





# **Optical Lattices and Artificial Gauge Potentials**

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# **Institute of Laser Physics**



Photo: AG Hammarich

### **Group Hemmerich**

We use ultracold atoms to study minimal laboratory models of quantum many-body physics. Our research covers ultracold atoms in optical cavities, topological optical lattices, and new concepts for quantum metrology.

Group Hemmerich >



Photo: AG Schmelcher

### Group Schmelcher

The theory group on 'Fundamental processes in quantum physics' focuses on the structure and dynamics in ultracold trapped systems but also on the development of novel fundamental concepts in quantum physics in general.

#### Group Schmelcher >



### Group Mathey

We investigate ultracold atom and solid-state systems, with emphasis on many-body phenomena such as superfluidity and superconductivity. Our primary research interest is many-body dynamics using novel theoretical concepts for quantum dynamics.

Group Mathey >



### Group Schnabel

We develop lasers for squeezed and entangled light and research new technologies for gravitational-wave detectors and quantum communication, and address fundamental questions of quantum physics.

Group Schnabel >



#### Group Moritz

We experimentally cool dilute gases to near absolute zero temperature. Here, quantum mechanical behaviour dominates, enabling us to study fundamental phenomena such as superfluidity, matter wave interference and correlated dynamics in highly tuneable model systems.

Group Moritz >



#### Group Sengstock

In our group we use ultracold quantum gases to study various kinds of interacting many-body systems, phenomena related to topology and hybrid quantum systems.

Photo: AG Sengstock Group Sengstock >



# Institute of Laser Physics





# Projects in Sengstock's group

#### $V_0(E_R)$ Unconventional superfluids in higher bands BEC J. Simonet / K. Sengstock Explore new orbital states. B Find new paths to higher bands. Interaction-induced topological properties. $\varepsilon(k)/E_{ m rec}$ $y/|\mathbf{a}_2|$ -0.5 -7.5 1 -1 -0.5 0.5 0 -1 $x/|\mathbf{a}_2|$ $x/|\mathbf{a}_2|$ $x/|\mathbf{a}_2|$ $k_x/|\mathbf{b_1}|$

### **Ultrafast & Ultracold**

J. Simonet / M. Drescher / K. Sengstock

- Instantaneous creation of ions and photoelectrons.
- Hybrid quantum systems.
- Cold electron wave-packets.
- Ultracold plasma.
- Coherence transfer in quantum matter.



# Projects in Sengstock's group



# **Optical Lattices and Artificial Gauge Potentials**

Some model Hamiltonians in solid state physics are still unsolved

$$\widehat{H} = -J \sum_{\langle ll' \rangle, \sigma} \widehat{a}_{l,\sigma}^{+} \widehat{a}_{l',\sigma} + \frac{U}{2} \sum_{l,\sigma} \widehat{n}_{l,\sigma} (\widehat{n}_{l,\sigma} - 1)$$

Numerical simulation Scales exponentially in size with N State of the art: 40 electrons Cold atoms simulator



Build up the Hamiltonian



"Look" at the ground state





# **Optical Lattices and Artificial Gauge Potentials**

## Part 1: Build up the Hamiltonian

Optical Lattices Non-interacting properties (band structure, wave functions) Hubbard models

### Part 2: Read out the quantum state

Probing quantum gases in optical lattice Mapping phase diagrams of Hubbard models

### Part 3: Beyond Hubbard models in optical lattices

Topological properties and transport Magnetic phenomena for neutral atoms

## Cold atoms simulator



# Optical Lattices and Artificial Gauge Potentials Part 1: Build up the Hamiltonian

Part 1

1.1 Periodic potentials from standing light waves

1.2 Bloch theorem and Bloch functions (single-particle properties)

1.3 Wannier functions and Hubbard models *(interacting gases)* 

## **1.1 Periodic Potentials from Standing Light Waves**

## **Optical Dipole Traps / Semi-classical description**



Far detuned laser + spatially varying intensity: Conservative trap

# **Optical Dipole Traps / Trapping Potential**

• Gaussian profile of a laser beam

$$I(x, y, z) = \frac{2P}{\pi W^2(z)} e^{-2(x^2 + y^2)/W^2(z)}$$

$$W(z) = W_0 \sqrt{1 + z^2/z_R^2} \quad z_R = W_0^2 \pi / \lambda$$

- Optical dipole potential of 1 beam
  - » Taylor expansion around the center

$$V(x, y, z) \approx -V_{\rm dip}^0 \left(1 - \frac{x^2 + y^2}{W_0^2/2} - \frac{z^2}{z_R^2}\right) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$$

- » Weak confinement in z direction ( $z_R \gg W_0$ )
- Crossed dipole trap
  - » Confinement in all dimensions
  - » Typical values:  $\omega \approx 1 \text{Hz}...3 \text{kHz}, \ V_{\text{dip}}^0/k_B \approx 10 \text{nK}...1 \text{mK}$
  - » Gravitational sag non negligible





# **Optical Lattices**

- 1D lattice
  - Each lattice site is a quasi-2D system (pancake-shaped, many particles per disc)
- 2D lattice
  - Each lattice site is a quasi-1D system (cigar shaped, many particle per tube)
- 3D lattice
  - » Each lattice site is a OD system (one or few particles per site)
- Perfect Lattices
  - » No defects (starting from perfect wave fronts)
  - » No phonons
  - » Typical values: 30 sites per dimensions, 10<sup>5</sup> atoms
- Weak external confinement (Gaussian lattice beams)  $V_C = \frac{1}{2}m\omega_x^2 x^2 + \frac{1}{2}m\omega_y^2 y^2 + \frac{1}{2}m\omega_z^2 z^2$



# **Optical Lattices / Beyond retro-reflection**

- Super-lattices
  - » Superposition of several lattices

(e.g. lattices with orthogonal polarization or different frequency)

- » 1D: Lattice of tunable double wells
- » 2D: Kagomé lattice (2 triangular lattices)
- Optical lattices in d dimensions
  - » Interference pattern of *d*+1 beams is independent of the laser phases, only global translation
  - » Interferences between more than d+1 beams: tunable lattice geometry

Grynberg et al., PRL 70, 2249 (1993)

- Aim
  - » Getting closer to the complexity of solid state crystals
  - » New physical properties: Dirac points, flat bands,...
  - » New probing protocols



# **Bloch theorem**

Non-interacting particle in an optical lattice (1D Schrödinger equation)

$$\left(\frac{\hat{p}^2}{2m} + V(x)\right)\psi(x) = E\psi(x)$$

- » Periodic lattice potential: V(x) = V(x+a)
- **»** Lattice vector:  $\mathbf{a} = (a, 0, 0)$
- » Reciprocal lattice vector  $\mathbf{G} = (G,0,0)$  with  $G = 2\pi/a$
- Bloch theorem for periodic potentials  $\psi_q^{(n)}(x) = e^{iqx}u_q^{(n)}(x)$ 
  - » with cell-periodic functions  $u_q^{(n)}(x)$  on [-a/2, a/2)
  - » Quasi momentum q  $-G/2 \le q \le G/2$
  - » Band index n



## **Eigenvalues / Band structure**

- Expand the periodic function  $u_q^{(n)}(x)$  as Fourier sum in (discrete) plane wave  $\psi_q^{(n)}(x) = e^{i\tilde{q}Gx} \sum_k c_k e^{ikGx}$ with dimensionless quasi momentum  $\tilde{q} = q/G$ ,
  reciprocal lattice vector  $G = 2\pi/a$  and Bloch coefficients  $c_k^{(n)}$
- Periodic potential as Fourier sum  $V_P(x) = \sum_m \nu_m e^{imGx}$
- Insert the Fourier sum into the Schrödinger equation  $\left(-\frac{\hbar^2}{2m\partial x^2}+V(x)\right)\psi_q^{(n)}(x) = E_q^{(n)}\psi_q^{(n)}(x)$   $\sum_k \left[\frac{\hbar^2 G^2}{2m}(k+\tilde{q})^2 c_k e^{i(k+\tilde{q})Gx} + e^{i\tilde{q}Gx}\sum_m c_k\nu_m e^{i(k+\tilde{q}+m)Gx}\right] = E_q^{(n)}\sum_k c_k e^{i(k+\tilde{q})Gx}$ by equating coefficients to  $e^{i(k+\tilde{q})Gx}$  we obtain  $\frac{\hbar^2 G^2}{2m}(k+\tilde{q})^2 c_k + \sum_m c_{k-m}\nu_m = E_q^{(n)}c_k$
- Eigenvalue equation for the coefficients

$$4E_{\rm R}(k+\tilde{q})^2c_k + \sum_m c_{k-m}\nu_m = E_q^{(n)}c_k \qquad E_R = \frac{\hbar^2 G^2}{8m} = \frac{\hbar^2}{8ma^2}$$

• Fourier coefficients for optical lattice potential

 $V(x) = -V_0 \cos^2(\pi x/a) \implies \nu_0 = -V_0/2, \quad \nu_{\pm 1} = -V_0/4 \quad \text{(the others vanish)}$  $\implies [4(k+\tilde{q})^2 - \frac{\tilde{V}_0}{2}]c_k - \frac{\tilde{V}_0}{4}c_{k-1} - \frac{\tilde{V}_0}{4}c_{k+1} = \tilde{E}_{\tilde{q}}c_k \quad \text{with } \tilde{E}_{\tilde{q}} = \frac{E_{\tilde{q}}}{E_R}, \tilde{V}_0 = \frac{V_0}{E_R}$ 

• Matrix equation can be calculated numerically (  $k=-k_0,...,k_0$  ,  $k_0\approx 5$  ) as eigenvalue equation for each  $\tilde{q}$  in units of  $E_{\rm R}$ 

$$\begin{pmatrix} 4(\tilde{q}-2)^2 & -\frac{\bar{V}_0}{4} & 0 & 0 & 0\\ -\frac{\tilde{V}_0}{4} & 4(\tilde{q}-1)^2 & -\frac{\tilde{V}_0}{4} & 0 & 0\\ 0 & -\frac{\bar{V}_0}{4} & 4(\tilde{q})^2 & -\frac{\bar{V}_0}{4} & 0\\ 0 & 0 & -\frac{\bar{V}_0}{4} & 4(\tilde{q}+1)^2 & -\frac{\bar{V}_0}{4}\\ 0 & 0 & 0 & -\frac{\bar{V}_0}{4} & 4(\tilde{q}+2)^2 \end{pmatrix} \mathbf{c} = (E_{\tilde{q}} + \frac{\bar{V}_0}{2}) \mathbf{c}$$

- Block diagonal matrix
  - » Optical lattice couples plane waves that differ by  $G = \frac{2\pi}{a} = 2k_L$
  - » Bragg transition from the two beams forming the standing wave yields momentum transfer  $k_1 k_2 = 2k_L$



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Figure: courtesy Dirk-Sören Lühmann

# **Eigenvectors / Bloch coefficients**

• Eigenvectors

$$\psi_q^{(n)}(x) = e^{i\tilde{q}Gx} \sum_k c_k e^{ikGx}$$

- Bloch coefficients versus lattice depth
  - Weak lattice: only one momentum, free space solution
  - Deep lattice: many momenta, more localized in real space
- Bloch wave functions at  $q=\pi/a$ 
  - » Wave function localized at  $q=\pi/a$  (QM expectation value)
  - » Tunneling  $(x \rightarrow x + a)$ :

Wave function acquires a phase of  $\boldsymbol{\pi}$ 



Figures from: Dalibard, cours CdF 2013. Greiner PhD Thesis , Munich (2003)

# **1.3 Wannier Functions and Hubbard Model**



Let us add ultracold gases

- What about quantum statistics? Ground state for bosons & fermions?
- What about interactions?

Potential created by standing light wave

C Atoms



# Wannier functions / Definition

- Bloch functions
  - » Orthonormal basis of eigenvalues of the single-particle Hamiltonian
  - » Completely delocalized over the lattice
- Ultracold quantum gases
  - » Local interactions between particles (on a lattice site)
  - » Best described in a basis localized in space!
- Wannier functions
  - » New orthonormal basis, maximally localized to individual lattice sites
  - » Wannier function at site  $x_j$ :  $\omega_{n,j}(x) = \left(\frac{a}{2\pi}\right)^{1/2} \int_{-\pi/a}^{+\pi/a} \psi_{n,q}(x) e^{-ijaq} dq$

• Inverse transformation:  $\psi_{n,q}(x) = \left(\frac{a}{2\pi}\right)^{1/2} \sum_{j \in Z} \omega_{n,0}(x - ja) e^{ijaq}$ 

# Wannier functions / Properties

- Wannier functions for the lowest band for increasing lattice depth
  - » Localization in space for large lattice depth  $V_0/E_r = (0, 0.5, 1, 2, 4, 8, 12, 16, 20)$
  - Orthonormal basis lattice sites
     (dashed blue line: Wannier function
     on the neighboring site )
- Wannier functions for higher bands
  - » Orthogonal to each other
  - » Similar to harmonic oscillator (nodes, alternating parity)





Figures: Dalibard, cours CdF 2013. Fölling PhD Thesis, Mainz (2008)

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1 -1

 $|\varphi_2\rangle'$ 

0

 $x/|\mathbf{a}_2|$ 

1

0.5

0

-1 -1

-0.5

 $y/|\mathbf{a}_2|$ 

» Similar to harmonic oscillator (nodes, alternating parity)

 $\langle \varphi_4 \rangle'$ 

0

 $x/|\mathbf{a}_2|$ 

1 -1



Figures: Dalibard, cours CdF 2013. Fölling PhD Thesis, Mainz (2008)

• Single-particle Hamiltonian in the Bloch basis

$$H = \sum_{n} \int_{-\pi/a}^{+\pi/a} dq E_n(q) |\psi_{n,q}\rangle \langle \psi_{n,q}| = \sum_{n} \int dq E_n(q) \hat{a}_{n,q}^{\dagger} \hat{a}_{n,q}$$

- Annihilation operators
  - »  $\hat{a}_{n,q}$  : Annihilation operator for particle in Bloch wave  $\psi_{n,q}$
  - »  $\hat{b}_{n,j}$ : Annihilation operator for particle in Wannier function  $\omega_{n,j}(x)$  $\hat{a}_{n,q} = \left(\frac{a}{2\pi}\right)^{1/2} \sum_{j} e^{ijaq} \hat{b}_{n,j}$
- Single-particle Hamiltonian in Wannier basis

$$\widehat{H} = \sum_{n} \sum_{j,j'} J_n(j-j') \widehat{b}_{n,j}^{\dagger} \widehat{b}_{n,j'}$$

• Tunneling between lattice sites

 $J_n(j-j')$ : matrix element of the Hamiltonian coupling two Wannier functions

$$J_{n}(j) = \int \omega_{n,j}^{*}(x) \left(\frac{\hat{p}^{2}}{2m} + V(x)\right) \omega_{n,0}(x) dx = \frac{a}{2\pi} \int_{-\pi/a}^{+\pi/a} dq E_{n}(q) e^{ijaq}$$

• The hopping amplitude is given by the overlap of the Wannier functions

$$J_n(j) = \int \omega_{n,j}^*(x) \left(\frac{\hat{p}^2}{2m} + V(x)\right) \omega_{n,0}(x) dx$$

- For increasing lattice depth, the Wannier functions become more localized and the hopping amplitude drops exponentially
- Hopping over longer distances is much weaker and can be neglected (smaller than 1% of the next-neighbor hopping for  $V_0 \gtrsim 10E_r$ )



# Hubbard Model / Definition

- Hubbard Model (deep lattices)
  - » Restriction to the lowest band(band index dropped from now on)
  - » Only next neighbor hopping J



Potential created by standing light wave

- Hubbard Hamiltonian  $\widehat{H} = -J \sum_{j} \widehat{b}_{j+1}^{\dagger} \widehat{b}_{j} + h.c.$
- Dispersion relation:  $E(q) = -2J\cos(aq)$ 
  - » Width: 1D lattice  $\rightarrow 4J$ , 2D square lattice  $\rightarrow 8J$ , 3D cubic lattice  $\rightarrow 12J$
- Approximate analytic formula for the tunneling
  - » Using the dispersion relation

$$\frac{J}{E_r} \approx \frac{4}{\sqrt{\pi}} \left(\frac{V_0}{E_r}\right)^{3/4} \exp\left[-2\left(\frac{V_0}{E_r}\right)^{1/2}\right]$$

» Exponential decrease with  $\sqrt{V_0/E_r}$ 



Figure: courtesy Dirk-Sören Lühmann

- Bosons (without dipolar interactions)
  - » Short-range interactions of strength g described by pseudo-potential

$$\widehat{H}_{int} = \frac{g}{2} \int \widehat{\Psi}^{\dagger}(x) \widehat{\Psi}^{\dagger}(x) \widehat{\Psi}(x) \widehat{\Psi}(x) dx \qquad \widehat{\Psi}(x) = \sum_{n,j} \omega_{n,j}(x) \widehat{b}_{n,j}$$

- » Simplify to on-site interactions in the Hubbard model (lowest band only)  $\widehat{H}_{int} \approx \frac{U}{2} \sum_{i} \widehat{n}_{j} (\widehat{n}_{j} - 1)$  with number operator  $\widehat{n}_{j} = \widehat{b}_{j}^{+} \widehat{b}_{j}$
- » Interaction energy of two particles on one lattice site  $U = g \int \omega_{0,j}^4(x) dx$
- » Analytical expression (Wannier function approximated by a Gaussian function)

$$U^{3D} = \frac{g^{3D}}{\left(\sqrt{2\pi}a_{ho}\right)^3} = \sqrt{\frac{8}{\pi}} k a_d \left(\frac{V_0}{E_r}\right)^{3/4} E_r \qquad g^{3D} = \frac{4\pi\hbar^2 a_d}{m}$$

• Spin-1/2 fermions (similar description)

$$\widehat{H}_{int} \approx U \sum_{j} \widehat{n}_{j,\uparrow} \widehat{n}_{j,\downarrow}$$



: Atoms

Potential created by standing light wave • Ultracold atoms in optical lattices are well descriped by Hubbard models

\* Bosons 
$$\widehat{H} = -J \sum_{j} \widehat{b}_{j+1}^{\dagger} \widehat{b}_{j} + h.c. + \frac{U}{2} \sum_{j} \widehat{n}_{j} (\widehat{n}_{j} - 1)$$



$$\widehat{H} = -J \sum_{j} \widehat{b}_{j+1}^{\dagger} \widehat{b}_{j} + h.c. + U \sum_{j} \widehat{n}_{j,\uparrow} \widehat{n}_{j,\downarrow}$$



Contraction

Potential created by standing light wave

• The Hubbard parameters *J* and *U* can be tuned via the lattice depth

• Phase diagram in the Hubbard model?



# **Bose-Hubbard Model**

- Superfluid phase
  - » Tunneling dominates

Minimization of the kinetic energy

- Delocalized in space, localized in momentum space
   "BEC in the lattice"
- » Coherent state on each lattice site (number fluctuations)



- Mott insulating phase
  - » Interactions dominate

Minimization of  $\frac{U}{2}\sum_{i}\hat{n}_{i}(\hat{n}_{i}-1)$ 

» Localized in real space, delocalized in momentum space

Number state on each lattice site

- » Gapped excitation spectrum
- » Incompressible  $\frac{\partial N}{\partial \mu} = 0$

Figure: Lühmann, PhD thesis, Hamburg (2009)

# **Bose-Hubbard Model / Non-interacting Superfluid**

- For *U*=0: superfluid phase
  - » BEC in the lowest Bloch state q=0

$$|\Psi_{\rm SF}\rangle = \frac{1}{\sqrt{N!}} \left(\hat{b}_{q=0}^{\dagger}\right)^N |0\rangle$$

» Rewriting in the Wannier basis yields

$$\phi_{q=0}^{(0)}(x) = \frac{1}{\sqrt{N_s}} \sum_j w^{(0)}(x - R_j)$$

(sum over j: ,coherence between all lattice sites')

- Coherent approximation
  - » Basis change

$$\hat{b}_{q=0}^{\dagger} = \frac{1}{\sqrt{N_s}} \sum_i \hat{b}_i^{\dagger} \quad \text{yields} \quad |\Psi_{\text{SF}}\rangle = \frac{1}{\sqrt{N!}\sqrt{N_s}^N} \left(\sum_i \hat{b}_i^{\dagger}\right)^N |0\rangle \approx \prod_i |\alpha\rangle_i$$

» At each site a coherent state

$$\begin{split} |\alpha\rangle_i &= \sum_{n=0}^\infty \sqrt{e^{-\bar{n}} \frac{\bar{n}^n}{n!}} \, |n\rangle_i \\ \text{with } |\alpha|^2 &= \bar{n} = N/N_s \end{split}$$

i.e. the square of the coefficients follows a Poisson distribution!

» Eigen state to the annihilation operator  $\hat{b}_i \left| \alpha \right\rangle_i = \alpha \left| \alpha \right\rangle_i$ 



# **Bose-Hubbard Model / Mott Insulator**

- Named after N. F. Mott, Nobel prize 1977 "for their fundamental theoretical investigations of the electronic structure of magnetic and disordered systems"
- For J=0 ("atomic limit") and repulsive U
  - » Double and multiple occupation energetically unfavorable!
  - » At each lattice site exactly n particles , state  $\ |n\rangle_i$
  - » Fluctuations  $\langle \hat{b}_i \rangle = \langle n |_i \, \hat{b}_i \, | n \rangle_i = 0$
  - » Manybody wave function  $|\Psi_{\rm MI}\rangle = \left(\prod_i \frac{1}{\sqrt{n!}} b_i^{\dagger n}\right) |0\rangle$
- Quantum phase also exists for finite J
  - » Correlated state with finite fluctuations between next neigbours  $\langle \hat{b}_j^{\dagger} \hat{b}_i \rangle \neq 0$ , but  $\langle \hat{b}_j^{\dagger} \hat{b}_i \rangle$  decays exponentially with the distance i j
  - » Ground state has an energy gap of size U





Sir Nevill Francis Mott



## **Bose-Hubbard Model / Phase diagram**

