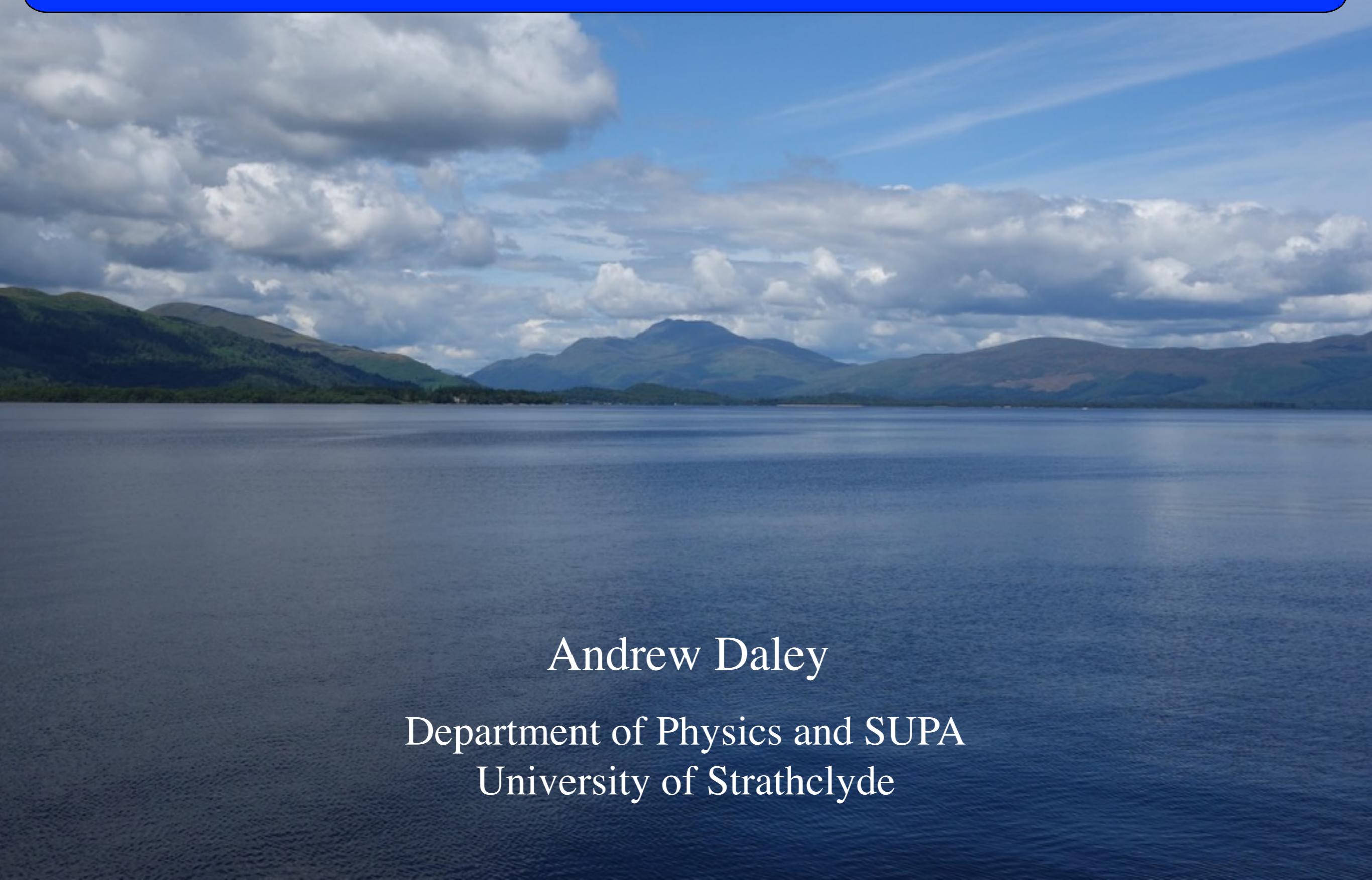


# Microscopic control of quantum gases and quantum simulation



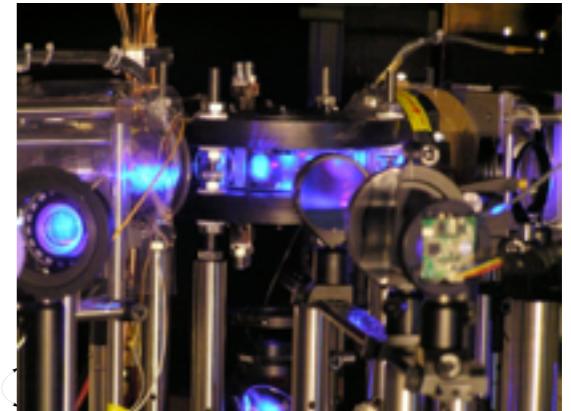
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# Outline

## Overview of Quantum Simulation

- Analogue and digital quantum simulators
- Microscopic description of cold atomic gases
- Example: The Bose-Hubbard Model
- Recent developments and extensions
- Perspectives

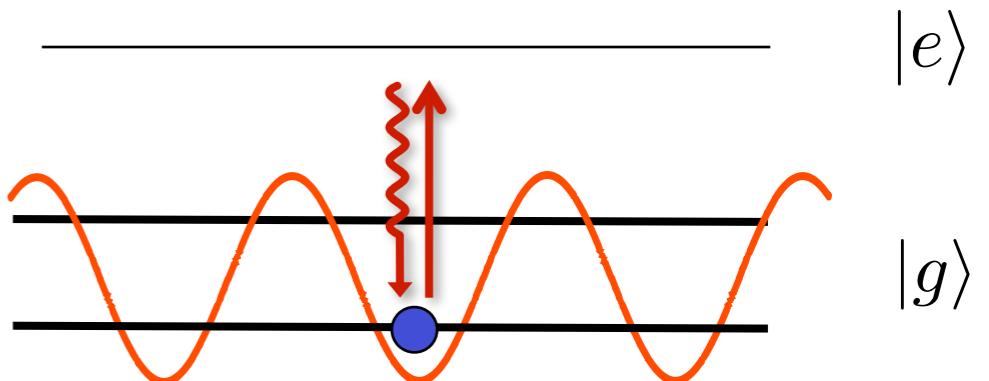
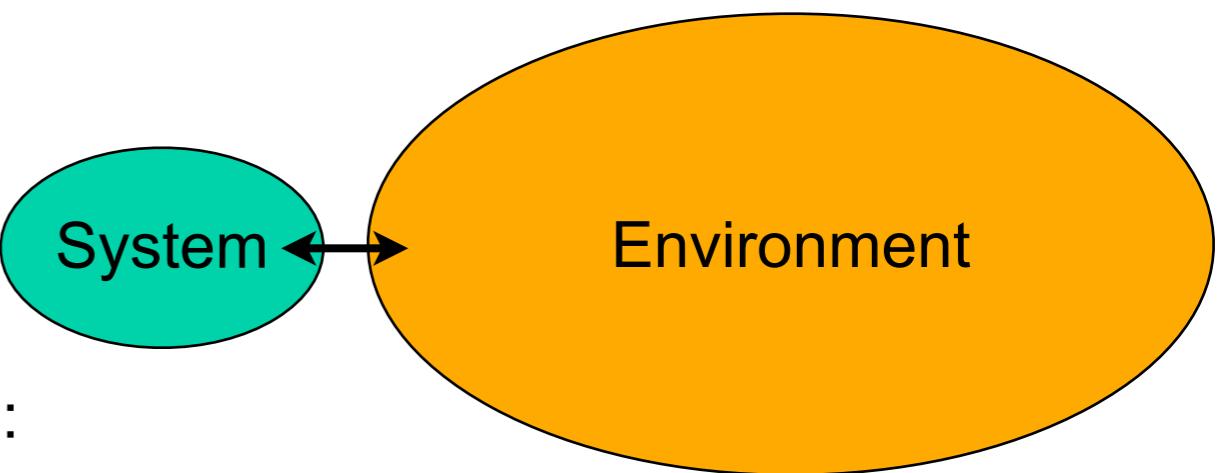
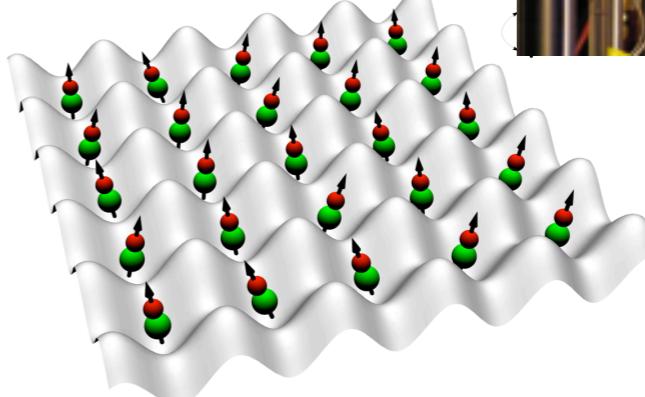


## Microscopic Details for optical lattices

- Microscopic treatment of interactions
- Band structure and the Bose-Hubbard model

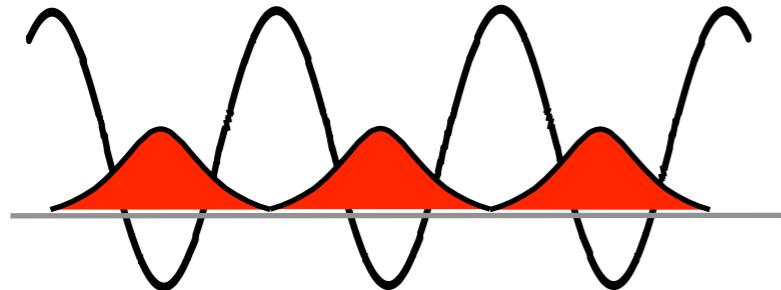
## Open many-body quantum systems

- Also decoherence is microscopically understood:  
Heating in optical lattices
- Decoherence can be your friend:  
Losses are good!  
Dark state cooling and state preparation



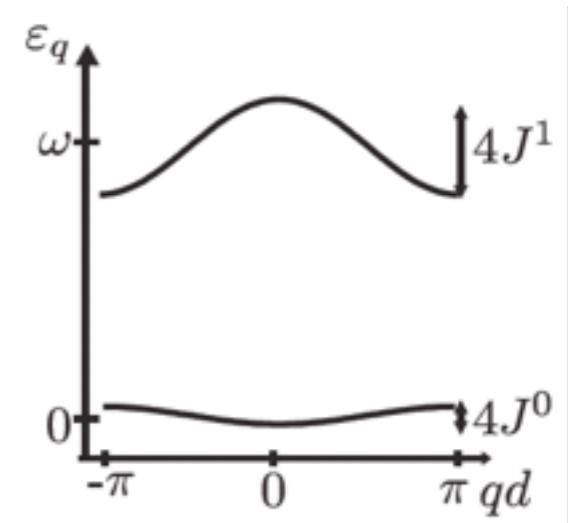
# Bose-Hubbard model

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



Wannier  
functions

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



Assume:

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

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

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

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

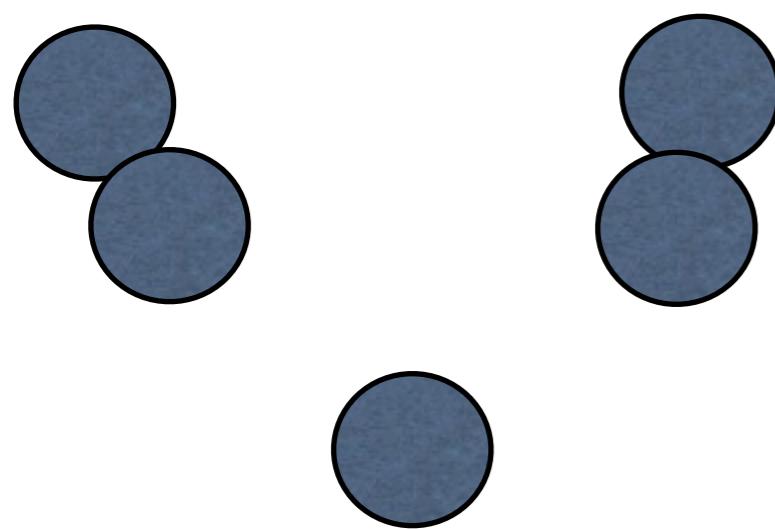
$$\longrightarrow H = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \sum_i \epsilon_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) \quad k_B T, J, U \ll \hbar\omega$$

# Microscopic Details for Optical Lattices

- Microscopic treatment of interactions
- Band structure and the Bose-Hubbard model

## Microscopic Control: Interactions:

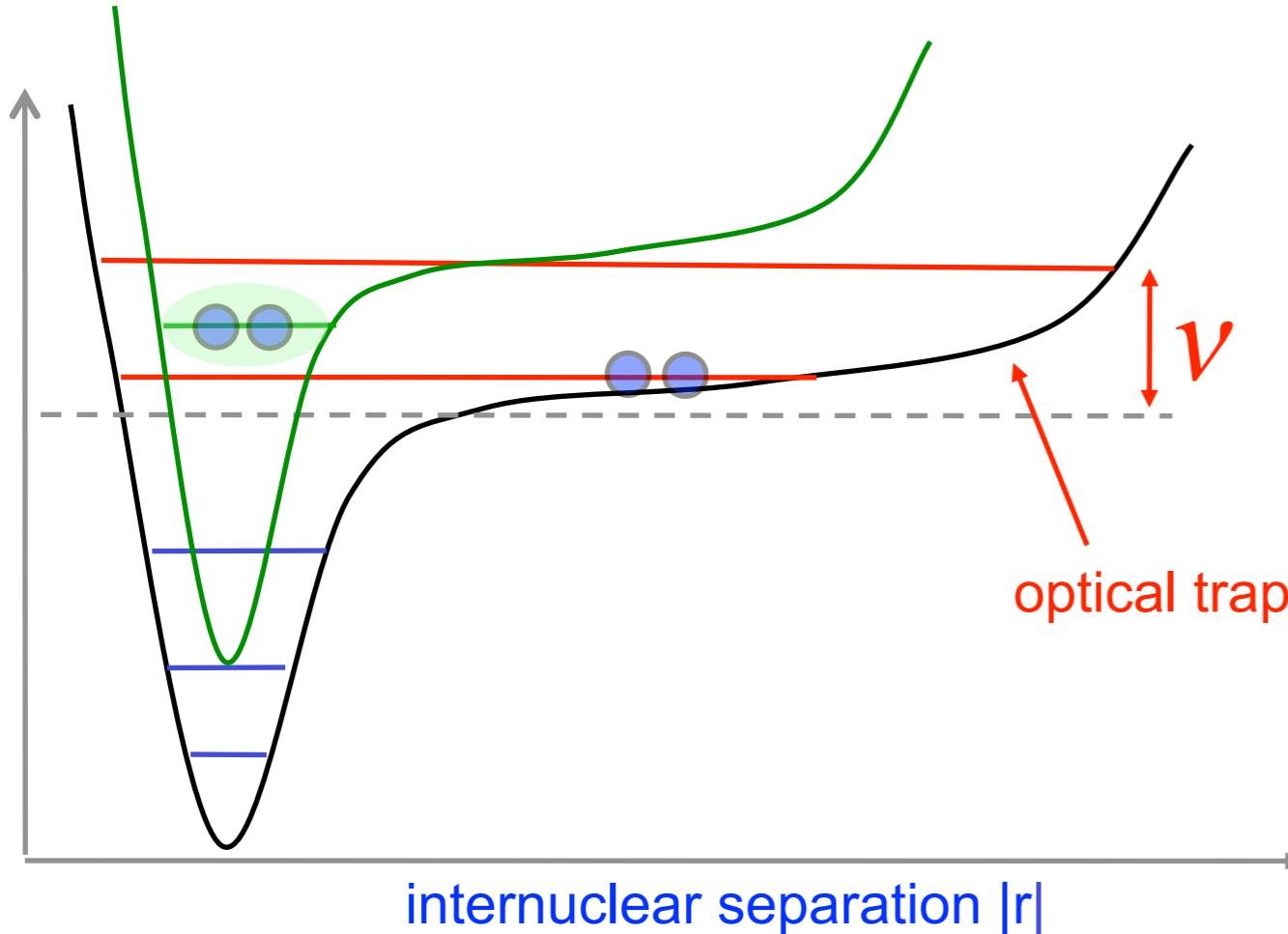
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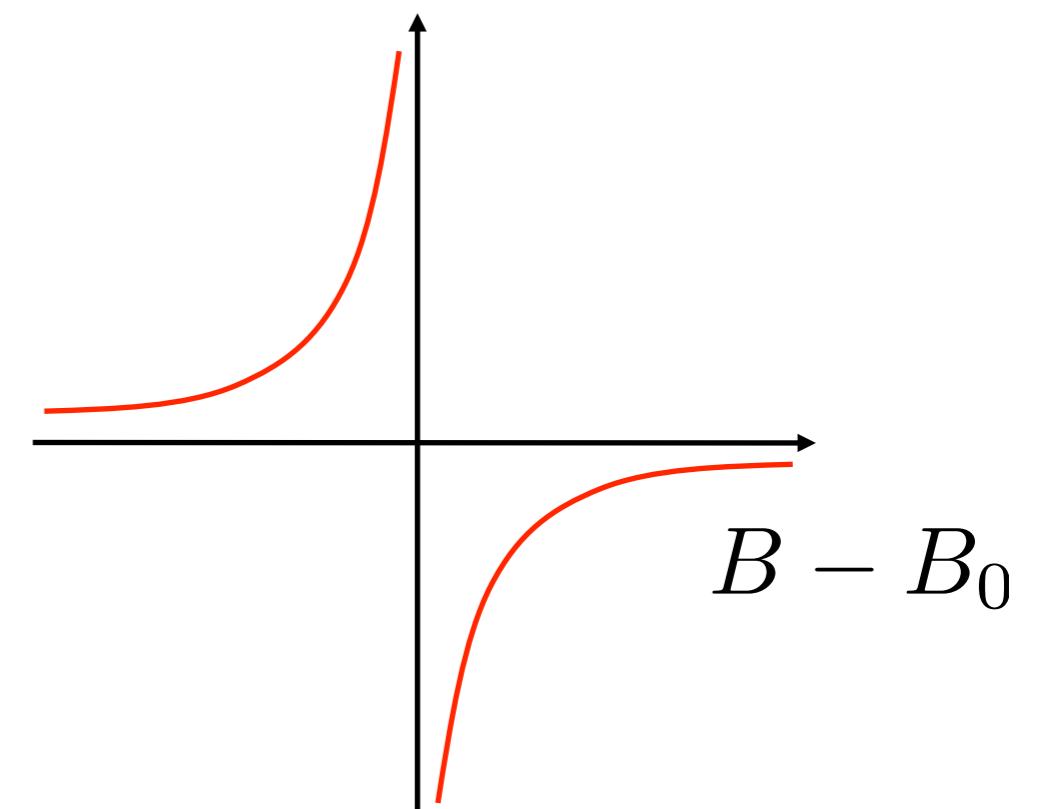
Microscopic understanding of interactions:

- Dilute gas - three body interactions weak
- Low-energy two-body interactions
- Simple microscopic description

## Microscopic Control: Feshbach Resonance



Scattering length  
(strength of interactions)



## Microscopic Model for Cold Bosons

- In terms of second quantised field operators  $\hat{\psi}(\mathbf{r})$ , the many-body Hamiltonian for a Bose gas, including the effects of an external trapping potential and two-body interactions may be written as

$$\hat{H} = \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) + \frac{1}{2} \int d^3r \int d^3r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r}' - \mathbf{r}) \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r})$$

- Here,  $V_{ext}(\mathbf{r})$  is an external potential (e.g., a magnetic trapping potential, or potential due to an AC-Stark shift from interaction with laser light).
- $V(\mathbf{r}' - \mathbf{r})$  is the two-body interaction Hamiltonian. Treating only two-body interactions is valid provided that the gas is sufficiently dilute that higher order interactions are not relevant on the timescale of the experiment.
- For low energy collisions between distinguishable particles or Bosons, we can write

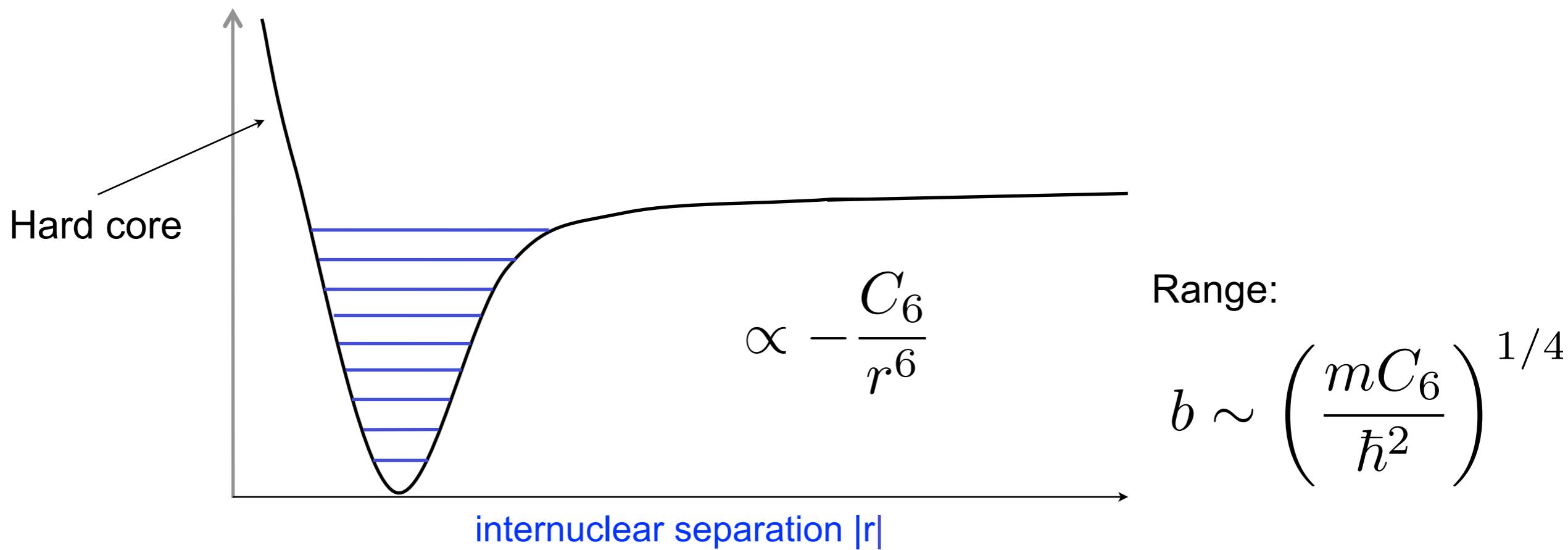
$$\hat{H} = \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) + \frac{g}{2} \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r})$$

- Note: The second-quantised field operators obey the commutation relation

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

## Interactions in a dilute Bose Gas

- In thermal equilibrium typical BECs in atomic gases would be solid (crystalline)
- Density of gas is sufficiently small that 3-body collisions are rare, and gas is metastable with lifetimes of the order of seconds
- Also because 3-body collisions are rare, interactions may be treated as two-body scattering.
- We see this metastability from the Born-Oppenheimer curve for the interaction potential, where the unbound state is a metastable state.



## Why use a pseudopotential?

- In the limit of low energies, the scattering properties are universal, and depend essentially on 1 parameter, the scattering length  $a$ . The details of the scattering potential are, in this sense not important. The scattering length will be measured experimentally, and this is the only data really required to describe 2-body interactions in the system.
- At the same time, it is difficult to determine the real potential  $V(r)$  precisely, and difficult to perform calculations with it.
- Any small error in  $V(r)$  could significantly change the scattering properties, when really the most relevant information is simply the value for the scattering length produced by the potential.
- The weakly interacting Bose gases we deal with are metastable. We thus cannot perform calculations assuming thermal equilibrium using the real potential.
- Because  $V(r)$  is strongly repulsive at short distances and has many bound states, the Born approximation (1st order perturbation theory) is not valid when used with the real potential.
- We thus replace exact interaction potential with a potential having the same scattering properties at low energy (i.e., the same scattering length), but that is treatable in the Born approximation and easier in general to work with mathematically.

- The pseudopotential with only the one necessary parameter is the zero-range pseudopotential, originally used by Fermi.

$$\langle \mathbf{r} | V(\mathbf{r}) | \psi(\mathbf{r}) \rangle = g \delta(\mathbf{r}) \left[ \frac{\partial}{\partial r} (r \psi(\mathbf{r})) \right]_{r=0}$$

with

$$g = \frac{2\pi\hbar^2 a}{m_r} = \frac{4\pi\hbar^2 a}{m}$$

## References:

- E. Fermi, La Ricerca Scientifica, VII-II (1936), 1352.
- K. Huang and C. N. Yang, Phys. Rev. 105 (1957), 767.
- K. Huang, Statistical Mechanics, Wiley, New York, 1963.
- “Bose-Einstein Condensation in Atomic Gases: simple theoretical results”  
Yvan Castin, <http://www.arxiv.org/abs/cond-mat/0105058>

## Results from Scattering Theory

- We can show that at large distances from the scattering centre,  $r = |\mathbf{r}| \gg b$ , where  $b$  is the range of the potential, the outgoing scattering wavefunctions for a local potential  $V(\mathbf{r})$  are written as the sum of an incoming plane wave and an outgoing spherical wave,

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} + f(\mathbf{k}, \mathbf{k}') \frac{e^{ikr}}{r}$$

$$f(\mathbf{k}, \mathbf{k}') = -\frac{2m_r}{4\pi\hbar^2} \int d\mathbf{r}' e^{-i\mathbf{k}' \cdot \mathbf{r}'} V(\mathbf{r}') \psi_{\mathbf{k}}^{(+)}(\mathbf{r}')$$

with  $m_r = m_1 m_2 / (m_1 + m_2)$  the reduced mass,

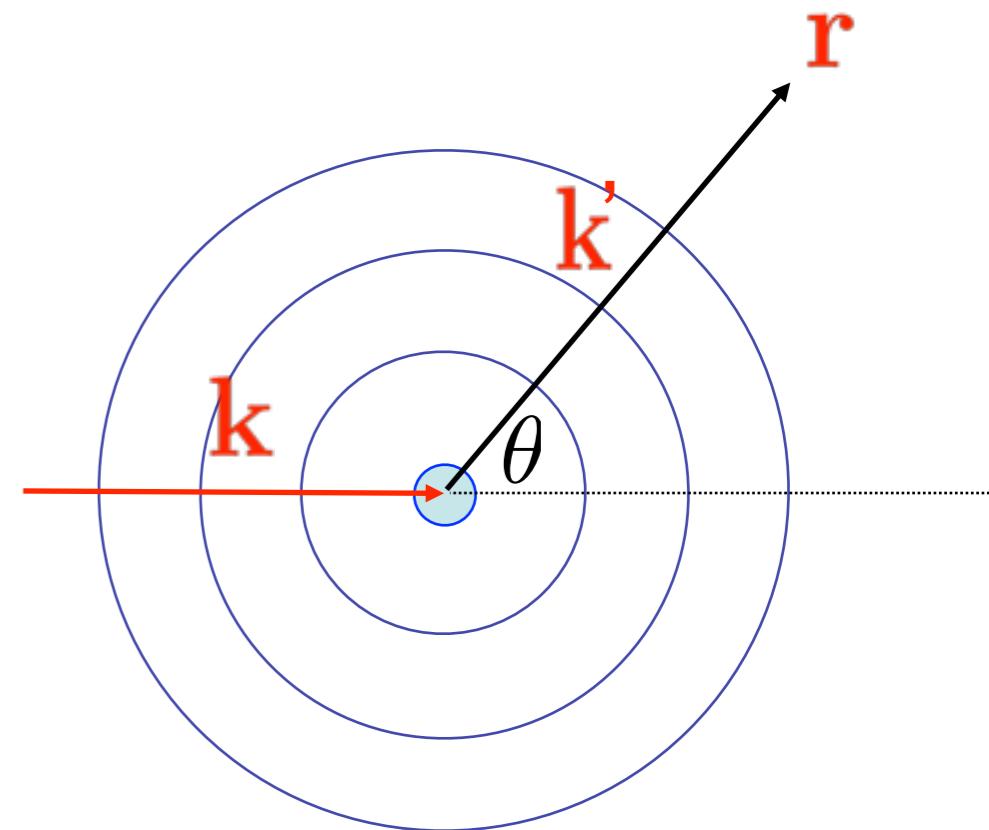
$$r = |\mathbf{r}|, \quad k = |\mathbf{k}| = \sqrt{\frac{2mE}{\hbar^2}}$$

and  $\mathbf{k}' = k \frac{\mathbf{r}}{|\mathbf{r}|}$ .

- For a spherically symmetric potential,  $V(\mathbf{r}) = V(r)$  and

$$f(\mathbf{k}, \mathbf{k}') = f(k, \theta)$$

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} + f(k, \theta) \frac{e^{ikr}}{r}$$



$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} + f(\mathbf{k}, \mathbf{k}') \frac{e^{ikr}}{r}$$

$$f(\mathbf{k}, \mathbf{k}') = -\frac{2m_r}{4\pi\hbar^2} \int d\mathbf{r}' e^{-i\mathbf{k}' \cdot \mathbf{r}'} V(\mathbf{r}') \psi_{\mathbf{k}}^{(+)}(\mathbf{r}')$$

## Born Approximation

- It is clear that one can iterate this solution in the sense of a perturbation expansion in the strength of the potential  $V(\mathbf{r})$ . The first order expansion, in which we substitute the incoming plane wave  $\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}}$  into the expression for the scattering amplitude yields:

$$f(\mathbf{k}, \mathbf{k}') = -\frac{2m_r}{4\pi\hbar^2} \int d\mathbf{r}' e^{-i\mathbf{k}' \cdot \mathbf{r}'} V(\mathbf{r}') \psi_{\mathbf{k}}^{(+)}(\mathbf{r}')$$

$$\approx -\frac{2m_r}{4\pi\hbar^2} \int d\mathbf{r}' e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}'} V(\mathbf{r}') + \frac{m_r^2}{4\pi^2\hbar^4} \int d\mathbf{r}' \int d\mathbf{r}'' e^{-i\mathbf{k}' \cdot (\mathbf{r}' + \mathbf{r}'')} V(\mathbf{r}'') V(\mathbf{r}') \psi_{\mathbf{k}}^{(+)}(\mathbf{r}'')$$

$$\approx -\frac{2m_r}{4\pi\hbar^2} \int d\mathbf{r}' e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}'} V(\mathbf{r}')$$

- This first order expansion is known as the Born approximation.

## Partial Wave expansion

- If the potential  $V(\mathbf{r}) = V(r)$  is spherically symmetric, then the Hamiltonian commutes with the total angular momentum operator,  $\hat{L}$  and  $\hat{L}^2$ .
- We can expand the wavefunction as a sum of states of definite angular momentum as

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty} \sqrt{\frac{2l+1}{4\pi}} P_l(\cos \theta) \frac{\chi_{kl}(r)}{r}$$

where we have chosen the incoming axis to be the  $z$ -direction,  $P_l(x)$  is a Legendre Polynomial and the scattering amplitude can be expressed as

$$f(k, \theta) = \sum_{l=0}^{\infty} (2l+1) f_l(k) P_l(\cos \theta),$$

and the radial functions are solutions of the radial Schrödinger equation

$$\frac{d^2 \chi_{kl}}{dr^2} - \frac{l(l+1)}{r^2} \chi_{kl} + \frac{2m_r}{\hbar^2} [E - V(r)] \chi_{kl} = 0$$

with  $E = \hbar^2 k^2 / (2m_r)$ .

- For  $V(r) = 0$ , the general solution to the radial Schrödinger equation,

$$\frac{d^2\chi_{kl}}{dr^2} - \frac{l(l+1)}{r^2}\chi_{kl} + \frac{2m_r}{\hbar^2}[E - V(r)]\chi_{kl} = 0$$

is given in terms of the so-called spherical Bessel and Von Neumann functions as

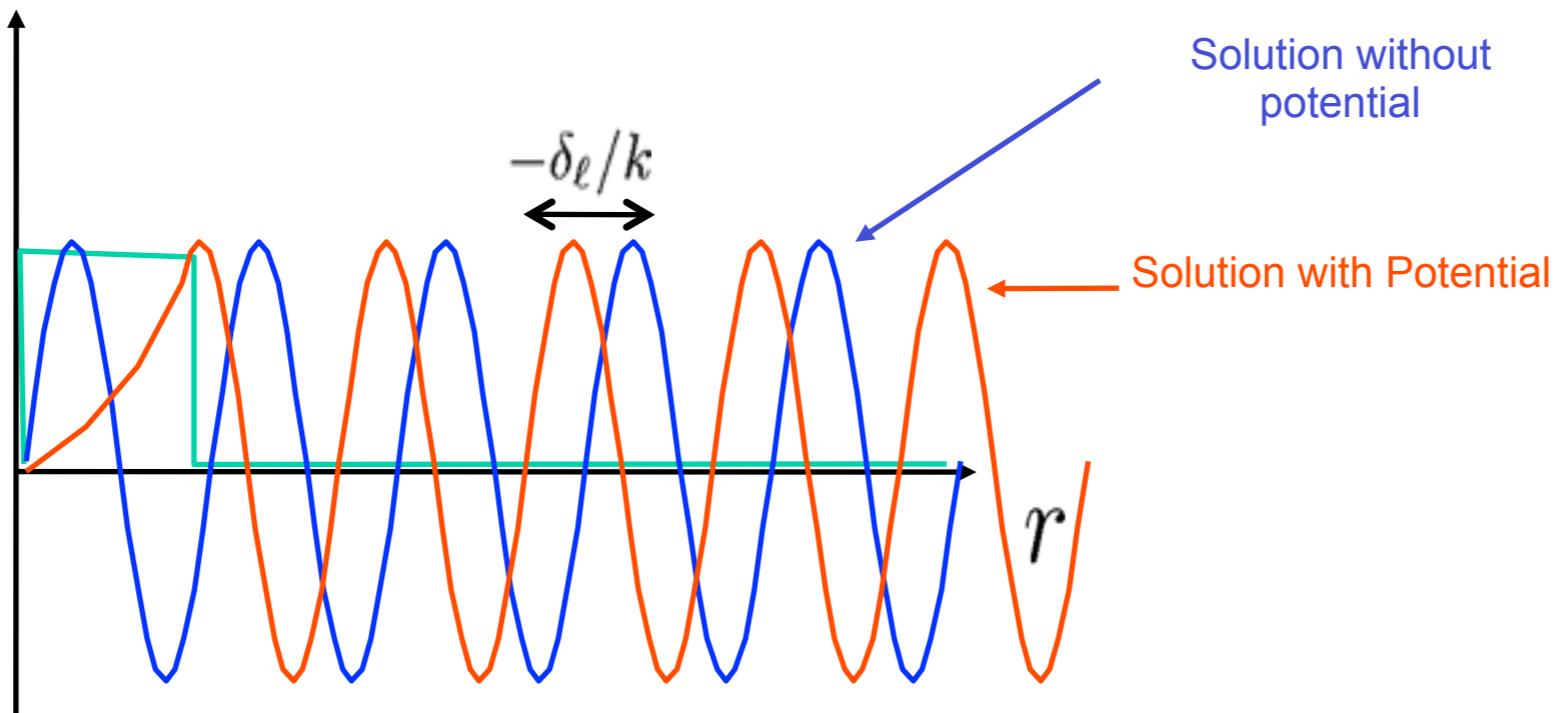
$$\chi_{kl} = A_l[\hat{j}_l(kr) \cos \delta_l + \hat{n}_l(kr) \sin \delta_l]$$

which reduces at large distances to

$$\chi_{kl}(r) = A_l[\sin(kr - \pi l/2) \cos \delta_l + \cos(kr - \pi l/2) \sin \delta_l] = A_l \sin\left(kr - \frac{\pi l}{2} + \delta_l\right)$$

where  $\delta_l(k)$  are the scattering phase shifts.

- These scattering phase shifts describe the full details of the scattering process, and are in general dependent on both the scattering potential and incident energy.



## Scattering from a Hard Sphere

- We consider the simple example of scattering from a hard sphere,

$$V(r) = \begin{cases} \infty, & r \leq a \\ 0, & r > a \end{cases}$$

- The general solution to the radial Schrödinger equation is given by

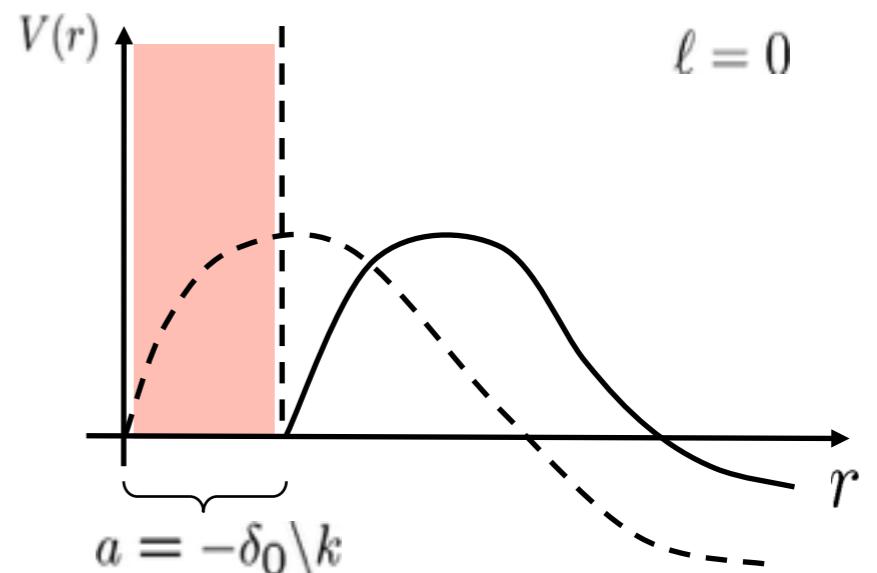
$$\chi_l(r) = \begin{cases} 0, & r \leq a \\ A_l [\hat{j}_l(kr) \cos \delta_l + \hat{n}_l(kr) \sin \delta_l], & r > a \end{cases}$$

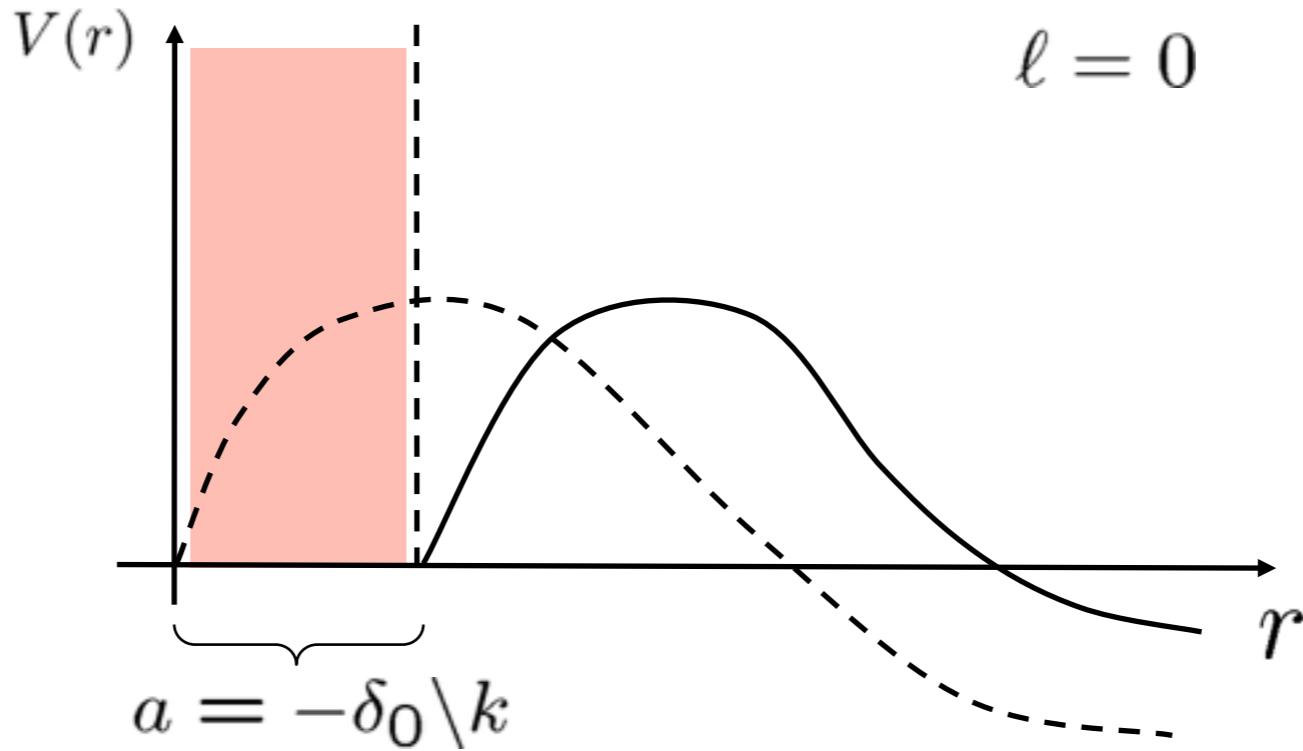
- Imposing continuity, we obtain  $\chi_l(a) = 0$ ,

$$\Rightarrow \tan \delta_l(k) = -\frac{\hat{j}_l(ka)}{\hat{n}_l(ka)}$$

- For s-wave scattering, taking  $ka \ll 1$ , we obtain

$$\delta_0(k) = -\frac{\sin(ka)}{\cos(ka)} = -ka$$





- In general at low energies,

$$\delta_l(k) = -\frac{\hat{j}_l(ka)}{\hat{n}_l(ka)} = \frac{(ka)^{l+1}}{(2l+1)!!} \frac{1}{(ka)^{-l}(2l-1)!!} \sim (ka)^{2l+1}$$

from which the dominance of s-wave scattering is clear.

- Note that as  $a \rightarrow 0$ ,  $\delta_l \rightarrow 0$ , and thus in the limit of a zero range delta function (in 3D), the scattering potential becomes transparent.

- We can express the plane wave component of  $\psi(\mathbf{r})$  in terms of Legendre Polynomials as

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l\left(\frac{\mathbf{k}\cdot\mathbf{r}}{kr}\right)$$

where  $j_l(kr)$  is the Bessel function of order  $l$ , and  $P_l(\cos \theta)$  are the Legendre Polynomials.

- For  $kr \gg 1$ ,

$$j_l(kr) \rightarrow \frac{e^{i(kr-l\pi/2)} - e^{-i(kr-l\pi/2)}}{2ikr}$$

writing  $i^l = e^{il\pi/2}$ , we see

$$\begin{aligned} \psi_{\mathbf{k}}^{(+)}(\mathbf{r}) &= e^{i\mathbf{k}\cdot\mathbf{r}} + f(k, \theta) \frac{e^{ikr}}{r} \\ &= \sum_{l=0}^{\infty} (2l+1) P_l(\cos \theta) \left( \frac{e^{i(kr)} - e^{-i(kr-l\pi)}}{2ikr} \right) + \sum_{l=0}^{\infty} (2l+1) f_l(k) P_l(\cos \theta) \frac{e^{ikr}}{r} \\ \psi_{\mathbf{k}}^{(+)}(\mathbf{r}) &= \sum_{l=0}^{\infty} (2l+1) \frac{P_l(\cos \theta)}{2ik} \left[ [1 + 2ik f_l(k)] \frac{e^{ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r} \right] \end{aligned}$$

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = \sum_{l=0}^{\infty} (2l+1) \frac{P_l(\cos \theta)}{2ik} \left[ [1 + 2ik f_l(k)] \frac{e^{ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r} \right]$$

- Thus, when no scattering occurs,  $f_l(k) = 0$ , the wavefunction is a sum of an incoming and outgoing spherical wave.
- Scattering changes the coefficient of the outgoing wave to  $1 + 2ik f_l(k)$ .
- Unitarity condition: As there is no source or sink of particles, the incoming flux must equal the outgoing flux, and therefore the modulus of the coefficients for the incoming and outgoing waves must be equal. Momentum conservation implies that this must be true for each partial wave separately.

$$|1 + 2ik f_l(k)| = 1$$

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = \sum_{l=0}^{\infty} (2l+1) \frac{P_l(\cos \theta)}{2ik} \left[ [1 + 2ik f_l(k)] \frac{e^{ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r} \right]$$

- By comparison with the general solution for  $\chi_{kl}$ ,

$$\chi_{kl}(r) = A_l \sin \left( kr - \frac{\pi l}{2} + \delta_l \right) = \frac{A_l}{2i} \left[ e^{i(kr-l\pi/2+\delta_l)} - e^{-i(kr-l\pi/2+\delta_l)} \right]$$

we write

$$[1 + 2ik f_l(k)] \frac{e^{ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r} = \frac{e^{+il\pi/2+i\delta_l}}{r} \left[ e^{i(kr-l\pi/2+\delta_l)} - e^{-i(kr-l\pi/2+\delta_l)} \right]$$

identifying

$$1 + 2ik f_l(k) = e^{2i\delta_l}.$$

so that

$$f_l(k) = \frac{e^{2i\delta_l} - 1}{2ik} = \frac{e^{i\delta_l} \sin \delta_l}{k} = \frac{1}{k \cot \delta_l - ik}$$

$$\frac{d^2\chi_{kl}}{dr^2} - \frac{l(l+1)}{r^2}\chi_{kl} + \frac{2m_r}{\hbar^2}[E - V(r)]\chi_{kl} = 0$$

## Low-Energy Scattering

- By matching the phase shifts  $\delta_l$  from the solutions to the radial Schrödinger equation with the amplitude,

$$f(k, \theta) = \sum_{l=0}^{\infty} \frac{2l+1}{k \cot \delta_l - ik} P_l(\cos \theta)$$

- Contribution of higher partial waves is important at high incident energies, but for a short range potential,  $\delta_l \propto k^{2l+1}$ , and contributions to the scattering amplitude approach zero as  $k^l$  when  $k \rightarrow 0$ . This is a result of the centrifugal barrier in the radial Schrödinger equation.
- Hence, at low energies (typically  $T < 100\mu\text{K}$ ), the scattering for distinguishable particles or identical Bosons is entirely dominated by contributions from s-wave,  $l = 0$ . (For Fermions, it is dominated by p-wave,  $l = 1$ ).

$$f(k, \theta) \approx \frac{1}{k \cot \delta_0 - ik}$$

- At sufficiently low energies, the s-wave phase shift can be expanded in powers of  $k$ . This effective-range expansion is given by

$$k \cot \delta_0(k) = -1/a + r_b k^2/2 - P_s k^4/4 + \dots$$

where  $r \sim b$  for a Van der Waals potential, and  $a$  is called the scattering length.

$$f(k, \theta) \approx \frac{1}{k \cot \delta_0 - ik}$$

$$k \cot \delta_0(k) = -1/a + r_b k^2/2 - P_s k^4/4 + \dots$$

- For small  $k$ , we thus write  $f(k, \theta)$  as

$$f(k) = \frac{1}{-1/a - ik + r_b k^2/2 + \dots}$$

- As  $k \rightarrow 0$ ,  $f(k) \rightarrow -a$ .
- Note that in this limit,

$$a \approx -\frac{1}{k \cot \delta_0(k)}$$

diverging scattering length,  $a \rightarrow \pm\infty$  can thus be understood in terms of a phase shift that becomes close to  $\pm\pi/2$ .

## The Zero-Range Pseudopotential

- We see at low energies that the description of the scattering process reduces to a single parameter. Thus, we can introduce a pseudopotential if it produces these same low energy scattering properties.
- The pseudopotential with only the one necessary parameter is the zero-range pseudopotential, originally used by Fermi.

$$\langle \mathbf{r} | V(\mathbf{r}) | \psi(\mathbf{r}) \rangle = g \delta(\mathbf{r}) \left[ \frac{\partial}{\partial r} (r \psi(\mathbf{r})) \right]_{r=0}$$

with

$$g = \frac{2\pi\hbar^2 a}{m_r} = \frac{4\pi\hbar^2 a}{m}$$

- The effect of regularisation here is to remove any part of the wavefunction that diverges as  $1/r$ . Any part of the wavefunction that does not diverge as  $1/r$  is unaffected by regularisation.
- Note that if we took only a  $\delta$ -function, then the potential would give rise to no scattering at all in three dimensions, as can be seen from a hard sphere in the limit  $b \rightarrow 0$ .
- The regularisation comes from the need to introduce the appropriate boundary conditions for  $r \rightarrow \infty$ .

# Scattering properties of the zero-range pseudopotential

- We can compute the resulting outgoing state exactly using this potential. Writing

$$C_\psi = \left[ \frac{\partial}{\partial r} (r \psi(\mathbf{r})) \right]_{r=0}, \text{ we obtain}$$

$$\langle \mathbf{r} | V(\mathbf{r}) | \psi(\mathbf{r}) \rangle = g \delta(\mathbf{r}) \left[ \frac{\partial}{\partial r} (r \psi(\mathbf{r})) \right]_{r=0}$$

$$f(\mathbf{k}, \mathbf{k}') = -\frac{2m_r}{4\pi\hbar^2} \int d\mathbf{r}' e^{-i\mathbf{k}' \cdot \mathbf{r}'} V(\mathbf{r}') \psi_{\mathbf{k}}^{(+)}(\mathbf{r}')$$

$$= -g \frac{2m_r}{4\pi\hbar^2} \int d\mathbf{r}' e^{-i\mathbf{k}' \cdot \mathbf{r}'} \delta(\mathbf{r}') \left[ \frac{\partial}{\partial r} (r \psi_{\mathbf{k}}^{(+)}(\mathbf{r})) \right]_{r=0}$$

$$= -a C_{\psi+}$$

as  $g = 4\pi\hbar^2 a/m = 2\pi\hbar^2 a/m_r$

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} - a C_{\psi+} \frac{e^{ikr}}{r}$$

thus,

$$C_{\psi+} = \frac{1}{1 + ika}$$

$$f(\mathbf{k}, \mathbf{k}') = -\frac{a}{1 + ika} = \frac{1}{-1/a - ik}$$

$$r \psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = r e^{i\mathbf{k} \cdot \mathbf{r}} - r a C_{\psi+} \frac{e^{ikr}}{r}$$

$$\left[ \frac{\partial}{\partial r} (r \psi_{\mathbf{k}}^{(+)}(\mathbf{r})) \right]_{r=0} = \left[ \frac{\partial}{\partial r} (r e^{i\mathbf{k} \cdot \mathbf{r}} - r a C_{\psi+} e^{ikr}) \right]_{r=0}$$

$$C_{\psi+} = [e^{i\mathbf{k} \cdot \mathbf{r}} + ikr e^{i\mathbf{k} \cdot \mathbf{r}} - ika C_{\psi+} e^{ikr}]_{r=0}$$

$$C_{\psi+} = 1 - ika C_{\psi+}$$

$$C_{\psi^+} = \frac{1}{1 + ika}$$

so that

$$f(\mathbf{k}, \mathbf{k}') = -\frac{a}{1 + ika} = \frac{1}{-1/a - ik}$$

which is the correct s-wave scattering amplitude that we obtained previously.

- Thus, we can describe scattering properties by replacing  $V(r)$  with this pseudopotential.
- This is valid whenever s-wave scattering dominates, and our scattering amplitude,

$$f(k) = \frac{1}{-1/a - ik + r_b k^2/2 + \dots} \approx \frac{1}{-1/a - ik}.$$

Thus, the pseudopotential is valid in the limit where  $kb \ll 1$ . It is **not** required that  $ka \ll 1$ .

- Therefore, the pseudopotential may be used near a Feshbach resonance, where  $a$  diverges, but  $b$  remains constant.

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - aC_{\psi^+} \frac{e^{ikr}}{r}$$

$$C_{\psi} = \left[ \frac{\partial}{\partial r} (r \psi(\mathbf{r})) \right]_{r=0}$$

## Zero-Range Pseudopotential and the Born Series

- The requirement for the use of the Born approximation to be valid with the pseudopotential (as is required for mean-field theories to be used) is, indeed  $ka \ll 1$  :
- The Born expansion reduces to iterations of the equation

$$C_{\psi^+} = 1 - ikaC_{\psi^+},$$

in order to specify the corresponding scattering states,

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - aC_{\psi^+} \frac{e^{ikr}}{r}.$$

The Born approximation is given by the first order iteration, i.e.,

$$C_1 = 1 - ikaC_0 = 1.$$

Similarly, higher order approximations are given by:

$$C_2 = 1 - ikaC_1 = 1 - ika$$

$$C_3 = 1 - ikaC_2 = 1 - ika + (ika)^2$$

and the Born expansion is a geometrical series of the exact result  $C_{\psi^+} = 1/(1 + ika)$  in powers of  $ika$ .

$$\langle \mathbf{r} | V(\mathbf{r}) | \psi(\mathbf{r}) \rangle = g \delta(\mathbf{r}) \left[ \frac{\partial}{\partial r} (r \psi(\mathbf{r})) \right]_{r=0}$$

$$C_\psi = \left[ \frac{\partial}{\partial r} (r \psi(\mathbf{r})) \right]_{r=0}$$

$$C_1 = 1 - ikaC_0 = 1.$$

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - aC_{\psi^+} \frac{e^{ikr}}{r}$$

$$C_2 = 1 - ikaC_1 = 1 - ika$$

$$C_3 = 1 - ikaC_2 = 1 - ika + (ika)^2$$

- The Born approximation is thus valid when the first order result is a small correction to the zeroth order result, which requires

$$k|a| \ll 1.$$

For the scattering state, we thus require

$$r \gg a.$$

- Substituting the Pseudopotential for  $V(\mathbf{r})$  in the many body Hamiltonian for the case where the Born approximation is valid (and thus the regularisation in the pseudopotential gives the constant 1), we thus obtain from

$$\hat{H} = \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{ext}(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) + \frac{1}{2} \int d^3r \int d^3r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r}' - \mathbf{r}) \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r})$$

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

## 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.

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

- That these operators represent Bosons is an approximation: our atoms are actually composed of Fermions. In fact, the commutator is actually

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

where the correction  $D(\mathbf{r} - \mathbf{r}')$  is small provided that  $|\mathbf{r} - \mathbf{r}'| \gg b_0$ , where  $b_0$  is the typical extent of the electronic wavefunctions for a single atom.

- Thus, these corrections play a small role provided that the typical size of the atoms (The Bohr radius,  $\sim 0.05$  nm) is small compared with the typical separation between atoms in the condensate (typically  $> 10$  nm, even in an optical lattice).
- EXERCISE:** Try computing  $D(\mathbf{r} - \mathbf{r}')$  for the Hydrogen atom,  $\hat{\psi}_H(\mathbf{R}) \approx \int d^3r \phi(\mathbf{r}) \hat{\psi}_e(\mathbf{R} + \mathbf{r}) \hat{\psi}_p(\mathbf{R})$  (where we take  $m_e/m_p \approx 0$ )

## Gross-Pitaevskii as a Classical Field Equation

- This replacement of the field operator with a classical wavefunction,

$$\hat{\psi}(\mathbf{r}) \approx \sqrt{N}\phi(\mathbf{r}) = \psi(\mathbf{r})$$

is analogous to treating quantum electrodynamics (photons) as the classical electromagnetic field.

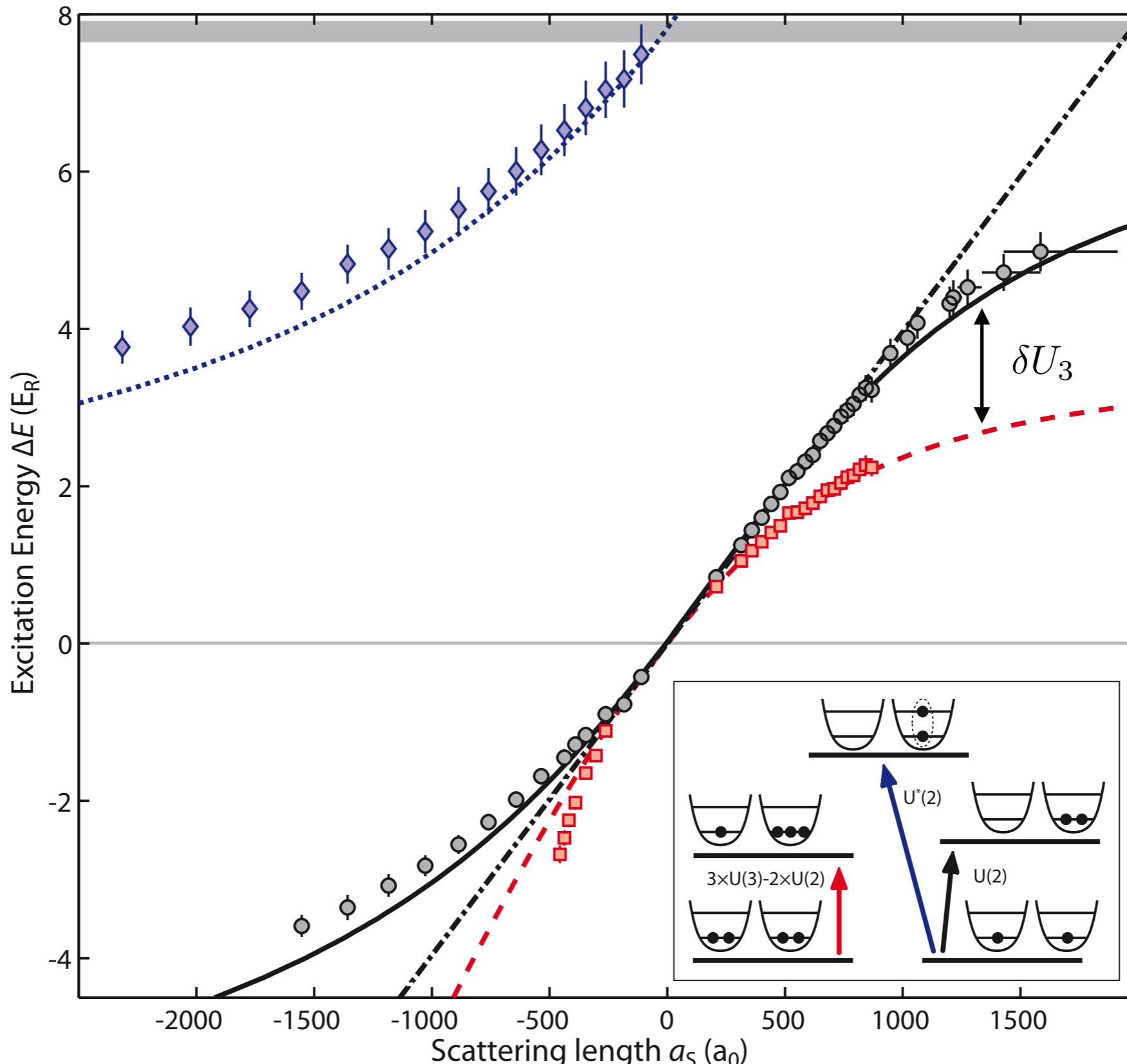
- This is valid if there are many photons in approximately the same quantum state, in which case the commutivity of the field operators is not important, and we can replace them by the classical electric and magnetic fields, obeying Maxwell's equations.
- Here, we similarly have many atoms in one quantum state, and we can neglect fluctuations on the single atom level.
- We can obtain the Gross-Pitaevskii equation, then, directly from the equation of motion for the field operator,

$$i\hbar \frac{\partial}{\partial t} \hat{\psi}(\mathbf{r}, \mathbf{t}) = [\hat{\psi}(\mathbf{r}, \mathbf{t}), \hat{H}] = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_0(\mathbf{r}) + g \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}, \mathbf{t})$$

by replacing the field operator with the classical condensate wavefunction,

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, \mathbf{t}) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_0(\mathbf{r}) + g |\psi(\mathbf{r})|^2 \right] \psi(\mathbf{r}, \mathbf{t})$$

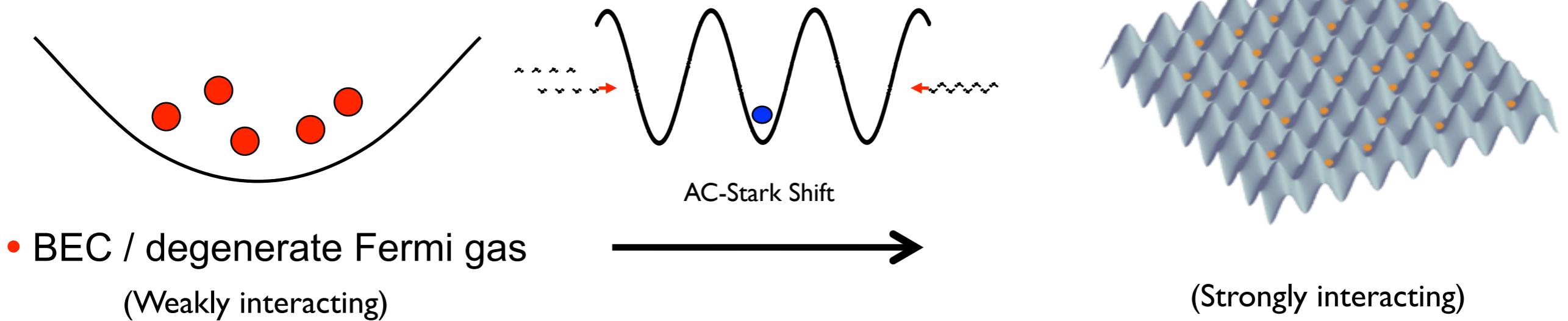
# Shifts beyond the Born approximation in the scattering:



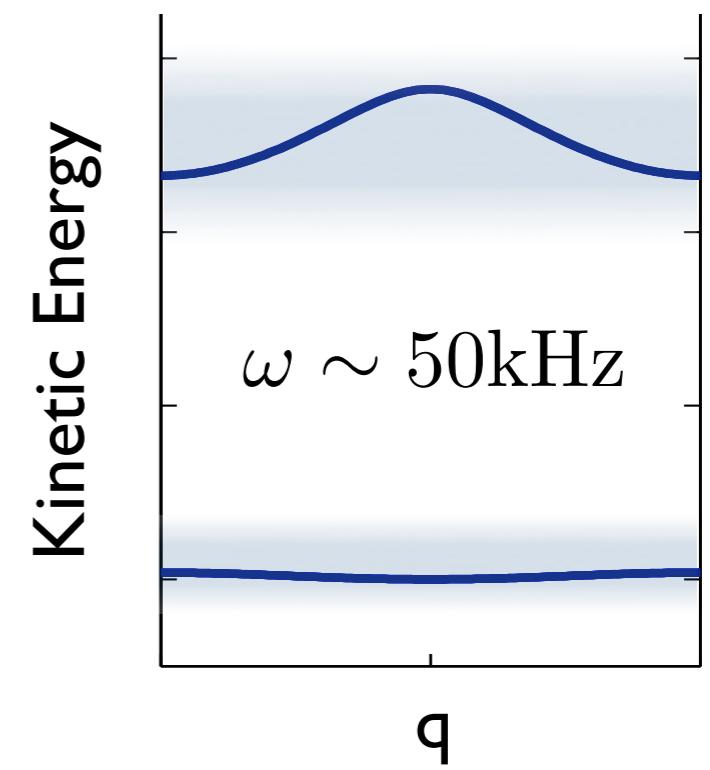
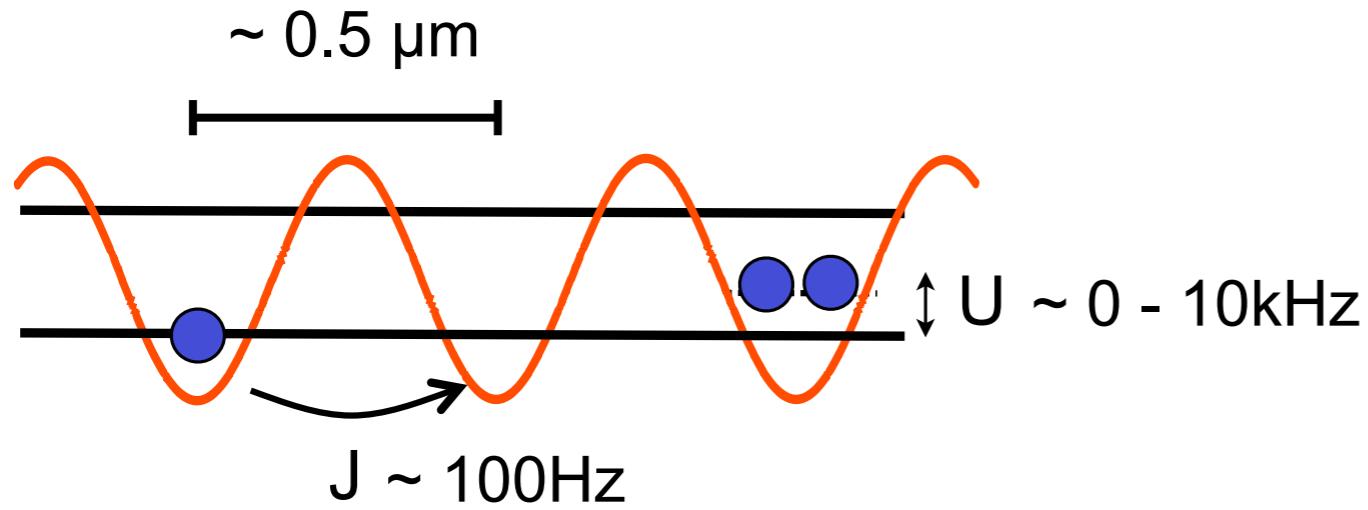
# Microscopic Details for Optical Lattices

- Microscopic treatment of interactions
- Band structure and the Bose-Hubbard model

# Atoms in 3D Optical Lattices (also 1D/2D geometries):



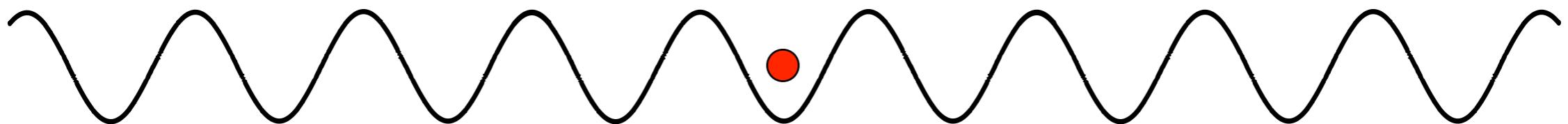
Bose-Hubbard: D. Jaksch et al. PRL '98



## 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  $\alpha \in [-\pi, \pi]$ .

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

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

- Because

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

we can write

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

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  $\hat{T}$ ,

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

## Bloch Functions

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

$$\phi_q^{(n)}(x) = e^{iqx} u_q^n(x),$$

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 ( $u_q^{(n)}(x + a) = u_q^{(n)}(x)$ ).

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

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

$$u_q^{(n)}(x) = \frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} c_j^{(n,q)} e^{i2k_l x j},$$

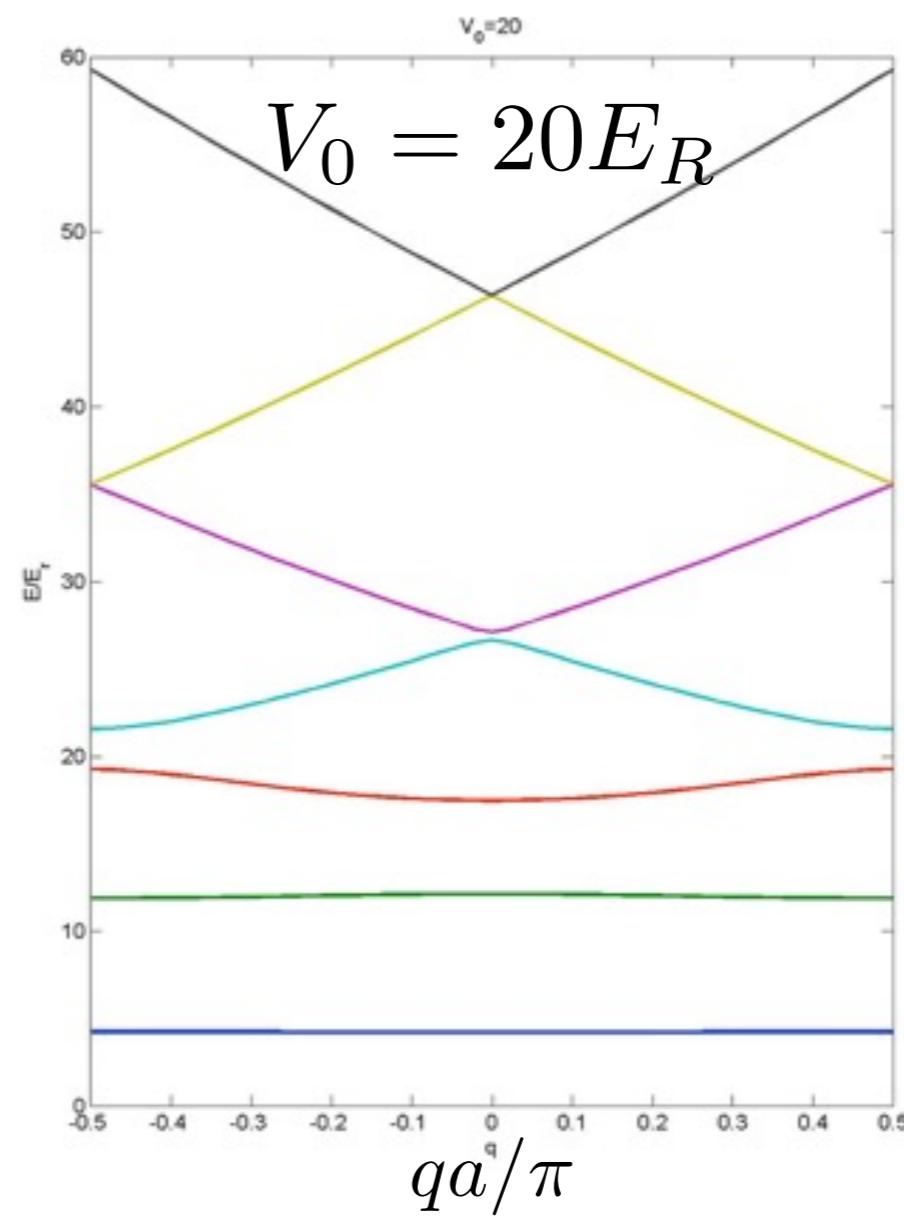
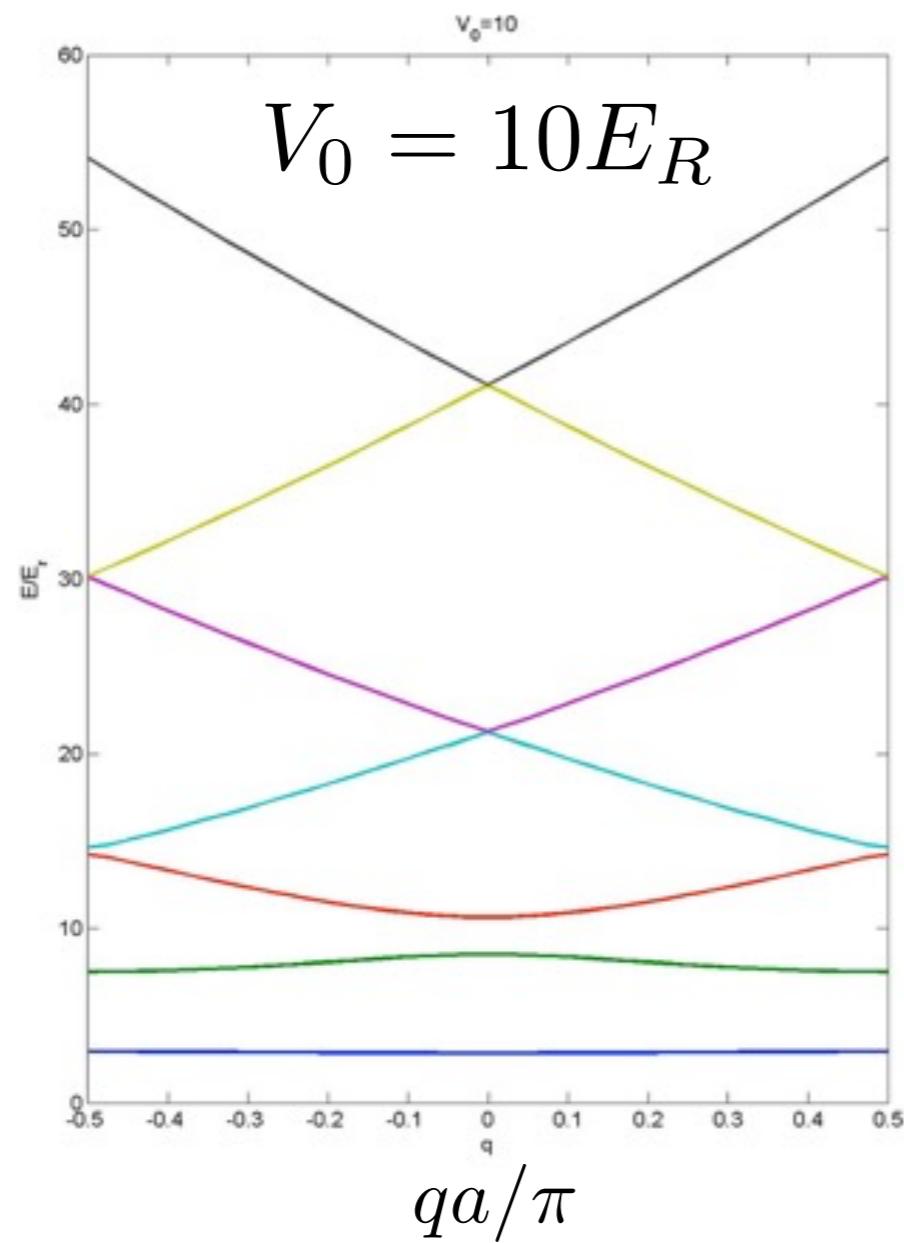
which allows us to reduce to a linear eigenvalue equation in the complex coefficients  $c_j$ ,

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

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

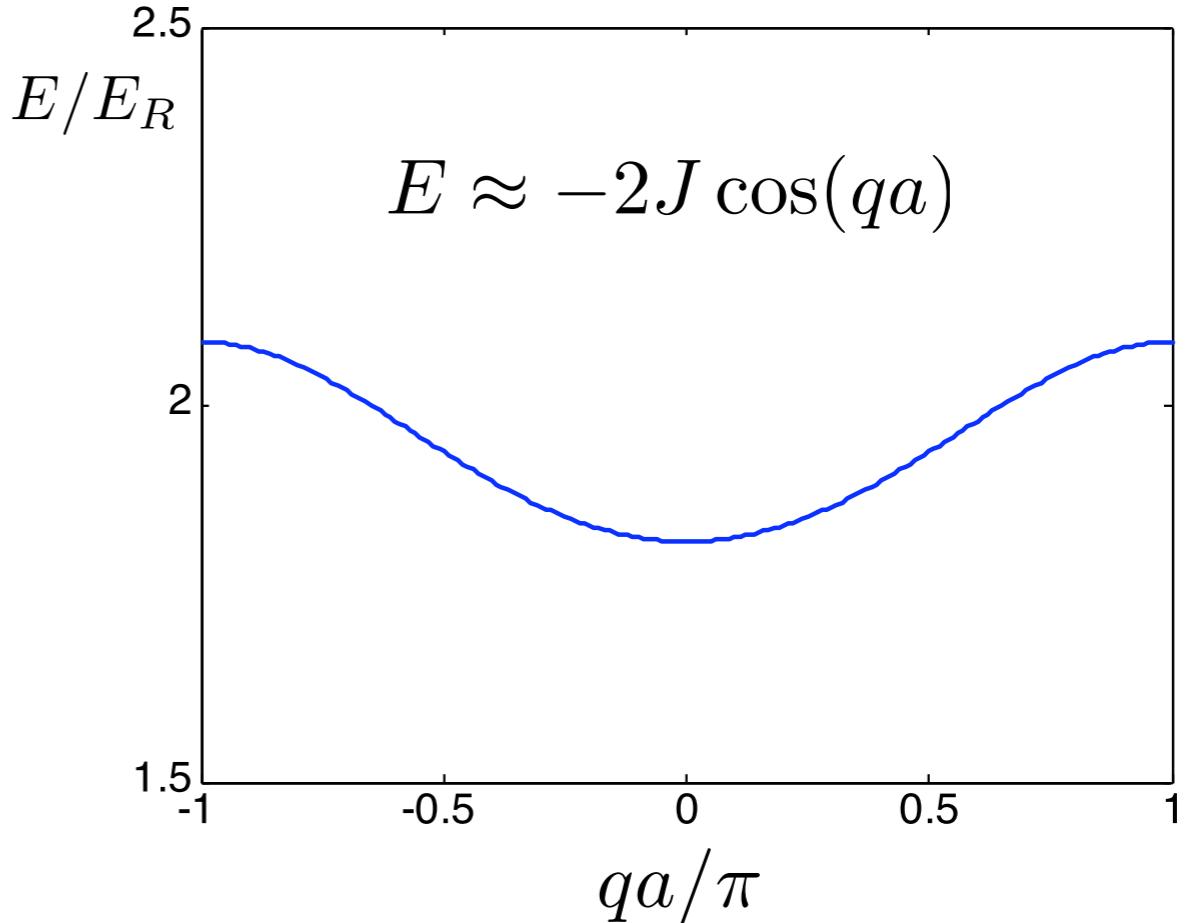
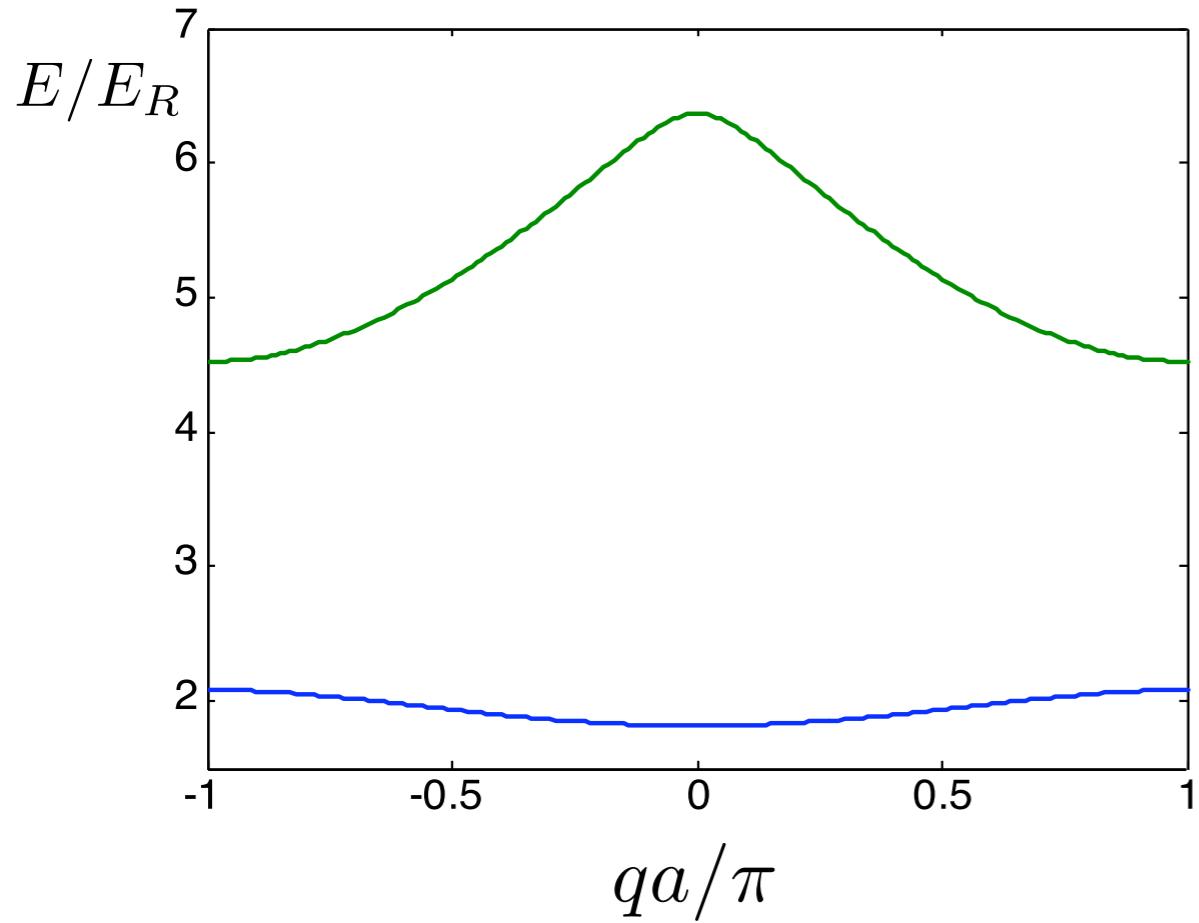
- This problem can be diagonalised numerically restricting  $j \in \{-l, \dots, l\}$ , and we find for the lowest few bands that good results are obtain for relatively small  $l \sim 10$ .
- The Bloch eigenstates are normalised so that

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



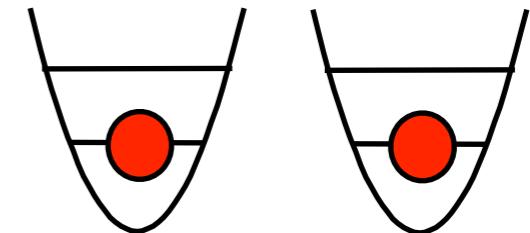
- Depending on the depth of the lattice, particles in the lowest bands, with  $E_q^{(n)} \lesssim V_0$  are in bound states of the potential, whilst the higher bands  $E_q^{(n)} > V_0$  correspond to free particles.

Lowest Two Bloch Bands,  
 $V_0=5 E_R$



- The lowest two bands are separated in energy by

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



approximately given by the trapping frequency from the Harmonic oscillator approximation,  $\omega_T$ .

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

## Wannier Functions

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

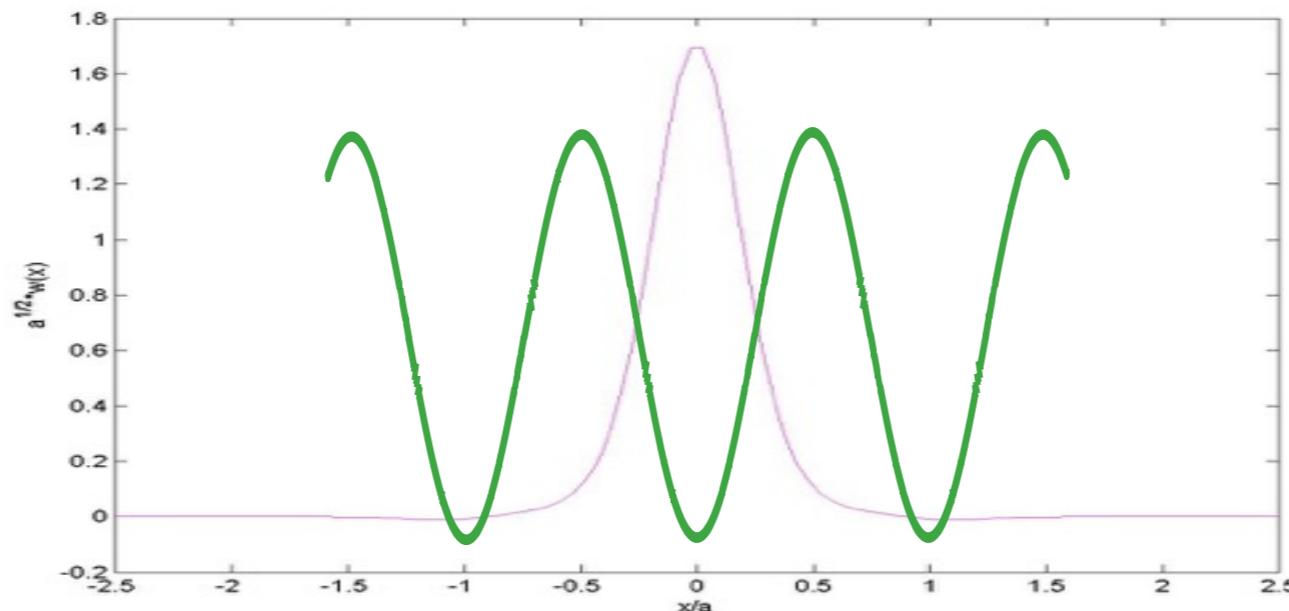
- It is often very convenient to express the Bloch functions in terms of Wannier functions, which also form a complete set of orthogonal basis states. The Wannier functions are given in 1D by

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

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,

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

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



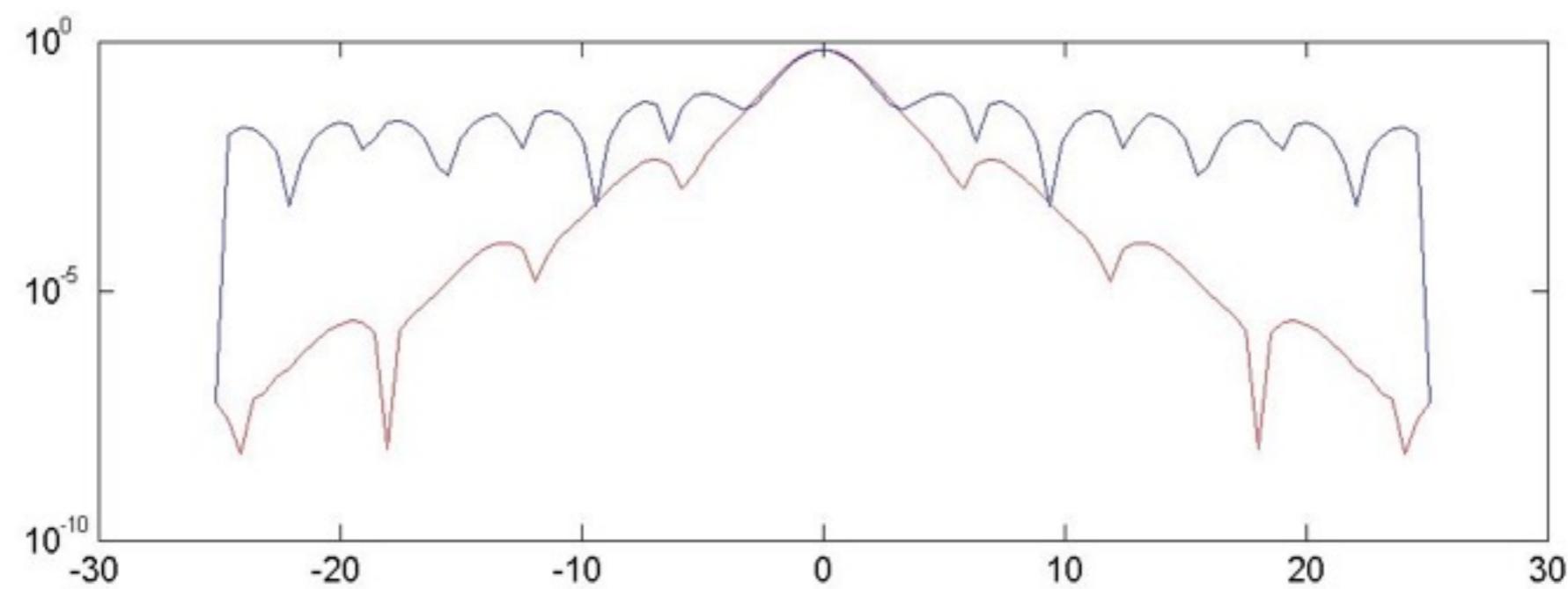
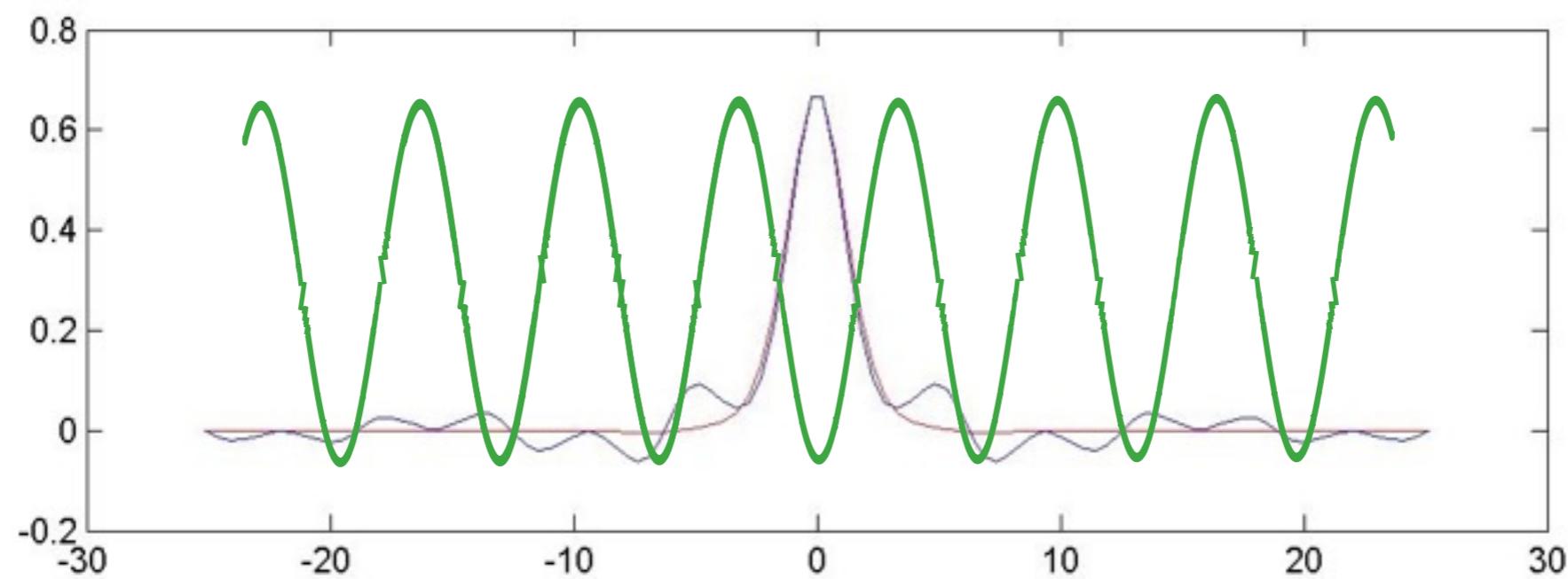
$$H_q = \frac{(p+q)^2}{2m} + V_0 \sin^2(k_l x), \quad \phi_q^{(n)}(x) = e^{iqx} u_q^n(x), \quad w_n(x - x_i) = \sqrt{\frac{a}{2\pi}} \int_{-\pi/a}^{\pi/a} dq u_q^n(x) e^{-iqx_i}$$

- 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  $x \rightarrow \infty$ .
- 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

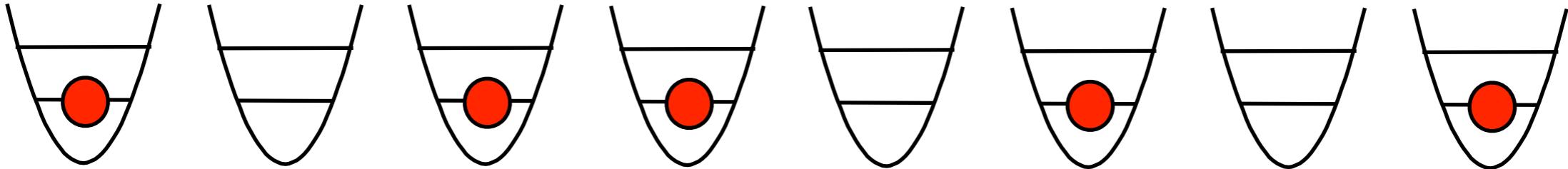
$$u_q^{(n)}(x) = \frac{1}{\sqrt{2\pi}} \sum_{j=-\infty}^{\infty} c_j^{(n,q)} e^{i2k_l x j}$$

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

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



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



- 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  $\exp[-x^2/(2a_0)^2]$ .

## 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

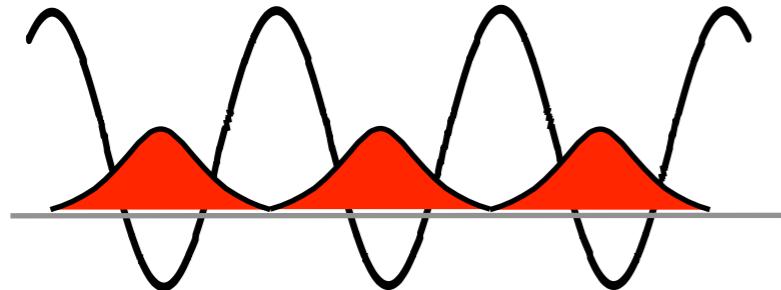
$$\hat{H} \approx \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_0(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) + \frac{g}{2} \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \hat{\psi}(\mathbf{r})$$

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.

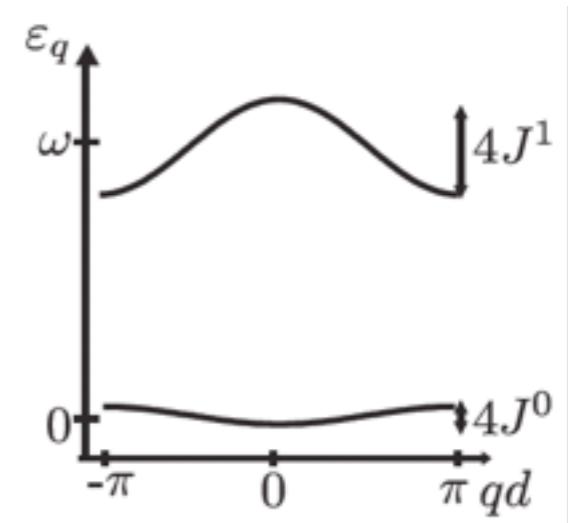
# Bose-Hubbard model

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



Wannier  
functions

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



Assume:

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

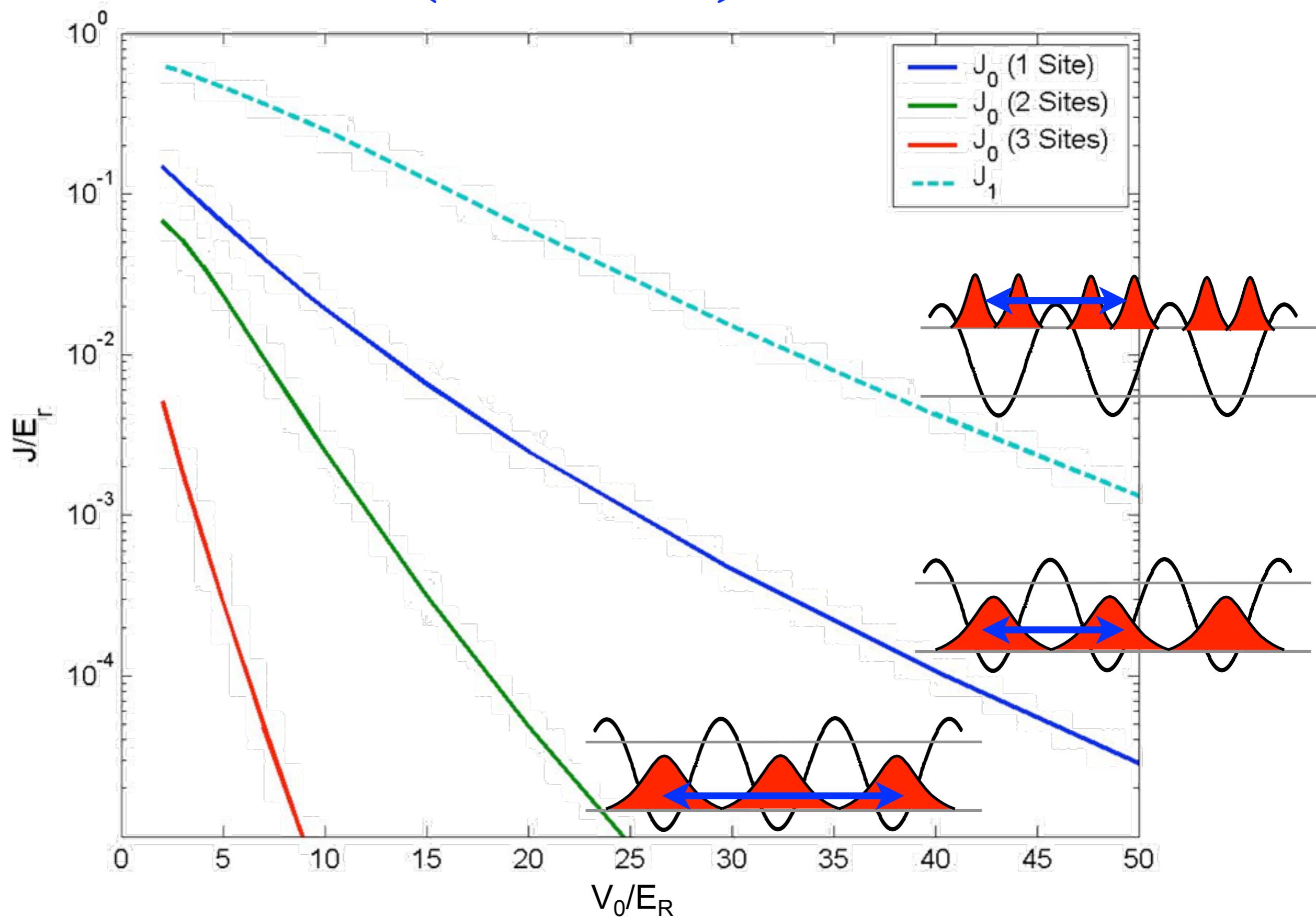
$$J = - \int dx w_0(x) \left( -\frac{\hbar^2}{2m} \nabla^2 + V_0 \sin^2(k_l x) \right) w_0(x - a),$$

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

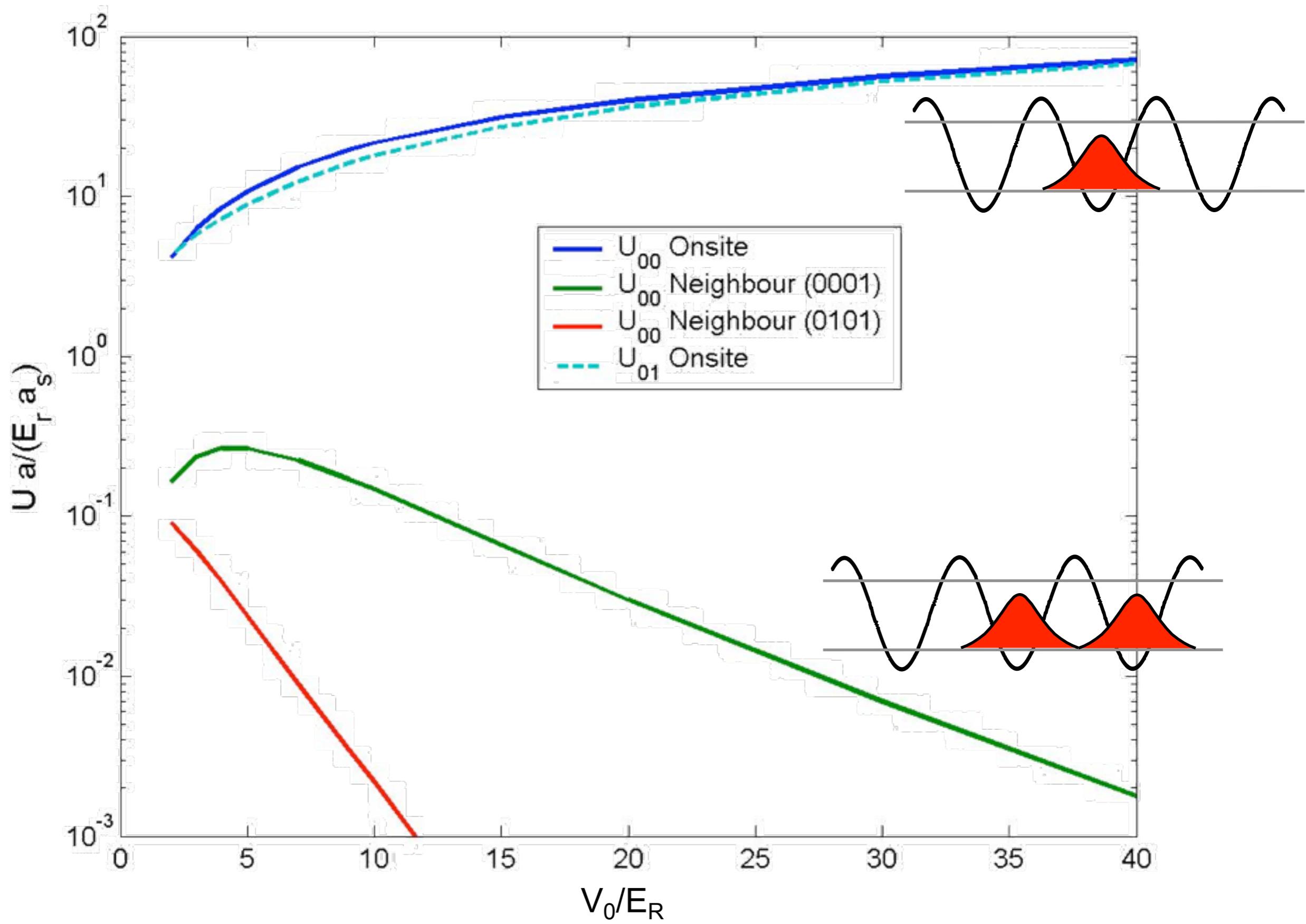
$$\epsilon_i = \int d\mathbf{x} |w_0(\mathbf{x} - \mathbf{x}_i)|^2 (V(\mathbf{x} - \mathbf{x}_i)),$$

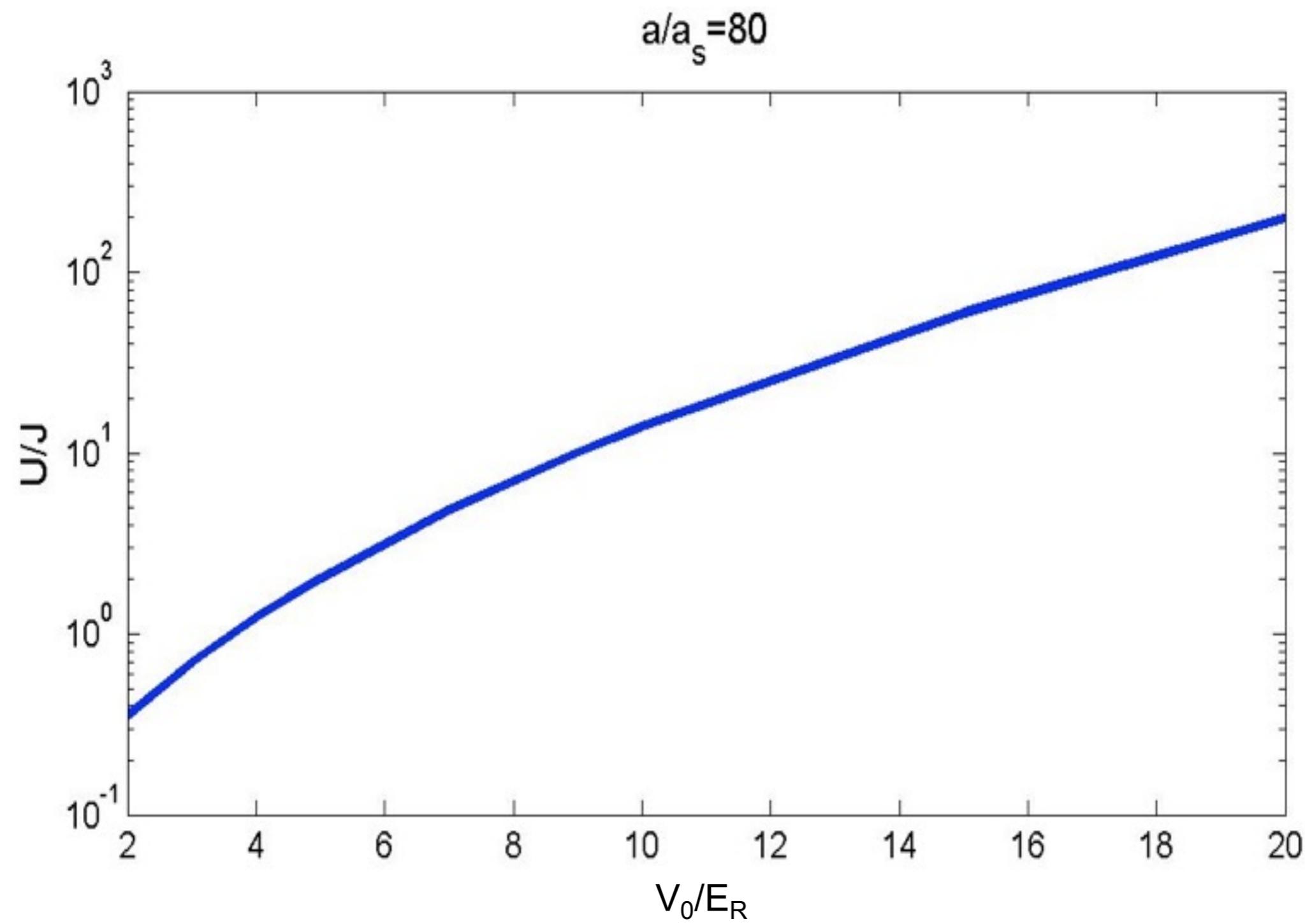
$$\longrightarrow H = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \sum_i \epsilon_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) \quad k_B T, J, U \ll \hbar\omega$$

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



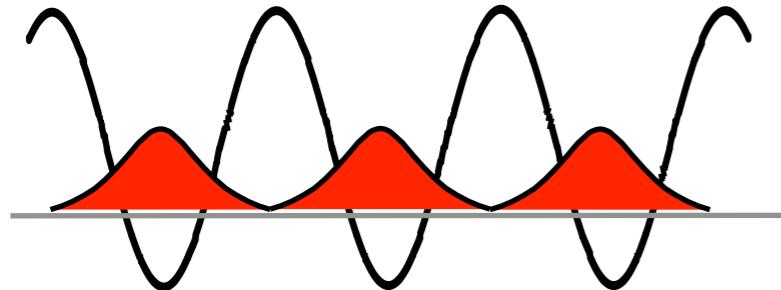
$$U_{ijkl} \propto \int d\mathbf{x} w_0(\mathbf{x} - \mathbf{x}_i) w_0(\mathbf{x} - \mathbf{x}_j) w_0(\mathbf{x} - \mathbf{x}_k) w_0(\mathbf{x} - \mathbf{x}_l) \hat{b}_{0,i}^\dagger \hat{b}_{0,j}^\dagger \hat{b}_{0,k} \hat{b}_{0,l}$$





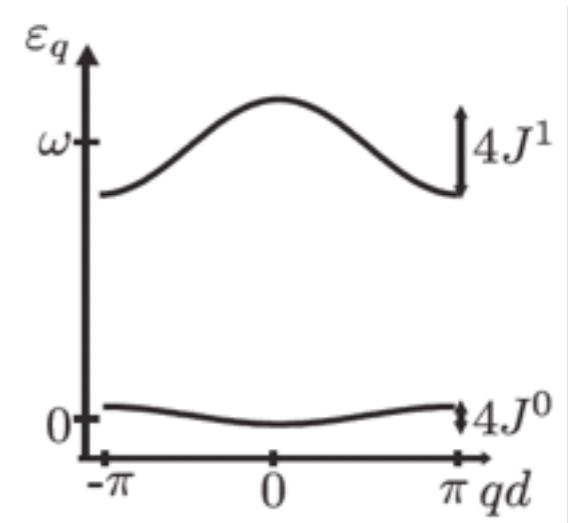
# Bose-Hubbard model

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



Wannier  
functions

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



Assume:

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

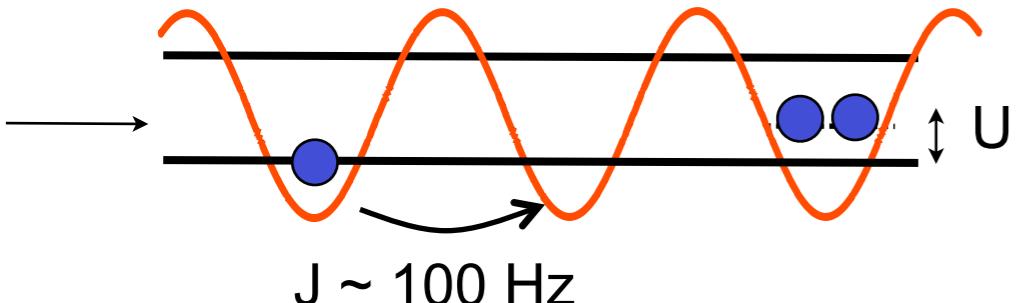
$$J = - \int dx w_0(x) \left( -\frac{\hbar^2}{2m} \nabla^2 + V_0 \sin^2(k_l x) \right) w_0(x - a),$$

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

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

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

# 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 ( $>1\text{s}$ ) (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, Zurich, NIST / JQI, MIT, Harvard, Innsbruck, Hamburg, Pisa, Florence, Oxford, Cambridge, Austin, Chicago, Penn State, Kyoto, Toronto, Stony Brook, Paris, Strathclyde, Illinois, Cornell .....

