Cold Atoms in Optical Lattices 1

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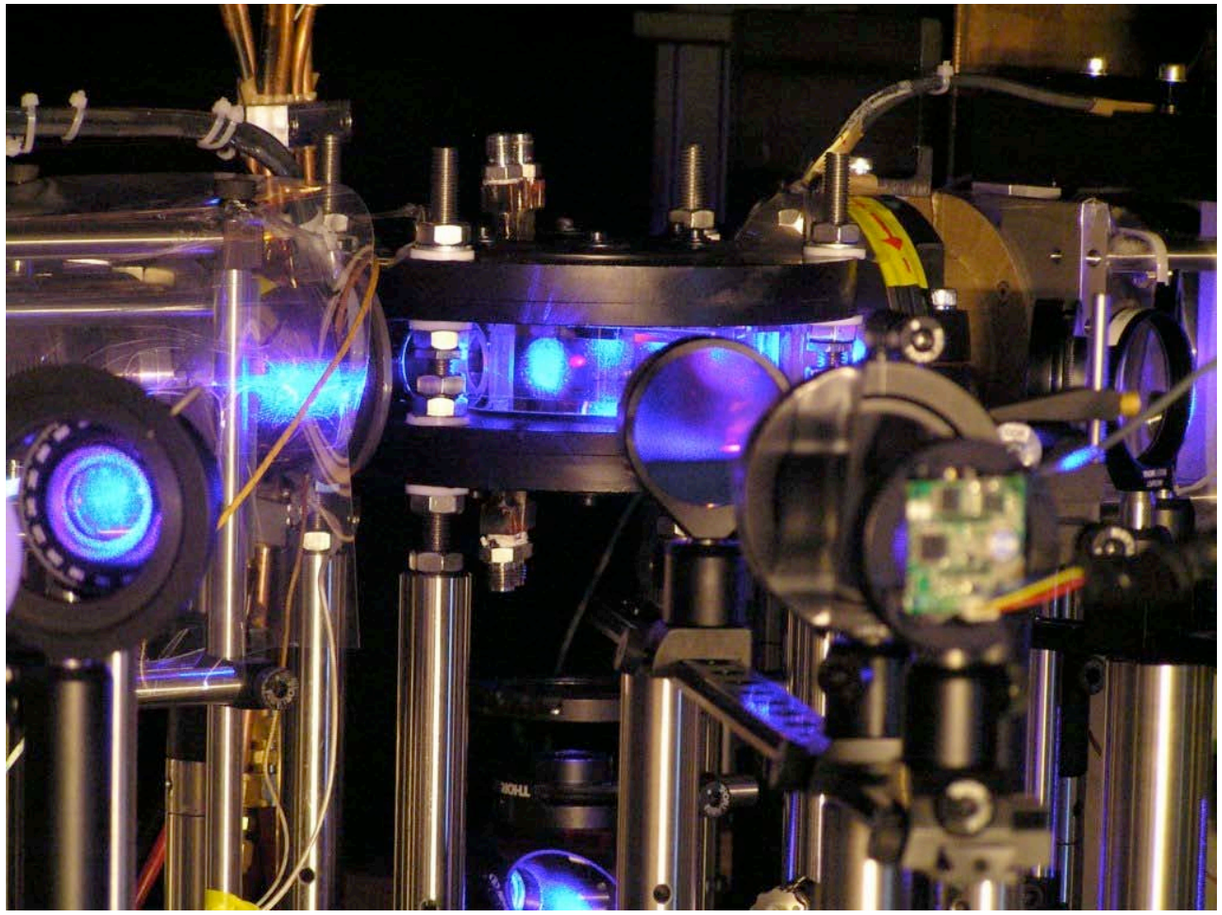
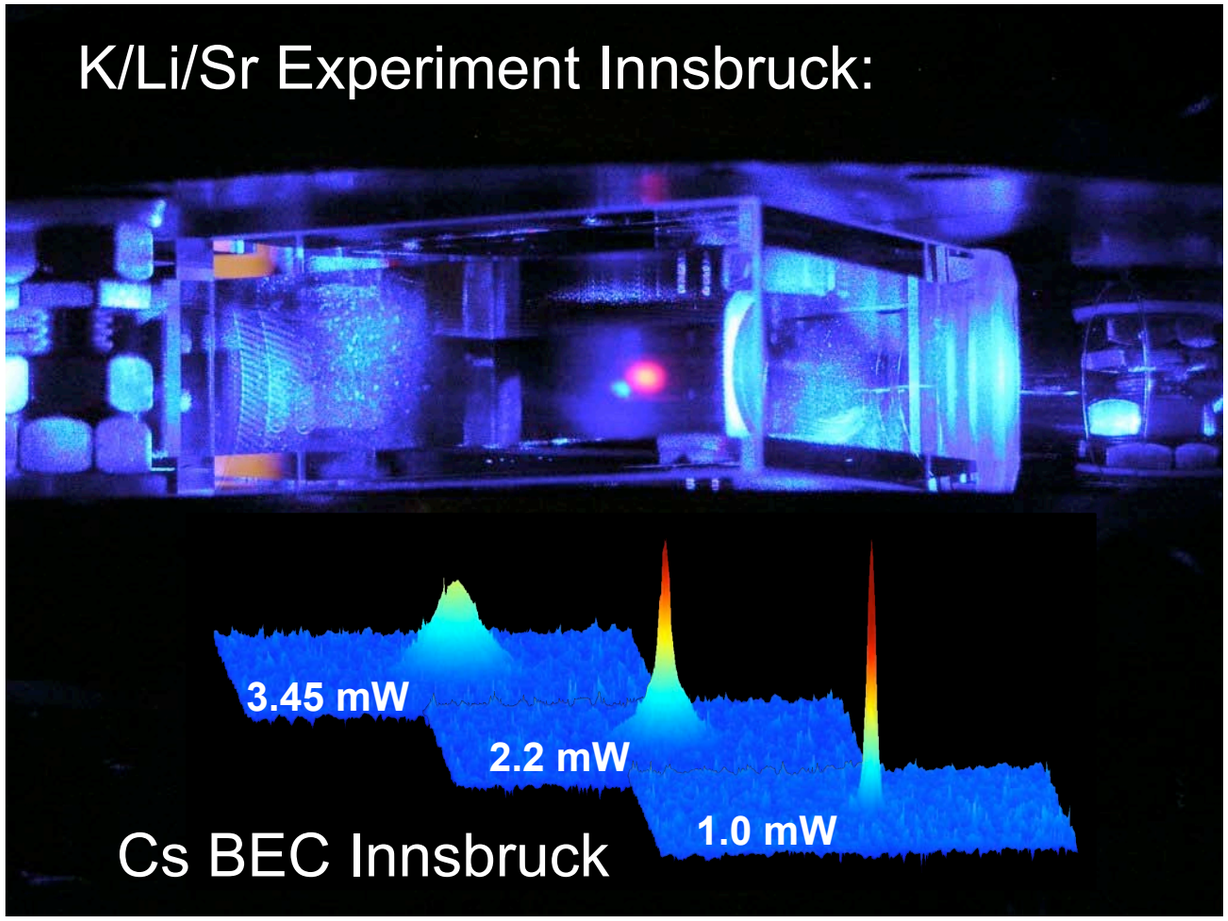
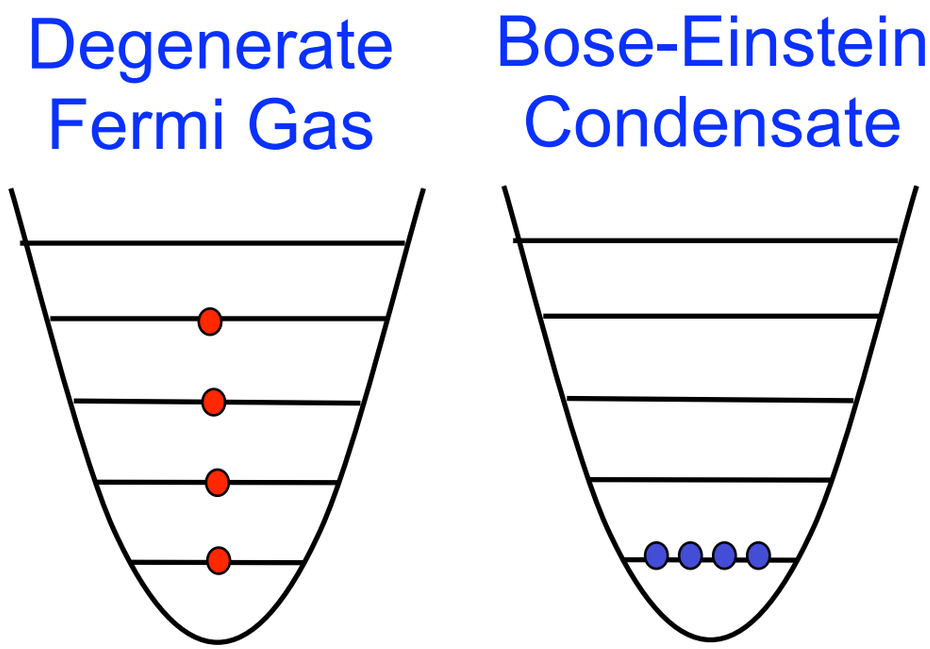
Degenerate Bose/Fermi Gases in the laboratory:

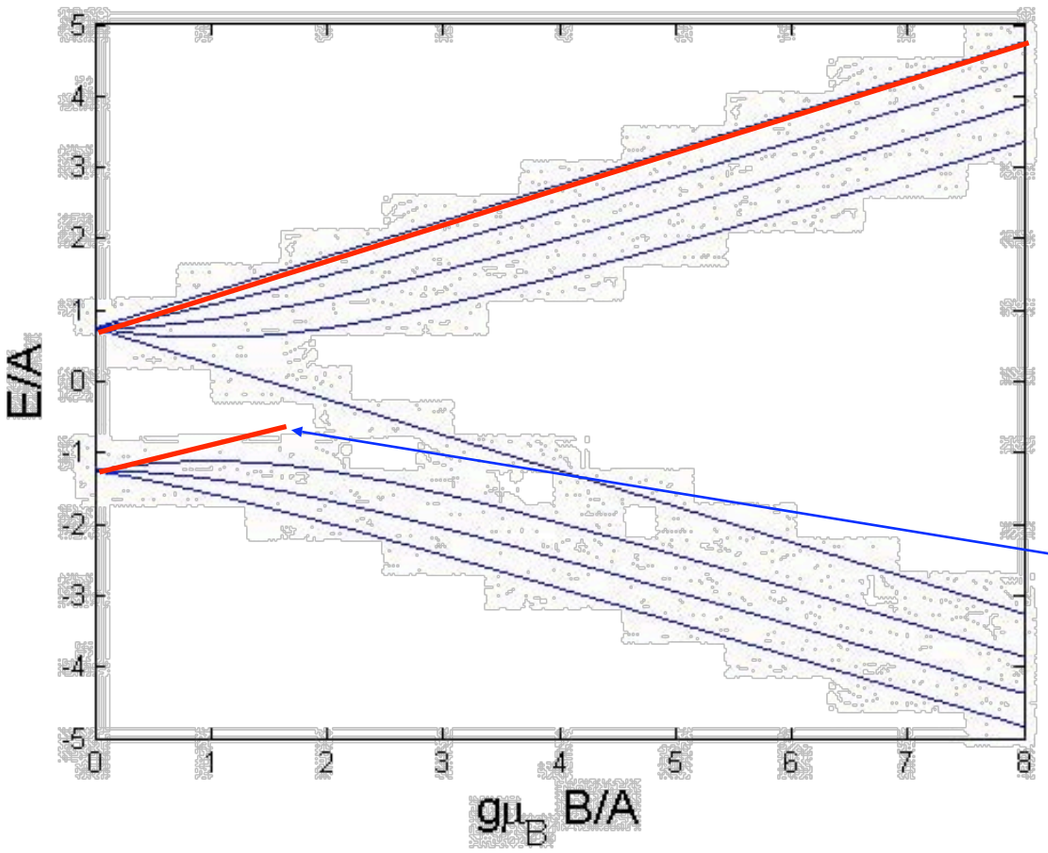


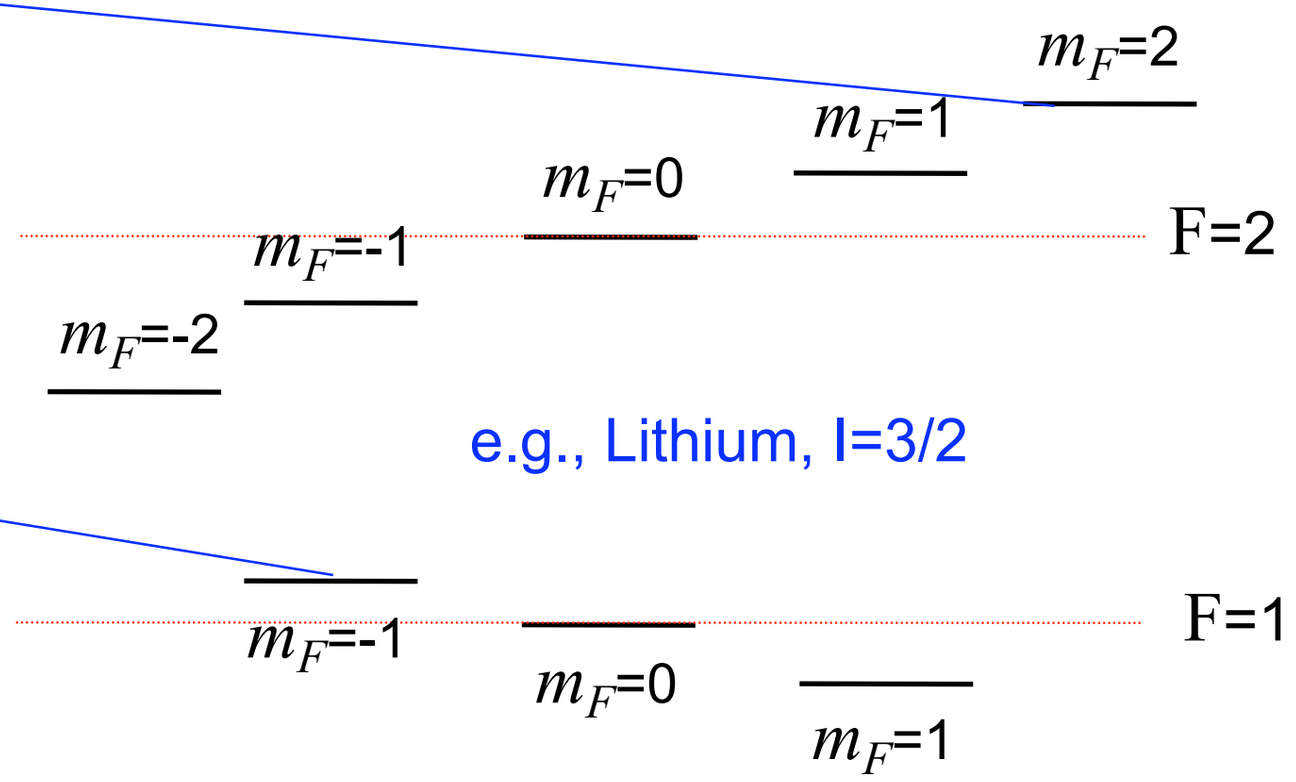


- Features:
  - Control via magnetic field / laser light
  - Microscopically well understood systems

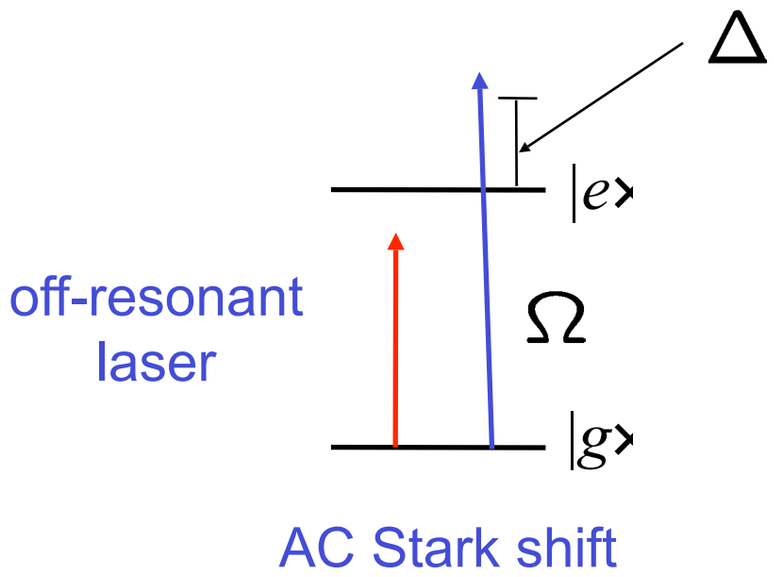


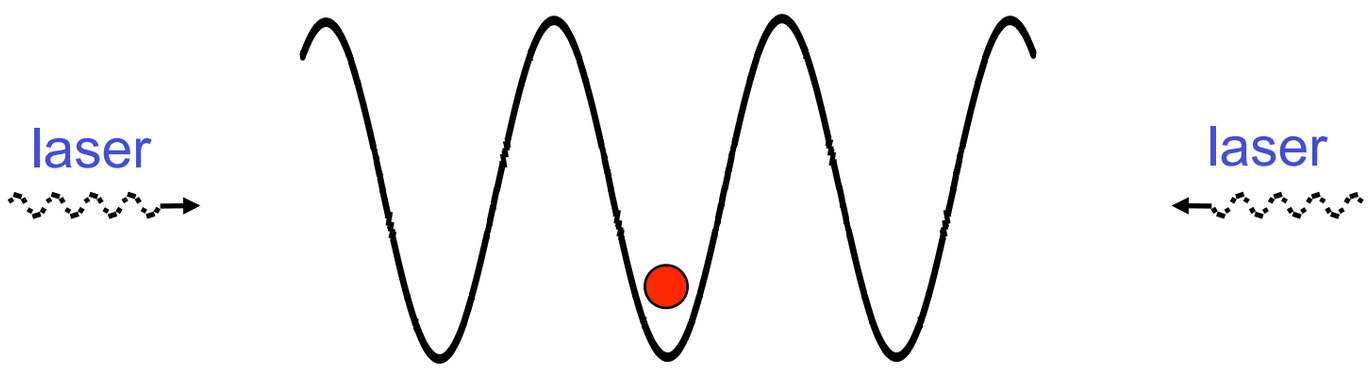
Microscopic Control: Magnetic Traps (Zeeman Shift):





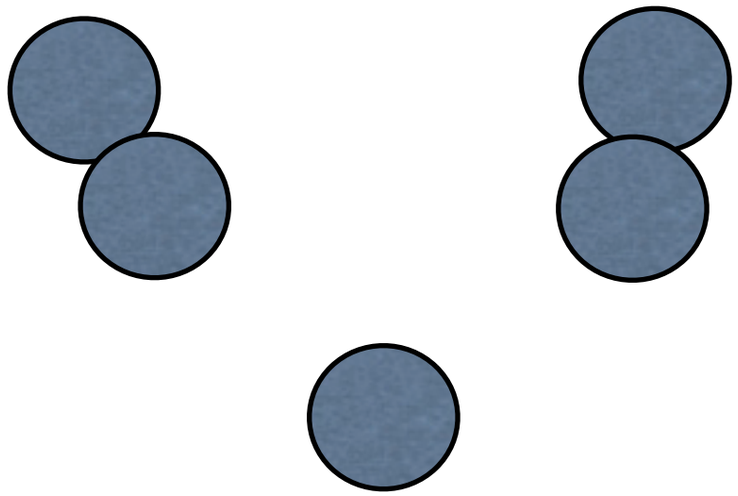
Microscopic Control: Optical Traps (AC-Stark Shift)





$$V(x) = \alpha(\omega) I = V_0 \sin^2(kx)$$

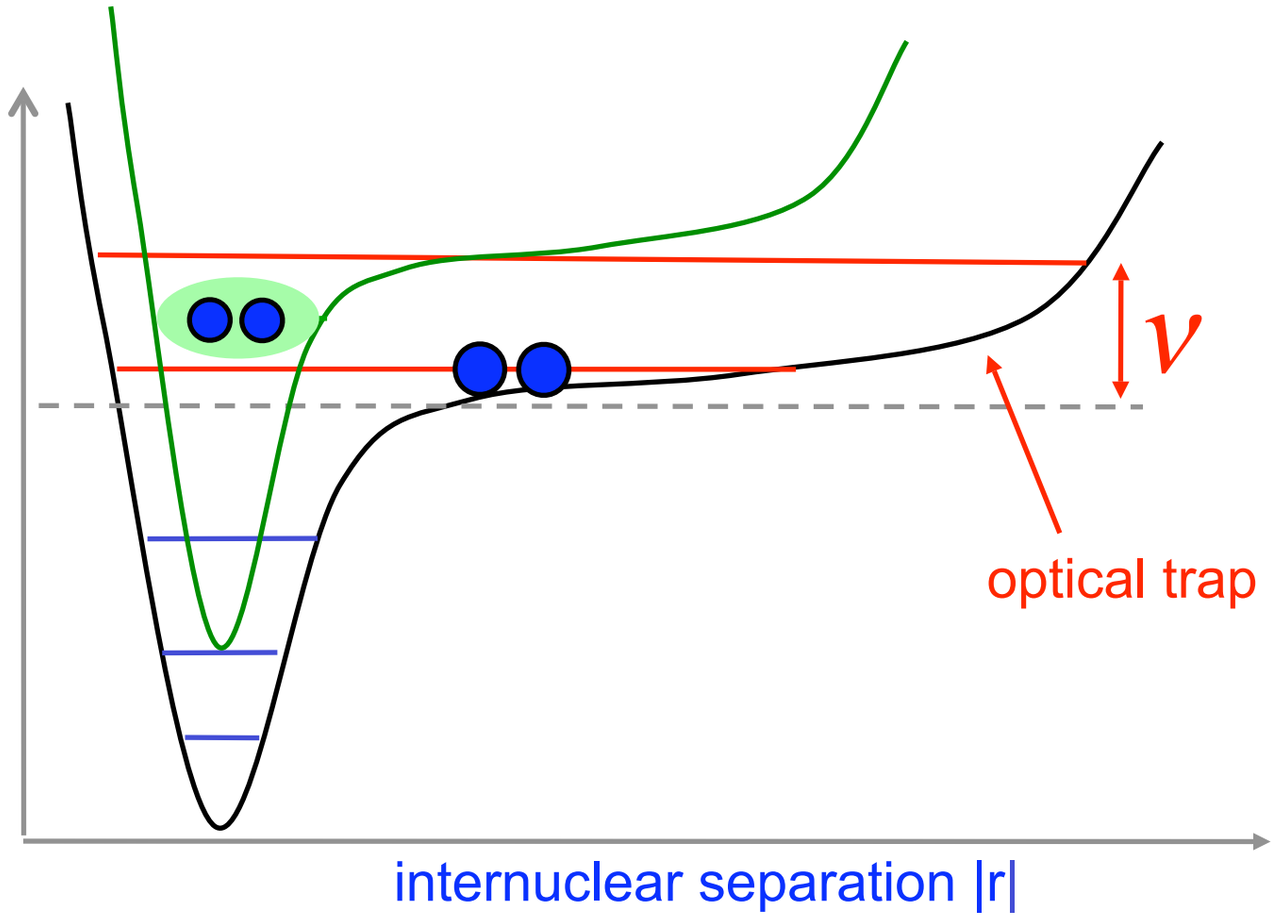
Microscopic Control: Interactions:



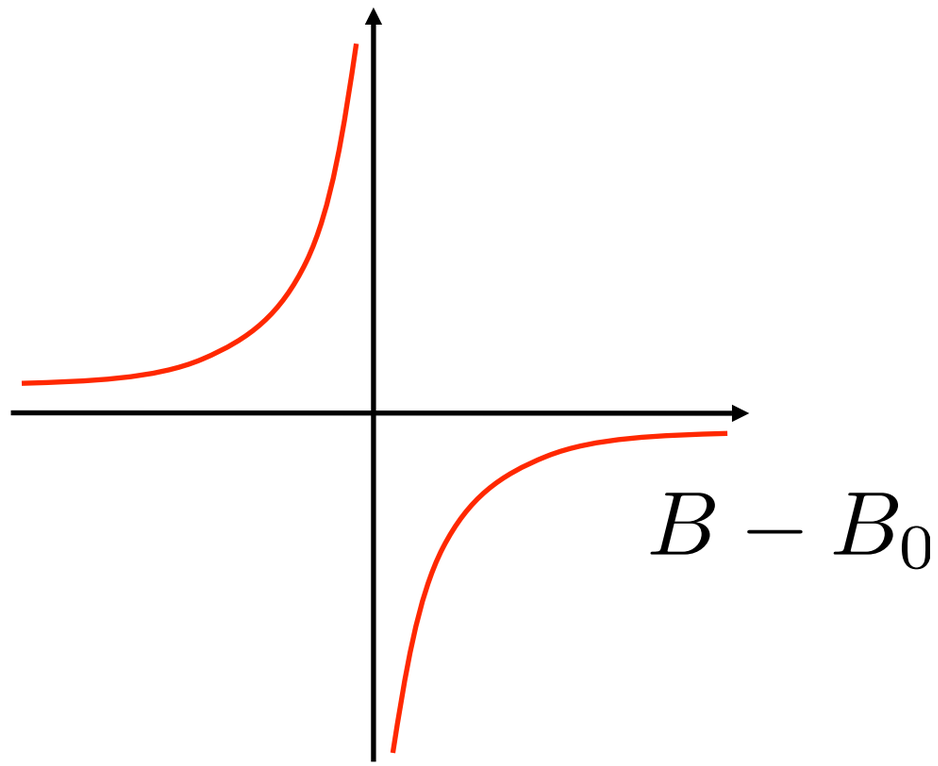
Microscopic understanding of interactions:

- Dilute gas - three body interactions weak
- Low-energy two-body interactions
- Simple microscopic description
  (see lecture on wednesday)

Microscopic Control: Feshbach Resonance

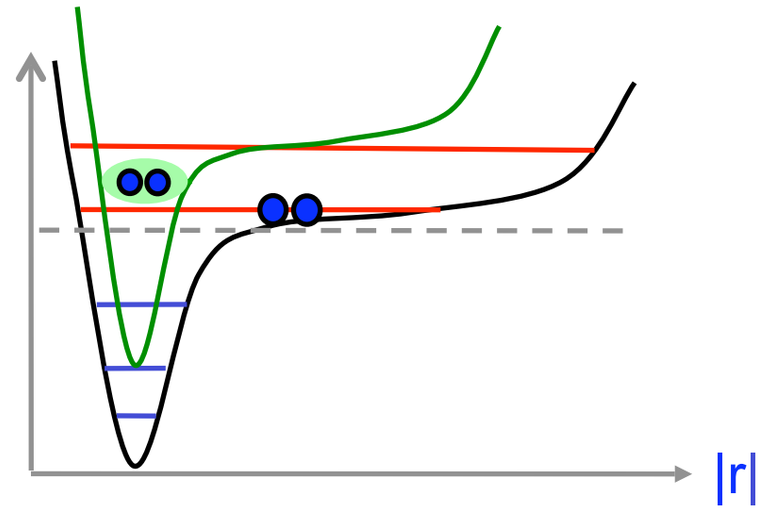


Scattering length
(strength of interactions)

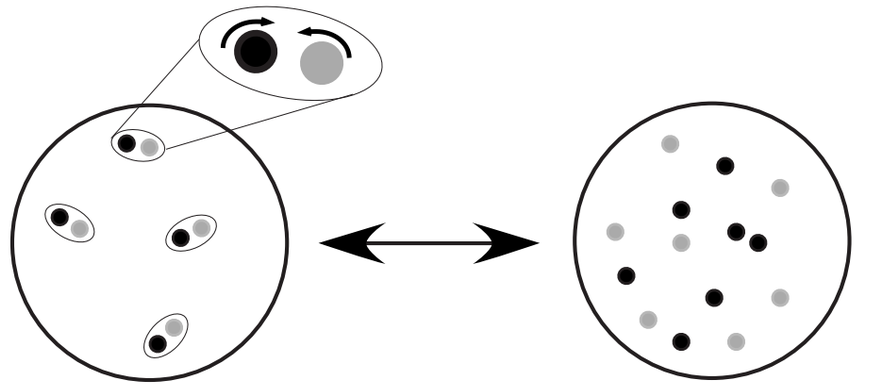


Goal: Use this control to study strongly interacting systems

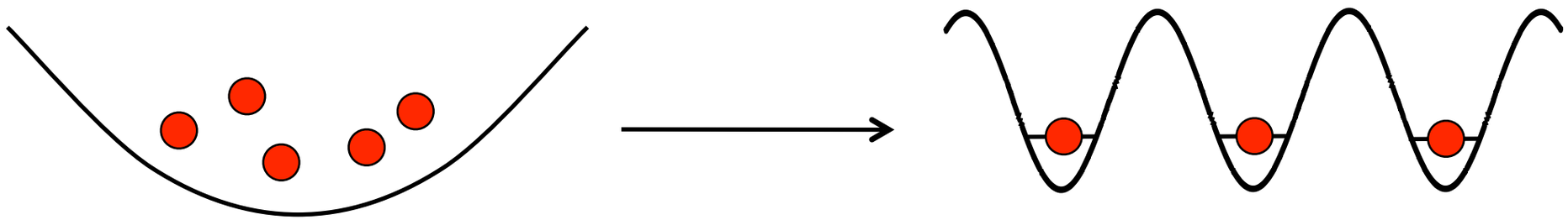
- Fermions near a Feshbach resonance



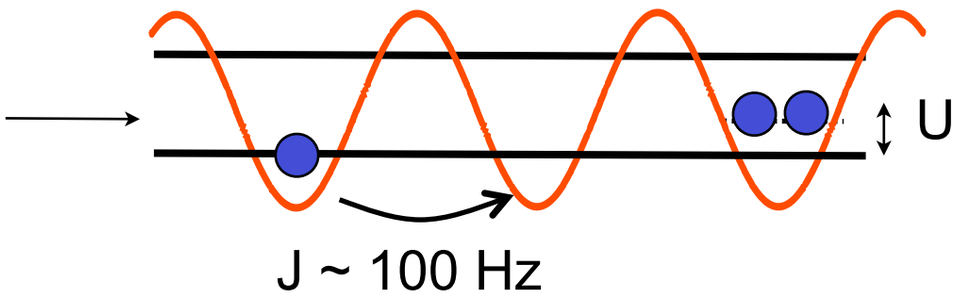
- Low-dimensional Gases



- Load BEC/Degenerate Fermi Gas into a 3D optical lattice



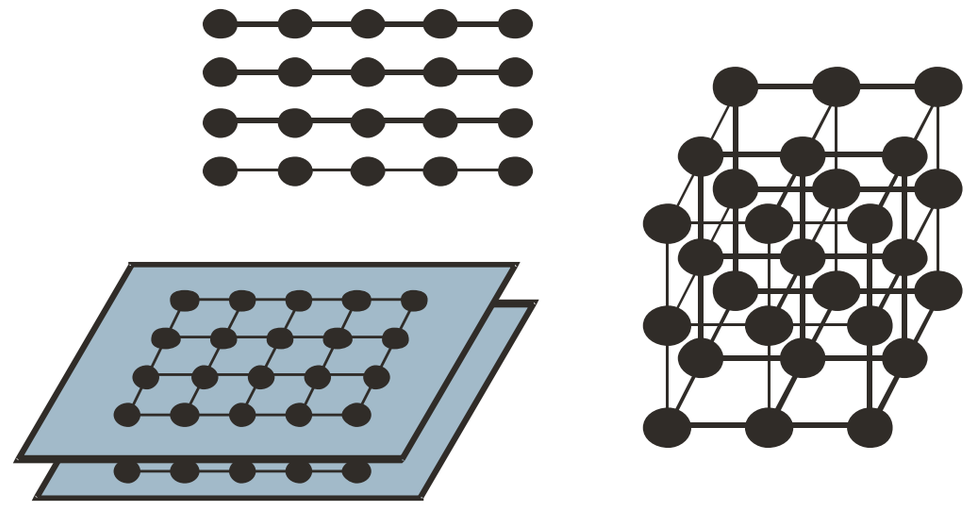
Cold atoms in an optical lattice and Strongly Correlated Systems:



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

Control:

- Modify Lattice structure, effective dimensionality
- Engineer interesting models from solid state physics with great control over system parameters



Clean system:

- No (uncontrollable) disorder
- Weak dissipation (>1s) (cf. phonons in solid state)

Measurements:

- (quasi-)momentum distribution, noise correlations by releasing atoms.
- Spectroscopy (e.g., lattice modulations / Bragg scattering).

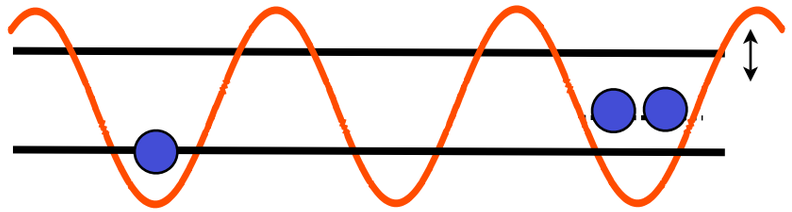
Experiments:

- Bosons, Superfluid-Mott Insulator transition (M. Greiner, I. Bloch et al., Munich, 2001)
- Fermions, (T. Esslinger et al., Zürich 2004)
- Munich, Mainz, Zurich, MIT, Harvard, Maryland, Innsbruck, Hamburg, Florence, Pisa, Oxford, Austin,.....

Outline of Lectures

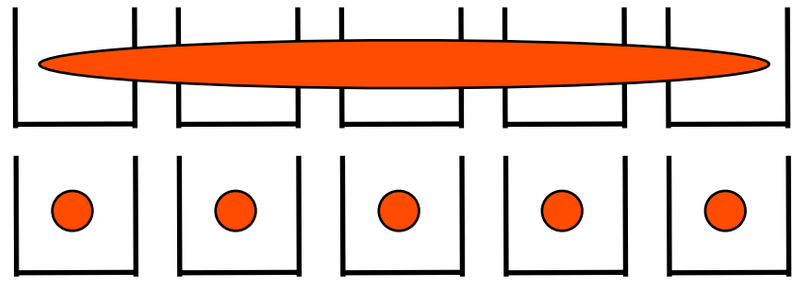
Now:

- Optical Lattices
- Band Structure, Bloch & Wannier functions
- Bose-Hubbard model



Later:

- Phase diagram of the Bose-Hubbard model: Superfluid, Mott-Insulator
- Single-Particle density matrix & correlations

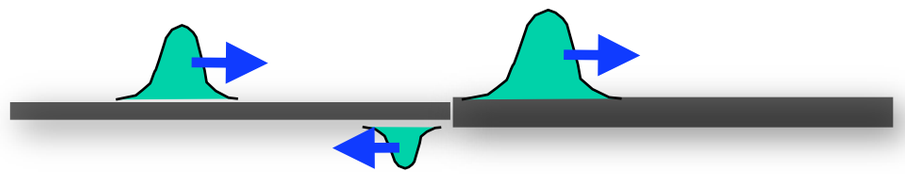


Wednesday:

- Microscopic model for interactions
- Zero-range pseudopotential and its properties

Friday:

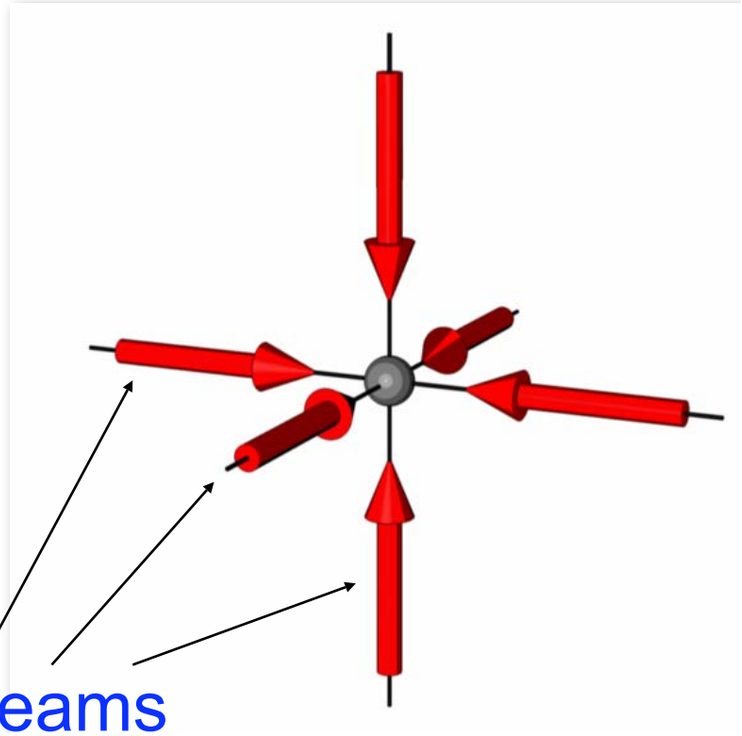
- Transport of atoms in optical lattices in 1D (Andreev Reflections, superfluidity)
- Dynamics of three-body loss in an optical lattice

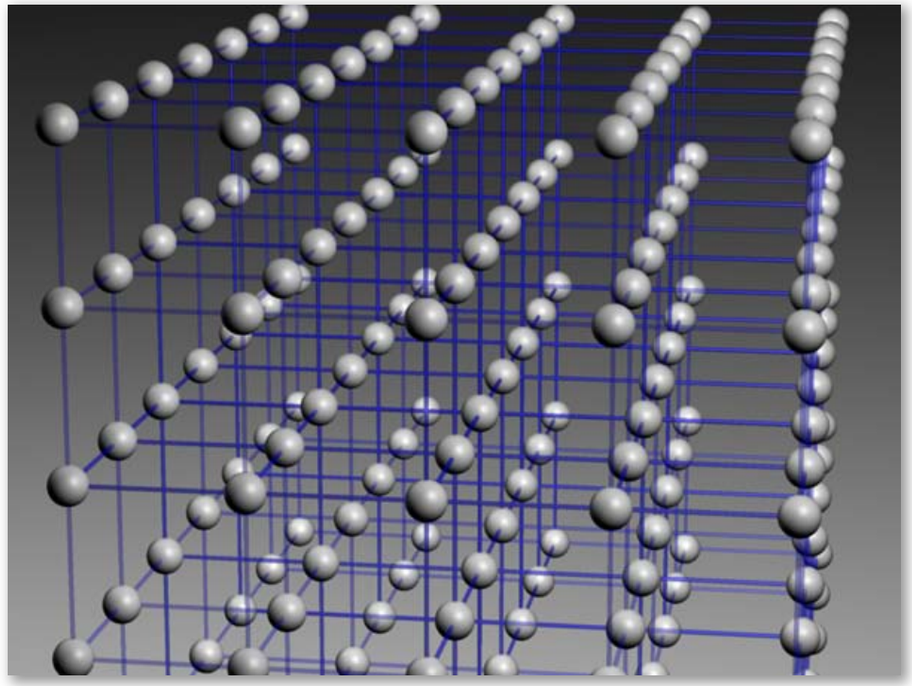


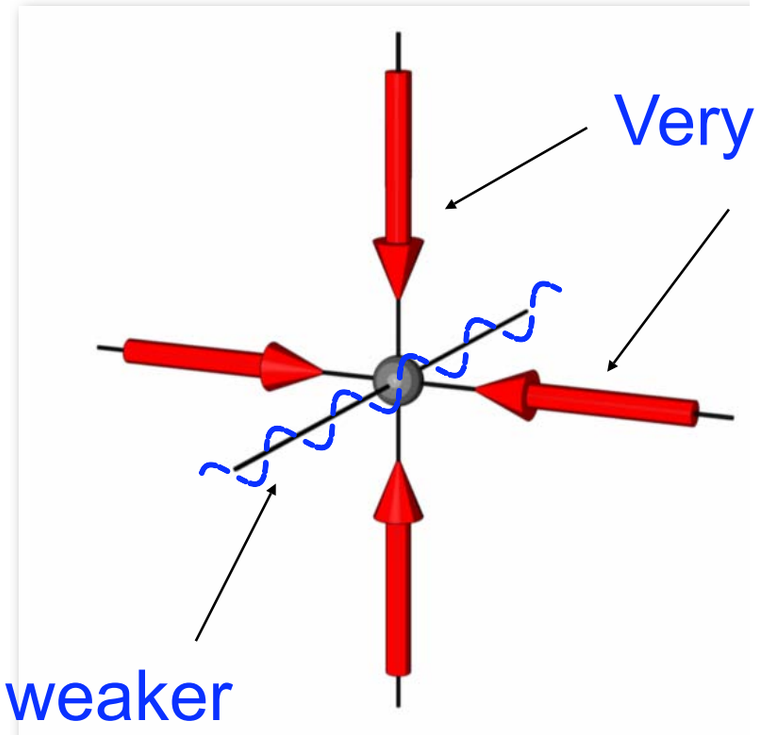
See also:

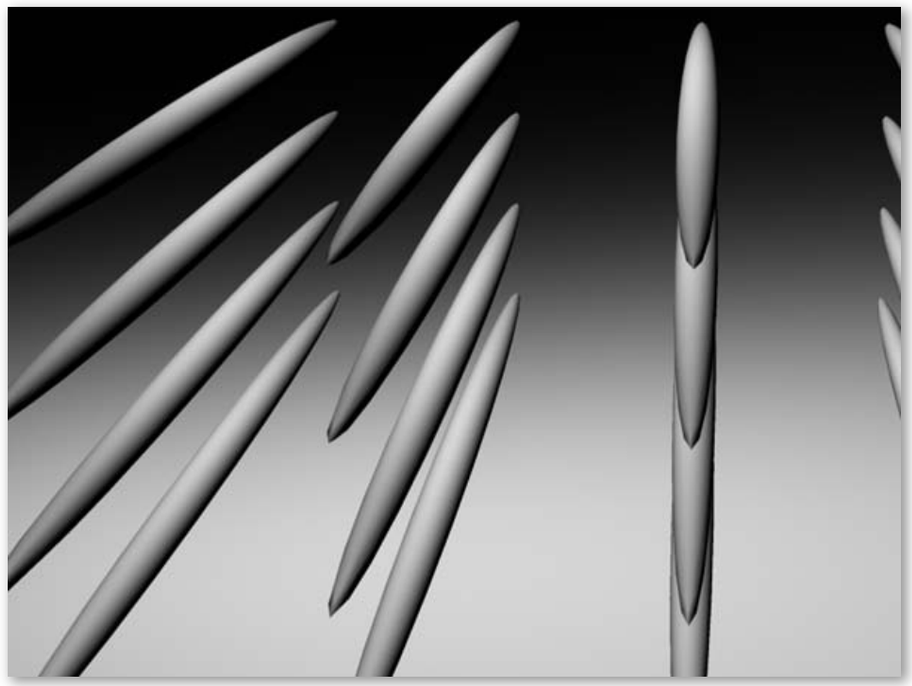
- Simon Fölling - more on Bosons in an optical lattice, experiments
- Michael Köhl - Fermions in an optical lattice
- Dieter Jaksch - Dynamics in 1D, immersion in a superfluid

Optical Lattice Potentials:

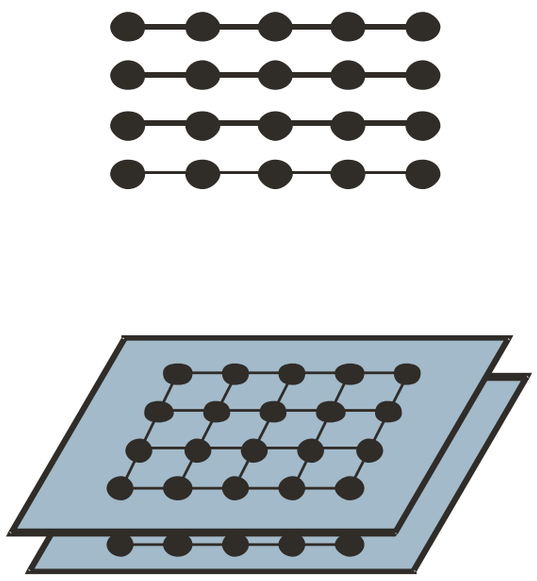


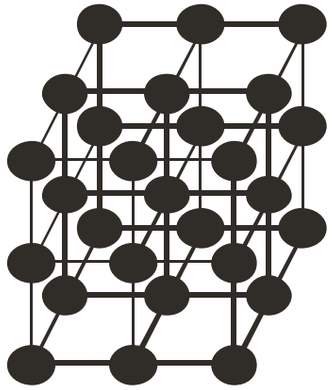




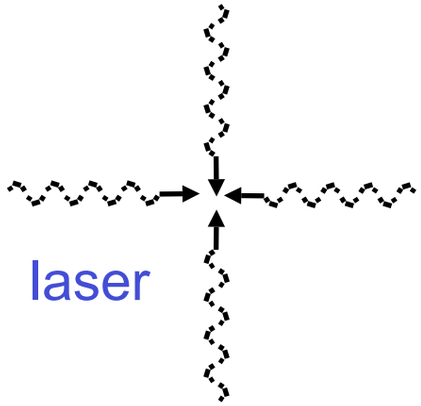


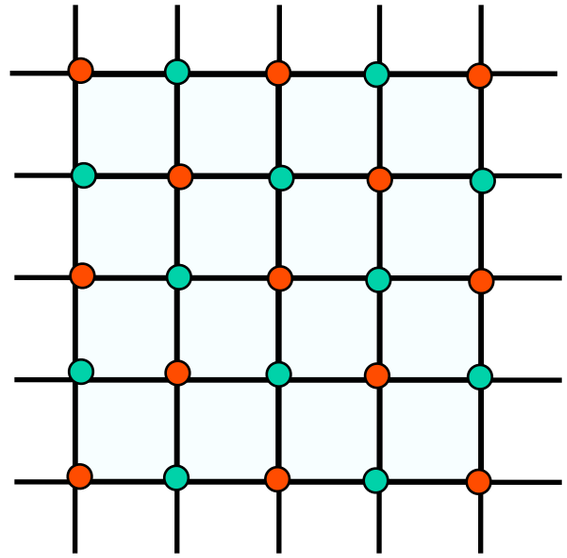
- 1D, 2D and 3D



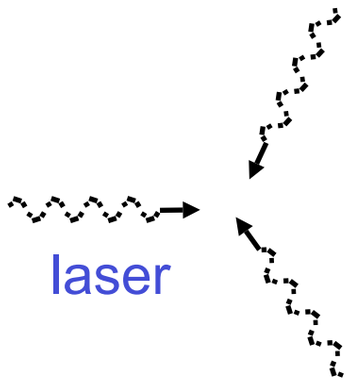


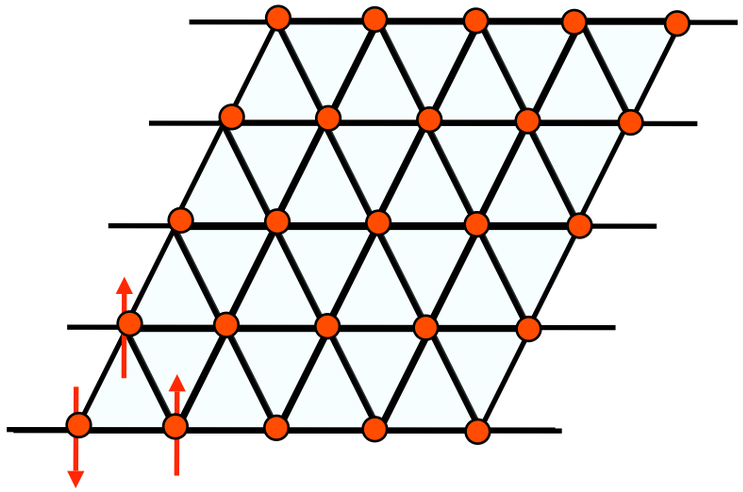
- lattice configurations





square lattice



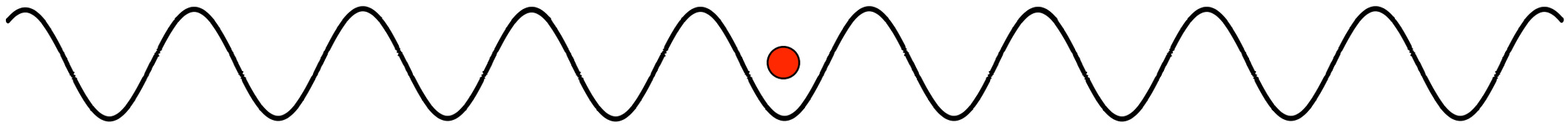


triangular lattice

Band Structure

- In 1D, the coherent dynamics of a single atom in the standing wave is described by the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + V_0 \sin^2(k_l x).$$



Bloch Theorem

- As the Hamiltonian is invariant under translation by one lattice period, a, it commutes with the translation operator:

$$\hat{T} = e^{i\hat{p}a/\hbar}, \quad \hat{T}\psi(x) = \psi(x+a)$$

- As T is unitary, it has eigenfunctions

$$\hat{T}\phi_\alpha(x) = e^{i\alpha}\phi_\alpha(x),$$

with real $\alpha \in [-\pi, \pi]$.

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with real $\alpha \in [-\pi, \pi]$.

- Because

$$\phi_\alpha(x+a) = e^{i\alpha}\phi_\alpha(x)$$

we can write

$$\phi_\alpha(x) = e^{i\alpha x}u_\alpha(x),$$

where $u_\alpha(x)$ is a periodic function with period a.

- Because $[\hat{H}, \hat{T}] = 0$, we can then find simultaneous eigenstates of $\hat{H}$ and $\hat{T}$,

$$\begin{aligned} H\varphi_q(x) &= E\varphi_q(x), \\ T\varphi_q(x) &= e^{iqa}\varphi_q(x), \end{aligned} \tag{1}$$

Bloch Functions

- The eigenstates of this Hamiltonian are then the Bloch eigenstates, which have the form

$$\phi_q^{(n)}(x) = \mathrm{e}^{\mathrm{i}qx}u_q^n(x),$$

where q is the quasimomentum of the eigenstate, $q \in [-\pi/a, \pi/a]$, and $u_q^{(n)}(x)$ are the eigenstates of the Hamiltonian

$$H_q = \frac{(p+q)^2}{2m} + V_0 \sin^2(k_l x),$$

and have the same periodicity as the potential ($u_q^{(n)}(x+a) = u_q^{(n)}(x)$).

$$H_q = \frac{(p+q)^2}{2m} + V_0 \sin^2(k_l x), \qquad \phi_q^{(n)}(x) = \mathrm{e}^{\mathrm{i}qx} u_q^n(x),$$

- Whilst $u_q(x)$ are, in general, complicated functions, they are relatively simple to compute numerically, e.g., by writing the Fourier expansion

$$u_q^{(n)}(x) = \frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} c_j^{(n,q)} \mathrm{e}^{\mathrm{i}2k_l x j},$$

which allows us to reduce to a linear eigenvalue equation in the complex coefficients c_j,

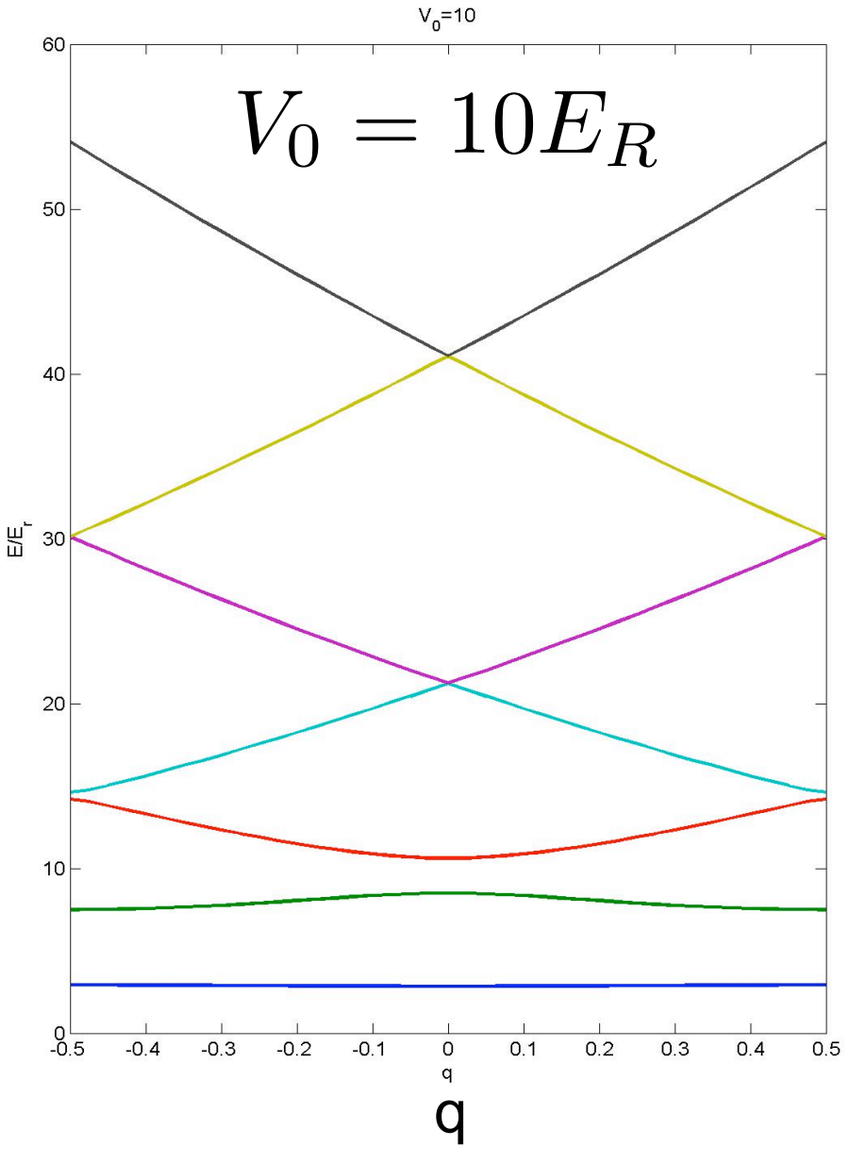
$$\sum_{j'=-l}^{l} H_{jj'} c_{j'}^{(n,q)} = E_q^{(n)} c_j^{(n,q)}$$

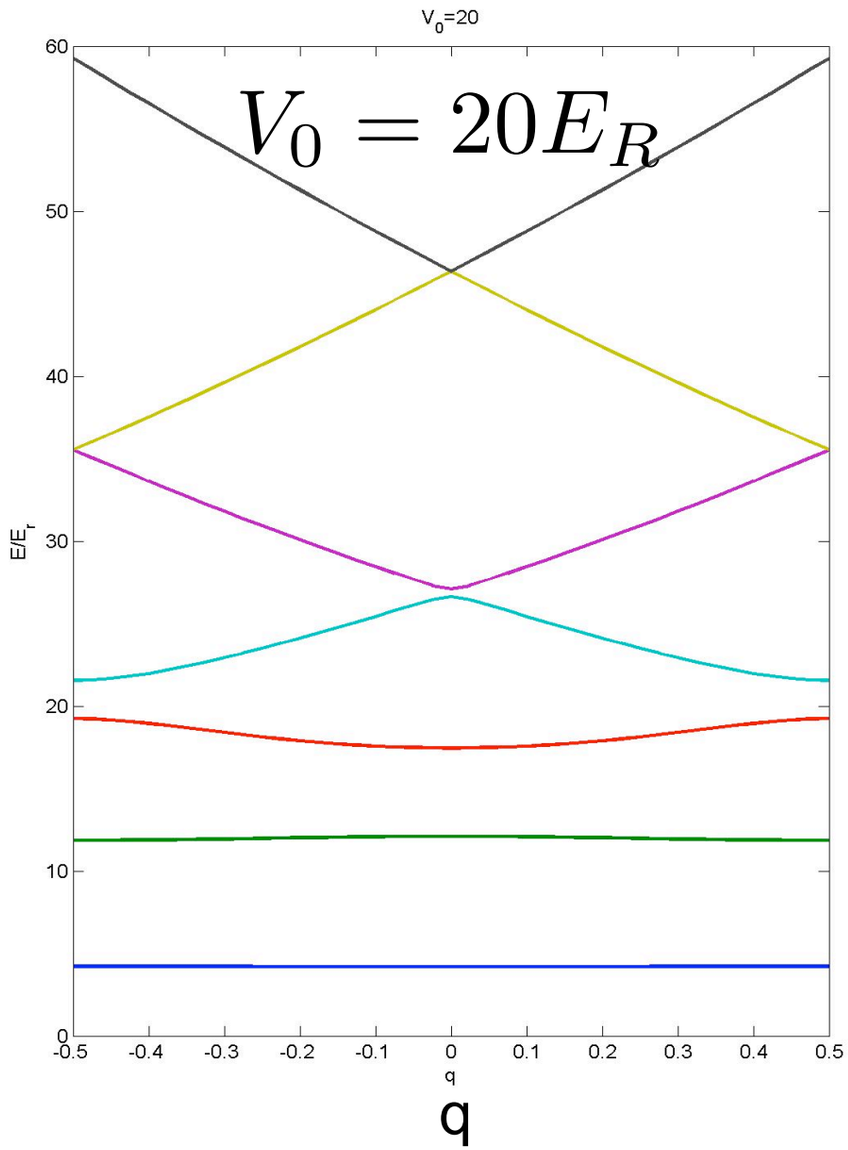
$$H_{jj} = \begin{cases} (2j + q/k_l)^2 E_R + V_0/2\,, & j = j' \\ -V_0/4 & |j - j'| = 1 \\ H_{jj'} = 0 & |j - j'| > 1 \end{cases}$$

- This problem can be diagonalised numerically restricting $j \in \{-l, \ldots, l\}$, and we find for the lowest few bands that good results are obtain for relatively small $l \sim 10$.

- The Bloch eigenstates are normalised so that

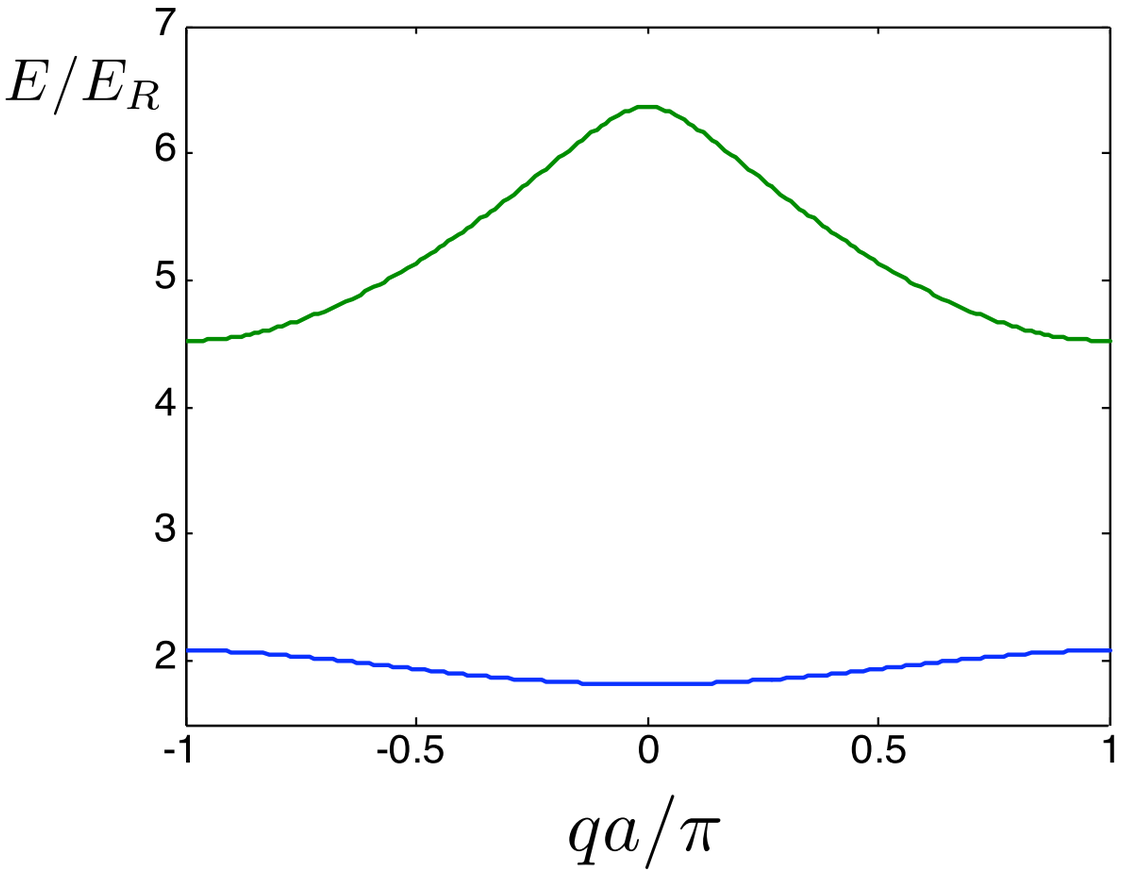
$$\frac{2\pi}{a} \int_0^a |\phi_q^{(n)}(x)|^2 \mathrm{d}x = 1.$$

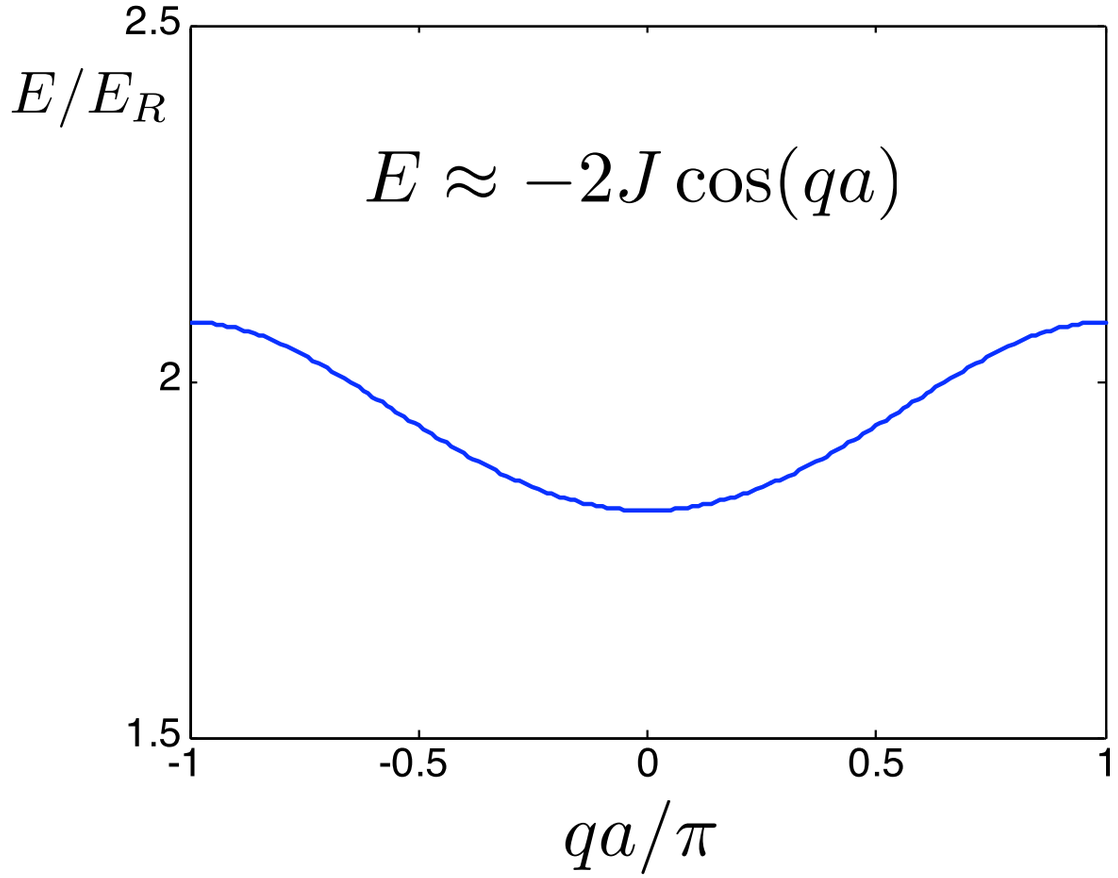




- Depending on the depth of the lattice, particles in the lowest bands, with $E_q^{(n)} \lesssim V_0$ are in bound states of the potential, whilst the higher bands $E_q^{(n)} > V_0$ correspond to free particles.

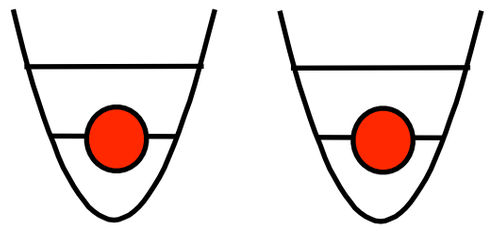
Lowest Two Bloch Bands, V_0=5 E_R





- The lowest two bands are separated in energy by

$$\Delta E = E^{(1)}_{q=\pi/a} - E^{(0)}_{q=\pi/a} = \hbar\omega \approx \hbar\omega_T$$



approximately given by the trapping frequency from the Harmonic oscillator approximation, ω_T.

- When we derive the Bose-Hubbard model we will assume that the temperature and all other energy scales in the system are smaller than ω_T, allowing us to restrict the system to the lowest Bloch band.

Wannier Functions

$$H_q = \frac{(p+q)^2}{2m} + V_0 \sin^2(k_l x), \qquad \phi_q^{(n)}(x) = \mathrm{e}^{\mathrm{i}qx} u_q^n(x),$$

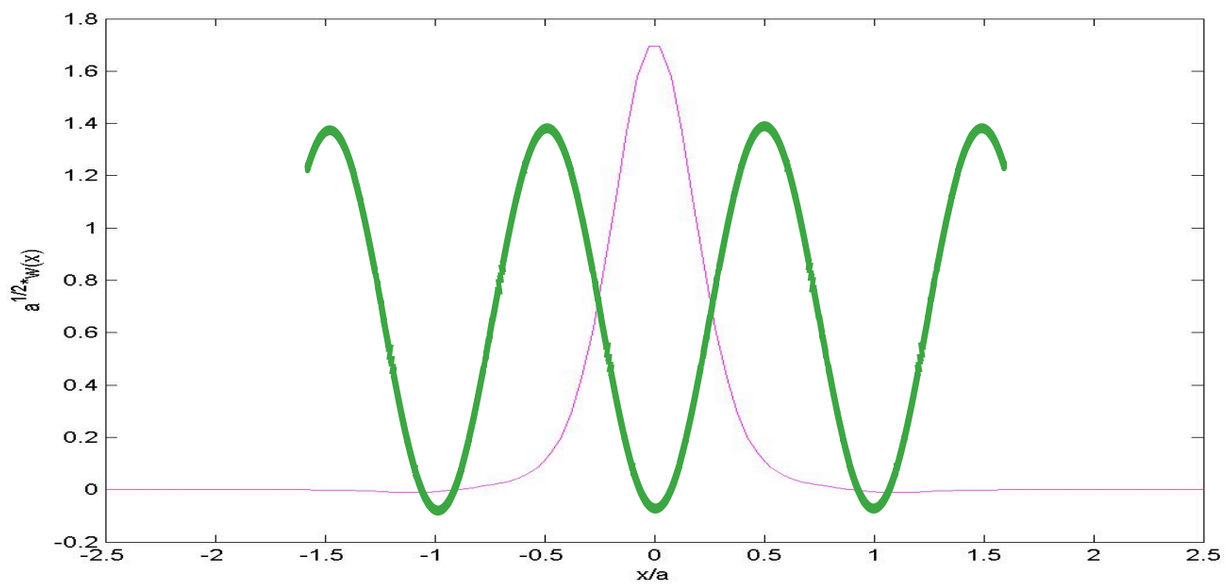
- It is often very convenient to express the Bloch functions in terms of Wannier functions, which also form a complete set of orthogonal basis states. The Wannier functions are given in 1D by

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

where x_i are the minima of the standing wave. Each set of Wannier functions for a given n can be used to express the Bloch functions in that band,

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

- The Wannier functions have the advantage of being localised on particular sites, which makes them useful for describing local interactions between particles.



$$H_q = \frac{(p+q)^2}{2m} + V_0 \sin^2(k_l x), \qquad \phi_q^{(n)}(x) = \mathrm{e}^{\mathrm{i}qx} u_q^n(x), \qquad w_n(x - x_i) = \sqrt{\frac{a}{2\pi}} \int_{-\pi/a}^{\pi/a} \mathrm{d}q \, u_q^n(x) \, \mathrm{e}^{-iqx_i}$$

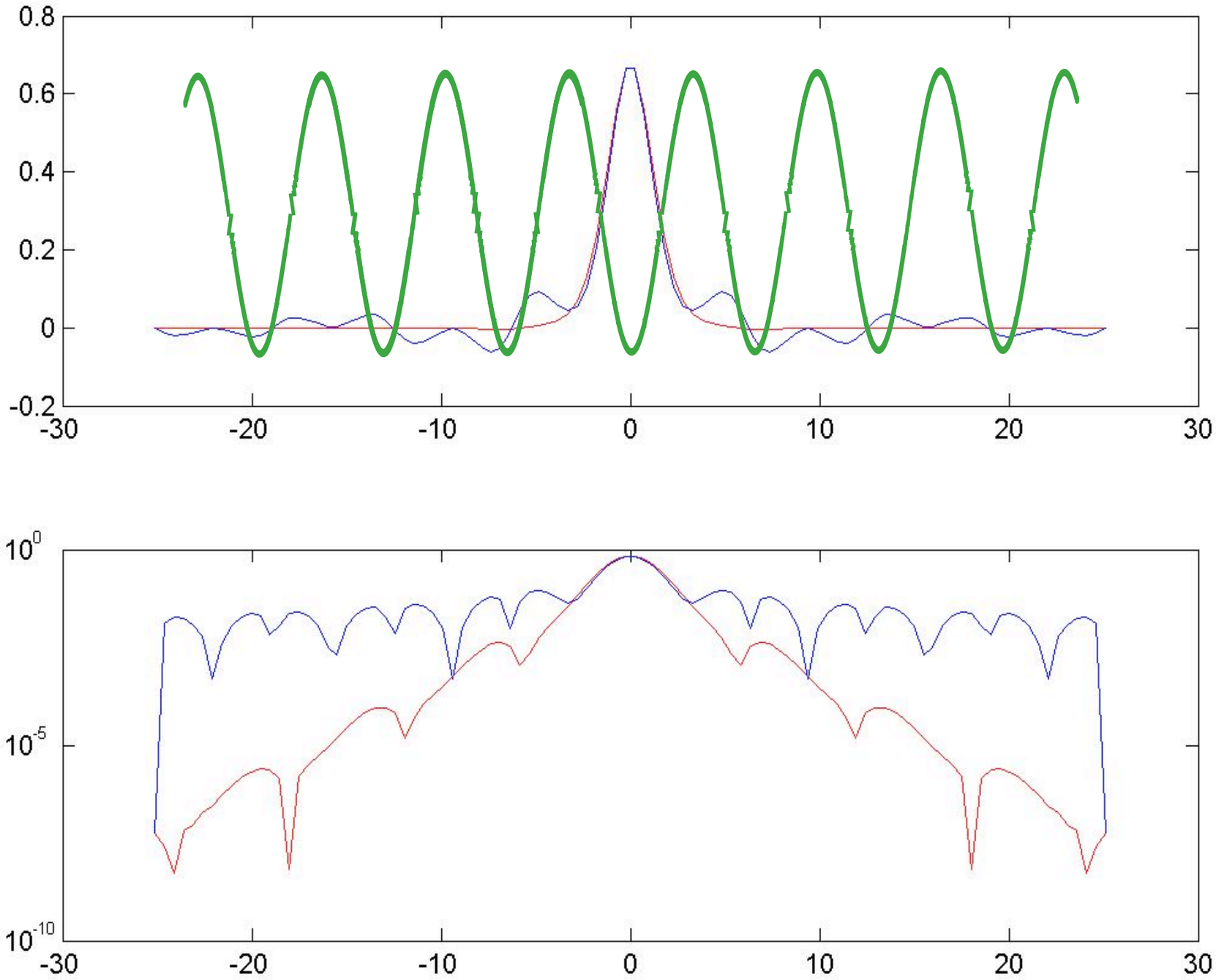
- The Wannier functions are not uniquely defined by the integral over the Bloch functions, as each wavefunction $\phi_q^{(n)}(x)$ is arbitrary up to a complex phase. However, as shown by Kohn [Phys. Rev. 115, 809 (1959)], there exists for each band only one real Wannier function $w_n(x)$ that is:
  - Either symmetric or antisymmetric about either $x = 0$ or $x = a/2$, and
  - Falls off exponentially, i.e., $|w_n(x)| \sim \exp(-h_n x)$ for some $h_n > 0$ as $x \to \infty$.
- These Wannier functions are known as the *maximally localised* Wannier functions, and we will use this choice for the Wannier functions in the rest of our discussions.

- If $u_q^{(n)}(x)$ is expanded as

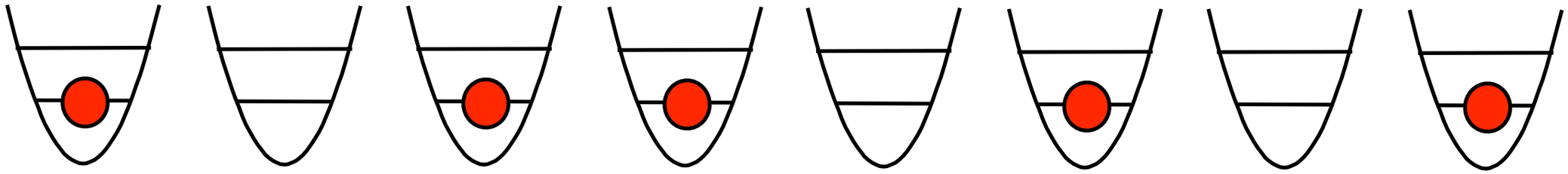
$$u_q^{(n)}(x) = \frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} c_j^{(n,q)} \mathrm{e}^{\mathrm{i}2k_l x j}$$

  the maximally localised Wannier functions can be produced if all $c_m^{n,q}$ are chosen to be purely real for the even bands, $n = 0, 2, 4, \ldots$, and imaginary for the odd bands $n = 1, 3, 5, \ldots$, and are smoothly varying as a function of q.

$$H_q = \frac{(p+q)^2}{2m} + V_0 \sin^2(k_l x), \qquad \phi_q^{(n)}(x) = \mathrm{e}^{\mathrm{i}qx} u_q^n(x), \qquad w_n(x - x_i) = \sqrt{\frac{a}{2\pi}} \int_{-\pi/a}^{\pi/a} \mathrm{d}q \, u_q^n(x) \, \mathrm{e}^{-iqx_i}$$



$$H_q = \frac{(p+q)^2}{2m} + V_0 \sin^2(k_l x), \qquad \phi_q^{(n)}(x) = \mathrm{e}^{\mathrm{i}qx} u_q^n(x), \qquad w_n(x - x_i) = \sqrt{\frac{a}{2\pi}} \int_{-\pi/a}^{\pi/a} \mathrm{d}q \, u_q^n(x) \, \mathrm{e}^{-iqx_i}$$



- Wannier functions for deeply bound bands are very close to the harmonic oscillator wavefunctions, and for many analytical estimates of onsite properties the Wannier functions may be replaced by harmonic oscillator wavefunctions if the lattice is sufficiently deep.

- The major difference between the two is that the Wannier functions are exponentially localised, $|w_n(x)| \sim \exp(-h_n x)$, whereas the harmonic oscillator wavefunctions decay more rapidly in the tails as $\exp[-x^2/(2a_0)^2]$.

Background: Second Quantisation

- When we deal with a system of identical particles, it becomes inconvenient to write the many-body wavefunction in the form

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, ..., \mathbf{r}_N).$$

- Instead, we make use of the fact that identical quantum mechanical particles are indistinguishable, and express the state in terms of the occupation numbers n_i of a complete set of single particle states, e.g., momentum states for free particles

$$|\psi\rangle = |n_{\mathbf{p}_1}, n_{\mathbf{p}_2}, ..., n_{\mathbf{p}_i}, ...\rangle = \prod_i |n_{\mathbf{p}_i}\rangle$$

Identical Bosons

- We now define the *annihilation* operator for mode $\mathbf{p}$ as

$$\hat{b}_{\mathbf{p}} |...n_{\mathbf{p}}...\rangle = \sqrt{n_{\mathbf{p}}} |...(n_{\mathbf{p}} - 1)...\rangle$$

- The adjoint of this operator is then the creation operator $b^\dagger_{\mathbf{p}}$, and it can be shown that

$$\hat{b}^\dagger_{\mathbf{p}} |...n_{\mathbf{p}}...\rangle = \sqrt{n_{\mathbf{p}} + 1} |...(n_{\mathbf{p}} + 1)...\rangle$$

- The relevant commutator relations are given by

$$[\hat{b}_{\mathbf{p}}, \hat{b}^{\dagger}_{\mathbf{p}'}] = \delta_{\mathbf{p},\mathbf{p}'}$$
$$[\hat{b}_{\mathbf{p}}, \hat{b}_{\mathbf{p}'}] = [\hat{b}^{\dagger}_{\mathbf{p}}, \hat{b}^{\dagger}_{\mathbf{p}'}] = 0$$

- Because

$$\hat{b}^{\dagger}_{\mathbf{p}} \hat{b}^{\dagger}_{\mathbf{p}'} \left|\phi\right\rangle = \hat{b}^{\dagger}_{\mathbf{p}'} \hat{b}^{\dagger}_{\mathbf{p}} \left|\phi\right\rangle$$

  these states are symmetric under interchange of particles, and we are dealing with a system of Bosons.

- These states are called Fock states, or number states, because they are eigenstates of the particle number operator

$$\hat{N}_{\mathbf{p}} = \hat{b}^{\dagger}_{\mathbf{p}} \hat{b}_{\mathbf{p}}$$
$$\hat{N}_{\mathbf{p}} \left|...n_{\mathbf{p}}...\right\rangle = n_{\mathbf{p}} \left|...n_{\mathbf{p}}...\right\rangle$$

- $\{N_{\mathbf{p}}\}$ forms a complete set of commuting observables, and thus all other possible many-body states can be constructed from superpositions of Fock states.
- Using the number operator, we can construct the momentum operator as

$$\hat{\mathbf{P}} = \sum_{\mathbf{p}} \mathbf{p} \hat{N}_{\mathbf{p}} = \sum_{\mathbf{p}} \mathbf{p}\, \hat{b}^{\dagger}_{\mathbf{p}} \hat{b}_{\mathbf{p}}$$

- The kinetic energy operator is then similarly written as

$$\hat{H}_{KE} = \sum_{\mathbf{p}} E_{\mathbf{p}} \hat{N}_{\mathbf{p}} = \sum_{\mathbf{p}} \frac{p^2}{2m}\, \hat{b}^{\dagger}_{\mathbf{p}} \hat{b}_{\mathbf{p}}$$

- Note the similarities between this formalism, and the formalism for the harmonic oscillator with creation and annihilation operators for the excitations. Here, each state behaves as an independent harmonic oscillator, and the number of particles in the state are the excitation level of that oscillator.

Identical Fermions

- The state for Fermions must be antisymmetric under interchange of particles, and therefore the fermion creation and annihilation operators must obey the relations

$$\hat{c}^\dagger_{\mathbf{p}}\hat{c}^\dagger_{\mathbf{p}'} = -\hat{c}^\dagger_{\mathbf{p}'}\hat{c}^\dagger_{\mathbf{p}}, \quad \hat{c}_{\mathbf{p}}\hat{c}_{\mathbf{p}'} = -\hat{c}_{\mathbf{p}'}\hat{c}_{\mathbf{p}}$$

  and

$$\hat{c}_{\mathbf{p}}\hat{c}^\dagger_{\mathbf{p}'} + \hat{c}^\dagger_{\mathbf{p}'}\hat{c}_{\mathbf{p}} = \delta_{\mathbf{p},\mathbf{p}'}$$

- These are so-called anticommutation relations, defined as

$$\{A, B\} = [A, B]_+ = AB + BA$$

- We can thus write the relations for Fermionic operators as

$$[\hat{c}_{\mathbf{p}}, \hat{c}^\dagger_{\mathbf{p}'}]_+ = \delta_{\mathbf{p},\mathbf{p}'}$$
$$[\hat{c}_{\mathbf{p}}, \hat{c}_{\mathbf{p}'}]_+ = [\hat{c}^\dagger_{\mathbf{p}}, \hat{c}^\dagger_{\mathbf{p}'}]_+ = 0$$

- Note that these operators obey the Pauli exclusion principle, as

$$\hat{c}_{\mathbf{p}}\hat{c}_{\mathbf{p}} = -\hat{c}_{\mathbf{p}}\hat{c}_{\mathbf{p}}, \Rightarrow \hat{c}^2_{\mathbf{p}} = 0,$$

  and thus

$$\hat{N}^2_{\mathbf{p}} = \hat{c}^\dagger_{\mathbf{p}}\hat{c}_{\mathbf{p}}\hat{c}^\dagger_{\mathbf{p}}\hat{c}_{\mathbf{p}} = \hat{c}^\dagger_{\mathbf{p}}\hat{c}_{\mathbf{p}} - \hat{c}^\dagger_{\mathbf{p}}\hat{c}^\dagger_{\mathbf{p}}\hat{c}_{\mathbf{p}}\hat{c}_{\mathbf{p}} = \hat{c}^\dagger_{\mathbf{p}}\hat{c}_{\mathbf{p}} = \hat{N}_{\mathbf{p}}$$

  so that the only allowed eigenvalues for $\hat{N}_{\mathbf{p}}$ for Fermions are 0 and 1.

Field Operators

- We define the field operators

$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{p}} \mathrm{e}^{i(\mathbf{k}.\mathbf{r} - \omega_p t)} \hat{a}_{\mathbf{p}}$$

  where $\mathbf{k} = \mathbf{p}/\hbar$, $\omega_p = E_p/\hbar = p^2/(2m\hbar)$.

- This operator obeys the commuator (or equivalent anticommutator for fermions)

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}')$$

- These operators can be interpreted as the creation and annihilation operators for a state in which a particle is located at the point $\mathbf{r}$, and are the Fourier transforms of the momentum space operators.

$$|\mathbf{r}\rangle = \hat{\psi}^\dagger(\mathbf{r}) |0\rangle$$

- Many useful forms involving the field operators can be proven using the wave-function for a particle of momentum $\mathbf{p}$ in a box of volume V,

$$\langle \mathbf{r} | \, \mathbf{p} \rangle = \frac{1}{\sqrt{V}} \mathrm{e}^{i(\mathbf{k}.\mathbf{r} - \omega_p t)}$$

  together with the identity

$$\int_V d^3r \; \mathrm{e}^{i\mathbf{k}.\mathbf{r}} = \begin{cases} V, & k = 0 \\ 0, & k \neq 0 \end{cases} = V \, \delta_{\mathbf{k},\mathbf{0}}$$

- For example,

$$\hat{H}_{KE} = \int d^3r \, \hat{\psi}^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 \right) \hat{\psi}(\mathbf{r})$$

$$\hat{P} = \int d^3r \, \hat{\psi}^\dagger(\mathbf{r}) \, (-i\hbar\nabla) \, \hat{\psi}(\mathbf{r})$$

$$\hat{N} = \int d^3r \, \hat{\psi}^\dagger(\mathbf{r}) \, \hat{\psi}(\mathbf{r})$$

- Interactions between two atoms described by a potential $V_2(\mathbf{r}_1 - \mathbf{r}_2)$ produce a Hamiltonian of the form $\hat{H} = \hat{H}_0 + \hat{H}_{int}$, with

$$\hat{H}_{int} = \frac{1}{2} \int d^3r \int d^3r' \, \hat{\psi}^\dagger(\mathbf{r}, t) \, \hat{\psi}^\dagger(\mathbf{r}', t) \, V_2(\mathbf{r}' - \mathbf{r}) \, \hat{\psi}(\mathbf{r}', t) \, \hat{\psi}(\mathbf{r}, t)$$

Many-body Hamiltonian:

- The many-body Hamiltonian for the dilute, weakly interacting Bose gas may be written in terms of bosonic operators, which obey

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}')$$

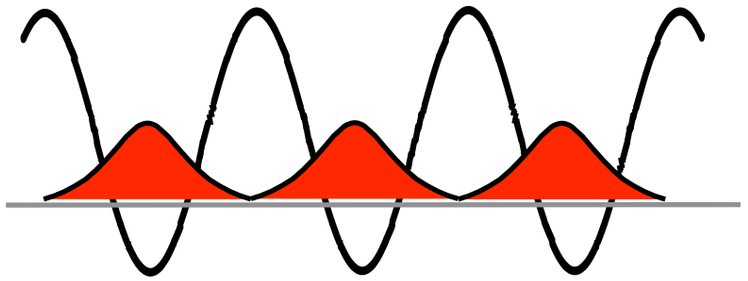
as

$$\hat{H} \approx \int d^3r\, \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V_0(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) + \frac{g}{2} \int d^3r \;\; \hat{\psi}^\dagger(\mathbf{r})\, \hat{\psi}^\dagger(\mathbf{r}) \;\, \hat{\psi}(\mathbf{r})\, \hat{\psi}(\mathbf{r})$$

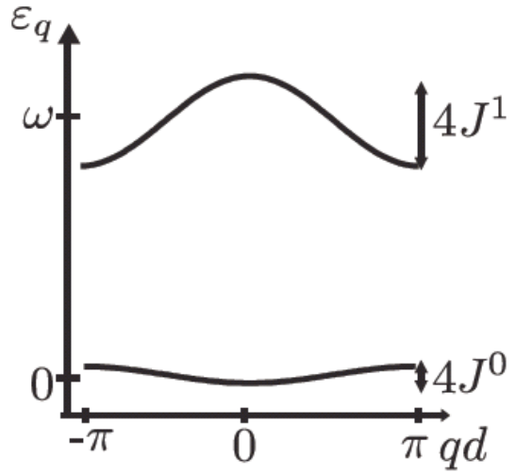
with $g = \frac{4\pi\hbar^2 a_s}{m}$, where a_s is the scattering length.

- This is valid under the assumptions:
  - The gas is sufficiently dilute that:
    - Only two-body interactions are important
    - We can treat the composite atoms as Bosons
  - The energy/temperature are sufficiently small that two-body scattering reduces to s-wave processes, parameterised by the scattering length.
  - That the scattering length a_s is sufficiently small that we can ignore corrections to g outside the Born approximation.
- These assumptions are typically satisfied when we load atoms from a BEC into an optical lattice. Thus, the same second-quantised Hamiltonian is valid.

The Bose-Hubbard Model

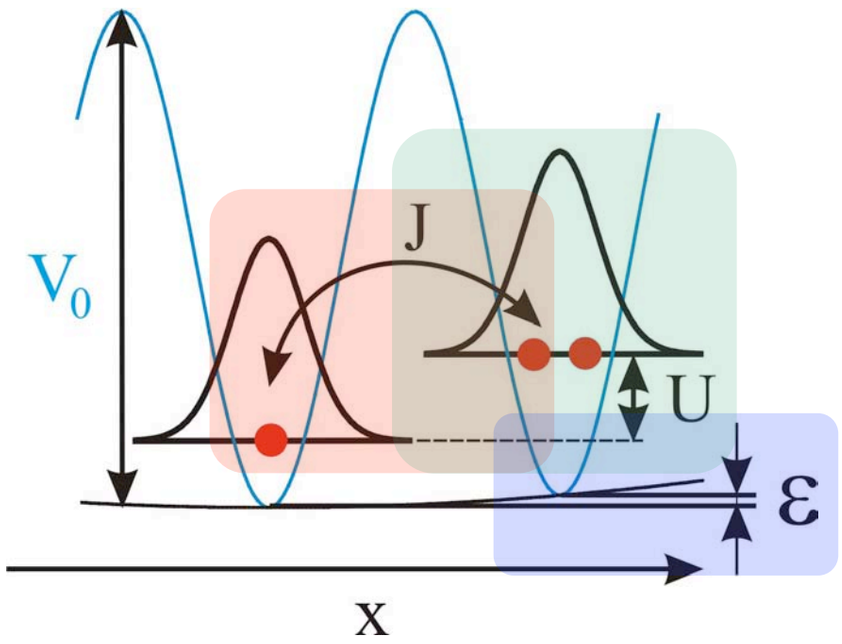


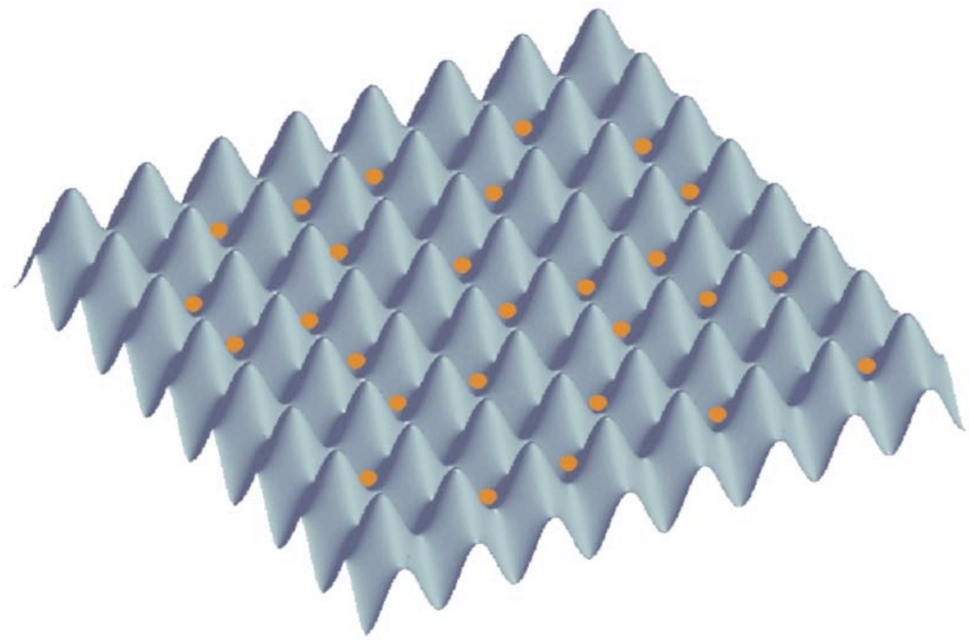
Wannier functions



- Our system is described by a Bose-Hubbard Model

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





D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys Rev. Lett. **81**, 3108 (1998)
M. Greiner, O. Mandel, T. Esslinger, T. Hänsch, and I. Bloch, Nature **415** 39 (2002) [& **419** 51 (2002)]
D. Jaksch and P. Zoller, "The Cold Atom Hubbard Toolbox", Annals of Physics **315**, 52 (2005).

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

- $\langle i, j \rangle$ denotes a sum over all combinations of neighbouring sites
- $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ and ϵ_i is the local energy offset of each site.
- ϵ_i can include, for example, the effects of background trapping potentials, superlattice, or fixed disorder.

Derivation of the Bose-Hubbard Hamiltonian

- The Bose-Hubbard Hamiltonian can be derived directly from the microscopic second-quantised Hamiltonian a cold atomic gas

$$\hat{H} = \int \mathrm{d}\mathbf{x} \hat{\Psi}^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}) \right) \hat{\Psi}(\mathbf{x}) + \frac{g}{2} \int \mathrm{d}\mathbf{x} \hat{\Psi}^\dagger(\mathbf{x}) \hat{\Psi}^\dagger(\mathbf{x}) \hat{\Psi}(\mathbf{x}) \hat{\Psi}(\mathbf{x})$$

- We expand the field operators in terms of Wannier functions,

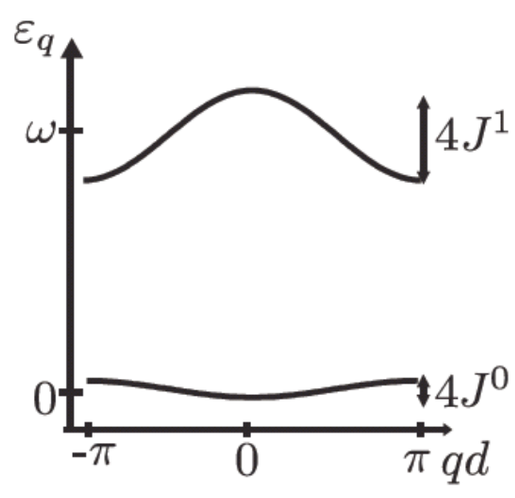
$$\hat{\Psi}(\mathbf{x}) = \sum_{i.n} w_n(\mathbf{x} - \mathbf{x}_i)\, \hat{b}_{n,i},$$

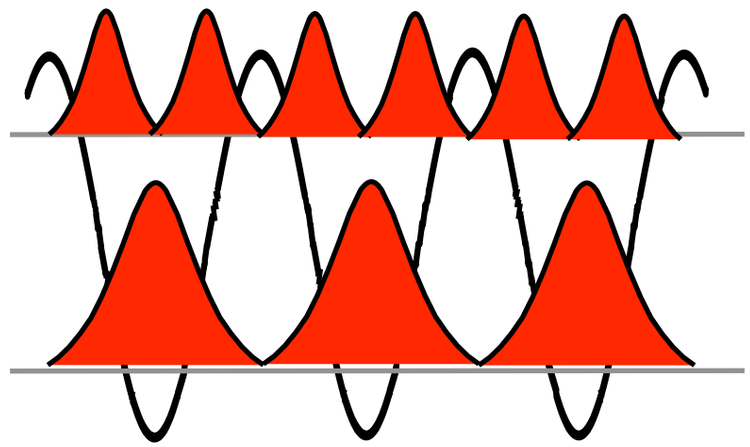
where for a 3D cubic lattice the Wannier function $w_n(\mathbf{x})$, $\mathbf{x} = (x, y, z)$ is a product of the 1D Wannier functions, $w_n(\mathbf{x}) = w_{n_x}(x) w_{n_y}(y) w_{n_z}(z)$.

$$\hat{H} = \int \mathrm{d}\mathbf{x}\hat{\Psi}^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) \right) \hat{\Psi}(\mathbf{x}) + \frac{g}{2} \int \mathrm{d}\mathbf{x}\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}(\mathbf{x})\hat{\Psi}(\mathbf{x})$$

$$\hat{\Psi}(\mathbf{x}) = \sum_{i.n} w_n(\mathbf{x} - \mathbf{x}_i)\, \hat{b}_{n,i}$$

- Approximation 1: That the Temperature T, and the interaction energies $U\langle\hat{n}\rangle/2$ are much less than the trapping frequency ω_T, which gives the separation between the Bloch Bands, so that we may restrict the system to Wannier states in the lowest band, eliminating the others in perturbation theory.
- Then we are left with terms involving $w_0(\mathbf{x})$ only.





Wannier functions

$$\hat{H} = \int \mathrm{d}\mathbf{x}\hat{\Psi}^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) \right) \hat{\Psi}(\mathbf{x}) + \frac{g}{2} \int \mathrm{d}\mathbf{x}\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}(\mathbf{x})\hat{\Psi}(\mathbf{x})$$

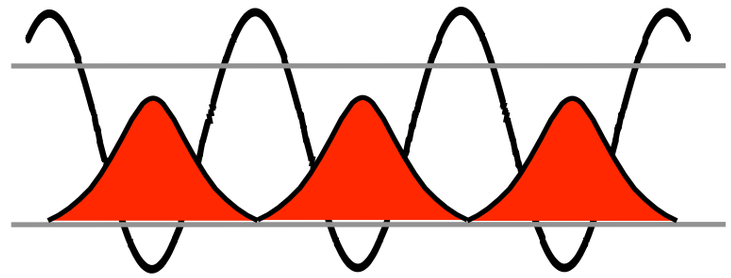
- Consider the First term,

$$\hat{\Psi}(\mathbf{x}) = \sum_{i.n} w_n(\mathbf{x} - \mathbf{x}_i)\, \hat{b}_{n,i}$$

$$\int \mathrm{d}\mathbf{x}\hat{\Psi}^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) \right) \hat{\Psi}(\mathbf{x})$$

- This produces onsite terms of the form

$$\epsilon_i = \int \mathrm{d}\mathbf{x}\, |w_0(\mathbf{x} - \mathbf{x}_i)|^2 \left(V(\mathbf{x} - \mathbf{x}_i) \right) \hat{b}^\dagger_{0,i}\hat{b}_{0,i}$$



and offsite terms of the form

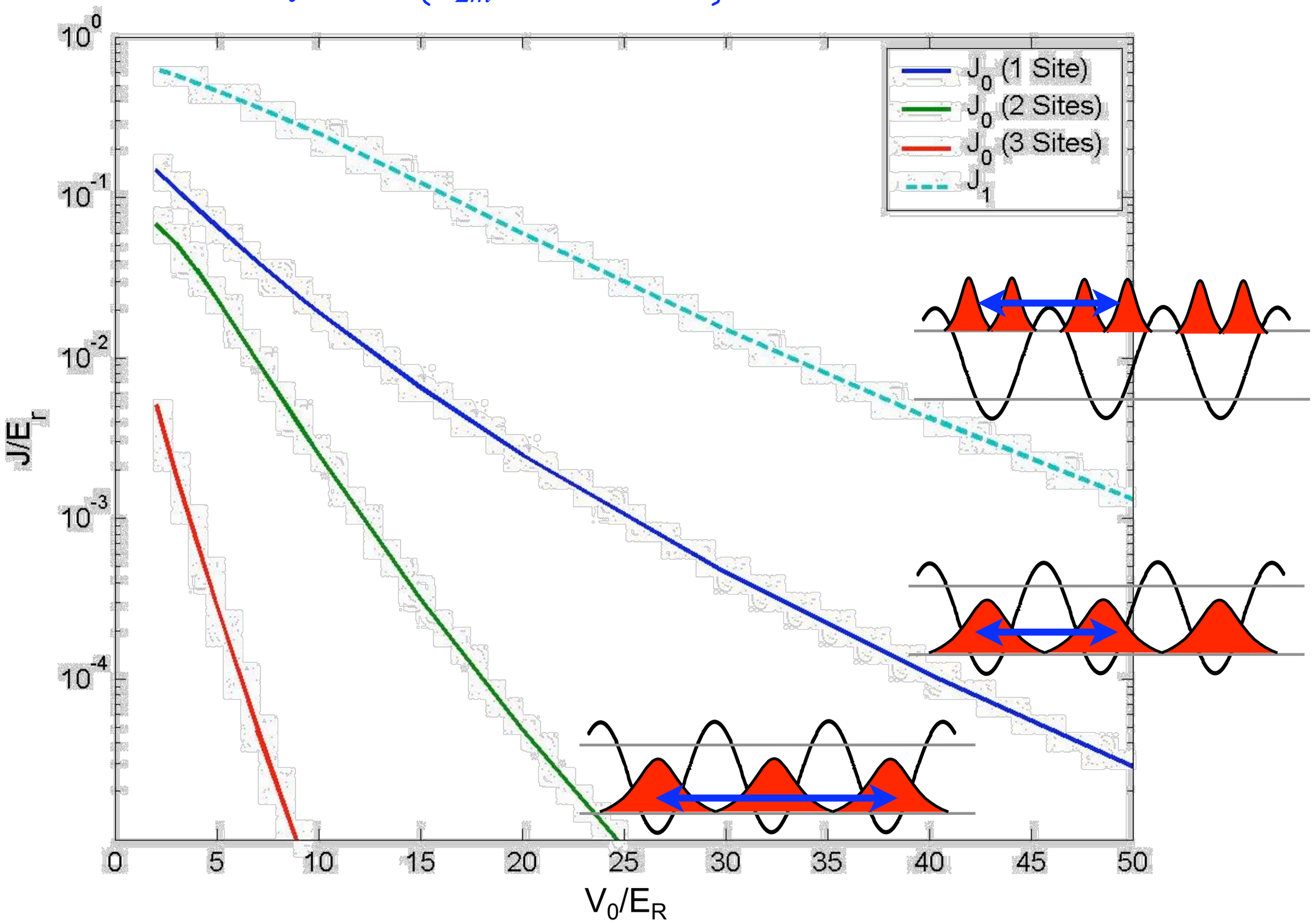
$$-\int \mathrm{d}x\, w_0(x) \left(-\frac{\hbar^2}{2m}\nabla^2 + V_0 \sin^2(k_l x) \right) w_0(x - la)\hat{b}^\dagger_{0,i}\hat{b}_{0,i+l},$$

where a is the distance between sites, and l is an integer.

- Approximation 2: That the tunnelling matrix elements between neighbouring sites $l = 1$ are much larger than those between next-nearest neighbours, $l > 1$, and that the remaining terms should be neglected. Then we write for the remaining terms,

$$J = -\int \mathrm{d}x\, w_0(x) \left(-\frac{\hbar^2}{2m}\nabla^2 + V_0 \sin^2(k_l x) \right) w_0(x - a)$$

$$-\int \mathrm{d}x\, w_0(x)\left(-\frac{\hbar^2}{2m}\nabla^2 + V_0 \sin^2(k_l x)\right) w_0(x - la)\hat{b}^{\dagger}_{0,i}\hat{b}_{0,i+l},$$



$$\hat{H} = \int \mathrm{d}\mathbf{x}\hat{\Psi}^\dagger(\mathbf{x})\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x})\right)\hat{\Psi}(\mathbf{x}) + \frac{g}{2}\int \mathrm{d}\mathbf{x}\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}(\mathbf{x})\hat{\Psi}(\mathbf{x})$$

$$\hat{\Psi}(\mathbf{x}) = \sum_{i.n} w_n(\mathbf{x} - \mathbf{x}_i)\,\hat{b}_{n,i}$$

- The Second Term

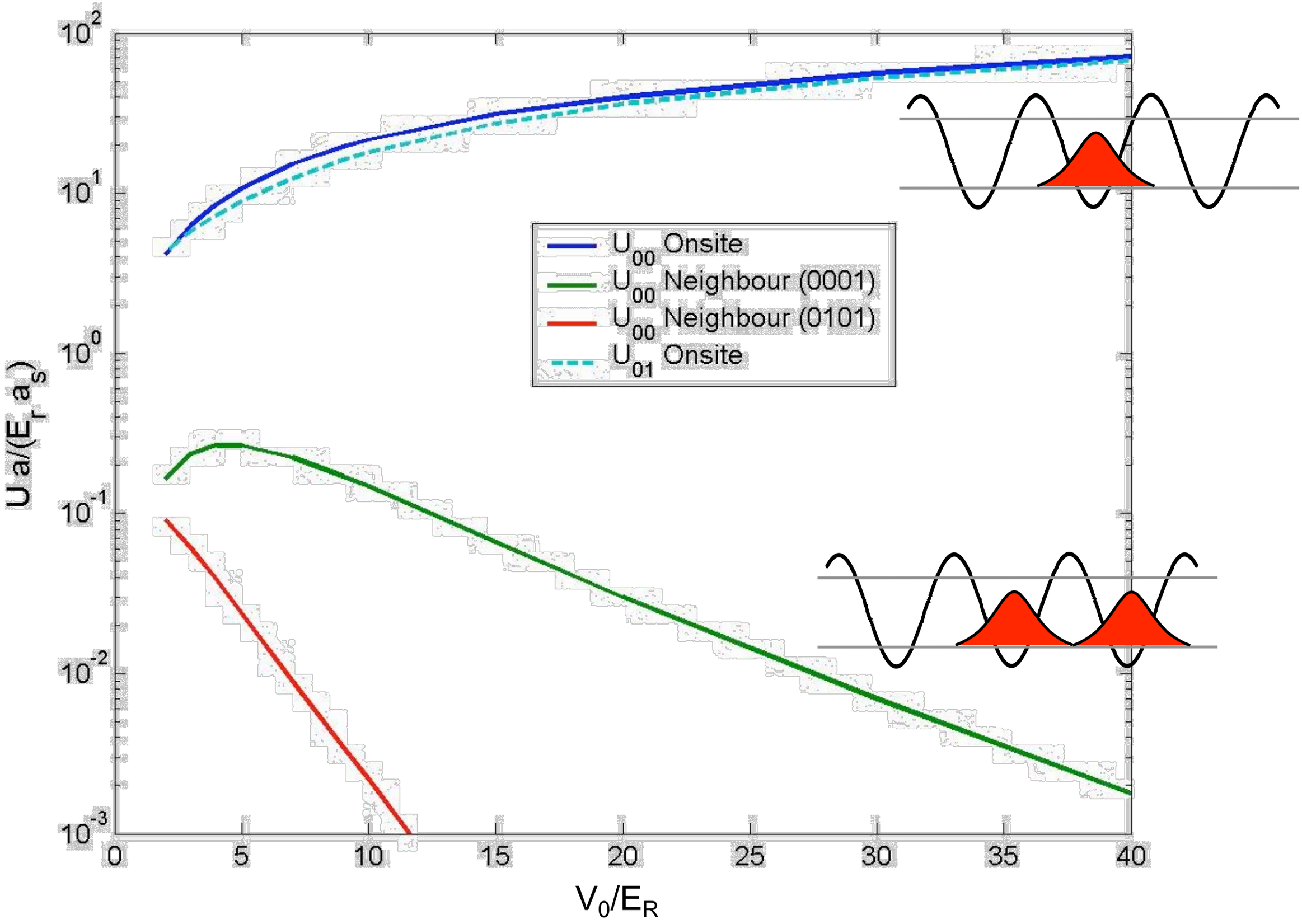
$$\frac{g}{2}\int \mathrm{d}\mathbf{x}\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}(\mathbf{x})\hat{\Psi}(\mathbf{x})$$

  produces interaction terms of the form

$$U_{ijkl} \propto \int \mathrm{d}\mathbf{x}\, w_0(\mathbf{x} - \mathbf{x}_i)w_0(\mathbf{x} - \mathbf{x}_j)w_0(\mathbf{x} - \mathbf{x}_k)w_0(\mathbf{x} - \mathbf{x}_l)\hat{b}^\dagger_{0,i}\hat{b}^\dagger_{0,j}\hat{b}_{0,k}\hat{b}_{0,l}$$

- Approximation 3: That the offsite interactions e.g., U_{1010} or tunneling, e.g., U_{0001} are small compared with $U = U_{0000}$ and can be neglected.

$$U_{ijkl} \propto \int \mathrm{d}\mathbf{x}\, w_0(\mathbf{x}-\mathbf{x}_i) w_0(\mathbf{x}-\mathbf{x}_j) w_0(\mathbf{x}-\mathbf{x}_k) w_0(\mathbf{x}-\mathbf{x}_l) \hat{b}^\dagger_{0,i} \hat{b}^\dagger_{0,j} \hat{b}_{0,k} \hat{b}_{0,l}$$



$$\hat{H} = \int \mathrm{d}\mathbf{x}\hat{\Psi}^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) \right) \hat{\Psi}(\mathbf{x}) + \frac{g}{2} \int \mathrm{d}\mathbf{x}\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}^\dagger(\mathbf{x})\hat{\Psi}(\mathbf{x})\hat{\Psi}(\mathbf{x})$$

$$\hat{\Psi}(\mathbf{x}) = \sum_{i.n} w_n(\mathbf{x} - \mathbf{x}_i)\, \hat{b}_{n,i}$$

- Then, our many-body Hamiltonian reduces to the Bose-Hubbard model

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

with

$$J = -\int \mathrm{d}x\, w_0(x) \left(-\frac{\hbar^2}{2m}\nabla^2 + V_0 \sin^2(k_l x) \right) w_0(x - a),$$

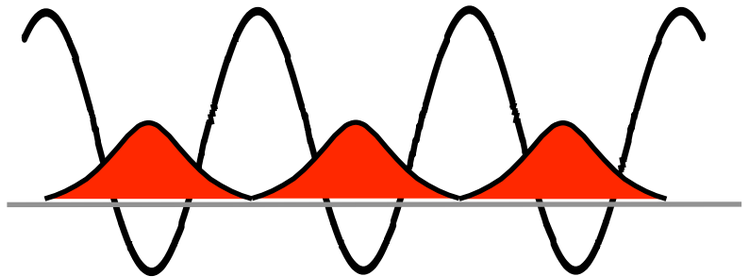
$$U = g \int \mathrm{d}\mathbf{x}\, |w_0(\mathbf{x})|^4,$$

$$\epsilon_i = \int \mathrm{d}\mathbf{x}\, |w_0(\mathbf{x} - \mathbf{x}_i)|^2 \left(V(\mathbf{x} - \mathbf{x}_i) \right),$$

$$\left[+ \int d\mathbf{x} w_0(\mathbf{x} - \mathbf{x}_i) \left(-\frac{\hbar^2}{2m}\nabla^2 + V_0 \sin^2(k_l x) \right) w_0(\mathbf{x} - \mathbf{x}_i) \right]$$

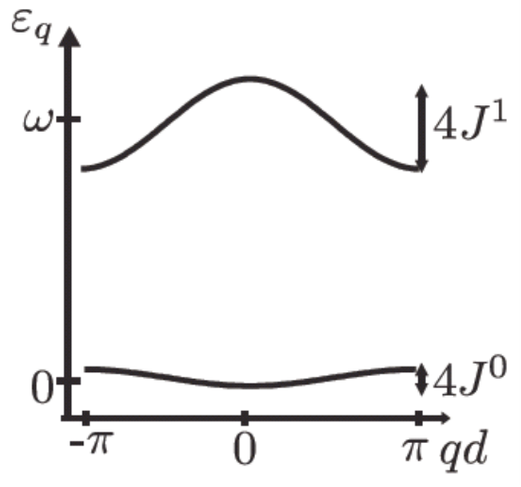
- All of these conditions are fulfilled provided that the lattice is deeper than $V_0 \sim 5\, E_R$
- Note that U/J can be varied by changing the depth of the lattice, or altering g via a Feshbach resonance.

Bose-Hubbard Model: Summary



Wannier functions

$$\psi(\vec{x}) = \sum_{\alpha} w(\vec{x} - \vec{x}_\alpha)\, b_\alpha$$



$$\hat{H} = \int \mathrm{d}\mathbf{x} \hat{\Psi}^\dagger(\mathbf{x}) \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) \right) \hat{\Psi}(\mathbf{x}) + \frac{g}{2} \int \mathrm{d}\mathbf{x} \hat{\Psi}^\dagger(\mathbf{x}) \hat{\Psi}^\dagger(\mathbf{x}) \hat{\Psi}(\mathbf{x}) \hat{\Psi}(\mathbf{x})$$

Assume:
- Only lowest band
- Only nearest neighbour tunneling
- Only onsite interactions

$$J = -\int \mathrm{d}x\, w_0(x) \left(-\frac{\hbar^2}{2m}\nabla^2 + V_0 \sin^2(k_l x) \right) w_0(x-a),$$

$$U = g \int \mathrm{d}\mathbf{x}\, |w_0(\mathbf{x})|^4,$$

$$\epsilon_i = \int \mathrm{d}\mathbf{x}\, |w_0(\mathbf{x} - \mathbf{x}_i)|^2 \left(V(\mathbf{x} - \mathbf{x}_i) \right),$$

$$\longrightarrow \quad H = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \sum_i \epsilon_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) \qquad k_B T, J, U \ll \hbar\omega$$

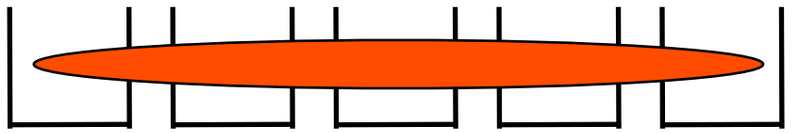
D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys Rev. Lett. **81**, 3108 (1998)

Basic Properties of the Bose-Hubbard Model

- Bose-Hubbard Model has a very interesting phase diagram, exhibiting a phase transition for commensurate filling (number of particles N is integer multiple of number of lattice sites M).

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

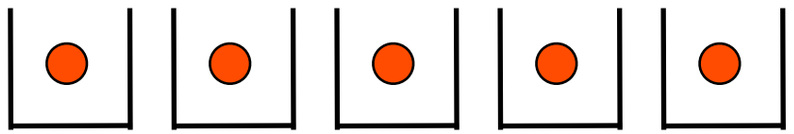
- **Superfluid** J>>U



delocalized atoms: BEC

$$\left(b_1^\dagger + \ldots + b_M^\dagger\right)^N |\text{vac}\rangle$$

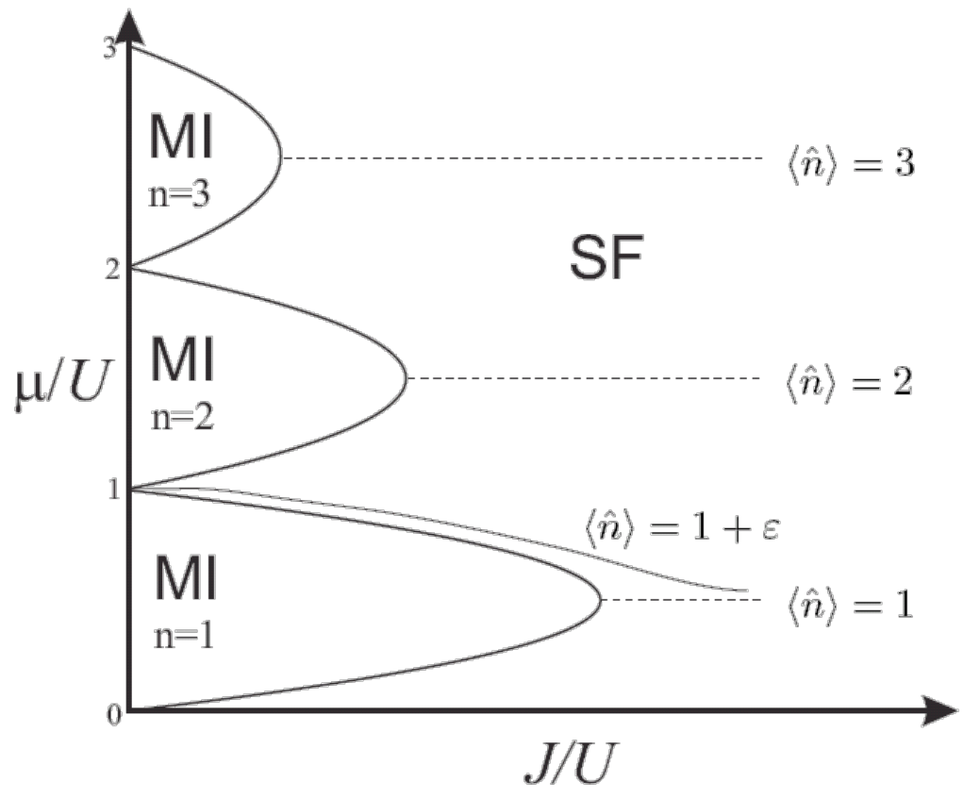
- **Mott Insulator Phase:** J<<U



$$b_1^\dagger b_2^\dagger \ldots b_M^\dagger |\text{vac}\rangle$$

"Fock states"

- Phase Diagram

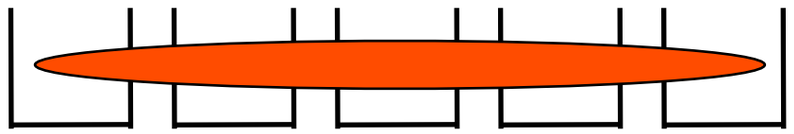


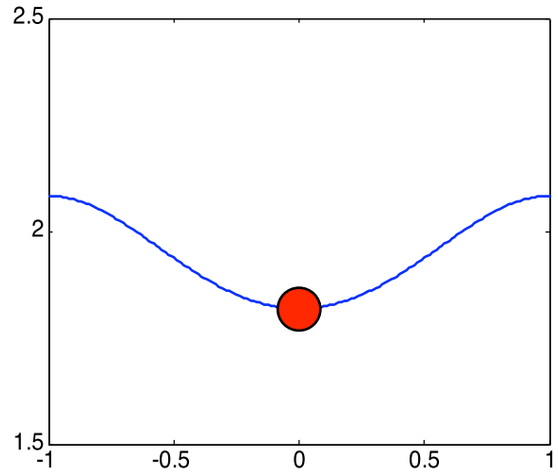
regular filling with exactly 1, 2 or 3 atoms per lattice site

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

- In the limit $(U/J) \to 0$, the ground state of the system is superfluid, and the atoms are delocalised around the lattice. For a lattice of M sites, this ideal superfluid state can be written as

$$|\Psi_{SF}\rangle = \left(\frac{1}{\sqrt{M}} \sum_{i=1}^{M} \hat{b}_i^\dagger \right)^N |0\rangle,$$





which for $N, M \to \infty$ at fixed N/M tends to

$$|\Psi_{SF}\rangle = \prod_{i=1}^{M} \left[\exp\left(\sqrt{\frac{N}{M}} \hat{b}_i^\dagger \right) |0\rangle_i \right],$$

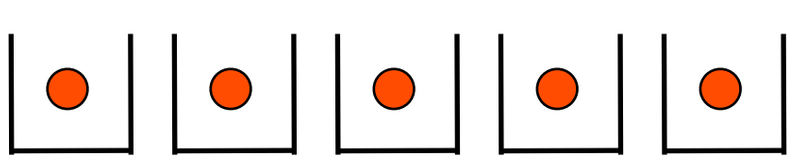
which is locally a coherent state with Poisson number statistics.

- In 3D, this state is an ideal BEC in which all N atoms are in the Bloch state $\phi_{\mathbf{q}=0}^{(n=0)}(x)$.

$$-J \sum_{\langle i,j \rangle} b_i^\dagger b_j = -2J \sum_q \cos(qa) a_q^\dagger a_q$$

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

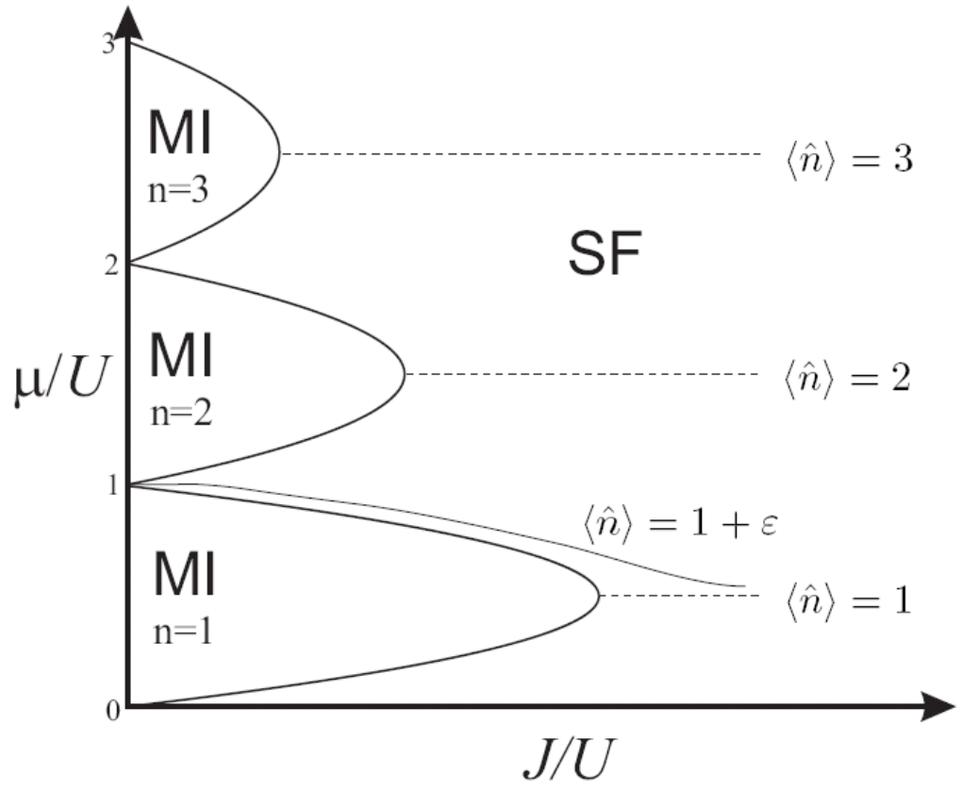
- As U/J increases, a regime exists in which the onsite interactions make it less favourable to particles to hop to neighbouring sites.
- Provided that the number of particles and lattice sites are commensurate, a phase transition then occurs to the Mott Insulator (MI) regime, in which particles are essentially localised at particular sites in the sense that their mean square displacement is finite.



- In the limit $J/U \to 0$, this state corresponds to a fixed number of atoms on each site,

$$|\Psi_{MI}\rangle = \prod_i |\bar{n}\rangle_i,$$

where $\bar{n} = \langle \hat{n} \rangle = N/M$ is the average filling factor. The MI regime appears as lobes in the phase diagram corresponding to an integer fixed filling factor.

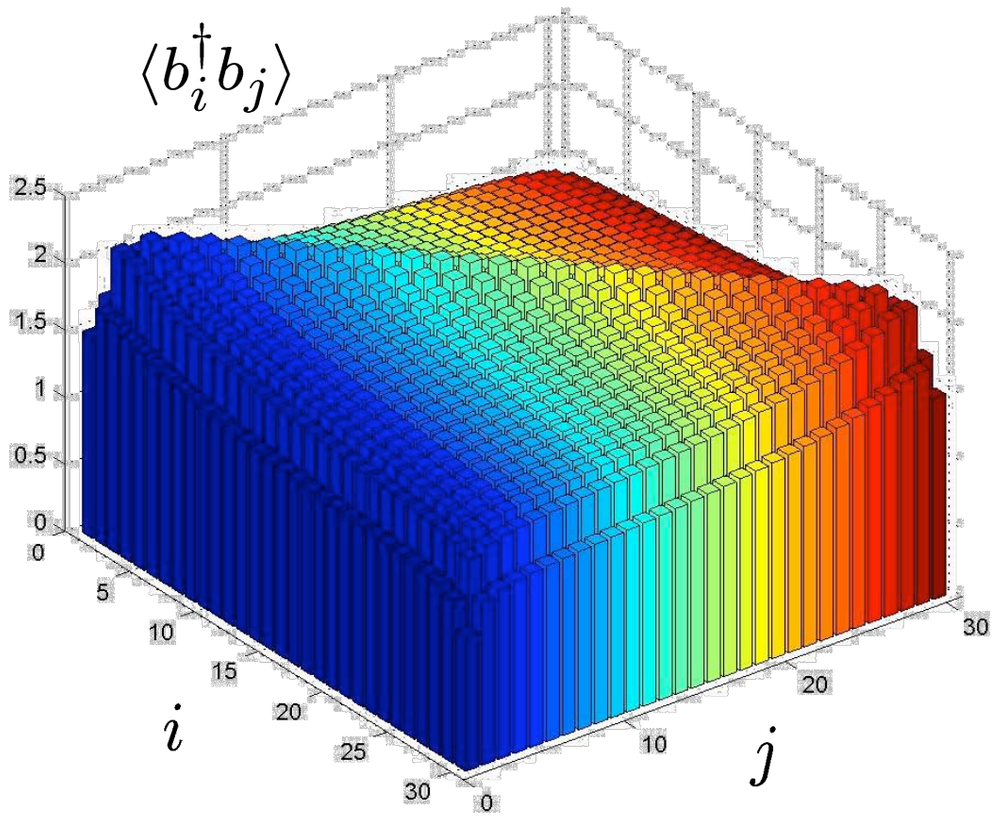


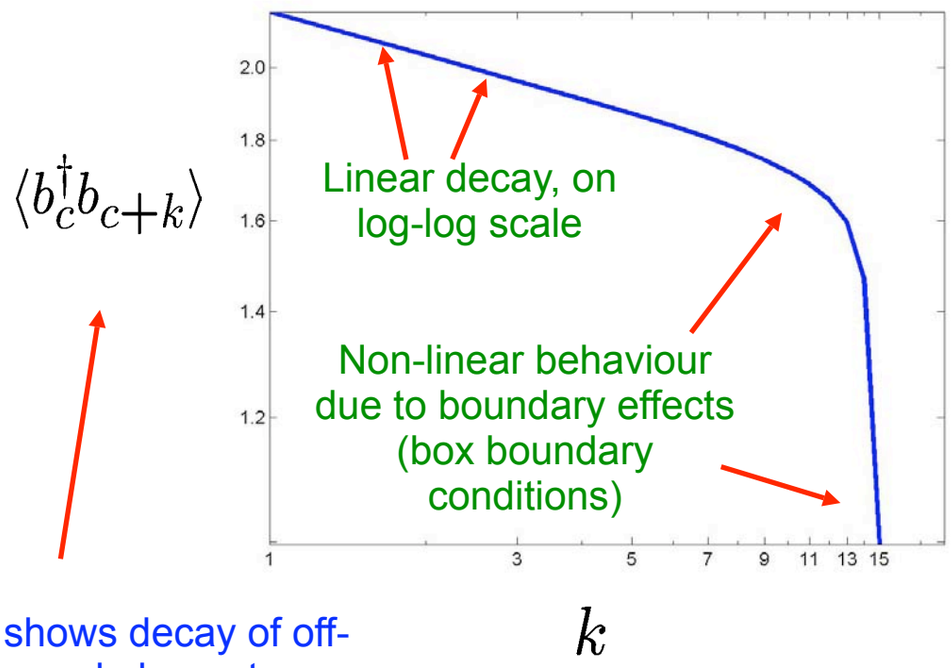
- Superfluid states at (T=0) exhibit off-diagonal long-range order (or quasi-long range order in 1D), with the off diagonal elements of the single particle density matrix, $\langle \hat{b}_i^\dagger \hat{b}_j \rangle$ decaying polynomially with $|i-j|$.
- For finite J/U, the off diagonal elements of the single particle density matrix, $\langle \hat{b}_i^\dagger \hat{b}_j \rangle$, decay exponentially for a MI state as a function of $|i-j|$.

Single Particle Density Matrix:

Superfluid (SF)
Ground State
U=1, J=1,
30 Sites, 66 Particles,

$\epsilon_i = 0$



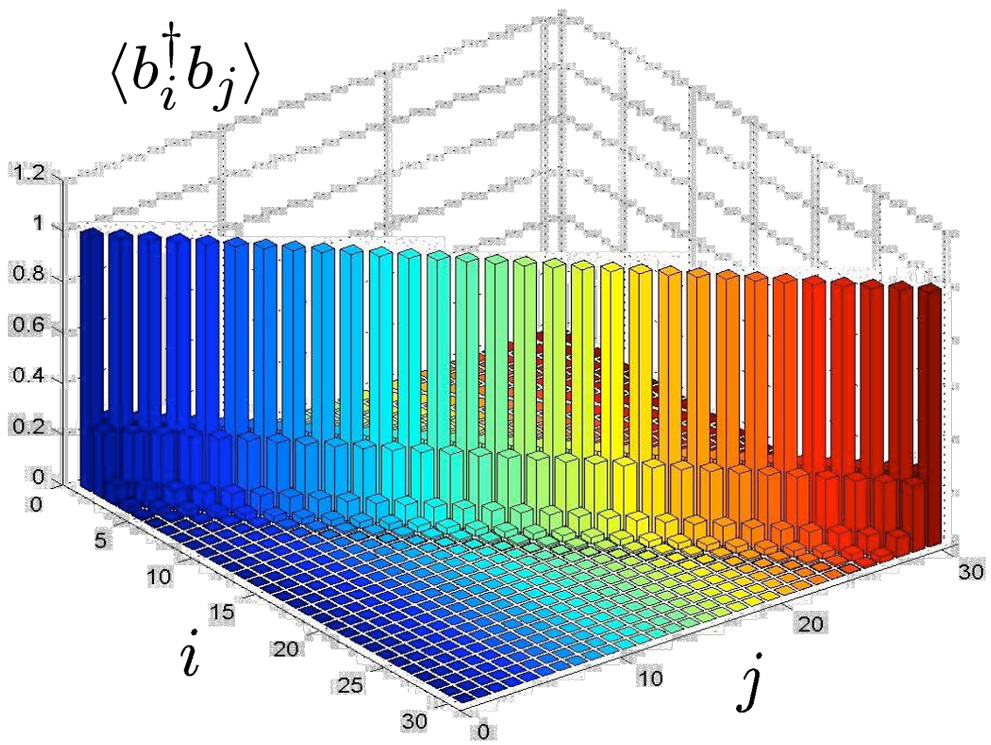


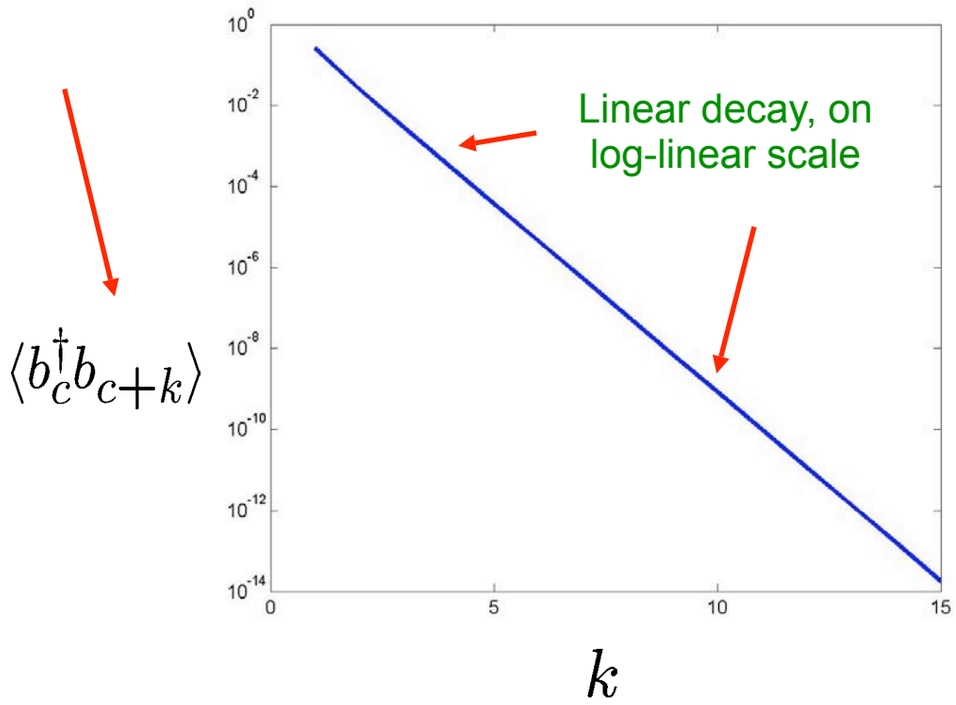
c=15, shows decay of off-diagonal elements.

- Polynomial for SF
- Exponential for MI

Mott Insulator (MI)
Ground State
U=15, J=1,
30 Sites,
30 Particles

$\epsilon_i = 0$





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Observation via momentum distribution:

- In a homogeneous system, the momentum distribution of atoms can be given as a function of the single particle density matrix at separation l,

$$\rho_1(l) = \langle \hat{b}_{\mathbf{i}}^{\dagger} \hat{b}_{\mathbf{i}+\mathbf{R}} \rangle$$

with $\mathbf{i} = (i_x, i_y, i_z)$, as

$$n(\mathbf{k}) = n|\tilde{w}(\mathbf{k})|^2 \sum_R e^{i\mathbf{k}.\mathbf{R}} \rho_1(\mathbf{R})$$

where n is the density, and $\tilde{w}(\mathbf{k})$ is the Fourier transform of the corresponding Wannier Function.

- The superfluid phase can be distinguished because as $l \to \infty$, $\rho_1(l) \to n_0/n$, where n_0 is the condensate density. Thus, the momentum distribution has a peak at reciprocal lattice vectors $\mathbf{k} = \mathbf{G}$, $\mathbf{G}.\mathbf{R} = 2\pi z$, where z is an integer. There,

$$n(\mathbf{k} = \mathbf{G}) = N.n_0|\tilde{w}(\mathbf{G})|^2$$

which scales as the number of particles, N.

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M. Greiner, I. Bloch, T. Hänsch et al., Nature 2002

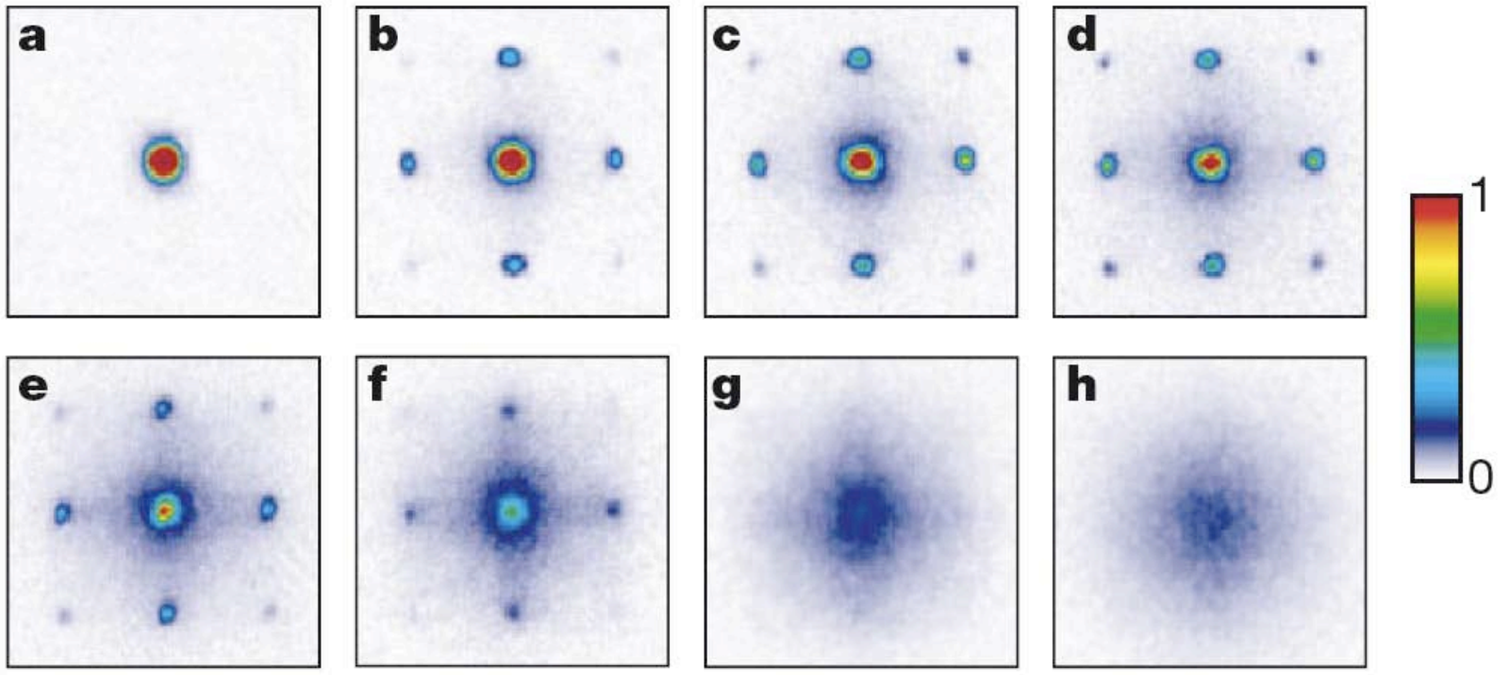


Figure 2 Absorption images of multiple matter wave interference patterns. These were obtained after suddenly releasing the atoms from an optical lattice potential with different potential depths V_0 after a time of flight of 15 ms. Values of V_0 were: **a**, 0 E_r; **b**, 3 E_r; **c**, 7 E_r; **d**, 10 E_r; **e**, 13 E_r; **f**, 14 E_r; **g**, 16 E_r; and **h**, 20 E_r.

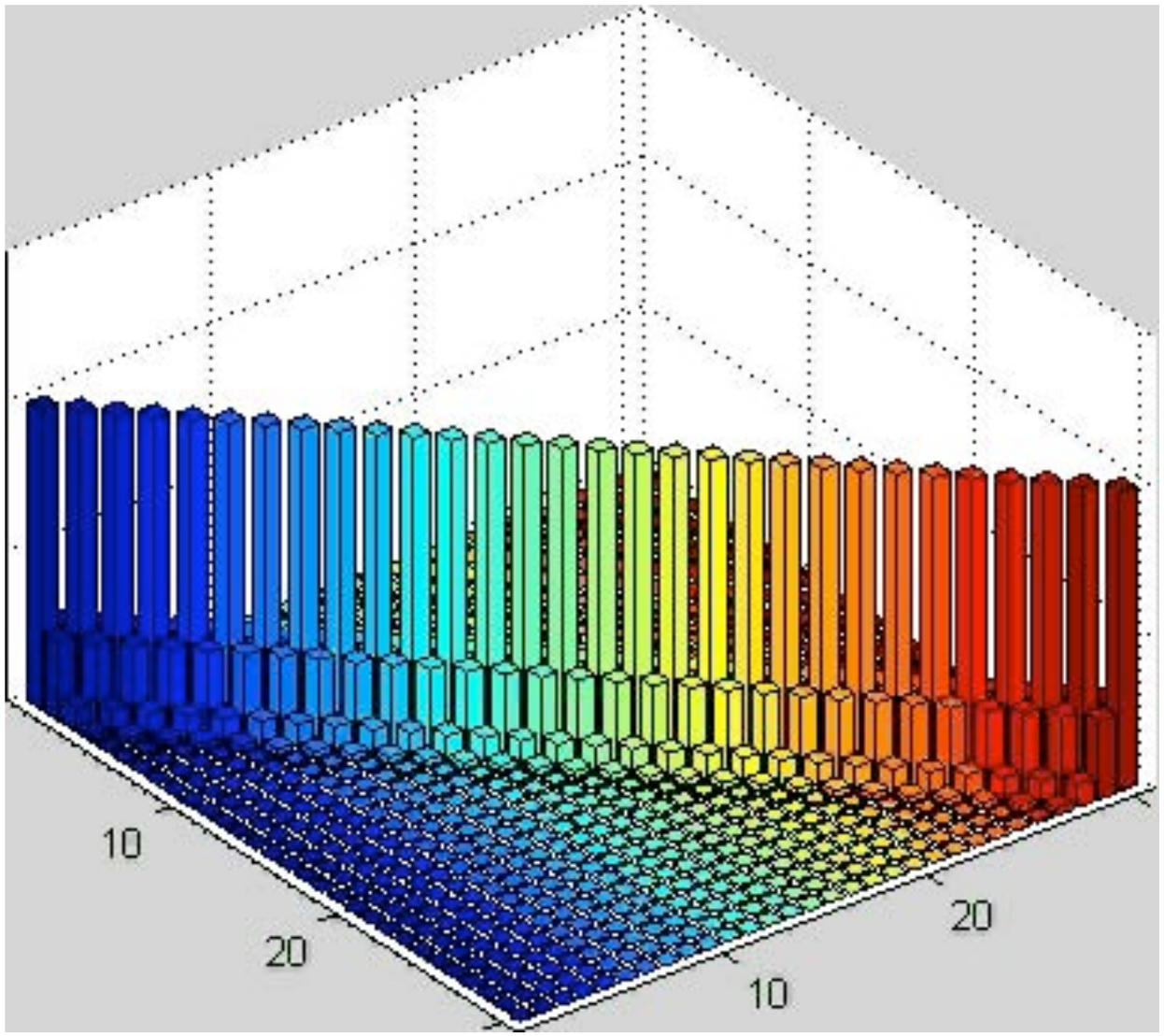
- For the MI phase, in the limit $U >> J$, $\rho_1(\mathbf{R}) = 0$ for $|R| \geq 1$, and thus no such peaks occur.
- For $U \sim J$, but in the MI phase, it is still possible to observe peaks in the momentum distribution at $\mathbf{k} = \mathbf{G}$, as the single particle denstiy matrix has non-zero off-diagonal elements, but the intensity of these peaks does not scale as N.

Time-dependent study of the Mott Insulator-Superfluid transition:

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

$$\langle b_i^\dagger b_j \rangle$$

$$\begin{aligned} J &= 1 \\ U &= 15 \rightarrow 1 \\ \epsilon_i &= 0 \end{aligned}$$



Gutzwiller mean field:

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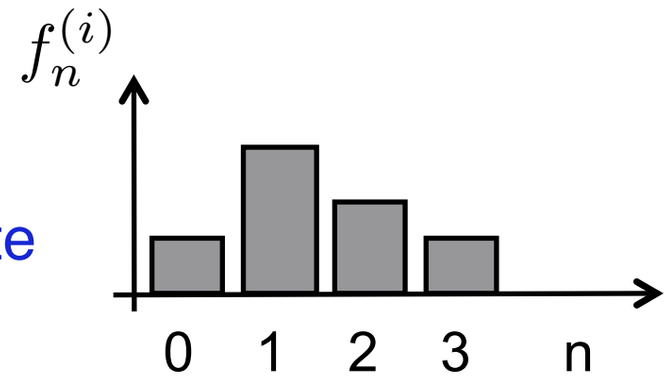
- Gutzwiller ansatz: $\langle H_{BH}\rangle - \mu\langle\hat{N}\rangle \rightarrow$ Minimise to find ground state

$$|\Psi\rangle = \prod_i |\phi_i\rangle \quad \text{with} \quad |\phi_i\rangle = \sum_{n=0}^{\infty} |n\rangle_i \, f_n^{(i)}$$

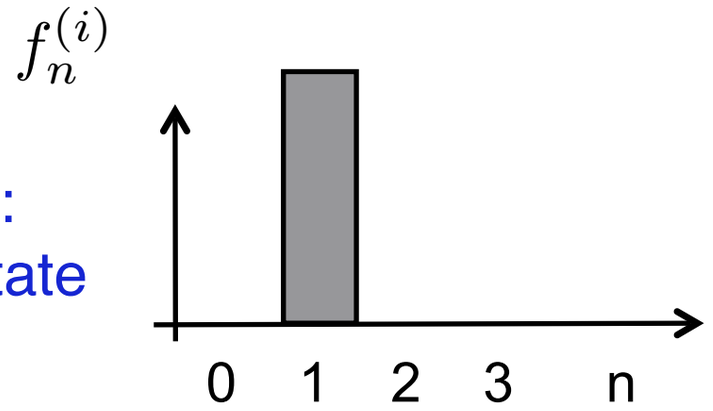
- product state
- Not number conserving

superfluid:
coherent state



$$f_n^{(i)} = \frac{\psi_i^n}{\sqrt{n!}} e^{-\frac{1}{2}|\psi_i|^2}$$

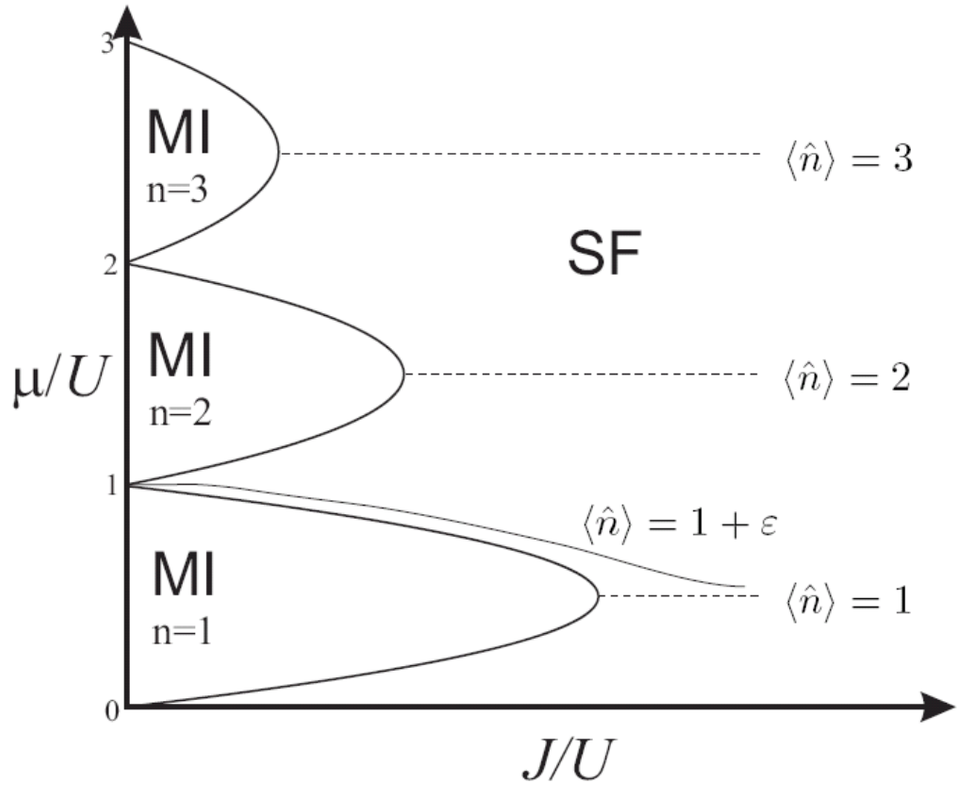
Mott:
Fock state



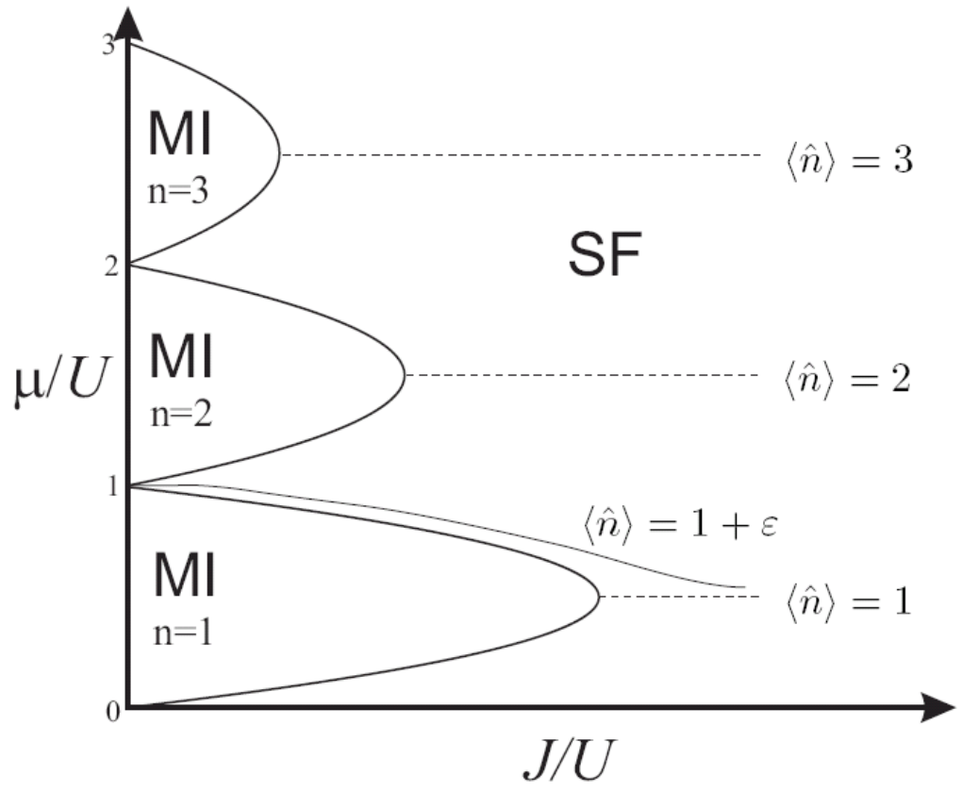
- Mean field Hamiltonian: sum of local Hamiltonians

$$H_{\mathrm{MF}} = \sum_i \left(-J \sum_{\langle j|i\rangle} \left(b_i^\dagger \psi_j + \psi_i^* b_j \right) + \frac{1}{2} U \sum_i \hat{n}_i(\hat{n}_i - 1) \right) \equiv \sum_i h_i$$

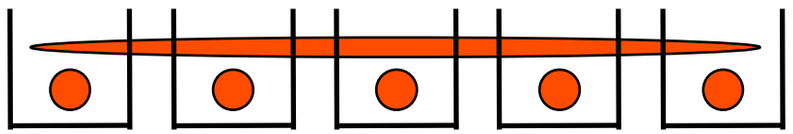
with mean field (SF order parameter) $\psi_i = \langle\Psi| \, b_i \, |\Psi\rangle \equiv \langle\phi_i| \, b_i \, |\phi_i\rangle$



- At fixed integer $\bar{n}$, the transition point in 2D or 3D is well described by mean-field theories, with $(U/J)_c = 5.8z$ for $\bar{n} = 1$ and $(U/J)_c = 4\bar{n}z$ for $\bar{n} > 1$, where z is the number of nearest neighbours for each lattice site (in a 3D cubic lattice, $\bar{n} = 6$).
- In 1D, the deviations from mean-field results are large, and $(U/J)_c = 3.37$ for $\bar{n} = 1$ and $(U/J)_c = 2.2\bar{n}$ for $\bar{n} > 1$.



- If $\bar{n}$ is fixed and non-integer (e.g., the line $\langle\hat{n}\rangle = 1 + \varepsilon$), then even in the limit $U \ll J$, there is a fraction of atoms which can remain superfluid on top of a frozen Mott-Insulator core (which will exist for $\bar{n} > 1$) provided $J > 0$.
- These atoms need not be affected by increasing U/J, as they can gain kinetic energy by delocalising over the lattice without two of them being present at the same site.



- In an external Harmonic trap, $\epsilon_l = \Omega l^2$ with a fixed number of particles, the local chemical

  potential, μ, varies across the trap, decreasing from the centre to the edges,

$$\mu \approx \mu_0 - V(\mathbf{r})$$

- As a result, regions exhibiting alternately the superfluid and MI phases appear
- This layer structure has recently been observed by two experimental groups (Mainz, MIT)

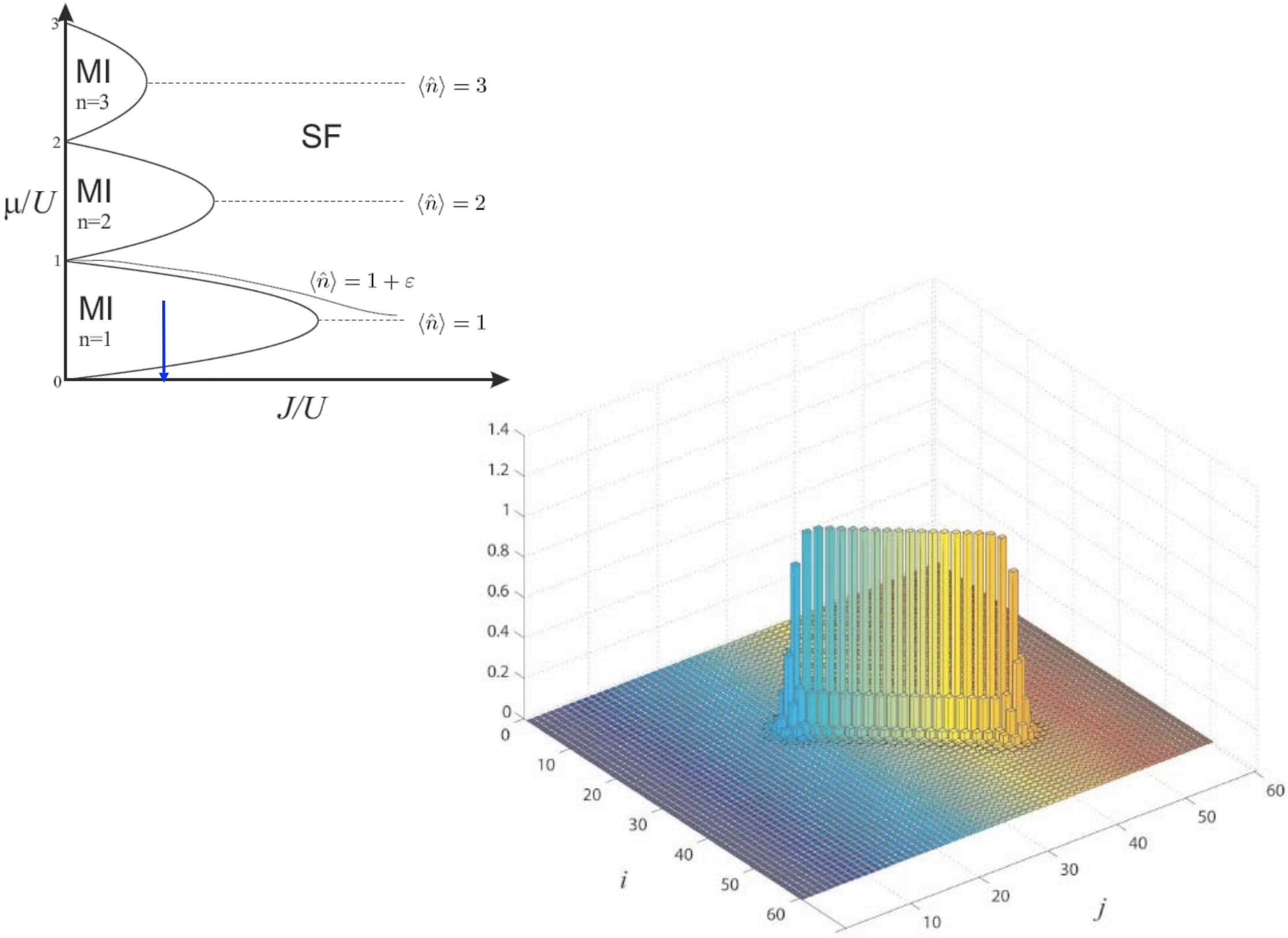


Figure 8.3. *Single particle density matrix, $\langle \hat{b}_i^\dagger \hat{b}_j \rangle$, for the ground state of the 1D Bose-Hubbard model with $N = 20$ particles, $U/J = 20$, $\epsilon_i/J = 0.1(i - i_0)^2$.*

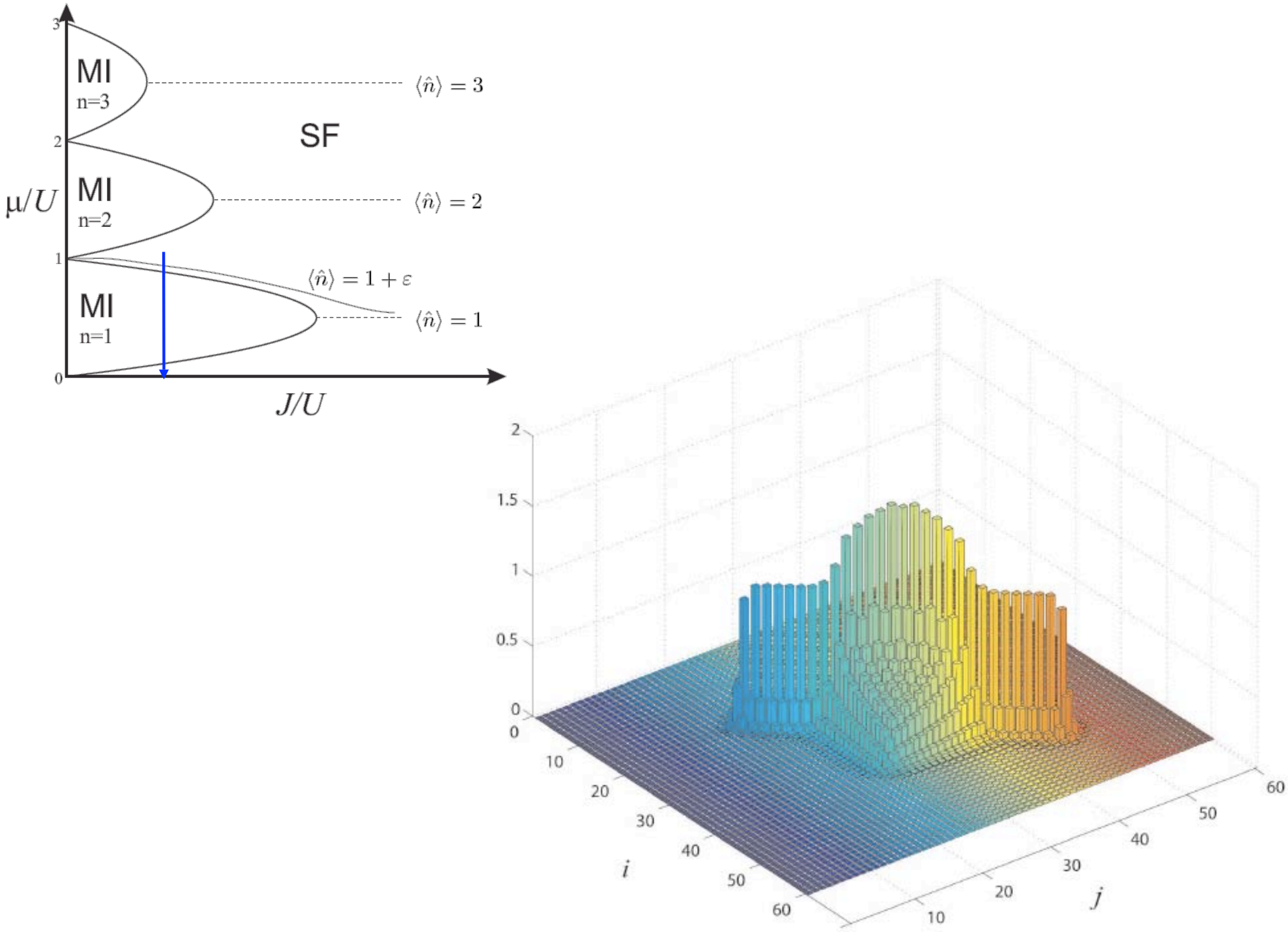
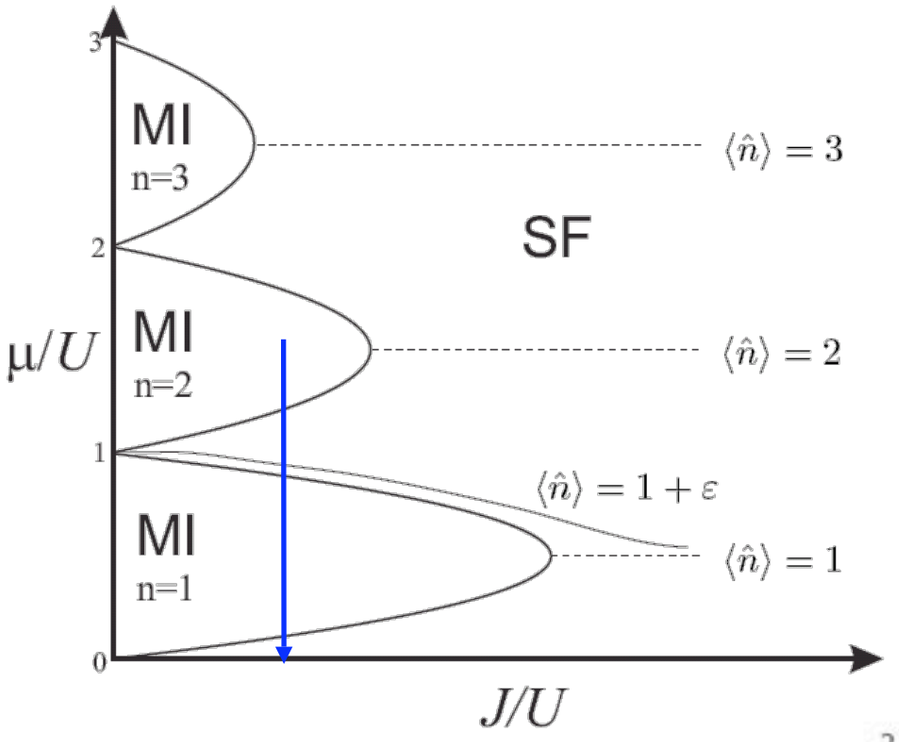


Figure 8.4. *Single particle density matrix, $\langle \hat{b}_i^\dagger \hat{b}_j \rangle$, for the ground state of the 1D Bose-Hubbard model with $N = 35$ particles, $U/J = 20$, $\epsilon_i/J = 0.1(i - i_0)^2$.*



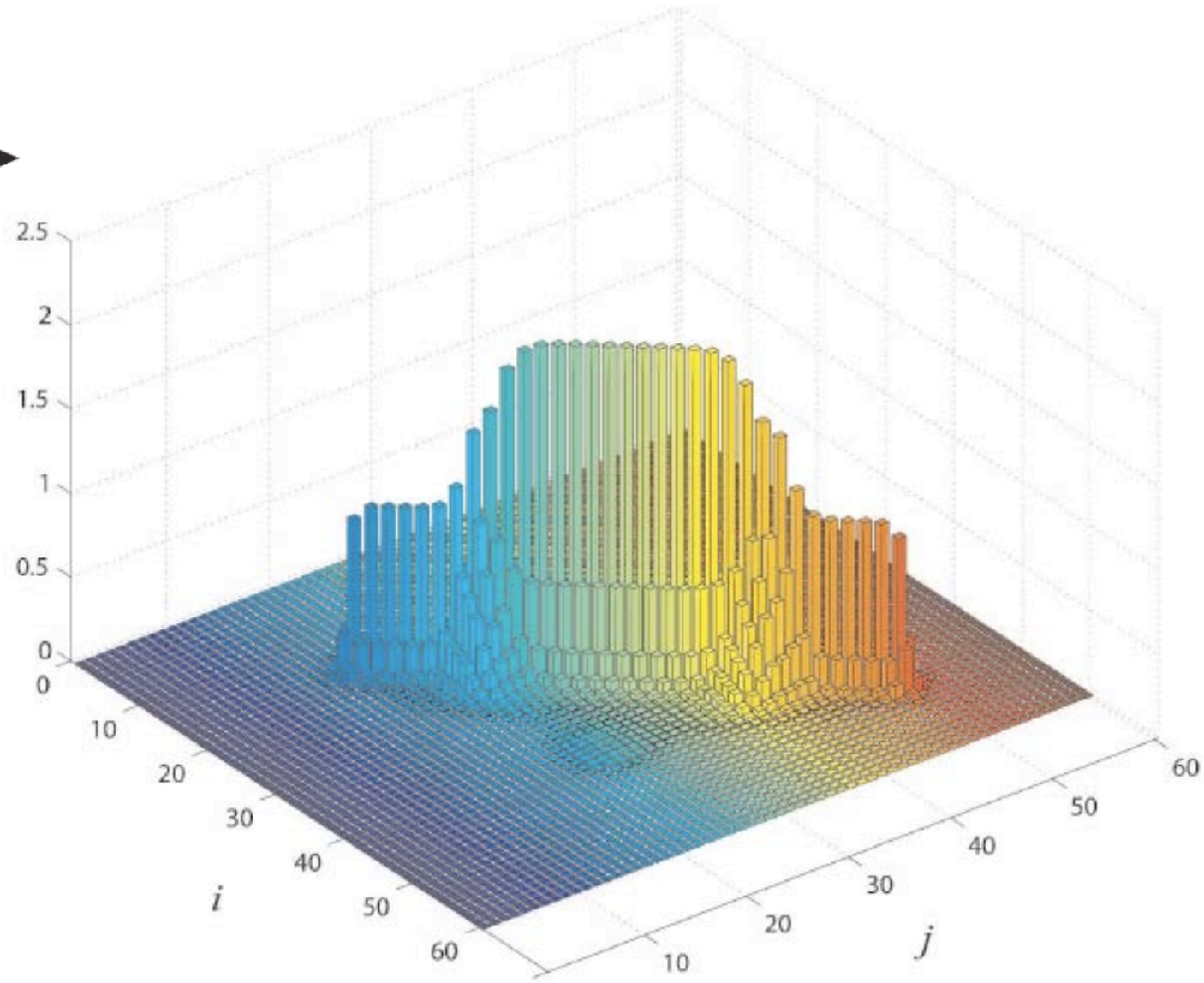


Figure 8.5. *Single particle density matrix, $\langle \hat{b}_i^\dagger \hat{b}_j \rangle$, for the ground state of the 1D Bose-Hubbard model with $N = 50$ particles, $U/J = 20$, $\epsilon_i/J = 0.1(i - i_0)^2$.*

Discussion

Example Applications

- Many other Hamiltonians can be implemented:
  - For strong interactions, we have only 0 or 1 atom at a lattice site
  - In perturbation theory this allows implementation of many spin models
  - Dipolar molecules in optical lattices would have long range interactions, and allow many possibilities for engineering different lattice models

- Such models are often extremely important in condensed matter systems
  - Many descriptions of superconductivity, including models for high-Tc superconductors are related to lattice models with the same form as the Hubbard model
  - Adding random potentials allows the study of disordered systems (Bose-Hubbard model was originally studied in this context).
  - Kondo problem, Luttinger Liquids, Exotic phases, Topological order, ...

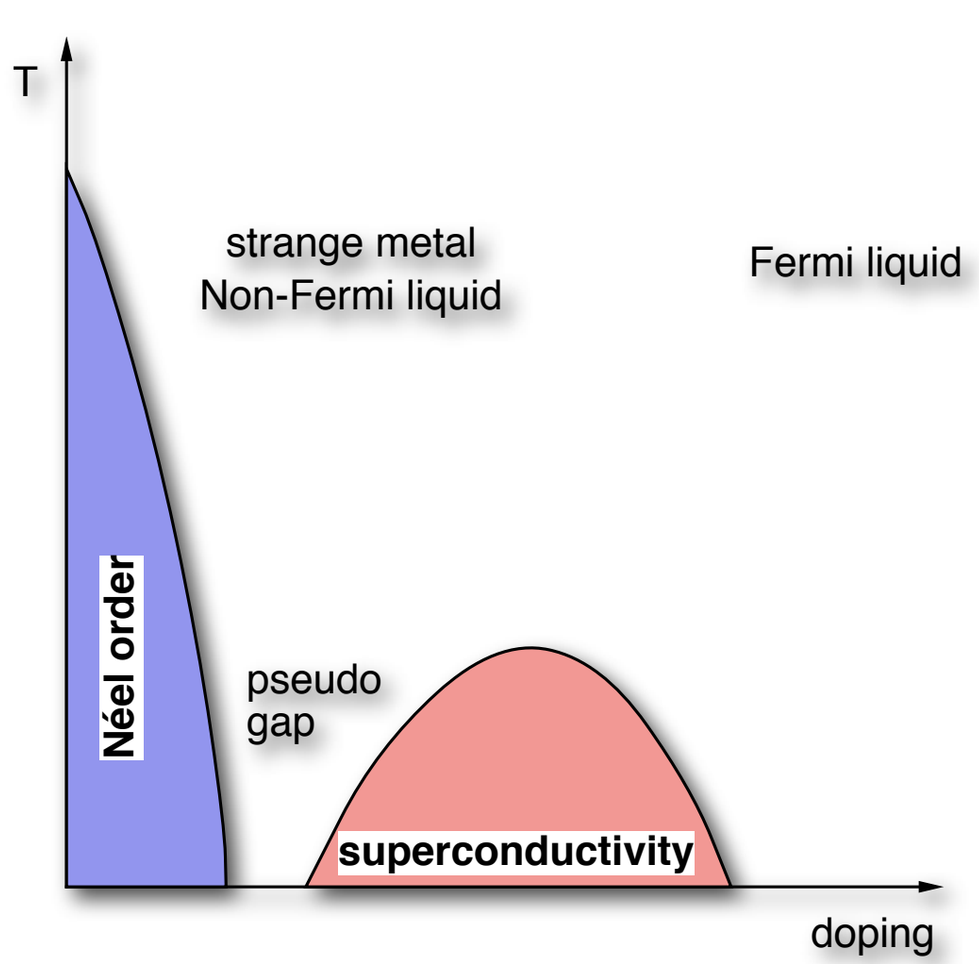
Related Models

- In a similar manner, one can show that the microscopic Hamiltonian for two fermionic spin species reduces to the original Hubbard model,

$$\hat{H} = -J \sum_{\langle i,j \rangle,\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{i,\sigma} \epsilon_i \hat{n}_{i\sigma}, ,$$

with fermionic operators $\hat{c}_i$, which obey the standard anti-commutator relations, and $\sigma \in \{\uparrow, \downarrow\}$. This is a simple example of the many two-species models that can be engineered with atoms in optical lattices.

Relationship to high Tc superconductivity for U>0:



- Can also, e.g., trap Bose-Fermi mixtures, and can produce spin-dependent or species-dependent lattices to tune U and J independently for different species.
- It is also possible to create multi-band Hubbard models, of the form

$$\hat{H}_{2:\mathrm{Band}} = -\sum_{\langle i,j\rangle}\left(J_0\hat{b}^\dagger_{0,i}\hat{b}_{0,j} + J_1\hat{b}^\dagger_{1,i}\hat{b}_{1,j}\right) + \frac{1}{2}\sum_i\left[U_{00}\hat{n}_{0,i}(\hat{n}_{0,i}-1) + U_{11}\hat{n}_{1,i}(\hat{n}_{1,i}-1)\right]$$
$$+ U_{10}\sum_i \hat{n}_{0,i}\hat{n}_{1,i} + \sum_{n,i}\epsilon_{n,i}\hat{n}_{n,i},$$

New Insight into Lattice Models

- The available control over the system means that these Hamiltonians can be engineered in experiments with unprecedented control over most relevant parameters.
- There are also many techniques available to make measurements on these systems (e.g., release of atoms from the lattice allows measurement of momentum and quasimomentum distributions).

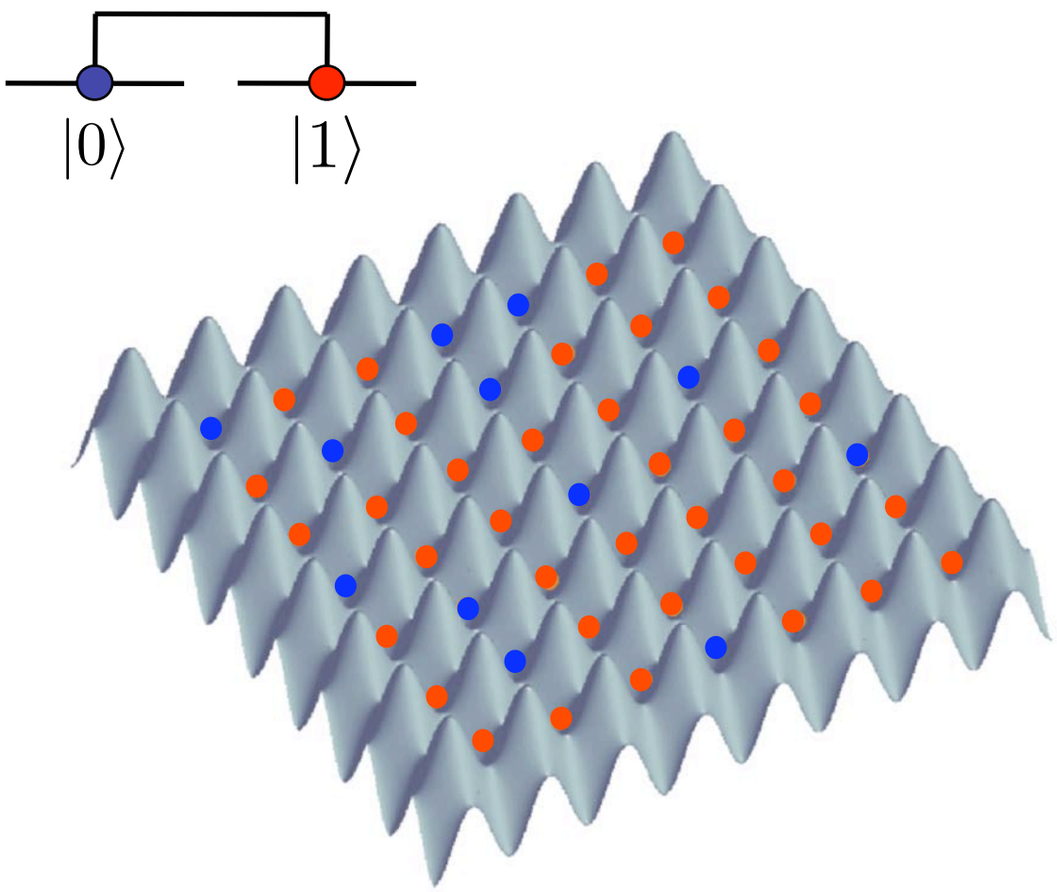
- This allows investigations of these models that would be impossible if the same system were realised in traditional condensed matter experiments.
- In this sense, atoms in optical lattices can act as a specialised quantum computer for simulation of lattice models.
- This may allow many "computations" to be performed on lattice models linked with important phenomena in condensed matter physics to be probed on a level that was previously impossible.

Coherent Phenomena and quantum computing

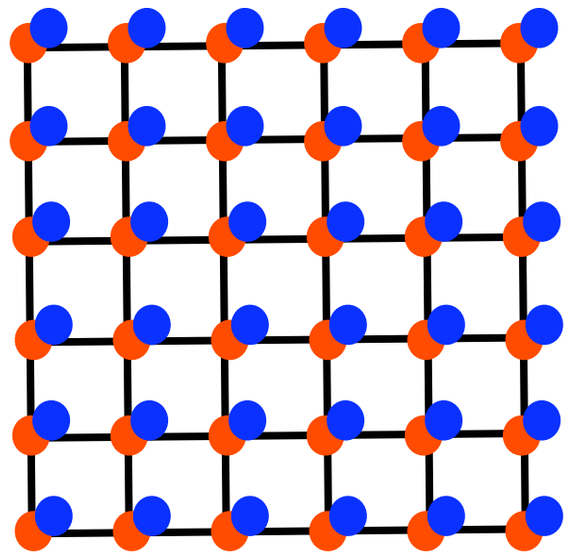
- These systems are strongly isolated from their environments: Typical parameters (J, U) are of the order of 100-10000Hz, whereas decoherence timescales are of the order of several seconds to tens of seconds (mainly from spontaneous emissions).
- These systems can thus be used to probe the coherent properties of these models

- In addition, the same setup offers many possibilities to engineer entanglement and has potential applications in quantum computing.
- Entanglement of a large array of atoms via controlled collisions has already been performed in an experiment
- A 1D version of the so-called cluster state required for measurement-based quantum computing schemes (such as the one-way quantum computer) has been demonstrated.

Applications to Quantum Information Processing:



- Array of singly occupied sites
- Qubits encoded in long-lived internal states.
- Entanglement, e.g., via controlled collisions in a spin-dependent lattice:



Cluster State,
1-way QC