33-755 Homework 9

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1 Schrodinger Equation for Bloch Function

The time independent Schrödinger equation for the Hamiltonian

$$\hat{\mathbf{H}} = \frac{\hat{\mathbf{P}}^2}{2m} + V(x),$$

with periodic potential $V(x+a) = V(x)$, has solutions of the form

$$\varphi(x) = e^{\imath qx} u_q(x)$$

where $u_q(x+a) = u_q(x)$ is periodic with the same periodicity as V. This function $u_q(x)$ obeys a Schrödinger equation with Hamiltonian H_q that depends on the Bloch index q. Determine H_q.

We can solve this problem by plugging the solution into the Schrödinger equation:

$$\begin{aligned}\hat{\mathbf{H}} e^{\imath qx} u_q(x) &= -\frac{\hbar^2}{2m}\partial_x^2 e^{\imath qx} u_q(x) + V(r) e^{\imath qx} u_q(x) \\ &= -\frac{\hbar^2}{2m}\left(-e^{\imath qx} q^2 u_q(x) + 2\imath q e^{\imath qx}\partial_x u_q(x) + e^{\imath qx}\partial_x^2 u_q(x)\right) + V(r) e^{\imath qx} u_q(x)\end{aligned}$$

Dividing out the exponential, we find the following equation for $u_q(x)$:

$$H_q u_q(x) = \left(\frac{\hbar^2 q^2}{2m} + V(r)\right) u_q(x) - \frac{\imath\hbar^2 q}{m}\partial_x u_q(x) - \frac{\hbar^2}{2m}\partial_x^2 u_q(x)$$

Writing this in terms of momentum operators, we find:

$$\hat{\mathbf{H}}_q = \frac{\hbar q \hat{\mathbf{P}}}{m} + \frac{\hat{\mathbf{P}}^2}{2m} + \left(V(r) + \frac{\hbar^2 q^2}{2m}\right)$$

2 The Kronig-Penney Model

The Kronig-Penney model is a model for electrons in crystalline solids. The square wells have width a and height V_0, and are placed periodically at intervals L, extending to $\pm\infty$. An electron of mass m and energy E is present.

(a) Determine the matrix M that relates the coefficients of plane waves $e^{\pm\imath kx}$ in one valley (region where $V(x) = 0$) to the next.

I will set up our potential as follows:

$$V = \begin{cases} 0 & x < -\frac{a}{2} \\ V_0 & -\frac{a}{2} < x < \frac{a}{2} \\ 0 & \frac{a}{2} < x \end{cases}$$

In these regions, the wave function can be described as

$$\psi(x) = \begin{cases} Ae^{\imath kx} + Be^{-\imath kx} & x < -\frac{a}{2} \\ Ce^{\imath k'x} + De^{-\imath k'x} & -\frac{a}{2} < x < \frac{a}{2} \\ Fe^{\imath kx} + Ge^{-\imath kx} & \frac{a}{2} < x \end{cases}$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$ and $k' = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$.
Let's first compute the matching conditions at $x = -\frac{a}{2}$. Continuity of the wave function implies

$$Ae^{-\imath k\frac{a}{2}} + Be^{\imath k\frac{a}{2}} = Ce^{-\imath k'\frac{a}{2}} + De^{\imath k'\frac{a}{2}}$$

Continuity of the derivative implies

$$kAe^{-\imath k\frac{a}{2}} - kBe^{\imath k\frac{a}{2}} = qCe^{-\imath k'\frac{a}{2}} - qDe^{\imath k'\frac{a}{2}}$$

We can describe these equations in terms of matrices:

$$P\begin{pmatrix} A \\ B \end{pmatrix} = Q\begin{pmatrix} C \\ D \end{pmatrix}$$

where

$$P = \begin{pmatrix} e^{-\imath k\frac{a}{2}} & e^{\imath k\frac{a}{2}} \\ ke^{-\imath k\frac{a}{2}} & -ke^{\imath k\frac{a}{2}} \end{pmatrix}$$

and

$$Q = \begin{pmatrix} e^{-\imath k'\frac{a}{2}} & e^{\imath k'\frac{a}{2}} \\ k'e^{-\imath k'\frac{a}{2}} & -k'e^{\imath k'\frac{a}{2}} \end{pmatrix}$$

We see that a transfer matrix is formed from the valley to inside the barrier: $M = P^{-1} \cdot Q$. We can use time-reversal symmetry to calculate the other half of the transfer function, from the barrier to the next valley.

$$\begin{aligned} M &= P^{-1} \cdot Q \cdot (Q^*)^{-1} \cdot P^* \\ &= \begin{pmatrix} e^{\imath ka}\left(\cos(k'a) - \imath\frac{(k^2+k'^2)\sin(k'a)}{2kk'}\right) & \imath\frac{(k^2-k'^2)\sin(k'a)}{2kk'} \\ -\imath\frac{(k^2-k'^2)\sin(k'a)}{2kk'} & e^{-\imath ka}\left(\cos(k'a) + \imath\frac{(k^2+k'^2)\sin(k'a)}{2kk'}\right) \end{pmatrix} \end{aligned}$$

(b) What condition must M satisfy in order for a propagating solution to exist?

M can be written as

$$M = \begin{pmatrix} \gamma & \delta^* \\ \delta & \gamma^* \end{pmatrix}$$

and

$$\begin{pmatrix} A \\ B \end{pmatrix} = M\begin{pmatrix} F \\ G \end{pmatrix}$$

To conserve the probability current, we want

$$|A|^2 - |B|^2 = |F|^2 - |G|^2$$

and using the above relation

$$|F|^2 - |G|^2 = (\gamma A + \delta^* B)(\gamma^* A^* + \delta B^*) - (\delta A + \gamma^* B)(\delta^* A^* + \gamma B^*)$$
$$= (|\gamma|^2 - |\delta|^2)(|A|^2 - |B|^2)$$

We want these to be equal, so

$$|\gamma|^2 - |\delta|^2 = 1$$

but this is just the determinant of M, so the condition to have a propagating solution is

$$\det(M) = 1$$

(c) Sketch the function $E(q)$ up to and slightly beyond the first band gap, taking $a = 2$, $L = 4$, $V_0 = \frac{\pi^2}{4}$, and setting $\frac{\hbar^2}{2m} = 1$. Here q is the wavenumber of the Bloch function that obeys $\varphi_q(L+x)/\varphi_q(x) = e^{\imath qL}$.

Now I will rephrase the problem by shifting the potential by $\frac{a}{2}$. The potential is infinitely periodic, so I am not changing anything by doing this. At $x = 0$, the wave function and its derivative are continuous, but now the system is slightly simpler:

$$A + B = C + D$$

and

$$k(A - B) = k'(C - D)$$

Next, we look at $x = L - a$. I found that in the end, when I solved this system, it simplified better if I rename this $L - a = b$ and then substitute back afterwards. On this boundary, we need to take into account the Bloch theorem condition

$$\varphi(-a)e^{\imath qL} = \varphi(L - a)$$
$$\varphi'(-a)e^{\imath qL} = \varphi'(L - a)$$

so

$$Ae^{\imath kb} + Be^{-\imath kb} = (Ce^{-\imath k'a} + De^{\imath k'a})e^{\imath qL}$$

and

$$k(Ae^{\imath kb} - Be^{-\imath kb}) = k'((Ce^{-\imath k'a} - De^{\imath k'a}))e^{\imath qL}$$

I solved this system using Mathematica and a bit of by-hand adjustment afterwards to get

$$\frac{(k-k')^2}{4kk'}\cos(k(L-a) - k'a) - \frac{(k+k')^2}{4kk'}\cos(k(L-a) + k'a) = \cos(qL)$$

I used the following Python code to graphically plot solutions to this system. This runs over a set of values for k and checks to see if they result in the left-hand side of the equation above gives an acceptable value. We require both sides of this equation to be bounded between -1 and $+1$ since we don't want imaginary q, so the cosine must be bounded.

```
import numpy as np
import matplotlib.pyplot as plt

a = 2
L = 4
b = L - a
V = np.pi * np.pi / 4


def kprime(k):
```

```
    k = k + 0j
    return np.sqrt(k * k - V)


def E(k):
    return k * k


def FofQ(k):
    k = k + 0j
    return np.real(
        (
            (k - kprime(k)) * (k - kprime(k)) * np.cos(b * k - a * kprime(k))
            -(k + kprime(k)) * (k + kprime(k)) * np.cos(b * k + a * kprime(k))
        )
        / (4 * k * kprime(k))
    )


ks = np.linspace(0.1, 4, 100000)
qs = np.zeros(len(ks))
for i in range(len(ks)):
    f = FofQ(ks[i])
    if np.abs(f) < 1:
        qs[i] = np.arccos(f) / L
    else:
        qs[i] = np.nan

plt.figure(figsize=(3, 6))
plt.plot(qs, E(ks))
plt.title("Kronig-Penney Model")
plt.xlabel("Bloch Wavenumber")
plt.ylabel("Allowed Energies")
plt.show()
```

This produced the attached figure found at the end of this document.

(d) Notice the discontinuities in your function that correspond to “forbidden energies”. What would happen if an electron with forbidden energy were incident on a crystal with this potential energy function?

Such an electron would be completely reflected off of the crystal. These forbidden regions cannot support the wave function, so it must destructively interfere inside, and there is no mechanism in this model for absorbing the energy from the electron, therefore it must be reflected.

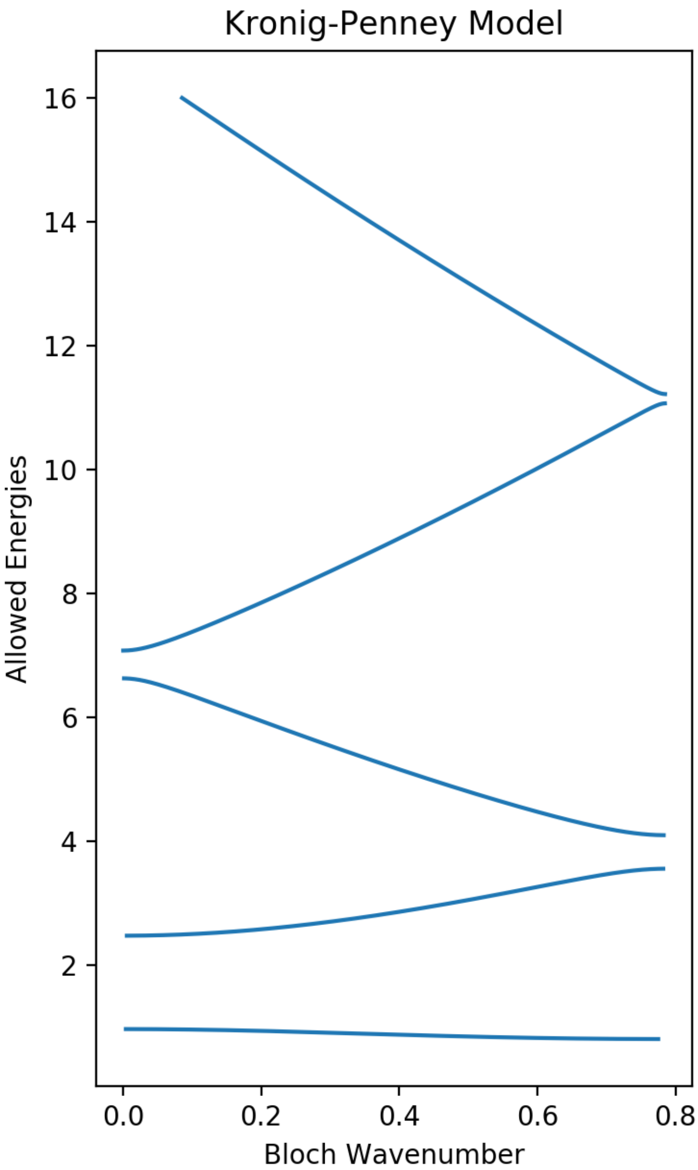

Figure 2.1: Band Structure of the Kronig-Penney Model