalized atoms - poisson statistic for number of atoms per lattice site

$$
\sim\sim\sim\sim\sim
$$

- localized particles
- integer particles per lattice site

Quantum phase transition

Mott insulator

- commensurate filling
- gapped phase
- incompressible



#### **Superfluid**

- long-range order
- finite superfluid stiffness
- linear excitation spectrum

Mean-field theory 
$$
(d = \infty)
$$

- critical value

$$
U/J\Big|_{\rm S-MI}=z\left(n+\sqrt{n+1}\right)^2
$$

- qualitative correct even at low dimensions
- no particle-hole fluctuations in the Mott insulator



### Experiments

Long-range order:



Disappearance of coherence for strong optical lattices (Greiner et al. '02)

$$
\frac{V}{E_r} > 13
$$

#### Structure factor



Appearance of well defined two particle excitations

### Bose-Hubbard Model



$$
b_i^{\dagger}b_j = \psi^*b_j + b_i^{\dagger}\psi - |\psi|^2 \quad \blacksquare
$$

 $H_{\text{\tiny BH}} = \sum H_i$ 



- ground state is a product state

$$
\rho = \prod_i \rho_i \underbrace{\qquad \qquad}_{\text{matrix}}^{\text{local density}}
$$
\n
$$
\psi = \langle b_i \rangle
$$

 $-$  self-com

Long-Range order condensate density - order parameter  $\langle b_i b_i^{\dagger}$ 

- mean-field result

$$
\langle b_i b_j^\dagger \rangle = |\psi|^2 \equiv n_0
$$

- zero-temperature

$$
\rho_i = |f\rangle\langle f|
$$

$$
|f\rangle = \sum_n f(n)|n\rangle
$$

- the mean-field  $\alpha$  breaks the  $U(1)$  symmetry

- order parameter of the quantum phase transition

#### Mott Insulator

- localized particles
- integer particles per lattice site

 $|f\rangle = |n_0\rangle$ 

- realistic Mott-Insulator has particle-hole fluctuations

#### Superfluid phase

- off-diagonal long range order

 $\psi \neq 0$ 

- weak interactions:
	- locally a coherent state
	- condensate involves all particles

$$
\ket{f}=\exp\left(-|\psi|^2/2\right)\exp\left(\psi b^\dagger\right)
$$

\°/ \°/`

"mean-field" Mott insulator

 $\cdot \wedge \cdot \wedge$ 

particle-hole fluctuations

Phase transition

- appearance of  $\psi \neq 0$ long-range order
- Ansatz across the transition

$$
\begin{aligned} |f\rangle &= \sqrt{1-2\epsilon^2}|n_0\rangle \\ &+ \epsilon\left(e^{i\phi}|n_0\!-\!1\rangle\!+\!e^{-i\phi}|n_0+1\rangle\right) \\ \psi &= 2e^{i\phi}\epsilon\sqrt{1-2\epsilon^2} \end{aligned}
$$



- energy

$$
\frac{E[\psi]}{U} = \left[1 - \frac{zJ}{U} \left(\sqrt{n_0} + \sqrt{n_0 + 1}\right)^2\right] |\psi|^2 + \beta |\psi|^4
$$
  
phase transition at the

change of the sign



#### Quantum phase transition

- critical value

$$
U/J\Big|_{\textrm{\tiny S-MI}} = z\left(n+\sqrt{n+1}\right)^2
$$

- qualitative correct even at low dimensions
- no particle-hole fluctuations in the Mott insulator



Partition function  
\n
$$
Z_{\rm B} = {\rm Tr}\left[\exp\left(-\frac{H_{\rm BH}}{T}\right)\right]^{\text{propagator in}}t = -i\tau\left(-\frac{itH_{\rm BH}}{\hbar}\right)
$$

- path integral formulation

$$
Z_{\scriptscriptstyle \text{B}} = \int \mathcal{D} \left[ b_i(\tau) \right] \mathcal{D} \left[ b_i^\dagger(\tau) \right] \exp \left( - \int_0^{1/T} d\tau \mathcal{L}_{\scriptscriptstyle \text{B}} \right)
$$

- Lagrangian of the Bose-Hubbard model

$$
\mathcal{L}_{\text{\tiny B}} = \sum_i \left[ b_i^\dagger \, \partial_\tau b_i - \mu b_i^\dagger b_i + \frac{U}{2} b_i^\dagger b_i^\dagger b_i b_i \right] - J \sum_{\langle i,j \rangle} \left( b_i^\dagger b_j + b_i b_j^\dagger \right)
$$
\n
$$
= \sum_i b_i^\dagger \, \partial_\tau b_i + H_{\text{\tiny BH}}
$$
\nopposite sign due to

imaginary time

Hubbard Stratonovich Transformation

- Decoupling of the non-local term

$$
\exp\left(\int_0^{1/T} d\tau \sum_{i,j} b_i^{\dagger} A_{i,j} b_j \right)
$$
\n
$$
= \int \mathcal{D} \left[ \psi_i(\tau) \right] \mathcal{D} \left[ \psi_i^{\dagger}(\tau) \right] \exp\left(-\int_0^{1/T} d\tau \left[ \sum_{i,j} \psi_i^{\dagger} A_{i,j}^{-1} \psi_j - \sum_i \left( \psi_i b_i^{\dagger} + \psi_i^{\dagger} b_i \right) \right] \right)
$$
\n
$$
= \int \mathcal{D} \left[ \psi_i(\tau) \right] \mathcal{D} \left[ \psi_i^{\dagger}(\tau) \right] \exp\left(-\int_0^{1/T} d\tau \left[ \sum_{i,j} \psi_i^{\dagger} A_{i,j}^{-1} \psi_j - \sum_i \left( \psi_i b_i^{\dagger} + \psi_i^{\dagger} b_i \right) \right] \right)
$$
\n
$$
\exp\left(-\int_0^{1/T} d\tau \left[ \sum_{i,j} \psi_i^{\dagger} A_{i,j}^{-1} \psi_j - \sum_i \psi_i b_i^{\dagger} \right] \right)
$$
\n
$$
= \int \mathcal{D} \left[ \psi_i(\tau) \right] \mathcal{D} \left[ \psi_i^{\dagger}(\tau) \right] \exp\left(-\int_0^{1/T} d\tau \left[ \sum_{i,j} \psi_i^{\dagger} A_{i,j}^{-1} \psi_j - \sum_i \psi_i b_i^{\dagger} + \psi_i^{\dagger} b_i \right] \right)
$$
\n
$$
= \int \mathcal{D} \left[ \psi_i(\tau) \right] \mathcal{D} \left[ \psi_i^{\dagger}(\tau) \right] \exp\left(-\int_0^{1/T} d\tau \left[ \sum_{i,j} \psi_i^{\dagger} A_{i,j}^{-1} \psi_j - \sum_i \psi_i b_i^{\dagger} + \psi_i^{\dagger} b_i \right] \right)
$$
\n
$$
= \int \mathcal{D} \left[ \psi_i(\tau) \right] \mathcal{D} \left[ \psi_i^{\dagger}(\tau) \right] \exp\left(-\int_0^{1/T} d\tau \left[ \sum_{i,j} \psi_i^{\dagger} A_{i,j}^{-1} \psi_j - \sum_i \psi_i b_i^{\dagger} \right] \right)
$$
\n

Integrating out the bosons

$$
\mathcal{L}_{\mathrm{B}} = \mathcal{L}_{0} - \sum_{i} \left[ \psi_{i} b_{i}^{\dagger} + \psi_{i}^{\dagger} b_{i} \right] + \sum_{i,j} \psi_{i}^{\dagger} A_{i,j}^{-1} \psi_{J}
$$

- local theory

$$
\mathcal{L}_0 = \sum_i \left[ b_i^\dagger\ \partial_\tau b_i - \mu b_i^\dagger b_i + \frac{U}{2} b_i^\dagger b_i^\dagger b_i b_i \right]
$$

- Greens function

$$
G(i\omega_s) = -\langle T_\tau b_i(\tau)b_i^\dagger(0)\rangle = \frac{n_0+1}{i\omega_s+\mu-Un_0} - \frac{n_0}{i\omega_s+\mu-U(n_0-1)}
$$

Effective theory

- continuum limes

$$
Z_{\scriptscriptstyle\rm B}=\int {\cal D}\left[\psi(\tau,{\bf x})\right] \left[\psi^\dagger(\tau,{\bf x})\right] \exp\left(-\int_0^{1/T} d\tau\, {\cal L}_{\scriptscriptstyle\rm B}\right)
$$

- lagrangian

$$
\mathcal{L}_{\text{B}} = \sum_{i} \psi_{i}^{\dagger} G(\tau) \psi_{i} + \sum_{i,j} \psi_{j}^{\dagger} A_{i,j}^{-1} \psi_{i} + O(|\psi|^{4})
$$
\n
$$
\approx \int d\mathbf{x} \left[ K_{1} \psi^{\dagger} \partial_{\tau} \psi + K_{2} |\partial_{\tau} \psi|^{2} + K_{3} |\nabla \psi|^{2} + r |\psi|^{2} + u |\psi|^{4} + \ldots \right]
$$
\n
$$
K_{1} = -\partial_{\mu} r
$$
\nsymmetry:

\n
$$
K_{1} = -\partial_{\mu} r
$$

- symmetry:

change of sign determines phase transition



holes



Quantum phase transition in cold gases

- optical lattices
- realization of the Bose-Hubbard model



#### Description of the Bose-Hubbard model

- mean-field theory
- effective theory
- 1D system



### **Bose-Hubbard model in 1D**



### Why one dimension?

#### Interaction potential

- pseudo potential in 1D

$$
V(x)=g\delta(x)=2\hbar\omega_{\perp}a_s\delta(x)
$$

- interaction strength

$$
\gamma = \frac{E_{\textrm{\tiny int}}}{E_{\textrm{\tiny kin}}} = \frac{mg}{\hbar^2 n}
$$

- homogoneous system is exactly solvable (Lieb and Liniger)
	- $\gamma \ll 1$  : weakly interacting bosons
		- mean field theory
		- Bogoliubov theory



 $\gamma \gg 1$ : Tonk gas limit





### Bose-Hubbard model

 $V_0>E_r$ 



### Hamiltonian

$$
H = \int dx \left[ \psi^{+}(x) \left( -\frac{\hbar^{2}}{2m} \Delta + V(x) \right) \psi(x) + \frac{g}{2} \psi^{+}(x) \psi^{+}(x) \psi(x) \psi(x) \right]
$$

• interaction strength

$$
g = 2\hbar\omega_r a_s \qquad \gamma = \frac{mg}{n\hbar^2}
$$
 scattering length

• external potential

$$
V(x) = V \sin^2(kx) + V_{trap}(x)
$$
  
\n
$$
E_r = \frac{\hbar^2 k^2}{2m}
$$
recoil energy  $\lambda = k/2\pi$ 



### Hydrodynamic description

• Bosonic field operator in terms of a long-wavelength density- and phase-field operator θ and φ (Haldane, '81)

commutation relation

$$
\psi(x) \approx \sqrt{n + \partial_x \theta / \pi} \exp(i\phi) \quad \text{[} \phi(x), \partial_y \theta \text{]} = i\pi \delta(x - y)
$$

• Hamiltonian (without optical lattice)

$$
H_0 = \frac{\hbar}{2\pi} \int dx \left[ v_J \left( \partial_x \phi \right)^2 + v_N \left( \partial_x \theta \right)^2 \right]
$$

 $v_s = \sqrt{v_J v_N}$ 

superfluid stiffness

inverse compressability

$$
v_J = \pi \, \hbar n/m
$$

$$
\boxed{v_N} = \partial_n \mu / \pi \hbar
$$

(Lieb and Liniger,'63)

 $V_0 \lesssim E_r$ 

• quasi long-range order

$$
\langle \psi(x)\psi^{\dagger}(0)\rangle \sim |x|^{-1/2K} \sim K = \sqrt{\nu_{J}/\nu_{N}}
$$

• sound velocity

$$
\frac{K \left(\gamma - \gamma^{3/2} / 2\pi\right)^{1/2}}{\gamma_c \approx 3.5}
$$

 $V_0 \lesssim E_r$ 

• Taking into account the discrete nature of the particles (Haldane, '81)



### Sine-Gordon model

$$
H = \frac{\hbar v_s}{\pi} \int dx \left\{ \frac{1}{2} \left[ K \left( \partial_x \phi \right)^2 + \frac{1}{K} \left( \partial_x \theta \right)^2 \right] - \frac{Q}{2K} \partial_x \theta + \frac{u}{a^2} \cos \left( 2\theta \right) \right\}
$$

• Three parameters



- Exactly solvable field theory
	- massive spinless fermions
	- U(1) symmetric Thirring model in a magnetic field

(Coleman, '75; Wiegmann, '78; Japardize et al., '84; Pokrovsky et al., '79; Kehrein, '99)

$$
V_0 \lesssim E_r
$$







### Commensurate density *Q*=0

• Instability in the sine-Gordon model (Coleman, '75)



• Kosterlitz-Thouless universality class

$$
K_c (u) = 2(1+u)
$$
  
  

$$
V_c (\gamma) \approx E_r (\gamma^{-1} - \gamma_c^{-1})/5.5
$$



### Tonks gas  $\gamma \rightarrow \infty$



• The bosons wave function maps to the wave function of free fermions in periodic potential (Girardeau,'60)

• At commensurate filling the fermions are a standard band insulator with a single particle gap  $2\Delta = V/2$ 





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