HW problem from "Conductivity Part 3"

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When U=0, the effects of the crystal disappear and there isn't any physical meaning to either the lattice spacing or the reciprocal lattice spacing. However, when intending to do perturbation theory, it's useful to pick the Bravais vectors $\mathbf{R}$ to match the crystal. In 1-D, $R = ma$ and their reciprocals are $\frac{2n\pi}{a}$ for integers m. This HW problem is all in 1D.

For every value of k (including negative values), the free Hamiltonian has one (unnormalized[1]) eigenfunction $\psi(x) = e^{ikx}$ with eigenvalue $E_k = \frac{\hbar^2 k^2}{2m}$.

Note that the following, for **positive** integers n, has the (unnormalized) Bloch form:

$$\psi_{nk}(x) = e^{ikx}\left[e^{i\left(2n\frac{\pi}{a}\right)x}\right]$$

where we identify $u_{nk}(x) = \frac{1}{\sqrt{2\pi}}e^{i\left(2n\frac{\pi}{a}\right)x}$. To prove this is of the Bloch form, we must show that $u_{nk}(x+R) = u_{nk}(x)$ where $R = ma$.

$$u_{nk}(x+R) = e^{i\left(2n\frac{\pi}{a}\right)(x+R)} = e^{i\left(2n\frac{\pi}{a}\right)(x+ma)} = e^{i\left(2n\frac{\pi}{a}\right)x}e^{i\left(2nma\frac{\pi}{a}\right)} = e^{i\left(2n\frac{\pi}{a}\right)x} = u_{nk}(x)$$

since $e^{i(2nm\pi)} = 1$. Notice that $\frac{2n\pi}{a}$ (for positive n) are reciprocal lattice vectors and usually written[2] K'. So what we've shown is that the above Bloch form looks like $e^{ikx}e^{iK'x} = e^{i(k+K')x}$ **but only for positive integers** n **– this will turn out to be an issue!**

It is customary to restrict the Bloch functions to a "canonical case" where (a) $-K/2 < k < K/2$ (a) $-K/2 < k < K/2$(a) $-K/2 < k < K/2$ and (b) there is exactly **one** eigenfunction for each combination (n, k). Does the

[1]The normalized functions require a factor of $\frac{1}{\sqrt{2\pi}}$.

[2]I'm using K' instead of K because I've reserved the symbol K to be equal $\frac{2\pi}{a}$.

above form meet that goal? First let's show that if there are two functions $\psi_{nk'}$ and ψ_{mk} such that $-K/2 < k, k' < K/2$, then those two functions be equal?. Solve

$$e^{i(k+2n\frac{\pi}{a})x} = e^{i(k'+2m\frac{\pi}{a})x},$$

Since the equation holds for all values of x, let $x = a$. then $e^{2in\pi} = e^{2in'\pi} = 1$ and we need only solve the equation

$$e^{ika} = e^{ik'a}$$

for $-K/2 < k, k' < K/2$, i.e. for $-\pi < ka, k'a < \pi$. But this can only be solved when $k = k'$. We've therefore proven that the set of solutions $e^{i(k+K')x}$ have the a canonical Bloch form and that for distinct values of the indices, the eigenfunctions are distinct. **However, these are NOT all the possible eigenfunctions.** The reason has to do with the fact that we've only allowed positive integers n for $\psi_{nk}(x)$. So, for example, consider the eigensolution $e^{ik'x}$ for $k' = -K/4 = -\pi/2a$. There is no combination of n and k (with positive n and $-K/2 < k < K/2$) so that $\psi_{nk}(x) = e^{-i\frac{\pi}{2}x}$. If there were, then we'd be able to show that $e^{i\left(k+2n\frac{\pi}{a}\right)x} = e^{ik'x}$. That is, we must solve $e^{i\left(k+2n\frac{\pi}{a}\right)x} = e^{-i\frac{\pi}{2a}x}$, which requires that $\left(2n+\frac{1}{2}\right)\frac{\pi}{a} = -k$ with $-\pi/a < k < \pi/a$. It's easy to see that there is no positive value of n which solves that equation.

1 Solution to HW problem

Start with the proposed set of (unnormalized) Bloch functions $\psi_{nk}(x) = e^{ikx}u_{nk}(x)$ where $(2\pi)^{\frac{1}{2}}\, u_{nk}(x) = e^{i\left(\mathrm{sgn}(k)(-1)^{n-1}\left[\frac{n}{2}\right]K\right)x}$.

- *First consider $n = 1$, and derive ψ_{1k}*

  $u_{1k}(x) = e^{i\left(\mathrm{sgn}(k)\frac{(n-1)K}{2}\right)x} = e^0 = 1$, so $\psi_{1k}(x) = e^{ikx}u_{1k}(x) = e^{ikx}$.

  Note that by our Brillouin-zone condition, $K/2 < k < K/2$.

- *Then apply the Hamiltonian operator to ψ_{1k} and show that $H\psi_{1k} = \frac{\hbar^2 k^2}{2m}\psi_{1k}$.*

$$
\begin{aligned}
H\psi_{1k} &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}e^{ikx} = -\frac{\hbar^2}{2m}\left[\frac{d}{dx}\left(ike^{ikx}\right)\right] \\
&= -\frac{\hbar^2}{2m}\left[ik\left(ik\frac{d}{dx}e^{ikx}\right)\right] = \frac{k^2\hbar^2}{2m}e^{ikx} \\
&= \frac{k^2\hbar^2}{2m}\psi_{1k}
\end{aligned}
$$

- *Since this is of the form $H\psi_{1k} = E\psi_{1k}$ say what the energy is as a function of k.*

  $E_k = \frac{k^2\hbar^2}{2m}$.

- *Compare to the standard form when $|k| < \frac{K}{2}$ to the lower half of the blue section*

  Look at the slide with title "Standard form" ψ_{1k} looks identical to the full blue part of the standard form (the blue part ranges from $-K$ to K.). Now look at the slide with title "Canonical form". ψ_{1k} looks identical to the lower half of the blue part of the canonical form (the lower blue part ranges from $-K/2$ to $K/2$.)

- *Now set $n = 2$ and derive ψ_{2k}.*

  $u_{2k}(x) = e^{i\left(\text{sgn}(k)(-1)^{2-1}\left[\frac{2}{2}\right]K\right)x} = e^{-i\ sgn(k)Kx}$, so

$$
\psi_{2k}(x) = e^{ikx}u_{2k}(x) = \begin{cases} e^{ikx}e^{-i\left(\frac{2\pi}{a}x\right)} = e^{i\left(k-\frac{2\pi}{a}\right)x} & \text{if } k > 0 \\ e^{ikx}e^{i\left(\frac{2\pi}{a}x\right)} = e^{i\left(k+\frac{2\pi}{a}\right)x} & \text{if } k < 0 \end{cases}
$$

- *Apply the Hamiltonian operator and, as before, derive the energy as a function of k.*

$$
\begin{aligned}
H\psi_{2k} &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}e^{i\left(k\pm\frac{2\pi}{a}\right)x} = \frac{\left(k\pm\frac{\pi}{a}\right)^2\hbar^2}{2m}e^{i\left(k\pm\frac{\pi}{a}\right)x} \\
&= \frac{\left(k\pm\frac{2\pi}{a}\right)^2\hbar^2}{2m}\psi_{2k}
\end{aligned}
$$

  so that $E_k = \frac{\left(k\pm\frac{2\pi}{a}\right)^2\hbar^2}{2m}$ where the $\pm$ sign is according to whether k is negative or positive.

- *Compare the upper blue graph (in the canonical form) to the standard form – but when $\frac{K}{2} < |k| < K$.*

From this we see that in the canonical form, when k ranges from 0 to $K/2$, the energy ranges from $4\left(\frac{\pi}{a}\hbar\right)^2$ to $\left(\frac{\pi}{a}\hbar\right)^2$ and also when k ranges from 0 to $-K/2$, the energy ranges from $4\left(\frac{\pi}{a}\hbar\right)^2$ to $\left(\frac{\pi}{a}\hbar\right)^2$.

On the other hand, in the standard form where $E_k = \frac{k^2\hbar^2}{2m}$ for all k, we see that when k ranges from $\pm K/2$ to $\pm K$, the energy ranges from $\left(\frac{\pi}{a}\hbar\right)^2$ to $4\left(\frac{\pi}{a}\hbar\right)^2$.

- *Pick some other random n (less than 5) to see how the rest of the graph works.*

  I'll leave the details to the "reader". However, for grins I'll summarize for $n = 3$.

  $u_{3k}(x) = e^{i\ sgn(k)Kx}$, so

$$\psi_{3k}(x) = e^{ikx}u_{3k}(x) = \begin{cases} e^{i\left(k+\frac{2\pi}{a}\right)x} & \text{if } k > 0 \\ e^{i\left(k-\frac{2\pi}{a}\right)x} & \text{if } k < 0 \end{cases}$$

$$\begin{aligned} H\psi_{3k} &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}e^{i\left(k\pm\frac{2\pi}{a}\right)x} = \frac{\left(k\pm\frac{\pi}{a}\right)^2\hbar^2}{2m}e^{i\left(k\pm\frac{\pi}{a}\right)x} \\ &= \frac{\left(k\pm\frac{2\pi}{a}\right)^2\hbar^2}{2m}\psi_{2k} \end{aligned}$$

  so that $E_k = \frac{\left(k\pm\frac{2\pi}{a}\right)^2\hbar^2}{2m}$ where the $\pm$ sign is according to whether k is positive or negative.

  In the canonical form, when k ranges from 0 to $\pm K/2$, the energy ranges from $4\left(\frac{\pi}{a}\hbar\right)^2$ to $9\left(\frac{\pi}{a}\hbar\right)^2$.

  in the standard form where $E_k = \frac{k^2\hbar^2}{2m}$ for all k, we see that when k ranges from $\pm K$ to $\pm\frac{3}{2}K$, the energy ranges from $4\left(\frac{\pi}{a}\hbar\right)^2$ to $9\left(\frac{\pi}{a}\hbar\right)^2$.