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# Lattice systems:
# Physics of the Bose-Hubbard Model

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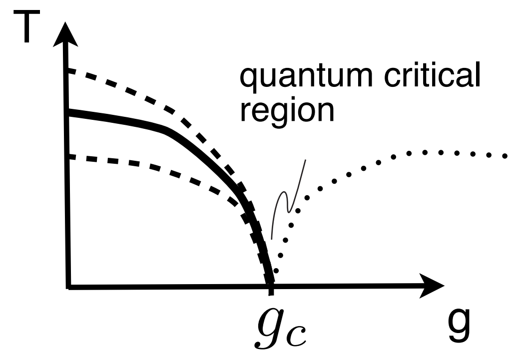
**SFB**
*Coherent Control of Quantum Systems*

# Outline

## Quantum Phase transitions: General Overview

- What is a Quantum Phase transition?
- Example: Mott Insulator -- Superfluid transition

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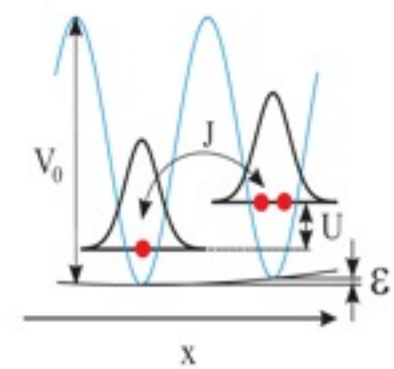
## Microscopic derivation of the Bose-Hubbard model

- Atoms in optical potentials
- Periodic potentials, Bloch theorem
- Bose-Hubbard model

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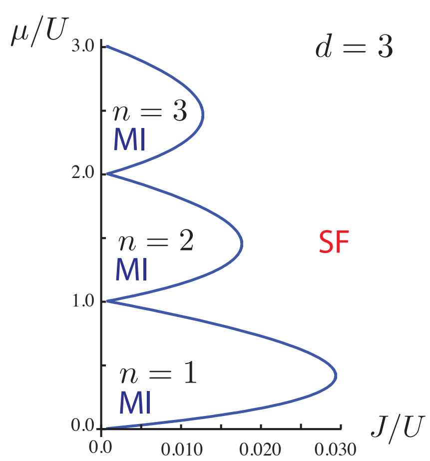
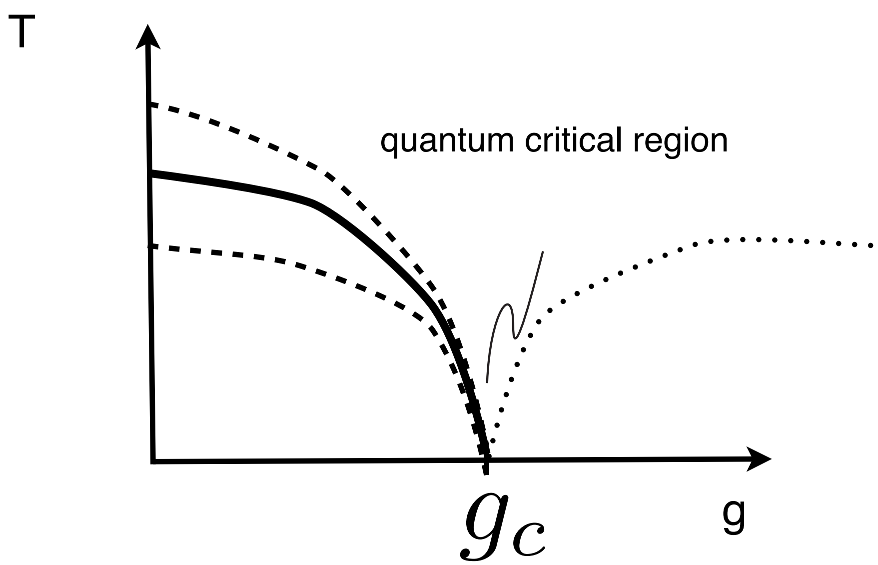
## Phase diagram of the Bose-Hubbard model

- Basic mean field theory: phase border and limiting cases
- Path integral formulation: excitation spectrum in the Mott phase and bicritical point



# Quantum Phase Transitions: General Overview



# What is a quantum phase transition?

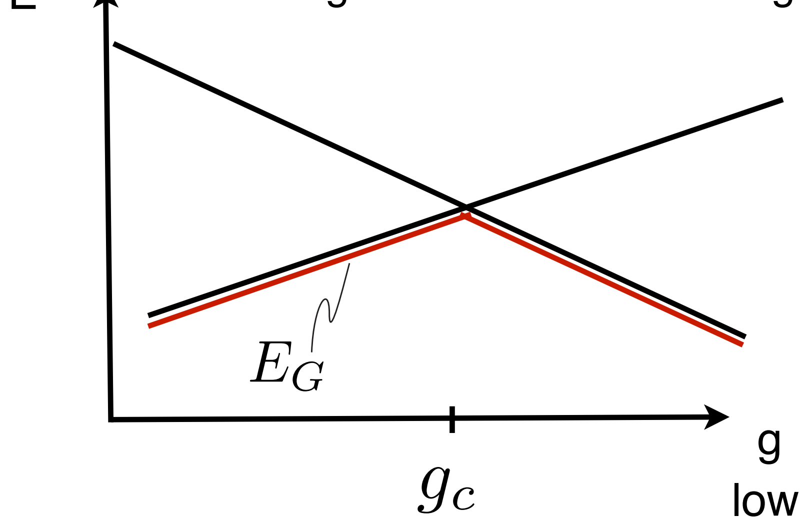
- Consider a Hamiltonian of the form:

$$H = H_1 + gH_2$$

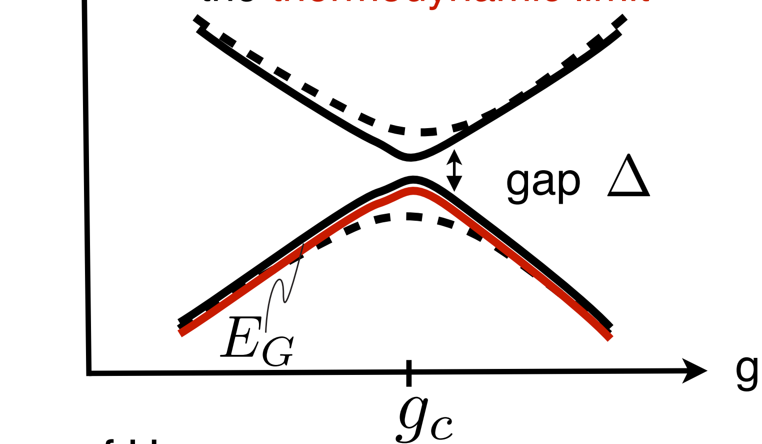
dimensionless parameter

- Study the ground state behavior of the energy $E(g) = \langle \mathrm{G}|H|G\rangle$
- Quantum phase transition: Nonanalytic dependence of the ground state energy on coupling parameter g
- Two possibilities:

  - parts commute, $[H_1, H_2] = 0$
  - but eigenvalues have crossing




  - parts do not commute, $[H_1, H_2] \neq 0$
  - eigenvalues crossing develops in the thermodynamic limit

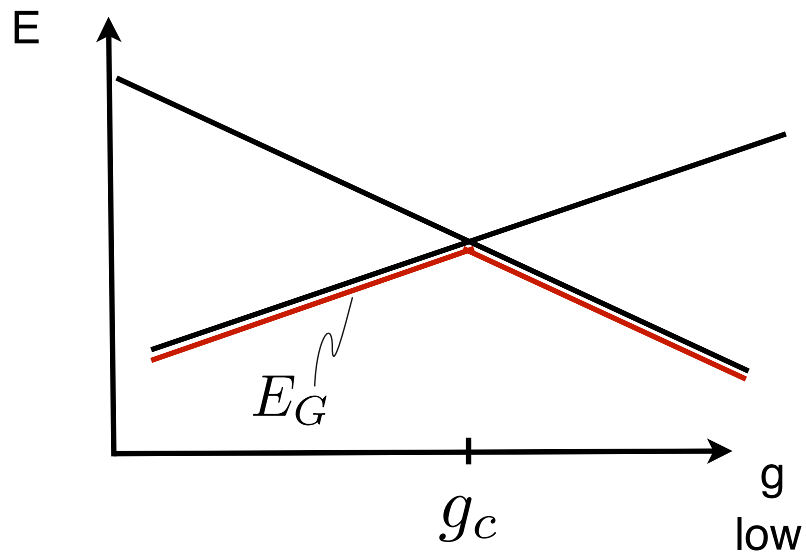


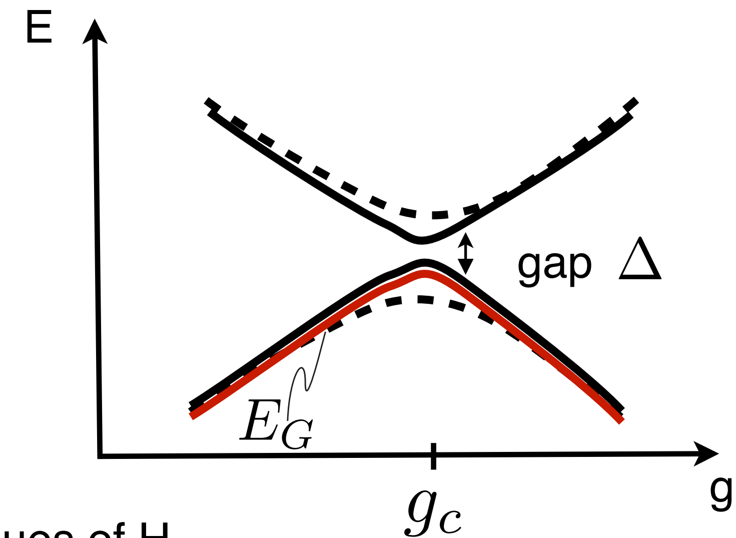

low eigenvalues of H

Literature: Subir Sachdev, Quantum Phase Transitions, Cambridge University Press (1999)

# What is a quantum phase transition?

$$H = H_1 + gH_2$$




low eigenvalues of H

- The second possibility is more common and closer to the situation in conventional classical phase transitions in the thermodynamic limit
- The first possibility often occurs only in conjunction with the second (ex: Bose-Hubbard phase diagram)
- The phase transition is usually accompanied by qualitative change in the correlations in the ground state

# What is a quantum phase transition?

- We concentrate on second order transitions (as those above)
- characteristic features:
  - vanishing of the energy scale separating ground from excited states (gap) at the transition point
  - universal scaling close to criticality,

critical exponent

$$\Delta \sim J|g - g_c|^{\nu z_d}$$

typical microscopic energy scale (in H)

- diverging length scale describing the decay of spatial correlations at the transition point

$$\xi^{-1} \sim \Lambda|g - g_c|^{\nu}$$

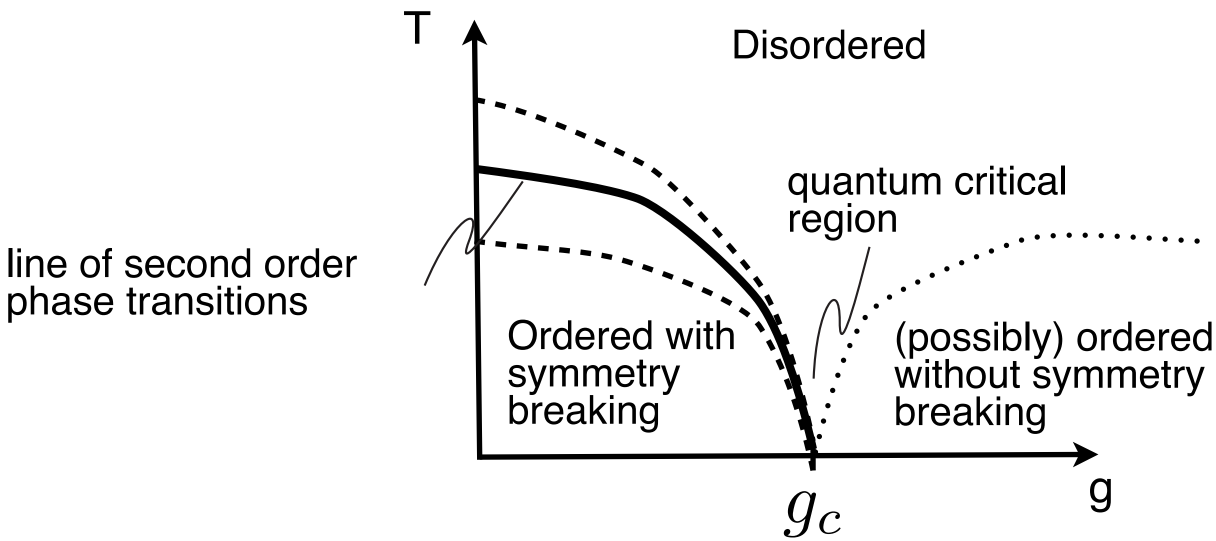
typical microscopic length scale (e.g. lattice spacing)

- the ratio defines the dynamic critical exponent,

$$\Delta \sim \xi^{-z_d}$$

# Quantum vs. Classical Phase Transition

- A quantum phase transition strictly occurs only at zero temperature T=0
- Temperature always sets a minimal energy scale, preventing scaling of $\Delta$
- Generic quantum phase diagram:




- classical description of critical behavior applies if

$$\hbar\omega_{typ} \ll k_B T$$

- This is always violated at low enough T: classical-quantum crossover

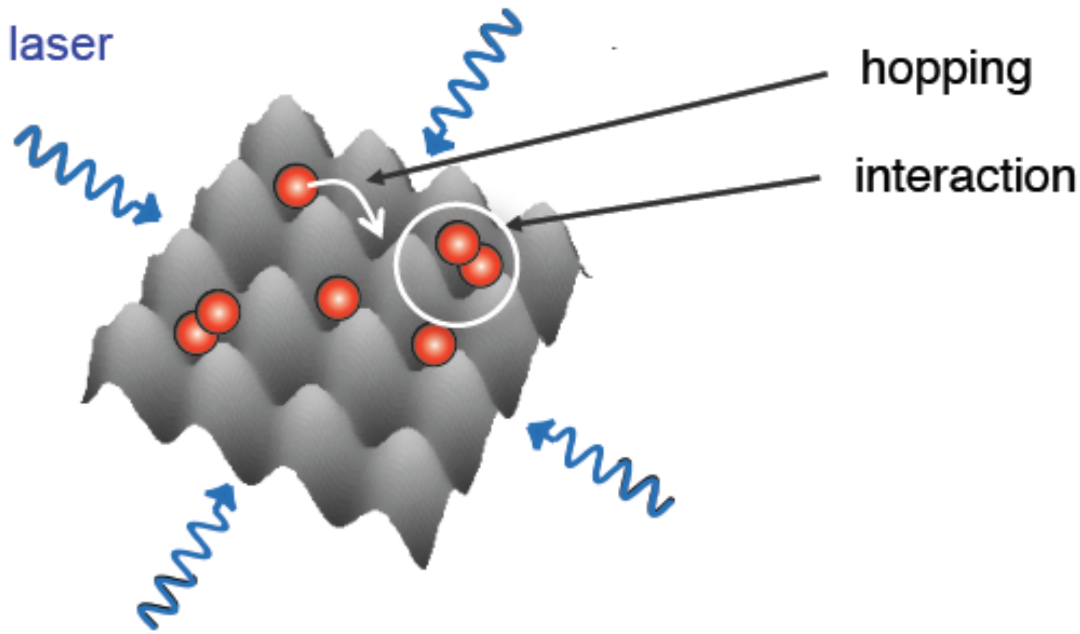
- Phase transitions in classical models are driven by statistical (thermal) fluctuations. They freeze to fluctuationless ground state at T=0
- Quantum models have fluctuations driven by Heisenberg uncertainty principle

➡ Quantum critical region features interplay of quantum (temporal) and statistical (spatial) fluctuations

# Bosons in the Optical Lattice

**System:** We consider $N$ bosonic particles moving on a lattice ("lattice gas") consisting of $M$ lattice sites. The essential ingredients of the dynamics are

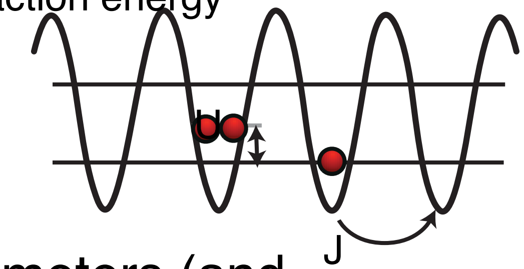
- hopping of the bosonic particles between lattice sites (kinetic energy)
- repulsive / attractive interaction between the particles (interaction energy)
- Bose statistics




cold atoms in an optical lattice (see below)

# Bose-Hubbard Model

$$H = \underbrace{-J \sum_{\langle i,j \rangle} b_i^\dagger b_j}_{\text{kinetic energy}} - \mu \sum_i \hat{n}_i + \underbrace{\sum_i \epsilon_i \hat{n}_i}_{\text{trapping potential}} + \underbrace{\tfrac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1)}_{\text{interaction energy}}$$




- Achieved via coherent manipulation of ultracold atoms.
- Ratio of kinetic and interaction energy tunable via lattice parameters (and Feshbach resonances). In particular, reach interaction dominated regime.
- Possible to penetrate high density regime $\langle \hat{n}_i \rangle = \mathcal{O}(1)$. Not possible in the continuum.
- The Bose-Hubbard model is an exemplary model for strongly correlated bosons. It is not realized in condensed matter.

- Remark: strong interactions and high density not in contradiction to earlier scale considerations:
    - strong interactions: $J/U \ll 1$ mainly from reduction of kinetic energy via lattice depth.
    - High density due to strong localization of onsite wave function.
    - For validity of lowest band approximation, it is however important that $a \ll \lambda$

# Kinetic vs. Interaction Domination - Limiting Cases

- Goal: Find the ground state (gs) phase diagram for Bose-Hubbard model (T=0)
- Strategy: (i) analyze limiting cases, (ii) find interpolation scheme
- Restrict to the homogeneous system $\epsilon_i = 0$

---

- Interaction dominated regime: set J = 0

number eigenstates
n=1

$$H = -\mu \sum_i \hat{n}_i + \tfrac{1}{2} U \sum_i \hat{n}_i(\hat{n}_i - 1) = \sum_i h_i$$

- Purely local Hamiltonian: gs many-body wavefunction takes product form

$$|\psi\rangle = \prod_i |\psi\rangle_i$$

$$\hat{n}_i |n\rangle_i = n|n\rangle_i$$

➡ Remains to analyze onsite problem only.

- Only onsite density operators occur, with (real space) occupation number eigenstates

➡ Onsite Hamiltonian also diagonal in this basis: Thus, minimize onsite energy and find the optimal n for given mu:

$$\begin{array}{ll} \text{for } \mu/U < 0 & n = 0 \\ \text{for } 0 < \mu/U < 1 & n = 1 \\ \text{for } 1 < \mu/U < 2 & n = 2 \end{array}$$

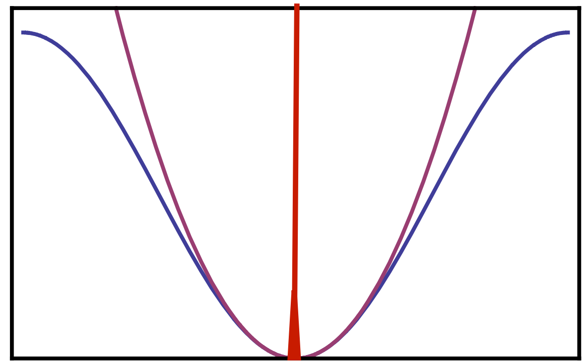
and so on

particle number quantization: for ranges of the chemical potential (particle reservoir), the system draws an integer number out or it: "Mott states"

# Kinetic vs. Interaction Domination - Limiting Cases

lattice direction

lattice dispersion $\epsilon_{\mathbf{q}} = -2J \sum_{\lambda} \cos \mathbf{q}\mathbf{e}_{\lambda}$



momentum eigenstate
q=0

- Kinetically dominated regime: set U=0

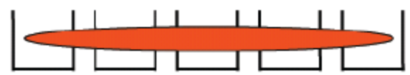
$$H = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j - \mu \sum_i \hat{n}_i$$

  - Free bosons at T=0: Bose Einstein condensation!
  - See that: Diagonalize with Fourier transformation

$$H = \sum_{\mathbf{q}} (\epsilon_{\mathbf{q}} - \mu) b_{\mathbf{q}}^\dagger b_{\mathbf{q}}$$

- Ground state wave function: fixed particle number N (M - no. of lattice sites)

$$b_{\mathbf{q}=0}^{\dagger\, N} |vac\rangle = (M^{-1/2} \sum_i b_i^\dagger)^N |vac\rangle$$



  - product state in momentum space, not in position space

- Work in grand canonical ensemble: coherent state with av. density $\langle \hat{n}_i \rangle = N/M$

$$e^{N^{1/2} b_{\mathbf{q}=0}^\dagger} |vac\rangle = e^{(N/M)^{1/2} \sum_i b_i^\dagger} |vac\rangle = \prod_i \left( e^{((N/M)^{1/2} b_i^\dagger)} |vac\rangle_i \right)$$

ensures av. particle no.

➡ grand canonical ground state can be written as a product of onsite coherent states

# Intermediate summary

- Hopping J favors delocalization in real space:
- Condensate (local in momentum space!)
- Fixed condensate phase: Breaking of phase rotation symmetry

$$\langle b_i \rangle \sim e^{\mathrm{i}\varphi}$$

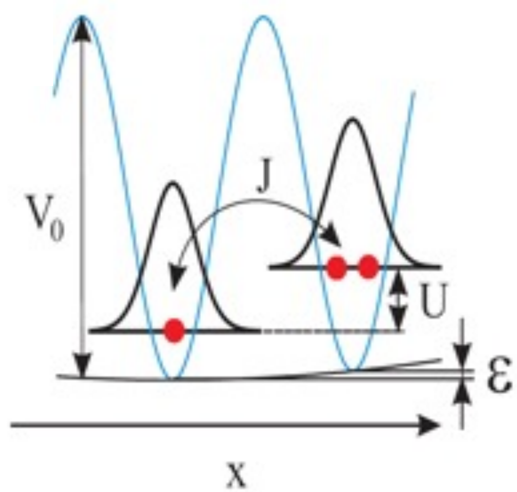
- Interaction U favors localization in real space for integer particle numbers:
- Mott state with quantized particle no.
- no expectation value: phase symmetry intact (unbroken)

➡ Competition gives rise to a quantum phase transition as a function of

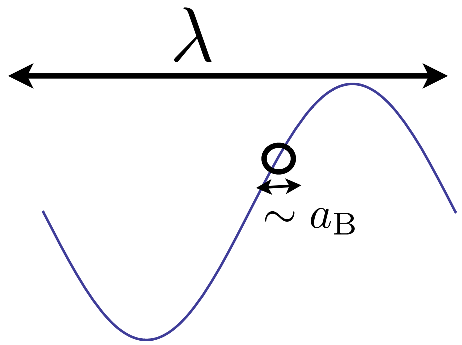
$$U/J$$

➡ Link between extremes: position space product ground states, respectively

# Microscopic Derivation of the Bose Hubbard Model



# Atoms in Optical Lattices




extent of atom much smaller than laser wavelength

$$a_{\mathrm{B}} \ll \lambda$$

- AC-Stark shift
  - Consider an atom in its electronic ground state exposed to laser light at fixed position $\vec{x}$.
  - The light be far detuned from excited state resonances: ground state experiences a second-oder *AC-Stark shift*

$$\delta E_g = \alpha(\omega) I$$

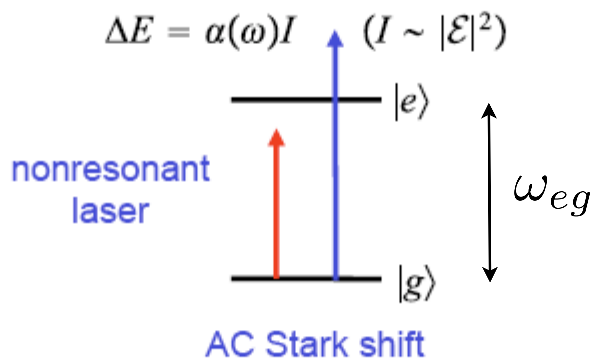
    with $\alpha(\omega)$ - dynamic polarizability of the atom for laser frequency $\omega$, $I \propto \vec{E}^2$ - light intensity.
  - Example: two-level atom $\{|g\rangle, |e\rangle\}$.

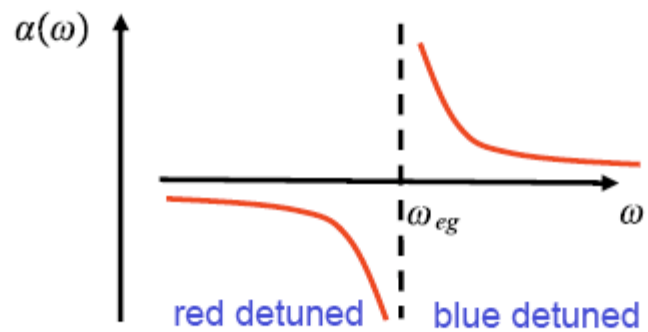
Rabi frequency

$$\delta E_g = \hbar \frac{\Omega^2}{4\Delta}$$

detuning from resonance $\Delta = \omega - \omega_{eg}$

$$\Omega \ll \Delta$$

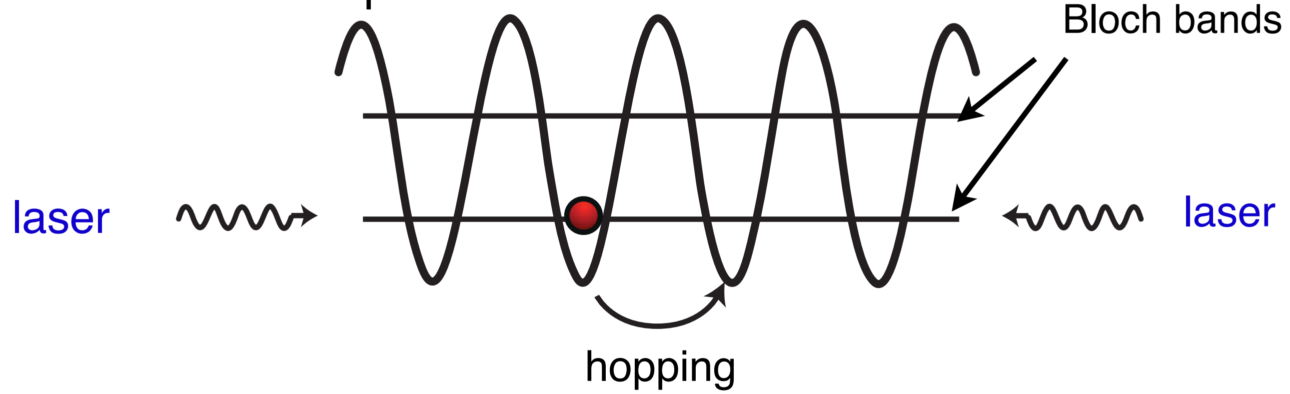



$\Delta < 0,\ \delta E_g < 0$ $\quad$ $\Delta > 0,\ \delta E_g > 0$

# Atoms in Optical Lattices

- standing wave laser configuration: $\vec{E}(\vec{x},t) = \vec{e}\mathcal{E}\sin kx\, e^{-i\omega t} + \text{h.c.}$
- AC Starkshift as a function of position




- The AC Starkshift appears as a conservative potential for the center-of-mass motion of the atom

$$i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{opt}}(\vec{x})\right)\psi(\vec{x},t) \qquad (V_{\text{opt}}(\vec{x}) \equiv \delta E_g(\vec{x}) = \hbar\frac{\Omega^2(\vec{x})}{4\Delta})$$

where the *position dependent AC-Stark* shift appears as a (conservative) "optical potential"

$$V_{\text{opt}}(x) = V_0 \sin^2 kx \qquad (k = 2\pi/\lambda)$$

for the center-of-mass motion of the atom.

- The potential is periodic with lattice period $\lambda/2$, and thus supports a band structure (Bloch bands). The depth of the potential is proportional to the laser intensity

# Bloch Theorem for Periodic Potentials

- Consider a Hamiltonian (in 1D) $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$ with periodic potential $V(x) = V(x+a)$. We are interested in the eigenfunctions $H\psi(x) = E\psi(x)$. (We set $\hbar = 1$).
- We define a translation operator $T = e^{-i\hat{p}a}$ so that $T\psi(x) = \psi(x+a)$.
  - $T$ is unitary, and thus has eigenfunctions $T\phi_\alpha(x) = e^{i\alpha}\phi_\alpha(x)$ with $\alpha = (-\pi, \pi]$ real.
  - Because $\phi_\alpha(x+a) = e^{i\alpha}\phi_\alpha(x)$ we can write $\phi_\alpha(x) = e^{i\alpha}u_\alpha(x)$ with periodic Bloch functions $u_\alpha(x) = u_\alpha(x+a)$ .
- We have $[H, T] = 0$, and we can find simultaneous eigenfunctions of $\{H, T\}$

$$
\begin{aligned}
H\varphi_q(x) &= E\varphi_q(x) \\
T\varphi_q(x) &= e^{iqa}\varphi_q(x)
\end{aligned}
$$

with $q \in [-\pi/a, \pi/a]$. We call $\hbar q$ quasimomentum.

# Bloch Theorem for Periodic Potentials

- Eigenstates of the Hamiltonian thus have the form

$$\boxed{\phi_q^{(n)}(x) = e^{iqx} u_q^{(n)}(x) \qquad q \in [-\pi/a, \pi/a]}$$

and the Bloch functions $u_q^{(n)}(x)$ are eigenstates of

$$\boxed{\hat{h}_q u_q^{(n)}(x) \equiv \left( \frac{(\hat{p}+q)^2}{2m} + V(\hat{x}) \right) u_q^{(n)}(x) = \epsilon_q^{(n)} u_q^{(n)}(x)}$$

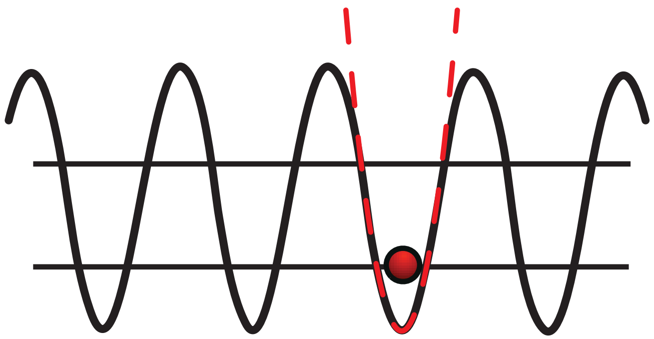
quantum number of the eigenstate (-> Bloch band index)

spatial dependence of wave function

$$u_q^{(n)}(x)$$

quasimomentum due to lattice periodicity

# Solution of Schroedinger Equation for 1D optical lattice



**Harmonic approximation (1D):** For deep lattices we can ignore tunneling. Assuming $V_0 > 0$ we have for the lowest states a *harmonic oscillator potential*

$$V(x) = V_0 \sin^2(kx) \approx V_0\,(kx)^2 \approx \frac{1}{2} m\nu^2 x^2$$

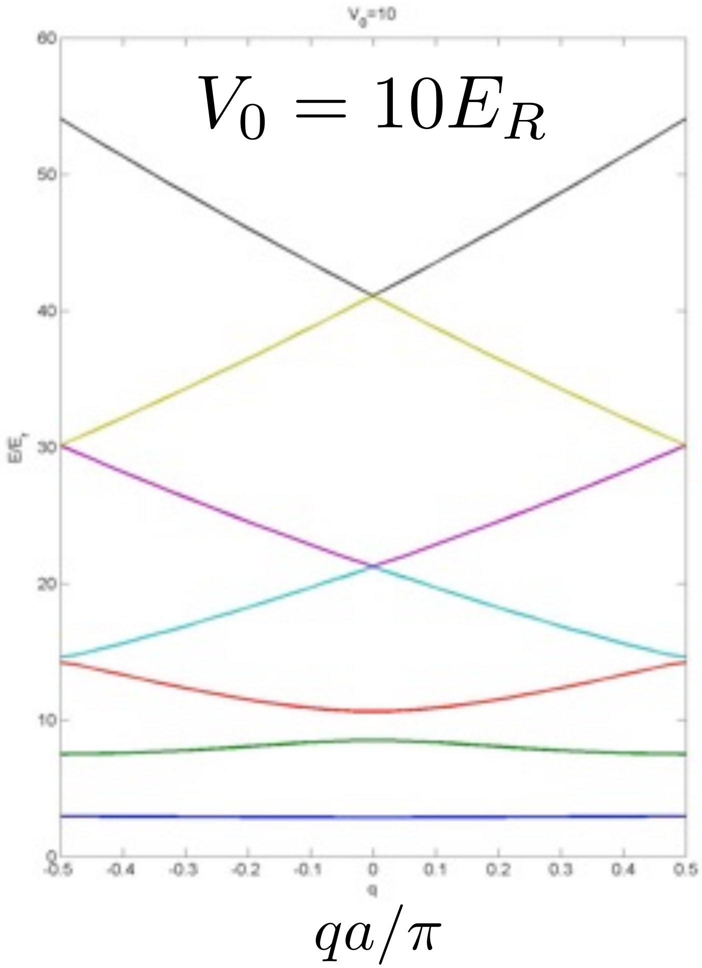
with *trapping frequency* $\nu = \sqrt{4V_0 E_R}/\hbar$ and with *recoil frequency / energy* $E_R \equiv \hbar^2 k^2/2m$. (Typcially$E_R \sim$ kHz, and $V_0 \sim$ few tens of kHz.)

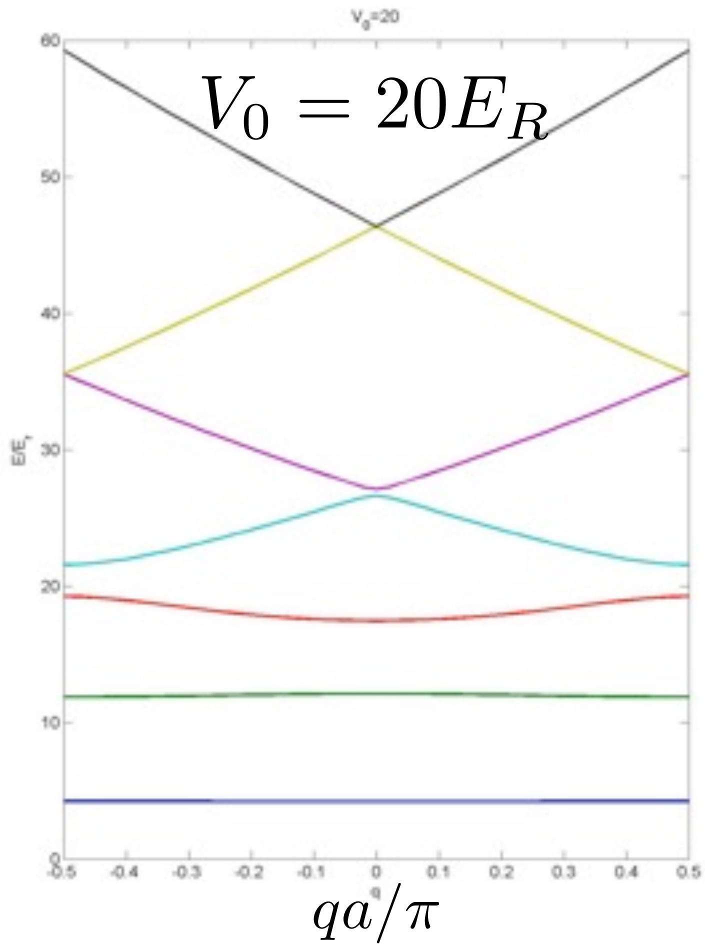
The ground state wave function

$$\psi_{n=0}(x) = \sqrt{\frac{1}{\pi^{1/2} a_0}}\mathrm{e}^{-x^2/(2a_0^2)}$$

$\mathrm{has}$ size $a_0 = \sqrt{\hbar/m\nu} \ll \lambda/2$, and we are in the Lamb-Dicke limit $\eta = 2\pi a_0/\lambda \ll 1$.

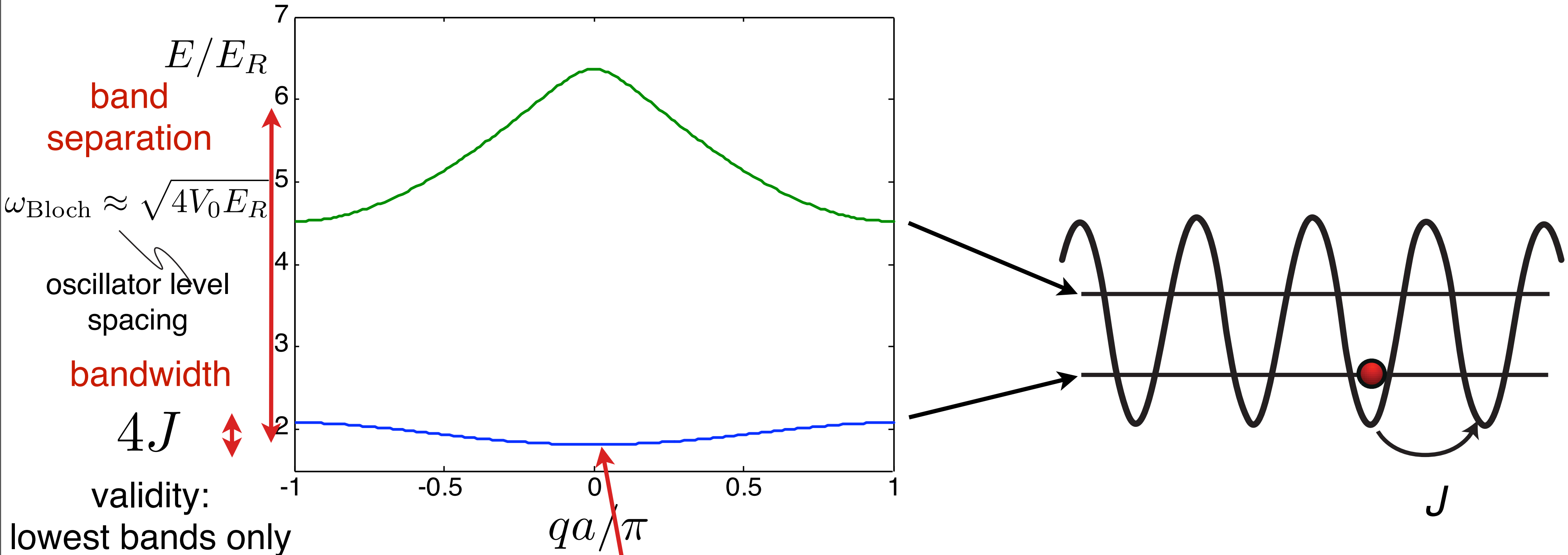
# Band Structure




**Bloch wave functions and bands (1D):** In general the eigen-solutions of the time-independent Schrödinger equation with periodic potential, $H\psi_{nq}(x) = \epsilon_{nq}\psi_{nq}(x$ has the form $\psi_{nq}(x) = e^{iqx}u_{nq}(x)$ with (periodic) Bloch wave functions $u_{nq}(x) = u_{nq}(x+a)$, $q$ the quasimomentum in the first Brillouin zone $-\pi/a < q \leq +\pi/a$, and $n = 0, 1, \ldots$ labelling the Bloch bands.

# Lowest Two Bloch Bands for $V_0$=5 $E_R$




**Compare: Bloch bands in tight binding approximation.** Above we introduced the Hamiltonian

$$\hat{H} = -J \sum_i \left( b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i \right) = \sum_q \epsilon_q b_q^\dagger b_q$$

with the tight-binding dispersion relation

$$\epsilon_q = -2J \cos qa \quad (-\pi/a < q \leq \pi/a).$$

For well separated bands the Bloch band calculation fits this relation well. This is typically fulfilled for the lowest bands.

# Wannier functions

**Wannier functions (1D):** Instead of Bloch wave functions we can also work with *Wannier wave functions*

$$u_q^{(n)}(x) = \sqrt{\frac{a}{2\pi}} \sum_{x_i = ia} w_n(x - x_i) \mathrm{e}^{\mathrm{i}x_i q},$$

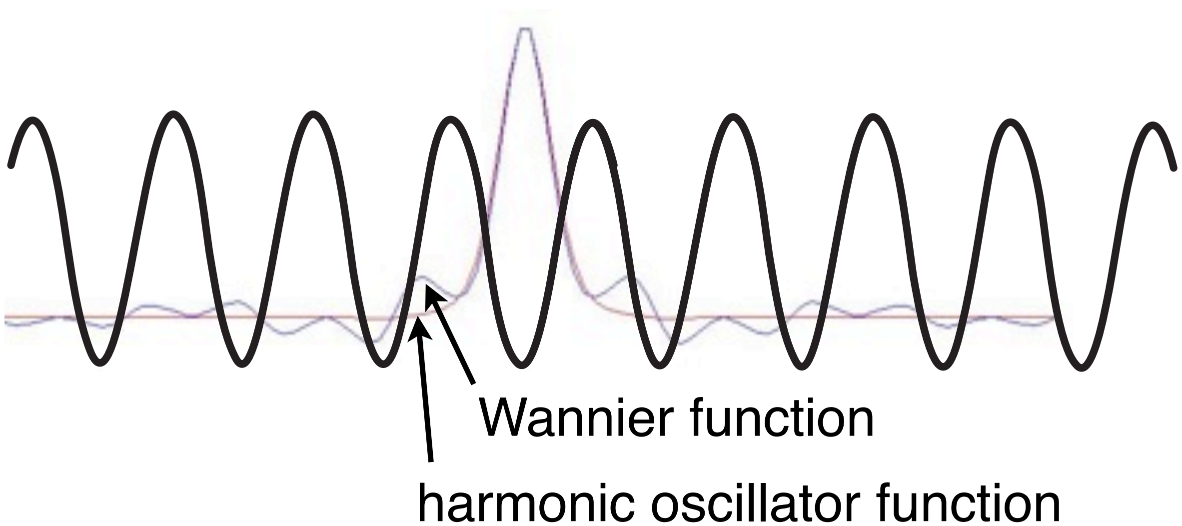
discrete Fourier transform

$$w_n(x - x_i) = \sqrt{\frac{a}{2\pi}} \int_{-\pi/a}^{\pi/a} \mathrm{d}q \, u_{nq}(x) \, \mathrm{e}^{-iqx_i}$$

trade quasimomentum for site index

which are *localized* around a particular lattice site $x_i = ia$ with $i = 0, \pm 1, \ldots$ .

The Bloch and Wannier wave functions are complete set of functions



# Bose Hubbard Hamiltonian

Starting point:

## Many body Hamiltonian of a dilute gas of bosonic atoms

Hamiltonian

$$H = \int d^3x \hat{\psi}^\dagger(\vec{x}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_0(\vec{x}) \right] \hat{\psi}(\vec{x}) + \frac{1}{2} g \int d^3x \hat{\psi}^\dagger(\vec{x}) \hat{\psi}^\dagger(\vec{x}) \hat{\psi}(\vec{x}) \hat{\psi}(\vec{x})$$

with $V_0(\vec{x})$ a single particle trapping potential (below: the optical lattice), and $g = \frac{4\pi\hbar a_s}{m}$, where $a$ is the scattering length.

This is valid under the assumption:

- The gas is sufficiently dilute so that only two body interactions are important, we can treat the composite atoms as bosons
- The enery / temperature are sufficiently small that two-body interactions reduce to s-wave scattering, parametrized by the scattering length $a_s$.

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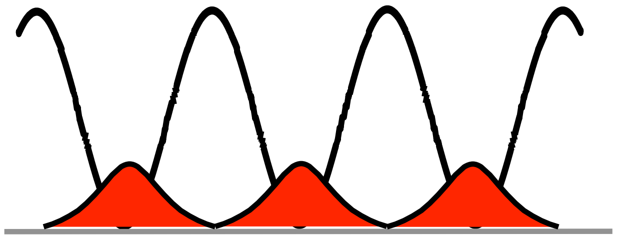
- Note: Fermions can be treated analogously: Fermi Hubbard model

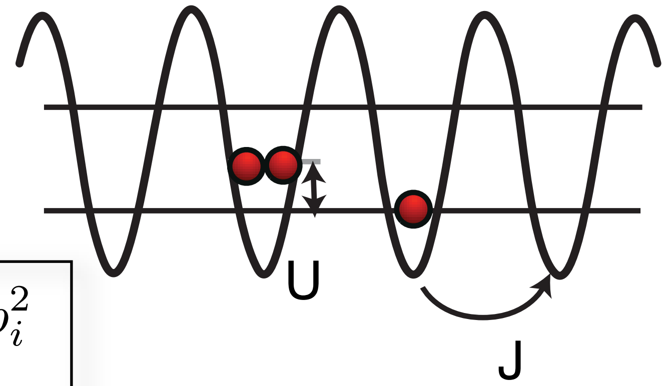
# Bose Hubbard Hamiltonian



spatially localized
Wannier functions

We expand the field operators in Wannier functions of the lowest band

$$\hat{\psi}(\vec{x}) = \sum_i w(\vec{x} - \vec{x}_i) b_i$$




to obtain the Bose Hubbard model

$$\boxed{\hat{H} \quad = \quad -\sum_{ij} J_{ij} b_i^\dagger b_j + \tfrac{1}{2} U \sum_i b_i^{\dagger 2} b_i^2}$$

with hopping $J_{ij} = \int d^3x w(\vec{x} - \vec{x}_i) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_0(\vec{x}) \right] w(\vec{x} - \vec{x}_j)$ and interaction $U = \frac{1}{2} g \int d^3x \, |w(\vec{x})|^4$ valid for $J, U, k_B T \ll \hbar\omega_{\mathrm{Bloch}}$.

(tight binding lowest band approximation)

---

additionally, we are bound to interactions
(scattering lengths)

extent of Wannier function

$$g \ll a_0, a$$

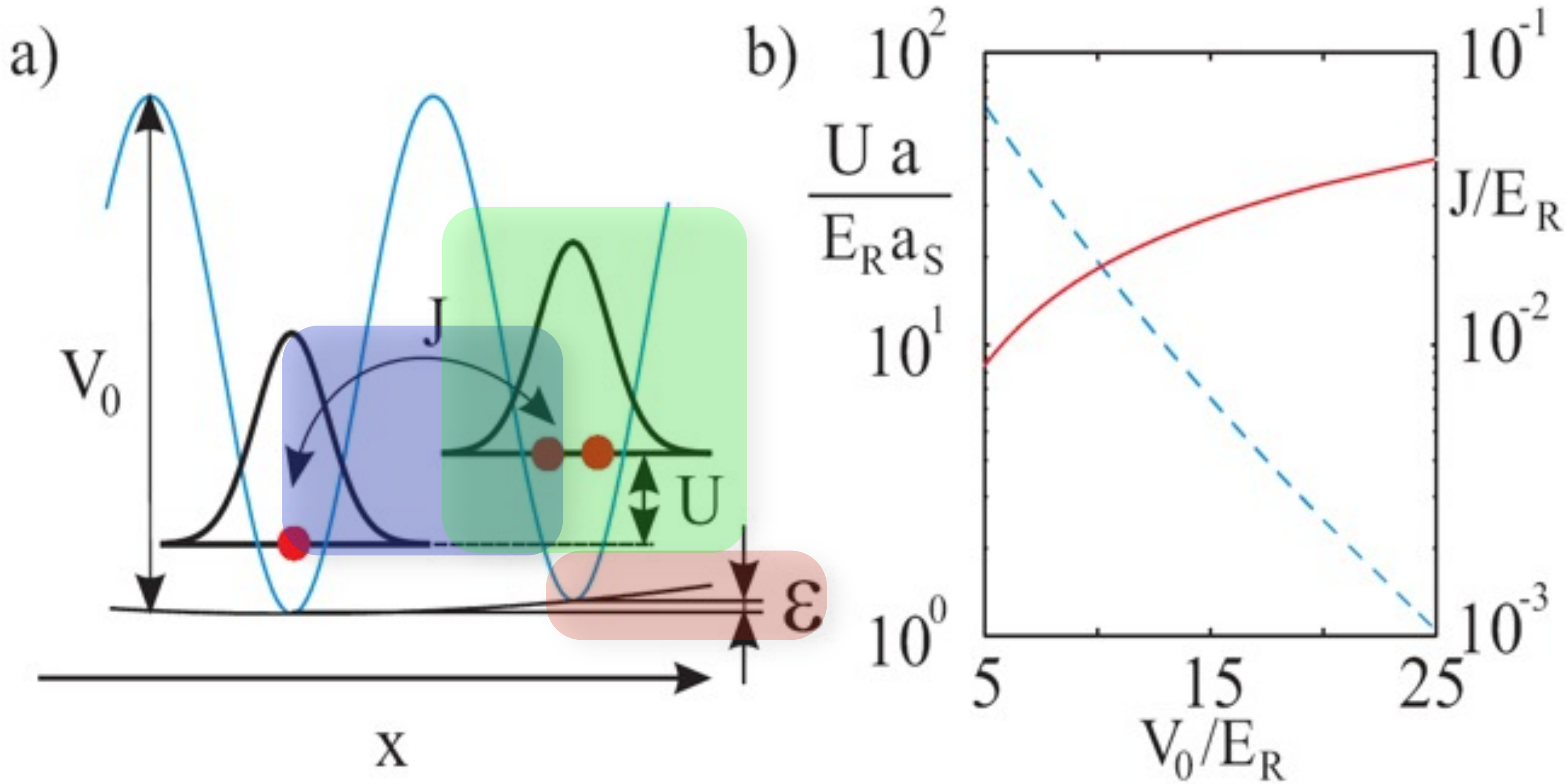
here, it means lattice spacing

This is not true close to
Feshbach resonances!

# Bose Hubbard Parameters

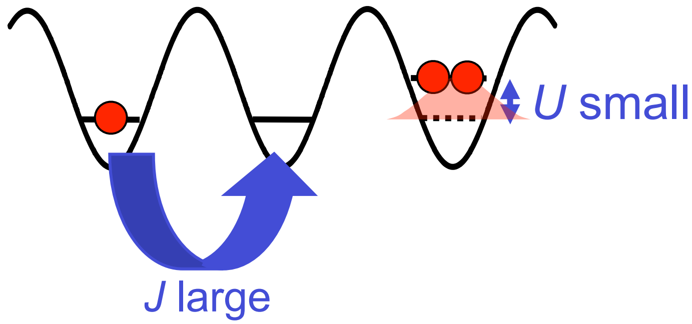
Parameters as function of laser intensity

$$H = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j + \sum_i \epsilon_i \hat{n}_i + \frac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1)$$

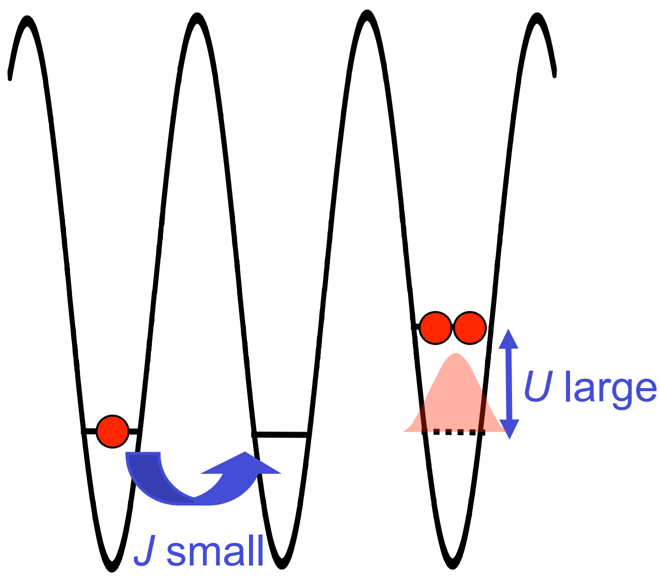


# Laser Control: Kinetic vs. Potential Energy

- **shallow lattice** : weak laser




- **deep lattice:** intense laser




**weakly interacting system:**

$J >> U$

*(kinetic energy >> interactions)*

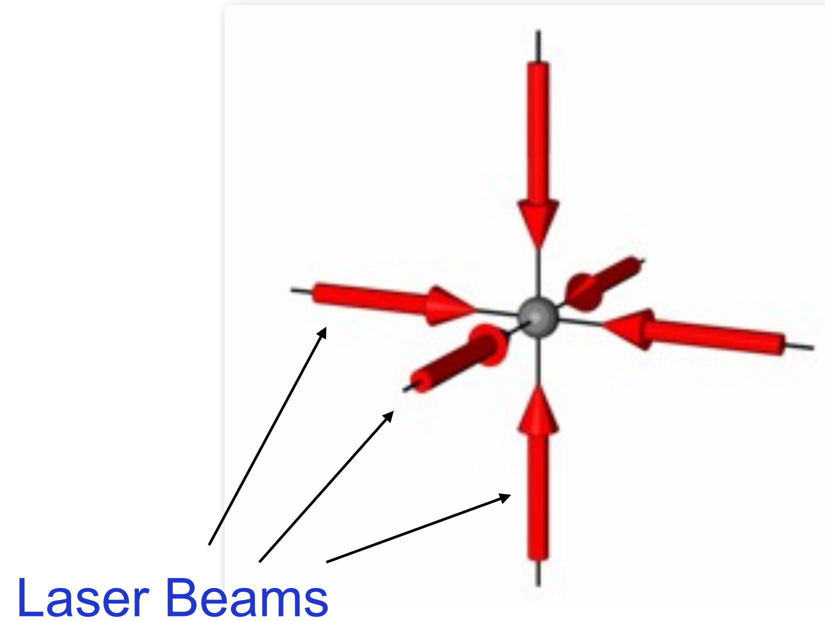
laser parameters
(time dependent)

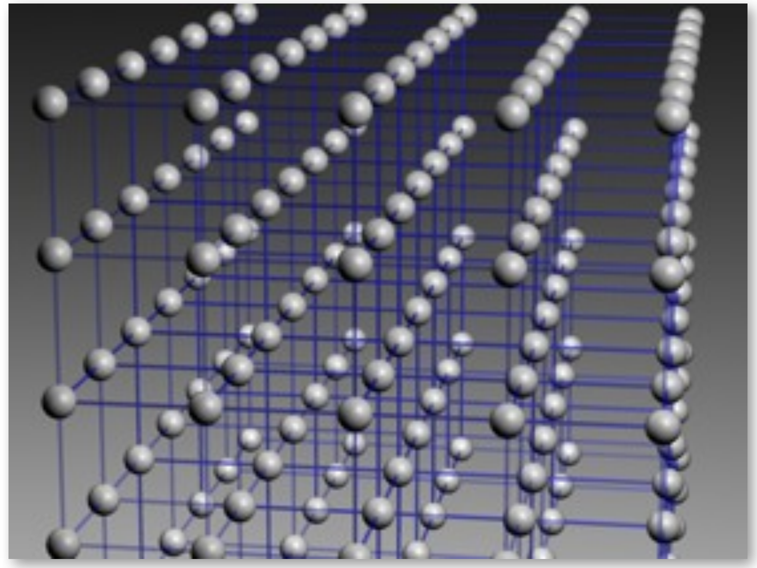
**strongly interacting system:**

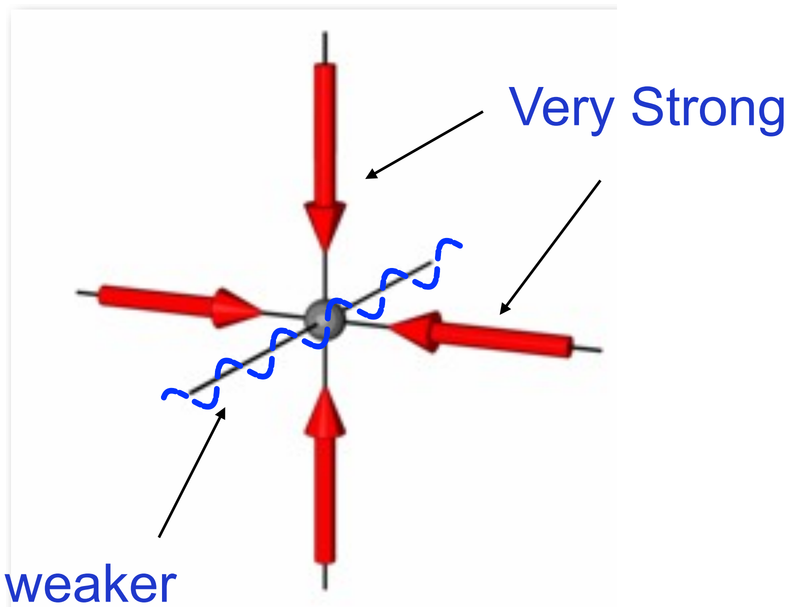
$J << U$

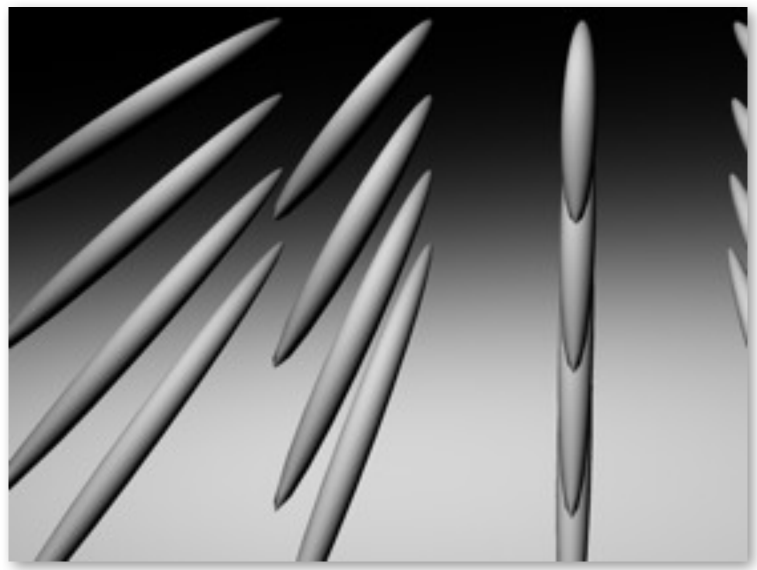
*(kinetic energy << interactions)*

# Optical Lattice Configurations

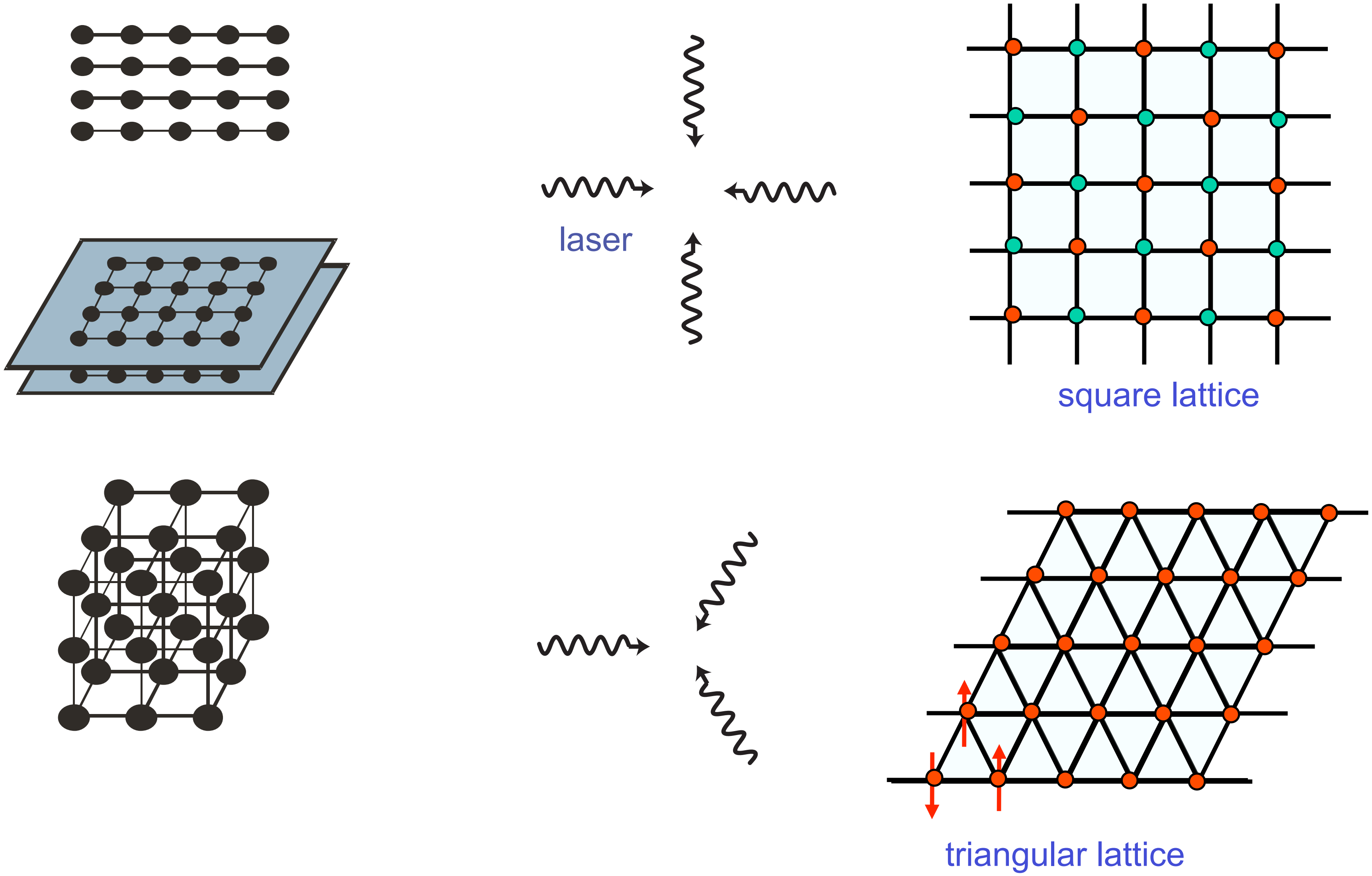


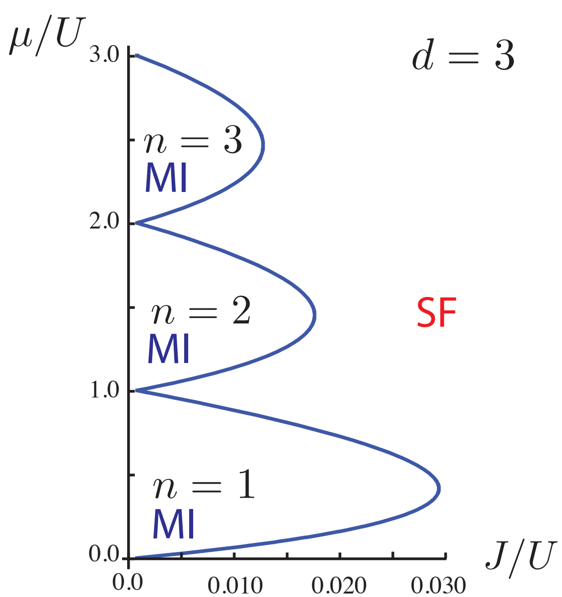


# Optical Lattice Configurations



# Phase Diagram
# of the
# Bose Hubbard Model



# Mean Field Theory

- Interpolation scheme encompassing the full range $J/U$.
- Main ingredient: Based on above discussion, construct local mean field Hamiltonian

$$H^{(\mathrm{MF})} = \sum_i h_i$$

$$H = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j - \mu \sum_i \hat{n}_i + \tfrac{1}{2} U \sum_i \hat{n}_i(\hat{n}_i - 1)$$

full Bose Hubbard Hamiltonian

$$h_i = -\mu \hat{n}_i + \tfrac{1}{2} U \hat{n}_i(\hat{n}_i - 1) - Jz(\psi^* b_i + \psi b_i^\dagger) + Jz\psi^*\psi$$

$$\hat{n}_i = b_i^\dagger b_i$$

coordination number

$z = 2d$ (cubic lattice)

- Discussion:
  - Derivation: Decompose $b_i = \psi + \delta b_i$, neglect $\delta b_i^\dagger \delta b_j$ terms, rewrite in terms of $b_i$
  - The problem is reduced to an onsite problem
  - $\psi$ is the “mean field”:
    - information on other other sites only via averages
    - if nonzero, assumes translation invariance but spontaneous phase symmetry breaking
  - Validity: approximation neglects spatial correlations via local form
    - becomes exact in infinite dimensions (Metzner and Vollhardt ’89)
    - reasonable in d=2,3 (T=0)

# Phase Diagram: Derivation

- Assume second order phase transition and follow Landau procedure:
  - Study ground state energy

$$E(\psi) = \text{const.} + m^2|\psi|^2 + \mathcal{O}(|\psi|^4)$$

  - Determine zero crossing of mass term

- Calculate E in second order perturbation theory

$$h_i = h_i^{(0)} + \psi V_i$$

smallness parameter close
to phase transition

$$h_i^{(0)} = -\mu\hat{n}_i + \tfrac{1}{2}U\hat{n}_i(\hat{n}_i - 1) + Jz\psi^*\psi$$

$$V_i = Jz(b_i + b_i^\dagger)$$

# Phase Diagram: Derivation

- Zero order Hamiltonian $h_i^{(0)}$ : diagonal in Fock basis $\{|n\rangle\}, n = 0, 1, 2, ...$
- The eigenvalues are $E_n^{(0)} = -\mu n + \frac{1}{2}Un(n-1) + Jz\psi^2$
- The ground state energies for given $\mu$ are

$$E_{\bar{n}}^{(0)} = \begin{cases} 0 & \text{for } \mu < 0 \\ -\mu\bar{n} + \frac{1}{2}U\bar{n}(\bar{n}-1) + Jz\psi^2 & \text{for } U(\bar{n}-1) < \mu < U\bar{n} \end{cases}$$

- The second order correction to the energy is

$$E_{\bar{n}}^{(2)} = \psi^2 \sum_{n \neq g} \frac{|\langle \bar{n}|V_i|n\rangle|^2}{E_{\bar{n}}^{(0)} - E_n^{(0)}} = (Jz\psi)^2 \left( \frac{\bar{n}}{U(\bar{n}-1) - \mu} + \frac{\bar{n}+1}{\mu - U\bar{n}} \right)$$

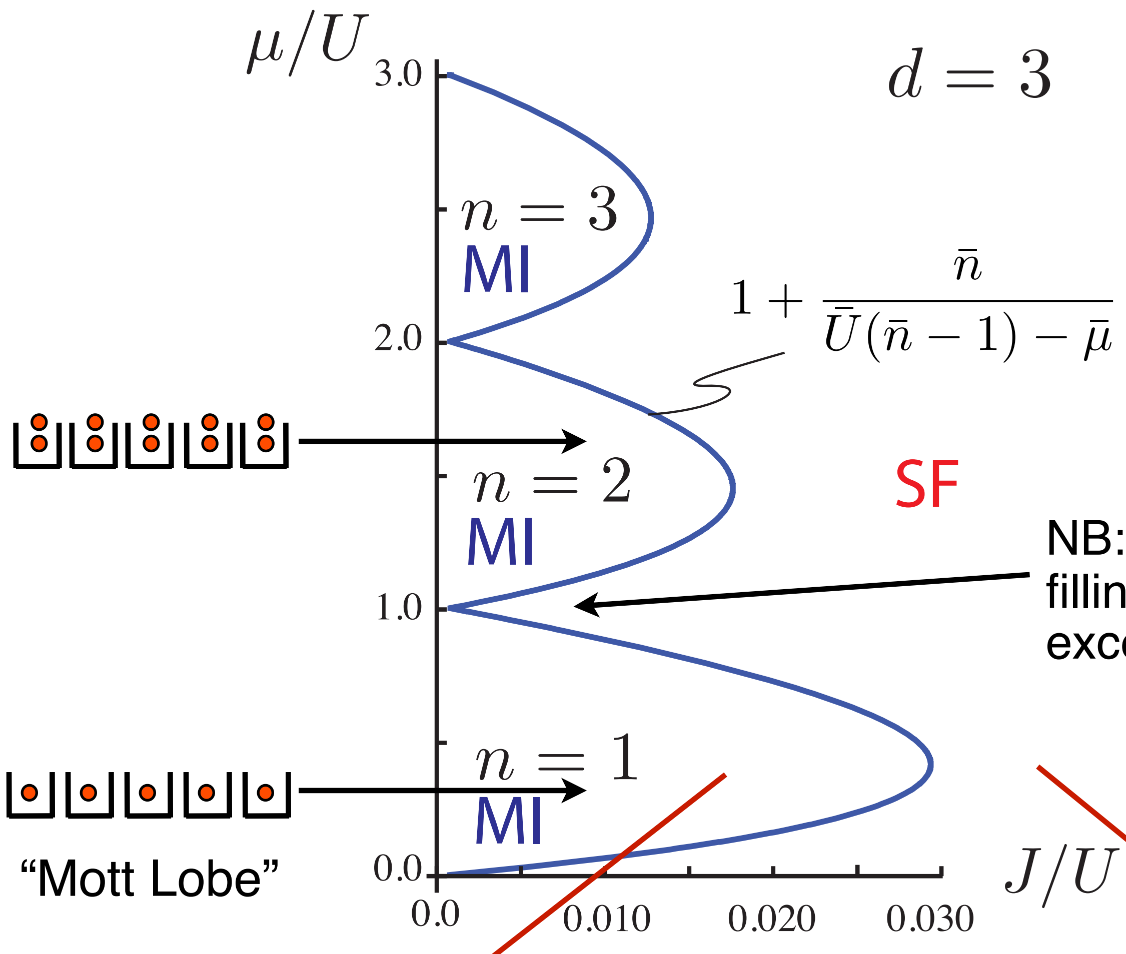
- For $E = \text{const.} + m^2\psi^2 + ...$ the phase transition happens at ($\bar{\mu} = \mu/Jz, \bar{U} = U/Jz$)

$$\frac{m^2}{Jz} = \boxed{1 + \frac{\bar{n}}{\bar{U}(\bar{n}-1) - \bar{\mu}} + \frac{\bar{n}+1}{\bar{\mu} - \bar{U}\bar{n}} = 0}$$

Bose-Hubbard phase border

# Phase Diagram: Overall Shape

This gives the phase diagram as a function of $\mu/U$ and $J/U$.




NB: for non-commensurate (= integer) fillings, superfluidity persists for U -> 0: excess particles condense.

Simple picture:

MI: Quantization of particle number

SF: Quantization of phase

$$"[\hat{N}, \hat{\varphi}] = \mathrm{i}"$$ - conjugate variables

# Limiting cases: Weak coupling, Superfluid

- Consider site dependent mean fields, $h_i = -\mu\hat{n}_i + \frac{1}{2}U\hat{n}_i(\hat{n}_i - 1) - J\sum_{\langle j|i\rangle}(\psi_j^* b_i + \psi_j b_i^\dagger) + \mathrm{const.}$
- Consider the equation of motion for the order parameter:
  - Heisenberg equation of motion for onsite Hamiltonian:

$$\partial_t \rho = -\mathrm{i}[h_i, \rho], \quad \rho = |\psi\rangle\langle\psi|, \quad |\psi\rangle = \prod_i |\psi\rangle_i$$

  - Equation of motion for the order parameter:

$$\mathrm{i}\partial_t \psi_i \equiv \mathrm{i}\partial_t \mathrm{tr}(b_i\rho) = -J\sum_{\langle j|i\rangle}\psi_i - \mu\langle\hat{n}_i\rangle + U\langle\hat{n}_i b_i\rangle$$

  - Weak coupling: assume coherent states $b_i|\psi\rangle_i = \psi_i|\psi\rangle_i$ $\quad |\psi_i\rangle = e^{-|\psi_i|^2/2}\sum_{n=0}^{\infty}\frac{\psi_i^n}{\sqrt{n!}}|n\rangle$

$$\mathrm{i}\partial_t\psi_i = -J\sum_{\langle j|i\rangle}\psi_i - \mu\psi_i^*\psi_i + U\psi_i^*\psi_i^2 = -J\triangle\psi_i - \mu'\psi_i^*\psi_i + U\psi_i^*\psi_i^2$$

$$\triangle f_i = \sum_{\langle j|i\rangle} f_j - f_i$$ lattice Laplacian

$$\mu' = \mu + Jz$$

shift: defines zero of kinetic energy

➡ At weak coupling, the (lattice) Gross-Pitaevski equation is reproduced

➡ certain spatial fluctuations are included: scattering off the condensate

➡ dispersion:

$$\omega_{\mathbf{q}} = \sqrt{\epsilon_{\mathbf{q}}(2U\psi^*\psi + \epsilon_{\mathbf{q}})} \qquad \epsilon_{\mathbf{q}} = 2J\sum_{\lambda}(1 - \cos aq_\lambda)$$

# Limiting cases: Strong coupling, Mott Insulator

- Mean field Mott state : $|\bar{n}\rangle = \prod_i |\bar{n}_i\rangle = \bar{n}^{-M/2} \prod_i b_i^{\dagger \bar{n}} |\text{vac}\rangle$: Quantization of particle number
- Discussion:
  - Within mean field, Mott-ness follows as a consequence of purity:
    - $*$ assume mechanism that suppresses SF off-diagonal order: $\rho$ diagonal, $1 = \mathrm{tr}\rho = \prod_i \mathrm{tr}_i \rho_i \overset{\text{hom.}}{=} (\sum p_m)^M$
    - $*$ Zero temperature: pure state, $1 = \mathrm{tr}\rho^2 = \prod_i \mathrm{tr}_i \rho_i^2 \overset{\text{hom.}}{=} (\sum p_m^2)^M$
    - $*$ only solution is $p_m = \delta_{n,\bar{n}}$
  - Quantization of particle number within MI is an exact result in the sense $\langle b_i^\dagger b_i \rangle = \bar{n}$
    - $*$ at $J=0$, Mott state $|\bar{n}\rangle$ is (i) exact ground state, (ii) eigenstate to particle number $\hat{N} = \sum_i \hat{n}_i$, (iii) separated from other states by gap $\sim U$
    - $*$ kinetic perturbation $H_{\text{kin}} = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j$
    - $*$ commutes with $\hat{N}$ , $[H_{\text{kin}}, \hat{N}] = 0$

➡ switching on J adiabatically, the ground state remains exact eigenstate to number operator. Assuming translation invariance gives exact result

$$\langle b_i^\dagger b_i \rangle = \bar{n}$$

- Implication: the Mott insulator is an incompressible state, $\dfrac{\partial \langle \hat{N} \rangle}{\partial \mu} = 0$

# Excitation spectrum in the Mott phase

- We are looking for the single particle dispersion relation $\omega_{\mathbf{q}}$
- This is a dynamical quantity: hard to get within Hamiltonian framework above
- Path integral formulation of the Bose-Hubbard model

$$Z = \mathrm{tr} e^{-\beta \hat{H}} = \int \mathcal{D}a \exp - S_{\mathrm{BH}}[a]$$

$$S_{\mathrm{BH}}[a] = S_{\mathrm{loc}}[a] + S_{\mathrm{kin}}[a]$$

$$S_{\mathrm{loc}}[a] = \int_{-\beta/2}^{\beta/2} d\tau \sum_i \left[ a_i^* (\partial_\tau - \mu) a_i + \tfrac{1}{2} U a_i^{*\,2} a_i^2 \right]$$

local contribution

$$S_{\mathrm{kin}}[a] = \int_{-\beta/2}^{\beta/2} d\tau \sum_{i,j} t_{ij} a_i^* a_j$$

bi-local contribution; for nearest-neighbour hopping

$$t_{ij} = -J \sum_{\sigma\lambda} \delta_{i,j+\sigma \mathbf{e}_\lambda}$$

$$\sigma = \pm 1$$
$$\lambda = x, y, z$$

spatial directions

- Discussion:
  - Nonrelativistic action (on the lattice)
  - Note symmetry (T=0): temporally local gauge invariance $a_i \to a_i e^{\mathrm{i}\phi(\tau)}, \;\; \mu \to \mu + \mathrm{i}\partial_\tau \phi(\tau)$
  - so far: weak coupling problems J>>U, decoupling in the interaction U
  - now: Mott physics, i.e. strong coupling problem U>>J: decoupling in J

# Decoupling in J: Hopping Expansion

$$S_{\rm BH}[a] = S_{\rm loc}[a] + S_{\rm kin}[a]$$

$$\sim U \qquad \sim J$$

- Goal: treat the strong coupling problem U>>J via decoupling in J

- Hubbard-Stratonovich transformation:

$$\begin{aligned}
Z &= \int \mathcal{D}a \exp - S_{\sf BH}[a] = \mathcal{N} \int \mathcal{D}a\mathcal{D}\psi \exp - S_{\sf BH}[a] + \int d\tau \sum_{ij} t_{ij}(\psi_i^* - a_i^*)(\psi_j - a_j) \\
&= \mathcal{N} \int \mathcal{D}a\mathcal{D}\psi \exp - S_{\sf loc}[a] + \int d\tau \sum_{ij} t_{ij}(\psi_i^*\psi_j - \psi_i^* a_j - \psi_j a_i^*) = \mathcal{N} \int \mathcal{D}\psi \exp - S_{\sf eff}[\psi] \\
S_{\sf eff}[\psi] &= \int d\tau \sum_{ij} t_{ij}\psi_i^*\psi_j - \log\langle \exp - \int d\tau \sum_{ij} (\psi_i^* a_j + \psi_j a_i^*\rangle_{S_{\sf loc}} \\
\langle \mathcal{O}\rangle_{S_{loc}} &= \int \mathcal{D}a\mathcal{O} \exp - S_{\sf loc}[a]
\end{aligned}$$

- Discussion
  - Form of intermediate action identical to mean field decoupling above (for site dependent mean fields)
  - The effective action $S_{\sf eff}[\psi]$ can now be calculated perturbatively

# Decoupling in J: Hopping Expansion

- expansion in powers of the hopping

$$\langle \exp - \int d\tau \sum_{ij} t_{ij}(\psi_i^* a_j + \psi_j a_i^*)\rangle_{S_{\text{loc}}} = 1 + \sum_{m=1}^{\infty} \langle [\int d\tau \sum_{ij} t_{ij}(\psi_i^* a_j + \psi_j a_i^*)]^{2m}\rangle_{S_{\text{loc}}}$$

$\rightarrow$ note: averages of odd powers of $a_i$ or $a_i^*$ vanish in the Mott state

- To lowest order, the effective action thus reads

$$S_{\text{eff}}[\psi] = \int d\tau \sum_{ij} t_{ij}\psi_i^*(\tau)\psi_j(\tau) + \int d\tau d\tau' \sum_{iji'j'} t_{ij}t_{i'j'}\psi_j^*(\tau)\psi_{j'}(\tau')\langle a_i(\tau)a_{i'}^*(\tau')\rangle_{S_{\text{loc}}}$$

- Discussion
  - the approach is inherently perturbative: no known closed form expression for above average
  - the hopping expansion does not lead to an exact solution of the problem: $Z = \int \mathcal{D}\psi \exp - S_{\text{eff}}[\psi]$ would need to be calculated for this purpose
  - the hopping expansion is closely related to the mean field approximation (see below)

# Quadratic Effective Action

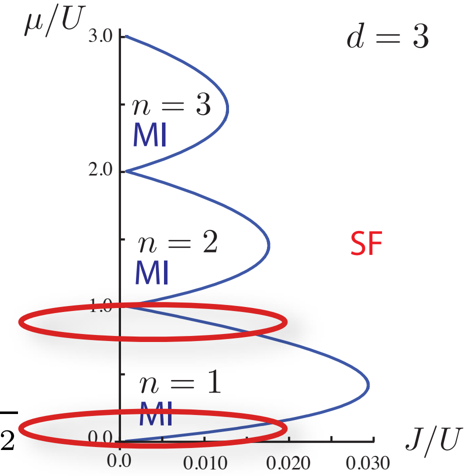
- The correlation functions $\langle a_i(\tau)a^*_{i'}(\tau')\rangle_{S_{\text{loc}}}$ can be evaluated explicitly since the local onsite problem is solved exactly
- The effective action is then, in frequency and momentum space and for nearest neighbour hopping

$$\begin{aligned} S^{(2)}_{\text{eff}}[\psi] &= \int \frac{d\omega}{2\pi}\frac{d^dq}{(2\pi)^d}\psi^*_{\mathbf{q}}(\omega)G^{-1}(\omega,\mathbf{q})\psi_{\mathbf{q}}(\omega) \\ G^{-1}(\omega,\mathbf{q}) &= \epsilon_{\mathbf{q}} - \epsilon^2_{\mathbf{q}}\left(\frac{\bar{n}+1}{-\mathrm{i}\omega-\mu+\bar{n}U} + \frac{\bar{n}}{\mathrm{i}\omega+\mu-(\bar{n}-1)U}\right), \quad \epsilon_{\mathbf{q}} = 2J\sum_\lambda \cos\mathbf{q}\mathbf{e}_\lambda \end{aligned}$$

- Evaluating $G^{-1}(\omega=0,\mathbf{q}=0)$ reproduces the above mean field result ($\epsilon_{\mathbf{q}} = Jz$): The fluctuations included here are the same, but their spatial and temporal dependence is resolved within the functional integral formulation
- The frequency dependence is dictated by the temporally local gauge invariance to $-\mathrm{i}\omega-\mu$
- The quasiparticle spectrum obtains from the poles of the Green's function analytically continued to real frequencies,

$$G^{-1}(\omega\to\mathrm{i}\omega,\mathbf{q}) \stackrel{!}{=} 0$$

# Excitation Spectrum: Particles and Holes




- Solving $G^{-1}(\omega \to \mathrm{i}\omega, \mathbf{q}) \overset{!}{=} 0$ yields the quasiparticle dispersion

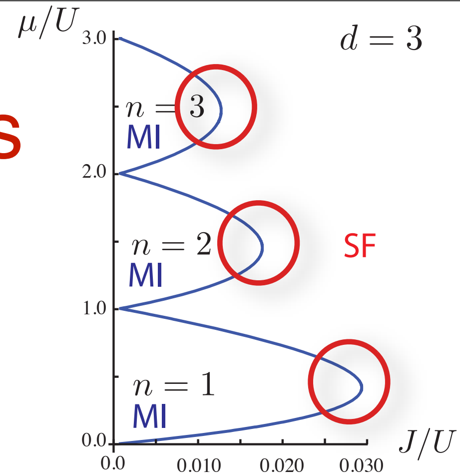
$$\omega^{\pm}_{\mathbf{q}} = -\mu + \tfrac{U}{2}(2\bar{n}-1) - \tfrac{\epsilon_{\mathbf{q}}}{2} \pm \tfrac{1}{2}\sqrt{\epsilon^2_{\mathbf{q}} - 2(2\bar{n}+1)U\epsilon_{\mathbf{q}} + U^2}$$

- For $\mu$ within the Mott phase, $\omega^+_{\mathbf{q}} \geq 0$ and $\omega^-_{\mathbf{q}} \leq 0$. They correspond to quasiparticle and quasihole excitations.
- If we are interested in the true excitation spectrum, we need to consider that the quasiholes are propagating backward in time. The true particle and hole excitation energies are therefore

$$E^{\pm}_{\mathbf{q}} = \pm\omega^{\pm}_{\mathbf{q}} = \pm\big(-\mu + \tfrac{U}{2}(2\bar{n}-1) - \tfrac{\epsilon_{\mathbf{q}}}{2}\big) + \tfrac{1}{2}\sqrt{\epsilon^2_{\mathbf{q}} - 2(2\bar{n}+1)U\epsilon_{\mathbf{q}} + U^2}$$

- Generically, both branches of the spectrum are gapped: $E^{\pm}_{\mathbf{q=0}} = \mathcal{O}(U) > 0$
- Study the phase border for $Jz \ll U$, defined with $G^{-1}(\omega=0, \mathbf{q}=0) \overset{!}{=} 0 \longrightarrow \mu_{\text{crit}}(U)$ in the upper branch of the lobe:
  - there is a gapless particle with quadratic dispersion for $\mathbf{q} \to 0$, $E^+_{\mathbf{q}} \approx (1 + \frac{(\bar{n}+1)U+Jz}{\Delta})\delta\epsilon_{\mathbf{q}}$, $\delta\epsilon_{\mathbf{q}} = 2J\sum_\lambda(1-\cos\mathbf{q}\mathbf{e}_\lambda) \approx J\mathbf{q^2}$
  - there is a gapped hole with gap $\Delta = E_{\mathbf{q=0}} = \sqrt{Jz^2 - 2(2\bar{n}+1)UJz + U^2}$
- For the lower branch of the lobe and $Jz \ll U$, the holes disperse $E^-_{\mathbf{q}} \approx J\mathbf{q^2}$ and the particles are gapped with $\Delta \approx U$

# Bicritical point: Change of Universality Class




- The interpretation in terms of particle and hole excitation only holds for $Jz \ll U$
- In general, at the phase transition there is one gapless mode. Choosing it to set the zero of energy, the gap of the other mode is given by

$$\Delta = E^{+}_{\mathbf{q}=\mathbf{0}} + E^{-}_{\mathbf{q}=\mathbf{0}} = \sqrt{Jz^2 - 2(2\bar{n}+1)UJz + U^2}$$

- At the tip of the lobe, $U/Jz = 2\bar{n} + 1 + \sqrt{(2\bar{n}+1)^2 - 1}$ and thus $\Delta = 0$: there are two gapless modes (particle-hole symmetry)
- The excitation spectrum at this point is dominanted by the square root for $\mathbf{q} \to 0$ and reads

$$E^{\pm}_{\mathbf{q}} = \tfrac{1}{2}\sqrt{(2(2\bar{n}+1)U + Jz)\delta\epsilon_{\mathbf{q}}} \sim |\mathbf{q}|$$

- The spectrum changes form a nonrelativistic spectrum $E \sim \mathbf{q}^2$ (dynamic exponent $z_d = 2$) to a relativistic spectrum $E \sim |\mathbf{q}|$ (dynamic exponent $z_d = 1$)

➡ At a generic point on the phase border, the system is in the z_d = 2 O(2) universality class
➡ At the tip of the lobe, the system is in the z_d = 1 O(2) universality class

# Bicritical point: Symmetry Argument

- We show that the change in universality class at the tip of the lobe is not an artifact of mean field theory
- The full effective action (including fluctuations) at low energies has a derivative expansion

$$\Gamma[\psi] = \int \psi^*[Z\partial_\tau + Y\partial_\tau^2 + m^2 + ...]\psi + \lambda(\psi^*\psi)^2 + ...$$

- At the phase transition, we have $m^2 = 0$. At the tip of the lobe, we have additionally(vertical tangent)

$$\frac{\partial m^2}{\partial \mu} = 0$$

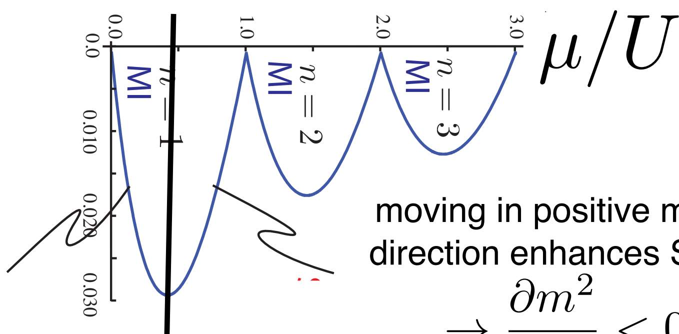
- Using the invariance under temporally the local symmetry$\psi \to \psi e^{\mathrm{i}\theta(\tau)}, \mu \to \mu + \mathrm{i}\partial_\tau\theta(\tau)$, we find the Ward identity ($q = (\omega, \mathbf{q})$)

$$-\frac{\partial m^2}{\partial \mu} = -\frac{\partial}{\partial \mu}\frac{\delta^2\Gamma}{\delta\psi^*(q)\delta\psi(q)}\Big|_{\psi=0;q=0} = \frac{\partial}{\partial(\mathrm{i}\omega)}\frac{\delta^2\Gamma}{\delta\psi^*(q)\delta\psi(q)}\Big|_{\psi=0;q=0} = Z$$

- Thus, there cannot be a linear time derivative ath the tip of the lobe, $Z = 0$. The leading frequency dependence is quadratic

moving in positive mu
direction suppresses SF

$$\to \frac{\partial m^2}{\partial \mu} > 0$$

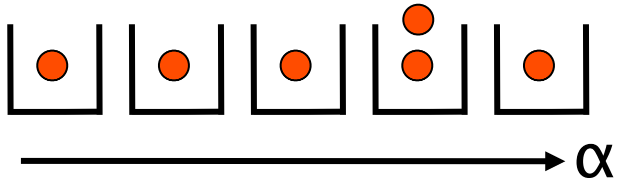



moving in positive mu
direction enhances SF

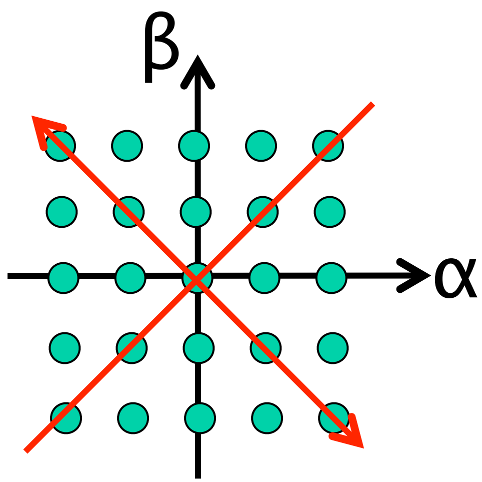
$$\to \frac{\partial m^2}{\partial \mu} < 0$$

# Experimental signatures 1: Interference

- spatial correlation function $\langle b_\alpha^\dagger b_\beta \rangle$




superfluid

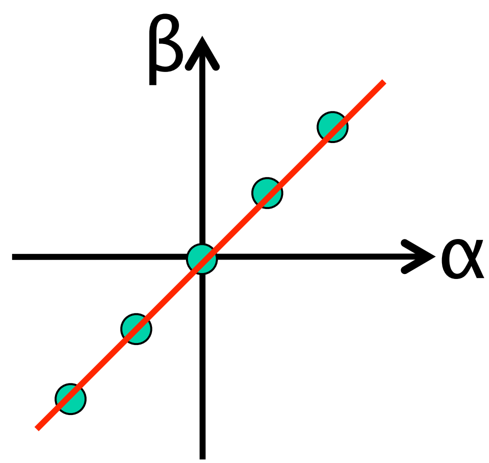



off-diagonal long range order:

interference

$$\langle b_\alpha^\dagger b_\beta \rangle \approx \psi_\alpha^* \psi_\beta$$

Mott

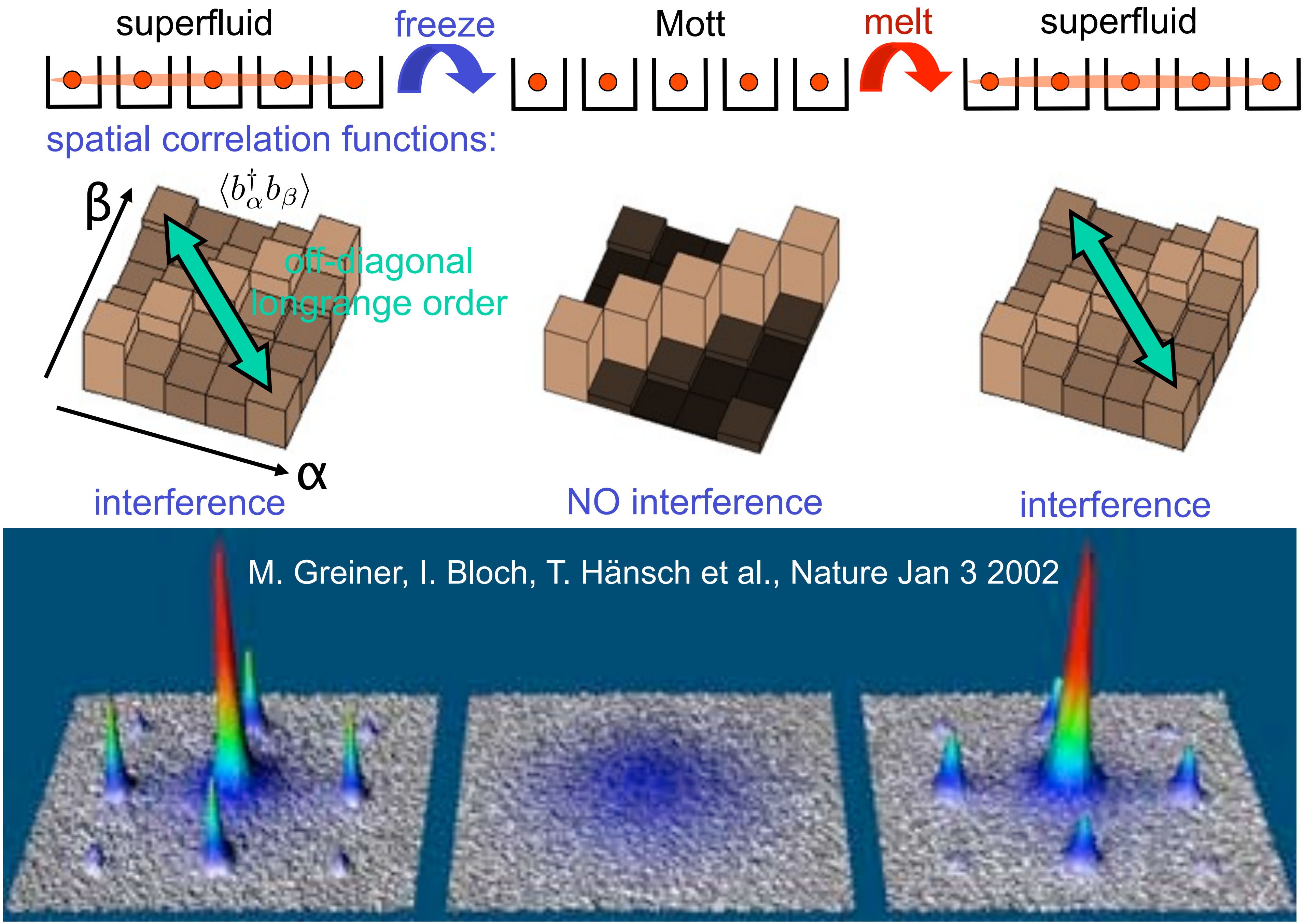



no interference

$$\langle b_\alpha^\dagger b_\beta \rangle \approx n_\alpha \delta_{\alpha\beta}$$

exp signature

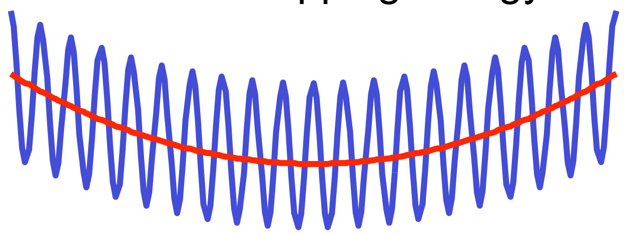
# Interference Patterns



# Experimental Signatures 2: Mott Gap

- The gap in the Mott phase causes staggered structure in density profile

(1) Consider situation

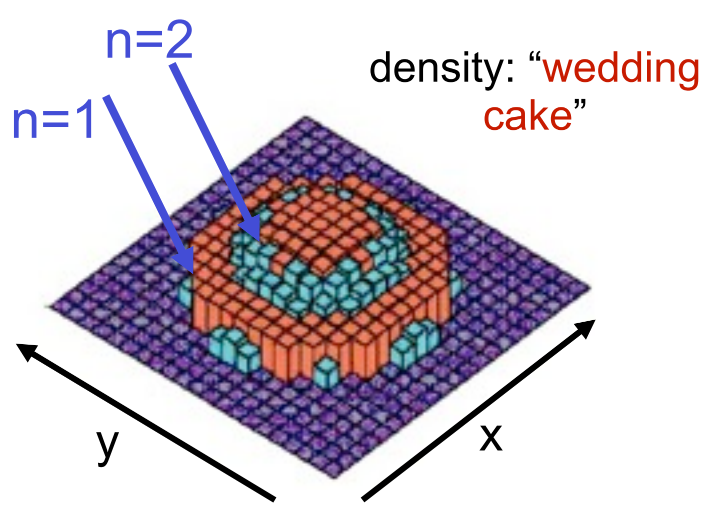



(2) Assume local density approximation: local applicability of mean field theory

$$\mu(x_i) = \mu - V(x_i), \;\; V(x_i) = \frac{k}{2} x_i^2$$

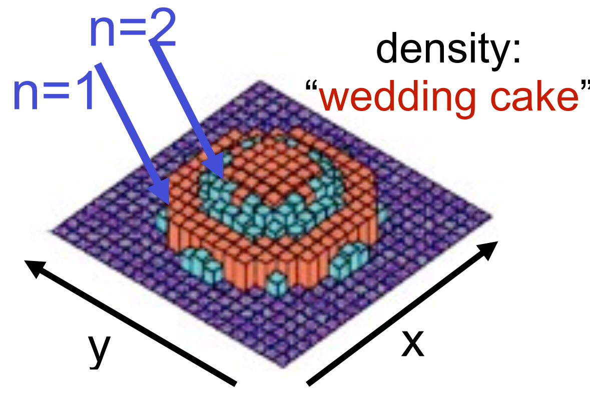
(3) The incompressibility within Mott state leads to  (2d)

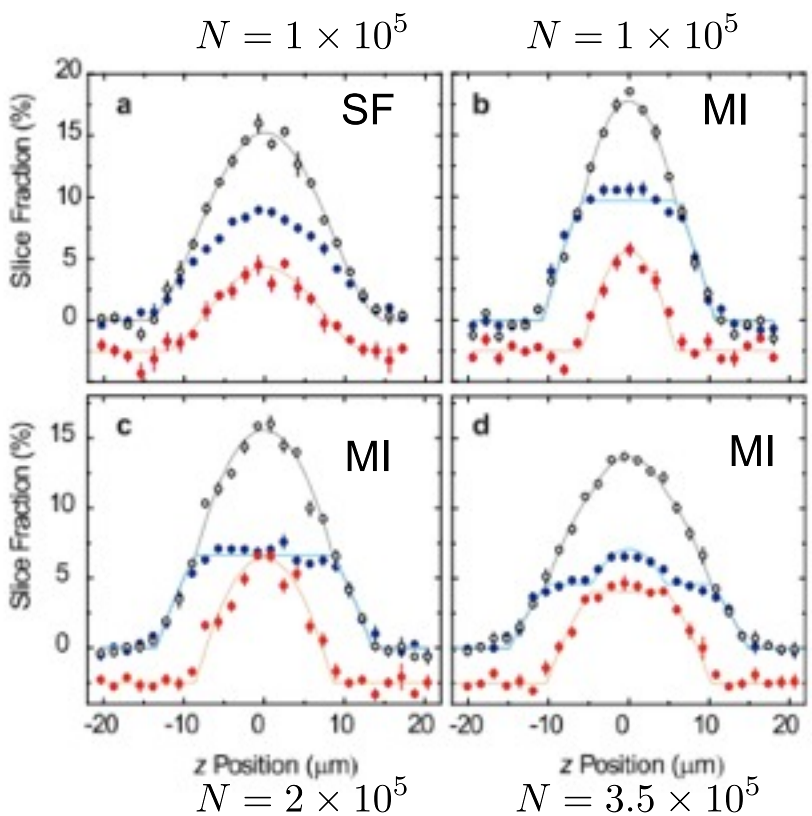
$$\frac{\partial \langle \hat{N} \rangle}{\partial \mu} = 0$$



# Experimental Signatures 2: Mott Gap

- Experiment:
  - 3D isotropic trap
  - resolve x-y-integrated density profile in z-direction
    - total density (grey)
    - singly occupied sites (red)
    - doubly occupied sites (blue)




Bloch group, 2006

- Superfluid region:
  - Thomas-Fermi quadratic shape
  - resolution of singly and doubly sites from Poissonian number statistics for SF state
- Mott insulator region
  - e.g. for spherical Mott shells of Radius R at the core of the trap, integrated profile:

$$\nu(R; z) = \text{const.} \times \max(0, R^2 - z^2)$$

  - profile for inner shell of radius R_2, n=2:

$$\nu(R_1; z) \quad \text{-- red line}$$

  - profile of outer shell of radius R_1, n=1

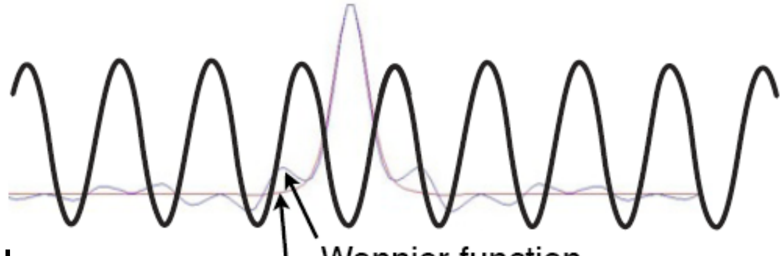
$$\nu(R_1; z) - \nu(R_2; z) \quad \text{-- blue line}$$

$$\int dx dy \theta(R^2 - (x^2 + y^2 + z^2)) = 2\pi \int dr r \theta((R^2 - z^2) - r^2) = \pi \max(0, R^2 - z^2)$$

# Summary

- Cold bosonic atoms loaded into optical lattices allow to implement an interacting many-body system with quantum phase transition with no counterpart in condensed matter physics
  - Optical lattices are standing wave laser configurations which couple to atoms via a position dependent AC Stark shift
  - In an accessible parameter regime the microscopic model for bosonic atoms reduces to a single band Bose-Hubbard model with parameters J (kinetic energy) and onsite interaction U
  - In such systems, it is possible to realize high densities (O(1)) and strong interactions U>J
  - The competition of kinetic and interaction energy g = J/U gives rise to a quantum phase transition for commensurate fillings n=1,2,...
  - The strong coupling “Mott phase” is an ordered phase (quantized particle number) without symmetry breaking
  - One characteristic property is incompressibility, which has been observed in experiments

# Effective Lattice Hamiltonian




- Start from our model Hamiltonian, add optical potential:

$$H = \int_{\mathbf{x}} [a^\dagger_{\mathbf{x}}( - \frac{\triangle}{2m} - \mu + V(\mathbf{x}) + V_{\rm opt}(\mathbf{x})\ )a_{\mathbf{x}} + g\hat{n}^2_{\mathbf{x}}]$$

- Periodicity of the optical potential suggests expansion of field operators into localized lattice periodic Wannier functions (complete set of orthogonal functions)

$$a_{\mathbf{x}} = \sum_{i,n} w_n(\mathbf{x} - \mathbf{x}_i) b_{i,n}$$

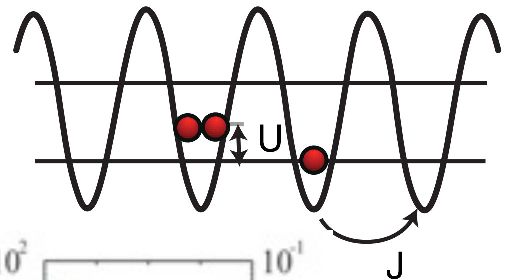
band index

minimum position

- For low enough energies (temperature), we can restrict to lowest band:

$$T, U, J \ll \sqrt{4V_0 E_R}, E_R = k^2/(2m) \to n = 0$$

- Then we obtain the single band (Bose-) Hubbard model

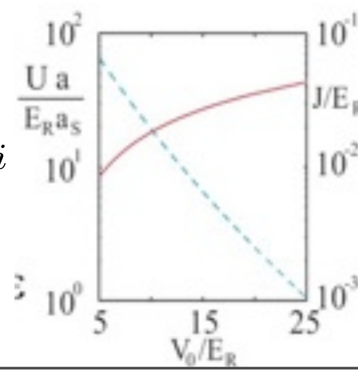



$$H = -J \sum_{\langle i,j \rangle} b^\dagger_i b_j - \mu \sum_i \hat{n}_i + \sum_i \epsilon_i \hat{n}_i + \tfrac{1}{2} U \sum_i \hat{n}_i(\hat{n}_i - 1)$$

$$\hat{n}_i = b^\dagger_i b_i$$

$$J = - \int dx w^*_0(x)(-\hbar^2/2m\triangle - V_{\rm opt}(x))w_0(x - \lambda/2)$$

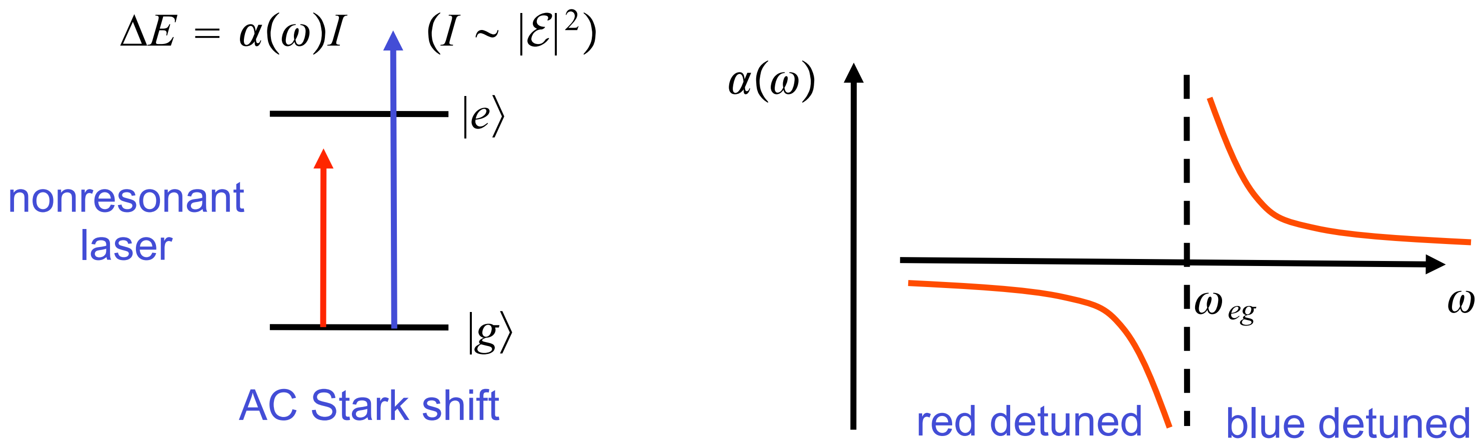
$$U = g \int dx |w_0(x)|^4$$



# Cold Atoms in Optical Lattices

## Optical Lattices

**AC-Stark shift:** We consider an atom in its electronic ground state exposed to laser light at fixed position $\vec{x}$. If the light is far detuned from excited state resonances, the ground state will experience a second-oder *AC-Stark shift* $\delta E_g(\vec{x}) = \alpha(\omega) I(\vec{x})$ with $\alpha(\omega)$ the dynamic polarizability of the atom for frequency $\omega$, and $I(\vec{x})$ the light intensity.




Example: for a two-level atom $\{|g\rangle, |e\rangle\}$ in the RWA the AC-Starkshift is given by $\delta E_g(\vec{x}) = \hbar \frac{\Omega^2(\vec{x})}{4\Delta}$ with Rabi frequeny $\Omega$ and detuning $\Delta = \omega - \omega_{eg}$ ($\Omega \ll \Delta$). Note that for red detuning ($\Delta < 0$) the ground state shifts down $\delta E_g < 0$, while for blue detuning ($\Delta > 0$) we have $\delta E_g > 0$.