### 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

#### 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



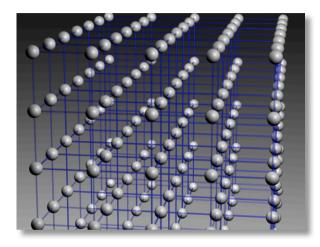
#### Theory groups

- ...

### 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



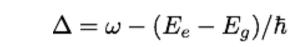


### Interaction between light and atoms

- Hamiltonian between atoms and light: dipole approximation

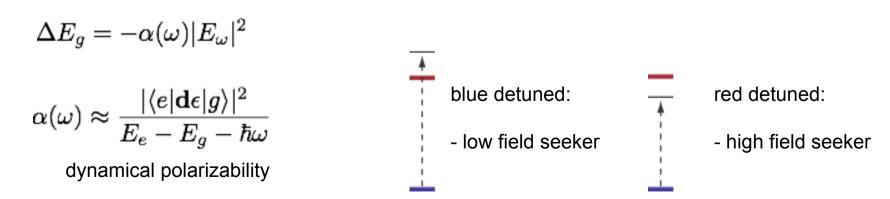
$$H = -\mathbf{d}\mathbf{E}(t, \mathbf{r})$$

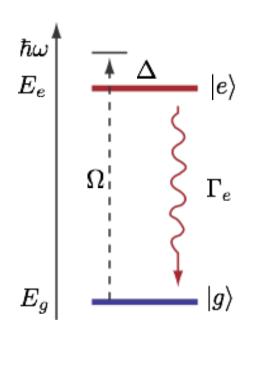
- external laser field:
- rabi frequency:  $\Omega = |\langle e | \mathbf{d} \mathbf{E}_\omega | g 
  angle | / \hbar$
- detuning:



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

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





### Interaction between light and atoms

- spontaneous emission:  $\Gamma_e$ 

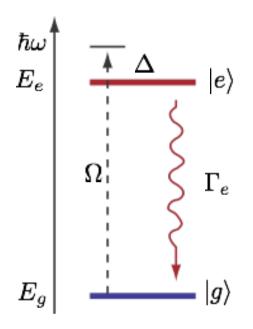
excited state has a finite life time due to spontaneous emission

- AC Stark shift

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

- loss of atoms from the ground state

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



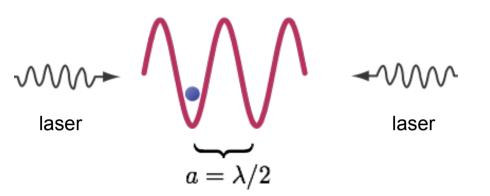
- limits life-time of a BEC in an optical lattice
- requires large detuning

 $\Delta \gg \Gamma_e$ 

- high laser power

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

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



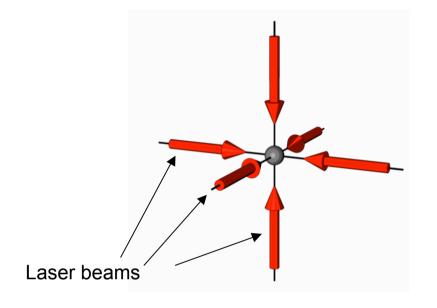
 $E_r = rac{\hbar^2 k^2}{2m}$ 

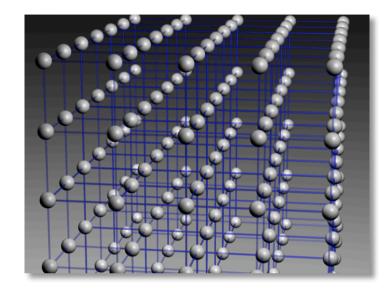
- structure in 3D

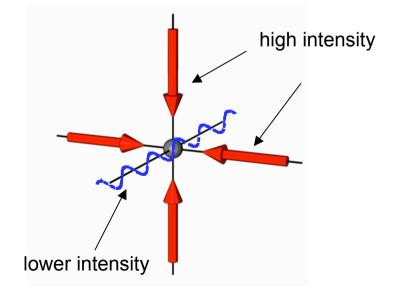
$$\mathbf{E}(t,\mathbf{r}) = \sum_{i} \mathbf{E}_{\omega_{i}}^{i} \cos(\mathbf{k}_{i}\mathbf{r}) e^{-i\omega_{i}t} + c.c.$$

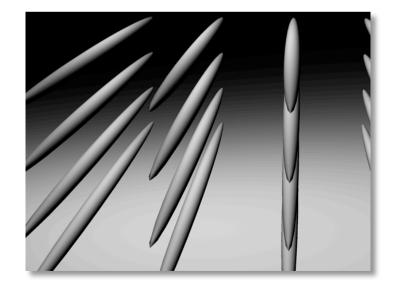
- $\mathbf{k}_i$ : wave length fixed by the atomic transition
- $\omega_i$  : slightly different frequencies to cancel cross terms
- $\mathbf{E}^i_\omega$ : polarization as additional degree of freedom

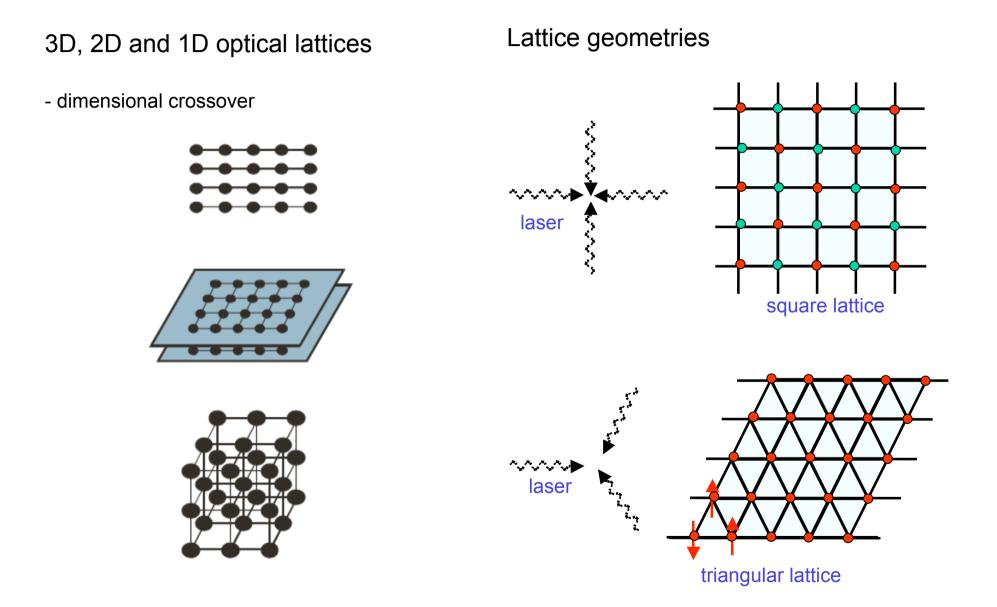
$$\bigvee V(\mathbf{x}) = \sum_{i} V_i \cos(\mathbf{k}_i \mathbf{r})^2$$





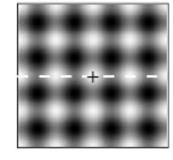






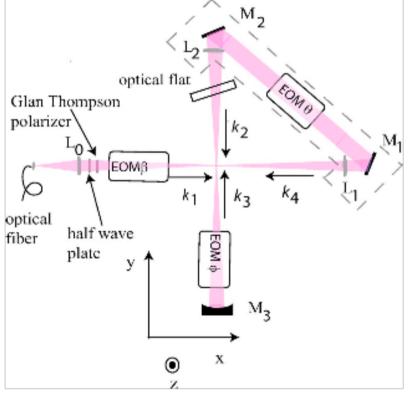
#### Tricks with 2D optical lattice

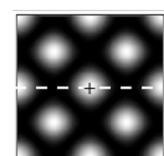
J. Sebby-Strabley, M. Anderlini, P.S. Jessen, and J.V. Porto, Phys Rev. A 73, 033605 (2006)



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

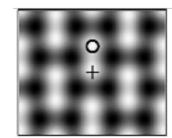
in plane polarization cross terms disappear



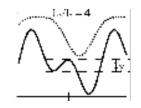


$$V(\mathbf{x}) = V_0 \left[\cos(kx) + \cos(ky)\right]^2$$

- 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
- field operator  $\psi(x), \psi^{\dagger}(x)$

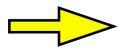
$$H = \int dx \ \psi^{+}(x) \left( -\frac{\hbar^{2}}{2m} \Delta + V(x) \right) \psi(x) + \frac{g}{2} \int dx \ \psi^{+}(x) \psi^{+}(x) \psi(x) \psi(x)$$
optical lattice 
$$g = \frac{4\pi \hbar^{2} a_{s}}{m} \quad \text{:interaction strength of the Pseudo potential}$$

Derivation of effective low energy theory:

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

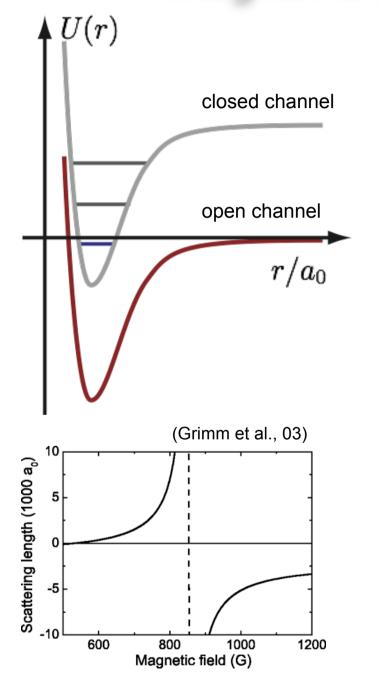
(i) Solve the single particle problem in an optical lattice

(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

$$a_{ ext{eff}} = a_s(1 + rac{\Delta 
u}{E-E_{ ext{res}}})$$

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

### Single particle problem

lattice vector

Hamiltonian

- particle in a periodic potential

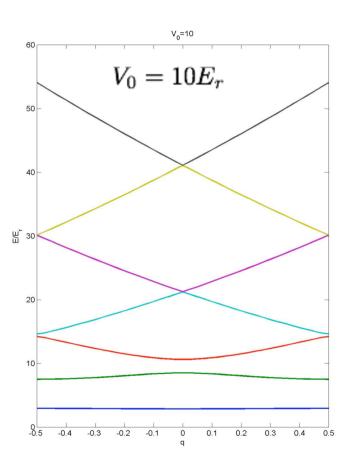
$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) \qquad V(\mathbf{r} + \mathbf{R}_i) = V(\mathbf{r})$$

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

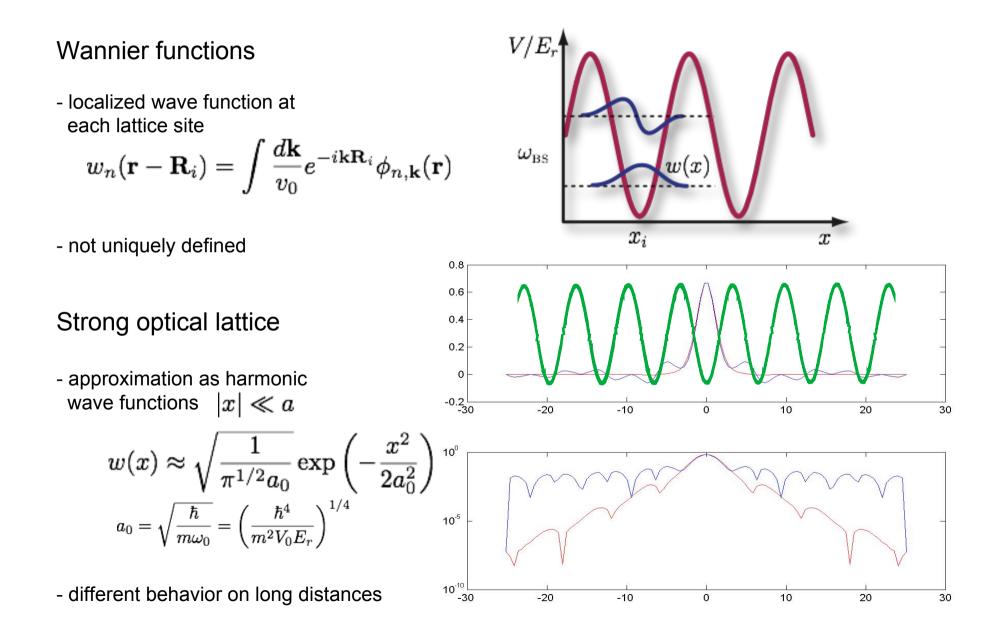
 $E_n(\mathbf{k})$ : energy dispersion $\mathbf{k}$ : quasi momentum within<br/>first Brillouine zone

- Bloch theorem

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



### Wannier functions



### Microscopic Hamiltonian

#### Hubbard model

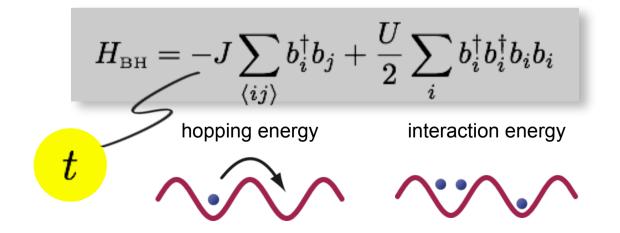
- express the bosonic field operator in terms of Wannier functions

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

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

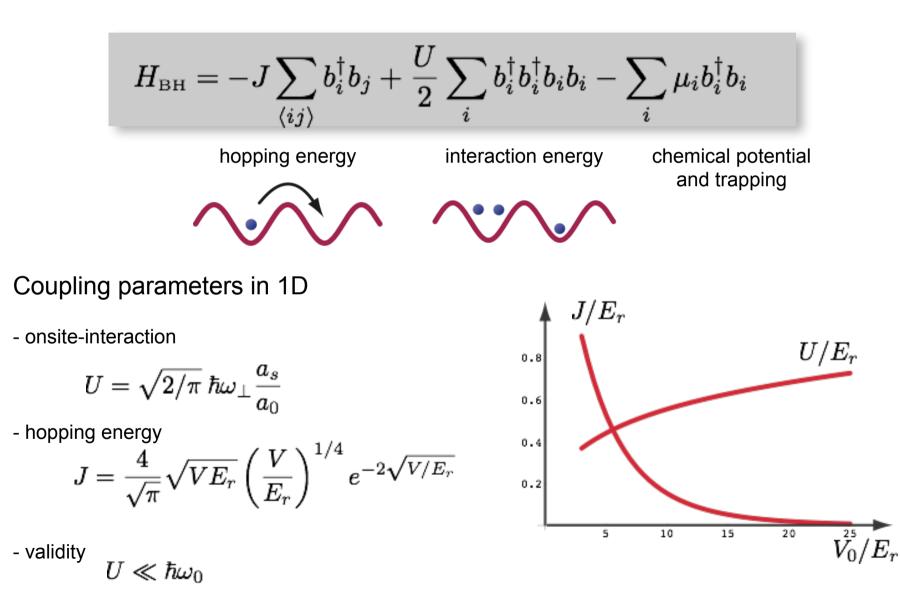
$$H = \int dx \ \psi^+(x) \left( -\frac{\hbar^2}{2m} \Delta + V(x) \right) \psi(x) + \frac{g}{2} \int dx \ \psi^+(x) \psi^+(x) \psi(x) \psi(x)$$

- restriction to lowest bloch bands
- only largest terms



### Bose-Hubbard Model

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



### Bose-Hubbard Model

#### Weak interactions

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

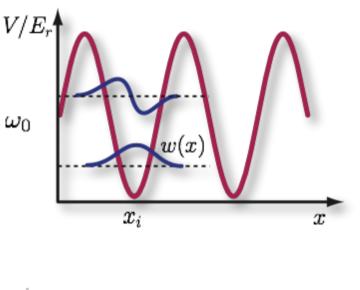
- Next-nearest-neighbor hopping
- small in the tight binding limit, but have to be included fore weak opitcal lattices

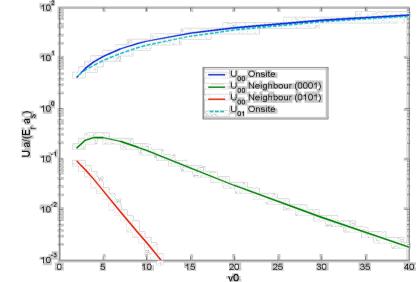
 $V_0 \lesssim E_r$ 

#### Nearest-neighbor interaction

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

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







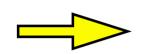
Characteristic parameters

- wave length

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

- lattice spacing

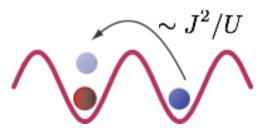
 $a\sim 500 {
m nm}$ 

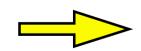


$$\begin{split} E_r = \frac{2\pi^2\hbar^2}{m\lambda^2} &\approx 9 \mathbf{k} \mathbf{H} \mathbf{z} \\ &\approx 430 \mathbf{n} \mathbf{K} \end{split}$$

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

- temperatures  $T_{\text{BEC}} \approx 1 \mu \mathbf{K}$   $T_{\text{min}} \sim 1 \mathbf{n} \mathbf{K}$   $(1 \mathbf{H} \mathbf{z} \equiv 50 \mathbf{p} \mathbf{K})$ 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

$$\phi_{\scriptscriptstyle
m BEC} \sim \left(\sum_i b_i^\dagger
ight)^N \ket{0}$$

- linear excitation spectrum
- off-diagonal long-range

$$\langle \psi(\mathbf{r})\psi^{\dagger}(0)
angle 
ightarrow n_{0}$$

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

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

$$\phi_{\scriptscriptstyle \rm Mott} = \prod_i b_i^\dagger |0\rangle$$

- -

 $\Delta \sim U$ 



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

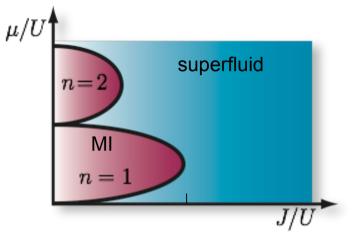
$$\widehat{}$$

- localized particles
- integer particles per lattice site

Quantum phase transition

#### Mott insulator

- commensurate filling
- gapped phase
- incompressible



#### Superfluid

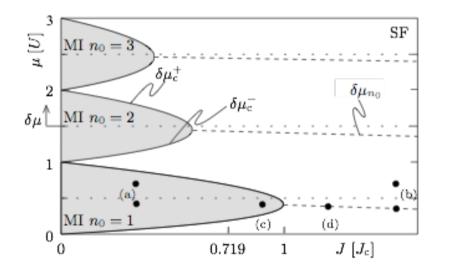
- long-range order
- finite superfluid stiffness
- linear excitation spectrum

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

- critical value

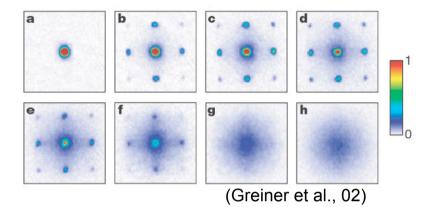
$$U/J\Big|_{\scriptscriptstyle \mathrm{S-MI}} = z\left(n+\sqrt{n+1}
ight)^2$$

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



### Experiments

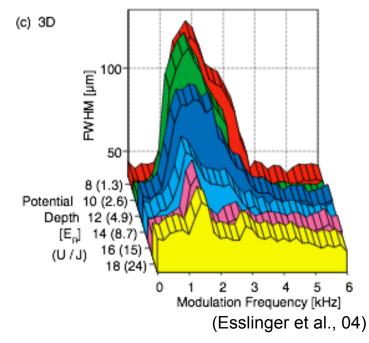
Long-range order:



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

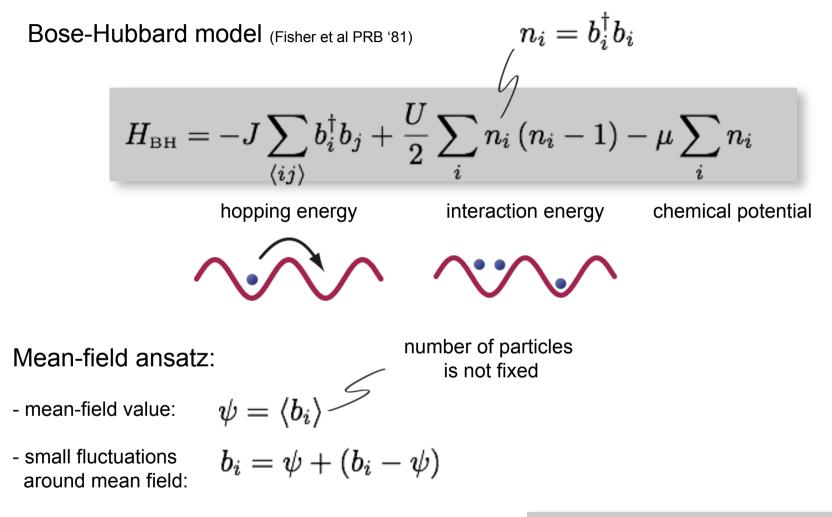
$$\frac{V}{E_r} > 13$$

#### Structure factor



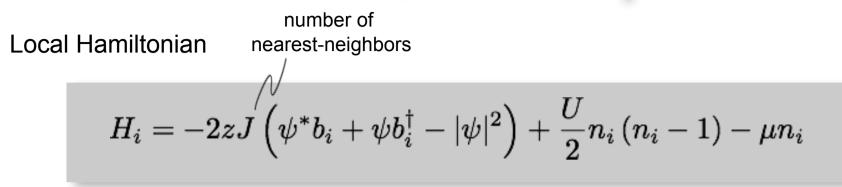
Appearance of well defined two particle excitations

### Bose-Hubbard Model



 $b_{i}^{\dagger}b_{j} = \psi^{*}b_{j} + b_{i}^{\dagger}\psi - |\psi|^{2}$ 

local Hamiltonian $H_{\scriptscriptstyle
m BH} = \sum_i H_i$ 



- ground state is a product state

condensate , density

$$ho = \prod_i 
ho_i \sim e_{ ext{matrix}} rac{1}{2} 
ho_i 
ightarrow e_{ ext{matrix}} \psi = \langle b_i 
angle$$

- self-consistency

Long-Range order

- order parameter

$$\langle b_i b_j^\dagger 
angle \longrightarrow n_0^{\prime}$$

- mean-field result

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

- zero-temperature

$$ho_i = |f
angle \langle f| \ |f
angle = \sum_n f(n) |n
angle$$

- the mean-field breaks the U(1) symmetry

- order parameter of the quantum phase transition

#### Mott Insulator

- localized particles
- integer particles per lattice site

 $|f
angle=|n_0
angle$ 

- 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

$$|f
angle = \exp\left(-|\psi|^2/2
ight)\exp\left(\psi b^\dagger
ight)$$

"mean-field" Mott insulator

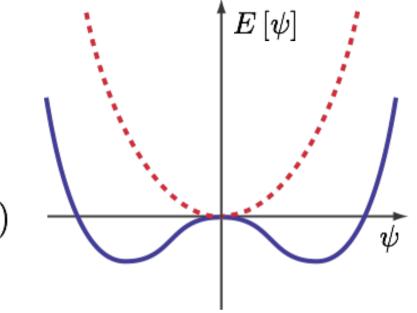
**\•**/

particle-hole fluctuations

Phase transition

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

$$egin{aligned} |f
angle &= \sqrt{1-2\epsilon^2} |n_0
angle \ &+\epsilon \left(e^{i\phi} |n_0-1
angle + e^{-i\phi} |n_0+1
angle 
ight) \ \psi &= 2e^{i\phi}\epsilon\sqrt{1-2\epsilon^2} \end{aligned}$$



- energy

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

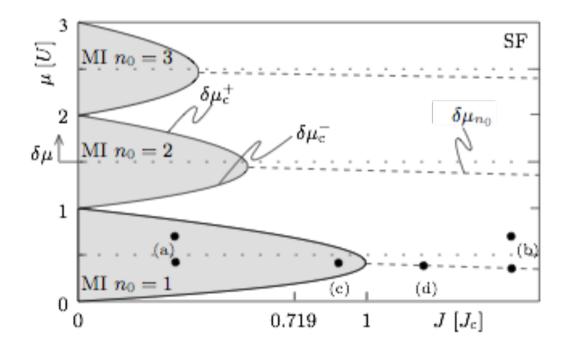


Quantum phase transition

- critical value

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

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



Partition functionpropagator in  
imaginary time
$$U = \exp\left(-\frac{itH_{\rm BH}}{\hbar}\right)$$
- $Z_{\rm B} = {\rm Tr}\left[\exp\left(-\frac{H_{\rm BH}}{T}\right)\right]$  $t = -i\tau$ 

- path integral formulation

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

- Lagrangian of the Bose-Hubbard model

$$\begin{split} \mathcal{L}_{\mathrm{B}} &= \sum_{i} \left[ b_{i}^{\dagger} \partial_{\tau} b_{i} - \mu b_{i}^{\dagger} b_{i} + \frac{U}{2} b_{i}^{\dagger} b_{i}^{\dagger} b_{i} b_{i} \right] - J \sum_{\langle i,j \rangle} \left( b_{i}^{\dagger} b_{j} + b_{i} b_{j}^{\dagger} \right) \\ &= \sum_{i} b_{i}^{\dagger} \partial_{\tau} b_{i} + H_{\mathrm{BH}} \\ & \swarrow \end{split}$$
opposite sign due to

imaginary time

Hubbard Stratonovich Transformation

- Decoupling of the non-local term

$$\exp\left(\int_{0}^{1/T} d\tau \sum_{i,j} b_{i}^{\dagger} A_{i,j} b_{j}\right) \xrightarrow{\text{non-local} \text{hopping term}} A_{i,j} = \begin{cases} J & \langle i,j \rangle \\ 0 & \text{else} \end{cases}$$
$$= \int \mathcal{D} \left[\psi_{i}(\tau)\right] \mathcal{D} \left[\psi_{i}^{\dagger}(\tau)\right] \exp\left(-\int_{0}^{1/T} d\tau \left[\sum_{i,j} \psi_{i}^{\dagger} A_{i,j}^{-1} \psi_{j} - \sum_{i} \left(\psi_{i} b_{i}^{\dagger} + \psi_{i}^{\dagger} b_{i}\right)\right]\right)$$
$$(j) = \int \mathcal{D} \left[\psi_{i}(\tau)\right] \exp\left(-\int_{0}^{1/T} d\tau \left[\sum_{i,j} \psi_{i}^{\dagger} A_{i,j}^{-1} \psi_{j} - \sum_{i} \left(\psi_{i} b_{i}^{\dagger} + \psi_{i}^{\dagger} b_{i}\right)\right]\right)$$
effective field: order parameter guadratic term local term

Integrating out the bosons

$$\mathcal{L}_{\scriptscriptstyle \mathrm{B}} = \mathcal{L}_0 - \sum_i \left[ \psi_i b_i^\dagger + \psi_i^\dagger b_i 
ight] + \sum_{i,j} \psi_i^\dagger A_{i,j}^{-1} \psi_J$$

- local theory

$$\mathcal{L}_0 = \sum_i \left[ b_i^\dagger \; \partial_ au b_i - \mu b_i^\dagger b_i + rac{U}{2} b_i^\dagger b_i^\dagger b_i b_i 
ight]$$

- 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

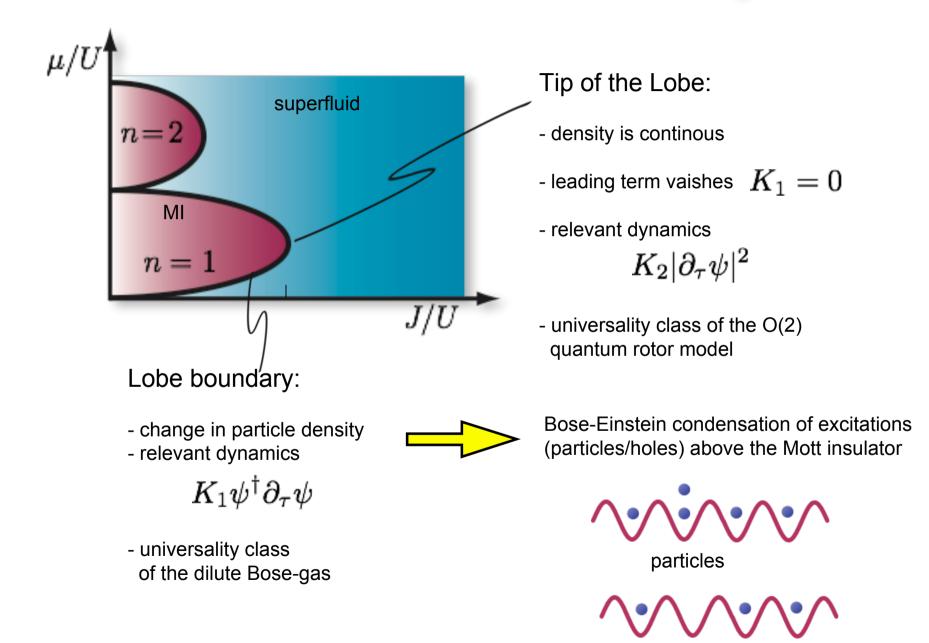
- continuum limes

$$Z_{\scriptscriptstyle \mathrm{B}} = \int \mathcal{D}\left[\psi( au, \mathbf{x})
ight] \left[\psi^{\dagger}( au, \mathbf{x})
ight] \exp\left(-\int_{0}^{1/T} d au \, \mathcal{L}_{\scriptscriptstyle \mathrm{B}}
ight)$$

- lagrangian

- symmetry:

change of sign determines phase transition

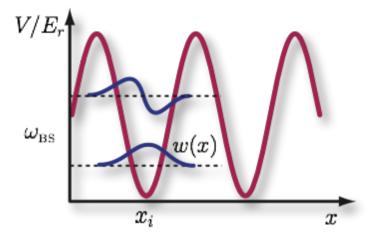


holes

### Conclusion

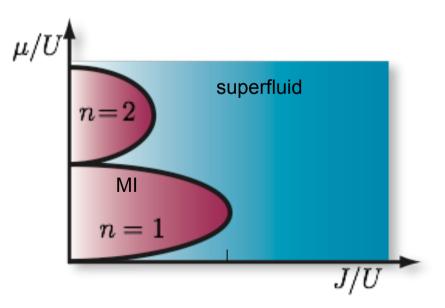
Quantum phase transition in cold gases

- optical lattices
- realization of the Bose-Hubbard model

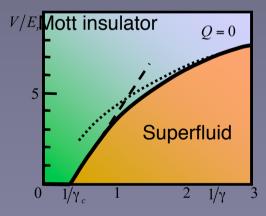


#### Description of the Bose-Hubbard model

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



### Bose-Hubbard model in 1D



### Why one dimension?

#### Interaction potential

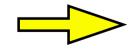
- pseudo potential in 1D

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

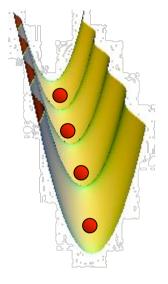
- interaction strength

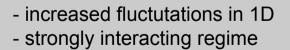
$$\gamma = \frac{E_{\rm int}}{E_{\rm kin}} = \frac{mg}{\hbar^2 n}$$

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



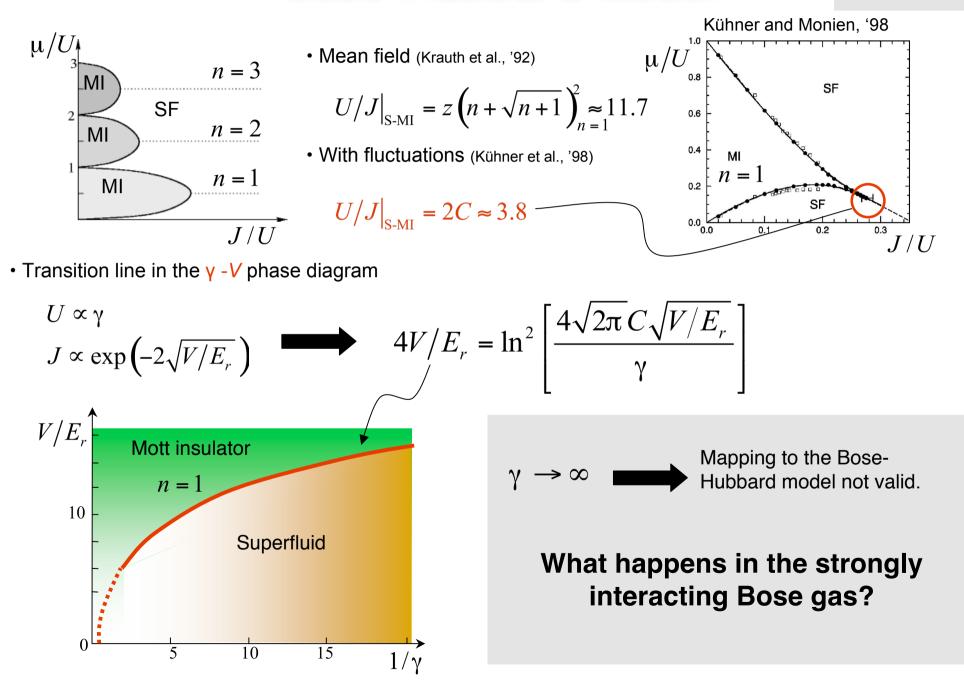
 $\gamma \gg 1$  : Tonk gas limit





### 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  $g = 2\hbar\omega_{T}a_{s}$   
• external potential  

$$V(x) = V \sin^{2}(kx) + V_{trap}(x)$$
  

$$E_{r} = \frac{\hbar^{2}k^{2}}{2m}$$
recoil energy  $\lambda = k/2\pi$   
Sine Gordon  
model  
 $V_{0} < E_{r}$   
Superfluid to Mott insulator quantum  
phase transition  
 $V_{0} > E_{r}$   
Bose-Hubbard  
model  
 $V_{0} > E_{r}$ 

### Hydrodynamic description

• Bosonic field operator in terms of a long-wavelength density- and phase-field operator  $\theta$  and  $\phi$  (Haldane, '81)

commutation relation

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

Hamiltonian (without optical lattice)

$$H_{0} = \frac{\hbar}{2\pi} \int dx \left[ \mathbf{v}_{J} \left( \partial_{x} \phi \right)^{2} + \mathbf{v}_{N} \left( \partial_{x} \theta \right)^{2} \right]$$

 $v_s = \sqrt{v_J v_N}$ 

superfluid stiffness

inverse compressability

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

$$v_N = \partial_n \mu / \pi \hbar$$

(Lieb and Liniger,'63)

• quasi long-range order

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

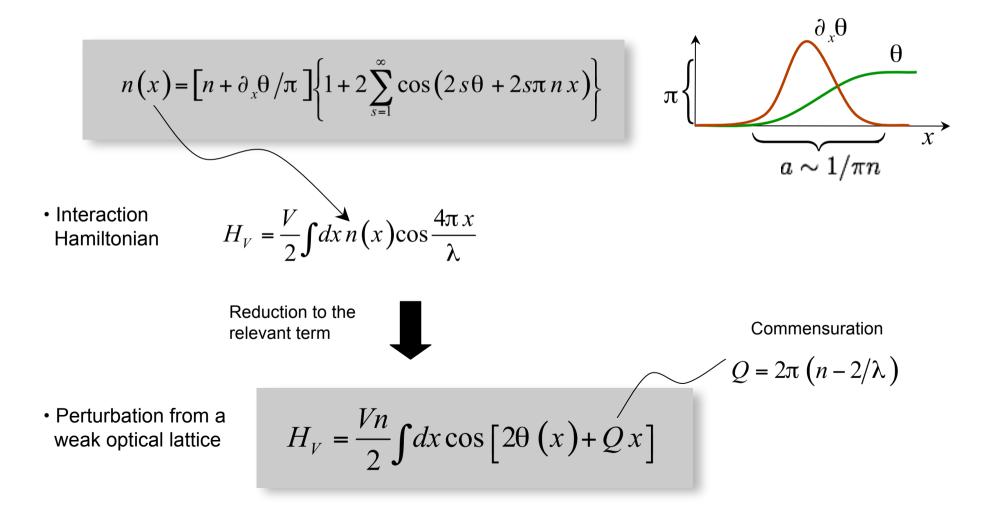
sound velocity

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

$$I \left( \frac{1 + 2/\gamma}{\gamma_c} \approx 3.5 \right)^{-1/2}$$

 $V_0 \lesssim E_r$ 

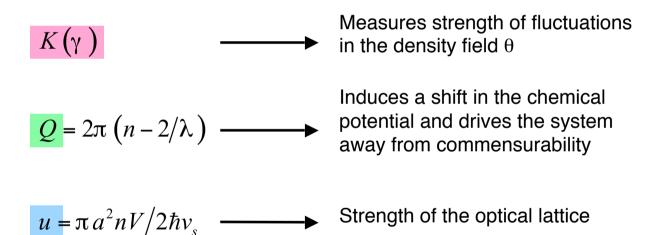
• Taking into account the discrete nature of the particles (Haldane, '81)



### Sine-Gordon model

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

Three parameters

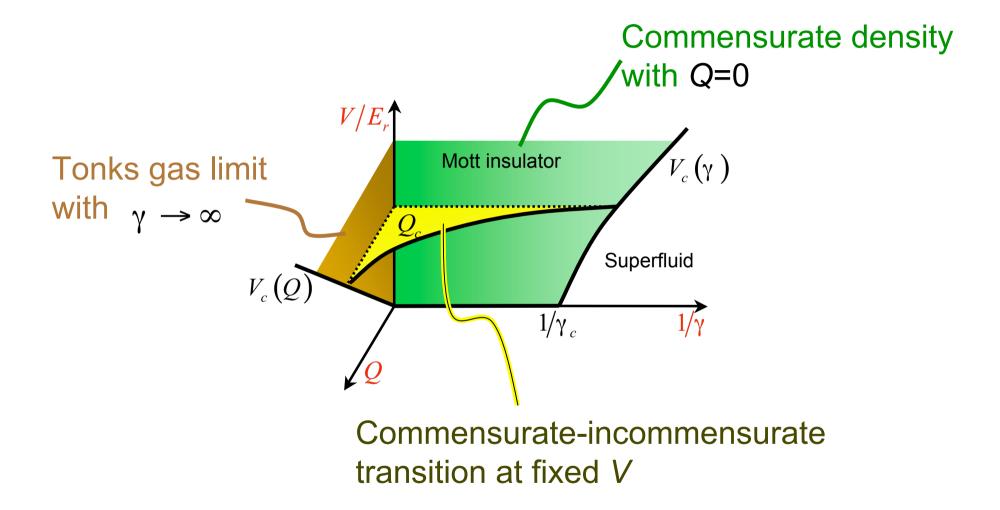


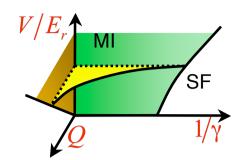
- Exactly solvable field theory
  - massive spinless fermions
  - U(1) symmetric Thirring model in a magnetic field

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

$$V_0 \lesssim E_r$$

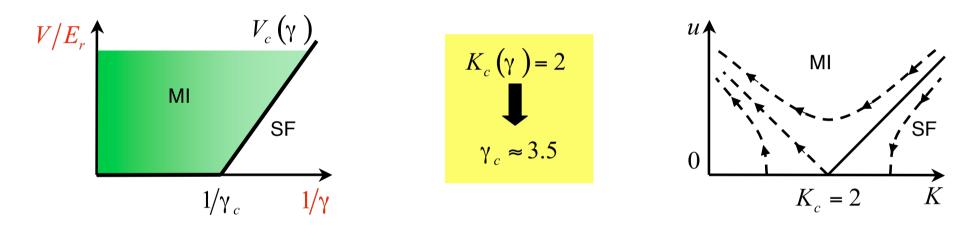






### Commensurate density Q=0

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

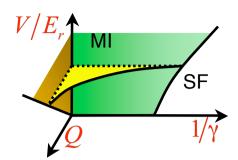


Kosterlitz-Thouless universality class

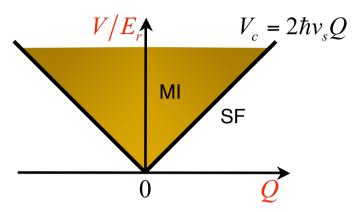
$$K_{c}(u) = 2(1+u)$$

$$\downarrow$$

$$V_{c}(\gamma) \approx E_{r}(\gamma^{-1} - \gamma_{c}^{-1})/5.5$$

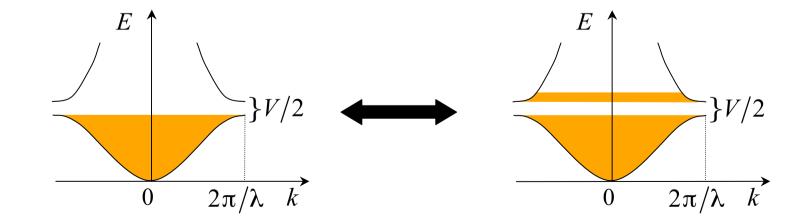


### Tonks gas $\gamma \rightarrow \infty$



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

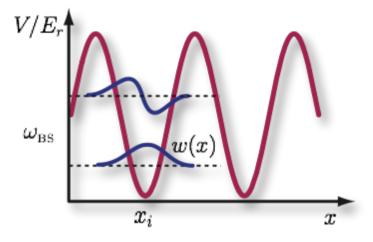
• At commensurate filling the fermions are a standard band insulator with a single particle gap  $2\Delta = V/2$ 



### Conclusion

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

