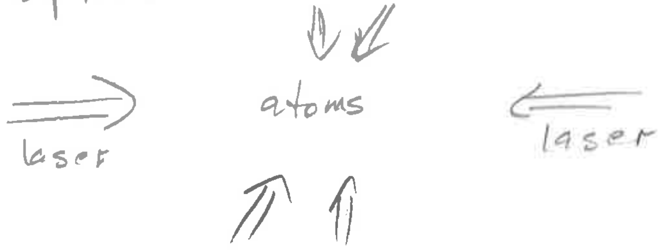
AMO perspective on band structure

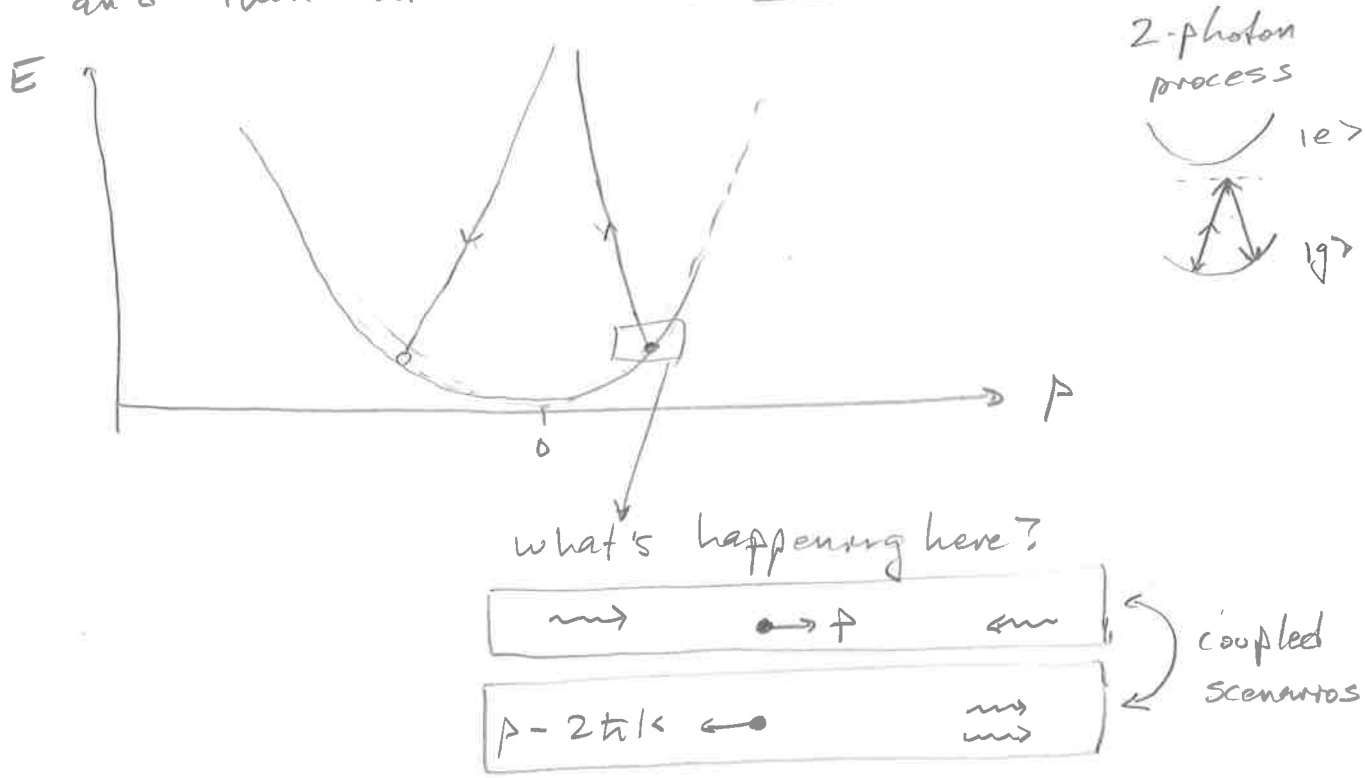
From the view of an optical table, laser cooling and optical lattices do not look that different:



and yet in analysis, the potential created by standing waves is treated much like a solid. However some parts of the resultant band structure can be identified with atom-photon processes used in other contexts.

Let's start with the free-particle dispersion

and then add coherent BRAGG SCATTERING:

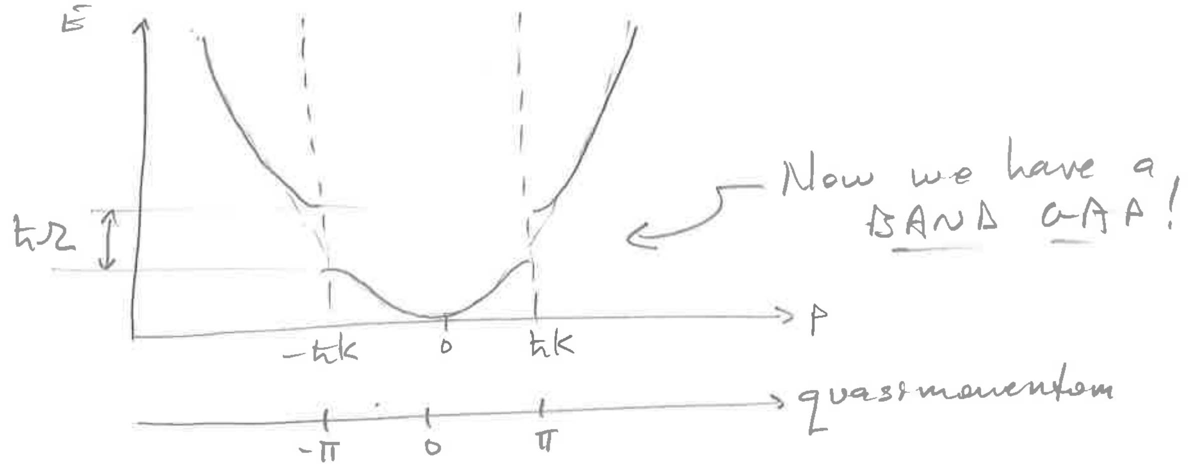


A simple Hamiltonian for this is

$$H \longrightarrow \begin{pmatrix} p^2/2m & \hbar\Omega/2 \\ \hbar\Omega/2 & \frac{(p-2\hbar k)^2}{2m} \end{pmatrix} \underset{p=+\hbar k}{\text{on-resonance,}} \begin{pmatrix} E_R & \hbar\Omega/2 \\ \hbar\Omega/2 & -E_R \end{pmatrix}$$

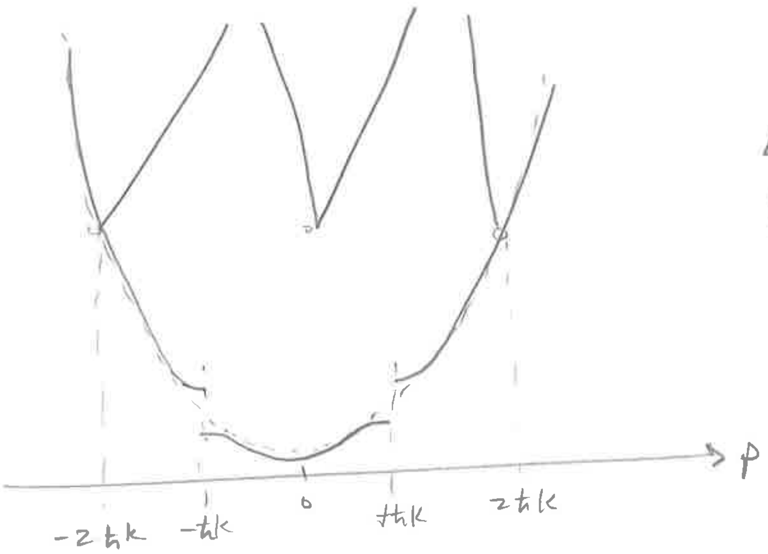
which is easy to diagonalise, $E = E_R \pm \hbar\Omega/2$

So the coupling opens a splitting $\hbar\Omega$ that is the strength of Bagg coupling between the $\pm\hbar k$ momenta.



The factors of 2 here are chosen such that the oscillation between an undressed $|+\hbar k\rangle$ state & $|-\hbar k\rangle$ state has oscillation frequency Ω. Later we will find that $\hbar\Omega = V_0/2$, where V_0 is the depth of the sinusoidal lattice potential.

What about other band gaps? So far we only have one. (Alexandra can't answer...)



4-photon Bragg scattering

In fact, we would anticipate this, and higher orders, simply by writing down the Bragg condition

$$2d \sin\theta = n\lambda$$

Here we have a de Broglie wave $\lambda_{dB} = \frac{h}{p} = \frac{2\pi a_L}{q}$

and retro-reflection $\theta = \pi/2$ or $\sin\theta = 1$

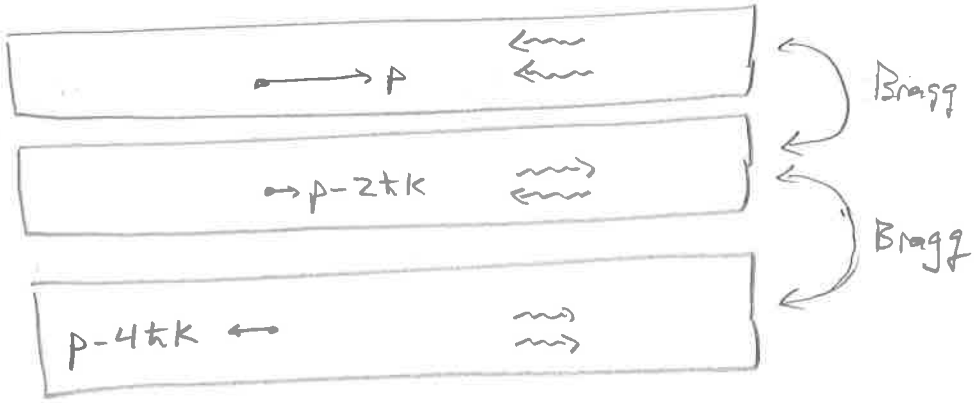
off a structure with period a_L (the optical lattice)

So,

$$2a_L = n\frac{2\pi a_L}{q} \longrightarrow \boxed{q = n\pi} \text{ for } n^{\text{th}} \text{ order Bragg}$$

However, higher-order processes have higher-power scaling with the coupling. We expect $\mathcal{O}(\Omega^2)$, & find $V_0^2/32$.

The Hamiltonian to describe this comes from



or in matrix language, using $\hbar\Omega = V_0/2$,

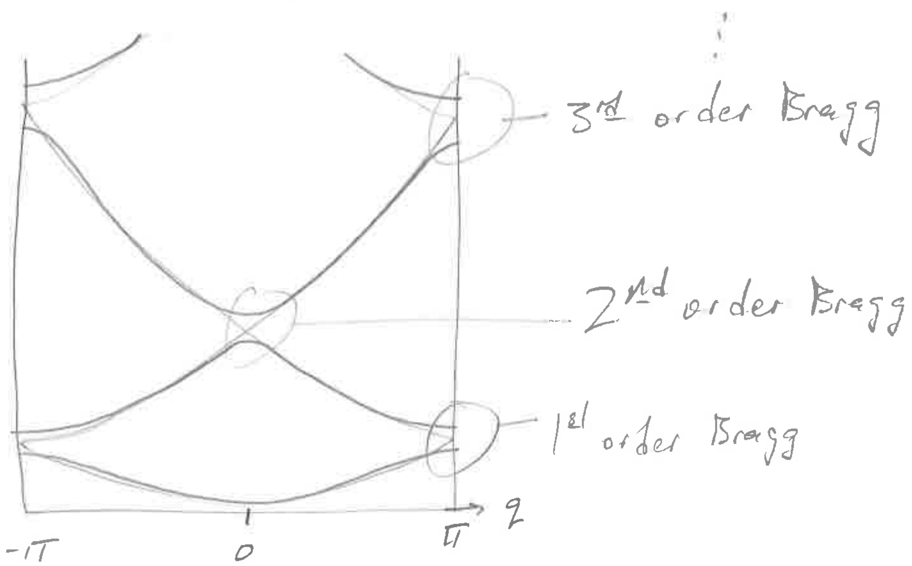
$$H \longrightarrow \begin{pmatrix} p^2/2m & V_0/4 & 0 \\ V_0/4 & \dfrac{(p-2\hbar k)^2}{2m} & V_0/4 \\ 0 & V_0/4 & \dfrac{(p-4\hbar k)^2}{2m} \end{pmatrix}$$

whose energy gap we again see at the resonant momentum, $p = 2\hbar k$:

$$\begin{pmatrix} 4E_R & V_0/4 & 0 \\ V_0/4 & 0 & V_0/4 \\ 0 & V_0/4 & 4E_R \end{pmatrix}$$

Diagonalise this, & find splitting of $V_0^2/32$.

Together these processes give us band structure:



One can find the effective H's I wrote down within a solution to the Schrodinger Equation as follows:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V_{lat}(\hat{x}) \quad , \quad \hat{H}\psi = \mathcal{E}\psi$$

use $\psi(x) = e^{iqx} u(x) = e^{iqx} \sum_{\ell} \alpha_\ell \left(e^{2ik_L x}\right)^{\ell}$

$$V_{lat} = V_0 \sin^2(k_L x) = \frac{V_0}{2} - \frac{V_0}{4} e^{-2ik_L x} - \frac{V_0}{4} e^{+2ik_L x}$$

Rescale everything by E_R, eg $s \equiv V_0/E_R$, & π/a_L, to get

$$\sum_{\ell'} \left[H(q)\right]_{\ell\ell'} \alpha_{\ell'} = \frac{\mathcal{E}}{E_R} \alpha_\ell$$

where
$$H(q) = \left(\left(\frac{q}{\pi} + 2\ell\right)^2 + \frac{s}{2}\right) \delta_{\ell\ell'} - \frac{s}{4} \delta_{\ell,\ell'-1} - \frac{s}{4} \delta_{\ell,\ell'+1}$$

Writing out this matrix we have

$$\begin{pmatrix} \ddots & & & & & & \\ & \left(\frac{q}{\pi}+4\right)^2 & -\frac{s}{4} & 0 & 0 & 0 & \\ & -\frac{s}{4} & \left(\frac{q}{\pi}+2\right)^2 & -\frac{s}{4} & 0 & 0 & \\ & 0 & -\frac{s}{4} & \left(\frac{q}{\pi}\right)^2 & -\frac{s}{4} & 0 & \\ & 0 & 0 & -\frac{s}{4} & \left(\frac{q}{\pi}-2\right)^2 & -\frac{s}{4} & \\ & 0 & 0 & 0 & -\frac{s}{4} & \left(\frac{q}{\pi}-4\right)^2 & \cdots \\ & \vdots & & & & \vdots & \ddots \end{pmatrix}$$

from which we can identify the smaller, near-resonant matrices considered previously. Even when calculating this numerically, you'll have to truncate the expansion $u = \sum_{\ell=-\infty}^{\infty} \alpha_\ell \left(e^{i2k_L x}\right)^\ell$ somewhere. This is done when

$$\left(q/\pi + 2\ell\right)^2 \gg \frac{s}{4}$$

so that plane-wave states are unaffected by Bragg scattering of the lattice.

In practice, $\ell_{max} = 3$ for weak lattices, $\ell_{max} = 10$ for deep lattices, works fine. Note $\sum |\alpha|^2 = 1$.

This discussion enforces an important distinction between Bloch states with q, and free-particle states with the same nominal momentum. The Bragg-dressed Bloch state is

$$|q\rangle = \alpha_0 \left| \bullet\!\!\rightarrow q/a \right\rangle + \alpha_{+1} \left| \begin{array}{l} \bullet\!\!\longrightarrow q/a + 2k_L \\ \text{and } \leftsquigarrow\leftsquigarrow \ 2\text{ ph.} \end{array} \right\rangle + \alpha_{-1} \left| \begin{array}{l} q/a - 2k_L \longleftarrow\!\!\bullet \\ \text{and } \rightsquigarrow\rightsquigarrow \ 2\text{ph} \end{array} \right\rangle$$

$$+ \alpha_{+2} \left| \begin{array}{l} \bullet\!\!\longrightarrow q/a + 4k_L \\ \leftsquigarrow\leftsquigarrow\leftsquigarrow\leftsquigarrow \ 4\text{ ph.} \end{array} \right\rangle + \alpha_{-2} \left| \begin{array}{l} q/a - 4k_L \longleftarrow\!\!\bullet \\ \rightsquigarrow\rightsquigarrow\rightsquigarrow\rightsquigarrow \ 4\text{ photons} \end{array} \right\rangle + \cdots$$

Light and atoms are coupled, in a way that conserves total momentum and energy, but that warns against identifying $|q\rangle$ with a particle momentum $\hbar q/a$. In fact, many momenta are contained within a single eigenstate! QUASIMOMENTUM AND MOMENTUM ARE NOT THE SAME. This will be particularly relevant when considering collisions, where we find that mass current, associated with bare-particle velocity p/m, is not conserved.

[→ slides]

From band structure to tunnelling & effective mass

So far, we have considered momentum states, finding that the single-particle Hamiltonian is

$$\hat{H} = \sum_q \varepsilon_q \hat{n}_q \quad , \text{ where } \hat{n}_q \text{ counts the \# particles in state } |q\rangle.$$

The number operator $\hat{n} = \hat{c}^\dagger \hat{c}$, where $\hat{c}$ = annihilation, $\hat{c}^\dagger$ = creation

Let's now define position-space operators at $x_\ell = \ell a_L$, where the centres of sites on the lattice, now taken to have M sites

$$\begin{cases} \hat{c}^\dagger_{k_n} = \dfrac{1}{\sqrt{M}} \displaystyle\sum_{\ell=1}^{M} e^{ik_n \cdot x_\ell} \hat{c}^\dagger_\ell \\ \hat{c}^\dagger_\ell = \dfrac{1}{\sqrt{M}} \displaystyle\sum_{n=1}^{M} e^{-ik_n \cdot x_\ell} \hat{c}^\dagger_{k_n} \end{cases}$$

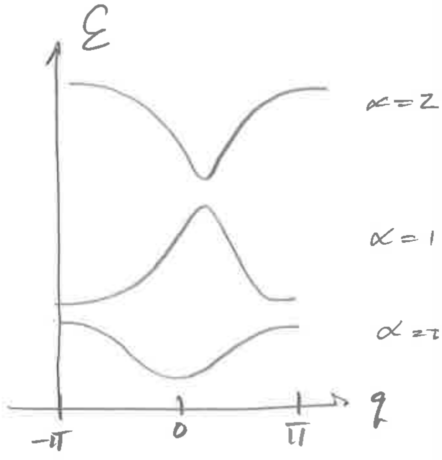
Here $x = \ell a_L$, and $k = (2\pi / M a_L)\, n$ or $q = \frac{2\pi}{M} n$

with max value $x_M = M a_L$. & $k_M = 2\pi$.

(Notice, $k_n \cdot x_\ell = (\ell a_L)(2\pi / M a_L)\, n = 2\pi \ell n / M$. Typical exponent in the discrete Fourier Transform.)

This unitary transformation preserves

$$\{\hat{c}^\dagger_r, \hat{c}_s\} = \delta_{rs}, \quad \{c^\dagger_r, c^\dagger_s\} = \{c_r, c_s\} = 0$$



Now consider the shape of the bands that we've been finding.
Since
- Periodic function of q, period 2π
- boundary conditions $d\mathcal{E}/dq = 0$

We can expand each band into a cosine series, $\mathcal{E}(q) = A + B\cos(q) + C\cos(2q) + \dots$

In fact we can show that the coefficients are the tunnelling rates between sites.

$$\mathcal{E}_\alpha(q) = -2\sum_{r=0}^{\infty} \underbrace{t_r^{(\alpha)}}_{\text{tunnel } r \text{ sites in } \alpha \text{ band.}} \cos(rq)$$

Dropping band index for simplicity:

$$\hat{H} = \sum_q \mathcal{E}(q)\,\hat{n}_q \quad , \text{ with } \hat{n}_q = \hat{c}_q^\dagger \hat{c}_q$$

$$= \sum_q \left(-2\sum_r t_r \cos(rq)\right)\left(\frac{1}{\sqrt{M}}\sum_{\ell=1}^{M} e^{iq x_\ell/a_L}\,\hat{c}^\dagger_{x_\ell}\right)\left(\frac{1}{\sqrt{M}}\sum_{\ell'=1}^{M} e^{-iq x'_{\ell'}/a_L}\,\hat{c}_{x'_\ell}\right)$$

collecting terms that depend on q, we have

$$\sum_q \left(e^{+iqr} + e^{-iqr}\right)\left(e^{iq(x_\ell - x'_\ell)/a_L}\right)$$

making the discrete q-sum explicit: $q = \frac{2\pi}{M}n$, $n: 0 \to M-1$,

so $\to \sum_{n=0}^{M-1} \exp\left[i2\pi(nr + \ell - \ell')/M\right] + \exp\left[i2\pi(-nr + \ell - \ell')/M\right]$

$$= M\,\delta_{\ell',\ell+r} + M\,\delta_{\ell',\ell-r} \qquad \text{since } -M < \ell - \ell' < M$$

Thus,

$$\hat{H} = -\sum_r t_r \sum_l \hat{c}_l^\dagger \hat{c}_{l+r} + h.c.$$

The simplest form of this is when only the nearest-neighbor hopping is nonzero, so-called "tight binding" (TB): then $t_1 = t$, and

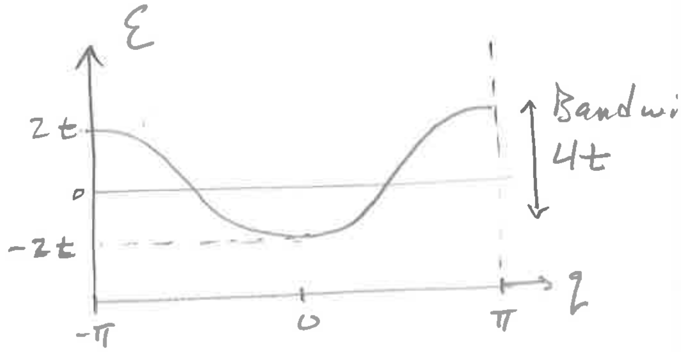
$$\hat{H} = -t \sum_l \hat{c}_l^\dagger \hat{c}_{l+1} + h.c.$$

Recall that we originally conjectured $\mathcal{E}_\alpha(q) = -2\sum_r t_r^{(\alpha)} \cos$

so here

$$\mathcal{E}(q) = -2t \cos q$$

Notice there is a constant shift here, so minimum is at $-2t$. This is dropping "t_0".



We'll make a lot of use of this TB dispersion relation.

Beyond TB, one can isolate each tunnelling coeffs from the dispersion relation/ band structure:

$$t_r^{(\alpha)} = -\frac{1}{2\pi} \int_{-\pi}^{\pi} dq \, \cos(rq) \, \mathcal{E}_\alpha(q)$$

|| THE $\{t_r\}$ ARE THE FOURIER COMPONENTS OF THE DISPERSION RELATION (OF THE BAND STRUCTURE). ||

Effective Mass

Let's apply our recipe for $\boxed{\mathcal{E}(q) \text{ dispersion}} \longrightarrow \boxed{t_r \text{ tunnelling}}$ to a few other dispersion relations you know. This helps us get a feeling for what t means.

Free particle: $\mathcal{E} = p^2/2m = \left(\frac{\hbar}{a_L} q\right)^2 / 2m$

Then $$t_1 = -\frac{1}{2\pi}\int_{-\pi}^{\pi} dq \, \cos(q) \cdot \frac{\hbar^2}{2m a_L^2} q^2 = \frac{\hbar^2}{2m a_L^2}$$

$$\left(\begin{array}{l} \text{and more generally, } \quad t_r = (-1)^{r+1} t_1 / r^2 , \quad r \geq 1 \\ \text{with an offset, } \quad t_0 = -\frac{\pi^2}{3} t_1 , \quad r = 0 \end{array} \right)$$

Turning this definition around, we can define an effective mass as

$$\frac{1}{m^*} = \frac{2 a_L^2}{\hbar^2} t \qquad \longleftrightarrow \qquad t = \frac{\hbar^2}{2 m a_L^2}$$

even when we don't have a free-particle dispersion. This provides a nice interpretation of the HM:

$$H_{HM} = \underbrace{-t \sum_{\ell} \hat{c}^{\dagger}_{\ell} \hat{c}_{\ell+1} + \text{h.c.}}_{\text{kinetic energy}} + \underbrace{U \sum \hat{n}_{\uparrow i} \hat{n}_{\downarrow i}}_{\text{interaction energy}}$$

with "t" telling us about $\frac{1}{m^*}$, inverse effective mass

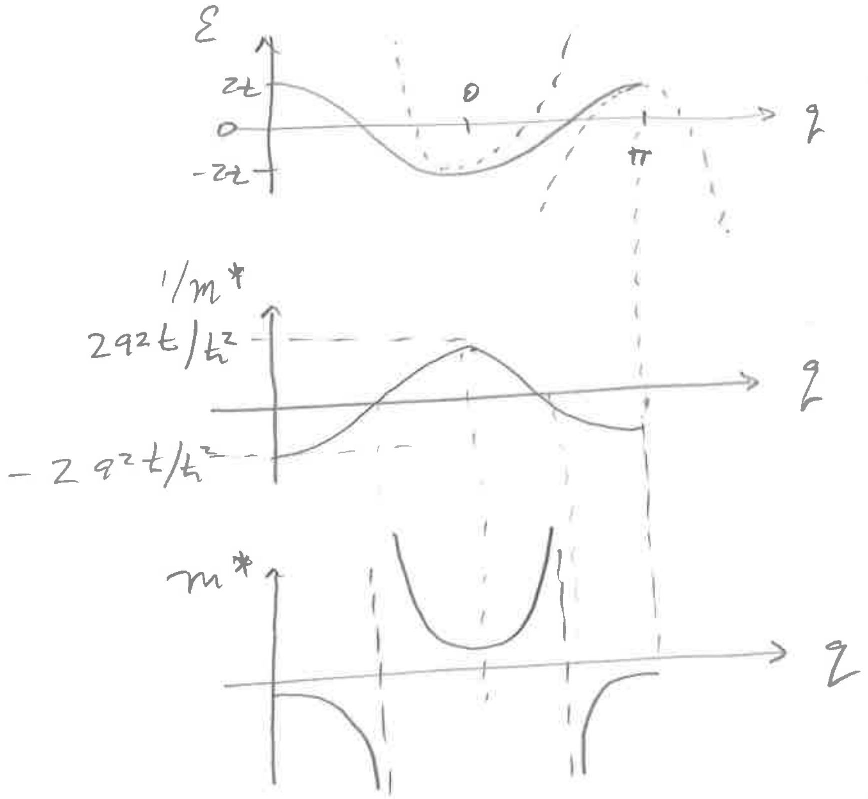
In fact, this is only the $q=0$ effective mass, in TB.
More generally, $\left.\frac{1}{m^*}\right|_q = \frac{a_L^2}{\hbar^2}\frac{\partial^2}{\partial q^2}\mathcal{E}(q)$

so that of $\mathcal{E} = -2\sum_r t_r \cos rq$

$$\left.\frac{1}{m^*}\right|_q = \frac{a_L^2}{\hbar^2}\sum_r 2 t_r\, r^2 \cos rq$$

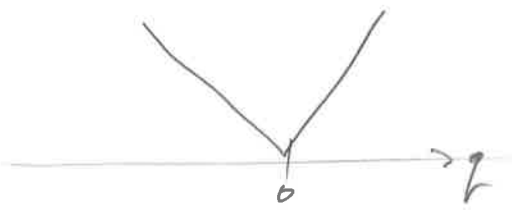
$$= \frac{2a_L^2}{\hbar^2}\left\{ t_1 \cos q + 4t_2 \cos 2q + 9 t_3 \cos 3q + \dots \right\}$$

Again taking $t = t_1$, & others zero, then



Effective mass diverges ($1/m^* = 0$) @ $q = \pm\pi/2$.
Quite relevant to DFG: at half filling, Fermi energy is located @ $q = \pi/2$!

Dirac dispersion



$$\mathcal{E} = c|p| = c\hbar^{-1} q_L |q|$$

Turn crank, to find $t_1 = 2/\pi$, $t_2 = 0$, $t_r = \frac{t_1}{r^2}$ for odd r

Now take sum: $\frac{1}{m^*(q=0)} = \frac{2 q_L^2}{\hbar^2} \sum_r t_r r^2 \to$ divergent

so that $1/m^* = \infty$ or, $\underline{\underline{m^* = 0}}$. Massless particles, as expected, @ $q=0$.

But this is a cautionary tale: the physics of your system may not, in fact, be well described by the tight binding approximation, that only includes nearest-neighbour hopping.

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btw: since $E_R = (\hbar^2/q_L^2 m)(\pi^2/2)$, another way to write the effective mass is in terms of $(t/E_R) = \frac{2 q_L^2}{\hbar^2} \frac{m}{\pi^2} t$, so that

$$\boxed{\frac{m}{m^*(q)} = \frac{1}{\pi^2} \sum_{r=1} \left(\frac{t_r}{E_R}\right) r^2 \cos(rq)}$$

now completely in terms of dimensionless ratios.