Lecture notes: Bose-Einstein condensates in optical lattice

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I. BACKGROUND, MOTIVATION, AND OUTLINE

This mini-lecture is intended to introduce you to how atomic physicists prepare ultracold atoms in optical lattice potentials. Many of the concepts required to understand this are at the heart of the control of atoms with laser light, which, in many ways, is the starting point for a number of interesting problems in quantum sensing, simulation, and computing with neutral atoms.

This lecture assumes that previous lectures have covered

- Atom trapping in laser fields (i.e., dipole trapping), including Gaussian beam propagation
- Cooling bosonic atoms down to Bose-Einstein condensation (BEC), including The Gross-Pitaevskii equation for describing ultracold bosons

The lecture is outlined as follows:

- First, we will define what an optical lattice is, as well as a Schrödinger equation for (single) atoms in an optical lattice.
- From this, we will derive the Bloch states and the band structure they give rise to, as well as the Wannier states that are comprised of sums of Bloch states. The utility of each of these representations will be elucidated.
- Finally, we will discuss the theory of BEC in optical lattices, particularly the Bose-Hubbard model.

Thus, at the end of this lecture, a student should be able to describe what an optical lattice is, how basic lattice potentials are made, and what the wavefunctions of atoms trapped in these lattices look like in the limits of low and high lattice depths.

Note that most of the content in this lecture is derived from Markus Greiner's PhD thesis [1]. It is a fantastic starting point for anyone looking to understand ultracold atoms in optical lattices. This reference also covers the basics of the aforementioned prerequisites (on atom trapping and cooling), and the interested reader can go into more depth by diving into the references therein.

Finally, if you have any questions regarding this lecture and the material contained within it (or if you find any typos or inaccuracies!), please email me at `c.weidner@bristol.ac.uk`.

II. THE ATOM WAVEFUNCTION IN AN OPTICAL LATTICE

If we take a single-mode, Gaussian laser beam and reflect it back onto itself, the laser (of wavelength λ_L) interferes with itself and creates a sinusoidal pattern of nodes and antinodes, with each node

separated by $\lambda_{\mathrm{L}}/2$. If we assume that the laser beam is relatively large, we can neglect variations in the potential due to the finite Rayleigh length of the laser. Restricting ourselves to one dimension (the direction of propagation of the laser beam), our potential takes the form

$$V(x) = -V_{\mathrm{L}} \cos^2(k_{\mathrm{L}} x) \tag{1}$$

where $k_{\mathrm{L}} = 2\pi/\lambda_{\mathrm{L}}$ and we have shoved all of our prefactors into V_{L}. We can also write this in the suggestive form

$$V(x) = -\frac{V_{\mathrm{L}}}{4}(e^{-2\imath k_{\mathrm{L}} x} + e^{2\imath k_{\mathrm{L}} x} + 2). \tag{2}$$

We can use this to define a Schrödinger equation

$$H\phi_q^{(n)}(x) = E_q^{(n)}\phi_q^{(n)}(x), \tag{3}$$

where

$$H = \frac{p^2}{2m} + V(x), \tag{4}$$

and the *Bloch state*

$$\phi_q^{(n)}(x) = e^{iqx/\hbar} u_q^{(n)}(x), \tag{5}$$

with $u_q^{(n)}(x)$ being a function with the same periodicity as the lattice. As will become clear in a moment, we refer to q as the *quasimomentum* and n will define our *energy band*. Both are needed to uniquely define a Bloch state in an optical lattice.

If we plug Eq. (5) into Eq. (3), we get

$$H_{\mathrm{B}} u_q^{(n)}(x) = E_q^{(n)}(x) u_q^{(n)}(x), \tag{6}$$

where

$$H_{\mathrm{B}} = \frac{(p+q)^2}{2m} + V(x). \tag{7}$$

From this, it should be clearer why we refer to q as the quasimomentum; this quasimomentum will define a *Brillouin zone* that is periodic with period $2\hbar k_{\mathrm{L}}$. If you've ever had any solid-state physics, you are probably aware of this concept.

The next step is to expand both our potential and $u_q^{(n)}(x)$ in a Fourier series. That is

$$V(x) = \sum_r V_r e^{2\imath k_{\mathrm{L}} r x}, \tag{8}$$

and

$$u_q^{(n)}(x) = \sum_\ell c_\ell^{(n,q)} e^{2\imath k_\mathrm{L} \ell x}. \tag{9}$$

This gives rise to the following Schrödinger equation:

$$\left[\frac{(p+q)^2}{2m} + V(x)\right] u_q^{(n)}(x) = \sum_\ell \frac{(2\hbar k_\mathrm{L}\ell + q)^2}{2m} c_\ell^{(n,q)} e^{2\imath k_\mathrm{L}\ell x} + \sum_{\ell,r} V_r e^{2\imath k_\mathrm{L}(r+\ell)x} c_\ell^{(n,q)}. \tag{10}$$

This looks kind of cumbersome, but if you remember the suggestive way in which we wrote $V(x)$ in Eq. (2), there are only three terms in the Fourier series. Furthermore, the last term in the series (with no exponential term) corresponds to an energy offset which can be set to zero.

Therefore, defining the photon recoil energy

$$E_\mathrm{r} = \frac{\hbar^2 k_\mathrm{L}^2}{2m}, \tag{11}$$

and setting the lattice depth to be $V_0 = V_\mathrm{L}/E_\mathrm{r}$ we can write Eq. (10) as

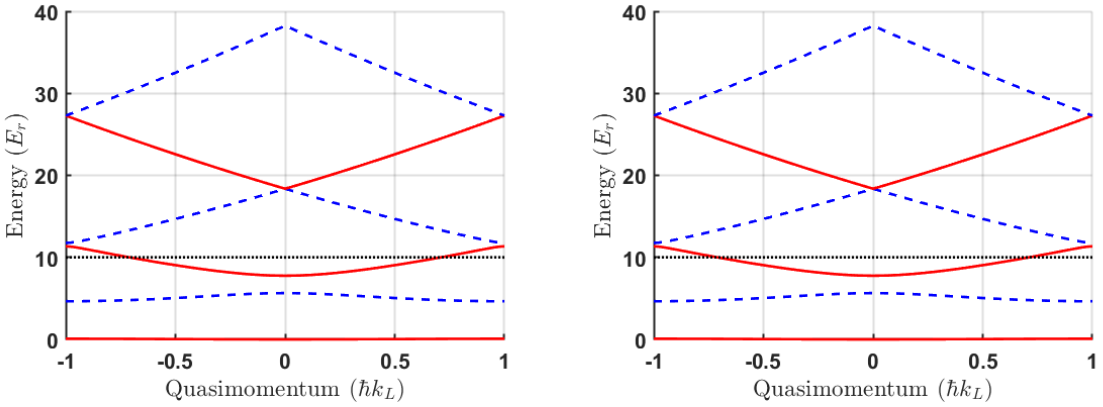
$$\sum_{\ell,\ell'} H_{\ell,\ell'} c_\ell^{(n,q)} = E_q^{(n)} c_\ell^{(n,q)} \tag{12}$$

where

$$H_{\ell,\ell'} = \begin{cases} \left(2\ell + \frac{q}{\hbar k_\mathrm{L}}\right)^2 E_\mathrm{r} & \text{if } \ell = \ell' \\ -\frac{V_0}{4} & \text{if } |\ell - \ell'| = 1 \\ 0 & \text{else,} \end{cases} \tag{13}$$

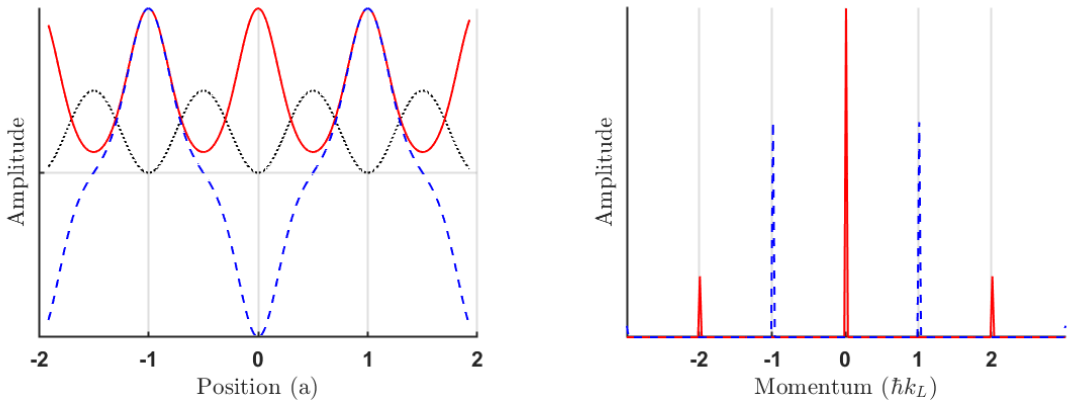
and we have rescaled the potential so the DC term is set to zero. This is just a matrix (albeit, right now, an infinite matrix, because we haven't put any restrictions on ℓ). In practice, if we are only concerned with the lowest energy states (which is typically the case when dealing with ultracold bosons), we can truncate ℓ such that $-5 \leq \ell \leq 5$. Then, for any given values of q and n, we can define a matrix and solve for its eigenvalues, which give us the eigenenergy of the state; these are plotted for various values of V_0 in Fig. 1. The eigenvectors are the $c_\ell^{(n,q)}$ that can be used to get the eigenstates of the system as a function of x by using Eqs. (5) and (9), which are plotted in Fig. 2(a). As will become important later, these states are periodic and thus delocalized in position, corresponding to an atom wavefunction spreading throughout the lattice, and because of this periodicity, they are quantized (localized) in momentum space.

However, we often want to prepare states such that they are localized to a given lattice site. These states, in contrast to the Bloch states, are localized in position and thus delocalized in momentum. This delocalization gives us a clue as to how to construct such states in that we need to sum over



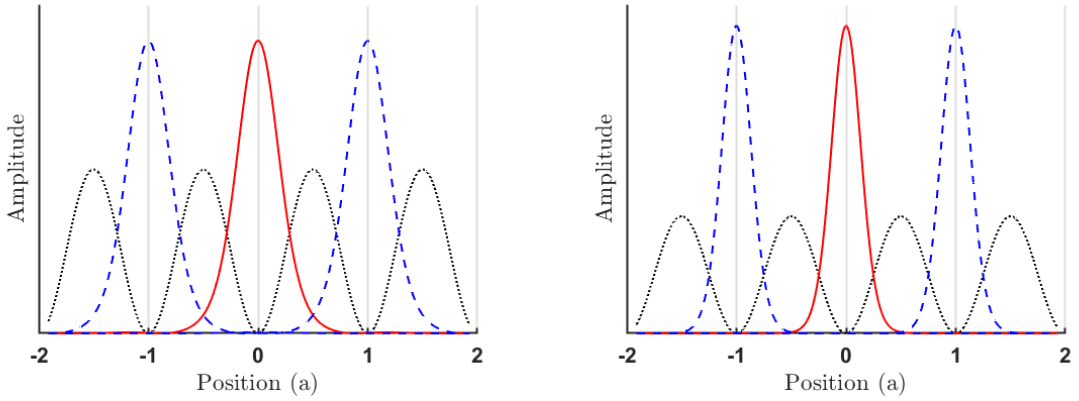
(a) $V_0 = 10E_\mathrm{r}$ (b) $V_0 = 20E_\mathrm{r}$

FIG. 1: Starting from the ground band $n = 0$, even (red) and odd (blue, dashed) Bloch bands plotted as a function of quasimomentum q within a single Brillouin zone for lattice depths of (a) $V_0 = 10E_\mathrm{r}$ and (b) $V_0 = 20E_\mathrm{r}$. The lattice depth is shown via a black, dotted line. We see that as the lattice depth increases, the lowest bands flatten out, and indeed, for a large lattice depth, these would approach the eigenenergies of a harmonic oscillator. Above the lattice energy, the gaps between the bands increasingly vanish due to the fact that the atom is effectively moving as a free particle in the continuum.



(a) (b)

FIG. 2: The (a) position- and (b) momentum-space representations of the ground Bloch states of an optical lattice with $V_0 = 10E_\mathrm{r}$ with $q = 0$ (red) and $q = \hbar k_\mathrm{L}$ (blue, dashed). The plots in (a) are of the real part of the wavefunction and are normalized such that the maximum amplitude of the state is one; the imaginary part of the wavefunctions are zero. For a spatial reference, the function $\cos(2kx)$ is plotted (blue), representing the lattice. In plot (b) the relative population in each of the $2n\hbar k_\mathrm{L}$ states (for integer n) is shown by the height of the peaks. This figure thus shows how the Bloch states are delocalized in position, but localized in momentum.



(a) $V_0 = 3E_\mathrm{r}$ (b) $V_0 = 10E_\mathrm{r}$

FIG. 3: Probability density of the Wannier function (red) for a lattice (black, dashed) of depth (a) $V_0 = 3E_\mathrm{r}$ and (b) $V_0 = 10E_\mathrm{r}$ as a function of x, showing how the wavefunction is much more localized for a deeper lattice. Wannier states localized to adjacent wells are shown with blue, dashed lines; the overlap of these states can be broadly related to a tunneling matrix element, as we shall see.

Bloch states for a given band n but with different quasimomenta. Thus, within a given band, we can define the so-called *Wannier states* localized to a given lattice site (with a minimum at x_j) as

$$w_n(x - x_j) = \mathcal{N}^{1/2} \sum_q e^{\imath q x_j/\hbar} \phi_q^{(n)}(x) \tag{14}$$

where $\mathcal{N}$ is a normalization factor. This works as-written for the lowest band in that we get a very nicely localized state (Fig. 3), but for higher bands, there is a phase freedom in how we write each $\phi_q^{(n)}(x)$ such that $\phi \to e^{\imath\Phi}\phi$. Thus, when performing the sum in practice, the states will be localized to one degree or another in the lattice. The definition of maximally localized Wannier states allows one to define the phase freedom $\Phi(q)$ such that the higher-excited Wannier states are localized to a given lattice site; more details are beyond the scope of this lecture but can be found via a literature search. Furthermore, while it may look like the Wannier states are basically Gaussians, the Gaussian has a larger tail and will lead to inaccuracies in calculations of quantities like tunneling matrix elements.

III. BECS IN OPTICAL LATTICES

Now we have set up the required background for discussing how BECs look in optical lattices. Note that for this section, we assume that we are working with a three-dimensional cubic lattice, and this will be represented by the vector nature of the spatial coordinate $\vec{x}$. Due to their low

temperature (about 100 nK in a typical rubidium-87 system), BECs are excellent for use in optical lattices, because they are straightforward to load into the lowest bands of the lattice. As we have seen before, we can produce a BEC in either a magnetic trap or an optical trap, and from there, we can simply overlap our lattice lasers with the BEC cloud and ramp up the lattice in such a way that the BEC atoms are loaded into the lowest bands. Specifically, we have to satisfy the specific adiabaticity criterion [2], representing a state in band n with quasimomentum q as $|n, q\rangle$:

$$|\langle n, q| \, d/dt \, |0, q\rangle| << |E_q^{(n)} - E_q^{(0)}|/\hbar. \tag{15}$$

For low lattice depths, the Bloch spectrum (similar to Fig. 1) will be effectively that of a free particle, which makes one think that the gap between bands would be deleteriously low, making this an exercise in futility. However, at $q = 0$, there is quite a large gap $E_0^{(1)} - E_0^{(0)} \approx 4E_\mathrm{r}$. Therefore, in practice, if one is working near zero quasimomentum, this criterion is straightforward to meet if one uses an exponential ramp when turning on the lattice lasers (empirically, the author has also found that a linear ramp will do in a pinch).

How do we describe BEC in optical lattices? For shallow lattices, the Bloch representation works, but the mean-field of the condensate changes the system such that the effective lattice depth (expressed in units of E_r) becomes [3]

$$V_\mathrm{eff} = \frac{V_0}{1 + C}, \tag{16}$$

where $C = gn_0/E_\mathrm{r}$ for a cloud with volume density n_0 and

$$g = \frac{4\pi\hbar^2 a_s}{m}. \tag{17}$$

However, for ultracold atoms in the lowest band of deeper lattices, one typically works in the basis of Wannier functions and thus uses the Bose-Hubbard Hamiltonian (although, in principle, one could use either basis regardless of depth, as long as one restricts themselves to the lowest band). For this, we will move from one dimension into 3D and assume that we have a cubic lattice of the form Eq. (1) in all three Cartesian dimensions. In second-quantization, we can describe the Hamiltonian of the atoms in a Bose-Einstein condensate as

$$\hat{H} = \int d\vec{r}\hat{\psi}^\dagger(\vec{r})\bigg(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\bigg)\hat{\psi}(\vec{r}) + g\int d\vec{r}\hat{\psi}^\dagger(\vec{r})\hat{\psi}^\dagger(\vec{r})\hat{\psi}(\vec{r})\hat{\psi}(\vec{r}) \tag{18}$$

where a_s is the s-wave scattering length of the atom (for Rb-87 this is $a_s \approx 95a_0$, where a_0 is the Bohr radius).

We can turn this into the Bose-Hubbard Hamiltonian by taking

$$\hat{\psi}(\vec{r}) = \sum_j \hat{a}_j w(\vec{r} - \vec{r}_j) \tag{19}$$

where the minima of the lattice potential are at the (periodic) positions $\vec{r}_j$ and $\hat{a}_j$ and $\hat{a}_j^\dagger$ are the annihilation and creation operators for an atom on site j. Plugging this into Eq. (18) gives the Bose-Hubbard Hamiltonian

$$\hat{H}_{\mathrm{BH}} = -J \sum_{\langle j,j' \rangle} \hat{a}_{j'}^\dagger \hat{a}_j + \sum_j \frac{U}{2} \hat{n}_j (\hat{n}_j - 1), \tag{20}$$

where $\hat{n} = \hat{a}^\dagger \hat{a}$ is the number operator. The first term describes tunneling from site j to site j', where the brackets indicate that j must be adjacent to j' (thus, this Hamiltonian describes only local interactions). The tunneling matrix element J can be written as

$$J = \int d\vec{x}\, w_0(\vec{x} - \vec{x}_j) \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right] w_0(\vec{x} - \vec{x}_{j'}), \tag{21}$$

effectively representing the overlap between the Wannier functions in adjacent sites j and j'. For lower lattice depths, this becomes larger, vanishing exponentially as the depth increases [4]. A plot of J and U (using the methods developed in Ref. [4]) as a function of the lattice depth can be found in Fig. 4(a). The second term in Eq. (20) represents the on-site interaction energy that an atom feels due to the other atoms on lattice site j. This term can be written as

$$U = g \int d\vec{x}\, |w_0(\vec{x} - \vec{x}_j)|^4. \tag{22}$$

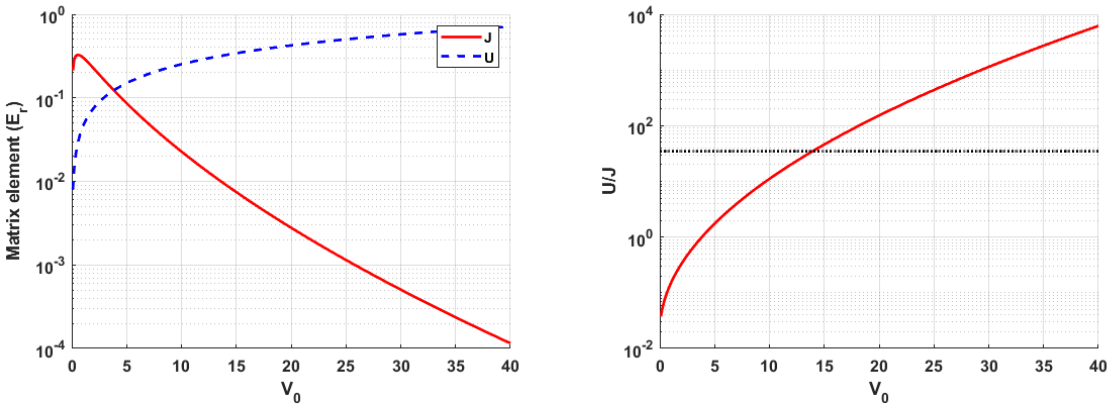
At low lattice depths, the tunneling term dominates the dynamics of the system, but as this term vanishes at increasing lattice depth, the on-site interaction term U dominates. Thus, for high lattice depths, atoms will prefer to localize to lattice sites, while at lower lattice depths, atoms will prefer to tunnel around, as the energy penalty paid by having multiple atoms on a single site will be overwhelmed by the tunneling term.

IV. PREPARING SUPERFLUID AND INSULATING STATES IN A LATTICE

The material in the last section was admittedly written somewhat suggestively, and we will find that the material here will likely fall out somewhat intuitively from the previous suggestive material. In a lattice, there are effectively two phases defined by whether or not the U or J terms are dominant in Eq. (20), and the knob that one turns to move between these states is the lattice depth.

More precisely, as U/J tends towards zero (at low lattice depths), we can write the many-body ground state of N bosons on a lattice of M sites as a product of identical Bloch states. This can be written as [1]

$$|\Psi_{\mathrm{SF}}\rangle \propto \left(\sum_{j=1}^{M} \hat{a}_j^\dagger \right)^N |0\rangle\,, \tag{23}$$



(a) (b)

FIG. 4: (a) Plot of the tunneling matrix element J (red) and the on-site interaction matrix element U (blue, dashed, see Ref. [4] for analytics) as a function of the lattice depth V_0 (in units of the recoil energy E_r), showing the exponential decay of the tunneling matrix element J as mentioned in the main text. The matrix element U rolls off as a function of the lattice depth but increases rapidly at lower lattice depths. (b) The ratio J/U, with the phase transition point $5.8z$ for $z = 6$ (the case of a 3D lattice) marked as a dotted black line. This marks the transition between the superfluid and the Mott insulating states.

which describes a coherent state on a given site. However, I find it far more instructive to simply write (for a given quasimomentum)

$$|\Psi_\mathrm{SF}\rangle \propto \prod_{j=1}^{M} \phi_q^{(0)}(x), \tag{24}$$

which is somewhat simplistic, but it exemplifies that the ground state of this superfluid state is simply the product of a set of identical Bloch states. As such, this state has a well-defined macroscopic phase, is localized in momentum, and we call this the *superfluid* state. However, as one can see from Eq. (23), the atom number per site is uncertain and will be distributed in a Poissonian manner, as we know from the behaviour of coherent states. This state has been used for a number of things, among them, the author was able to develop a quantum sensor via atom interferometry [5].

As we increase the lattice depth, the ratio U/J increases, as shown in Fig. 4(b), and as we approach $U/J >> 1$, atoms tend to localize to single lattice sites. For a cubic lattice, the phase transition will occur around $U/J = 5.8z$, where z is the number of neighboring sites (for a 3D lattice, $z = 6$). In practice, this occurs around $V_0 = 20E_\mathrm{r}$ for a 3D lattice. For our simple model, the system will tend towards one atom per site, and this can be written as

$$|\Psi_\mathrm{MI}\rangle \propto \prod_{j=1}^{M} \hat{a}_j^\dagger |0\rangle \,. \tag{25}$$

This so-called *Mott insulating state* does not have a coherent macroscopic phase (because the atoms simply do not talk to one another), but the atom number per site is very well-defined. This is an excellent starting point for many quantum simulators, as it provides a clean means of preparing one atom per site.

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