5. Population oscillation fit

This section investigates how the periodic potential of the standing optical wave results in band structure and calculates the wavefunctions

[1] We start by considering the time-independent Schrödinger eq. on a one-dimensional lattice wavefunction

1 $H\,\phi_q^{(n)}(x) = E\,\phi_q^{(n)}(x)$ where $H = \frac{1}{2m}p^2 + V(x)$

Since the potential $V(x)$ is periodic the wavefunction must satisfy Bloch's theorem

2 $\phi_q^{(n)}(x) = e^{ikx}\,u_q^{(n)}(x)$

Bloch's theorem states that the wavefunction in a periodic potential will be a plane wave modulated by the underlying periodicity of the lattice. We also see that $\phi_q^{(n)}(x)$ is dependent on the band, n, and quasimomentum q.

Energy bands arise naturally from Bloch's theorem, (Complete proof in Bloch theorem section.) These bands denote by $n = 0, 1, \ldots$ index the accesible energy values with each band separated by an energy gap.

Similarly, the concept of quasimomentum (also crystal momentum) is also a consequence of the periodic potential. Quasimomentum is not the same as momentum but should instead be thought of as a quantum number which is characteristic of the translational symmetry of the periodic potential, much as momentum is a quantum number characteristic of the complete translational symmetry of free space.[2]

We must note that, in the absence of external forces, momentum (p) can only be changed by $2\hbar k$ in an optical lattice since the momentum transfer due to absorbtion and reemission of a photon.

Since the real momentum can only change by units of $2\hbar k$ then we can define the available momentum states as

3 $p = q + 2l\hbar k$ with $l = 0, \pm 1, \pm 2, \ldots$

[1] Greiner, PhD thesis section 3.1.3
[2] Rey, PhD thesis

Given these definitions we now evaluate the Bloch wavefunction in the Schrödinger eq.

$$4 \quad H e^{ikx} u_q^{(n)}(x) = E_q^{(n)} e^{ikx} u_q^{(n)}(x) \Rightarrow \left(\frac{(p+q)^2}{2m} + V(x)\right) u_q^{(n)}(x) = E_q^{(n)} u_q^{(n)}(x)$$

Remembering that the lattice wavefunction modulation $(u_q^{(n)}(x))$ is dependent on the underlying harmonic potential, V_{Lat}. Then these functions must share the same periodicity and can be expanded as a discrete Fourier transform.

$$5 \quad V(x) = \sum_{r=-\infty}^{\infty} V_r e^{i2rkx} \quad \text{and} \quad u_q^{(n)}(x) = \sum_{l=-\infty}^{\infty} a_{n,q}(l)\, e^{i2lkx}$$

expansion coefficients onto each plane wave

The Schrödinger eq. now reads

$$6 \quad \sum_{l=-\infty}^{\infty} \frac{(q+2l\hbar k)^2}{2m} a_{n,q}(l)\, e^{i2lkx} + \sum_{l=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} V_r\, a_{n,q}(l)\, e^{i2(r+l)kx} = \sum_{l=-\infty}^{\infty} E_q^{(n)} a_{n,q}(l) e^{i2lkx}$$

From our calculation of the intensity profile of the standing optical wave we know that $V(x)$ will be of the form

$$7 \quad V(x) = \underbrace{-\alpha\left[\left(\frac{2P_1}{\pi\omega_{x_1}\omega_{y_1}}\right) + \left(\frac{2P_2}{\pi\omega_{x_2}\omega_{y_2}}\right) - \frac{4}{\pi}\left[\frac{P_1 P_2}{\omega_{x_1}\omega_{y_1}\omega_{x_2}\omega_{y_2}}\right]^{1/2}\right]}_{V_{off}} + \underbrace{\alpha\frac{8}{\pi}\left[\frac{P_1 P_2}{\omega_{x_1}\omega_{y_1}\omega_{x_2}\omega_{y_2}}\right]^{1/2}}_{V_{lat}} \cos^2(kz)$$

Eq. 7 is the general form of a 1D standing wave potential of unequal powers. For simplification we take $P_1 = P_2 \Rightarrow V_{off} = 0$ then the lattice contribution can be written as

$$8 \quad V(x) = -V_{lat}\cos^2(kx) = -V_{lat}\left(\frac{\cos(2\theta)+1}{2}\right) = -\frac{V_{lat}}{2} - \frac{V_{lat}}{4}\left(e^{i2kx} + e^{-i2kx}\right)$$

This form of $V(x)$ explicitly shows how to define the Fourier transform of $V(x)$ since

$$9 \quad V(x) = \sum_{r=-\infty}^{\infty} V_r e^{i2kx} = -\frac{V_{lat}}{2} - \frac{V_{lat}}{4}\left(e^{i2kx} + e^{-i2kx}\right) \Rightarrow V_{r=0} = -\frac{V_{lat}}{2} \quad \text{and} \quad V_{r=1} = V_{r=-1} = -\frac{V_{lat}}{4}$$

Finally, we can simplify the Schrödinger eq. and write the Hamiltonian as

$$10 \quad \sum_{l} H_{l,l'} a_{n,q}(l) = E_q^{(n)} a_{n,q}(l) \quad \text{where} \quad H_{ll'} = \begin{cases} \left(2l + q/\hbar k\right)^2 + S/2 \\ S/4 \\ 0 \end{cases}$$

Plan to elaborate further

Following the Philips paper we start by decomposing the Bloch eigenstates ($|n,q\rangle$) into the momentum plane wave states ($|\phi_p\rangle$)

11 $$|n,q\rangle = \sum_p |\phi_p\rangle\langle\phi_p|n,q\rangle$$

Since $p = q + 2l\hbar k$ then we can rewrite eq. 10 as

12 $$|n,q\rangle = \sum_{l=-\infty}^{\infty} |\phi_{q+2l\hbar k}\rangle\langle\phi_{q+2l\hbar k}|n,q\rangle$$

this allows us to define the amplitude coefficients of the projection of the Bloch states in the plane wave basis

13 $$a_{n,q}(l) = \langle\phi_{q+2l\hbar k}|n,q\rangle$$

These amplitudes may be found by truncating the plane waves to some l and diagonalizing the Hamiltonian found in eq. 10.

Furthermore, we can now describe the time-evolution after a sudden turn of the lattice by finding the initial state and letting it evolve in time under the new lattice Hamiltonian. Starting with a plane wave state $|\psi\rangle$ at $t=0$ projected onto the Bloch states

$$|\psi(t=0)\rangle = |\phi_q\rangle$$ => $p = q + 2l\hbar k$ => $p = q$ assuming one initial momentum state

14 $$|\psi(t=0)\rangle = \sum_{n=0}^{\infty} |n,q\rangle\langle n,q|\phi_q\rangle = \sum_{n=0}^{\infty} a^*_{n,q}(0)\,|n,q\rangle$$

The time evolution of this state is given by

15 $$|\psi(t)\rangle = e^{-iE_n(q)t/\hbar}|\psi(t=0)\rangle = \sum_{n=0}^{\infty} a^*_{n,q}(0)\, e^{-iE_n(q)t/\hbar}|n,q\rangle$$

Sudden turn off of the lattice will once more project the state $|\psi(t)\rangle$ back onto the plane wave states.

16 $$|\Theta(t)\rangle = \sum_{l=-\infty}^{\infty} |\phi_{q+2l\hbar k}\rangle\langle\phi_{q+2l\hbar k}|\psi(t)\rangle$$

$$|\Theta(t)\rangle = \sum_{l=-\infty}^{\infty}\sum_{n=0}^{\infty} |\phi_{q+2l\hbar k}\rangle\langle\phi_{q+2l\hbar k}|n,q\rangle\, a^*_{n,q}(0)\, e^{-iE_n(q)t/\hbar}$$

$$|\Theta(t)\rangle = \sum_{l=-\infty}^{\infty}\sum_{n=0}^{\infty} a_{n,q}(l)\, a^*_{n,q}(0)\, e^{-iE_n(q)t/\hbar}\,|\phi_{q+2l\hbar k}\rangle$$

We can simplify the above definition of $|\Theta(t)\rangle$ by defining

17 $$b_q(l) = \sum_{n=0}^{\infty} a_{n,q}(l)\, a^*_{n,q}(0)\, e^{-iE_n(q)t/\hbar} \Rightarrow |\Theta(t)\rangle = \sum_{l=-\infty}^{\infty} b_q(l)\,|\phi_{q+2l\hbar k}\rangle$$

Consider the particular case of following the population in the $l=0$ and $l=\pm 1$ ($p=\pm 2\hbar k$) plane wave states after time evolution in the lattice. We will assume that only the lowest two bands will be accesible in the lattice ($n=0$ and $n=2$ => due to symmetry of the wavefunction $a_{1q}(l)=0$)

$$|\Psi(t)\rangle = \sum_{l=-\infty}^{\infty}\left[a_{0q}(l)\,a_{0q}^*(0)\,e^{-iE_0(q)t/\hbar} + a_{2q}(l)\,a_{2q}^*(0)\,e^{-iE_2(q)t/\hbar}\right]|\phi_{q+2l\hbar k}\rangle$$

We will start from a $p=q=0$ initial plane wave state, thus the probability of finding a particle in the $l=0$ state is given by

18 prob. to be in $l=0$ $= |b_0(0)|^2 = \left|a_{0,0}(0)\,a_{0,0}^*(0)\,e^{-iE_0(0)t/\hbar} + a_{2,0}(0)\,a_{2,0}^*(0)\,e^{-iE_2(0)t/\hbar}\right|^2$

$$|b_0(0)|^2 = [a_{0,0}(0)\,a_{0,0}^*(0)]^2 + [a_{2,0}(0)\,a_{2,0}^*(0)]^2 + a_{0,0}(0)\,a_{0,0}^*(0)\,a_{2,0}(0)\,a_{2,0}^*(0)\,e^{-iE_0(0)t/\hbar}\,e^{iE_2(0)t/\hbar}$$
$$+ a_{0,0}(0)\,a_{0,0}^*(0)\,a_{2,0}(0)\,a_{2,0}^*(0)\,e^{-iE_2(0)t/\hbar}\,e^{iE_0(0)t/\hbar}$$

$$= [a_{0,0}(0)\,a_{0,0}^*(0)]^2 + [a_{2,0}(0)\,a_{2,0}^*(0)]^2 + a_{0,0}(0)\,a_{0,0}^*(0)\,a_{2,0}(0)\,a_{2,0}^*(0)\left[e^{-i(E_2(0)-E_0(0))t/\hbar} + e^{-i(E_2(0)-E_0(0))t/\hbar}\right]$$

Using the identity: $e^{ix}+e^{-ix} = 2\cos(x)$

19 $$|b_0(0)|^2 = [a_{0,0}(0)\,a_{0,0}^*(0)]^2 + [a_{2,0}(0)\,a_{2,0}^*(0)]^2 + 2\,a_{0,0}(0)\,a_{0,0}^*(0)\,a_{2,0}(0)\,a_{2,0}^*(0)\cos\left(\frac{E_2(0)-E_0(0)}{\hbar}t\right)$$

Similarly, the probability of being in $l=1$ is

20 $$|b_0(1)|^2 = \left|a_{0,0}(1)\,a_{0,0}^*(0)\,e^{-iE_0(0)t/\hbar} + a_{20}(1)\,a_{20}^*(0)\,e^{-iE_2(0)t/\hbar}\right|^2$$

$$= [a_{0,0}(1)\,a_{0,0}^*(0)]^2 + [a_{2,0}(1)\,a_{2,0}^*(0)]^2 + a_{0,0}(1)\,a_{0,0}^*(0)\,a_{2,0}(1)\,a_{2,0}^*(0)\left[e^{-iE_0(0)t/\hbar}\,e^{iE_2(0)t/\hbar} + e^{-iE_2(0)t/\hbar}\,e^{iE_0(0)t/\hbar}\right]$$

$$= [a_{0,0}(1)\,a_{0,0}^*(0)]^2 + [a_{2,0}(1)\,a_{2,0}^*(0)]^2 + a_{0,0}(1)\,a_{0,0}^*(0)\,a_{2,0}(1)\,a_{2,0}^*(0)\,(2)\cos\left(\frac{E_2(0)-E_0(0)}{\hbar}t\right)$$

due to only populating even bands, then
$b_0(1) = b_0(-1)$
thus we can find the fitting function by summing

21 $$|b_0(1)|^2 + |b_0(-1)|^2$$

$$= 2\underbrace{\left\{[a_{0,0}(1)\,a_{0,0}^*(0)]^2 + [a_{2,0}(1)\,a_{2,0}^*(0)]^2\right\}}_{A} + \underbrace{4\,a_{0,0}(1)\,a_{0,0}^*(0)\,a_{2,0}(1)\,a_{2,0}^*(0)}_{B}\cos\Big(\underbrace{\frac{E_2(0)-E_0(0)}{\hbar}}_{\omega}t\Big)$$

So ~~we will use the fit~~ the normalized $2\hbar k$ population using

22 $\boxed{P_{\pm 2\hbar k} = A + B\cos(\omega t)}$

Once we have found the frequency of oscillation ω, which is proportial to the $n=2 \rightarrow n=0$ bandgap then we use a minimization routine to find the lattice depth, s, such that the calculated bandgap between $n=0$ and $n=2$ matches the measured bandgap, ω. We find the theoretical bandgap by finding the eigenvalues of $\hat{H}_{lattice}$ (eq. 16). The implementation is below

23 $$\text{Lattice Depth}(s_{calc}) = \text{Minimize}\left[\,\left|\text{Bandgap}(H_{Lattice}) - \hbar\omega_{fit}\right|\,\right]$$

Verify that the state is normalized

For 2 bands $(n=0, n=2)$

$$|\Theta(t)\rangle = \sum_{l=-\infty}^{\infty}\left[a_{0q}(l)\,a_{0q}^*(0)\,e^{-iE_0(q)t/\hbar} + a_{2q}(l)\,a_{2q}^*(0)\,e^{-iE_2(q)t/\hbar}\right]|\phi_{q+2l\hbar k}\rangle$$

Assume all population in $-1, 0, +1$ peaks (and $q=0$)

$$|\Theta(t)\rangle = \left[a_{00}(-1)\,a_{00}(0)\,e^{-iE_0(0)t/\hbar} + a_{20}(-1)\,a_{20}^*(0)\,e^{-iE_2(0)t/\hbar}\right]|\phi_{-2\hbar k}\rangle$$
$$+\left[a_{00}(0)\,a_{00}(0)\,e^{-iE_0(0)t/\hbar} + a_{20}(0)\,a_{20}^*(0)\,e^{-iE_2(0)t/\hbar}\right]|\phi_0\rangle$$
$$+\left[a_{00}(1)\,a_{00}(0)\,e^{-iE_0(0)t/\hbar} + a_{20}(1)\,a_{20}^*(0)\,e^{-iE_2(0)t/\hbar}\right]|\phi_{2\hbar k}\rangle$$

$|\langle\Theta(t)|\Theta(t)\rangle|^2 = 1 \Rightarrow$ all cross terms between states cancel so

$$1 = \left[a_{00}(-1)\,a_{00}(0)\,e^{-iE_0(0)t/\hbar} + a_{20}(-1)\,a_{20}^*(0)\,e^{-iE_2(0)t/\hbar}\right]$$
$$\times\left[a_{00}^*(-1)\,a_{00}^*(0)\,e^{iE_0(0)t/\hbar} + a_{20}^*(-1)\,a_{20}(0)\,e^{iE_2(0)t/\hbar}\right]$$
$$+\left[a_{00}(0)\,a_{00}(0)\,e^{-iE_0(0)t/\hbar} + a_{20}(0)\,a_{20}^*(0)\,e^{-iE_2(0)t/\hbar}\right]$$
$$\times\left[a_{00}^*(0)\,a_{00}^*(0)\,e^{iE_0(0)t/\hbar} + a_{20}^*(0)\,a_{20}(0)\,e^{iE_2(0)t/\hbar}\right]$$
$$+\left[a_{00}(1)\,a_{00}(0)\,e^{-iE_0(0)t/\hbar} + a_{20}(1)\,a_{20}^*(0)\,e^{-iE_2(0)t/\hbar}\right]$$
$$\times\left[a_{00}^*(1)\,a_{00}^*(0)\,e^{iE_0(0)t/\hbar} + a_{20}^*(1)\,a_{20}(0)\,e^{iE_2(0)t/\hbar}\right]$$

I know the amplitudes are all real so

$$1 = [a_{00}(-1)a_{00}(0)]^2 + [a_{20}(-1)a_{20}(0)]^2 + 2a_{00}(-1)a_{00}(0)a_{20}(-1)\,a_{20}(0)\cos\left(\frac{E_2(0)-E_0(0)}{\hbar}t\right)$$
$$+[a_{00}(0)a_{00}(0)]^2 + [a_{20}(0)a_{20}(0)]^2 + 2a_{00}(0)a_{00}(0)a_{20}(0)\,a_{20}(0)\cos\left(\frac{E_2(0)-E_0(0)}{\hbar}t\right)$$
$$+[a_{00}(1)a_{00}(0)]^2 + [a_{20}(1)a_{20}(0)]^2 + 2a_{00}(1)a_{00}(0)a_{20}(1)\,a_{20}(0)\cos\left(\frac{E_2(0)-E_0(0)}{\hbar}t\right)$$

$$= \left[a_{00}(-1)^2 + a_{00}(0)^2 + a_{00}(1)^2\right]a_{00}^2(0) + \left[a_{20}(-1)^2 + a_{20}^2(0) + a_{20}(1)^2\right]a_{20}^2(0)$$

$$+\,2\,a_{00}(0)\,a_{20}(0)\left[a_{00}(-1)\,a_{20}(-1) + a_{00}(0)\,a_{20}(0) + a_{00}(1)\,a_{20}(1)\right]\cos\left(\frac{E_2(0)-E_1(0)}{\hbar}t\right)$$

Checking amplitudes this term $=0$ at $t=0$

With the cross terms eliminated we verify that $\sum_l\sum_n |b_q(l)|^2 = 1$ when $n=0,2$ and $l=-1,0,1$