Ultacold Atoms in Optical Lattices

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I. WHAT IS AN OPTICAL LATTICE?

These notes were prepared for the 2023 ICTP school on ultracold atoms, in Sao Paulo. Their intent is to introduce graduate students to ultracold atoms in optical lattices. As a pedagogical document, no attempt is made to capture

the state of the art in research using optical lattices; the reader is instead referred to a number of published reviews for this (Bloch, 2005; Georges and Giamarchi, 2012; Gross and Bloch, 2017; Jessen and Deutsch, 1996; Lewenstein *et al.*, 2012). Jean Dalibard's lectures at the College de France include a pedagogical set of notes on optical lattices (2013), an historical review of cold atoms (2014), and more. Absent from our discussion are two developing themes: periodically driven optical lattices (Eckardt, 2017) and topological effects.

This introductory section discusses how a periodic potential is made using interference patterns of laser light. Subsequent sections discuss the eigenvalue problem of non-interacting particles in a lattice (§II), how to think of a particle "at" a particular lattice site (§III), the deep-lattice limit (§V), and an introduction to many-body physics in a lattice (§VI).

A. Two traveling waves

The light emitted by a continuous-wave laser is typically collimated into a beam that is 0.5 mm to 5 mm in diameter. Within the intensity envelope of these beams, laser beams can be treated as monochromatic traveling waves of light. At position **r** and time *t*, the electric field of a travelling wave can be written

$$\boldsymbol{E}(\mathbf{r},t) = E_0 \hat{\boldsymbol{\epsilon}} \exp(i\boldsymbol{k} \cdot \mathbf{r} - i\omega t) \tag{1}$$

where \mathbf{k} is the wave vector, $\hat{\mathbf{c}}$ is the polarization unit vector, and E_0 is the peak electric field. We have adopted complex notation, but the electric field is a physical observable and thus must be real-valued! The complex notation is used just for convenience (e.g., to avoid sinusoids), and maps back onto the (observed) electric field as $\mathbf{E}_{real} = \text{Re}\{\mathbf{E}\}$. In fact, since we will typically assume a monochromatic $e^{-i\omega t}$ time dependence of the field, we will drop this as $\mathbf{E} = \tilde{\mathbf{E}}e^{-i\omega t}$, from which $\mathbf{E}_{real} = \text{Re}\{\tilde{\mathbf{E}}e^{-i\omega t}\}$.

The energy density of an electromagnetic wave is $u = \epsilon_0 |\mathbf{E}_{real}|^2$. This will oscillate on a time scale not visible to ordinary detectors, so it is convenient to take the time average and multiply by c to get units of intensity, power per area: $I(\mathbf{r}) = c\epsilon_0 |\mathbf{E}(\mathbf{r},t)|^2$. Applying this to Eq. 1, we see that each travelling wave has an intensity $I_0 = \frac{1}{2}c\epsilon_0 E_0^2$.

Now, we are ready to construct a one-dimensional optical lattice by forming a standing wave from two equal-intensity overlapping travelling waves:

$$\tilde{\boldsymbol{E}}_{\rm sw}(\mathbf{r}) = E_0 \hat{\boldsymbol{\epsilon}}_1 e^{i\boldsymbol{k}_1 \cdot \mathbf{r}} + E_0 \hat{\boldsymbol{\epsilon}}_2 e^{i\boldsymbol{k}_2 \cdot \mathbf{r}} \,. \tag{2}$$

The intensity of the standing wave is

$$I_{\rm sw}(\mathbf{r}) = 2I_0 + \underbrace{2I_0 \operatorname{Re}\{\hat{\boldsymbol{\epsilon}}_1 \cdot \hat{\boldsymbol{\epsilon}}_2^* e^{i(\boldsymbol{k}_1 - \boldsymbol{k}_2) \cdot \mathbf{r}}\}}_{\text{interference}}$$
(3)

The first term on the r.h.s. is what would be expected if the power of the consituant travelling waves added incoherently. The second term in Eq. 3 is an interference term. It appears for two beams that are phase-coherent. With sub-10-MHz frequency stability easily achieved in a modern laser, the coherence length $(\ell_{\rm coh} \sim c/\Delta f)$ of light is in excess of 10 m. State-of-the art sources are kHz-line-width fibre lasers, so that the coherence lengths are many kilometres. Thus, we will assume for now that the relative phase of any two interfering laser beams is under perfect experimental control.

The only remaining question is one of polarization. Figure 1 gives several possibilities for linearly polarized beams: that $\hat{\epsilon}_1$ and $\hat{\epsilon}_2$ are parallel, or crossed linearly; and that the local magnetic field is parallel or perpendicular to the electric field. The reason the B-field matters is that atoms respond differently to σ and π polarized light, as discussed in Sec. A.2. If $\hat{\epsilon}_1$ and $\hat{\epsilon}_2$ are parallel, then an intensity pattern will develop. The linear polarization of \tilde{E}_{sw} addresses the π matrix element if B||E (right column of Fig. 1) or equal parts σ^+ and σ^- if $B \perp E$ (centre column of Fig. 1). On the other hand, if $\hat{\epsilon}_1$ and $\hat{\epsilon}_2$ are perpendicular, the interference term in Eq. 3 vanishes, and there is no intensity pattern. The local polarization in \tilde{E}_{sw} has a pattern that goes from purely σ^+ to purely σ^- and back again, in one wavelength (left column of Fig. 1).

What response do these standing-wave fields induce for atoms? This depends critically on the detuning $\Delta = \omega - \omega_0$ of the light from the resonant transition frequency of the atom ω_0 . Typical detunings for OLs are tens to hundreds of nm, in order to minimize Rayleigh scattering, which can cause atom heating or loss. For alkali atoms (⁶Li, ⁸⁷Rb, ⁴⁰K, etc.) that are commonly used ultracold atoms, and in the limit where Δ is much larger than the fine-structure splitting $\Delta_{\rm FS}$, the induced potential in this limit can be written, at low magnetic field (Grimm *et al.*, 2000), as

$$U(\mathbf{r}) \approx \frac{3\pi c^2}{2\omega_0^3} \frac{\Gamma}{\Delta} \left(1 + \frac{1}{3} \mathcal{P}g_F m_F \frac{\Delta_{FS}}{\Delta} \right) I(\mathbf{r}), \qquad \text{(intermediate detuning } \Delta_{FS} \lesssim |\Delta| \ll \omega_0)$$
(4)



FIG. 1 Polarizations of standing waves. Starting with linear polarizations, two equal-intensity counter-propagating travelling waves create a standing wave of intensity or polarization gradient. Left: The "lin \perp lin" configuration creates no net intensity gradient, but does create an alternating $\sigma + / \sigma -$ polarization standing wave when the magnetic field is oriented in z, parallel to the k vectors of the light. Centre: The lin \parallel lin configuration creates a linear polarization and a standing wave in intensity. When the magnetic field is perpendicular to the electric field, that linear polarization is an equal superposition of $\sigma +$ and $\sigma -$ fields. Right: When the magnetic field is parallel to the electric field polarization, the lin \parallel lin standing wave is π polarized. Not shown here is a fourth possibility: lin perp lin polarization, like in the left-most column, but a B-field along x or y. In that case, there is neither a polarization gradient nor an intensity gradient.

where $\mathcal{P} = \pm 1$ for σ^{\pm} light and = 0 for linearly polarized light, g_F is the gyromagnetic ratio of the ground state, m_F is the magnetic quantum number. A beam that has equal parts σ^+ and σ^- creates two potentials, with $\mathcal{P} = +1$ and -1, such that the polarization effects cancel out. A magnetic potential is only created by an imbalance between σ^+ and σ^- intensities, which can be created with a "lin perp lin" configuration (first column in Fig. 1). Even then, the polarization sensitivity scales as the ratio of the fine-structure splitting $\Delta_{\rm FS}$ to the detuning (in alkali atoms). Going forward, we will neglect optically induced magnetic potentials. The force on an atom is just the gradient of this potential — i.e., the dipole force on an atom is proportional to the gradient in local intensity, and independent of the direction of propagation of the beam.

A contribution to the optical potential not included in Eq. 4 is the counter-rotating term. When magnetic terms are negligible (either because $\mathcal{P} = 0$ or when $|\Delta| \gg \Delta_{FS}$), the potential is

$$U(\mathbf{r}) \approx \frac{3\pi c^2}{2\omega_0^3} \Big(\underbrace{\frac{\Gamma}{\omega - \omega_0}}_{=\Gamma/\Delta} + \underbrace{\frac{\Gamma}{\omega + \omega_0}}_{\text{counter-rotating}}\Big) I(\mathbf{r}) \qquad \text{(large-detuning limit)} \tag{5}$$

assuming that a single strong dipole transition dominates the static polarizability. In the quasi-static limit $\omega \ll \omega_0$, which describes lattices made by CO₂ lasers at 10 μ m for instance, we see that the counter-rotating term contributes equally to the potential depth, so that Eq. 4 under-estimates the optical potential but as much as a factor of two.

In the true DC limit, electric fields create a static Stark shift:

$$U_{\text{Stark}}(\mathbf{r}) \equiv -\frac{1}{2}\alpha_0 |\mathbf{E}|^2(\mathbf{r}) \qquad \text{where} \qquad \alpha_0 = 2\sum_k \frac{\left|\langle 0|\hat{d} \cdot \hat{\boldsymbol{\epsilon}}|k\rangle\right|^2}{E_k - E_0} \tag{6}$$

Extending this treatment to an oscillating electric field, we can replace α_0 by a frequency-dependent polarizability $\alpha(\omega)$. Indeed the first-order perturbative treatment of a time-varying electric field has a similar form to Eq. 6, as



FIG. 2 The polarisability α/α_0 is plotted versus ω/ω_0 . The contributions of the resonant enhancement (8) is shown as a dashed green line; and the counter-rotating term is shown as a solid red line. These add to give the solid black line. Notice that the $1/\Delta$ scaling over-estimates polarisability for the ultraviolet limit $\omega \gg \omega_0$, because the counter-rotating term partially counteracts it, resulting in a $1/\Delta^2$ scaling. In the infrared $\omega \ll \omega_0$ limit, the polarisability approaches a constant α_0 , and the field can be treated as quasi-electrostatic.

shown in App. A. Several characteristics of the static Stark shift carry forward to the effect of a far-detuned laser beam on an atom: in both cases, the energetic shift of the ground state is proportional to E^2 , and thus proportional to intensity I.

Equation (5) would predict that in the limit $\omega \to 0$, the polarizability $(-2U/E^2)$ approaches

$$\alpha_0 \approx \frac{6\pi c^3 \epsilon_0 \Gamma}{\omega_0^4} \,. \tag{7}$$

Table I compares this to experimentally measured polarizabilities from several alkali metals. We see that at least for the alkali metals, the agreement is better than 5%.

However, the static polarizability $\alpha_0 \approx 3 \times 10^{-39} \,\mathrm{Cm^2/V}$ of atoms is not promising for static electric fields, since fields greater than $10^5 \,\mathrm{V/m}$ typically cause electrode discharge. This would limit a Stark shift to $|\Delta E_{\mathrm{Stark}}| \lesssim k_B 2 \,\mu\mathrm{K}$, which is only marginally operable for ultracold atoms. Of course, laser light is at a finite frequency ω_L , so offers some resonant enhancement over the static limit. This enhancement factor (again in the far-detuned limit) is clear from Eq. (5):

$$\frac{U_{\rm dip}}{U_{\rm Stark}} = \frac{1}{1 - (\omega_L/\omega_0)^2} = \frac{1}{1 - (\lambda_0/\lambda_L)^2}$$
(8)

This is plotted in Fig. 2. A commonly used trapping wavelength is $\lambda_L = 1064 \text{ nm}$ due to the availability of strong sources at the YAG wavelength. The resonant enhancement factor for the alkali then varies between ~1.4 (for Na) and ~2.9 (for Cs).

For far-detuned optical lattices, more significant than this resonant enhancement is the *accessible magnitude* of the electric field (i.e., intensity) that one can achieve using a focused laser beam. For a single-mode Gaussian laser beam

TABLE I Static electric polarizability of alkali atoms. The measured value [ref] is compared to values calculated from (7). Since the strongest dipole line in alkali is split by hyperfine interactions in the excited state, we use $\omega = \bar{\omega}$, where $\bar{\omega}$ is a weighted sum of the fine-structure-split lines: $\bar{\omega} = (1/3)\omega_1 + (2/3)\omega_2$, where ω_1 and ω_2 are the D1 and D2 lines, respectively. Also, $\bar{\Gamma} = (1/3)\Gamma_1 + (2/3)\Gamma_2$, where Γ_1 and Γ_2 are the line widths of the D1 and D2 lines, respectively. The listed wavelengths are $\bar{\lambda} = 2\pi c/\bar{\omega}$.

Element	$\bar{\Gamma}/h$	$ar{\lambda}$	α from Eq. (7)	measured α
	(MHz)	(nm)	($10^{-39}{\rm C}{\rm m}^2/{\rm V}$)	($10^{-39}\mathrm{Cm^2/V}$)
Lithium	5.9	671	2.7	2.7
Sodium	9.8	589	2.6	2.6
Potassium	6.0	768	4.7	4.8
Rubidium	6.1	785	5.1	5.3
Cesium	5.0	864	6.3	6.6

$$I(x, y, z) = \frac{2P}{\pi w^2(z)} \exp\left\{ \left[-2\frac{x^2 + y^2}{w^2(z)} \right] \right\} \quad \text{where} \quad w(z) = w_0 \left(1 + \frac{z^2}{z_R^2} \right)^{1/2} \quad \text{and} \quad z_R = \pi w_0^2 / \lambda \tag{9}$$

Here P is the optical power (in Watts), w(z) is the beam waist, w_0 is the minimum beam waist, and z_R is the Rayleigh Range. Notice the easily confused (but commonly used) symbols: w refers to beam radius, while ω_L is an optical frequency. At the focus of the beam, the intensity is

$$I_{\rm max} = 2P/\pi w_0^2 \,, \tag{10}$$

which for a 5-W beam focused to a waist of $35 \,\mu\text{m}$ creates an intensity of $5 \times 10^9 \,\text{W/m^2}$. This is an rms electric field of $1.4 \times 10^6 \,\text{V/m}$, a very difficult field to create with physical electrodes. A single YAG beam with these parameters creates a traveling-wave potential depth of $680 \,\mu\text{K}$ for Potassium, for instance.

Finally, let's put all this back in the context of OLs. Two travelling waves with parallel polarizations and peak intensity I_0 will make a standing-wave intensity pattern

$$I_{\rm sw}(\mathbf{r}) = 2I_0 + 2I_0 \cos(\mathbf{k}_{\rm rel} \cdot \mathbf{r}) \tag{11}$$

where $\mathbf{k}_{rel} = \mathbf{k}_1 - \mathbf{k}_2$. For two beams with $\mathbf{k}_{1,2} = \pm k_L \hat{\boldsymbol{x}}$, $\mathbf{k}_{rel} \cdot \mathbf{r} = 2k_L \boldsymbol{x}$. Using trig identities, we can also write

$$I_{\rm sw}(\mathbf{r}) = 4I_0 \left(\frac{1}{2} + \frac{1}{2}\cos(2k_L x)\right) = 4I_0 \cos^2(k_L x)$$
(12)

Where did this "factor of 4" come from? One doubling comes from the use of two traveling waves; one doubling comes from the interference effect. The latter does not increase the total power, of course: the spatially averaged intensity is still $2I_0$.

Using Eq. 5, this intensity $4I_0$ translates into a potential depth that we will define as V_L . Whether the potential minimum is at highest or lowest light intensity will depend on Δ ; whichever the case, it's mathematically convenient to locate x = 0 at the bottom of the potential. So we will typically write

$$V(x) = V_L \sin^2(k_L x) = V_L (1 - \cos 2k_L x) \qquad (1D \text{ optical lattice potential})$$
(13)

The period of this standing wave is $\lambda_L/2$, which is $2\pi/|\mathbf{k}_{rel}| = \pi/k_L$. It will be useful to rename this as a, the lattice periodicity. For arbitrary angle between laser beams θ ,

$$a = \frac{\lambda_L}{2\sin(\theta/2)} \qquad \text{(Lattice period)} \tag{14}$$

which reduces to the minimum length $\lambda_L/2$ for $\theta = \pi$.

B. Interference patterns of multiple traveling waves

So far, we have shown that two traveling waves can create a sinusoidal confining potential. What happens if we add additional beams?

To start with, let's consider three equal-intensity beams. If their polarizations are parallel, then

$$\tilde{\boldsymbol{E}}(\mathbf{r}) = E_0 \hat{\boldsymbol{\epsilon}} e^{i\boldsymbol{k}_1 \cdot \mathbf{r}} + E_0 \hat{\boldsymbol{\epsilon}} e^{i\boldsymbol{k}_2 \cdot \mathbf{r}} + E_0 \hat{\boldsymbol{\epsilon}} e^{i\boldsymbol{k}_3 \cdot \mathbf{r}}$$
(15)

and the intensity is

$$I(\mathbf{r}) = I_0 \left| e^{i\mathbf{k}_1 \cdot \mathbf{r}} + e^{i\mathbf{k}_2 \cdot \mathbf{r}} + e^{i\mathbf{k}_3 \cdot \mathbf{r}} \right|^2 \tag{16}$$

We will see that the intensity patterns produced are not evident from what seems to be such a simple geometric structure. For three beam at equal angles, we can calculate the intensity pattern in the (x, y) plane with $\mathbf{k}_1 \cdot \mathbf{r} = k_L x$, $\mathbf{k}_2 \cdot \mathbf{r} = k_L x \cos(2\pi/3) + k_L y \sin(2\pi/3)$, and $\mathbf{k}_3 \cdot \mathbf{r} = k_L x \cos(2\pi/3) - k_L y \sin(2\pi/3)$. The result is a *honeycomb* or hexagonal pattern. Would you have guessed this?

The situation gets even more complicated with *four* lattice beams in a co-planar arrangement. Now the geometry of the intensity pattern *depends on the relative phase of the beams*. In general, one can show that the geometry of n + 1 beams in n dimensions is robust to the relative phase, but no more than that. In other words, a tetrahedral configuration of four beams in three dimensions creates a predictable pattern; but the geometry of the interference pattern of five or more beams depends on phase.

A common "trick" used by experimentalists is to wash out interference patterns by using *slightly different optical frequencies* for each 1D standing wave. Frequencies that are offset by tens of MHz (where 1 MHz = 10^6 cycles per second = $2\pi \times 10^6 \text{ s}^{-1}$) will not substantially change the period of the standing waves, since ω_L is typically in the 10^{14} s^{-1} regime. However, the interference terms will "walk" at a rate that is too fast for the atoms to follow¹. A related approach is to use polarizations of standing waves that are mutually orthogonal. In either case, one can create a 2D potential that is

$$V(\mathbf{r}) = V(x) + V(y) = V_{L,x} \sin^2(k_L x) + V_{L,y} \sin^2(k_L y) \qquad (2D \text{ square lattice potential}) \tag{17}$$

which is a separable potential with a square structure. Extending to three pairs of beams, for which cross-interferences have been eliminated, we can create

$$V(\mathbf{r}) = V(x) + V(y) + V(z) = V_{L,x} \sin^2(k_L x) + V_{L,y} \sin^2(k_L y) + V_{L,z} \sin^2(k_L z)$$
(3D cubic lattice potential)
= $V_L (3 - \cos(2k_L x) - \cos(2k_L y)) - \cos(2k_L z))$ in the isotropic case

(18)

which is a separable potential with a simple cubic structure. Due to its experimental and theoretical simplicity, this is the "default" OL potential for ultracold atoms, used in the vast majority of labs. Natural crystals do not have the same bias: simple cubic crystals are rare. The second line of Eq. 18 emphasizes that V_L is not the peak depth, but the modulation depth of each individual lattice.

Even without cross-interference patterns, multi-beam lattices can make surprising patterns. Consider laying two potentials like Eq. 17 on top of each other at an angle of $\pi/4$. If all pairs have equal intensity, then the potential is

$$V(\mathbf{r}) = V_L \sin^2(k_L x) + V_L \sin^2(k_L y) + V_L \sin^2(k_L (x+y)/\sqrt{2}) + V_L \sin^2(k_L (x-y)/\sqrt{2})$$
(19)

It turns out that this *is not a periodic potential*! Although it has long-range order, there is no unit cell. Such a potential is called a *quasi-crystal*. Famously, and incorrectly, Linus Pauling said, "there is no such thing as quasi-crystals, only quasi-scientists." Years later, a Nobel was awarded for work on quasi-crystals. In 2D, the only possible crystalline orders are rectangular (of which cubic is a special case), centered rectangular, hexagonal, and oblique (of which triangular is a special case). All of them can be made by optical lattices, but only the square lattice has been well explored.

II. BAND STRUCTURE

The treatment of a non-interacting particles in a periodic potential is familiar to anyone who has studied solid state physics. "Band structure" is the starting point for understanding electronic properties of metals and semiconductors. The new perspective offered by cold atom are that the particles might have bosonic statistics (unlike electrons), and eigenstates of the problem can now be understood as atoms dressed by photons. There are also some simplifications: the crystal is completely rigid, since single atoms have negligible back-action on the standing waves, so there are no lattice phonons. Also, the spacing between lattice sites far exceeds the range of inter-particle potentials, at least of dipole-dipole interaction are weak. We shall discuss interactions in \S VI; in this section and the next, we focus on the non-interacting problem.

The essence of the problem is the Hamiltonian

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + V(\hat{\boldsymbol{r}}) \tag{20}$$

where $V(\mathbf{r})$ is the single-particle lattice potential. We will ignore the usual confining potential present in most coldatom experiments; for a treatment of this, see (Rey *et al.*, 2005), and references therein. For simplicity we treat only

¹ In the limit of deep lattices, the time scale of motional response of a single atom is set by the band gap, $\sim \hbar/\sqrt{E_R V_L}$, which for typical atomic mass and lattice configurations is tens of microseconds. Washing out interference between optical beams is safely accomplished with a $\sim 10^2$ MHz frequency difference, such that the optical pattern walks through a full period on the nanosecond scale.

the 1D sinusoidal problem in these notes, i.e.,

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + V_L \sin^2(k_L \hat{x})$$
(21)

and refer the reading to numerous solid-state physics textbooks for a systematic treatment of three-dimensional band structure.

A. Symmetry of the eigenstates: quasi-momentum

A periodic potential breaks the continuous translational symmetry that is present in free space. Noether's Theorem states that for every continuous symmetry, there is a conserved quantity. For the continuous translational symmetry, it is *momentum* that is conserved, even in a many-body system. For instance, if two particles collide in free space, they can exchange momentum, but the total momentum of the two particles is the same before and after the collision.

The optical lattice ruins all this and more: $V(\mathbf{r})$ is not translationally invariant, so momentum is not conserved. Seen another way: momentum can be transferred between the light and matter, so the atoms' momentum is not conserved. Furthermore, the lattice potential provides a fixed reference frame that destroys Galilean invariance: we can always compare the speed of an atom to the (stationary) lattice potential, which now defines a natural choice for v = 0.

However, a periodic potential does have a discrete translational symmetry. Shifting the potential by one spatial period returns us to the original scenario. A natural question to ask is whether there is some conserved quantity that is the complement of this newly restricted symmetry. Bloch (1929) and Floquet (1883) found that indeed, there is a new quantity, "crystal momentum" or "quasi-momentum", which characterizes the eigenstates $|\Phi\rangle$ of Eq. 20. We will first show the structure of the solution for the 1D case, and then return to the 3D case.

The translation operator \hat{T}_a is defined by

$$\hat{T}_a |x\rangle = |x+a\rangle$$
 such that $\hat{T}_a \Phi(x) = \langle x | \hat{T}_a | \Phi \rangle = \langle x-a | \Phi \rangle = \Phi(x-a_L)$. (22)

Since momentum operator \hat{p}_x is (also defined as) the generator of translations in x, we can write

$$\hat{T}_a = e^{-ia\hat{p}_x/\hbar}$$
. (Spatial translation operator) (23)

Our 1D Hamiltonian $\hat{H}_x = \hat{p}_x^2/2m + V(\hat{x})$ commutes with \hat{T}_a when *a* is the period of the lattice because $V(x) = V(x \pm a)$, and \hat{p}_x commutes with \hat{T}_a for any *a*. Thus, when looking for the eigenvalues of \hat{H}_x , we know they should also be eigenstates of \hat{T}_a .

First, let's show that \hat{T}_a is a unitary operator, whose inverse is its hermetian conjugate:

$$\hat{T}_a^{-1} = (e^{-ia\hat{p}_x/\hbar})^{-1} = e^{+ia\hat{p}_x/\hbar} = \hat{T}_a^{\dagger}$$
(24)

Hermetian operators have the nice property that their eigenvalues have unity modulus², we can write them as $\lambda = e^{i\theta}$, and label the eigenstates with θ ; or, we could choose to write $\lambda = e^{-iqa_L}$, where a_L is fixed (the period of the lattice), and associate each eigenstate with a new variable q, a wave number that must have units of inverse length. Our eigenstates are now $|q\rangle$, with eigenvalues of \hat{T}_a that are $\hat{T}_a |q\rangle = e^{-iqa} |q\rangle$.

Without loss of generality, we can write these eigenstates in the form

$$\langle x|q\rangle = \Phi_q(x) = e^{iqx}u_q(x)$$
 where $u_q(x-a) = u_q(x)$ (Bloch waves) (25)

where we still need to find the form of the periodic function $u_q(x)$. Note that the full function $\Phi_q(x)$ is not periodic: there is a phase difference e^{iqa} between between one period and the next. This reminds of us a plane wave, whose phase also evolves by e^{ika} between any two points a apart, and thus q is called the quasi-momentum³.

What is the relationship between quasi-momentum and true momentum? The relationship is not simple. $\Phi_q(x)$ is a plane wave times a spatial modulation $u_q(x)$ that is periodic in x, and whose momentum components are non-trivial:

$$u_q(x) = \sum_j c_j^q e^{2ijk_L x} \tag{26}$$

² Proof of this is as follows. Let's take an eigenstate ϕ of operator \hat{U} , with eigenvalue λ , i.e., $\hat{U}\phi = \lambda\phi$. The modulus $|\lambda\phi|^2 = |\hat{U}\phi|^2 = \phi^* \hat{U}^{\dagger} \hat{U}\phi$. But for unity operators, $\hat{U}^{\dagger} \hat{U} = 1$, so $|\lambda\phi|^2 = |\phi|^2$. However, this can only be true if $|\lambda|^2 = 1$. QED.

 $^{^{3}}$ No relation to the quasi-crystals discussed in §I.B

for integer j and (recall) $k_L = \pi/a$. The Fourier-series representation of u_q ensures its periodicity: replacing x by x + a modifies the phase factor to be $e^{2ijk_La} = e^{ij2\pi} = 1$.

The physical interpretation of Eqs. 25 and 26 is useful: the eigenstates of an atom in an optical lattice is a massive particle in which several momentum eigenstates are coupled. This wave function might be visualized as

$$c_0 | \bigotimes \stackrel{\bullet}{q} \rangle + c_{+1} | \bigotimes \stackrel{\bullet}{q+2k_L} \rangle + c_{-1} | \bigotimes \stackrel{\bullet}{q-2k_L} \rangle + c_{+2} | \bigotimes \cdots$$

where the c_j coefficients give the amplitudes of the coupled plane-wave states. The reason the coupling occurs with pairs of photons is that these are off-resonant Raman-type events, where a photon is taken from one beam and put into the other. This is discussed further in the next section.

Another perspective is to *dress* the uncoupled states to equal-momentum eigenstates. If we keep track of the momentum in the light field, then total momentum is conserved. In this dressed picture, we have

$$c_0 \left| \bigotimes \begin{array}{c} q \\ q \end{array} \right\rangle + c_{+1} \left| \bigotimes \begin{array}{c} q + 2k_L \\ \Leftarrow 2 \text{ photons} \end{array} \right\rangle + c_{-1} \left| \bigotimes \begin{array}{c} q - 2k_L \\ \Rightarrow 2 \text{ photons} \end{array} \right\rangle + c_{+2} \left| \bigotimes \begin{array}{c} q \\ \Rightarrow 4 \end{array} \right\rangle$$

This picture is useful because it includes the light in the eigenstate. (Of course, there is a background of N photons, and we are only counting from that baseline.) In either picture, the important point is that *quasi-momentum is not* momentum: the Bloch state with q has other momenta in its "entourage".

B. The eigenvalue problem

Solving the eigenvalue problem for each q entails finding the $\{c_i^q\}$. Then,

$$\Phi_q(x) = \sum_j c_j^q e^{i(q+2jk_L)x} \quad \text{or} \quad |q\rangle = \sum_j c_j^q |k = q + 2jk_L\rangle$$
(27)

We see that each quasi-momentum state consists of a *comb of real momenta* q, $q \pm 2k_L$, $q \pm 4k_L$, etc. whose momentum spacing is $2\hbar k_L$, i.e., the momenta of two photons at the wavelength of the lattice.

The eigenstates and precise eigenvalues of the problem can be found by substituting Eq. 27 into Eq. 20. We have already discussed why these states are labelled $|q\rangle$; the remaining unknown function is $u_q(x)$, described by a series of coefficients c_j . It is convenient to rescale everything in the problem by the energy scale $E_R = \hbar^2 k_L^2/2m$, length a_L , and wave vector $k_L = \pi/a_L$. The eigenvalue problem now distills down to a single matrix equation

$$\sum_{\ell'} [H_q]_{\ell\ell'} c_{\ell'} = \frac{E_q}{E_R} c_\ell \tag{28}$$

where

$$[H_q]_{\ell\ell'} = \left(\left(\frac{qa_L}{\pi} + 2\ell\right)^2 + \frac{s}{2}\right)\delta_{\ell,\ell'} - \frac{s}{4}\delta_{\ell,\ell'-1} - \frac{s}{4}\delta_{\ell,\ell'+1}$$
(29)

which is a tri-diagonal matrix that looks like

$$H_q \rightarrow \begin{pmatrix} (qa_L/\pi + 4)^2 & -s/4 & 0 & 0 & 0 \\ -s/4 & (qa_L/\pi + 2)^2 & -s/4 & 0 & 0 \\ 0 & -s/4 & (qa_L/\pi)^2 & -s/4 & 0 \\ 0 & 0 & -s/4 & (qa_L/\pi - 2)^2 & -s/4 \\ 0 & 0 & 0 & -s/4 & (qa_L/\pi - 4)^2 \end{pmatrix}$$
(30)

where we have only written out the central 5x5 elements of this infinite matrix. The eigenvectors are column vectors of the coefficients $\{c_\ell\}$. From these, you can assemble the previously unknown function $u(x) = \sum_{\ell} c_\ell \exp(2i\ell k_L x)$. Note that $\sum |c_\ell|^2 = 1$.

Practically speaking, you will have to truncate this matrix to some $\pm \ell_{\text{max}}$. This can be safely down when $(qa_L/\pi + 2\ell_{\text{max}})^2 \gg s/4$, so that the plane-wave states are unaffected by Bragg scattering of the lattice. In practice, $\ell_{\text{max}} = 3$ can work for weak lattices, and $\ell_{\text{max}} = 10$ can work for deep lattices. This matrix approach is general, and can be generalized to complex and multi-dimensional lattice structure.

$$\frac{d^2}{dz^2}y + \left[\varepsilon - 2\mathbf{v}\cos(2z)\right]y = 0\tag{31}$$

and yields periodic solutions of even parity when $\varepsilon = \mathbf{a}(r, \mathbf{v})$, and odd parity when $\varepsilon = \mathbf{b}(r, \mathbf{v})$, where r is a "characteristic exponent" that maps onto the quasi-momentum in our problem: $r \to q/k_L = \pi q/a_L$. The solutions to this differential equation are special functions: "cosine-elliptic" $y = \operatorname{ce}(r, \mathbf{v}, z)$ and "sine-elliptic" $y = \operatorname{se}(r, \mathbf{v}, z)$, respectively. For $\mathbf{v} = 0$, $\operatorname{ce} \to \cos(\sqrt{\varepsilon}z)$ and $\operatorname{se} \to \sin(\sqrt{\varepsilon}z)$.

Mapping Eq. 31 to Eq. 21 with $\langle x | \hat{H} | \psi \rangle = \langle x | E | \psi \rangle$ uses $\mathbf{v} \to -V_L/4E_R$ and $\varepsilon \to E/E_R - V_L/2E_R$. We are left with two continua of possible solutions:

$$\Phi_q(x) = \operatorname{ce}(q/k_L, \mathbf{v}, k_L x) \quad \text{with} \quad E_q = \mathbf{a}(q/k_L, \mathbf{v})E_R + V_L/2 \quad (\text{even parity})$$

$$\Phi_q(x) = \operatorname{se}(q/k_L, \mathbf{v}, k_L x) \quad \text{with} \quad E_q = \mathbf{b}(q/k_L, \mathbf{v})E_R + V_L/2 \quad (\text{odd parity})$$
(32)

where we have not specified the normalization. That there are two solutions to this equation poses a problem in a sense: are there two eigenvalues for each q? In fact, **a** and **b** are different only for *integer* r, i.e., $q = n k_L$. As we shall see in the next section, these critical points are *Bragg planes* that correspond to gaps in the energy spectrum, where for a single q, there are two possible eigenstates. The *n*th energy gap (between those eigenstates) is $|\mathbf{a}(n, \mathbf{v}) - \mathbf{b}(n, \mathbf{v})| E_R$. Apart from those gaps, $\mathbf{a}(r, \mathbf{v}) = \mathbf{b}(r, \mathbf{v})$, however we still need to choose between the two parity of solutions (which are different even for non-integer r). As we discuss in the next section, this is resolved by partitioning the eigenspectrum into *bands*, enumerated with positive integers n. The band index n, shared by all quasi-momenta in the band, is the number of Bragg planes (and thus gaps) crossed in going from q = 0 to the q in that band. Once the band is established, one can choose the correct solution: odd n have odd-parity $\Phi_q(x)$, and even n have even-parity $\Phi_q(x)$.

C. Bragg scattering and band gaps

Before proceeding further to discuss the solutions of the eigenvalue problem, let's pause to consider the physical picture. Why does the $|q\rangle$ state in Eq. 27 consist of a comb of momenta spaced by *two* photon momenta?

The explanation comes from considering the wave-like properties of matter: the structure of $|q\rangle$ reflects the diffraction of matter waves from a periodic potential. nth-order Bragg scattering occurs for a wave of wavelength λ interacting with a periodic structure of period a, when the (equal) incident and reflected angle θ satisfy

$$2a\sin\theta = n\lambda\,.\tag{33}$$

In our case, the wave is a de-Broglie wave with $\lambda \to \lambda_{dB} = h/|p_x|$ and retro-reflection in the standing wave has $\theta = \pi/2$, so that $\sin \theta = 1$. This gives $|p_x| = n\frac{h}{2a} = nh/(2\pi/k_L) = n\hbar k_L$ since $a = \pi/k_L$. Thus

$$p_x = \pm n\hbar k_L \tag{34}$$

are the resonant momenta at which atoms Bragg scatter off of the optical lattice.

When Bragg scattering does occur, both momentum and energy are conserved. The first-order process is as follows: an atom moving at momentum $p_{x,i} > 0$



is converted to a final momentum $p_{x,i} - 2\hbar k_L$,

which conserves momentum because the number of photons moving in the -x direction decreases by one, and the number of photons moving in the +x direction increases by one. The optical field absorbs the momentum of the scattered atom. If all photons have the same frequency, the energy of the light field is unchanged, so the energy of the atom must also be unchanged; this can only happen when $p_{x,f}^2 = p_{x,i}^2$, i.e., $p_{x,f} = -p_{x,i}$. Putting energy and momentum conservation together, we find again the condition in Eq. 34 for n = 1.

Bragg scattering is a two-photon process⁴. Two-photon coupling generally occurs at a strength $\hbar\Omega_{\text{Ram}}$ that is given

⁴ Note that this is not the same as a time-ordered sequence of two single-photon processes. Bragg scattering is also fully coherent, and it does not involve spontaneous emission.



FIG. 3 Opening of band gaps. A free-particle dispersion relation $(V_L = 0)$ is shown as a black dashed line. The eigenvalues of H_q are shown for $V_L = 2E_R$ (blue solid line) and for $V_L = 5E_R$ (red solid line). Here we have offset the curves such that all energies to overlap at q = 0.

by the 2-photon (or Raman) Rabi frequency,

$$\Omega_{\rm Ram} = \frac{\Omega_1 \Omega_2}{2\Delta} \,, \tag{35}$$

where Ω_1 and Ω_2 are single-photon Rabi frequencies, given by Eq. A9. In this case, these single-photon Rabi frequencies are (separately) based on the electric field for a travelling-wave beam and the electric dipole moment of the ground-toexcited-state transition. The standing-wave lattice potential is *also* created from a second-order process in the electric field, $V_L = \hbar \Omega_L^2/4\Delta$, but where Ω_L comes from the *total* electric field, including all the interference terms discussed in §I.A; whereas Ω_{Ram} , Ω_1 , and Ω_2 are spatially constant. Thus $\Omega_{1,2} = \Omega_L/2$, and $\Omega_{\text{Ram}} = V_L/2\hbar$. Check factors.

Bragg scattering is the process in which a two-photon (or 2n-photon) transition changes the momentum of the atom. Wave-function overlap requires momentum conservation, such that Bragg processes can only be driven by the part of the optical field that provides the needed $2n\hbar k$. We can find what is needed for a $\pm 2\hbar k_L$ change directly in the standing-wave potential, by writing it as

$$V_L \sin^2(k_L x) = \frac{V_L}{2} - \frac{V_L}{4} e^{2ik_L x} - \frac{V_L}{4} e^{-2ik_L x}.$$
(36)

We see that only the $V_L/4$ components could couple momentum states that differ by $2\hbar k_L$; the spatially uniform $V_L/2$ provides an energy offset to eigenstates. Since coupling strengths are always $\pm \hbar \Omega_{\text{Rabi}}/2$, we read off the first-order Bragg scattering Rabi frequency as

$$\Omega_{B,1} = \frac{-V_L}{2\hbar} = \Omega_{\text{Ram}} \,. \tag{37}$$

Higher-order Bragg scattering also requires considering the detunings of intermediate states. Going from $-2\hbar k_L$ to $+2\hbar k_L$ is a second-order process (so proportional to $(-V_L/2)^2$), through the intermediate virtual state $|p = 0\rangle$, whose detuning is $4E_R$. We'd thus expect the $\hbar\Omega_{B,2}$ to be $(V_L/2)^2/(4E_R) = 2^{-4}V_L^2/E_R$. Indeed, more careful treatments(Giltner *et al.*, 1995; Müller *et al.*, 2008) find that

$$\Omega_{B,n} = \frac{\Omega_{\text{Ram}}^n}{(8E_R/\hbar)^{n-1}((n-1)!)^2} = \frac{(-V_L/2\hbar)^n}{(8E_R/\hbar)^{n-1}((n-1)!)^2}$$
(38)

is the Rabi frequency for *n*th-order Bragg scattering, which couples $p_{x,i}$ to $p_{x,i} \pm 2n\hbar k_L$, through a 2*n*-photon coherent process. The first-order $\hbar\Omega_{B,1} = V_L/2$, the second-order process is $\hbar\Omega_{B,2} = V_L^2/32E_R$, etc.

Let's now discuss how Bragg scattering breaks the energy continuum of a free-particle dispersion relation into distinct energetic bands. The eigenvalues of Eq. 20 with V(x) = 0 are simply $E = p_x^2/2m$, shown as a dashed line in Fig. 3. The addition of a weak lattice will shift this curve by $V_L/2$ (see Eq. 36), and leave most of the curve unaffected, expect for places where the resonance condition Eq. 34 is met. The strongest modification occurs for the first-order Bragg resonance, so let's consider that first.



FIG. 4 Band structure The same band structure plotted in Fig. 3 is shown here again, but for the "reduced zone scheme", where q goes only from $-\hbar k_L = \pi/a_L$ to $+\hbar k_L$, but now $E_q^{(n)}$ also contains a band index. The first three bands are labelled; diagrams are shown for $V_L = 0$, $V_L = 2$, and $V_L = 5$. Unlike in Fig. 3, we have not shifted energy curves to overlap at q = 0.

A simple Hamiltonian for this is

$$H_{B,1} = \begin{pmatrix} p_i^2/2m & \hbar\Omega_{B,1}/2\\ \hbar\Omega_{B,1}/2 & p_f^2/2m \end{pmatrix} = \begin{pmatrix} E_R & -V_L/4\\ -V_L/4 & E_R \end{pmatrix}$$
(39)

This is easy to diagonalize: $E = E_R \pm \hbar \Omega_{B,1}/2$, such that an *energy gap* opens up with a width $\hbar |\Omega_{B,1}| = V_L/2$ (see $\pm \hbar k_L$ in Fig. 3). This is a radical change to the structure of allowed energy eigenstates: none may exist with this gap. We call the continuum of q and energies leading up to this first gap the *lowest band*, and the continuum above this gap the *first excited band*. We will assign these bands the indices n = 0 and n = 1, respectively.

A similar phenomenon happens at $p = -2\hbar k_L$ and $p = +2\hbar k_L$. These two states are coupled through second-order Bragg scattering. Since the p = 0 virtual state is involved in this second-order process, we can find the gap by diagonalizing

$$H_{B,2} = \begin{pmatrix} p_i^2/2m & -V_L/4 & 0\\ -V_L/4 & 0 & -V_L/4\\ 0 & -V_L/4 & p_f^2/2m \end{pmatrix} = \begin{pmatrix} 4E_R & -V_L/4 & 0\\ -V_L/4 & 0 & -V_L/4\\ 0 & -V_L/4 & 4E_R \end{pmatrix}$$
(40)

or by using Eq. 38, which has already eliminated the off-resonant states:

$$H_{B,2} \to \begin{pmatrix} p_i^2/2m & \hbar\Omega_{B,2}/2\\ \hbar\Omega_{B,2}/2 & p_f^2/2m \end{pmatrix}$$
(41)

In either case, in the limit $V_L \ll E_R$, we find eigenvalues near $4E_R$ that are split by $V_L^2/(32E_R)$, i.e., at $\pm \hbar \Omega_{B,2}/2$ given by Eq. 38. For a weak optical lattice, this second gap is smaller than the first gap: see $\pm 2\hbar k_L$ in Fig. 3. However the same *structural* change occurs in the eigenspectrum, i.e., a *first excited band* of continuous energies below $4E_R$ is gapped from a *second band* of continuous energies above it. This is the dividing point between the n = 1 and n = 2 bands.

In sum, we find that coherent coupling of atomic momentum states breaks the continuum of $p^2/2m$ free-particle energies into an infinite number of bands. The gaps between the bands are proportional to atom-photon coupling strengths required to couple the $\pm 2n\hbar k_L$ momenta at the edges of the bands. In the next section, we discuss the structure of these bands.

D. Band structure

A property of the infinite-dimensional matrix H_q is that the same eigenspectrum results when considering q or any $q + 2n\pi/a$, for integer n. We can see this by examining the on-diagonal elements of Eq. 30: adding $2\pi/a_L$ to q simply shifts those entries down by one diagonal step. But since this is an infinite matrix, this leaves the Hamiltonian unchanged. A similar property applies to the eigenstates: notice that the eigenvalues of \hat{T}_{a_L} , $\lambda = e^{-iqa_L}$, are unchanged for $q \to q + 2\pi/a_L$. The eigenstates $|q\rangle$ are always arbitrary up to an overall phase, but clearly the



FIG. 5 Bandwidths and band gaps. The range of solutions $\{E_q^{(n)}\}\$ is shown for a range of lattice depths. At one particular depth, a panel from Fig. 4 is repeated, but this time labelling the widths W_0 , W_1 , and W_2 , as well as the first two gaps, $BG_{0\to 1}$ and $BG_{1\to 2}$. For comparison, the lattice depth is shown (red dashed line). We see that gaps appear even for energies above V_L .

eigenvalue problem is only distinct within a range $q = (-\pi/a_L, +\pi, a_L)$. For this reason, the eigenspectrum is only shown for q up to $\pm \pi/a_L$. This is called the "folded band" representation, and shown in Fig. 4.

Notice that the energies shown are identical for q and -q. This is due to time-reversal symmetry of the Hamiltonian. Time reversal changes \hat{p} to $-\hat{p}$, but leaves \hat{r} unchanged. Since there is no magnetic field under consideration (which would have contributed a $\hat{p} \cdot A$ term), \hat{H} is quadratic in \hat{p} and therefore unchanged. This carries through to quasimomentum, as E(-q) = E(q). For this reason, applying a "modulo 2π " to qa_L when plotting the E(q) spectrum makes it looks as if the energy diagram were "folded"; hence the name.

At each q, the solutions to Eq. 28 can be sorted by increasing energy, and labelled with the band index n = 0, 1, 2, ...We will refer to them as $E_q^{(n)}$. Figure 5 shows the range of solutions within each band as a function of depth. The range of energies within each band is the band width W_n :

$$W_n = \max_q E_q^{(n)} - \min_q E_q^{(n)} \tag{42}$$

We will show below that for deep lattices, W_n is proportional to the site-to-site tunnelling strength. The gaps between bands are BG_n, defined as

$$BG_{n \to n+1} = \min_{q} E_{q}^{(n+1)} - \max_{q} E_{q}^{(n)}$$
(43)

We note that for more complex lattice structure than the one considered here, full band gaps may not exist between bands.

A feature of Fig. 4 is that the dispersion is flat at the edges of each band, i.e., $dE_q^{(n)}/dq = 0$. This feature arises from the nature of the avoided crossing, as follows. As discussed in §II.C, *n*th-order Bragg resonances occur near resonant momenta $q_n = nk_L$. Consider a small displacement $\delta_k = q - q_n$: here $q_i = q_n + \delta_k$ is coupled to $q_f = q_i - 2q_n = \delta_k - q_n$. The effective Hamiltonian is

$$H \to \begin{pmatrix} \frac{\hbar^2}{2m} (q_n + \delta_k)^2 & \hbar\Omega_{B,n}/2\\ \hbar\Omega_{B,n}/2 & \frac{\hbar^2}{2m} (-q_n + \delta_k)^2 \end{pmatrix} \approx n^2 E_R + \begin{pmatrix} 2n E_R (\delta_k/k_L)^2 & \hbar\Omega_{B,n}/2\\ \hbar\Omega_{B,n}/2 & -2n E_R (\delta_k/k_L)^2 \end{pmatrix}$$
(44)

where we have dropped terms of order δ_k^2 . Diagonalizing this Hamiltonian, we find that for small δ_k ,

$$E_{q}^{(n)} \approx n^{2} E_{R} - \frac{\hbar\Omega_{B,n}}{2} \left(1 + \frac{1}{2} (\frac{2n\hbar k_{L}}{m\Omega_{B,n}})^{2} \delta_{k}^{2} \right) \quad \text{and} \quad E_{q}^{(n+1)} \approx n^{2} E_{R} + \frac{\hbar\Omega_{B,n}}{2} \left(1 + \frac{1}{2} (\frac{2n\hbar k_{L}}{m\Omega_{B,n}})^{2} \delta_{k}^{2} \right) \tag{45}$$

This shows that energy is quadratic in $\delta_k = q - q_n$ near the band edge, and thus that $dE^{(n)}/dq = 0$ at $\delta_k = 0$.

E. Bloch states

Having solved the eigenvalue problem numerically, we can calculate both $u_q^{(n)}(x)$ and $\Phi_{n,q}(x)$. As mentioned before, the overall phase of each eigenfunction can be chosen freely. A standard convention is to choose $\Phi_{n,q}(x=0)$ to be

The simplest example of a Bloch state is the q = 0 state in the lowest band:

here shown for $V_L = 20E_R$. We see that the amplitude of $|\Phi_{n,q}|^2$ is maximal at the bottom of the lattice potential (which has been shifted downwards for clarity). For the n = 1 band, the on-site function aquires a node:

$$\left| \Phi_{n=1,q=0}(x) \right|^2 \underbrace{\bigwedge_{V(x)}}_{V(x)} \underbrace{\bigvee_{V(x)}}_{V(x)} \underbrace{\bigvee_{V($$

and for the n = 2 band, two nodes:

$$\left| \Phi_{n=2,q=0}(x) \right|^2 \bigwedge_{V(x)} \bigwedge_{V($$

here shown for $V_L = 50E_R$. We will see in §III.E that in the limit of a deep lattice, the wave function at each site approaches a harmonic oscillator. Already, these Bloch wavefunctions resemble the $n = \{0, 1, 2\}$ harmonic oscillator eigenstates.

As eigenstates of a Hermetian operator, the Bloch states form an orthogonal basis:

$$\langle n, q | n', q' \rangle = \delta_{n,n'} \delta(q - q') \tag{46}$$

or, inserting $1 = \int |x\rangle \langle x|$, an equivalent relation in the spatial domain is:

$$\int_{-\infty}^{+\infty} dx \,\Phi_{n,q}^*(x) \Phi_{n',q'}(x) = \delta_{n,n'} \delta(q-q') \tag{47}$$

In this way Bloch states behave much like momentum eigenstates. For the examples of q = 0 states given above, the orthogonality of different bands is already suggested in the nodal structure of the on-site wavefunction.

For different q states within the same band, it is instead the long-range structure that shows the character of the eigenvector. We see this in the following sequence for n = 0 band Bloch functions (shown for $V_L = 50E_R$) at variable q:



Note that negative q solutions are identical to positive q solutions for parity-symmetric lattices (V(-x) = V(x)), so we only show examples of $q \ge 0$. In each plot, $\operatorname{Re}\{\Phi_q\}$ is compared to $\cos qx$, which is the real part of the e^{iqx} prefactor from Eq. 25.

At the largest quasi-momentum in the lowest band, $q = k_L = \pi/a_L$, the period of the wave function is $2a_L$, which may at first seem strange. (Did you expect half this period, a_L ?) Going back to smaller lattice depths lets us see why this is natural. As $V_L \to 0$, the Bloch function becomes a plane-wave function. For example, at $V_L = E_R$,

 $\operatorname{Re}\{\Phi_{n=0,q=k_{L}}(x)\}$

In this limit, a plane wave at the maximum q is $\Phi_{q=k_L} \to \exp(ik_L x)$. It cannot have any higher momentum, without being outside of the first band. But with $q = k_L$, the period of this function is $2\pi/k_L$, which is $2a_L$. Another argument for why it would be nonsensical for the phase to a period of a_L is that it is only the *difference between adjacent sites* that matters. If the phase-modulation factor were $e^{i2\pi x/a_L}$, then one lattice site away the phase will have wrapped by 2π , which is no change at all. The fastest change of phase is a π phase shift between adjacent sites, which is what is shown above, and has a period of $2a_L$. A final argument returns to the Bragg condition. At the edge of the Brillouin zone, Bragg scattering should be resonanent, and indeed from Eq. 33, we expect $\lambda = 2a_L$. i.e., $\operatorname{Re}\Phi_{n=1,q=k_L} \sim \sin k_L x$ instead of $\operatorname{Re}\Phi_{n=0,q=k_L} \sim \cos k_L x$, so that the two Bloch functions at the avoided crossing (see Eq. 39) are orthogonal.

F. Band mapping

III. LOCALIZATION AND TUNNELLING

Let's now put individual atoms into the modes derived in §II, and try to understand their spatial motion. Of course, an atom in a Bloch state has no dynamics: Bloch state are eigenstates. However initializing particles in delocalized states is not always natural for an experiment. For instance, interactions (discussed in §VI) may localize particles. In this section we show how tunnelling – one of the most iconic quantum phenomona – is already present in band structure.

A. Localization

How do we describe a localized particle in an optical lattice? As a warm-up, let's ask this question without the periodic potential; and then return to a system with band structure.

In an infinite system, the plane-wave eigenstates with $E = \hbar^2 k^2/2m$ are $\phi(x) = \exp(ikx)$, neglecting normalization for now. A localized wave function, centred at x_c , has a position-space representation⁵

$$\psi_{x_c}(x) = \langle x | x_c \rangle = \delta(x - x_c) \tag{48}$$

where $\delta(\cdot)$ is the Dirac delta function. In momentum space,

$$\psi_{x_c}(k) = \langle k | x_c \rangle = \exp(-ikx_c) \tag{49}$$

This uses all momentum states: *localization to a single point in position space requires delocalization in momentum space.* We expect this, of course, from the Heisenberg uncertainly principle, which is just a consequence of Fourier relations.



We can summarize this as

$$|x_c\rangle = \int_{k=-\infty}^{k=+\infty} dk \, e^{i\phi(k)} \, |k\rangle \qquad \text{with} \quad \left[\phi(k) = -kx_c\right] \tag{50}$$

The particular phase chosen for each momentum state, $\phi(k) = -kx_c$, is essential to coherently sum to the delta function at x_c .

For a particle in a single band of an optical lattice, we don't have all momenta: only q (which for $V_L = 0$, is the same thing as k) between $-\pi/a_L$ and $\pi/a_L = k_L$. Using these, how localized can the state be? What's unclear is which phases $\phi(q)$ give the optimal localization. Kohn (Kohn, 1959) showed that the optimal choices can give exponential localization, so long as band gaps exist.

⁵ In this section and the next, we will neglect the normalization of wave functions, and restore them in §III.D.

$$|\psi_{x_c}\rangle = \int_{k=-\pi/a_L}^{k=+\pi/a_L} dk \, e^{i\phi(k)} \, |k\rangle \tag{51}$$

If we choose $\phi(k) = 0$, then

$$\langle x|\psi_0\rangle = \psi_0(x) = \frac{2\sin k_L x}{x} = \mathcal{N}\operatorname{sinc}(k_L x)$$
(52)

where \mathcal{N} is a normalization factor (which we are going to neglect for now). This is a "sinc" function, whose nodes (given by $k_L x = \pm \pi, \pm 2\pi$, etc.) are $\pm a_L, \pm 2a_L$, etc. We could displace this wavefunction by choosing $\phi(k) = -kx_c$, which is equivalent to applying the translation operator $\hat{T}(x_c) = e^{-i\hat{p}x_c/\hbar}$, to $|\psi_0\rangle$. Together, this gives

$$|\psi_{x_c}\rangle = \int_{k=-\pi/a_L}^{k=+\pi/a_L} dk \, e^{-ikx_c} \, |k\rangle \qquad \text{such that} \quad \psi_{x_c}(x) = \mathcal{N}\operatorname{sinc}(k_L(x-x_c)) \tag{53}$$

whose momentum and position representations are as follows:

$$\left(\begin{array}{c|c} |\psi_{x_c}(k)|^2 \\ \hline \\ \hline \\ -k_L & 0 & k_L \end{array}\right) \leftrightarrow \left(\begin{array}{c|c} |\psi_{x_c}(x)|^2 \\ \hline \\ \hline \\ x_c \end{array}\right) \left(\begin{array}{c|c} |\psi_{x_c}(x)|^2 \\ \hline \\ x_c \end{array}\right)$$

In summary, we find that although we cannot make a wavefunction localized to a point (Eq. 48), we can still make a "bump" at $x = x_c$, using the range of momenta in the lowest band. The form of $\psi_{x_c}(x)$ will recognized by anyone familiar with the diffraction-limited optics: a cylindrical lens creates an electric field at its foucus that has the same qualitative form.

A remarkable feature of $|x_c\rangle$ us that the displaced wave function is *orthogonal* to the original one at specific displacements:

$$\langle \psi_0 | \psi_{\Delta x} \rangle = \left(\int_{-\pi/a_L}^{+\pi/a_L} dk' \langle k' | \right) \left(\int_{-\pi/a_L}^{+\pi/a_L} dk \, e^{-ik\Delta x} \, |k\rangle \right) = 2 \frac{\sin(\pi \Delta x/a_L)}{\Delta x} \tag{54}$$

which is = 0 when $\Delta x = \pm a_L, \pm 2a_L, \pm 3a_L, \ldots$ So even though this function is only "approximately localized", and has amplitude beyond a single lattice site, the $|\psi_{x_c}\rangle$ at any one site is orthogonal to the $|\psi_{x'_c}\rangle$ at any other site.

B. Wannier functions

In a standing wave, certain positions are privileged: the locations at which the potential V(x) is minimized, $x_j = a_L j$ (with integer j), which we will call the "locations" of the *lattice sites*. This is a fuzzy notion, since all quantum-mechanical wave functions are extended, or more precisely, localization is energetically expensive. In the limit $V_L \gg E_R$, the amplitudes of low-energy Bloch states are peaked around the $\{x_j\}$, as seen in §II.E.

At lattice sites, the idea of "diffraction limited localization" carries to a nonzero lattice, when using the Bloch basis instead of plane waves. Motivated by the discussion of the previous section, we define the *Wannier state* localized at $x = x_j = ja_L$ as

$$|w_j\rangle = \int_{-k_L}^{k_L} dq \, e^{-iqx_j} \, |q\rangle \tag{55}$$

where $|q\rangle$ is the Bloch state, and we consider only the lowest band for now. Applying the translation operator T_{a_L} , Eq. 23, and using the defining characteristic of $|q\rangle$ that $\hat{T}_{a_L} |q\rangle = e^{-iqa_L} |q\rangle$, we find that

$$\hat{T}_{a_L} |w_j\rangle = |w_{j+1}\rangle \tag{56}$$

localized at $x = x_j - a_L$. Because of this, we can reference all Wannier functions to the j = 0 one, so that each band has a unique Wannier function, which we will call $|w\rangle$ (without reference to position). Including band indices explicitly, we have

$$\left|w^{(n)}\right\rangle = \int_{-k_L}^{k_L} dq \left|q,n\right\rangle \quad \text{and} \quad \left|w_{n,j}\right\rangle = \hat{T}_{x_j} \left|w^{(n)}\right\rangle$$

$$\tag{57}$$



FIG. 6 Wannier States of the lowest band. Spatial representations of the Wannier states, Eq. 58, are shown here for lattice depths $V_L/E_R = 0, 4, 20$. The solid line shows $w_{0,0}(x)$ which (as discussed in the text) is has a functional form identical to all other $w_{0,j}(x)$, apart from a translation from x = 0 to $x = x_j = ja_L$. The yellow curves show $w_{0,j=1}(x)$, for example. The lattice potential is shown (dashed, offset, and with unity amplitude) for reference.



FIG. 7 Momentum representation of Wannier States. The first row shows $w^{(0)}(x)$ and $w^{(1)}(x)$, which are the spatial representation of the Wannier states for the lowest and first excited bands. The second row shows (as a grey dashed line) the Fourier transform, of those, compared to the "comb teeth" of two particular Bloch states (of the same band): q = 0.5, n = 0 on the left, and q = 0.1, n = 1 on the right. The spatial representation of those states are shown on the final row (boxed in blue).

The spatial representation of the Wannier state is

$$w_{n,j}(x) = \langle x | \hat{T}_{x_j} | w^{(n)} \rangle = \langle x | \left(\int dx' | x' \rangle \langle x' | \right) \int_{-k_L}^{k_L} dq \, \hat{T}_{x_j} | q \rangle = \int_{-k_L}^{k_L} dq \, e^{-ix_j q} \Phi_{n,q}(x) \tag{58}$$

Examples of these are shown in Fig. 6. Again, note that $w_{n,j}(x) = w_{n,0}(x - x_j)$ so that there is a unique Wannier function for each band, copied at each lattice site. Because of this, we will sometimes drop the j index here too, and write $w^{(n)}(x)$. As mentioned above, one can show that there is a unique choice of the phases of Bloch states $\{\Phi_{n,q}(x)\}$ that results in Wanner functions that decay exponentially fast at infinity.⁶ If our goal is to represent spatially localized particles, this is an important property! Two further properties may be useful: $w^{(n)}(x)$ are real, and have definite parity, i.e., $w^{(n)}(-x) = \pm w^{(n)}(x)$.

We can find a useful perspective on the Bloch states by considering the momentum-space representation of the Wannier states. At first you might think that the Bloch states are *already* this; after all, we emphasized the Fourier-like relations between $|q\rangle$ and $|w_j\rangle$ at the end of the previous section. However, instead of $|q\rangle \langle w_j|$, we will ask about

⁶ For the sinusoidal potential we consider here, this choice is the same as was mentioned in §II.E: that $\Phi_{n,q}(x=0)$ to be real and positive for even n, and $d\Phi_{n,q}(x)/dx|_{x=0}$ to be real and positive for odd n. (Kohn, 1959) can find such a choice for a lattice potential with mirror symmetry, and whose energy bands are disjoint.

 $|k\rangle \langle w_i|$ (i.e., projections onto eigenstates of \hat{p} , not \hat{H}). From Eq. 57 and 27,

$$\tilde{w}^{(n)}(\kappa) = \langle \kappa | w^{(n)} \rangle = \int_{-k_L}^{k_L} dq \sum_j c_j^q \langle \kappa | q + 2jk_L \rangle \quad \text{i.e.,} \quad c_j^q = \tilde{w}^{(n)}(\kappa = q + 2jk_L)$$
(59)

In other words, $\tilde{w}^{(n)}(\kappa)$ is the continuous function that *includes all the "comb teeth" of the Bloch functions*. For $V_L \to 0$, $\tilde{w}^{(0)}(\kappa)$ would only be a square function of unity between $-k_L$ and k_L ; see Fig. 7 for some examples at finite lattice depth.

We can then rewrite any Bloch function in terms of \tilde{w} :

$$|q,n\rangle = \sum_{j} \tilde{w}^{(n)}(q+2jk_L) |q+2jk_L\rangle$$
(60)

i.e., we can simply draw from \tilde{w} at discrete momenta to form the Bloch state. Figure 7 shows two examples of this. Since $|u_{q,n}\rangle = e^{-iqx} |q,n\rangle$, we can also write the periodic function u(x) in the Bloch wave (see Eq. 25):

$$|u_{q,n}\rangle = \sum_{j} \tilde{w}^{(n)}(q+2jk_L) |2jk_L\rangle \tag{61}$$

So, even though the momentum components of $|u\rangle$ are not displaced by q, the amplitude of their coefficients is still drawn from \tilde{w} at κ which are displaced by q. This is why $|u_{q,n}\rangle$ is in general dependent on q.

In what limit might $u_{q,n}$ be independent of q? Only when $\tilde{w}^{(n)}(q+2jk_L) \approx \tilde{w}^{(n)}(2jk_L)$. This would require that $\tilde{w}(\kappa)$ is broad compared to k_L , which implies that it is w(x) is narrow compared to a_L . We shall discuss in §V that such a limit is realized for $(V_L/E_R)^{1/4} \gg 1$.

Returning to the distinction between u(x) and w(x): from $|u_q\rangle = e^{-iq\hat{x}} |q\rangle$, we can write

$$|u_{q,n}\rangle = \sum_{j} e^{iq(x_j - \hat{x})} |w_{j,n}\rangle \tag{62}$$

This means that the probability density is

$$|u_{q,n}(x)|^{2} = \sum_{j,j'} e^{iq(x_{j}-x_{j'})} w_{j',n}^{*}(x) w_{j,n}(x)$$

$$= \sum_{j} w_{j,n}^{2}(x) + 2\sum_{j} \cos(a_{L}q) w_{j}(x) w_{j}(x-a_{L}) + 2\sum_{j} \cos(2a_{L}q) w_{j}(x) w_{j}(x-2a_{L}) + \dots$$
(63)

where we have used w * (x) = w(x), and assumed even n in the second line. (A similar expression can be found for odd n.) If $|w_j(x-2a_L)| \ll |w_j(x)|$, due to the localization of $w_j(x)$, then we can neglect the cross terms; in this limit, $|u(x)|^2$ is just the sum of Wannier probability densities at each site. Looking back to the plots of Bloch waves shown in §II.E, the periodic u(x) part does look a lot like a sum of the Wannier functions, displaced over each site. However this is only strictly true in the deep lattice limit, where w(x) is narrow compared to a_L . Note that this is the same condition discussed in the previous paragraph for $u_{q,n}$ to be independent of q.

C. A spatially localized basis for atoms in a lattice

Like Bloch functions, the Wannier basis forms an orthonormal set:

$$\int dx \, w_{n,j}(x) \, w_{n',j'}(x) = \delta_{n,n'} \delta_{j,j'} \tag{64}$$

(compare to Eqs. 46 and 47). The proof is left as an exercise (see App. C).

Notice that $|q\rangle$ and $|w_i\rangle$ are Fourier transform pairs. We can invert Eq. 55, such that

$$|q\rangle = \sum_{j} e^{iqx_{j}} |w_{j}\rangle \qquad \text{or} \qquad |q,n\rangle = \sum_{j} e^{iqx_{j}} \left|w_{j}^{(n)}\right\rangle \tag{65}$$

The key relation is

$$\langle q|w_j \rangle = \exp(-iqx_j) \quad \text{and} \quad \langle w_j|q \rangle = \exp(iqx_j)$$
(66)

This, along with inserting complete sets $\int dq |q\rangle \langle q|$ or $\sum |w_j\rangle \langle w_j|$, is the basis of all transformations between these two bases. Also, this reinforces the analogy to plane-wave states of the continuum, where $\langle k|x\rangle = \exp(-ikx)$.

It may bother you that we are replacing a continuum (of Bloch states across a range of q) by a discrete set (of Wannier states at each site). Are the number of states in these two bases the same? Some insight can be gained by putting the lattice in a box of length Ma_L . Here, M is the number of lattice sites, and a_L is the lattice period. Within this box, quasi-momentum become discretized

$$q = \frac{\pi}{Ma_L} \ell = k_L \frac{\ell}{M} \qquad \text{with} \quad \ell \in -M/2 + 1, \dots, M/2$$
(67)

with a maximum value $\pi/a_L = k_L$. The locations of lattice sites are $x_j = ja_L$, with j taking the range $-M/2 + 1, \ldots, M/2$ (or 0 to M-1, if preferred). In any case, we see that there are M discrete values of q_ℓ for quasi-momentum, which matches the number of sites x_j . For larger lattices, these both approach infinity at the same rate. Of course, this range of q covers only one Brillouin zone, and complete sets will also require a summation over bands. Discretization has two further appeals: it simplifies units, and is also immediately amenable to numerical algorithms (which always require discretization). The continuum limit $\sum_q \to a_L \int dq/(2\pi)$ can always be taken.

D. Tunnelling

Returning to the question of atomic motion: how does a particle in "one place" – which we now know means, *initialized in a Wannier state at one lattice site* – evolves in time. In order to approach that problem, we will adopt the formalism of second quantization (App. B). This formalism is convenient since it lets us talk about single particles; more importantly, it lays the ground-work for a discussion of many particles in §VI, where particles interact, and where we will need particles to obey the correct exchange statistics.

We have already diagonalized the single-particle Hamiltonian. The total energy of a system the

$$E = \sum_{n,q} E_q^{(n)} \bar{N}_{n,q} \quad \text{or} \quad E = \sum_n \frac{a_L}{2\pi} \int_{-k_L}^{k_L} dq \, E_q^{(n)} \bar{N}_{n,q}$$
(68)

where $E_q^{(n)}$ are the eigenvalues of the (first quantized) Hamiltonian Eq. 20, and $\bar{N}_{n,q}$ is the number of particles at momentum q in the *n*th band. We are simply adding up the number of particles in each of these states. This total E is the expectation value of the many-body Hamiltonian

$$\hat{H} = \sum_{n} \frac{a_L}{2\pi} \int_{-k_L}^{k_L} dq \, E_q^{(n)} \hat{N}_{n,q} = \sum_{n} \frac{a_L}{2\pi} \int_{-k_L}^{k_L} dq \, E_q^{(n)} \hat{a}_{n,q}^{\dagger} \hat{a}_{n,q}$$
(69)

where $\hat{N} = \hat{a}^{\dagger}\hat{a}$ is the number operator, and \hat{a}^{\dagger} and \hat{a} are the creation and anihilation operators for particles. Here $\hat{N}_{n,q}$, $\hat{a}^{\dagger}_{n,q}$, and $\hat{a}_{n,q}$ are dimensionless. Notice a shift in perspective here: until now, by \hat{H} we meant the Hamiltonian of a single particle; now, by \hat{H} we mean the *total energy of a many-body system*, so that E is extensive.

Since \hat{H} clearly breaks into bands, we can consider each band separately,

$$\hat{H} = \sum_{n} \hat{H}_{\text{band}}^{(n)} \quad \text{with} \quad \hat{H}_{\text{band}}^{(n)} = \frac{a_L}{2\pi} \int_{-k_L}^{k_L} dq \, E_q^{(n)} \hat{a}_q^{\dagger} \hat{a}_q$$
(70)

and often suppress the band index on \hat{a}_q^{\dagger} and \hat{a}_q for simplicity of notation, when discussing a single-band problem.

If \hat{a}_q^{\dagger} creates a Bloch state, what is its relation to the operator that creates a Wannier state? Let's call it \hat{b}_j^{\dagger} , such that $|w_j\rangle = \hat{b}_j^{\dagger} |\text{vac}\rangle$. From Eq. 55, with $|q\rangle = \hat{a}_q^{\dagger} |\text{vac}\rangle$, we have

$$\hat{b}_{j}^{\dagger} |\text{vac}\rangle = \frac{a_{L}}{2\pi} \int_{-k_{L}}^{k_{L}} dq \, e^{-iqx_{j}} \hat{a}_{q}^{\dagger} |\text{vac}\rangle \tag{71}$$

These operators are thus Fourier Transform pairs. In discrete form, a symmetric representation is

$$\hat{b}_{j}^{\dagger} = \frac{1}{\sqrt{M}} \sum_{q} e^{-iqx_{j}} \hat{a}_{q}^{\dagger} \quad \text{and} \quad \hat{a}_{q}^{\dagger} = \frac{1}{\sqrt{M}} \sum_{j} e^{iqx_{j}} \hat{b}_{j}^{\dagger}$$
(72)

A spatially localized creation operator is the sum of all delocalized creation operators. Similarly, the creation of a particle in a single momentum state involves the (phased) creation of particles on all lattice sites. For the infinite lattice, we instead write these in a somewhat asymmetric way:

$$\hat{b}_{j}^{\dagger} = \frac{a_{L}}{2\pi} \int_{-k_{L}}^{\kappa_{L}} dq \, e^{-iqx_{j}} \hat{a}_{q}^{\dagger} \qquad \text{and} \qquad \hat{a}_{q}^{\dagger} = \sum_{j} e^{iqx_{j}} \hat{b}_{j}^{\dagger} \tag{73}$$

In either case, the normalization factors are chosen such that any commutation relations between the \hat{a}_q operators is preserved for the \hat{b}_i operators, and vice versa.

We can now rewrite our Hamiltonian in terms of spatially local operators \hat{b}_i and \hat{b}_i^{\dagger} .

$$\hat{H}_{n} = \frac{a_{L}}{2\pi} \int_{-k_{L}}^{k_{L}} dq \, E_{q} \hat{a}_{q}^{\dagger} \hat{a}_{q} \\
= \frac{a_{L}}{2\pi} \int_{-k_{L}}^{k_{L}} dq \, E_{q} \left(\sum_{j} e^{iqx_{j}} \hat{b}_{j}^{\dagger} \right) \left(\sum_{j'} e^{-iqx_{j'}} \hat{b}_{j'} \right) \\
= \sum_{j,j'} \underbrace{\left(\frac{a_{L}}{2\pi} \int_{-\pi/a_{L}}^{\pi/a_{L}} dq \, E_{q} \, e^{iqa_{L}(j-j')} \right)}_{\equiv -t(\Delta j)} \hat{b}_{j}^{\dagger} \hat{b}_{j'}$$
(74)

where $t(\Delta j)$ has units of energy, and depends only on $\Delta j = j - j'$. (We will justify the minus sign in its definition shortly.) In order to understand its meaning, consider the action of $\hat{b}_j^{\dagger}\hat{b}_{j'}$ for $j \neq j'$. This operator pair *anihiliates a particle at* $x_{j'}$ and creates a particle at x_j . This is what is meant by "hopping" from site j' to site j. For states whose energy is less than the lattice depth, such motion is classically forbidden: it is quantum-mechanical tunnelling.

The rate of tunnelling is related to the matrix element of \hat{H}_n between two Wannier functions. We can see this by writing

$$\langle w_{\ell} | \hat{H}_n | w_{\ell'} \rangle = -\sum_{j,j'} t(j-j') \langle w_{\ell} | \hat{b}_j^{\dagger} \hat{b}_{j'} | w_{\ell'} \rangle = -t(\ell - \ell')$$

$$\tag{75}$$

such that

$$-t(\ell - \ell') = \langle w_{\ell} | \left(\frac{\hat{p}_x^2}{2m} + V_L \sin^2(k_L \hat{x}) \right) | w_{\ell'} \rangle = \int dx \, w_{\ell}(x)^* \left(\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + V_L \sin^2(k_L x) \right) w_{\ell'}(x) \tag{76}$$

From this, and since \hat{H} is hermetian, we can see that

$$t(-\Delta j) = t^*(\Delta j) \tag{77}$$

If the Wannier functions can be chosen to be real (see earlier discussion) then furthermore $t(-\Delta j) = t(\Delta j)$.

We do not need to use Eq. 76 to find the tunnelling coefficients. It is already evident in the dispersion relation for each band! From the definition of $t(\Delta j)$ in Eq. 74,

$$-t(\Delta j) = \frac{a_L}{\pi} \int_{-\pi/a_L}^{\pi/a_L} dq \, E_q \, \cos(iqa_L\Delta j) \tag{78}$$

where we have additionally used the fact that $E_{-q} = E_q$. In fact, since $E_q^{(n)}$ are periodic functions of q, with period $2\pi/a_L$, and have boundary conditions dE/dq = 0 at band edges, we can invert this relation to write E_q as a cosine Fourier series:

$$E_q = \overline{E_q} - 2t(1)\cos(a_L q) - 2t(2)\cos(2a_L q) - \dots \quad \text{or} \quad E_q - \overline{E_q} = -2\sum_{\Delta j=1} t(\Delta j)\cos(a_L q\Delta j)$$
(79)

In sum, the dispersion relation $E_q^{(n)}$ for the *n*th band reveals the tunnelling rates between sites in real space.



FIG. 8 **Tunnelling beyond nearest neighbour.** The tunnelling energies , calculated using Eq. 78, are shown as a function of lattice depth. The main figure shows a linear scale, and the inset shows the same data on a log scale. In principle, atoms can tunnel at infinitely long range. However the relative strength of any Δj greater than 1 is suppressed at a faster exponential rate than nearest-neighbour tunnelling. The dashed line is Eq. 82.

E. The tight-binding limit

As an optical lattice becomes deeper, nearest-neighbour tunnelling becomes more and more dominant. We can see this in Fig. 8, where t(1) t(2), and t(3) are shown for the lowest band, as a function of lattice depth. We see that t(1)dominates, by a factor of 10 already at $V_L \approx 3E_R$, and by a factor of 100 at $V_L \approx 10E_R$.

In the limit where only $t(\Delta j)$ is significant, then we drop the Δj argument, such that the lowest-band energy is

$$E_q \approx \overline{E_q} - 2t\cos(a_L q)$$
 "Tight-binding limit", $t(2) \ll t(1)$ (80)

Notice, looking at Fig. 4, that $E_q^{(0)}$ looks like an inverted cosine, with is minimum at q = 0, and thus t > 0 as defined here. As defined in Eq. 42, the band width is the difference between maximum and minimum energy. Thus

$$W_0 = 4t$$
 (Tight binding) (81)

which is useful rule of thumb to remember.

In the deep-lattice limit, one can show (Campbell, 1955) that its tunnelling strength in the ground band is

$$t \approx \frac{W}{4} \approx \frac{4s^{3/4}}{\sqrt{\pi}} \exp\left(-2s^{1/2}\right) E_R \quad \text{for } s \gg 1 \tag{82}$$

with $s = V_L/E_R$. The exponential decrease is characteristic of quantum tunnelling through a high barrier. This approximation is shown as a dashed line in Fig. 8

In the tight-binding limit, one typically shifts zero energy to coincide with $\bar{E}_q^{(n=0)}$, and writes

$$\hat{H}_{TB} = -t \sum_{\langle j,j' \rangle} \hat{b}_{j'}^{\dagger} \hat{b}_j = -t \sum_j (\hat{b}_{j+1}^{\dagger} \hat{b}_j + \hat{b}_j^{\dagger} \hat{b}_{j+1}) = -t \sum_j \hat{b}_{j+1}^{\dagger} \hat{b}_j + \text{h.c.}$$
(83)

where each of these forms is equivalent: $\langle j, j' \rangle$ is a notation that means "neighbouring sites" (useful when going to higher dimensions or more complex geometries); and h.c. means "hermetian conjugate".

Another insightful form of the TB hamiltonian comes from recognizing that $\hat{b}_{j+1}\hat{b}_j^{\dagger}$ is one-site discrete translation operator, which could also be written (back into first-quantized form) as $|w_{j+1}\rangle \langle w_j|$. In either case, we can then write the one-site translation operator as $\hat{T}_+ = \sum \hat{b}_{j+1}\hat{b}_j^{\dagger}$ or $\sum |w_{j+1}\rangle \langle w_j|$, which now acts on all sites. The TB Hamiltonian is then

$$\hat{H}_{TB} = -t(\hat{T}_{+} + \hat{T}_{+}^{\dagger}) \tag{84}$$

Bloch states in the TB limit take a particularly simple form. The periodic u(x) function is just the sum of all on-site Wannier functions, such that

$$|u\rangle = \sum_{j} |w_{j}\rangle$$
 and $|q\rangle = \sum_{j} e^{iqa_{L}j} |w_{j}\rangle$ (Tight binding) (85)



FIG. 9 **Tunnelling of a single particle.** In a two-dimensional optical lattice, particles are localized to a central column and restricted to tunnel only horizontally (along x, as labelled). Each atom undergoes a coherent quantum random walk; a single image collapses the wave function of each row, enabling a statistical measurement of occupations. (Preiss *et al.*, 2015)

We can solve for the energy of this eigenstate with $\hat{H}_{TB} |q\rangle = E_q |q\rangle$, such that

$$E_q = -t(e^{iqa_L} + e^{-iqa_L}) = -2t\cos(a_L q) \qquad \text{(Tight binding)} \tag{86}$$

Thus we recover the single-cosine dispersion relation of Eq. 80.

F. Quantum Random Walks

If a single atom is initialized in a lattice site at x_j , what are the populations at later times? Let's write out a quantum "register" that has the occupations of the first five sites:

$$|\text{init}\rangle = |0\rangle_{-2} |0\rangle_{-1} |1\rangle_{0} |0\rangle_{+1} |0\rangle_{+2} \tag{87}$$

Applying the TB hamiltonian, Eq. 83, the particle can either hop to the left or hop to the right:

$$\hat{H}\left|\text{init}\right\rangle = -t\left|0\right\rangle_{-2}\left|1\right\rangle_{-1}\left|0\right\rangle_{0}\left|0\right\rangle_{+1}\left|0\right\rangle_{+2} - t\left|0\right\rangle_{-2}\left|0\right\rangle_{-1}\left|0\right\rangle_{0}\left|1\right\rangle_{+1}\left|0\right\rangle_{+2} \tag{88}$$

Taking one more discrete "step":

$$\hat{H}^{2} |\text{init}\rangle = -t^{2} |1\rangle_{-2} |0\rangle_{-1} |0\rangle_{0} |0\rangle_{+1} |0\rangle_{+2} + 2t^{2} |0\rangle_{-2} |0\rangle_{-1} |1\rangle_{0} |0\rangle_{+1} |0\rangle_{+2} - t^{2} |0\rangle_{-2} |0\rangle_{-1} |0\rangle_{0} |0\rangle_{+1} |1\rangle_{+2}$$

$$(89)$$

etc.

Remarkably, this experiment has been done. Fig. 9 shows a measurement of the time evolution of an atom in a single free direction, as a function of time (Preiss *et al.*, 2015). The occupations of sites are measured as a function of time. Atoms can be thought of as hopping from site to site with a characteristic time is $2\pi/t$.

IV. CURRENTS

We saw in the last section that a particle initialized in a single Wannier state will hop from site to site via tunnelling. Microscopically, movement of particles will alway rely on this process. However bulk transport of electrons through a crystal is not usually caused by initialization in a single Wannier state; rather, the movement of charge is induced by an electric field, whose force on particles induces a mass current. In this section, we will consider the speed at which non-equilibrium distributions move, and also find the equivalent of Newton's laws for particles in a lattice.

A. Currents and transport

For neutral particles, the analogue of electrical current is transport of mass. In free space, spatial velocity is related to the center-of-mass momentum by v = p/m. Things are not so simple in a lattice: as discussed in §II, momentum p and quasi-momentum q are not the same, such that $v \neq q/m$. Sometimes (such as in the first band), these two quantities do not even have the same sign! More generally, a single $|q\rangle$ state has multiple components with the same total momentum only if one includes the dressing by the photon field; however the momentum of photons is *not* associated with any mass-current. This makes the discussion of mass transport in optical lattices complex – and interesting!

We will define the total current as the particle number (N) times the velocity of the centre of mass (CM): $J = Nv_{CM}$, where

$$\hat{v}_{\rm CM} = \frac{i}{\hbar} [\hat{H}, \hat{X}_{\rm CM}] \qquad \qquad \hat{J} = \frac{iN}{\hbar} [\hat{H}, \hat{X}_{\rm CM}] \tag{90}$$

in which the CM position operator is

$$\hat{X}_{\rm CM} = \frac{1}{N} \sum_{\ell} x_{\ell} \hat{n}_{\ell} = \sum_{\ell} x_{\ell} \hat{b}_{\ell}^{\dagger} \hat{b}_{\ell} \,. \tag{91}$$

This definition of \hat{J} gives the correct time dependence of expectation values, which we can see from the Ehrenfest Theorem,

$$\frac{d}{dt}\langle\hat{\mathcal{O}}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{\mathcal{O}}]\rangle + \langle\frac{\partial\hat{\mathcal{O}}}{\partial t}\rangle \tag{92}$$

applied to $\hat{\mathcal{O}} = \hat{X}_{CM}$. Since there is no explicit time dependence to \hat{X}_{CM} , we need only to calculate the commutator of $[\hat{H}, \hat{X}_{CM}]$.

$$\hat{J} = \frac{i}{\hbar} \sum_{\langle jk \rangle} \sum_{\ell} [t_{jk} \hat{b}_j^{\dagger} \hat{b}_k, x_{\ell} \hat{b}_{\ell}^{\dagger} \hat{b}_{\ell}] = \frac{i}{\hbar} \sum_{\langle jk \rangle} t_{jk} (x_k - x_j) \hat{b}_j^{\dagger} \hat{b}_k$$
(93)

where we have used $[\hat{b}_{j}^{\dagger}\hat{b}_{k},\hat{b}_{\ell}^{\dagger}\hat{b}_{\ell}] = (\delta_{k,\ell} - \delta_{j,\ell})\hat{b}_{j}^{\dagger}\hat{b}_{k}$. For the general case, we can now use the site-independence of $t_{jk} = t(j-k) = t(k-j)$ and write a simpler form. We will here just write down the tight-binding limit,

$$\hat{J}_{\mathrm{TB}} = -\frac{ita_L}{\hbar} \sum_{\ell} (\hat{b}_{\ell} \hat{b}^{\dagger}_{\ell+1} - \hat{b}_{\ell+1} \hat{b}^{\dagger}_{\ell}) = -\frac{ta_L}{\hbar} \sum_{\ell} i\hat{b}_{\ell} \hat{b}^{\dagger}_{\ell+1} + \text{h.c.} = \frac{ta_L}{\hbar} (i\hat{T}_{+} - i\hat{T}_{-})$$
(94)

which has the units of ta_L/\hbar , a velocity. Notice that, apart from units, \hat{J} has a form much like \hat{H}_{TB} itself, but with a minus sign between hopping terms. This means there must be an asymmetry between neighbouring site occupations for there to be a net current – which makes sense!

One also write down a *local* current operator, $\hat{j}_{\ell} = -i(ta_L/\hbar)\hat{b}_{\ell}\hat{b}^{\dagger}_{\ell+1} + h.c.$, which satisfies a continuity equation

$$\frac{d}{dt}\hat{n}_{\ell} + a_L^{-1}(\hat{j}_{\ell} - \hat{j}_{\ell-1}) = 0$$
(95)

where $(d/dt)\hat{n}_{\ell} = (i/\hbar)[\hat{H}, n_{\ell}]$. This has the form of a typical continuity equation: the rate of change of local density is given by the spatial gradient of a current. If the current from the left and right are balanced, then the local density does not change. We will not work further with the local current in these notes, but instead consider the extensive transport that come from a global force.

B. Group velocity of a wave packet

The band structure energy diagrams we have derived, giving E_q , are also called "dispersion relations", which refers to the spatial dynamics of a wave packet. Let us consider a coherent superposition of Bloch states that are clustered about a central q_0 with a width of σ_q . A typical treatment considers a gaussian weighting, for example:

$$|\psi(t=0)\rangle = \sum f(q) |q\rangle \qquad \text{with} \quad f(q) = \exp\left[-(q-q_0)^2/\sigma_q^2\right]$$
(96)

Important for this discussion is that

$$\sigma_q \ll k_L$$
 such that $\sigma_x \gg a_L$ (97)

ie, this must be a delocalized wave packet. We can therefore expand the local energy about q_0 :

$$E_q^{(n)} \approx E_q^{(n)} + (q - q_0) \underbrace{\frac{dE_q^{(n)}}{dq}}_{=\hbar v_g} + \frac{1}{2}(q - q_0)^2 \underbrace{\frac{d^2 E_q^{(n)}}{dq^2}}_{=\hbar^2/m_q^*},$$
(98)

As we will explain in the remainder of this section and the next, each of these terms has a physical implication: the initial energy of $|\psi\rangle$; the velocity of its propagation, v_g ; and its inertial response to an external force, m_q^* .

Let's first consider the spatial displacement of $|\psi\rangle$. We define the group velocity of the wave packet to be

$$v_g^{(n)}(q_0) = \frac{1}{\hbar} \left. \frac{dE_q^{(n)}}{dq} \right|_{q=q_0} .$$
(99)

The time evolution of ψ is

$$\hat{U}|\psi(t=0)\rangle = \sum_{q} f(q)e^{i\hat{H}t/\hbar}|q\rangle = e^{-i\omega_0 t} \sum_{q} f(q)e^{iv_g qt}|q\rangle$$
(100)

where we have pulled out the common phase factor $\omega_0 = E_{q_0}/\hbar - q_0 v_g$. The remaining phase is equivalent to a discrete translation of each $|q\rangle$ state every $\tau = a_L/v_g$, which we can see by substituting $t = \tau \Delta j$ for integer Δj :

$$e^{iv_g qt} |q\rangle = e^{iv_g q\tau \Delta j} |q\rangle = e^{iqa_L \Delta j} |q\rangle = \hat{T}_{a_L \Delta j} |q\rangle \tag{101}$$

The time evolution of the wave packet is thus a pure translation at these intervals, plus a phase factor

$$|\psi(t=\tau\Delta j)\rangle = e^{-i\omega_0 t} \hat{T}_{a_L\Delta j} |\psi(t=0)\rangle \qquad \text{for} \quad \tau = a_L/v_g \tag{102}$$

Seen stroboscopically at these time intervals, $|\psi\rangle$ propagates at the group velocity v_g defined in Eq. 99. Note that a wave packet made in different bands will have a different v_g even if at the same quasi-momentum q_0 .

So far, this discussion has been quite different in style from the discussion of \hat{J} in §IV. Why is dE/dq related to current? Consider

$$\frac{dE_q}{dq} = \frac{d}{dq} \langle q | \hat{H} | q \rangle = \left(\frac{d}{dq} \langle q |\right) \hat{H} | q \rangle + \langle q | \hat{H} \left(\frac{d}{dq} | q \rangle\right)$$
(103)

where we have used the fact that \hat{H} has no explicit dependence on q, and used a product rule. We can evaluate each derivative by inserting a complete set of Wannier states:

$$\frac{d}{dq}|q\rangle = \frac{d}{dq}\sum_{j}e^{ix_{j}q}|w_{j}\rangle = i\sum_{j}x_{j}e^{ix_{j}q}|w_{j}\rangle = i\sum_{j}x_{j}|w_{j}\rangle\langle w_{j}|q\rangle = iN\hat{X}_{CM}\hat{q}$$
(104)

where we have used Eq. 91. This gives us,

$$\frac{dE_q}{dq} = \left(-iN\left\langle q\right|\hat{X}_{CM}\right)\hat{H}\left|q\right\rangle + \left\langle q\right|\hat{H}\left(iN\hat{X}_{CM}\left|q\right\rangle\right) = iN\left\langle q\right|\left[\hat{H},\hat{X}_{CM}\right]\left|q\right\rangle = \hbar\left\langle q\right|\hat{J}\left|q\right\rangle \tag{105}$$

Comparing to the definition of group velocity above, where E_q was the dispersion relation for a single particle, we have

$$v_g = \langle \hat{J} \rangle / N \tag{106}$$

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C. External forces

Consider the modification of our original Hamiltonian Eq. 20 by the addition of an external force:

$$\hat{H}_F = \frac{\hat{p}^2}{2m} + V_L \sin^2(k_L \hat{x}) - F \hat{x}$$
(107)

This is no longer a translationally invariant hamiltonian, and thus Bloch states $|q\rangle$ are not longer eigenstates. Instead, for a weak force, one can show that the quasi-momentum of each Bloch state changes in time as

$$\frac{d}{dt}q(t) = \frac{1}{\hbar}F\tag{108}$$

In other words, quasi-momentum changes linearly in time with an applied external force. In this way, $\hbar q$ again behaves like free-space momentum p.

This problem was originally considered by Zener, who also found that if the force (or resultant \dot{q}) was too large, the problem became more complex: a particle that began in one band could end up in another one, due to non-adiabatic evolution of the quantum state, especially near small band gaps. Let's ignore this for now, and continue to work in the paradigm of a problem that can be broken into bands.

An intuitive picture for why $dq/dt = F/\hbar$ comes from considering the relative phase evolution of adjacent lattice sites. For a weak gradient, we can approximate the on-site Wannier functions as unchanged apart from a site-to-site phase evolution. For two quantum states shifted in energy by ΔE , their relative phase evolution is $\phi(t) = -(\Delta E)t/\hbar$, which in this case is $\phi(t) = Fa_L t/\hbar$. Across the entire lattice, we then have phases at x_j evolving as $\phi_j(t) = Fx_j t/\hbar$. The time dependence of a particular Bloch state is then

$$\hat{U}(t)|q\rangle = \sum_{j} e^{iqx_{j}} \hat{U}(t)|w_{j}\rangle = \sum_{j} e^{iqx_{j}} e^{iFx_{j}t/\hbar}|w_{j}\rangle = \sum_{j} e^{i(q+Ft/\hbar)x_{j}}|w_{j}\rangle = |q+Ft/\hbar\rangle$$
(109)

agreeing with Eq. 108.

In fact, this intuitive picture can be made more rigorous by considering the following unitary transformation of the problem:

$$\hat{U}_1(t) = \exp\{-i\hat{x}p_0(t)/\hbar\}$$
 with $p_0(t) = Ft$ (110)

and we will also call $p_0(t) = -A(t)$, for reasons that become clear in a moment. In general, through a unitary transformation, the wave function is transformed to $\left|\tilde{\psi}\right\rangle = U \left|\psi\right\rangle$, which obeys the Schrödinger equation under a new Hamiltonian,

$$\widetilde{H} = UHU^{\dagger} + i\hbar \frac{dU}{dt}U^{\dagger}$$
(111)

In our case

$$U_1 \hat{x} U_1^{\dagger} = \hat{x} , \qquad U_1 \hat{p} U_1^{\dagger} = \hat{p} + p_0(t) , \qquad i\hbar \frac{dU_1}{dt} U_1^{\dagger} = \hat{x} \frac{d}{dt} p_0(t)$$
(112)

such that

$$H_F \to \tilde{H}_F = \frac{(\hat{p} - A(t))^2}{2m} + V(\hat{x}) - F\hat{x} + \dot{p}_0\hat{x}$$

= $\frac{(\hat{p} + Ft)^2}{2m} + V(\hat{x})$ (113)

Now that we have \widetilde{H}_F , we have recovered a periodic problem again. We can apply everything as we did before, for instance making use of Bloch functions, quasi momentum, etc. What do those eigenstates say about the solutions in our original frame of reference? We can, for instance, take $|\widetilde{q}\rangle$ and transform it back to $|q\rangle$ using U_1^{\dagger} :

$$|q\rangle = U_1^{\dagger} |\tilde{q}\rangle = e^{+i\hat{x}p_0(t)/\hbar} \sum_j c_j |\tilde{q} + 2n\hbar k_L\rangle = \sum_j c_j |\tilde{q} + 2n\hbar k_L + p_0(t)\rangle = |\tilde{q} + p_0(t)\rangle = |\tilde{q} + Ft/\hbar\rangle$$
(114)

where we have used the fact that $e^{i\hat{x}p_0(t)/\hbar}$ is a translation operator in momentum. Since \tilde{q} is time-independent in the transformed frame, we see that under \hat{H}_F , solutions are of the form $q_{\rm in} + Ft/\hbar$. QED.

It's interesting to note that in the frame created by U_1 , one can also write out a Tight-Binding Hamiltonian:

$$H_{F,TB} = -t \sum_{j} (\hat{b}_{j+1}^{\dagger} \hat{b}_{j} + \text{h.c.}) - F(t) \sum_{j} (ja_L) \hat{b}_{j}^{\dagger} \hat{b}_{j} \longleftrightarrow \widetilde{H}_{F,TB} = -t \sum_{j} (e^{ia_L A(t)/\hbar} \hat{b}_{j+1}^{\dagger} \hat{b}_{j} + \text{h.c.})$$
(115)

where again, A(t) = -Ft when the force is static. This looks like we've made a complex tunnelling strength,

$$t \longrightarrow t e^{-ia_L F t/\hbar} = t e^{-\phi(t)} \tag{116}$$

again following our intuitive picture that adjacent sites acquire a time-dependent phase in the presence of a force.

D. Effective mass

If an external force changes q, what current can it cause? We have already seen that $\hbar \dot{q} = F$ and $\hbar v_g = dE_q/dq$. Combining these,

$$\frac{dv_g}{dt} = \frac{dv_g}{dq}\frac{dq}{dt} = \frac{1}{\hbar}\frac{d^2E_q}{dq^2}\frac{dq}{dt} = \frac{1}{\hbar^2}\frac{d^2E_q}{dq^2}F$$
(117)

This gives us the lattice equivalent of "F = ma", which we will write a = F/m:

$$\frac{dv_g}{dt} = (m_q^*)^{-1} F \qquad \text{with} \quad \frac{1}{m_q^*} \equiv \frac{1}{\hbar^2} \frac{d^2 E_q}{dq^2} \quad \text{(effective mass)}$$
(118)

We can best see the relationship between the second derivative of the dispersion relation and mass when considering a free particle: if $E = p^2/2m = \hbar^2 q^2/2m$ (for zero lattice depth), then $m^* = m$ for all q. For deeper lattices, we can characterize the lowest band by m_0^* , the band curvature at q = 0. For tight banding, for instance,

$$(m_q^*)^{-1} = \frac{1}{\hbar^2} \frac{d^2}{dq^2} (-2t \cos q a_L) = \frac{2t a_L^2}{\hbar^2} \cos q a_L \qquad \text{such that} \qquad m_0^* = \frac{\hbar^2}{2t a_L^2} \qquad \text{(tight binding)} \qquad (119)$$

Note that one comes the same conclusion when finding t(1) from Eq. 78 applied to a free-particle dispersion relation. The fact that t can be written proportionally to an inverse mass emphasizes the identification of tunnelling as a kinetic energy in the problem.

A strange thing about effective mass is that it does not need to be positive, or even finite. Since $m_q^* \sim 1/\cos(qa_L)$, it diverges at $qa_L = \pi/2$, halfway across the band, and comes to a value of $-m_0^*$ at the band edges. The dispersion relation at the band edges can be approximated as an *inverted parabola*, such that an interpretation as a "normal" massive particle breaks down. Perhaps a $q \approx \pm k_L/2$ things make a bit more sense: a small change in q (induced by an external F) will not change v_g here, because $v_g \sim \sin(qa_L)$ at its maximum there.

Finally, consider a thermal distribution of Bloch states, such as one would expect to find in equilibrium. We'll call this distribution f^{eq} . If an external impluse shifts the *entire distribution* by some $\Delta q = F\Delta t$, then a new distribution will deviate from the old one by

$$f^{\text{dev}}(q) = f^{\text{eq}}(q + \Delta q) - f^{\text{eq}}(q) \approx \frac{\partial f^{\text{eq}}}{\partial q} \Delta q$$
 (120)

What current results? Notice that in equilibrium, there is no current, because f(q) = f(-q), so an group velocity a that |q| will cancel out. Thus

$$J = \int dq \, v_g f(q) = \int dq \, v_g f^{\text{dev}}(q) = \int dq \, v_g \frac{\partial f^{\text{eq}}}{\partial q} \Delta q \tag{121}$$

Using integration by parts, and the fact that $f^{eq}v_g = 0$ at the band edges, we can replace $v_g \partial f^{eq} / \partial q$ by $f^{eq} \partial v_g / \partial q$ under the integral. This gives,

$$J = \Delta q \int dq \, f^{\rm eq} \frac{\partial v_g}{\partial q} = \Delta q \int dq \, f^{\rm eq} \hbar \frac{1}{m_q^*} = \hbar \Delta q \left\langle \frac{1}{m_q^*} \right\rangle \tag{122}$$

where by $\langle 1/m_q^* \rangle$ we are indicating the *thermally averaged effective mass* across the band. When temperature is high enough that the occupation is equal everywhere in the band, then $\langle 1/m_q^* \rangle \to 0$, since any shift in q creates balanced positive and negative currents.



FIG. 10 **Deep-lattice limit.** (a) The band structure of a 1D optical lattice for depths of $6E_R$, $60E_R$ and $600E_R$. In each plot, $E^{(n)}(q)$ is shown for n = 0 (blue), n = 1 (green), n = 2 (red), and n = 3 (lavender). The dashed lines indicate the harmonic approximation of energy levels, $(n + \frac{1}{2})\hbar\omega_0$, which overestimate the lattice energy levels at all depths. (b) The on-site Wannier functions for the lowest three bands are shown at $V_L = 60E_R$. Here, the Wannier functions are well approximated by the harmonic-oscillator wavefunctions (dashed lines). [figure credit: V. Venu (Venu, 2022)]

V. THE ISOLATED-SITE LIMIT

For a sufficiently deep optical lattice, all tunnelling shuts down, and one is left with an array of isolated sites. A single particle in such a site experiences a harmonic oscillator potential (§V.A).

A. Harmonic approximation

When strongly confined in a single optical lattice site, the excursion of the atoms is much smaller than the lattice period: $k_L x \ll 1$. Because of this, we can expand the lattice potential:

$$V_L \sin^2(k_L x) \approx V_L (k_L x)^2 - \frac{1}{3} V_L (k_L x)^4 + \frac{2}{45} V_L (k_L x)^6 + \dots$$
 (123)

The first term is simply a quadratic confinement. When comparing to $V_{\rm ho} = \frac{1}{2}m\omega_0^2 x^2$, we see that

$$\omega_0 = \sqrt{\frac{2V_L k_L^2}{m}} = 2\sqrt{V_L E_R} = 2\omega_R s^{1/2} \tag{124}$$

where $\omega_R = E_R/\hbar$ is the recoil energy in frequency units. and For ⁴⁰K in a 1064 nm lattice, $\omega_R = 2\pi \times 4.5$ kHz; so the characteristic oscillation frequency is tens to hundreds of kHz.

The energy of a harmonic oscillator is

$$E_{\rm ho}^{(n)} = \omega_0 (n + \frac{1}{2}) \tag{125}$$

and becomes a reasonable prediction of $\bar{E}_q^{(n)}$, the average energy of each band. Figure 10 compares them.

Similarly, we know that the wave functions in a harmonic oscillator are given by Hermite polynomials. The final panel in Fig. 10 compares the Wannier states of the deep lattice to these. In particular, the ground state is

1 10

$$w^{(0)} \approx (\pi a_{\rm ho}^2)^{-1/4} \exp\left\{\frac{-x^2}{2a_{\rm ho}^2}\right\}$$
 (126)

where the harmonic oscillator length is

$$a_{\rm ho} = \sqrt{\frac{\hbar}{m\omega_0}} = \left(\sqrt{\frac{\hbar^2}{2mE_R}}\right)^{1/2} s^{-1/4} = \frac{a_L}{\pi s^{1/4}}$$
(127)



FIG. 11 Anharmonicity. The difference between the expected energy gap, $\hbar\omega_0$, and the actual band gap is shown versus lattice depth. We find that even in the deep-lattice limit, a remnant anharmonicity of $-(n+1)E_R$ remains, shown as dashed lines.

We see that self-consistency of the original approximation, $k_L x \ll 1$, requires that $s^{1/4} \gg 1$.

This leaves us with a characteristic hierarchy of energy and length scales:

$$E_R \ll \{\hbar\omega_0 \approx \mathrm{BG}\} \ll V_L \quad \text{and} \quad a_L \gg a_{\mathrm{ho}}$$

$$\tag{128}$$

We can also use this to estimate the number of bound states in a deep lattice. If the spacing is $\hbar\omega_0$, then

number of deeply bound states
$$\approx \frac{V_L}{\hbar\omega_0} = \frac{sE_R}{2E_R s^{1/2}} = \frac{1}{2}s^{1/2}$$
 (129)

where we have neglected the zero-point energy. Looking back at Fig. 5, we can see that as V_L exceeds the energy of a particular energy range, the gaps are perhaps larger, but it would not be evident from the band structure, a priori, which energies were "trapped". Perhaps the $E_q^{(n)} < V_L$ vs. $E_q^{(n)} > V_L$ distinction is instead that particles with energies above the lattice depth can move classically between sites; whereas those with energies below must tunnel. The appearance of gaps above V_L reminds us that quantum reflection can occur even for purely attractive potentials. In this case, we have already outlined how the Bragg scattering an every integer multiple of $\hbar k_L$ is a polynomial function of V_L (see Eq. 38).

The depiction of an entire band with a single energy level can only be true if $W_n \to 0$, which is called a "flat band". In deep lattices, this is a reasonable approximation, especially for the lowest bands. As seen in Fig. 13, the width of the n = 0 band becomes small more quickly than the next band. So, even after the ground band is "frozen out", the first excited band may still be active. Whether one can neglect any of these small but finite W_n depends on the time scale of a particular experiment, and the other competitive energy scales in the problem.

Anharmonicity of sinusoidal confinement provides the first deviation from the predictions laid out above. Through perturbation theory, one finds

$$V_{\rm OL}^{(n)} \equiv \langle n | V_L \sin^2(k_L x) | n \rangle = V_L k_L^2 \langle n | x^2 | n \rangle - \frac{1}{3} V_L k_L^4 \langle n | x^4 | n \rangle + \frac{2}{45} V_L k_L^6 \langle n | x^6 | n \rangle + \dots$$

$$= \underbrace{2\sqrt{E_R V_L}(n+1/2)}_{\text{harmonic}} - \underbrace{E_R \left(\frac{2n(n+1)+1}{4}\right)}_{\text{ind. of } V_L} - \mathcal{O}\left(\sqrt{\frac{E_R^2}{V_L}}n^3\right) \tag{130}$$

We can then see that the band gap between two successive bands is, neglecting terms that fall off as $V_L^{-1/2}$ or faster,

$$V_{\rm OL}^{(n+1)} - V_{\rm OL}^{(n)} \approx \hbar\omega_0 - (n+1)E_R$$
 (131)

such that it is always less than $\hbar\omega_0$. A comparison is shown in Fig. 11.

B. Creation of low-dimensional gasses

An optical lattice is made of counter-propagating laser beams. As discussed in §I.B, a cubic lattice is typically formed from pairs of counter-propagating beams that are independent from other axes, creating a potential such as

$$V(\mathbf{r}) = V_{L,x} \sin^2(k_L x) + V_{L,y} \sin^2(k_L y) + V_{L,z} \sin^2(k_L z)$$



FIG. 12 Creation of low-dimensional gases. (a) For a balanced set of beams in three spatial directions, a cubic optical lattice can be formed. (b) Reducing or eliminating the optical lattice along one direction while increasing lattice depth along the other two directions enables quasi-one-dimensional ensembles to be formed. [Source: (Bloch, 2005)]

Now if only one of these lattice depths, say $V_{L,z}$, is $\gg E_R$, then we can apply the paradigm of §V.A along that direction, and write the optical confining potential for each plane in z as

$$V(\mathbf{r}) = V_{L,x} \sin^2(k_L x) + V_{L,y} \sin^2(k_L y) + \frac{1}{2} m \omega_{0,z}^2 z^2 \qquad (\text{quasi-2D configuration})$$
(132)

where $\omega_{0,z} = 2\sqrt{V_{L,z}E_R}$. Here, we have neglected tunnelling in the z direction, assuming that $\{t_x, t_y\} \gg t_z$. This configuration creates a *quasi-two-dimensional* geometry, in which particles are confined a single spatial plane. Typically, because the BG_{0,z} is so much larger than all energy scales in the xy plane, atoms are in the ground band of the harmonic 2D confining potential.

This same approach can also create quasi-one-dimensional ensembles. If $V_{L,y} = V_{L,z} \gg V_{L,x}$, then we can approximate the confining potential along every minimum along the yz potential as

$$V(\mathbf{r}) \approx V_{L,x} \sin^2(k_L x) + \frac{1}{2} m \omega_{\perp}^2 (y^2 + z^2) \qquad \text{(quasi-1D configuration)}$$
(133)

where $\omega_{\perp} = 2\sqrt{V_{L,yz}E_R}$. Here, we have neglected tunnelling in the y and z directions, assuming that $t_x >> \{t_y, t_z\}$. The same remarks apply to these quasi-1D ensembles as were made for quasi-2D. These approaches are shown schematically in Fig. 12.

VI. MANY PARTICLES IN AN OPTICAL LATTICE

When optical lattices were first developed, they were made with near-resonant laser light, loaded with laser-cooled atoms, and explored at low filling: i.e., one atom every ten to hundred sites. As the field (and laser technology) advanced, quantum degenerate gases were loaded into the lattice, which could be made with powerful and far-detuned lasers. The natural question to ask is then, What happens when two atoms are on the same lattice site? The answer depends both on quantum statistics and on the interactions between the particles.

A. Quantum statistics

Even before we consider interactions, let's establish the Hilbert space of possible many-body states. We have discussed the creation and anihilation operators so far without reference to whether the particles we were trying to create were bosons or fermions. But now, this matters, for the following reason. For bosons,

$$\hat{b}_{j}^{\dagger} |\text{vac}\rangle = |1\rangle_{j} \quad , \hat{b}_{j}^{\dagger} |1\rangle_{j} = 2^{1/2} |2\rangle_{j} \quad , \hat{b}_{j}^{\dagger} |2\rangle_{j} = 3^{1/2} |3\rangle_{j} , \dots$$
(134)

so that any occupation number on a single site is possible. However for fermions,

$$\hat{c}_{j}^{\dagger} |\text{vac}\rangle = |1\rangle_{j} \quad , \text{but} \hat{c}_{j}^{\dagger} |1\rangle_{j} = \hat{c}_{j}^{\dagger} \hat{c}_{j}^{\dagger} |0\rangle_{j} = 0 |\text{vac}\rangle$$
(135)

so that the only allowed occupations are 0 and 1, which results in the Pauli exclusion principle. One can prove that this restriction in occupation is a direct result of the anti-commutation relations between fermionic operators (see App. B) as follows: Since $\{\hat{c}_r^{\dagger}, \hat{c}_s^{\dagger}\} = 0$, then for any single site, s, $\hat{c}_s^{\dagger} \hat{c}_s^{\dagger} + \hat{c}_s^{\dagger} \hat{c}_s^{\dagger} = 0$, which can only be true if $\hat{c}_s^{\dagger} \hat{c}_s^{\dagger} = 0$.

So far I have implicitly assumed a single band and a single spin. Both of these become important for fermions, because we can create a second, but non-identical, particle on an occupied site by putting it in the next band.



FIG. 13 Width of the lowest bands. The bandwidth of the lowest band drops more quickly than the bandwidth of the first excited band. Since each of these is dominated by nearest-neighbour tunnelling, population in the first band is far more mobile than the ground band at large depths.

Replicated across the entire lattice, a Fermi surface is formed at the first unoccupied band. If there are multiple spin species, they each have their own Fermi energy, i.e., individual chemcial potentials μ_{\uparrow} and μ_{\downarrow} that are conjugate to the number of spins, N_{\uparrow} and N_{\downarrow} . At "half filling", there is one atom of each spin type in every second site, such that (on average) each lattice site will have either a \uparrow fermion or a \downarrow fermion.

We can view the filling of a lattice from a band-structure perspective as well. Once again, although bosons can multiply occupy a single $|q\rangle$ eigenstate – for instance, all atoms at q = 0 – at most one fermions can occupy each qstate. This means that the band structure is filled up to the Fermi energy. Since the number of $|q\rangle$ states is equal to the number of $|w_j\rangle$ states, the band filling $n = N_{\text{atoms}}/N_{sites}$ tells us about what fraction of each band is filled. For the example of "half filling" (n = 0.5) of the lowest band, the Fermi energy is half the bandwidth. For a 1D lattice, this is $E_F = 2t$; for a 3D lattice, this is $E_F = 6t$, or in general,

$$E_F = 2 dt$$
 (half filling, tight binding, d dimensions) (136)

For higher fillings, one can fill the lowest band. The Fermi energy moves into the first excited band, which (as shown in Fig. 13) has a higher band width and thus higher mobility than the ground band. This is the situation commonly found in metals, where a higher band is not fully filled, and provides an opportunity for electrons to tunnel across the lattice. A basic accomplishment of band theory was to understand the nature of metals and insulators.

Bosons, on the other hand, can Bose condense and easily occupy the lowest energies of the band structure. Adding interactions, however, we will find that the superfluid can be destroyed by localization of particles. A phase transition to an insulator due purely to interactions is a dramatic demonstration of the failing of single-particle picture.

B. On-site interactions

Consider now the interactions on a single site of an optical lattice. A perturbative calculation would use the non-interacting wave function with the interaction potential $U(\mathbf{r})$, such that

$$U = \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 U(\mathbf{r}_1 - \mathbf{r}_2) |w^{(0)}(\mathbf{r}_1)|^2 |w^{(0)}(\mathbf{r}_1)|^2$$
(137)

If we use the contact potential $U(\mathbf{r}) = g\delta(\mathbf{r})$, with $g = 4\pi\hbar^2 a_S/m$, and s-wave scattering length a_S , and the harmonicoscillator limit of the Wannier function in the lowest band, Eq. 126, then we find

$$U = g \left(\frac{\pi\hbar}{2}\right)^{3/2} (m\omega_0)^{3/4} = \frac{2^{3/2}}{\pi^{1/2}} k a_S s^{3/4}$$
(138)

How strong are these interactions? A comparison to single-particle energies can be made. For the lowest band, ignoring its width (and any anharmonicity), we could write

$$\hat{H} \approx \sum_{j} \frac{1}{2} \hbar \omega_0 \hat{b}_j^{\dagger} \hat{b}_j \tag{139}$$

If we add interactions, are these on-site interactions weak or strong? We can evaluate them with a ratio of the on-site interaction, U, to the on-site single-particle energy, $\hbar\omega_0/2$. From Eqs. 124 and 138, we find a dimensionless ratio

$$\gamma_{\rm on-site} = \frac{E_{\rm int}}{E_{\rm s.p.}} = \frac{U}{\hbar\omega_0/2} \sim \frac{E_R k_L a_S s^{3/4}}{E_R s^{1/2}} \sim \frac{a_S}{a_L} s^{1/4}$$
(140)

Since a_S is typically of the order of the van der Waals length in atoms, which is a few nm, whereas $a_L = \lambda_L/2$ is set by the optical length scale, we see that on-site interactions are typically weak. This validates the perturbative approach used to calculate U in Eq. 138.

On the other hand, if we consider the single-particle energy to be not what happens on the site of a single lattice site, but what happens between them – i.e., the tight-binding \hat{H} , Eq. 83 – then from Eq. 82 we find an altogether different picture:

$$\gamma_{\text{inter-site}} = \frac{U}{t} \sim \frac{E_R k_L a_S s^{3/4}}{E_R s^{3/4} \exp(-2s^{1/2})} \sim \frac{a_S}{a_L} \exp\left(2s^{1/2}\right) \tag{141}$$

Here we find an exponential increase of the dimensionless interaction strength with lattice depth. A perturbative approach is quickly invalid!

C. The Hubbard Model

Tunnelling and interactions in a lattice are combined in the Hubbard hamiltonian. There are two flavours: the Bose Hubbard Model and the Fermi Hubbard Model. Let's start with bosons:

$$\hat{H}_{BH} = -t \sum_{j} (\hat{b}_{j+1}^{\dagger} \hat{b}_j + \text{h.c.}) + \frac{1}{2} U \sum_{j} \hat{n}_j (\hat{n}_j - 1) \qquad \text{(bosons, tight banding)}$$
(142)

Here, the on-site interaction term is zero when there is only one atom, and U if there are two atoms. Since there is no limit to the number of particles on a single site, we can also have 3U for three particles, 12U for four particles, etc!

For fermions, a single-band model with interactions required two spin types, $\sigma = \{\uparrow, \downarrow\}$:

$$\hat{H}_{FH} = -t \sum_{j} (\hat{c}_{j+1}^{\dagger} \hat{c}_{j} + \text{h.c.}) + U \sum_{j} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} \qquad \text{(fermions, tight banding)}$$
(143)

Here, no factor of two is required, but the only possibilities in a single band are U for a site with $|1_{\uparrow}1_{\downarrow}\rangle$ and zero interaction energy for all other possibilities, $|0_{\uparrow}1_{\downarrow}\rangle$, $|1_{\uparrow}0_{\downarrow}\rangle$, and $|0_{\uparrow}0_{\downarrow}\rangle$.

With these hamiltonians as a starting point, one can investigate, both theoretically and experimentally, basic manybody phenomena in optical lattices. The reader is referred to further discussion in review papers, such as (Bloch, 2005; Georges and Giamarchi, 2012; Gross and Bloch, 2017).

D. Scattering of Bloch waves

In momentum space, we can show that the FHM is

$$H = \sum_{\boldsymbol{q}_n\sigma} \epsilon_{\boldsymbol{q}} \hat{N}_{\boldsymbol{q}_n\sigma} + \frac{U}{M} \sum_{\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3} \hat{c}^{\dagger}_{\boldsymbol{q}_4\uparrow} \hat{c}^{\dagger}_{\boldsymbol{q}_3\downarrow} \hat{c}_{\boldsymbol{q}_2\uparrow} \hat{c}_{\boldsymbol{q}_1\downarrow} \quad \text{where} \quad \boldsymbol{q}_4 = \boldsymbol{q}_1 + \boldsymbol{q}_2 - \boldsymbol{q}_3 \operatorname{mod} 2\pi/a \tag{144}$$

where we are using the discrete $\{q_n\}$ here and for the remainder of this section. Notice the change back to the eigenstate basis: while in position space, the tunnelling t term couples adjacent sites. However in momentum space, we find that this term does *not* couple different modes, but simply gives the momentum space modes their kinetic energy,

$$\epsilon_q = -2t\cos a_L q \quad (1D) \qquad \epsilon_q = -2t\cos \left(a_L q_x\right) - 2t\cos \left(a_L q_y\right) \quad (2D) \tag{145}$$

The independence of momentum-space modes is the starting point for thermodynamic expressions describing the non-interacting HM. In momentum space, H_U describes a scattering event: an \downarrow atom with q_1 scatters off an \uparrow atom with q_2 , and they emerge with momenta q_3 and q_4 respectively.

The relation of momentum-space operators to position-space operators is

$$\hat{c}_{q_n\sigma}^{\dagger} = \frac{1}{\sqrt{M}} \sum_{\ell}^{M} e^{iq_n \cdot x_{\ell}} \hat{c}_{\ell\sigma}^{\dagger} \quad \text{and} \quad \hat{c}_{\ell\sigma}^{\dagger} = \frac{1}{\sqrt{M}} \sum_{n}^{M} e^{-iq_n \cdot x_{\ell}} \hat{c}_{q_n\sigma}^{\dagger}$$
(146)

where $q_n = (2\pi/Ma)n$ in 1D, and $x_{\ell} = \ell a$. Notice that as M gets larger, the range of q_n remains 0 to $2\pi/a$, whereas x_{ℓ} has a larger range but fixed spacing. The factors of $1/\sqrt{M}$ in front of the sum makes this transform pair unitary.

Let's see how this interaction term arises, by applying Eq. 146 to the (normally ordered) interaction term:

$$H_{U} = U \sum_{\ell} \left(\frac{1}{\sqrt{M}} \sum_{\boldsymbol{q}_{4}} e^{-i\boldsymbol{q}_{4}\cdot\mathbf{x}_{\ell}} \hat{c}^{\dagger}_{\boldsymbol{q}_{4}\uparrow} \right) \left(\frac{1}{\sqrt{M}} \sum_{\boldsymbol{q}_{3}} e^{-i\boldsymbol{q}_{3}\cdot\mathbf{x}_{\ell}} \hat{c}^{\dagger}_{\boldsymbol{q}_{3}\downarrow} \right) \left(\frac{1}{\sqrt{M}} \sum_{\boldsymbol{q}_{2}} e^{i\boldsymbol{q}_{2}\cdot\mathbf{x}_{\ell}} \hat{c}_{\boldsymbol{q}_{2}\uparrow} \right) \left(\frac{1}{\sqrt{M}} \sum_{\boldsymbol{q}_{1}} e^{i\boldsymbol{q}_{1}\cdot\mathbf{x}_{\ell}} \hat{c}_{\boldsymbol{q}_{1}\downarrow} \right) \\ = \frac{U}{M^{2}} \sum_{\boldsymbol{q}_{1},\boldsymbol{q}_{2},\boldsymbol{q}_{3},\boldsymbol{q}_{4}} \hat{c}^{\dagger}_{\boldsymbol{q}_{4}\uparrow} \hat{c}^{\dagger}_{\boldsymbol{q}_{3}\downarrow} \hat{c}_{\boldsymbol{q}_{2}\uparrow} \hat{c}_{\boldsymbol{q}_{1}\downarrow} \sum_{\ell} e^{-i(\boldsymbol{q}_{4}+\boldsymbol{q}_{3}-\boldsymbol{q}_{2}-\boldsymbol{q}_{1})\cdot\mathbf{x}_{\ell}}$$
(147)

and the sums over momentum are still discrete, such as $q_1/(2\pi/a) = \langle n_{1x}/M_x, n_{1y}/M_y \rangle$, and M appearing in (147) is the total number of sites, $M = M_x M_y$. The second sum is nearly a kronecker delta function, but modulo 2π in $a_L q_\alpha$:

$$\sum_{\ell} e^{-i(\boldsymbol{q}_{4}+\boldsymbol{q}_{3}-\boldsymbol{q}_{2}-\boldsymbol{q}_{1})\cdot\boldsymbol{x}_{\ell}} = \left(\sum_{\ell=1}^{M_{x}} e^{i(\boldsymbol{q}_{4x}+\boldsymbol{q}_{3x}-\boldsymbol{q}_{2x}-\boldsymbol{q}_{1x})\boldsymbol{x}_{\ell}}\right) \left(\sum_{\ell'=1}^{M_{y}} e^{i(\boldsymbol{q}_{4y}+\boldsymbol{q}_{3y}-\boldsymbol{q}_{2y}-\boldsymbol{q}_{1y})\boldsymbol{y}_{\ell'}}\right) \left(\sum_{\ell''=1}^{M_{z}} e^{i(\boldsymbol{q}_{4z}+\boldsymbol{q}_{3z}-\boldsymbol{q}_{2z}-\boldsymbol{q}_{1z})\boldsymbol{z}_{\ell''}}\right)$$
$$= \left(\sum_{\ell=1}^{M_{x}} e^{i2\pi(n_{4x}+n_{3x}-n_{2x}-n_{1x})\ell}\right) \left(\sum_{\ell'=1}^{M_{y}} e^{i2\pi(n_{4y}+n_{3y}-n_{2y}-n_{1y})\ell'}\right) \left(\sum_{\ell''=1}^{M_{z}} e^{i2\pi(n_{4z}+n_{3z}-n_{2z}-n_{1z})\ell''}\right)$$
(148)

Each of the sums is

$$\sum_{\ell=1}^{M_x} e^{i2\pi(n_{4x}+n_{3x}-n_{2x}-n_{1x})\ell} = M_x \sum_{r=-1,0,1} \delta(n_{4x}+n_{3x}-n_{2x}-n_{1x},rM_x)$$
$$= M_x \sum_{r=-1,0,1} \delta(q_{4x}+q_{3x}-q_{2x}-q_{1x},2\pi r)$$
(149)

since $q_{1x,n} = (2\pi/M_x a)n_{1x}$, etc., in each direction. The inclusion of r = -1, 0, 1 is because each n is only defined from 0 to $M_x - 1$, so that $n_{4x} + n_{3x} - n_{2x} - n_{1x}$ has a full range of $-2M_x + 2 \rightarrow 2M_x - 2$, allowing only $-M_x$, 0, and M_x as possible values. These $r = \pm 1$ values are "Umklapp" collisions; in comparison, r = 0 are "normal" collisions. Together,

$$H_U = \frac{U}{M} \sum_{\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3} \hat{c}^{\dagger}_{\boldsymbol{q}_4 \uparrow} \hat{c}^{\dagger}_{\boldsymbol{q}_3 \downarrow} \hat{c}_{\boldsymbol{q}_2 \uparrow} \hat{c}_{\boldsymbol{q}_1 \downarrow} \quad \text{where} \quad \boldsymbol{q}_4 = \boldsymbol{q}_1 + \boldsymbol{q}_2 - \boldsymbol{q}_3 \mod 2\pi/a.$$
(150)

We conclude that in momentum space, H_U describes a scattering event: an \downarrow atom with q_1 scatters off an \uparrow atom with q_2 , and they emerge with momenta q_3 and q_4 respectively. Notice that conservation of quasi-momentum appears naturally.

VII. CONCLUSION

In sum, we have discussed the basic concepts of ultracold atoms in optical lattices. In §I, we discussed how to a periodic potential arises from the interference of coherent laser light. In §II, we discussed the eigenstates and eigenvalues of a single particle in a sinusoidal potential. The discrete translational symmetry of the problem is reflected in the Bloch states, each of which can be characterized by a quasi-momentum. Coherent Bragg scattering was seen to fracture the energy continuum of a free particle into distinct bands of energy and single-atoms eigenstates have a structure that reflects their dressing by the light field. In §III, we described how to describe a particle localized to a single lattice site. The Wannier states formed a basis in which to discuss tunnelling of particles between sites. For lattices of moderate depth, nearest-neighbour tunnelling dominates. In §IV, we discussed how currents in the lattice can be characterized, and how they are induced by external forces. For a delocalized wave packet with a well defined quasi-momentum, the expectation value of the current operator is its group velocity. The optical lattice modifies the inertia of an atom, such that it acquires an effective mass that depends on both depth and quasi-momentum. In V, we considered the limit of deep optical lattices, where the particles are so strongly confined that each lattice site can be treated as a harmonic oscillator potential. In this limit, the Wannier wave functions and level spacings also approach the well known solutions of the simple harmonic oscillator. Deep lattices were presented as a tool to form low-dimensional systems. Finally, in VI, we introduced the problem of many particles in a lattice. Both exchange statistics and interactions become important. The canonical Hubbard Models were introduced. We hope these notes can serve as a foundation to learn further about ongoing research involving optical lattices.

Appendix A: Light-matter interactions

The interaction of the optical field with the atom is considered in second-order perturbation theory:

$$U_g(\mathbf{r}) = \sum_e \frac{\left|\langle e|\hat{H}_{\rm E1}|g\rangle\right|^2}{\hbar(\omega - \omega_{eg})} \tag{A1}$$

where ω_{eg} is the resonant frequency of each transition. The states $|e\rangle$ and $|g\rangle$ are eigenstates of $\hat{H}_{at} + \hat{H}_{hf}$. To the same level of approximation, the photon scattering rate is due to the excited state fraction due to the perturbation: $\gamma_{sc} = \Gamma \sum_{e} \left| \langle e | \hat{H}_{E1} | g \rangle \right|^2 / \hbar^2 (\omega - \omega_{eg})^2.$

We consider a spatially varying light fields (standing waves) but a homogeneous magnetic field. The atom is then a test particle following the changing first-order mixing of its internal states and feeling the second-order shift of its energies. The rate of optical pumping must be negligible for this approximation to be true, so we are implicitly assuming that an experiment is done quickly compared to γ_{sc}^{-1} .

In order to evaluate the dipole matrix element in Eq. (A1), it is convenient to project the electric field polarization written in the lab (xyz) coordinates onto a polarization basis, π , σ^+ , and σ^- — for which unit vectors are e_Z and $(e_X \pm i e_Y)/\sqrt{2}$, where e_X is the direction aligned with the magnetic field (and otherwise rotations about this axis are equivalent to a uniform time delay, unimportant for the static potential).

Let's define a rotation $[R_{at}]$ that takes the atomic basis (XYZ) and rotates it into the lab basis xyz. This rotation takes the X axis and rotates it parallel to B written out in the xyz basis. Defining $\mathbf{b} = \mathbf{B}/|\mathbf{B}|$, then the rotation should be a rotation by $-\theta$ about \mathbf{n} , where

$$\mathbf{n} = \frac{\mathbf{b} \times \mathbf{e}_z}{|\mathbf{b} \times \mathbf{e}_z|} = [b_y, -b_x, 0] / \sqrt{b_x^2 + b_y^2}$$

Using Rodrigues' rotation formula, this rotation is

$$[R_{\rm at}] = \mathbb{I} + [\mathbf{n}_{\times}]\sin\theta + (1 - \cos\theta)[\mathbf{n}_{\times}]^2 \tag{A2}$$

where $\cos \theta = b_z = B_z / |\mathbf{B}|$ and $\sin \theta = -\sqrt{1 - b_z^2}$. The cross-product matrix is

$$[\mathbf{n}_{\times}] = \begin{bmatrix} 0 & -n_z & n_y \\ n_z & 0 & -n_x \\ -n_y & n_x & 0 \end{bmatrix} = \frac{1}{\sqrt{b_x^2 + b_y^2}} \begin{bmatrix} 0 & 0 & -b_x \\ 0 & 0 & -b_y \\ b_x & b_y & 0 \end{bmatrix},$$
(A3)

such that $[\mathbf{n}_{\times}]\mathbf{v} = \mathbf{n} \times \mathbf{v}$ for any vector \mathbf{v} .

With this rotation matrix we can express the atomic polarization basis in the xyz frame, and take their dot products to find the desired polarizations of **E**:

$$\tilde{E}_{\pi} = \tilde{\boldsymbol{E}}(\mathbf{r}) \cdot [R_{\rm at}] \boldsymbol{e}_{Z} = \tilde{\boldsymbol{E}}(\mathbf{r}) \cdot \mathbf{b}$$
(A4)

$$\tilde{E}_{\sigma\pm} = \tilde{\boldsymbol{E}}(\mathbf{r}) \cdot [R_{\rm at}] (\boldsymbol{e}_X \pm i \boldsymbol{e}_Y) / \sqrt{2} \tag{A5}$$

1. Rotating Wave Approximation

The optical frequencies are high enough that they are unimportant to near-resonant problems, so we will go to a rotating frame and discard high-frequency terms. This rotating-wave approximation results in a time-independent interaction hamilton, which can then be treated with time-independent perturbation theory.

To first order in the fine structure constant, the interaction of an optical field with an atom is an electric dipole

$$\hat{H}_{\rm E1} = -\hat{\boldsymbol{d}} \cdot \tilde{\boldsymbol{E}},\tag{A6}$$

which has no on-diagonal component. The time-dependent problem is then a Hamiltonian of the form

$$\hat{H} = \hat{H}_0 + \hat{H}_1(t)$$
 (A7)

$$=\frac{\hbar\omega_{eg}}{2}\{|e\rangle\langle e|-|g\rangle\langle g|\} + \operatorname{Re}\{\hbar\Omega_R e^{-i\omega t}\}\{|e\rangle\langle g|+|g\rangle\langle e|\},\tag{A8}$$

where Ω_R is the (complex) Rabi frequency

$$\hbar\Omega_R = \langle e|\hat{H}_{\rm E1}|g\rangle = -\langle e|\hat{d}|g\rangle \cdot \tilde{E}.$$
(A9)

Going into the rotating frame with a unitary transform $\hat{U}(t) = \exp\left(-i\hat{H}_0 t/\hbar\right)$, and neglecting the counter-rotating terms (which rotate at roughly 2ω when $\omega \approx \omega_{eg}$), we find

$$\hat{H} \to \frac{\hbar}{2} \begin{pmatrix} \Delta & \Omega_R \\ \Omega_R^* & -\Delta \end{pmatrix} = \operatorname{Re}\{\Omega_R\} \hat{S}_x - \operatorname{Im}\{\Omega_R\} \hat{S}_y + \Delta \hat{S}_z,$$
(A10)

where the spin matrices do not refer to spatial axes, but the axes of the Bloch picture. (Each of the spin operators is a Pauli matrix in the $\{|e\rangle, |g\rangle\}$ basis: $\hat{S}_i = (\hbar/2)\hat{\sigma}_i$.) We see that the complex phase of the Rabi frequency (that can appear as a complex E-field amplitude) determines the projection of the drive vector onto the XY plane of the Bloch sphere. This is important for Ramsey sequences and other interferometric protocols, but does not appear in the induced potential or the scattering rate.

In sum, the second-order energy shift of the ground state is

$$\Delta E_q^{(2)} = \hbar |\Omega_R|^2 / 4\Delta, \tag{A11}$$

and the excited state fraction is

$$\rho_{ee} = |\Omega_R|^2 / 4\Delta^2. \tag{A12}$$

2. Polarizability

Our next task is to express the matrix element $|\Omega_R|^2$ in terms of field and atomic properties. Since we are working in the $|I m_I J m_J\rangle$ basis, we have direct access to the electronic degrees of freedom (unlike in the low-field basis, where m_J needs to be extracted from the m_F eigenstates). The optical field does not affect nuclear degrees of freedom, and thus all matrix elements will have $m'_I = m_I$.

Since the atomic basis are eigenstates of angular momentum, it is useful to break the vector dipole operator \hat{d} into π , σ^+ , and σ^- components,

$$\hat{\boldsymbol{d}} = \sum_{q} \hat{d}_{q} \boldsymbol{e}_{q} \tag{A13}$$

with the unit vectors $\mathbf{e}_0 = \mathbf{e}_z$ and $\mathbf{e}_{\pm 1} = \mathbf{e}_{\sigma\pm} = (\mathbf{e}_x \pm i\mathbf{e}_y)/\sqrt{2}$. Matrix elements of the dipole hamiltonian can then be expressed as sums of the atomic matrix elements weighted by the field polarization components:

$$\hbar\Omega_R = \langle e|\mathbf{d}|g\rangle \cdot \mathbf{E} = E_{\sigma-} \langle d_{-1} \rangle + E_{\pi} \langle d_0 \rangle + E_{\sigma+} \langle d_1 \rangle$$

= $E \sum_q \tilde{\epsilon}_q \langle \hat{d}_q \rangle$ (A14)

$$\left| \langle m'_J | \hat{d}_q | m_J \rangle \right|^2 = \frac{\hbar c \epsilon_0 \sigma_{0e}}{2\omega_{eg}} \Gamma_e \left| \begin{pmatrix} J & 1 & J' \\ m_J & q & -m'_J \end{pmatrix} \right|^2, \tag{A15}$$

where $\sigma_{0e} = 3\lambda_{eg}^2/2\pi$ is the resonant cross-section for a J = 1/2 to J' = 3/2 transition (Bransden and Joachain, 2003). Since the excited and ground states are not necessarily eigenstates of J_z , the matrix element will need to be

$$\langle \hat{d}_q \rangle = \langle \Psi_e | \hat{d}_q | \Psi_g \rangle = \sum_{m_J, m'_J} \langle \Psi_g | m_J \rangle \langle m'_J | \Psi_e \rangle \langle m'_J | \hat{d}_q | m_J \rangle.$$
(A16)

The values of the Clebsch-Gordan coefficients $|(...)|^2$ are given in Fig. 14.

Adding the contributions of multiple excited states, the induced potential is $U = \sum_{e} \Delta E_g^{(2)} \equiv \alpha I$, with

$$\alpha = \sum_{e} \frac{\Gamma_e \sigma_{0e}}{4\omega_{eg}(\omega - \omega_{eg})} \left| \sum_{m_J, m'_J} \langle \Psi_g | m_J \rangle \langle m'_J | \Psi_e \rangle \begin{pmatrix} J & 1 & J' \\ m_J & q & -m'_J \end{pmatrix} \right|^2.$$
(A17)

Here α has the units $[m^2 \cdot s]$, and depends on the frequency of light and the state of the atom.⁷

The scattering rate is also proportional to $|\Omega_R|^2$ and can be evaluated in a similar way. Defining the cross section σ as $\gamma_{sc} = (\sigma/\hbar\omega)I$, one finds

$$\sigma = \sum_{e} \frac{\Gamma_e^2 \sigma_{0e}}{4\omega_{eg}(\omega - \omega_{eg})^2} \left| \sum_{m_J, m'_J} \langle \Psi_g | m_J \rangle \langle m'_J | \Psi_e \rangle \begin{pmatrix} J & 1 & J' \\ m_J & q & -m'_J \end{pmatrix} \right|^2.$$
(A18)

For a cycling transition, where the ground state is $|\Psi_g\rangle = |m_J = 1/2\rangle$, the excited state is $|\Psi_e\rangle = |m'_J = 1/2\rangle$, and the transition is σ^+ polarized (q = 1), the matrix element is = 1 so that equations (A17) and (A18) take a simple form:

$$\alpha_{2L} = \sigma_0 \Gamma / 4\omega \Delta \quad \text{and} \quad \sigma_{2L} = \sigma_0 \Gamma^2 / 4\Delta^2.$$
 (A19)

The scattering rate can be put in dimensionless form as

$$\frac{\sigma_{2\mathrm{L}}}{\alpha_{2\mathrm{L}}\omega_0} = \frac{\Gamma}{\Delta},\tag{A20}$$

which shows the motivation to use far-detuned optical traps and lattices. The "sustain" of an optical potential (the time it takes to heat as much as the depth (LeBlanc and Thywissen, 2007)) is $\mathbf{s} = U/\dot{E} = \tau_R (\sigma/\alpha\omega)^{-1}$, where $\tau_R = \hbar/E_R$, $E_R = \hbar^2 k^2/2M$ is the recoil energy, $k = 2\pi/\lambda = \omega/c$ is the wave number, M is atomic mass. So the smaller the ratio $\sigma/\alpha\omega$, the longer atoms can be confined in an optical potential.

Appendix B: Second quantization: Mode and field operators

Consider the creation and annihilation operators \hat{a} and \hat{a}^{\dagger} , which for fermions obey the anticommutation relations

$$\{\hat{a}_r, \hat{a}_s^{\dagger}\} = \delta_{rs}, \quad \{\hat{a}_r, \hat{a}_s\} = \{\hat{a}_r^{\dagger}, \hat{a}_s^{\dagger}\} = 0$$
 (B1)

and for bosons obey similar commutation relations $[\hat{a}_r, \hat{a}_s^{\dagger}] = \delta_{rs}$, etc.

⁷ This is not the typical definition of polarizability. The standard notation is that $\tilde{p} = \alpha \tilde{E}$, where α is the complex polarizability, such that $U_{\text{dipole}}/I = -\text{Re}\{\alpha\}/2\epsilon_0 c$. So we have absorbed the factor of $-2\epsilon_0 c$ into our definition. In plots we will use "atomic units", for which the conversion factor is $2\pi a_B^3/c$ for the definition used here, and $4\pi\epsilon_0 a_B^3$ for the standard definition.



FIG. 14 Effective m_J model & magnetic level shifts. In the decoupled limit, such a diagram exists for each value of m_I , which is unaffected by optical transitions. In the intermediate or low-field limit, the ground state is a superposition of $|mJ = +1/2\rangle$ and $|mJ = -1/2\rangle$. The values in bubbles are the squares of the Clebsh-Gordon coefficients, and only shown for half of the transitions for clarity. (They are symmetric for a joint sign flip of m_J , m'_J , and q.) \mathcal{E} is a magnetic and hyperfine shift that depends on m_I .

⁶ Li	Ground $(2^2 S_{1/2})$	Excited $(2^2 P_{1/2})$	Excited $(2^2 P_{3/2})$		
$A_{\rm hf}~({\rm MHz})$	152.1368407	17.386	-1.155		
$B_{\rm hf}~({\rm MHz})$	n/a	n/a	-0.10		
g_J	$pprox g_S$	$\approx 2/3$	$\approx 4/3$		
g_I					
Г	stable	27.11(6) ns	27.11(6) ns		
40 K	Ground $(4^2 S_{1/2})$	Excited $(4^2 P_{1/2})$	Excited $(4^2 P_{3/2})$		
$A_{\rm hf}~({\rm MHz})$	-285.731(16)	-34.49(11)	-7.48(6)		
$B_{\rm hf}~({\rm MHz})$	n/a	n/a	-3.23(50)		
g_J	2.00229421(24)	0.665885	1.334102228		
g_I	0				
Γ	stable	26.79(7) ns	26.45(7) ns		
⁸⁷ Rb	Ground $(5^2 S_{1/2})$	Excited $(5^2 P_{1/2})$	Excited $(4^2 P_{3/2})$		
$A_{\rm hf}~({\rm MHz})$	3417.34130545215	408.328	84.7185		
$B_{\rm hf}~({ m MHz})$	n/a	n/a	12.4965		
g_J	$pprox g_S$	$\approx 2/3$	$\approx 4/3$		
g_I	-0.000 995 141 4				
Γ	stable	27.70(4) ns	26.24(4) ns		

TABLE II Atomic data to evaluate equations for α

These operators create or destroy particles from a complete orthonormal set of functions $\{\phi_r(\mathbf{x})\}$, describing the spatial distribution of a state such as momentum or trap eigenfunctions. These have the property that

$$\int \mathbf{dx} \,\phi_r(\mathbf{x})\phi_s(\mathbf{x}) = \delta_{r,s} \to \text{orthonormal}$$
(B2)

$$\sum_{r} \phi_r(\mathbf{x}) \phi_r^*(\mathbf{y}) = \delta(\mathbf{x} - \mathbf{y}) \to \text{complete}$$
(B3)

The number of particles in a particular mode is $\hat{N}_s = \hat{a}_s^{\dagger} \hat{a}_s$, and only has two possible eigenvalues, 0 or 1.

If instead we would like to know the density of particles at a particular location, we need to use a *field operator*,

$$\hat{\psi}(\mathbf{x}) = \sum_{r} \hat{a}_{r} \phi_{r}(\mathbf{x}) \quad \text{and} \quad \hat{\psi}^{\dagger}(\mathbf{x}) = \sum_{r} \hat{a}_{r}^{\dagger} \phi_{r}^{*}(\mathbf{x}).$$
 (B4)

The field operators take on the same (anti)commutation relations as the mode operators:

$$\{\hat{\psi}(\mathbf{x}), \hat{\psi}^{\dagger}(\mathbf{y})\} = \delta(\mathbf{x} - \mathbf{y}), \quad \{\hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{y})\} = \{\hat{\psi}^{\dagger}(\mathbf{x}), \hat{\psi}^{\dagger}(\mathbf{y})\} = 0$$
(B5)

or $[\hat{\psi}(\mathbf{x}), \hat{\psi}^{\dagger}(\mathbf{y})] = \delta(\mathbf{x} - \mathbf{y})$ etc. for bosons.

We can also express field operators in terms of mode operators:

$$\hat{a}_r = \int \mathbf{d}\mathbf{x} \,\phi_r(\mathbf{x})\hat{\psi}(\mathbf{x}) \quad \text{and} \quad \hat{a}_r^{\dagger} = \int \mathbf{d}\mathbf{x} \,\phi_r^*(\mathbf{x})\hat{\psi}^{\dagger}(\mathbf{x}). \tag{B6}$$

In fact, there is no reason to regard the mode operators as primary, even though they are usually introduced first: if we define the mode operators by Eq. (B6), they will automatically obey the correct (anti)commutation relations.

The density operator $\hat{\rho}(\mathbf{x}) \equiv \hat{\psi}^{\dagger}(\mathbf{x})\hat{\psi}(\mathbf{x})$ gives the local particle density. When acting on the vacuum state $|0\rangle$, it gives zero. The density operator obeys a *commutation* relation with the field operator for fermions:

$$\left[\hat{\rho}(\mathbf{x}), \hat{\psi}(\mathbf{y})\right] = -\hat{\psi}(\mathbf{x})\delta(\mathbf{x} - \mathbf{y}) \tag{B7}$$

Appendix C: Exercises

1. For a single traveling wave, trap frequencies can be found from Taylor expansion about the bottom of the trap. Expanding Eq. (9) and comparing to a simple harmonic oscillator potential, show that

$$\omega_x = \omega_y = \left(\frac{4U_{\text{max}}}{Mw_0^2}\right)^{1/2} \qquad \text{and} \qquad \omega_z = \left(\frac{2U_{\text{max}}}{Mz_R^2}\right)^{1/2} \tag{C1}$$

How does ω_{xy} and ω_z scale with beam power and with beam waist? Remember that U_{max} also depends on beam waist.

- 2. Create your own numerical code to calculate the band structure of the 1D sinusoidal lattice. You can do this in just a few lines with a mathematical package/library that has the Mathieu characteristic functions; or, if you prefer, you can solve a matrix equation as described in §II.B. In Wolfram Alpha or Mathematica, for instance, these are MathieuCharacteristicA[] and MathieuCharacteristicB[]. In Python, these are scipy.special.mathieu_a and scipy.special.mathieu_b.
- 3. Prove Equation (64): Show that for the ground band, $|w_j\rangle$ and $|w_{j'}\rangle$ are orthogonal for $j \neq j'$.
- 4. Find the spatial wavefunction of the Wannier state for the first band, $w^{(1)}(x)$, in the case of $V_L = 0$. Plot the function, and give the location of its nodes.
- 5. Derive Eq. 138.
- 6. For bosonic particles, what is the corresponding relation to Eq. (B7)?

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