Advanced Quantum Mechanics

Tutorials 2024–2025

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Please ask me MANY questions!

Wednesday, November 13th, 2024

Homework: BCS theory

The homework is not mandatory, it will not be marked

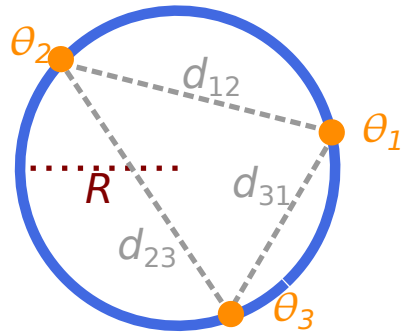
If you wish to do so, hand in a complete or partial solution at your convenience

before or on Sunday, December 22nd, 2024

so as to benefit from my correction and advice.

Rydberg atoms: chaos & semiclassical physics

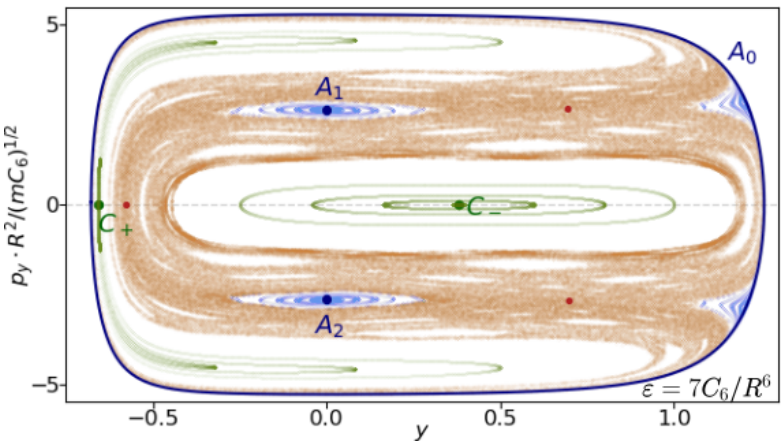
- **Non–ergodicity** of 3 **interacting** Rydberg atoms in a circular trap



This conceptually simple system is **experimentally accessible**
due to recent progress in Rydberg atom trapping in Paris and Palaiseau

[D.J. Papoular & B. Zumer, Phys. Rev. A **107**, 022217 (2023)]

[D.J. Papoular & B. Zumer, Phys. Rev. A **110**, 012230 (2024)]



Two mechanisms impeding ergodicity in the absence of disorder:

1. quantum mechanism: **quantum scar** [Heller PRL 1984]
2. classical mechanism: **KAM tori** (**K**olmogorov, **A**rnold, **M**oser)
   [Arnold, *Mathematical Methods of Classical Mechanics*, Springer (1989)])

Both mechanisms yield quantum eigenstates
localised near classical periodic trajectories

- Telling them apart requires a detailed understanding of the **classical system** and accurate **numerical calculations** of the quantum eigenstates (not ground state!)
- **Semiclassical analysis** which goes beyond the WKB approach

Gutzwiller's trace formula, Einstein–Brillouin–Keller theory

[M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics*, Springer (1990)]

Spontaneous applications for a PhD position with me are welcome

Outline of the tutorials for the first half ot the semester

- **Problem 1:** two–particle interference
- **Problem 2:** coherence and correlations in quantum gases
- **Problem 3:** lattice models, superfluid/Mott insulator transition

All problems describe experiments that have actually been performed

They all contain elements of theory and introduce calculation techniques

They all contain both standard questions and (very?) hard questions

A bird's eye view of the problem

Problem #3: Quantum Lattice Models

The Bose–Hubard Hamiltonian

- Brief review of periodic potentials and lattice models

  Bloch's theorem, Bloch and Wannier functions, energy bands

  Hubbard Hamiltonian

- A quantum phase transition: Superfluid to Mott insulator

  Gutzwiller ansatz, mean–field description of the phase transition

- Collapse and revival of coherence

Review: Periodic potentials, lattice models

Mostly single–particle physics (no identical particles)

[Ziman, *Principles of the Theory of Solids*, CUP (1972), §1.4]

[Ashcroft & Mermin, *Solid State Physics*, Harcourt (1976), chap. 8]

Example 1/3: discretised Schrödinger equation

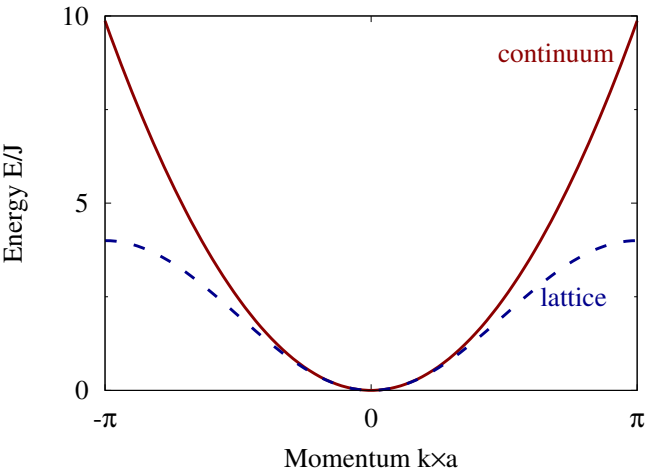
- Start from the 1D Schrödinger equation in continuous 1D space:

$$h\,|\psi\rangle = \varepsilon\,|\psi\rangle \qquad \text{with} \qquad h = +\frac{p^2}{2m} + v(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + v(x)$$

- Sample x every a: $x_n = n\,a$ (a sets the spatial resolution) and keep N values $(x_n)_{1\le n\le N}$

  Finite–Differencing (FD) *approximation*: $\psi''(x_n) \approx [\psi(x_{n+1}) - 2\psi(x_n) + \psi(x_{n-1})]\,/a^2$

$$h_{\mathrm{FD}} = +\frac{\hbar^2}{ma^2}\mathbb{1} - \frac{\hbar^2}{2ma^2}\begin{bmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & \ddots & 1 & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 1 & \ddots & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix} + \begin{bmatrix} v_1 & 0 & 0 & 0 & 0 \\ 0 & \ddots & 0 & 0 & 0 \\ 0 & 0 & \ddots & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & v_N \end{bmatrix}$$



- What are the chosen boundary conditions for h_{FD}?

  Then, for $v_1 = \cdots = v_N = 0$, h_{FD} is a *circulant matrix*

- Free particle dispersion relation:

  $\varepsilon_p^{\mathrm{FD}} = 2J[1 - \cos(k_p a)]$ with $k_p = p\,2\pi/a$, $p \ge 0$ integer

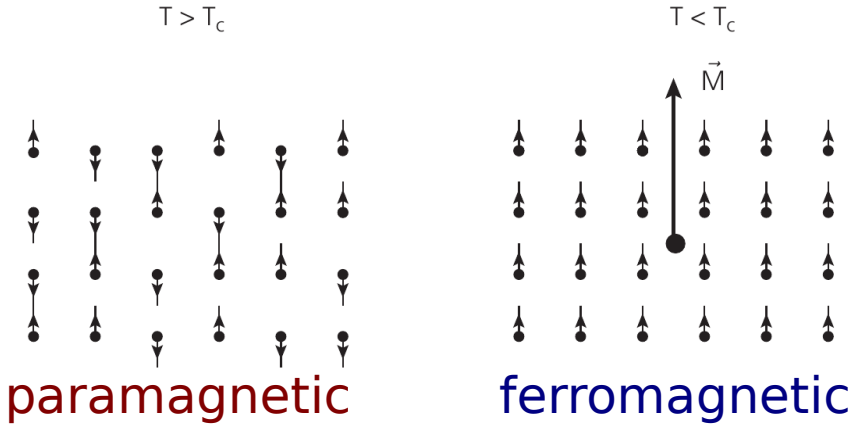
1. For which wavelengths is h_{FD} a good approximation to h?

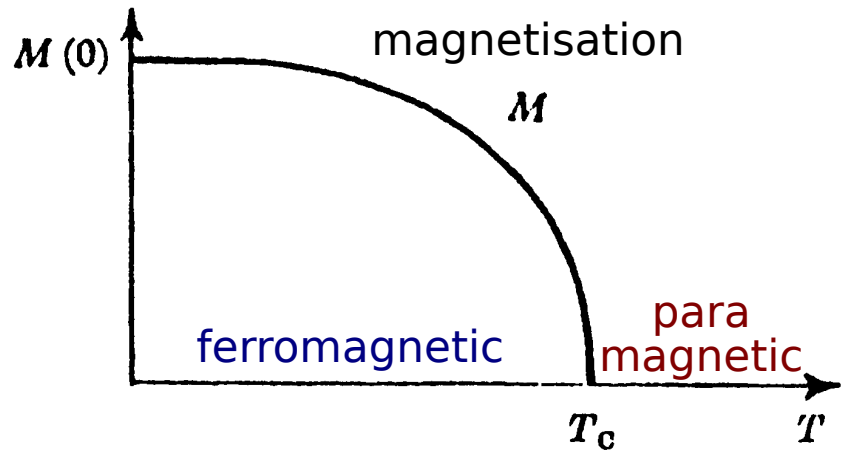
2. Express J in terms of a

Example 2/3: magnetism in a crystal: spin models

- Atomic spins fixed at lattice sites, exchange interaction between nearest neighbours

  Heisenberg Hamiltonian: $H = -J \sum_{\langle \mathbf{l},\mathbf{l}' \rangle} \mathbf{s}_\mathbf{l} \cdot \mathbf{s}_{\mathbf{l}'}$ ($J > 0$ favours ferromagnetism)





- Ordered ferromagnetic phase below the Curie temperature T_c

  The order parameter is the magnetisation $\mathbf{M} = \langle \mathbf{s} \rangle$

  Spontaneous symmetry breaking: $\mathbf{M} = \mathbf{0}$ for $T > T_c$, $\mathbf{M} \neq \mathbf{0}$ for $T < T_c$

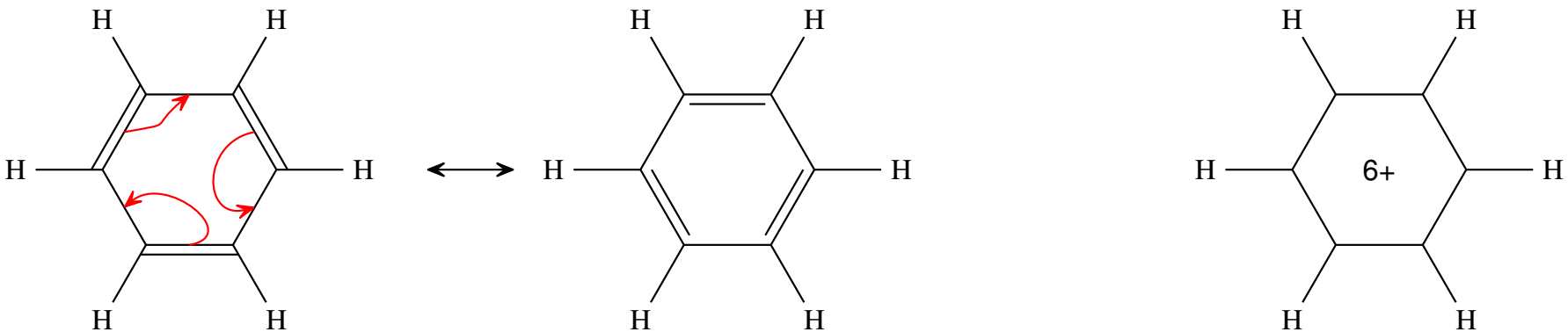
- First–order or second–order phase transition?

- For Bose–Einstein condensation, what plays the role of the magnetisation $\mathbf{M} = \langle \mathbf{s} \rangle$?

Example 3/3: benzene molecule C_6H_6

- Standard picture for the **ground state**:

  Two–state system with different positions for the two double bonds



- More refined picture, allowing for the description of **excited states**:

  Start from molecule without the 3 double bonds: ion charged 6+

  Lattice model: each C atom is a site which may accommodate up to 2 electrons

- What is the dimensionality of this lattice model? Which boundary conditions?

[*Feynman Lectures on Physics,* Basic Books (2010), vol. III, §15.4]

Review: Bloch's theorem for a periodic potential

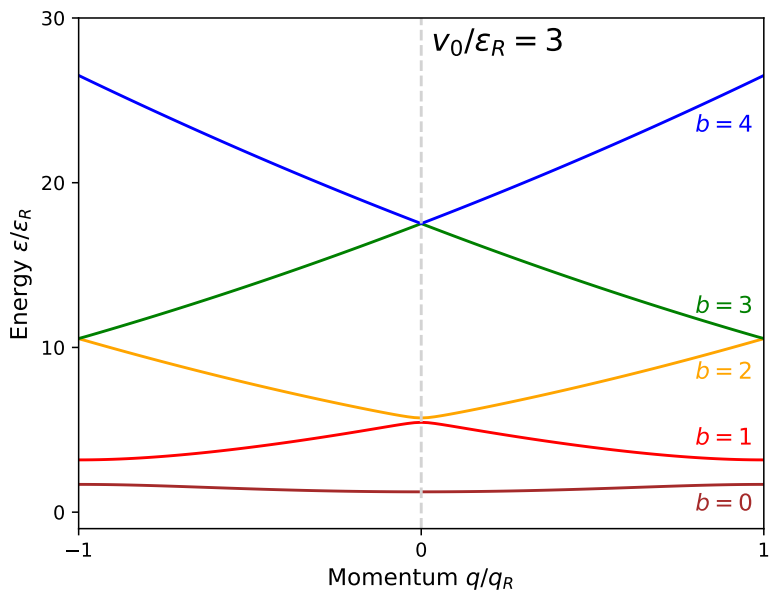
- If the **single–particle** trapping potential $v(\mathbf{r})$ is spatially periodic,
  seek the eigenstates of $h = \mathbf{p}^2/(2m) + v(\mathbf{r})$ as Bloch waves $\psi_{b,\mathbf{q}}(\mathbf{r}) = e^{i\mathbf{q}\mathbf{r}}\, u_{b,\mathbf{q}}(\mathbf{r})$,
  where the function $u_{b,\mathbf{q}}(\mathbf{r})$ has the **same spatial periodicity as the potential** $v(\mathbf{r})$
  The quasi–momenta $\mathbf{q}$ are in the Brillouin zone; the band index b is discrete.

- For example, 1D optical lattice with spatial period a: $v(x) = v_0 \sin^2(\pi\, x/a)$
  Typical scales: recoil momentum $q_R = \pi/a$, recoil energy $\varepsilon_R = \hbar^2 q_R^2/(2m)$:

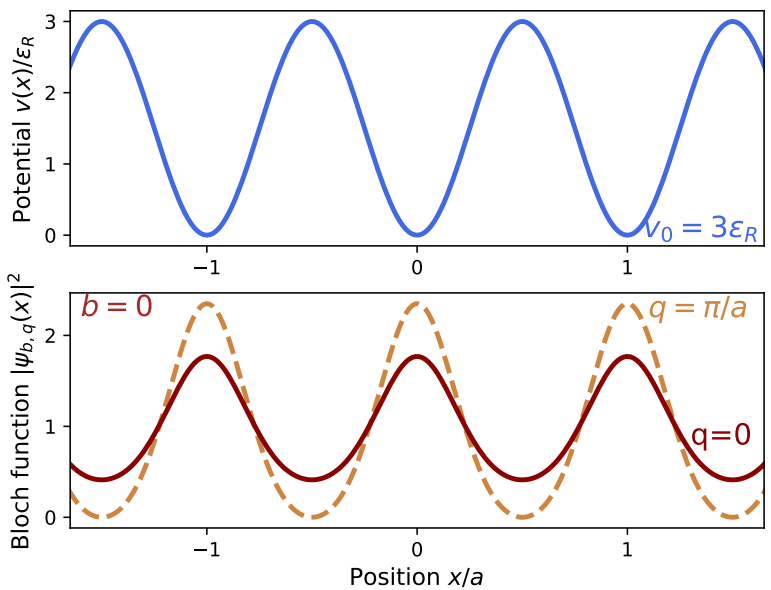
changes in momentum and energy for an atom at rest upon absorbing 1 photon of wavelength $2a$

The energy spectrum $\varepsilon = \hbar^2 q^2/(2m)$ is replaced by one with **band structure**

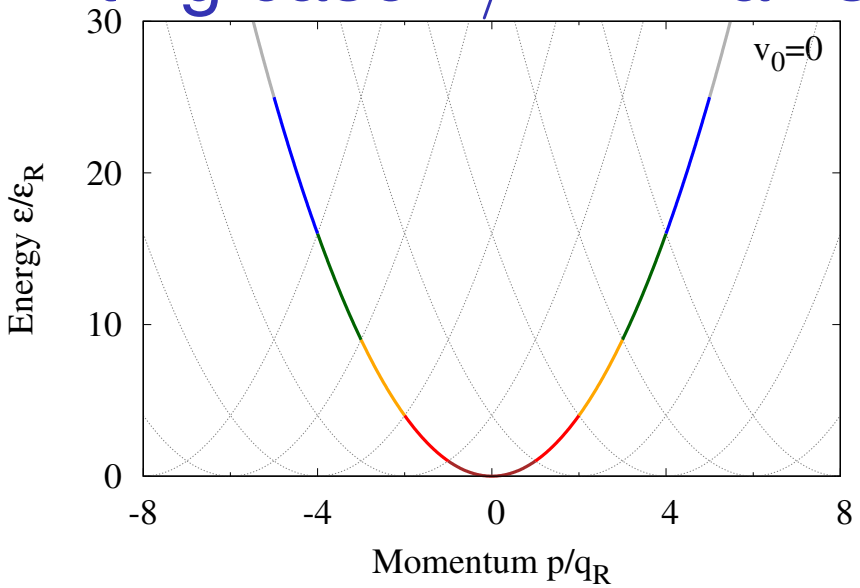
Energy spectrum with band structure

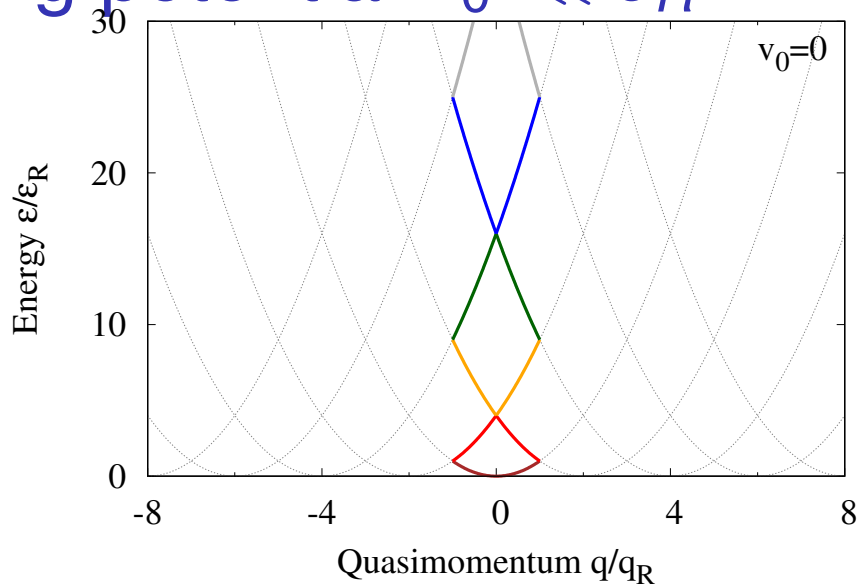


Potential and Bloch functions



Limiting case 1/2: vanishing potential $v_0 \ll \varepsilon_R$





The gray parabolas correspond to $(p - n2\pi/a)^2/(2m)$, n integer, $a =$ spatial period of $v(x)$

- The dispersion relation may be understood in two equivalent ways:

  1. The single complete parabola for a single particle in free space

  defined for all momenta p, single branch ('extended zone scheme')

  2. Dispersion relation for a single particle in a periodic potential $(q_R = \pi/a)$

  quasimomenta in Brillouin zone $-q_R < q \leq q_R$, multiple branches ('reduced zone scheme')

- Express the plane wave e^{ipx} in terms of a Bloch wave $e^{iqx}u_{b,q}(x)$

  HINT: The 'ceiling' integer parts $\lceil p/(2q_R) - 1/2 \rceil$ play a role; $x \leq \lceil x \rceil < x + 1$

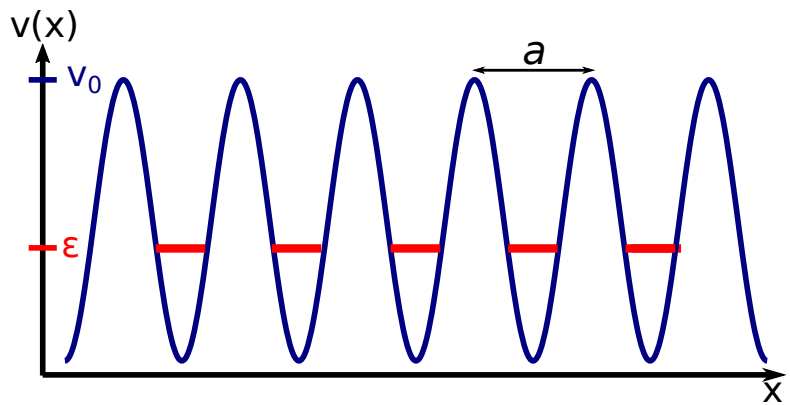
Limiting case 2/2: very deep band $v_0 \gg \varepsilon_0$

- If the energies of all states in the band are much smaller than v_0,

  tunnelling is negligible: all sites are uncoupled 'atomic limit'

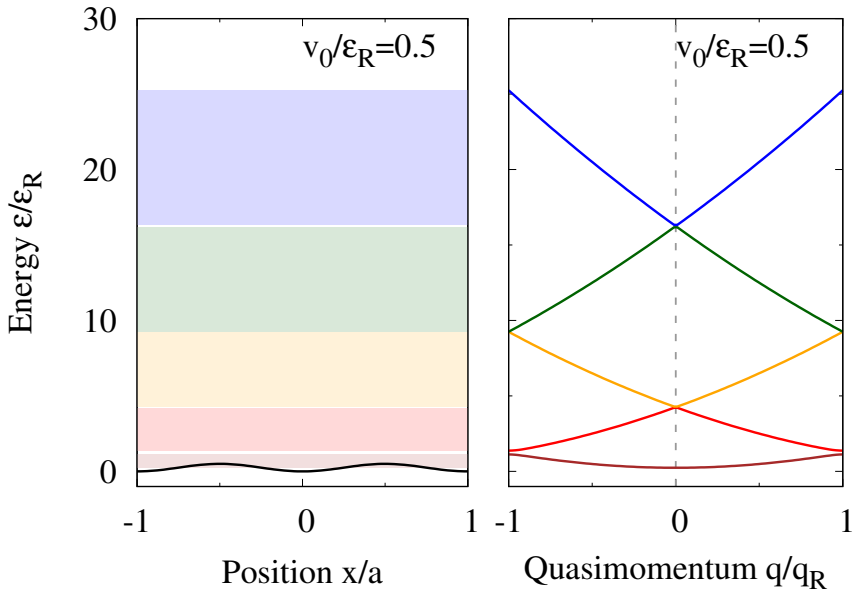
  Each well supports an individual bound state with energy ε_0

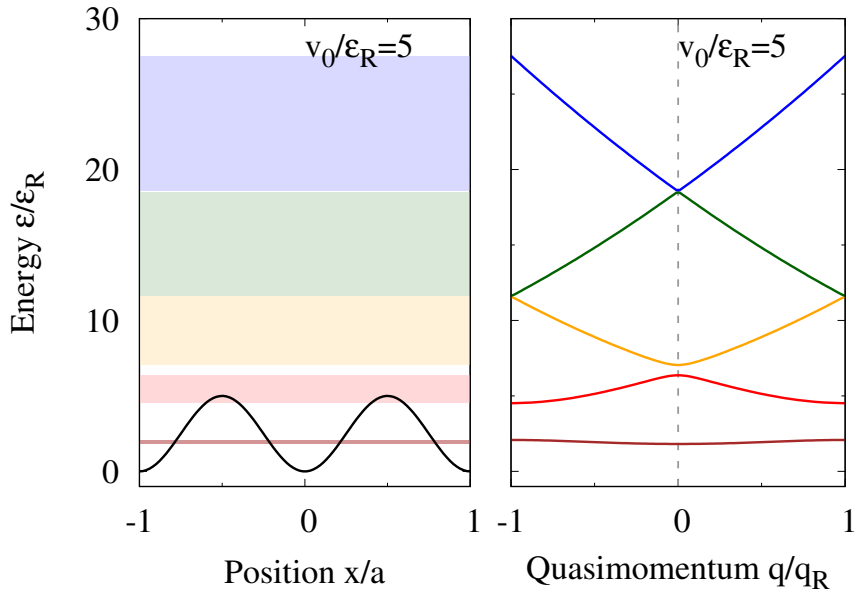
  They are all degenerate and form a flat band

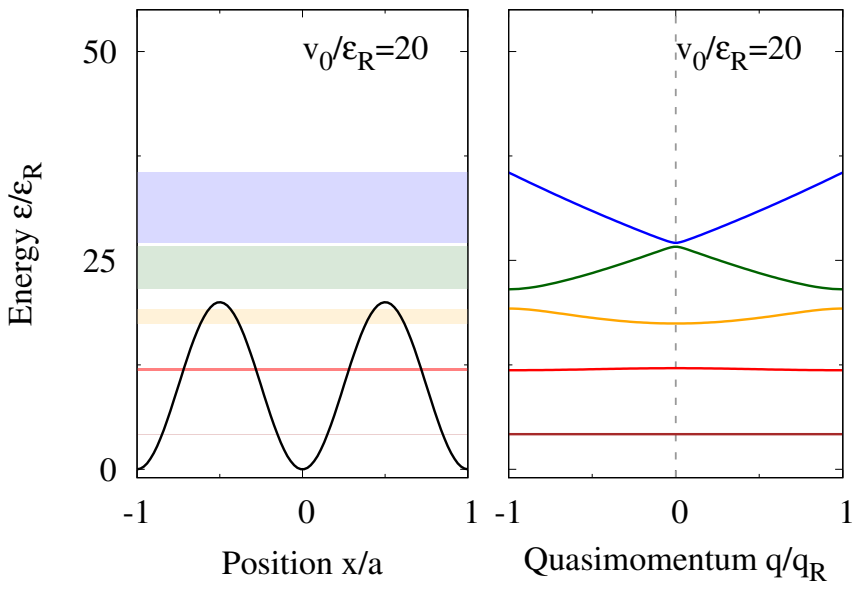


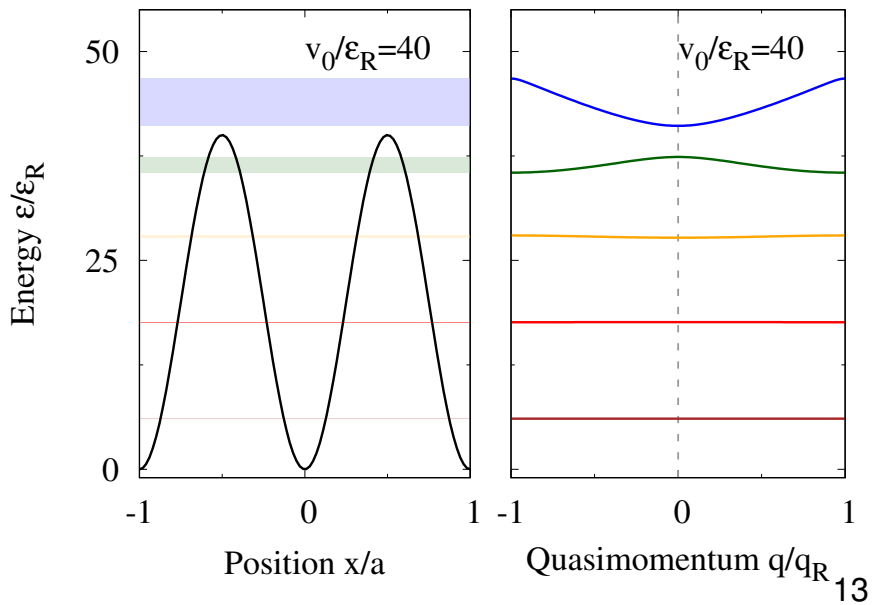
- Write the Bloch function $\psi_{0,q}(x) = e^{iqx} u_{0,q}(x)$ in terms of the single–well state $w_0(x)$

Band structure as a function of the lattice depth









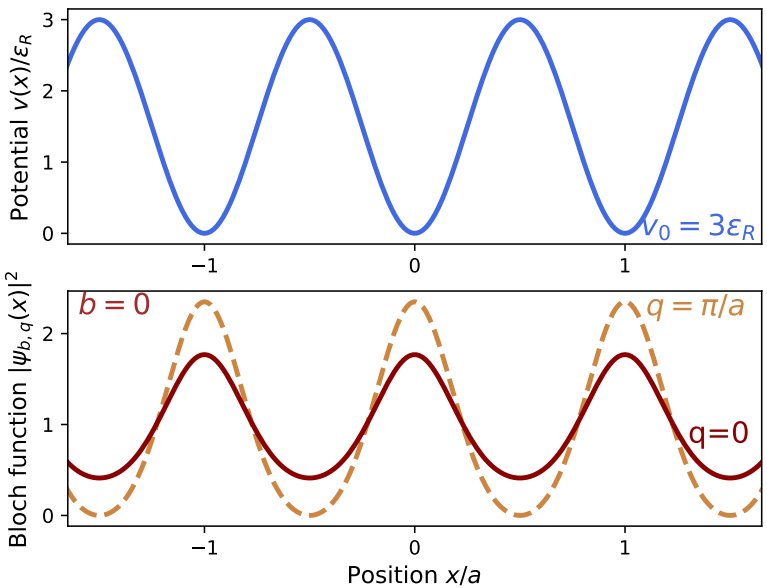
Wannier functions: localised at the lattice sites

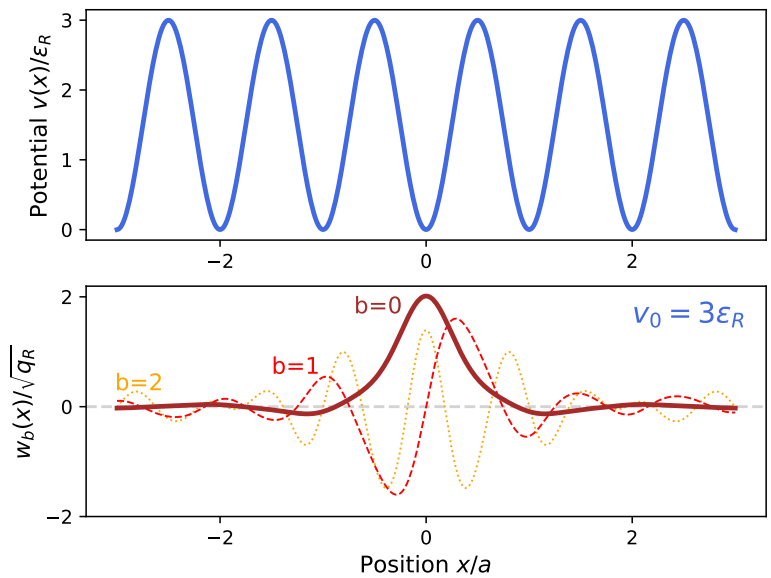
- Free particle: $h = p^2/(2m)$ eigenstates are plane waves $|k\rangle$ with $\langle x|k\rangle = e^{ikx}/\sqrt{2\pi}$

  $|x\rangle = \int dk\ |k\rangle\langle k|x\rangle = \int dk\ |k\rangle\, e^{-ikx}/\sqrt{2\pi}$ is localised, but *not an eigenstate* of h

- Similarly, Wannier functions are sums over all Bloch states **in a given band:**

$$w_{b,j}(x) = \left(\frac{a}{2\pi}\right)^{1/2} \int_{-q_R}^{q_R} dq\ \psi_{b,q}(x)\, e^{-i\,jaq} \quad \text{so that} \quad w_{b,j}(x) = w_{b,0}(x - ja)$$





- The Wannier functions are a normalised basis of single–particle wavefunctions

  For well chosen phases of the Bloch functions, they are localised on the lattice sites

  Beware: they are not Gaussians! their wings change signs

Numerical calculation of Bloch and Wannier functions

- The Bloch wave $\psi_{b,q}(x) = e^{iqx} u_{b,q}(x)$ is defined by two conditions:

1. $\psi_{b,q}$ is an eigenstate of $h = p^2/(2m) + v$:

$$\varepsilon\, \psi_{b,q} = -\hbar^2 \psi''_{b,q}/(2m) + v_0 \sin^2(q_R x)\, \psi_{b,q}$$

2. $u_{b,q}(x)$ is spatially periodic with period a:

expand it into a Fourier **series** involving the plane waves with period a/j:

$$u_{b,q}(x) = \sum_{j\in\mathbb{Z}} c_j \exp\left(i\,\frac{2\pi}{a/j}\,x\right), \qquad \text{so that} \qquad \psi_{b,q}(x) = \sum_{j\in\mathbb{Z}} c_j \exp\left[i\left(q + j\frac{2\pi}{a}\right)x\right]$$

- Combine the two conditions: [recoil momentum $q_R = \pi/a$, energy $\varepsilon_R = \hbar^2 q_R^2/(2m)$]

$$\frac{\varepsilon}{\varepsilon_R}\, c_j \;=\; \left[\left(2j + \frac{q}{q_R}\right)^2 + \frac{v_0}{2\varepsilon_R}\right] c_j \;-\; \frac{v_0}{4\varepsilon_R}(c_{j-1} + c_{j+1})$$

- Eigenvalue problem for real, symmetric, tridiagonal 'infinite matrix'
  Truncate to $|j| \le j_M \sim 20$ coefficients, and diagonalise numerically for given q

- The band structure, Bloch functions, and Wannier functions shown today have been calculated and visualised with a Python script of $\sim$ 200 lines

[Bloch & Greiner, Adv. At. Mol. Opt. Phys. **52**, 1 (2005), Sec. 3.1]

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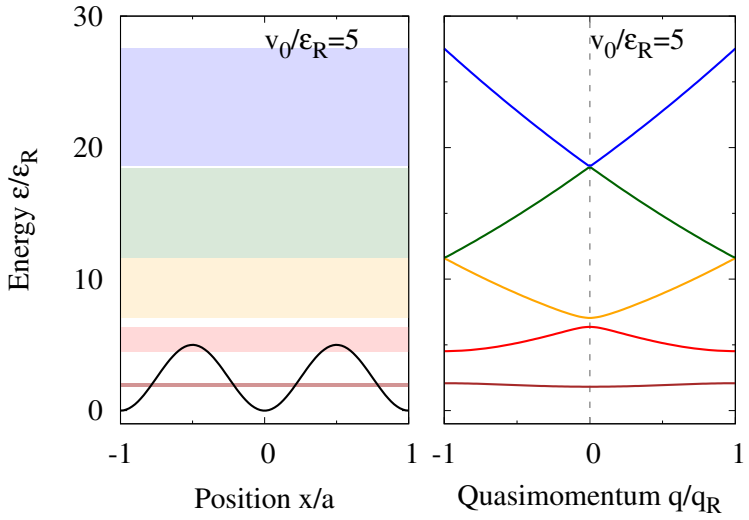
Wednesday, November 20$^{\text{th}}$, 2024

Summary: band structure, Bloch & Wannier functions



- If the potential is spatially periodic,

  e.g. $v(x) = v_0 \sin^2(\pi x/a)$ (1D optical lattice)

  the dispersion relation within the first Brillouin zone exhibits band structure

- Eigenstates may be sought as **Bloch waves** $\psi_{b,q}(x) = e^{iqx}\, u_{b,q}(x)$

  where the band function $u_{b,q}(x)$ has the same spatial periodicity as the potential

  They satisfy $\psi_{b,q}(x+a) = e^{iqa}\, \psi_{b,q}(x)$ and extend over the whole lattice

- **Wannier functions:** basis of normalised wavefunctions which are NOT eigenstates

  $$w_{b,j}(x) = \left(\frac{a}{2\pi}\right)^{1/2} \int_{-q_R}^{q_R} dq\, \psi_{b,q}(x)\, e^{-ijaq} \quad \text{so that} \quad w_{b,j}(x) = w_{b,0}(x - ja)$$

  The Wannier function $w_{b,n}$ is a linear combination of all Bloch functions of band b

- Bloch and Wannier functions play the roles of $|p\rangle$ and $|x\rangle$ states for a free particle

The Hubbard model

It is the simplest model

for identical bosons or fermions on a lattice

in the presence of interactions

Bosons: [Cohen–Tannoudji & Guéry–Odelin, *Advances in Atomic Physics*, World Scientific (2011), §26.3]

Fermions: [Georges, *Condensed Matter Physics with Light and Atoms*, in Proceedings of the Varenna School of Physics Enrico Fermi CLXIV, IOS (2007)]

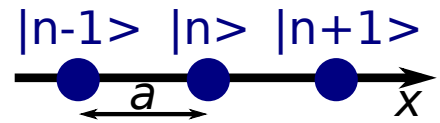
The single–band approximation: **Hubbard model**

- 1D lattice with the spatial period a: discrete sites at positions $x_n = n\,a$

  The discrete sites are represented by the single–particle states $\{|n\rangle\}$

  A particle may hop from site $|n\rangle$ to one of its 2 nearest neighbours: $|n-1\rangle$ or $|n+1\rangle$

$$h \;=\; -J \sum_{n=1}^{N_l} \left(\,|n-1\rangle\langle n| \;+\; |n+1\rangle\langle n| \,\right)$$



Possible geometries: infinite 1D lattice or ring (see next slide)

- Look for eigenstates of h in the form of Bloch waves $\psi_{b,q}(x) = e^{iqx}\,u_{b,q}(x)$

  $u_{b,q}(x)$ has period a and it is sampled every a therefore it is constant:

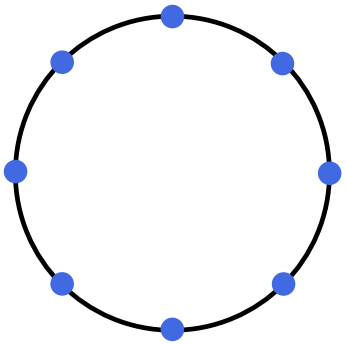
$$\psi_q(x_n) = \frac{e^{inqa}}{\sqrt{N_l}} \quad \text{or equivalently:} \quad |\psi_q\rangle \;=\; \frac{1}{\sqrt{N_l}} \sum_{n=1}^{N_l} e^{inqa}\,|n\rangle \qquad (N_l = \text{number of sites})$$

- The Hubbard model supports a single band

  It is applicable if both temperature and interaction energy $\ll$ band spacing

  This requires a lattice which is deep enough: $v_0 \gtrsim \varepsilon_R$ $\left(\varepsilon_R = \dfrac{\hbar^2 k_R^2}{2m},\; k_R = \dfrac{\pi}{a}\right)$

Hubbard model: number of independent states



- N_l sites on a line with periodic boundary conditions

  that is, N_l sites on a ring

- 'Plane–wave' states: $|\psi_q\rangle = \frac{1}{\sqrt{N_l}} \sum_{n=1}^{N_l} e^{inqa} |n\rangle$

All $|\psi_q\rangle$ are actually Bloch states belonging to the same band with $u_b(x) = 1$

The number of independent states $|\psi_q\rangle$ is determined by two effects:

1. Periodic boundary conditions: $\langle N_l|\psi_q\rangle = \langle 0|\psi_q\rangle$, so that $q = \frac{p}{N_l}\frac{2\pi}{a}$ (p integer)

2. Bloch wave structure: $\langle n+1|\psi_q\rangle = e^{iqa}\langle n|\psi_q\rangle$

q and $q + 2\pi/a$ yield the same Bloch state: the independent values of q are chosen in Brillouin Zone

- Combining the two conditions, we find N_l independent values of q

  For instance, one may choose $q = \frac{p}{N_l}\frac{2\pi}{a}$ with $0 \leq p < N_l$

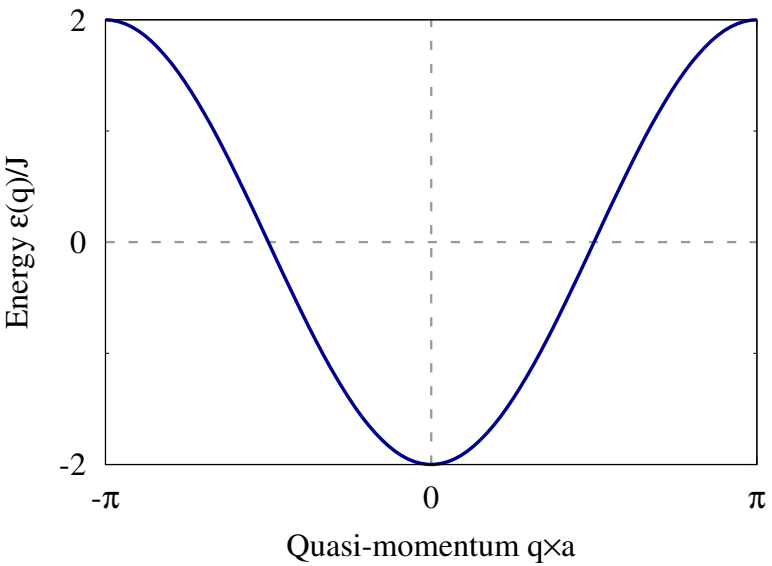
With a **single band,** there are as many Bloch states $|\psi_q\rangle$ as there are sites

Hubbard model: 1–particle dispersion relation (qu. 5)

$$h = -J \sum_{n=1}^{N_l} \left(|n-1\rangle\langle n| + |n+1\rangle\langle n| \right) \quad \text{and} \quad |\psi_q\rangle = \frac{1}{\sqrt{N_l}} \sum_{n=1}^{N_l} e^{inqa} |n\rangle$$

- Act with h on $|\psi_q\rangle$ to get the corresponding energy:

$$\begin{aligned} h|\psi_q\rangle &= -J \sum_n (|n-1\rangle\langle n| + |n+1\rangle\langle n|) \frac{1}{\sqrt{N_l}} \sum_m e^{imqa} |m\rangle \\ &= -\frac{J}{\sqrt{N_l}} \sum_n e^{inqa} (|n-1\rangle + |n+1\rangle) \\ &= -J\, e^{iqa} \left(\frac{1}{\sqrt{N_l}} \sum_n e^{i(n-1)qa} |n-1\rangle \right) - J\, e^{-iqa} \left(\frac{1}{\sqrt{N_l}} \sum_n e^{i(n+1)qa} |n+1\rangle \right) \end{aligned}$$



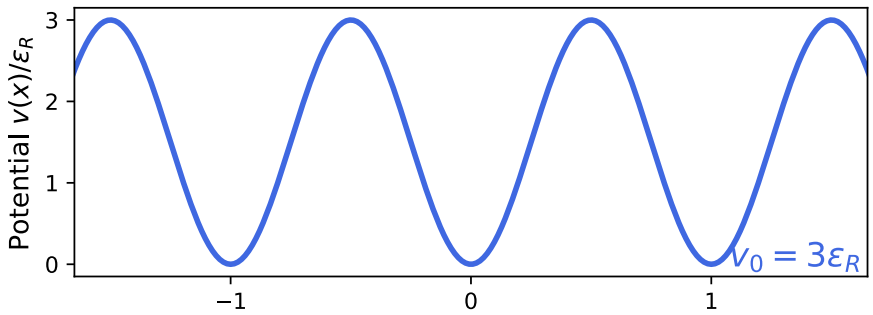
Thanks to the periodic boundary condition:

$$h|\psi_q\rangle = -J(e^{iqa} + e^{-iqa})|\psi_q\rangle = -2J\cos(qa)\,|\psi_q\rangle$$

$$\varepsilon(q) = -2J\cos(qa)$$

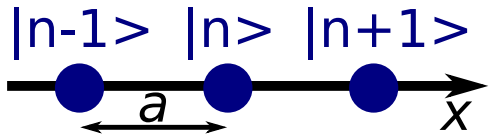
From the full lattice Hamiltonian to the Hubbard model

- Spatially periodic lattice potential:



$$h = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + v(x)$$

- Single–band Hubbard approximation:



$$h_{\text{Hubbard}} = -J \sum_{n=1}^{N_l} \left(|n-1\rangle\langle n| + |n+1\rangle\langle n| \right)$$

- We wish to choose J such that $h \approx h_{\text{Hubbard}}$

  The sites $|n\rangle$ in h_{Hubbard} are the Wannier functions $w_0(x - na)$ of the first band of h

$$-J = \langle n+1|\, h\, |n\rangle = \int dx\, w_0(x-a) \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + v(x) \right) w_0(x)$$

Exercise: Beyond the Hubbard model

1. Show that, if the 1D Hamiltonian h is spatially periodic with the period a,
   it may be presented in the following form
   in terms of its Wannier functions $|w_{b,n}\rangle$ related to the band b and the site n:

$$h = -\sum_{\text{band } b} \sum_{j,n\in\mathbb{Z}} J_{b,n} \, |w_{b,j+n}\rangle \langle w_{b,j}| \qquad \text{with} \qquad J_{b,n} = -\langle w_{b,n}| \, h \, |w_{b,0}\rangle = J^*_{b,-n}$$

   HINT: Justify that the bands are not mixed: there is a single sum on the band index b.

2. What is the physical meaning of the coefficients $J_{b,n}$?

3. Express these coefficients
   in terms of the Fourier components of the dispersion relation $\varepsilon_b(q)$ for the band b:

$$-J_{b,n} = \int_{-\pi/a}^{\pi/a} \frac{dq}{2\pi/a} \, \varepsilon_b(q) \, e^{inaq}$$

   HINT: $\langle w_{b,j}|\psi_{b,q}\rangle = [a/(2\pi)]^{1/2} \, e^{ijqa}$

- This exercise shows that the Hubbard Hamiltonian relies on two approximations:
  (i) a single band is retained *(ii)* nearest–neighbour hopping

Hubbard model: second quantisation (qu. 5)

$$h = -J \sum_{n=1}^{N_l} \left(|n-1\rangle\langle n| + |n+1\rangle\langle n| \right), \qquad |\psi_q\rangle = \frac{1}{\sqrt{N_l}} \sum_{n=1}^{N_l} e^{inqa} |n\rangle, \qquad \varepsilon(q) = -2J\cos(qa)$$

- "Creation operators transform like kets" the many–body Hamiltonian reads:

$$H = -J \sum_{n=1}^{N_l} \left(a_{n-1}^\dagger a_n + a_{n+1}^\dagger a_n \right) = -J \sum_{\langle i,j \rangle} a_i^\dagger a_j \qquad (\ \langle i,j \rangle : \text{nearest neighbours}\ )$$

- **Ground state $|\mathrm{SF}_{N_a}\rangle$ for bosons:** all N_a atoms in lowest–energy state $|\psi_{q=0}\rangle$

$$|\psi_{q=0}\rangle = \frac{1}{\sqrt{N_l}} \sum_{n=1}^{N_l} |n\rangle \qquad \text{hence:} \qquad a_{q=0}^\dagger = \frac{1}{\sqrt{N_l}} \sum_{n=1}^{N_l} a_n^\dagger$$

$$|\mathrm{SF}_{N_a}\rangle = \frac{1}{\sqrt{N_a!}} a_{q=0}^{\dagger N_a} |\mathrm{vac}\rangle = \frac{1}{\sqrt{N_a!}} \left(\frac{1}{\sqrt{N_l}} \sum_{n=1}^{N_l} a_n^\dagger \right)^{N_a} |\mathrm{vac}\rangle \qquad \text{"superfluid state"}$$

N_l = number of lattice sites; N_a = number of atoms; filling factor $\nu = N_a/N_l$ atoms per site

- What is the ground state for N_a fermions all in the same spin state?

Bosons: annihilating an atom in superfluid state (qu. 6)

$$|\mathrm{SF}_{N_a}\rangle = \frac{a_{q=0}^{\dagger N_a}}{\sqrt{N_a!}}\,|\mathrm{vac}\rangle \qquad \text{with} \qquad a_{q=0}^{\dagger} = \frac{1}{\sqrt{N_l}}\sum_{n=1}^{N_l} a_n^{\dagger}, \qquad [A, B\,C] = [A,B]\,C + B\,[A,C]$$

- Write $a_j\,|\mathrm{SF}_{N_a}\rangle$ in terms of a commutator:

$$a_j\,|\mathrm{SF}_{N_a}\rangle = a_j\,\frac{1}{\sqrt{N_a!}}\,a_{q=0}^{\dagger N_a}\,|\mathrm{vac}\rangle = \frac{1}{\sqrt{N_a!}}\left([a_j, a_{q=0}^{\dagger N_A}] + a_{q=0}^{\dagger N_A}\,a_j\right)|\mathrm{vac}\rangle = \frac{1}{\sqrt{N_a!}}\,[a_j, a_{q=0}^{\dagger N_A}]\,|\mathrm{vac}\rangle$$

$$[a_j, a_{q=0}^{\dagger}] = \frac{1}{\sqrt{N_l}}$$

$$[a_j, a_{q=0}^{\dagger 2}] = [a_j, a_{q=0}^{\dagger}]\,a_{q=0}^{\dagger} + a_{q=0}^{\dagger}\,[a_j, a_{q=0}^{\dagger}] = \frac{2}{\sqrt{N_l}}\,a_{q=0}^{\dagger}$$

$$[a_j, a_{q=0}^{\dagger 3}] = [a_j, a_{q=0}^{\dagger}]\,a_{q=0}^{\dagger 2} + a_{q=0}^{\dagger}\,[a_j, a_{q=0}^{\dagger 2}] = \frac{1}{\sqrt{N_l}}\,a_{q=0}^{\dagger 2} + a_{q=0}^{\dagger 2}\,\frac{2}{\sqrt{N_l}} = \frac{3}{\sqrt{N_l}}\,a_{q=0}^{\dagger 2}$$

Then, by recursion: $[a_j, a_{q=0}^{\dagger N_a}] = \dfrac{N_a}{\sqrt{N_l}}\,a_{q=0}^{\dagger (N_a-1)}$

$$a_j\,|\mathrm{SF}_{N_a}\rangle = \frac{1}{\sqrt{N_a!}}\,\frac{N_a}{\sqrt{N_l}}\,a_{q=0}^{\dagger (N_a-1)}\,|\mathrm{vac}\rangle = \sqrt{\frac{N_a}{N_l}}\,\frac{1}{\sqrt{(N_a-1)!}}\,a_{q=0}^{\dagger (N_a-1)}\,|\mathrm{vac}\rangle = \sqrt{\frac{N_a}{N_l}}\,|\mathrm{SF}_{N_a-1}\rangle$$

The result does not depend on the site index j

- Alternative derivation: first, show $|\mathrm{SF}_{N_a}\rangle = \displaystyle\sum_{n_1+\cdots+n_{N_l}=N_a} \left(\frac{1}{N_l^{N_a}}\,\frac{N_a!}{n_1!\cdots n_{N_l}!}\right)^{1/2} |n_1,\ldots,n_{N_l}\rangle$

Bose–Hubbard model: on–site interactions (qu. 1)

- The bosonic atoms interact only if they are at the same lattice site:

$$\frac{U}{2}\, a_i^\dagger\, a_i^\dagger\, a_i\, a_i \quad = \quad \frac{U}{2}\, a_i^\dagger (a_i\, a_i^\dagger \, - \, 1) a_i \quad = \quad \frac{U}{2}\, n_i\, (n_i - 1)$$

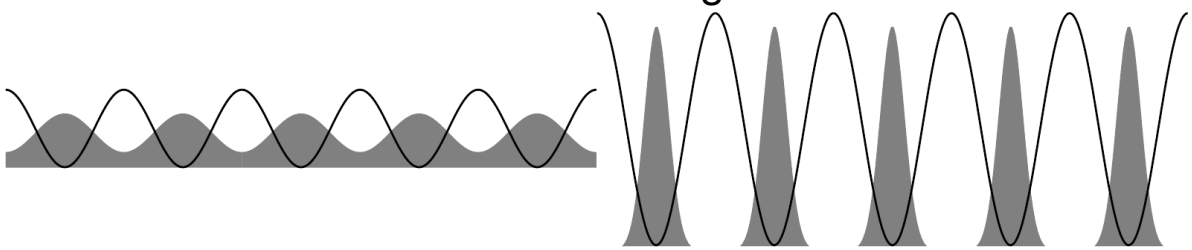
$$H_{\text{Hubbard}} \quad = \quad -J \sum_{<i,j>} a_i^\dagger\, a_j \quad + \quad \frac{U}{2} \sum_i n_i\, (n_i - 1)$$

- Two typical energies: tunnelling between sites $J > 0$, interaction $U > 0$

  One single dimensionless parameter: the ratio U/J

Shallow lattice $U/J \ll 1$: macroscopic coherent wavefunction delocalised over the whole lattice

Deep lattice $U/J \gg 1$: each atom is localised at a given site



- For bosons interacting via the contact interaction $g\,\delta(\mathbf{r})$, express U in terms of the Wannier function $w_0(\mathbf{r})$: $U = g \int d^3 r\, |w_0(\mathbf{r})|^4$

  HINT: Expand the field operator $\hat{\Psi}^\dagger(\mathbf{r})$ into the single–particle Wannier functions $|w_{bn}\rangle$

- Fermions present in 2 internal states: show the interaction term is $U\, n_{i\uparrow}\, n_{i\downarrow}$

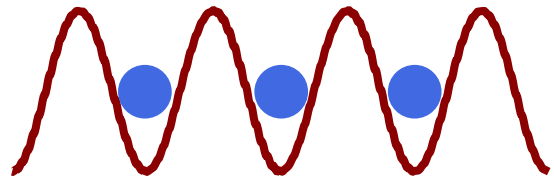
Mott–Insulator state: one–body density matrix (qu. 2)

- $a_i^\dagger$ creates an atom on the site i.
  We assume that there are as many atoms as there are lattice sites:

  $$N_a = N_l \qquad \text{filling factor } \nu = N_a/N_l = 1$$

- **Mott insulator $|\mathrm{MI}\rangle$: one atom localised in each site**

  $$|\mathrm{MI}\rangle = a_1^\dagger \cdots a_{N_l}^\dagger \, |\mathrm{vac}\rangle$$



- $|\mathrm{MI}\rangle$ is a many–particle state (with the fixed number of particles $N_a = N_l$)
  1–body density matrix $\langle \mathbf{r}|\rho^{(1)}|\mathbf{r}'\rangle = \langle \hat\Psi^\dagger(\mathbf{r}')\hat\Psi(\mathbf{r})\rangle$ becomes $\langle i|\rho^{(1)}_{\mathrm{MI}}|j\rangle = \langle \mathrm{MI}|a_j^\dagger a_i|\mathrm{MI}\rangle$
- For $i = j$: mean atom number in site i $\quad \langle i|\rho|i\rangle = \langle \mathrm{MI}|n_i|\mathrm{MI}\rangle = 1$
- For $i \neq j$, $\quad a_i\,|\mathrm{MI}\rangle = |1,\cdots,0_i,\cdots,1\rangle$ and $a_j\,|\mathrm{MI}\rangle = |1,\cdots,0_j,\cdots,1\rangle$
  $a_i\,|\mathrm{MI}\rangle$ and $a_j\,|\mathrm{MI}\rangle$ are orthogonal: $\quad \langle i|\rho|j\rangle = 0$
  $|\mathrm{MI}\rangle$ exhibits **no off–diagonal long–range order**
- For any i, $\quad |\mathrm{MI}\rangle$ is an eigenstate of $n_i = a_i^\dagger a_i$: $\quad n_i\,|\mathrm{MI}\rangle = |\mathrm{MI}\rangle$
  No atom number fluctuations on any site.

Mott–insulator state: average energy (qu. 3 and 4)

$$H_{\text{Hubbard}} = -J \sum_{<i,j>} a_i^\dagger a_j + \frac{U}{2} \sum_i n_i (n_i - 1) \quad \text{and} \quad |\text{MI}\rangle = a_1^\dagger \cdots a_{N_l}^\dagger |\text{vac}\rangle$$

- For each site i, $n_i |\text{MI}\rangle = |\text{MI}\rangle$, so $|\text{MI}\rangle$ **is an eigenstate of the interaction term:**

$$\left(\frac{U}{2} \sum_i n_i (n_i - 1) \right) |\text{MI}\rangle = 0$$

- The *average* kinetic energy is $\langle \text{MI}| \left(-J \sum_{<i,j>} a_i^\dagger a_j \right) |\text{MI}\rangle$

  It involves $\langle \text{MI}| a_i^\dagger a_j |\text{MI}\rangle = \langle j| \rho^{(1)}_{\text{MI}} |i\rangle$ for i,j nearest neighbours

  We have shown that $\langle j| \rho^{(1)}_{\text{MI}} |i\rangle = 0$ for $i \neq j$, so **average kinetic energy vanishes**

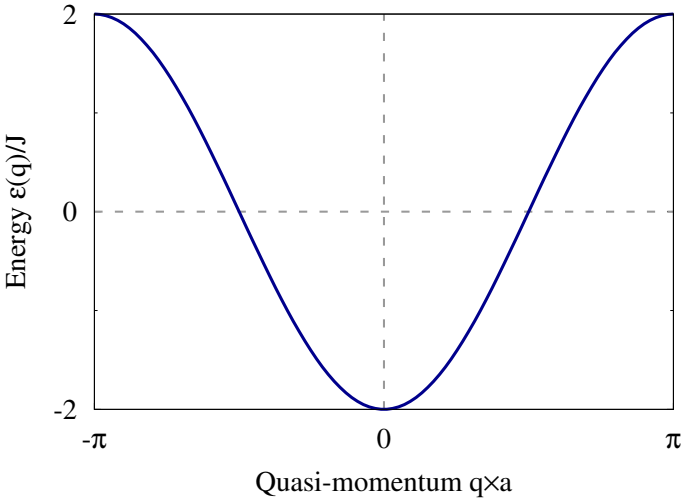
  Hence, the **average (kinetic + interaction) energy** is zero: $\langle \text{MI}| H_{\text{Hubbard}} |\text{MI}\rangle = 0$

- $|\text{MI}\rangle$ is NOT an eigenstate of the kinetic energy term

  It generates terms like $|1, \cdots, 1, 2_i, 0, 1, \cdots, 1\rangle$ and $|1, \cdots, 1, 0, 2_i, 1, \cdots, 1\rangle$

$|\text{MI}\rangle$ is an eigenstate of H_{Hubbard} **in the deep lattice limit** $U \gg J$

Superfluid state: summary of its properties (qu. 5)



- Shallow lattice $U \ll J$: $H_{\text{Hubbard}} = -J \sum_{<i,j>} a_i^\dagger a_j$

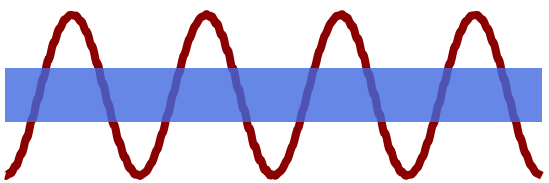
Dispersion relation for the single band: $\varepsilon(q) = -2J\cos(qa)$

1–atom ground state energy: $-2J$ (TYPO in the printed text!)

N_a–atom ground state: all atoms in $|\psi_0\rangle = \sum_{n=1}^{N_l} |n\rangle / \sqrt{N_l}$

Each atom is delocalised over the whole lattice

No interaction: N_a–atom ground state energy is $-2J\,N_A$



$$|\mathrm{SF}_{N_a}\rangle = \frac{1}{\sqrt{N_a!}} a_{\mathbf{k}=\mathbf{0}}^{\dagger N_a} |\mathrm{vac}\rangle = \frac{1}{\sqrt{N_a!}} \left(\frac{1}{\sqrt{N_l}} \sum_{n=1}^{N_l} a_n^\dagger \right)^{N_a} |\mathrm{vac}\rangle$$

- Annihilate an atom in $|\mathrm{SF}_{N_a}\rangle$: $a_j |\mathrm{SF}_{N_a}\rangle = \sqrt{\frac{N_a}{N_l}} |\mathrm{SF}_{N_a-1}\rangle$

$a_j |\mathrm{SF}_{N_a}\rangle$ does not depend on the site j on which the atom is annihilated

Superfluid state: coherence between sites (qu. 6)

For the filling factor $\nu = N_a/N_l$, $a_j \,|\mathrm{SF}_{N_a}\rangle = \sqrt{\nu}\,|\mathrm{SF}_{N_a-1}\rangle$

- 1–body density matrix in superfluid state: $\langle i|\,\rho^{(1)}_{\mathrm{SF}}\,|j\rangle = \langle \mathrm{SF}|\,a_j^\dagger a_i\,|\mathrm{SF}\rangle = \nu$

- Average atom number per site: $\langle \mathrm{SF}|\,n_i\,|\mathrm{SF}\rangle = \langle i|\,\rho^{(1)}_{\mathrm{SF}}\,|i\rangle = \nu$

- Fluctuations on the atom number on site i:

$$\begin{aligned}\langle \mathrm{SF}|\,n_i^2\,|\mathrm{SF}\rangle &= \langle \mathrm{SF}|\,a_i^\dagger a_i a_i^\dagger a_i\,|\mathrm{SF}\rangle = \langle \mathrm{SF}|\,a_i^\dagger(1+a_i^\dagger a_i)a_i\,|\mathrm{SF}\rangle \\ &= \langle \mathrm{SF}|\,n_i\,|\mathrm{SF}\rangle + \langle \mathrm{SF}|\,a_i^\dagger a_i^\dagger a_i a_i\,|\mathrm{SF}\rangle = \nu+\nu^2\end{aligned}$$

The last step uses the thermodynamic limit: $N_a \to \infty$ and $N_l \to \infty$ with $N_a/N_l = \nu$

Variance of atom number on each site: $\Delta n_i^2 = \langle n_i^2\rangle - \langle n_i\rangle^2 = \nu$

The atom number variance satisfies $\Delta n_i^2 = \langle n_i\rangle$

- In the thermodynamic limit, show that n_i obeys a Poisson distribution

HINT: justify that the superfluid state is nearly a tensor product of coherent states on each site.

- For any two sites i and j, $\langle i|\rho^{(1)}_{\mathrm{SF}}|j\rangle \neq 0$: quantum coherence between the two sites

$\lim \langle i|\rho^{(1)}_{\mathrm{SF}}|j\rangle \neq 0$ for $|i-j| \to \infty$: **Off–diagonal long–range order!**

Advanced Quantum Mechanics

Tutorials 2024–2025

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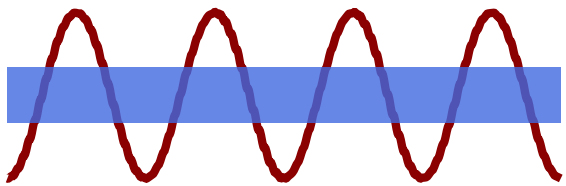
Please ask me MANY questions!

Wednesday, November 27$^{\text{th}}$, 2024

SUMMARY: Bose–Hubbard Hamiltonian

$$H_{\text{Hubbard}} = -J \sum_{<i,j>} a_i^\dagger a_j + \frac{U}{2} \sum_i n_i (n_i - 1)$$

SHALLOW LATTICE LIMIT $U/J \ll 1$



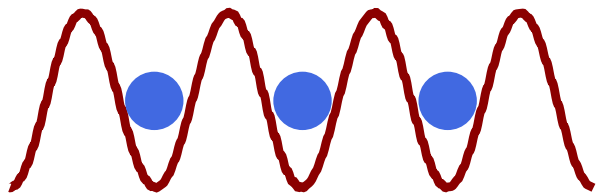
Superfluid state $|\text{SF}\rangle$

$$|\text{SF}_{N_A}\rangle = \frac{1}{\sqrt{N_A!}} a_{\mathbf{k}=\mathbf{0}}^{\dagger N_A} |\text{vac}\rangle$$

- Filling factor $\langle n_i \rangle = N_A/N_L = \nu$
- Variance $\Delta n_i^2 = \nu$
- $\langle \text{SF}| a_j^\dagger a_i |\text{SF}\rangle = \nu$

  Off–diagonal long–range order

DEEP LATTICE LIMIT $U/J \gg 1$



Mott Insulator state $|\text{MI}\rangle$

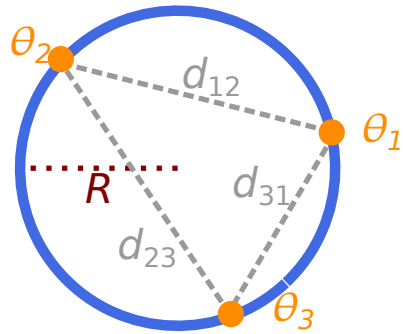
$$|\text{MI}\rangle = a_1^\dagger \cdots a_{N_L}^\dagger |\text{vac}\rangle$$

- Filling factor $\langle n_i \rangle = N_A/N_L = 1$
- No atom number fluctuations $\Delta n_i = 0$
- $\langle \text{MI}| a_j^\dagger a_i |\text{MI}\rangle = \delta_{ij}$

  NO off–diagonal long–range order

Rydberg atoms: chaos & semiclassical physics

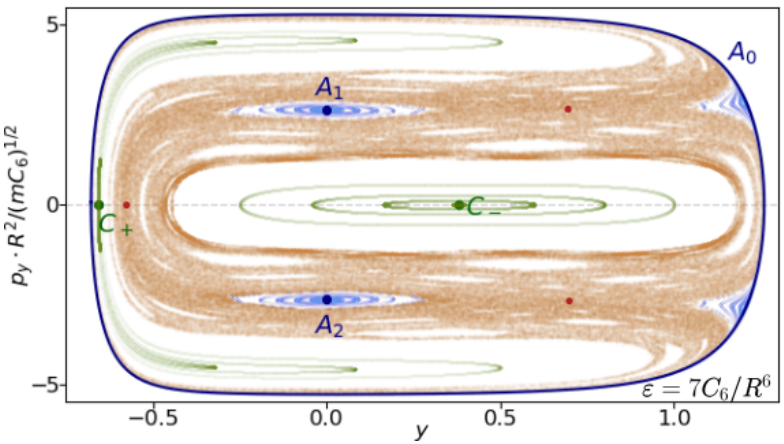
- **Non–ergodicity** of 3 **interacting** Rydberg atoms in a circular trap



This conceptually simple system is **experimentally accessible**
due to recent progress in Rydberg atom trapping in Paris and Palaiseau

[D.J. Papoular & B. Zumer, Phys. Rev. A **107**, 022217 (2023)]

[D.J. Papoular & B. Zumer, Phys. Rev. A **110**, 012230 (2024)]



Two mechanisms impeding ergodicity in the absence of disorder:

1. quantum mechanism: **quantum scar** [Heller PRL 1984]
2. classical mechanism: **KAM tori** (**K**olmogorov, **A**rnold, **M**oser)
   [Arnold, *Mathematical Methods of Classical Mechanics*, Springer (1989)])

Both mechanisms yield quantum eigenstates
localised near classical periodic trajectories

- Telling them apart requires a detailed understanding of the **classical system** and accurate **numerical calculations** of the quantum eigenstates (not ground state!)
- **Semiclassical analysis** which goes beyond the WKB approach

Gutzwiller's trace formula, Einstein–Brillouin–Keller theory

[M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics*, Springer (1990)]

Spontaneous applications for a PhD position with me are welcome

The Quantum Phase Transition between the Superfluid and Mott–Insulator phases

Phase transition at zero temperature

driven by quantum vacuum fluctuations

(this problem presents Gutzwiller's mean–field theory for bosons)

[Cohen–Tannoudji & Guéry–Odelin, *Advances in Atomic Physics*, World Scientific (2011), §7.5.4, §14.4.3, §26.3]

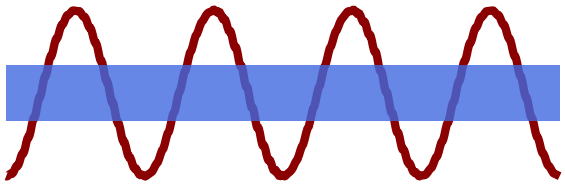
Mott insulators in condensed–matter physics (i.e. involving fermions):

[Mott, Physics Today **31**, 11, 42 (1978)]

Site–factorised wavefunctions: Gutzwiller ansatz

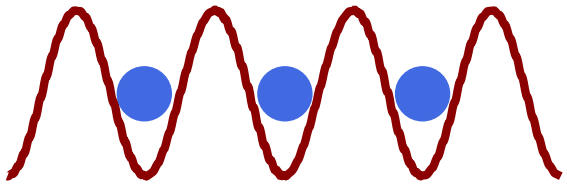
- We have described the system in two opposite limits:

SHALLOW LATTICE LIMIT $U/J \ll 1$



Superfluid state $|\mathrm{SF}\rangle$

DEEP LATTICE LIMIT $U/J \gg 1$



Mott Insulator state $|\mathrm{MI}\rangle$

- Now, we turn to the intermediate regime $U \sim J$

  Variational approach using a family of trial wavefunctions $|\Psi_{\theta,\phi}\rangle$

The family $\{|\Psi_{\theta,\phi}\rangle\}$ is indexed by two real parameters: $0 \le \theta \le \pi/4$ and $-\pi < \phi < \pi$

$$|\Psi_{\theta,\phi}\rangle = \bigotimes_{i=1}^{N_l} |\chi^{(i)}_{\theta,\phi}\rangle \qquad \text{where} \qquad |\chi^{(i)}_{\theta,\phi}\rangle = \cos\theta\ |1\rangle + \sin\theta\ \frac{e^{-i\phi}\,|0\rangle + e^{i\phi}\,|2\rangle}{\sqrt{2}}$$

1. $|\Psi_{\theta,\phi}\rangle$ = tensor product of wavefunctions $|\chi^{(i)}_{\theta,\phi}\rangle$ representing **single sites**

Hartree–type ansatz: **neglect correlations between sites**

2. All sites are represented by the same wavefunction $|\chi^{(i)}_{\theta,\phi}\rangle$ (translational invariance)

- Where have you encountered a similar (but different!) Hartree–type ansatz?

Gross–Pitaevskii equation as a Hartree–type ansatz

$$H = \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} + V_{\text{trap}}(\mathbf{r}_i) \right] + \frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i} V_{\text{int}}(|\mathbf{r}_i - \mathbf{r}_j|) \quad \text{with} \quad V_{\text{int}}(\mathbf{r}) = g\,\delta(\mathbf{r})$$

Beware: Dirac peak 'potentials' should be handled with care! (problem if $\lim_{r \to 0} (r\psi) \neq 0$)

- Hartree ansatz factorised in terms of **particles** all in the same quantum state $|\psi\rangle$

  $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \psi(\mathbf{r}_1) \cdots \psi(\mathbf{r}_N)$ neglects correlations between the atoms

- Minimise $\langle \Psi | H | \Psi \rangle$ under the constraint $\langle \Psi | \Psi \rangle = 1$

  The Lagrange multiplier is the chemical potential μ

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V_{\text{trap}}(\mathbf{r})\,\psi(\mathbf{r}) + g\,N\,|\psi(\mathbf{r})|^2\,\psi(\mathbf{r}) = \mu\,\psi(\mathbf{r})$$

- Link with the order parameter: $\psi(\mathbf{r}) = \frac{1}{\sqrt{N}} \langle \hat{\Psi}(\mathbf{r}) \rangle$

Gutzwiller ansatz: atom number statistics (qu. 7)

$$|\Psi_{\theta,\phi}\rangle = \bigotimes_{i=1}^{N_l} |\chi^{(i)}_{\theta,\phi}\rangle \qquad \text{where} \qquad |\chi^{(i)}_{\theta,\phi}\rangle = \cos\theta\,|1\rangle + \sin\theta\,\frac{e^{-i\phi}\,|0\rangle + e^{i\phi}\,|2\rangle}{\sqrt{2}}$$

- $|\chi^{(i)}\rangle$ is not an eigenstate of $\hat{n}_i$: the atom number on each site fluctuates

$$\langle\Psi_{\theta,\phi}|\hat{n}_i\,|\Psi_{\theta,\phi}\rangle = \langle\chi^{(i)}_{\theta,\phi}|\hat{n}_i\,|\chi^{(i)}_{\theta,\phi}\rangle = \cos^2\theta\times 1 + \frac{\sin^2\theta}{2}\times 0 + \frac{\sin^2\theta}{2}\times 2 = 1$$

$$\langle\Psi_{\theta,\phi}|\hat{n}_i^2|\Psi_{\theta,\phi}\rangle = \langle\chi^{(i)}_{\theta,\phi}|\hat{n}_i^2|\chi^{(i)}_{\theta,\phi}\rangle = \cos^2\theta\times 1^2 + \frac{\sin^2\theta}{2}\times 0^2 + \frac{\sin^2\theta}{2}\times 2^2 = 1+\sin^2\theta$$

Variance: $(\Delta n_i)^2 = \langle n_i^2\rangle - \langle n_i\rangle^2 = \sin^2\theta$ and mean square deviation: $\Delta n_i = \sin\theta$

- $|\Psi_{\theta,\phi}\rangle$ is factorised with respect to the sites: $n_i =$ independent random variables

$$\langle N\rangle = \sum_{i=1}^{N_l}\langle n_i\rangle = N_l, \qquad \langle\Delta N^2\rangle = \sum_{i=1}^{N_l}\langle\Delta n_i^2\rangle = N_l\sin^2\theta, \qquad \Delta N = \sqrt{N_l}\,\sin\theta$$

- The fluctuations vanish for $\theta = 0$ (and any ϕ). $|\Psi_{\theta=0,\phi}\rangle = |\mathrm{MI}\rangle$ exactly!

Gutzwiller ansatz: order parameter (qu. 8)

$$|\Psi_{\theta,\phi}\rangle = \bigotimes_{i=1}^{N_l} |\chi^{(i)}_{\theta,\phi}\rangle \qquad \text{where} \qquad |\chi^{(i)}_{\theta,\phi}\rangle = \cos\theta\,|1\rangle + \sin\theta\,\frac{e^{-i\phi}\,|0\rangle + e^{i\phi}\,|2\rangle}{\sqrt{2}}$$

- In the continuum: $\Psi(\mathbf{r}) = \langle\hat{\Psi}(\mathbf{r})\rangle$ On the lattice: $\psi_i = \langle\Psi_{\theta,\phi}|\, a_i\, |\Psi_{\theta,\phi}\rangle$

- $|\Psi_{\theta,\phi}\rangle$ is factorised sitewise, all sites have the same wavefunction $|\chi_{\theta,\phi}\rangle$

$$\psi_i = \langle\chi^{(i)}_{\theta,\phi}|\, a_i\, |\chi^{(i)}_{\theta,\phi}\rangle = \left[\cos\theta\,\langle 1| + \frac{\sin\theta}{\sqrt{2}}\left(e^{i\phi}\,\langle 0| + e^{-i\phi}\,\langle 2|\right)\right]\left[\cos\theta\,|0\rangle + \sin\theta\,e^{i\phi}\,|1\rangle\right]$$

$$\psi = \frac{1}{2}\left(1 + \frac{1}{\sqrt{2}}\right)\sin(2\theta)\,e^{i\phi} \qquad \text{and} \qquad |\psi|^2 = \frac{1}{4}\left(\frac{3}{2} + \sqrt{2}\right)\sin^2(2\theta)$$

The order parameter $\psi = \psi_i$ does not depend on the site i

- $\psi = 0$ for $\theta = 0$: Mott–insulator state $|\mathrm{MI}\rangle$

  $\psi \neq 0$ for all θ such that $0 < \theta \leq \pi/4$: 'superfluid phase'

  $|\psi|$ is maximal for $\theta = \pi/4$: deep superfluid state

$$|\Psi_{\theta=\pi/4,\phi}\rangle = \bigotimes_{i=1}^{N_l}\left[\frac{1}{\sqrt{2}}\,|1^{(i)}\rangle + \frac{1}{2}\left(e^{-i\phi}\,|0^{(i)}\rangle + e^{i\phi}\,|2^{(i)}\rangle\right)\right] \approx |\mathrm{SF}\rangle$$

Gutzwiller ansatz: 1–body density matrix (qu. 8 & 10)

$$|\Psi_{\theta,\phi}\rangle = \bigotimes_{i=1}^{N_l} |\chi^{(i)}_{\theta,\phi}\rangle \qquad \text{where} \qquad |\chi^{(i)}_{\theta,\phi}\rangle = \cos\theta\ |1\rangle + \sin\theta\ \frac{e^{-i\phi}\,|0\rangle + e^{i\phi}\,|2\rangle}{\sqrt{2}}$$

- Mean–field one–body density matrix: $\langle i|\rho_{\mathrm{MF}}|j\rangle = \langle\Psi_{\theta,\phi}|\, a_j^\dagger a_i\, |\Psi_{\theta,\phi}\rangle$

  Gutzwiller wavefunction neglects correlations between different sites: mean–field approach

We have already calculated $\langle i|\rho_{\mathrm{MF}}|i\rangle = \langle i|n_i|i\rangle = 1$

Off–diagonal element: $\langle i|\rho_{\mathrm{MF}}|j\rangle = \langle\chi^{(i)}\chi^{(j)}|a_j^\dagger a_i|\chi^{(i)}\chi^{(j)}\rangle = \langle\chi^{(j)}|a_j^\dagger|\chi^{(j)}\rangle\,\langle\chi^{(i)}|a_i|\chi^{(i)}\rangle$

$$\langle i|\rho_{\mathrm{MF}}|j\rangle = |\psi|^2 = \frac{1}{4}\left(\frac{3}{2}+\sqrt{2}\right)\sin^2(2\theta)$$

- $\rho^{(1)}_{\mathrm{MF}}$ does not depend on ϕ

  Its off–diagonal elements $\langle i|\rho_{\mathrm{MF}}|j\rangle$ vanish for $\theta = 0$ (state $|\mathrm{MI}\rangle$)

  $\langle i|\rho_{\mathrm{MF}}|j\rangle \neq 0$ for $0 < \theta \leq \pi/4$, off–diagonal long–range order: SF phase

  $\langle i|\rho_{\mathrm{MF}}|j\rangle$ is maximal for $\theta = \pi/4$ ($\approx$ state $|\mathrm{SF}\rangle$)

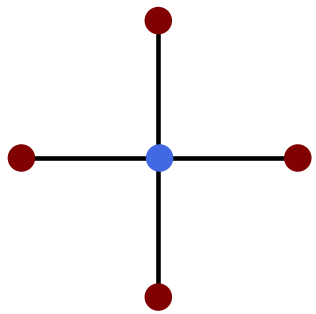
Number of nearest–neighbouring sites (qu. 9 & 13)

- Coordination number z = number of nearest neighbours for a given lattice site

  z depends on the dimensionality and the considered lattice

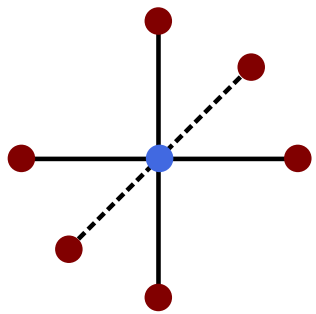
1D lattice, one atom per unit cell

$z = 2$



2D square lattice, one atom per unit cell

$z = 4$



3D cubic lattice, one atom per unit cell

$z = 6$

- For higher z, mean–field theory is more accurate

  1. cf. Ising model: mean–field theory is exact on a fully–connected graph

  2. In lower dimensions, the role of fluctuations is enhanced

  e.g. Mermin–Wagner theorem 'forbids' long–range order in 2D and 1D

  [Peierls, *Surprises in Theoretical Physics*, Princeton Univ. Press (1979), §4.1]

Gutzwiller ansatz: average energy (qu. 10)

$H_{\text{Hubbard}} = -J \sum_{<i,j>} a_i^\dagger a_j + \frac{U}{2} \sum_i n_i (n_i - 1)$, $\quad \langle \Psi_{\theta,\phi} | \hat{n}_i | \Psi_{\theta,\phi} \rangle = 1$, $\quad \langle \Psi_{\theta,\phi} | \hat{n}_i^2 | \Psi_{\theta,\phi} \rangle = 1 + \sin^2\theta$

- Hopping: $\langle \Psi_{\theta,\phi} | (-J\, a_i^\dagger a_j) | \Psi_{\theta,\phi} \rangle = -J \langle j | \rho_{\text{MF}} | i \rangle = -\frac{J}{4} \left(\frac{3}{2} + \sqrt{2} \right) \sin^2(2\theta)$

$\sum_{\langle i,j \rangle}$: first choose site (among N_l), then choose nearest neighbour (among z): $N_l\, z$ such terms

- Interaction: $\langle \Psi_{\theta,\phi} | \frac{U}{2} n_i (n_i - 1) | \Psi_{\theta,\phi} \rangle = \frac{U}{2} \left(\langle \Psi_{\theta,\phi} | n_i^2 | \Psi_{\theta,\phi} \rangle - \langle \Psi_{\theta,\phi} | n_i | \Psi_{\theta,\phi} \rangle \right)$

$= \frac{U}{2} (1 + \sin^2\theta - 1) = \frac{U}{2} \sin^2\theta$

$\sum_i$: choose a site (among N_l): N_l such terms. Reminders: $\langle n_i \rangle = 1$ and $\langle n_i^2 \rangle = 1 + \sin^2\theta$

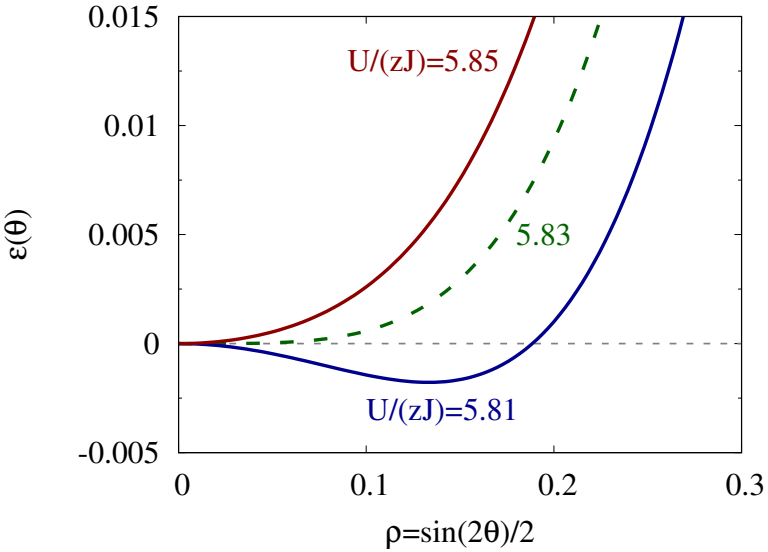
- Total average energy:

$$\frac{2}{N_l\, z\, J} \langle \Psi_{\theta,\phi} | H_{\text{Hubbard}} | \Psi_{\theta,\phi} \rangle = \sin^2\theta \left[\frac{U}{z\, J} - \left(3 + 2\sqrt{2} \right) \cos^2\theta \right] = \varepsilon(\theta)$$

- Mean–field result: for given $U/(zJ)$, find the phase by minimising $\varepsilon(\theta)$

No dependence on ϕ: **spontaneously broken symmetry**

Gutzwiller ansatz: phase diagram (qu. 11)



- For given $U/(z\,J)$,
  phase determined by minimising:

$$\varepsilon(\theta) \quad = \quad \sin^2\theta \left[\frac{U}{z\,J} - \left(3 + 2\sqrt{2}\right) \cos^2\theta \right]$$

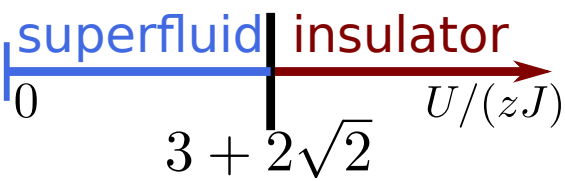
- Plot ε against $\rho = \sin(2\theta)/2$, directly related to order parameter $\psi = (1 + 1/\sqrt{2})\, e^{i\phi}\, \rho$

- If $U/(zJ) > (3 + 2\sqrt{2})$: the term in the brackets is always > 0,
  minimum reached for $\theta = 0$: Mott–Insulator phase with $\psi = 0$

- If $U/(zJ) < (3 + 2\sqrt{2})$: introduce $0 < \theta_0 \leq \frac{\pi}{4}$ such that $\cos(2\theta_0) = \frac{U/(zJ)}{3 + 2\sqrt{2}}$

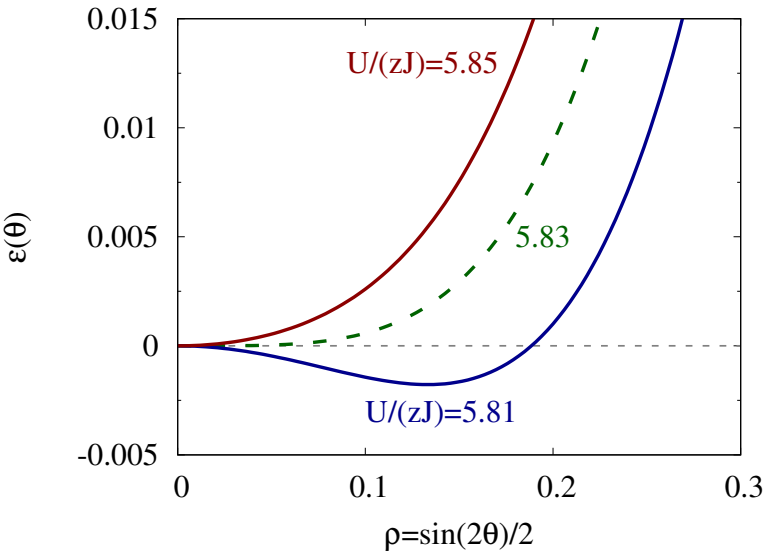
  $d\varepsilon/d\theta = (3 + 2\sqrt{2})\, \sin(2\theta)\, [\cos(2\theta_0) - \cos(2\theta)]$ minimum reached for $\theta = \theta_0$

  $\psi = \frac{1}{2}\left(1 + \frac{1}{\sqrt{2}}\right) \sin(2\theta_0)\, e^{i\phi} \neq 0$ superfluid phase



- In mean–field theory, dimensionality and lattice geometry are encoded in the coordination number z

Superfluid to insulator: 2nd order phase transition (qu. 12)



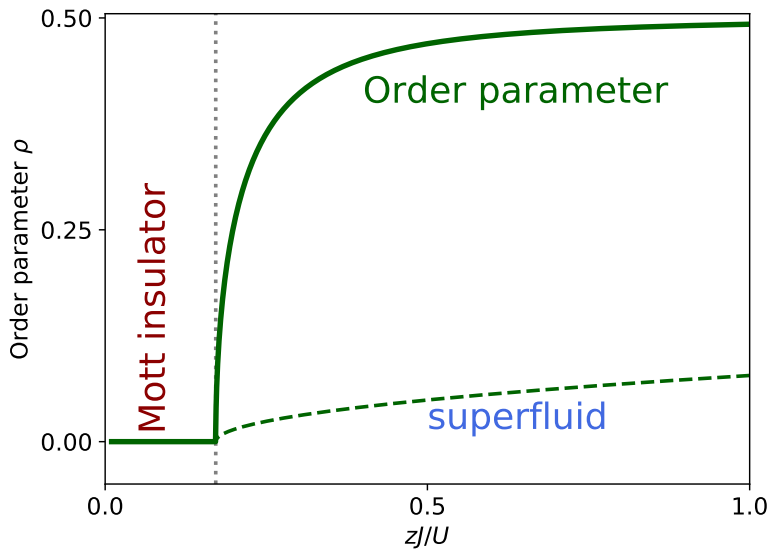
$$\rho \quad = \quad \sin(2\theta)/2 \quad = \quad \psi\, e^{-i\phi}/(1+1/\sqrt{2})$$

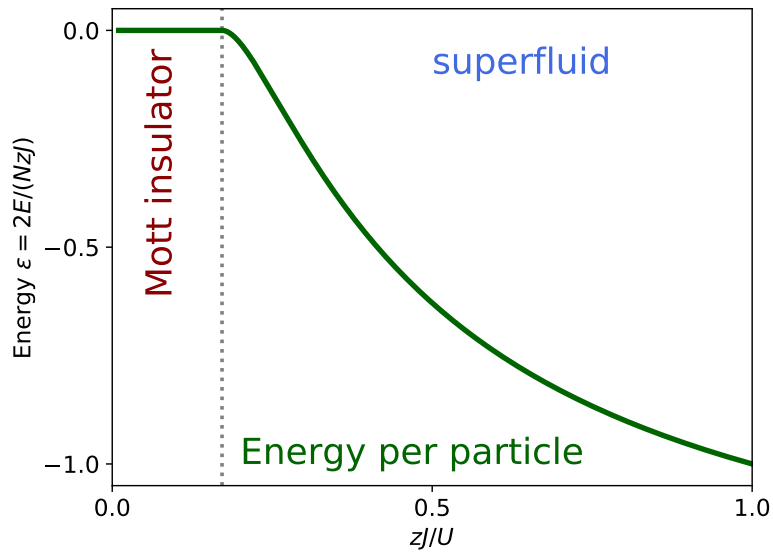
- For given $(z\,J)/U$,
  phase determined by minimising:

$$\varepsilon(\rho) \quad = \quad \frac{1}{2}\,\frac{U}{zJ}\left[1-(1-4\rho^2)^{1/2}\right]-(3+2\sqrt{2})\,\rho^2$$

Value ρ at which minimum is reached sets order parameter

- Plot ρ and $\varepsilon = 2E/(NJz)$ as a function of $(z\,J)/U$

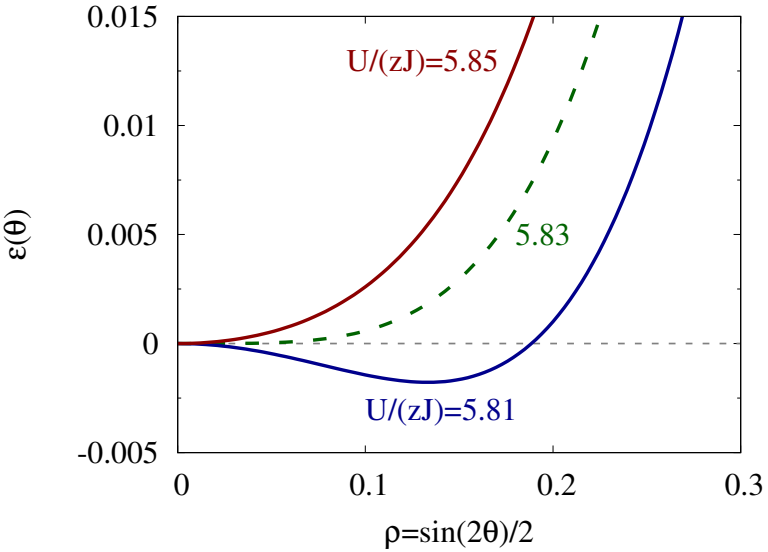




Energy is continuous across transition at $\dfrac{U}{zJ} = 3+2\sqrt{2}$: **$2^{\text{nd}}$–order transition**

- Which quantity does the dashed green line illustrate ?

Superfluid to insulator: critical exponent (qu. 12)



- For given $(zJ)/U$, phase determined by minimising:

$$\varepsilon(\rho) = \frac{1}{2}\frac{U}{zJ}\left[1-(1-4\rho^2)^{1/2}\right] - (3+2\sqrt{2})\,\rho^2$$

- ρ is small on both sides of transition: expand $\varepsilon(\rho)$

$$\varepsilon(\rho) = \rho^2\left(\frac{U}{zJ} - \left[\frac{U}{zJ}\right]_{\rm crit}\right) + \rho^4\,\frac{U}{zJ}$$

- No term $\propto \rho$: for $U/(zJ) > [U/(zJ)]_{\rm crit}$, energy is minimal for $\rho = 0$, i.e. $|{\rm MI}\rangle$ phase
  The term $\propto \rho^2$ changes signs at transition: $\rho = 0$ is a local maximum for $U/(zJ) < [U/(zJ)]_{\rm crit}$
  No term $\propto \rho^3$ to avoid first–order phase transition
  The term $\propto \rho^4$ is positive to ensure stability of $|{\rm MI}\rangle$ at transition point $U/(zJ) = [U/(zJ)]_{\rm crit}$

- In the superfluid phase $(U/(zJ) < 3+2\sqrt{2})$, solve for ρ as a function of zJ/U:

$$\rho = \left[\frac{3+2\sqrt{2}}{2}\right]^{1/2}\left[\frac{zJ}{U} - \frac{1}{3+2\sqrt{2}}\right]^{1/2}$$

so the critical exponent is $\beta = 1/2$

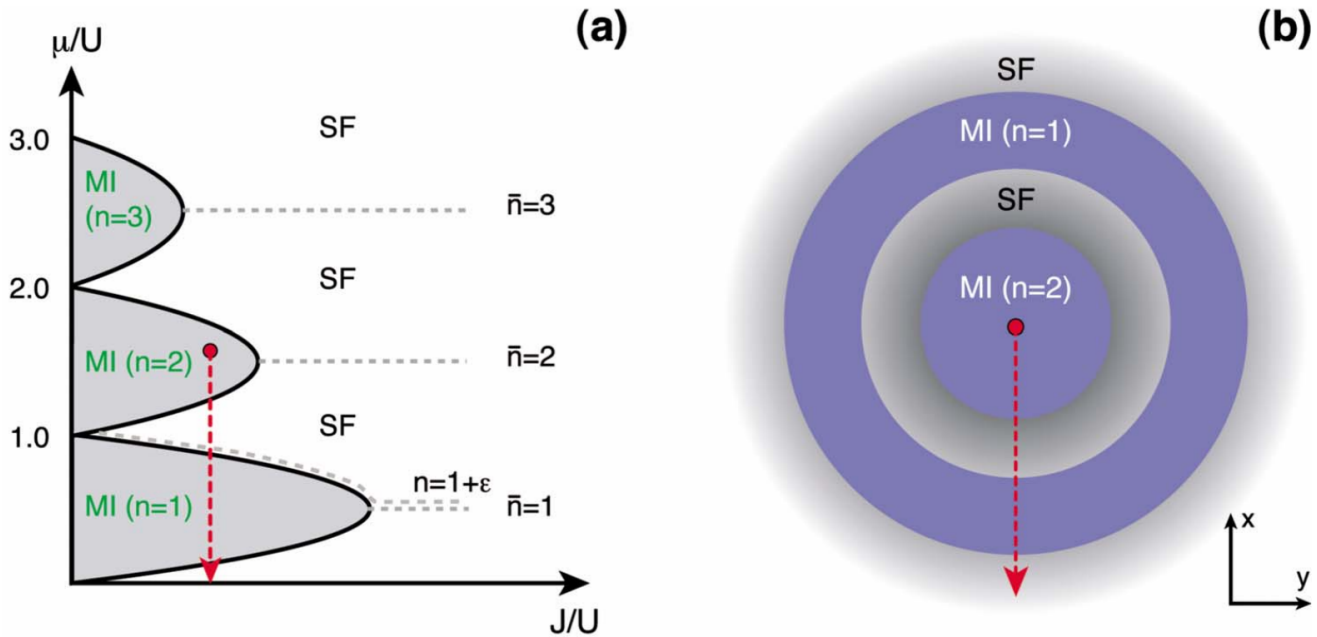
- Beyond–mean–field calculations confirm the transition is second–order; in 2D, $\beta = 0.348$, like the Λ transition in liquid ^{4}He [Sanders & Holthaus, J. Phys. A **55**, 255001 (2019)]

Bosons: grand–canonical phase diagram; trapped gas

$$H_{\text{Hubbard}} - \mu N = -J \sum_{<i,j>} a_i^\dagger a_j + \frac{U}{2} \sum_i n_i (n_i - 1) - \mu N$$

- **Homogeneous system:** chemical potential μ sets average filling factor $\bar{n} = N_a/N_l$

  Three energies J, U, μ yield two independent adimensional parameters: J/U, μ/U



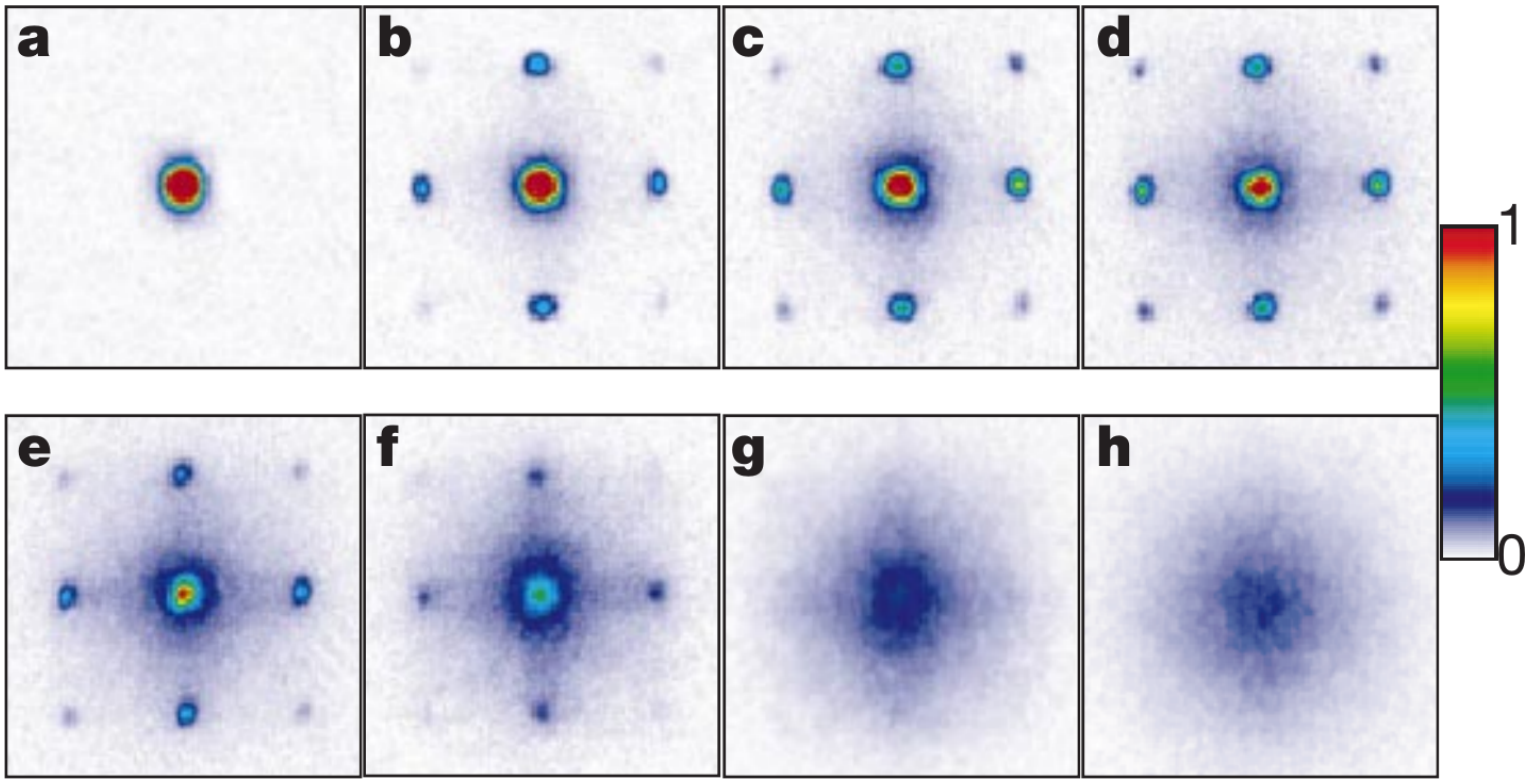
- **Trapped system:** local density approximation $\mu = V(\mathbf{r}) + \mu(\mathbf{r})$

  Corresponds to the Thomas–Fermi approximation for the Gross–Pitaevskii equation

1 experiment probes many values of μ: vertical segment of homogeneous phase diagram

[Bloch, Dalibard, Zwerger, Rev. Mod. Phys. **80**, 885 (2008), §IV]

Time–of–flight expansion from a lattice

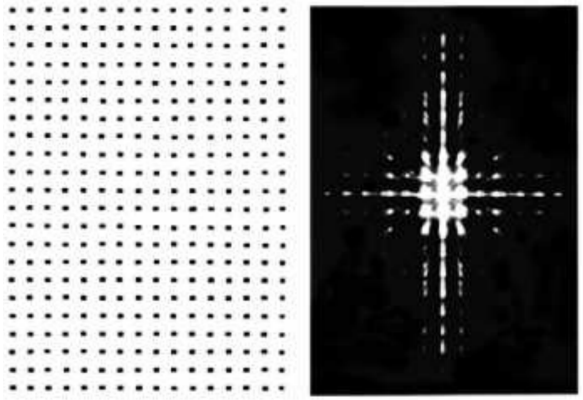


[original experimental figure from: Greiner et al, Nature **419**, 51 (2002)]

[Bloch, Dalibard, Zwerger, Rev. Mod. Phys. **80**, 885 (2008), §II.C & §IV.B]

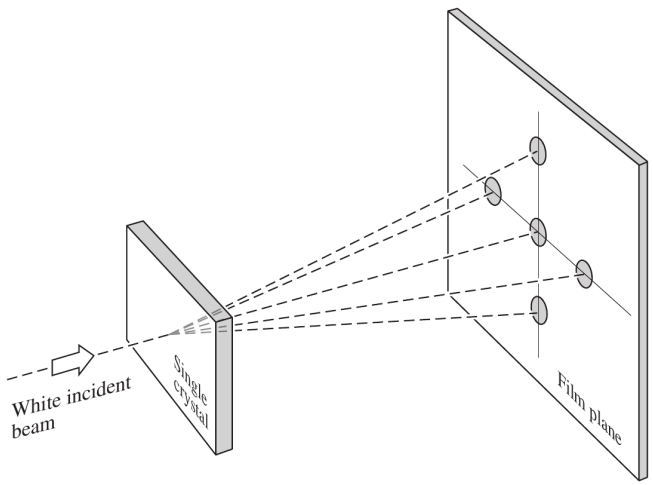
Diffraction of optical waves by a **periodic structure**

- Diffraction by a **2D grating**

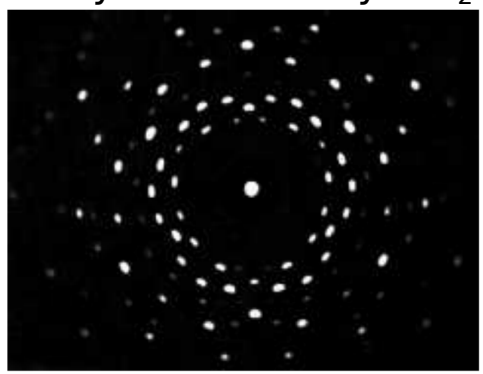


- Diffraction by a **3D crystal**

Bragg's law: $2d \sin\theta = n\lambda$



X-ray diffraction by SiO_2



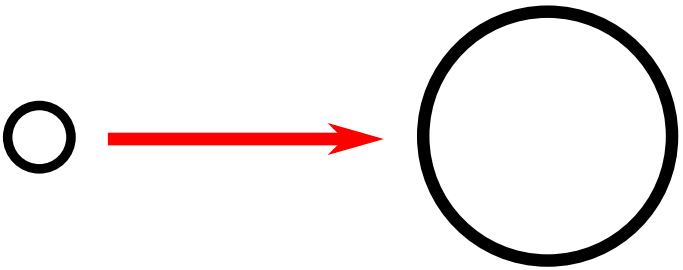
Diffraction figure = (background due to one scatterer)×(spots due to grating)

The position of the spots is dictated by the reciprocal lattice of the grating

[Hecht, *Optics*, 5th edition, Pearson (2016), chap. 10]

Time–of–flight expansion (qu. 14)

- We prepare the system in a stationary state inside a trap and a lattice
  At $t = 0$, we switch off both trap and lattice: the gas undergoes **free expansion**



- Matter waves from lattice wells expand and interfere
- Expansion from an isotropic trap conserves isotropy
- What happens if the trap is not isotropic?

- We make two assumptions, both well satisfied in Greiner's experiment (2002):
  1. Long expansion time: the initial size of the cloud is negligible
  2. During the expansion, interactions between atoms play no role

Interactions do play a key role before the expansion!

- Then, after the expansion time T,
  an atom that initially had the momentum $\hbar\mathbf{k}$ is at the position $\mathbf{r}_f = \mathbf{v}\,t = \hbar\,\mathbf{k}t/m$
  Probing final density distribution amounts to probing initial momentum distribution

Analogous to optical diffraction

Expanding a plane wave onto the Wannier functions

- We need the momentum distribution $\langle n_{\mathbf{k}} \rangle = \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle$ in the state $|\Psi\rangle$ before expansion

  No lattice during expansion, hence, $\hbar\mathbf{k}$ is the *true* momentum (NOT quasi–momentum)

  To obtain $a_{\mathbf{k}}^\dagger$, we first calculate $|\mathbf{k}\rangle$ in terms of the Wannier functions $w_{b,\mathbf{j}}(\mathbf{r}) = w_{b,\mathbf{0}}(\mathbf{r} - \mathbf{a}_{\mathbf{j}})$

$$
\begin{aligned}
|\mathbf{k}\rangle &= \sum_{b,\mathbf{j}} |w_{b,\mathbf{j}}\rangle \langle w_{b,\mathbf{j}}|\mathbf{k}\rangle = \sum_{b,\mathbf{j}} |w_{b,\mathbf{j}}\rangle \int d^3r \, \langle w_{b,\mathbf{j}}|\mathbf{r}\rangle \, \langle \mathbf{r}|\mathbf{k}\rangle \\
&= \sum_{b,\mathbf{j}} |w_{b,\mathbf{j}}\rangle \int d^3r \, w^*_{b,\mathbf{0}}(\mathbf{r} - \mathbf{r}_{\mathbf{j}}) \frac{\exp(i\,\mathbf{k}\cdot\mathbf{r})}{(2\pi)^{3/2}} \\
&= \sum_{b,\mathbf{j}} |w_{b,\mathbf{j}}\rangle \int d^3r \, w^*_{b,\mathbf{0}}(\mathbf{r} - \mathbf{r}_{\mathbf{j}}) \frac{\exp[i\,\mathbf{k}\cdot(\mathbf{r} - \mathbf{r}_{\mathbf{j}})]}{(2\pi)^{3/2}} \exp(i\,\mathbf{k}\cdot\mathbf{r}_{\mathbf{j}}) \\
&= \sum_{b} \left(\sum_{\mathbf{j}} |w_{b,\mathbf{j}}\rangle \exp(i\,\mathbf{k}\cdot\mathbf{r}_{\mathbf{j}}) \right) w^*_{b,\mathbf{0}}(\mathbf{k})
\end{aligned}
$$

  b = band index, $\mathbf{r}_{\mathbf{j}}$ = position of site $\mathbf{j}$, $w_{b,\mathbf{0}}(\mathbf{k}) = \langle \mathbf{k}|w_{b,\mathbf{0}}\rangle$

- The contribution of each band b has
  the same structure as the electromagnetic field diffracted from a grating:

  Product of the interference of plane waves originating from all lattice sites
  and the Fourier transform of a single slit or lattice site

The momentum distribution $\langle\Psi|n_{\mathbf{k}}|\Psi\rangle$

For a single band, $|\mathbf{k}\rangle = \left(\sum_{\mathbf{j}} |w_{\mathbf{j}}\rangle \exp(i\,\mathbf{k}\cdot\mathbf{r}_{\mathbf{j}})\right) w_0^*(\mathbf{k})$

- Creation operators transform like kets

$$a_{\mathbf{k}}^\dagger = \left(\sum_{\mathbf{j}} a_{\mathbf{j}}^\dagger\, e^{i\,\mathbf{k}\cdot\mathbf{r}_{\mathbf{j}}}\right) w_0^*(\mathbf{k}) \quad \text{and} \quad a_{\mathbf{k}} = \left(\sum_{\mathbf{j}'} a_{\mathbf{j}'}\, e^{-i\,\mathbf{k}\cdot\mathbf{r}_{\mathbf{j}}}\right) w_0(\mathbf{k})$$

- $n_{\mathbf{k}} = a_{\mathbf{k}}^\dagger\, a_{\mathbf{k}} = |w_0(\mathbf{k})|^2 \sum_{\mathbf{j},\mathbf{j}'} e^{i\mathbf{k}\cdot(\mathbf{r}_{\mathbf{j}}-\mathbf{r}_{\mathbf{j}'})}\, a_{\mathbf{j}}^\dagger\, a_{\mathbf{j}'}$

- The momentum distribution $\langle\Psi|n_{\mathbf{k}}|\Psi\rangle$ is the expectation value of $n_{\mathbf{k}}$ at $t = 0$, i.e. just before the expansion in the many–body quantum state $|\Psi\rangle$

$$\langle\Psi|n_{\mathbf{k}}|\Psi\rangle = |w_0(\mathbf{k})|^2 \sum_{\mathbf{j},\mathbf{j}'} e^{i\mathbf{k}\cdot(\mathbf{r}_{\mathbf{j}}-\mathbf{r}_{\mathbf{j}'})}\, \langle\mathbf{j}'|\rho^{(1)}|\mathbf{j}\rangle$$

The density matrix $\langle\mathbf{j}'|\rho^{(1)}|\mathbf{j}\rangle = \langle\Psi|a_{\mathbf{j}}^\dagger\, a_{\mathbf{j}'}|\Psi\rangle$ reflects the phase (superfluid or insulator)

$\langle j'|\rho^{(1)}_{\mathrm{SF}}|j\rangle = \delta_{j,j'} + |\psi|^2(1-\delta_{j,j'})$ | $\langle j'|\rho^{(1)}_{\mathrm{MI}}|j\rangle = \delta_{j,j'}$

Expansion starting from Mott-Insulator phase (qu. 14)

$$\langle \Psi | n_{\mathbf{k}} | \Psi \rangle \quad = \quad |w_0(\mathbf{k})|^2 \sum_{\mathbf{j},\mathbf{j}'} e^{i\mathbf{k}\cdot(\mathbf{r}_\mathbf{j} - \mathbf{r}_{\mathbf{j}'})} \; \langle \mathbf{j}' | \rho^{(1)} | \mathbf{j} \rangle$$

- In the Mott–Insulator phase $|\mathrm{MI}\rangle$ (filling factor $\nu = N_a/N_l = 1$)

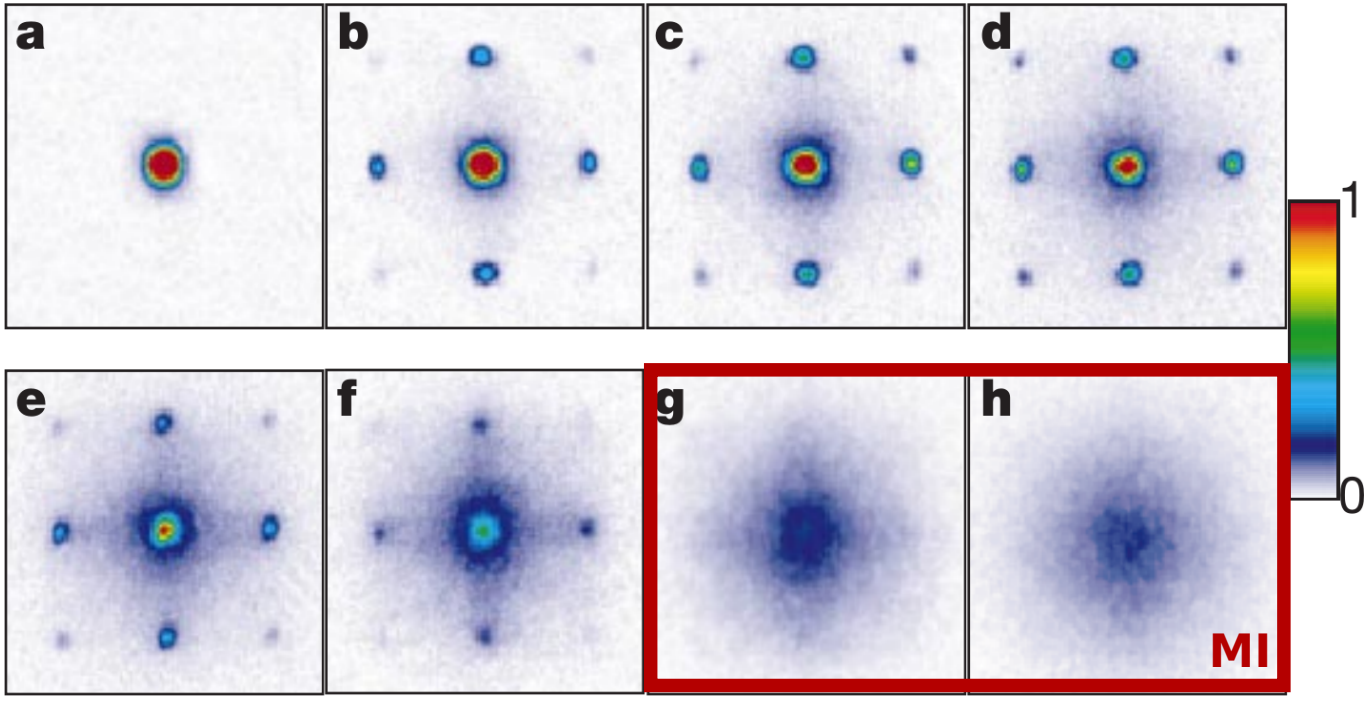
  only the diagonal density matrix elements are non–zero: $\langle \mathbf{j}' | \rho^{(1)}_{\mathrm{MI}} | \mathbf{j} \rangle = \delta_{\mathbf{j},\mathbf{j}'}$

$$\langle \mathrm{MI} | n_{\mathbf{k}} | \mathrm{MI} \rangle \quad = \quad N \, |w_0(\mathbf{k})|^2$$

- After a long expansion time T, the density distribution reflects $\langle n(\mathbf{k}) \rangle$

  Signal dictated by Fourier transform $w_0(\mathbf{k})$ of the Wannier function

  'Incoherent', i.e. no constructive interference, scales with N



Expansion starting from superfluid phase (qu. 14)

$$\langle\Psi|n_{\mathbf{k}}|\Psi\rangle = |w_0(\mathbf{k})|^2 \sum_{\mathbf{j},\mathbf{j}'} e^{i\mathbf{k}\cdot(\mathbf{r}_\mathbf{j}-\mathbf{r}_{\mathbf{j}'})} \langle\mathbf{j}'|\rho^{(1)}|\mathbf{j}\rangle \quad \text{and} \quad |\psi|^2 = \frac{1}{4}\left(\frac{3}{2}+\sqrt{2}\right)\sin^2(2\theta) < 0.73$$

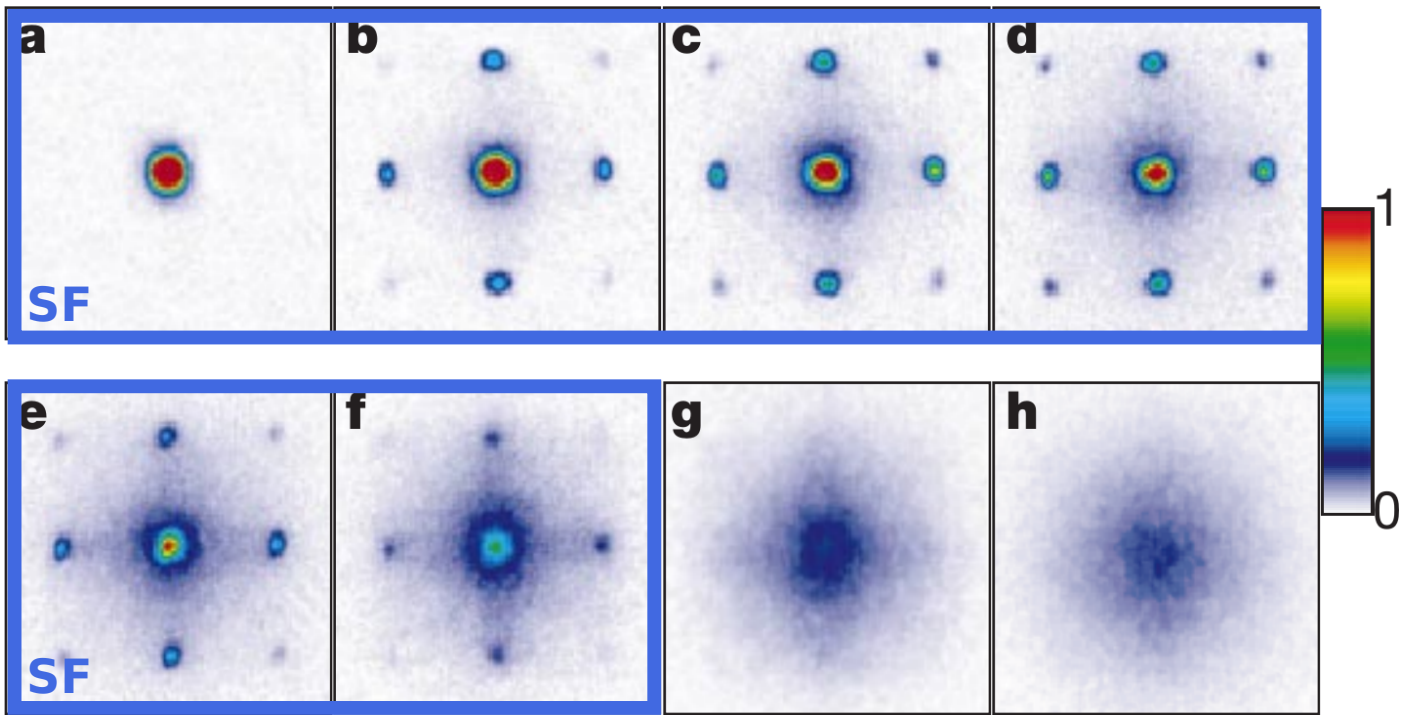
- In the superfluid phase $|\mathrm{SF}\rangle$ (filling factor $\nu = N_a/N_l = 1$)

All density matrix elements $\neq 0$: $\langle\mathbf{j}'|\rho^{(1)}_{\mathrm{SF}}|\mathbf{j}\rangle = \delta_{\mathbf{j},\mathbf{j}'} + |\psi|^2(1-\delta_{\mathbf{j},\mathbf{j}'}) = (1-|\psi|^2)\delta_{\mathbf{j},\mathbf{j}'} + |\psi|^2$

$$\langle\Psi_{\theta,\phi}|n_{\mathbf{k}}|\Psi_{\theta,\phi}\rangle = N\,|w_0(\mathbf{k})|^2\,(1-|\psi|^2) + |w_0(\mathbf{k})|^2\,|\psi|^2 \sum_{\mathbf{j},\mathbf{j}'} e^{i\mathbf{k}\cdot(\mathbf{r}_\mathbf{j}-\mathbf{r}_{\mathbf{j}'})}$$

If **k** is not a reciprocal lattice vector: $N\,|w_0(\mathbf{k})|^2\,(1-|\psi|^2)$ incoherent background

If **k is a reciprocal lattice vector:** $N^2\,|w_0(\mathbf{k})|^2\,|\psi|^2$ constructive interference **peak**



Collapse and revival of the coherence of a matter wave

- Prepare the system deep in the superfluid phase
  At time $t = 0$, abruptly increase the height of the wells to isolate them
  At $t = 0$, the state of each well i is almost a coherent state for a_i
  Study the quantum dynamics for $t > 0$: piloted by interactions U

- **Collapse:** coherence vanishes at short times, i.e. order parameter ψ goes to 0
  Revivals: ψ returns to its maximum value periodically in time ($T = h/U$)

- The experimental approach is similar: time–of–flight expansion from a lattice
  [Greiner et al, Nature **419**, 51 (2002)]
  Theory: description of the state of a single site using the Husimi function
  i.e. a quantum state ρ is fully determined by its average value in *all* coherent states $\langle\beta|\rho|\beta\rangle$

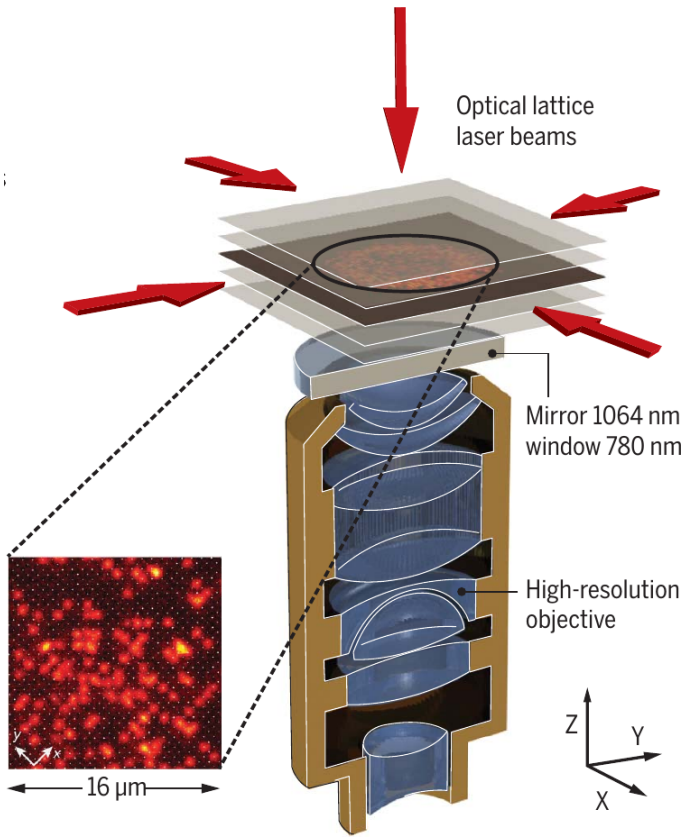
- This experiment involving many atoms in an optical lattice (2002)
  is closely related to a previous experiment (1996) involving
  1 Rydberg atom in a cavity containing a coherent EM field [Brune PRL **76**, 1800 (1996)]

- **Good luck!** I shall post a detailed solution.

A new observation scheme: Quantum gas microscope

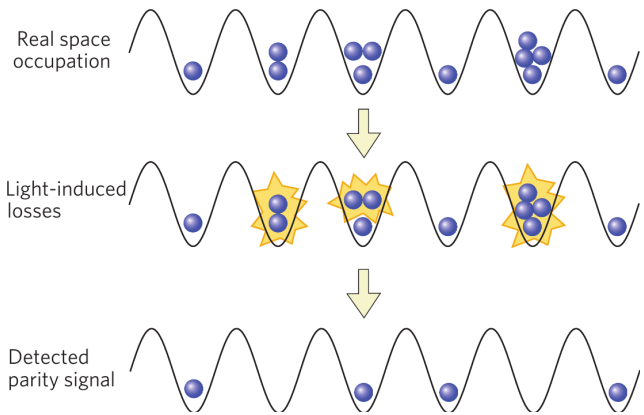
- Site–resolved measurement in a 2D optical lattice, both for bosons and for fermions

  No time–of–flight expansion; averages & fluctuations extracted from single image



- Shine near–resonant light onto the trapped atoms and collect multiple fluorescence photons using a high–resolution microscope objective

  High resolution allows for site–resolved detection

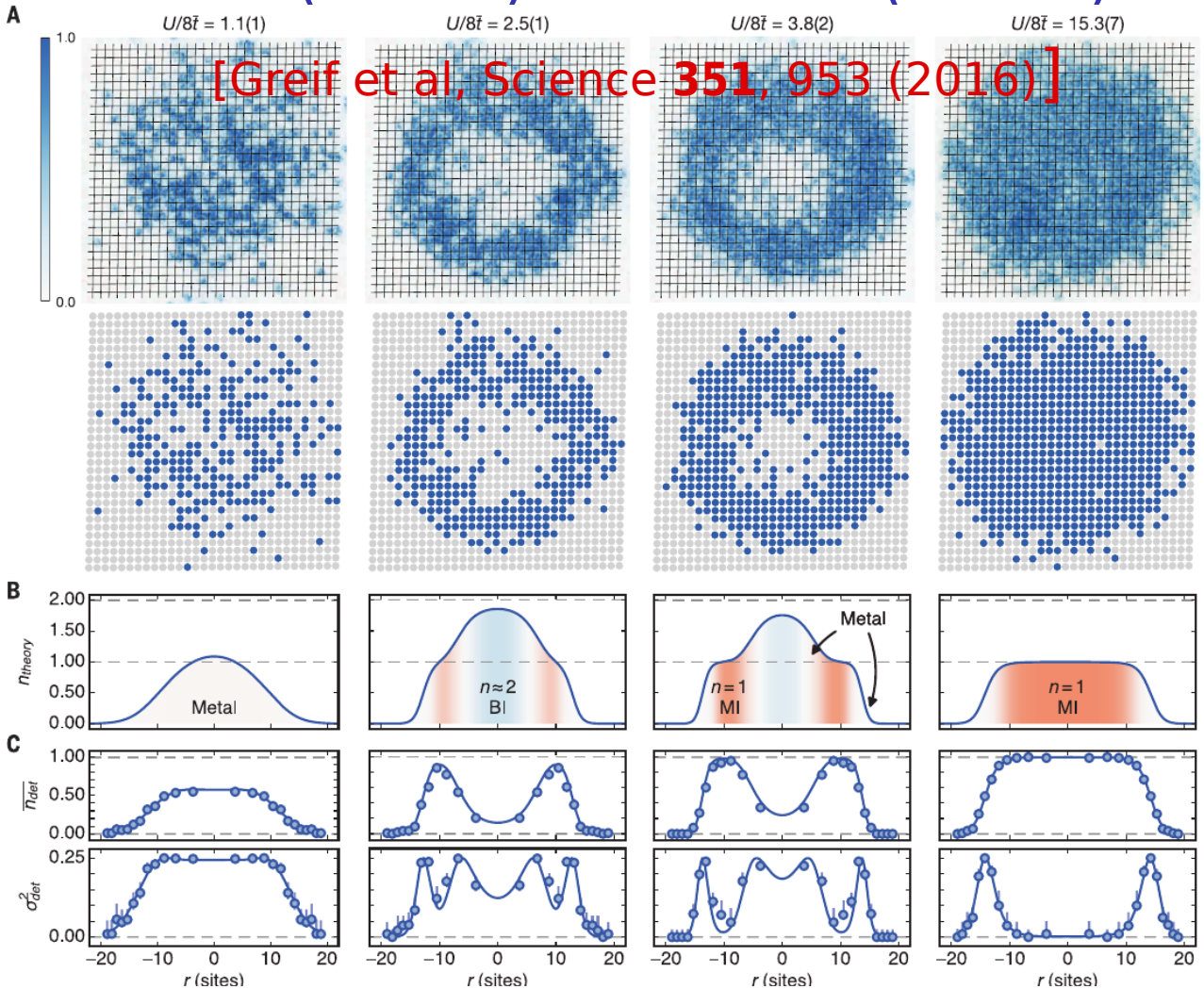


- Light–induced collisions cause atoms on the same lattice site to be lost by pairs:

  Measurement of parity of the occupation of each site

[Bloch, Dalibard, Nascimbène, Nature Physics **8**, 267 (2012)]

FERMIONS: Mott ($n = 1$) and band ($n = 2$) insulators



- Metallic / Insulator phases told apart through atom–number fluctuations $\sigma^2 = \Delta n^2$ on each site:
  metallic phases have larger fluctuations; insulator phases have smaller fluctuations.
- Which of the two insulator phases is/are due to the presence of interactions?
  HINT: the free–particle band structure plays a key role.