PH4101 Assignment — 3
22MS037

Problem 1 — Kronig Penny Model

a) Done in Class.

b) The Kronig Penny Dispersion relation is given by

$$\cos(ka) = \cos(\alpha(a-b))\cosh(\beta b) + \left(\frac{\alpha^2 - \beta^2}{2\alpha\beta}\right)\sinh(\beta b)\sin(\alpha(a-b)) \tag{1}$$

where $\alpha = \sqrt{(2mE)/(\hbar^2)}$ and $\beta = \sqrt{(2m(U-E))/(\hbar^2)}$.

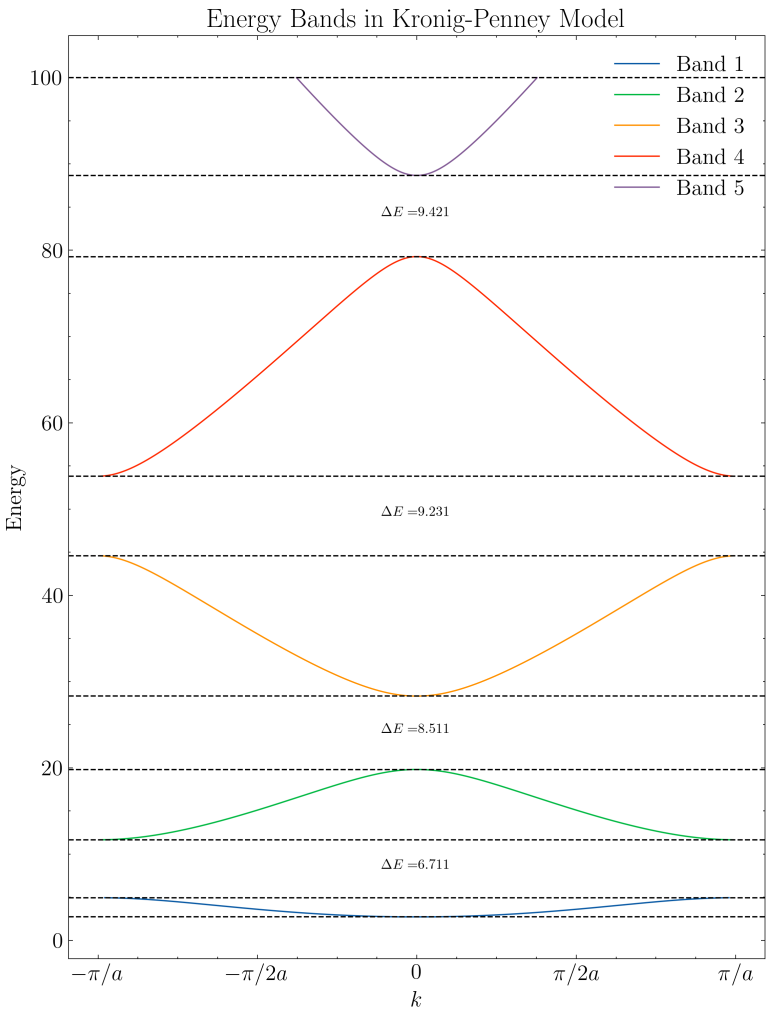

Figure 1: The bands in the Kronig Penny Model

c) In the limiting case when $b \longrightarrow 0$ and $E \longrightarrow \infty$ such that $V_0 = Ub$ is constant, we have,

$$\begin{aligned}\beta &= \sqrt{\frac{2m(U-E)}{\hbar^2}} \approx \sqrt{\frac{2mU}{\hbar^2}} = q \\ \beta b &= \sqrt{\frac{2m(U-E)b^2}{\hbar^2}} \longrightarrow 0\end{aligned} \tag{2}$$

Then we can approximate the hyperbolic functions as

$$\begin{aligned}\cosh(\alpha b) &\approx 1 \\ \sinh(\alpha b) &\approx \alpha b\end{aligned} \tag{3}$$

Then the dispersion relation becomes,

$$\begin{aligned}\cos(ka) &= \cos(\alpha a) + \frac{1}{2\alpha}\sqrt{\frac{2mU}{\hbar^2}}(\beta b)\sin(\alpha a) \\ &= \cos(\alpha a) + \frac{mV_0}{\hbar^2\alpha}\sin(\alpha a)\end{aligned} \tag{4}$$

Note that if the RHS in the dispersion relation is greater than 1 or less than -1, there are no real solutions for k. However, if we allow for complex K, we can find solutions in these regions as well.

Problem 2 — 2D tight binding

The tight binding Hamiltonian for a two- dimensional square lattice is given by

$$H = -t\sum_{n,m}[|m+1,n\rangle\langle m,n| + |m,n+1\rangle\langle m,n| + h.c.] + \epsilon_0\sum_{n,m}|m,n\rangle\langle m,n| \tag{5}$$

a) Using Bloch's theorem, the Bloch states are given by

$$|\psi(\boldsymbol{k})\rangle = \frac{1}{\sqrt{N}}\sum_{n,m} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{m,n}}|m,n\rangle \text{ where } \boldsymbol{r}_{m,n} = ma\hat{x} + na\hat{y} \tag{6}$$

where $|m,n\rangle$ are the orthonormal localized basis states at site (m,n) and N is the total number of lattice sites. The basis states satisfy the orthonormality condition $\langle m',n',m,n|m',n',m,n\rangle = \delta_{m',m}\delta_{n',n}$. Using these states we can evaluate the action of the Hamiltonian on the bloch states. Let's consider the hopping term in the x direction first,

$$
\begin{aligned}
-t\sum_{n,m}[|m+1,n\rangle\langle m,n| + h.c.]|\psi(\boldsymbol{k})\rangle &= -t\sum_{n,m}[|m+1,n\rangle\langle m,n|\psi(\boldsymbol{k})\rangle + |m,n\rangle\langle m+1,n|\psi(\boldsymbol{k})\rangle] \\
&= -t\sum_{n,m}\left[|m+1,n\rangle\left(\frac{1}{\sqrt{N}}\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{m,n}} + |m,n\rangle\left(\frac{1}{\sqrt{N}}\right)e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{m+1,n}}\right] \\
&= -t\left(\frac{1}{\sqrt{N}}\right)\sum_{n,m}\left[e^{i\boldsymbol{k}\cdot(m+1)a\hat{x}+na\hat{y}} + e^{i\boldsymbol{k}\cdot(m)a\hat{x}+na\hat{y}}e^{ik_x a}\right]|m,n\rangle \quad (7) \\
&= -t\left(e^{ik_x a} + e^{-ik_x a}\right)\left(\frac{1}{\sqrt{N}}\right)\sum_{n,m}e^{i\boldsymbol{k}\cdot\boldsymbol{r}_{m,n}}|m,n\rangle \\
&= -2t\cos(k_x a)|\psi(\boldsymbol{k})\rangle
\end{aligned}
$$

Similarly, for the hopping term in the y direction, we have

$$-t\sum_{n,m}[|m,n+1\rangle\langle m,n| + h.c.]|\psi(\boldsymbol{k})\rangle = -2t\cos\left(k_y a\right)|\psi(\boldsymbol{k})\rangle \quad (8)$$

The on-site potential term gives

$$\epsilon_0\sum_{n,m}|m,n\rangle\langle m,n||\psi(\boldsymbol{k})\rangle = \epsilon_0|\psi(\boldsymbol{k})\rangle \quad (9)$$

The Time independent Schrodinger equation $H|\psi(\boldsymbol{k})\rangle = E(\boldsymbol{k})|\psi(\boldsymbol{k})\rangle$ then gives us the following equation,

$$E(\boldsymbol{k})|\psi(\boldsymbol{k})\rangle = \left[-2t\cos(k_x a) - 2t\cos\left(k_y a\right) + \epsilon_0\right]|\psi(\boldsymbol{k})\rangle \quad (10)$$

This gives us the dispersion relation for the two dimensional tight binding model as

$$E(\boldsymbol{k}) = \epsilon_0 - 2t\left[\cos(k_x a) + \cos\left(k_y a\right)\right] \quad (11)$$

The Equal energy contours can be found by solving the equation

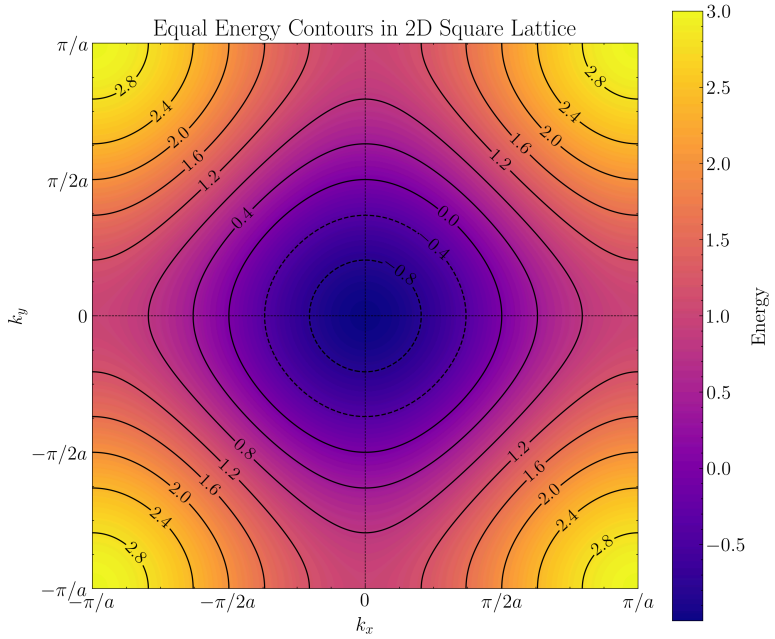

Figure 2: Equal energy contours for the 2D tight binding model at various energies

b) The density of states can be found out using the formula,

$$g(E) = \frac{1}{(2\pi)^2}\int_{BZ} d^2\boldsymbol{k}\delta(E - E(\boldsymbol{k})) \tag{12}$$

The integral is over the first Brillouin zone given by $-\frac{\pi}{a} \leq k_x, k_y \leq \frac{\pi}{a}$. The dispersion relation is given by,

$$\begin{aligned}\delta(E - E(\boldsymbol{k})) &= \delta\big(E - \epsilon_0 + 2t\big[\cos(k_x a) + \cos\big(k_y a\big)\big]\big) \\ &= \frac{1}{2t}\delta\big(\mathrm{E} - \cos(k_x a) - \cos\big(k_y a\big)\big) \text{ where } \mathrm{E} = \frac{\epsilon_0 - E}{2t}\end{aligned} \tag{13}$$

Now change the variables of integration from k_x, k_y to $x = k_x a, y = k_y a$. The limits of integration change from $-\pi$ to π. Also note that both $\cos(.)$ and $\delta(.)$ are symmetric functions. The density of states becomes

$$\begin{aligned}g(E) &= \frac{1}{(2\pi a)^2}\left(\frac{1}{2t}\right)\int_{-\pi}^{\pi} dx \int_{-\pi}^{\pi} dy \delta(\mathrm{E} - \cos(x) - \cos(y)) \\ &= \frac{1}{(2\pi a)^2}\left(\frac{1}{2t}\right)\int_{-\pi}^{\pi} dx \int_{-\pi}^{\pi} dy \delta(\cos(y) - (\mathrm{E} - \cos(x))) \\ &= \frac{1}{(2\pi a)^2}\left(\frac{2}{t}\right)\int_{0}^{\pi} dx \left[\frac{1}{|\sin(y_0)|}\right] \text{ where } y_0 = \arccos(\mathrm{E} - \cos(x)) \\ &= \frac{1}{(2\pi a)^2}\left(\frac{2}{t}\right)\int_{0}^{\pi} dx \left[\frac{1}{\sqrt{1 - (\mathrm{E} - \cos(x))^2}}\right]\Theta(1 - |\mathrm{E} - \cos(x)|)\end{aligned} \tag{14}$$

where $\Theta(.)$ is the Heaviside step function which is required since the $\arccos(.)$ function is only defined for inputs between -1 and 1. Using a variable $z = \cos(x)$, we can write the density of states as

$$\begin{aligned}g(E) &= \frac{1}{(2\pi a)^2}\left(\frac{2}{t}\right)\int_{-1}^{1} \frac{dz}{\sqrt{1 - z^2}\sqrt{1 - (\mathrm{E} - z)^2}}\Theta(1 - |\mathrm{E} - z|) \\ &= \frac{1}{(2\pi a)^2}\left(\frac{2}{t}\right)\int_{\max(-1, \mathrm{E}-1)}^{\min(1, \mathrm{E}+1)} \frac{dz}{\sqrt{1 - z^2}\sqrt{1 - (\mathrm{E} - z)^2}}\end{aligned} \tag{15}$$

and $g(E) = 0$ otherwise. The integral can be evaluated in terms of elliptic integrals. The final expression for the density of states is given by

$$\begin{gathered}g(E) = \frac{1}{2\pi^2 a^2 t} K\left(\frac{\sqrt{4 - \mathrm{E}^2}}{2}\right) \text{ for } |\mathrm{E}| \leq 2 \\ g(E) = 0 \text{ otherwise}\end{gathered} \tag{16}$$

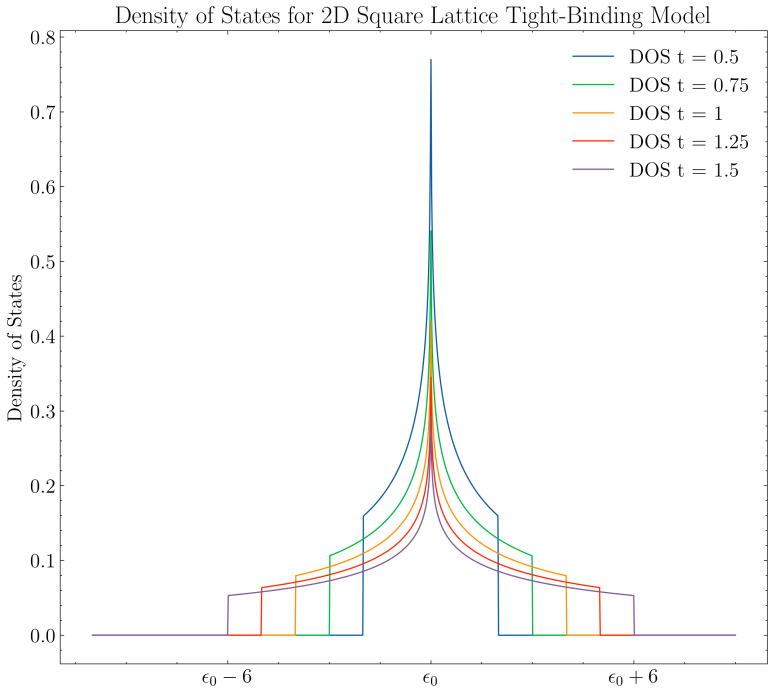

Figure 3: Density of states for the 2D tight binding model

We can observe from the plot, that the Van Hove singularities take place at E = 0 or $E = \epsilon_0$. At these energies, the density of states diverges logarithmically.

c) We now need to find the Fermi momentum and Fermi energy. Note the transformation from $\boldsymbol{k} = (k_x, k_y)$ to $\boldsymbol{k}' = \left(k_x + \frac{\pi}{a}, k_y + \frac{\pi}{a}\right)$ changes the energy as

$$\begin{aligned} E(\boldsymbol{k}') &= \epsilon_0 - 2t\left[\cos\left(\left(k_x + \frac{\pi}{a}\right)a\right) + \cos\left(\left(k_y + \frac{\pi}{a}\right)a\right)\right] \\ &= \epsilon_0 - 2t\left[-\cos(k_x a) - \cos\left(k_y a\right)\right] = 2\epsilon_0 - E(\boldsymbol{k}) \end{aligned} \tag{17}$$

We will now show that the DOS is symmetric about $E = \epsilon_0$. This allows us to obtain the Fermi energy and momentum without calculating the total number of states explicitly. The density of states is given by

$$\begin{aligned} g(E) &= \frac{1}{(2\pi)^2}\int_{BZ} d^2\boldsymbol{k}\,\delta(E - E(\boldsymbol{k})) \\ &= \frac{1}{(2\pi)^2}\int_{BZ} d^2\boldsymbol{k}'\,\delta(E - (2\epsilon_0 - E(\boldsymbol{k}'))) \text{ where } \boldsymbol{k}' = \left(k_x + \frac{\pi}{a}, k_y + \frac{\pi}{a}\right) \\ &= \frac{1}{(2\pi)^2}\int_{BZ} d^2\boldsymbol{k}'\,\delta((2\epsilon_0 - E) - E(\boldsymbol{k}')) \\ &= g(2\epsilon_0 - E) \end{aligned} \tag{18}$$

Let's consider the fully filled band case first. Here, the Fermi energy E_F is at the top of the band. The maximum energy in the band is given by

$$E_{\max} = \epsilon_0 - 2t[\cos(\pi) + \cos(\pi)] = \epsilon_0 + 4t \tag{19}$$

We also get

$$2N = \int_{\epsilon_0-4t}^{\epsilon_0+4t} g(E)dE = \int_{\epsilon_0}^{\epsilon_0+4t} g(E)dE + \int_{\epsilon_0-4t}^{\epsilon_0} g(E)dE \tag{20}$$

Using the symmetry of the DOS about $E = \epsilon_0$, we have

$$\int_{\epsilon_0-4t}^{\epsilon_0} g(E)dE = \int_{\epsilon_0}^{\epsilon_0+4t} g(E)dE \tag{21}$$

Therefore, we have,

$$\begin{aligned} 2N &= 2\int_{\epsilon_0-4t}^{\epsilon_0} g(E)dE \\ \implies N &= \int_{\epsilon_0-4t}^{\epsilon_0} g(E)dE \end{aligned} \tag{22}$$

Comparing this with the half filled case, we see that the Fermi energy for the half filled case is given by

$$E_F = \epsilon_0 \tag{23}$$

The corresponding Fermi momentum can be found by solving the equation,

$$\begin{aligned} E_F &= \epsilon_0 - 2t\left[\cos\left(k_{F_x}a\right) + \cos\left(k_{F_y}a\right)\right] \\ \implies \cos\left(k_{F_x}a\right) &+ \cos\left(k_{F_y}a\right) = 0 \end{aligned} \tag{24}$$

Within the first Brillouin zone, the Fermi surface is given by the square connecting the points $\left(\pm\frac{\pi}{a}, 0\right)$ and $\left(0, \pm\frac{\pi}{a}\right)$, which is given by the 4 equations,

$$\begin{aligned} k_{F_y} &= \pm\left(\frac{\pi}{a} - k_{F_x}\right) \text{ for } 0 \leq k_{F_x} \leq \frac{\pi}{a} \\ k_{F_y} &= \pm\left(-\frac{\pi}{a} - k_{F_x}\right) \text{ for } -\frac{\pi}{a} \leq k_{F_x} \leq 0 \end{aligned} \tag{25}$$

The Fermi surface is shown below.

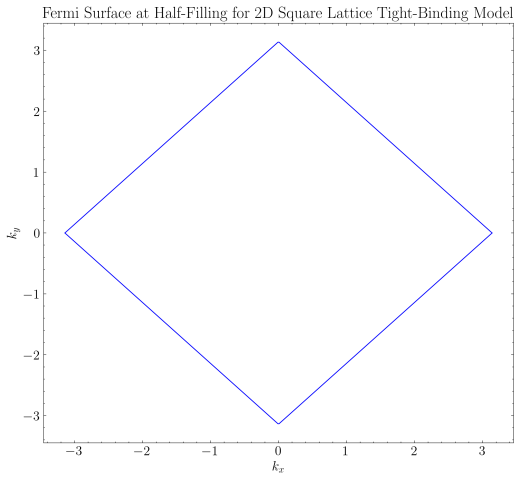

Figure 4: Fermi surface for the half filled 2D tight binding model

Problem 3 — Tight Binding with Staggered Potential

The Hamiltonian for a one dimensional with staggered potential is given by

$$H = -t\sum_n [|n\rangle\langle n+1| + h.c.] + U\sum_n |n\rangle\langle n| + V\sum_n (-1)^n |n\rangle\langle n| \tag{26}$$

We divide the chain into two sublattices A and B such that even sites belong to A and odd sites belong to B. All "A" sites have on-site potential $U+V$ and all "B" sites have on-site potential $U-V$. One other change takes place, the periodicity of the lattice changes from a to $2a$. This makes the unit cell contain two sites, one from sublattice A and one from sublattice B.

We can now rewrite the Hamiltonian as

$$\begin{aligned} H = -t\sum_n \Bigg[\underbrace{|n\rangle_A\langle n|_B + h.c.}_{1} + \underbrace{|n+1\rangle_B\langle n|_A + h.c.}_{2} \Bigg] \\ + \sum_n \Bigg[\underbrace{(U+V)|n\rangle_A\langle n|_A}_{3} \Bigg] + \sum_n \Bigg[\underbrace{(U-V)|n\rangle_B\langle n|_B}_{4} \Bigg] \end{aligned} \tag{27}$$

where n_A and n_B denote the site index for sublattice A and B respectively. The terms (1) and (2) denote hopping between A and B sublattices while terms (3) and (4) denote on-site potentials for A and B sublattices respectively. (1) and (2) are hopping terms where (1) denotes hopping from A to B within the same unit cell while (2) denotes hopping from B to A in the next unit cell.

a) We now need to find the dispersion relation for this system. To do this, we write the Hamiltonian in the k-space basis. The position basis states can be written in terms of the k-space basis states as

$$|n\rangle_A = \left(\frac{1}{\sqrt{N/2}}\right)\sum_k e^{-ikn(2a)}|k\rangle_A \tag{28}$$

$$|n\rangle_B = \left(\frac{1}{\sqrt{N/2}}\right)\sum_k e^{-ikn(2a)}|k\rangle_B \tag{29}$$

where N is the total number of sites in the chain. Using these relations, we can rewrite each term in the Hamiltonian in the k-space basis. To do this we consider the Hamiltonian term by term. Note that there are only two types of terms: terms between same index sublattices and terms between different index sublattices. Terms (1), (3) and (4) are between same index sublattices while term (2) is between different index sublattices.

Term (1):

$$\begin{aligned} T_1 &= -t\sum_n [|n\rangle_A\langle n|_B + |n\rangle_B\langle n|_A] \\ &= -t\sum_{k,k'}\left[\left(\frac{1}{\sqrt{N/2}}\right)\sum_n e^{-i(k-k')n(2a)}\right]|k\rangle_A\langle k'|_B + h.c. \\ &= -t\sum_{k,k'}\left[\delta_{k,k'}\right]|k\rangle_A\langle k'|_B + h.c. \\ &= -t\sum_k [|k\rangle_A\langle k|_B + |k\rangle_B\langle k|_A] \end{aligned} \tag{30}$$

Term (2):

$$\begin{aligned} T_2 &= -t\sum_n [|n+1\rangle_B\langle n|_A + |n\rangle_A\langle n+1|_B] \\ &= -t\sum_{k,k'}\left[\left(\frac{1}{\sqrt{N/2}}\right)\sum_n e^{-i(k-k')n(2a)}e^{-ik'(2a)}\right]|k\rangle_B\langle k'|_A + h.c. \\ &= -t\sum_{k,k'}\left[\delta_{k,k'}e^{-ik'(2a)}\right]|k\rangle_B\langle k'|_A + h.c. \\ &= -t\sum_k \left[e^{-ik(2a)}|k\rangle_B\langle k|_A + e^{ik(2a)}|k\rangle_A\langle k|_B\right] \end{aligned} \tag{31}$$

The Hamiltonian (27) can then be written in the k-space basis as

$$\begin{aligned} H = \sum_k \big[&-t\big(1+e^{-ik(2a)}\big)|k\rangle_B\langle k|_A - t\big(1+e^{ik(2a)}\big)|k\rangle_A\langle k|_B \\ &+(U+V)|k\rangle_A\langle k|_A + (U-V)|k\rangle_B\langle k|_B\big] \end{aligned} \tag{32}$$

Note that $\left(1+e^{\pm ik(2a)}\right) = 2\cos(ka)e^{\pm ika}$. Using this, we can write the Hamiltonian as,

$$\begin{aligned} H(k) = \sum_k \big[&-2t\cos(ka)e^{-ika}|k\rangle_B\langle k|_A - 2t\cos(ka)e^{ika}|k\rangle_A\langle k|_B \\ &+(U+V)|k\rangle_A\langle k|_A + (U-V)|k\rangle_B\langle k|_B\big] \end{aligned} \tag{33}$$

Note in our unit cell, we have two basis states, $|k\rangle_B$ and $|k\rangle_A$. Therefore, the Hamiltonian can be represented as a 2×2 matrix in this basis $\{|k\rangle_B, |k\rangle_A\}$ as

$$\begin{aligned} H &= \sum_k (|k\rangle_B \;\; |k\rangle_A) H(k) \begin{pmatrix} |k\rangle_B \\ |k\rangle_A \end{pmatrix} \text{ where} \\ H(k) &= \begin{pmatrix} U-V & -2t\cos(ka)e^{ika} \\ -2t\cos(ka)e^{-ika} & U+V \end{pmatrix} \end{aligned} \tag{34}$$

The dispersion relates the energy eigenvalues $E(k)$ of the Hamiltonian $H(k)$ to the momentum k. To find the energy eigenvalues, we need to solve the characteristic equation given by

$$\det(H(k) - E\mathbb{I}) = 0 \tag{35}$$

We obtain,

$$\begin{aligned} &\begin{vmatrix} U-V-E & -2t\cos(ka)e^{ika} \\ -2t\cos(ka)e^{-ika} & U+V-E \end{vmatrix} = 0 \\ \implies &(U+V-E)(U-V-E) - 4t^2\cos^2(ka) = 0 \\ \implies &(U-E)^2 - V^2 - 4t^2\cos^2(ka) = 0 \\ \implies &E(k) = U \pm \sqrt{V^2 + 4t^2\cos^2(ka)} \end{aligned} \tag{36}$$

b) The Brillouin zone for this system is given by $-\frac{\pi}{2a} \leq k \leq \frac{\pi}{2a}$. This is smaller than the original Brillouin zone $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$ due to the doubling of the unit cell size from a to $2a$. The energy levels in the Brillouin zone are shown below.

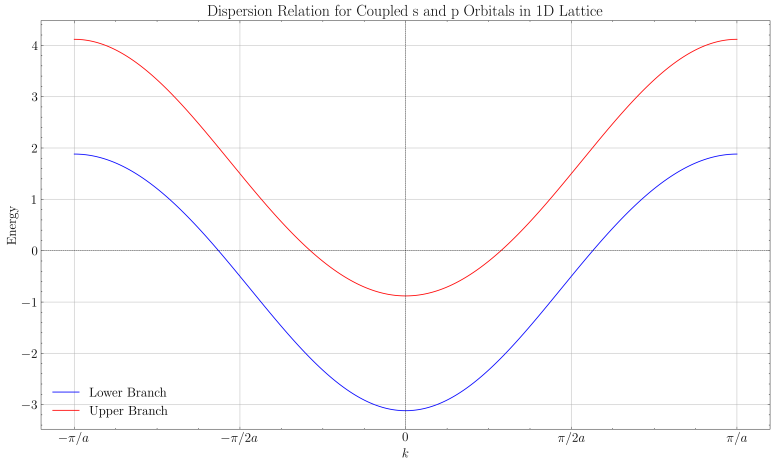

Figure 5: Energy bands for the 1D tight binding model with staggered potential

Problem 4 — Parallel Chains

The two parallel chain system have a tight binding Hamiltonian given by

$$\begin{aligned} H = &-t\sum_n (|n,s\rangle\langle n+1,s| + h.c.) - t'\sum_n (|n,p\rangle\langle n+1,p| + h.c.) \\ &-\Omega\sum_n |n,s\rangle\langle n,p| + h.c. + \epsilon_p\sum_n |n,p\rangle\langle n,p| + \epsilon_s\sum_n |n,s\rangle\langle n,s| \end{aligned} \tag{37}$$

a) We now need transform the Hamiltonian to the k-space basis. The bloch states are given as

$$|k,s\rangle = \frac{1}{\sqrt{N}}\sum_n e^{ikna}|n,s\rangle \quad ; \quad |k,p\rangle = \frac{1}{\sqrt{N}}\sum_n e^{ikna}|n,p\rangle \tag{38}$$

Taking the inverse fourier transform, we have

$$|n,s\rangle = \frac{1}{\sqrt{N}}\sum_k e^{-ikna}|k,s\rangle \quad ; \quad |n,p\rangle = \frac{1}{\sqrt{N}}\sum_k e^{-ikna}|k,p\rangle \tag{39}$$

We then plug these into the Hamiltonian term by term. Note that there are three types of terms: hopping within same chain, hopping between different chains and on-site potential terms.

$$\begin{aligned}
-t\sum_n(|n,s\rangle\langle n+1,s|+h.c.) &= -t\sum_{k,k'}\left[\left(\frac{1}{\sqrt{N}}\right)\sum_n e^{-i(k-k')na}e^{-ik'a}\right]|k,s\rangle\langle k',s|+h.c.\\
&= -t\sum_{k,k'}\left[\delta_{k,k'}e^{-ik'a}\right]|k,s\rangle\langle k',s|+h.c.\\
&= -t\sum_k\left[e^{-ika}|k,s\rangle\langle k,s|+e^{ika}|k,s\rangle\langle k,s|\right]\\
&= -2t\sum_k\cos(ka)|k,s\rangle\langle k,s|
\end{aligned} \tag{40}$$

Similarly, for the p chain hopping term, we have

$$-t'\sum_n(|n,p\rangle\langle n+1,p|+h.c.) = -2t'\sum_k\cos(ka)|k,p\rangle\langle k,p| \tag{41}$$

The inter-chain hopping term gives

$$\begin{aligned}
-\Omega\sum_n(|n,s\rangle\langle n,p|+h.c.) &= -\Omega\sum_{k,k'}\left[\left(\frac{1}{\sqrt{N}}\right)\sum_n e^{-i(k-k')na}\right]|k,s\rangle\langle k',p|+h.c.\\
&= -\Omega\sum_{k,k'}\left[\delta_{k,k'}\right]|k,s\rangle\langle k',p|+h.c.\\
&= -\Omega\sum_k[|k,s\rangle\langle k,p|+|k,p\rangle\langle k,s|]
\end{aligned} \tag{42}$$

The on-site potential terms give, similarly,

$$\begin{aligned}
\epsilon_s\sum_n|n,s\rangle\langle n,s| &= \epsilon_s\sum_k|k,s\rangle\langle k,s|\\
\epsilon_p\sum_n|n,p\rangle\langle n,p| &= \epsilon_p\sum_k|k,p\rangle\langle k,p|
\end{aligned} \tag{43}$$

Combining all these terms, we can write the Hamiltonian in the k-space basis as

$$\begin{aligned}
H = \sum_k\big[&(-2t\cos(ka)+\epsilon_s)|k,s\rangle\langle k,s|+\big(-2t'\cos(ka)+\epsilon_p\big)|k,p\rangle\langle k,p|\\
&-\Omega(|k,s\rangle\langle k,p|+|k,p\rangle\langle k,s|)\big]
\end{aligned} \tag{44}$$

In the basis $\{|k,s\rangle,|k,p\rangle\}$, the Hamiltonian can be written in a matrix form as

$$\begin{aligned}
H &= \sum_k(|k,s\rangle\quad|k,p\rangle)H(k)\begin{pmatrix}|k,s\rangle\\|k,p\rangle\end{pmatrix}\text{ where}\\
H(k) &= \begin{pmatrix}-2t\cos(ka)+\epsilon_s & -\Omega\\ -\Omega & -2t'\cos(ka)+\epsilon_p\end{pmatrix}
\end{aligned} \tag{45}$$

b) Similar to the previous problem, we can find the dispersion relation by solving the characteristic equation given by

$$\det(H(k)-E\mathbb{I})=0 \tag{46}$$

. We obtain,

$$\begin{aligned}
&\begin{vmatrix} -2t\cos(ka)+\epsilon_s-E & -\Omega \\ -\Omega & -2t'\cos(ka)+\epsilon_p-E \end{vmatrix} = 0 \\
\implies &(-2t\cos(ka)+\epsilon_s-E)\big(-2t'\cos(ka)+\epsilon_p-E\big)-\Omega^2=0 \\
\implies E_{\pm}(k) &= \frac{\epsilon_s+\epsilon_p-2(t+t')\cos(ka)}{2} \pm \sqrt{\left(\frac{\epsilon_s-\epsilon_p}{2}-(t-t')\cos(ka)\right)^2+\Omega^2}
\end{aligned} \tag{47}$$

Problem 5 — Bloch Theorem

The wavefunction in a lattice with lattice constat a can be obeys the Bloch theorem,

$$\psi_{n,k}(x) = e^{ikx}u_{n,k}(x) \text{ where } u_{n,k}(x+a) = u_{n,k}(x) \tag{48}$$

a) We need to show that

$$h_k u_{n,k}(x) = E_{n,k}u_{n,k}(x) \text{ where } h_k = \left(-\frac{\hbar^2}{2m}\right)(p_x+ik)^2 + V(x) \tag{49}$$

We start with the time independent schrodinger equation,

$$H\psi_{n,k}(x) = E_{n,k}\psi_{n,k}(x) \text{ where } H = \left(-\frac{\hbar^2}{2m}\right)p_x^2 + V(x) \tag{50}$$

Note that $p_x = -i\ \hbar\ \frac{\partial}{\partial x}$. p_x acting on $\psi_{n,k}(x)$ gives

$$\begin{aligned}
p_x\psi_{n,k}(x) &= -i\ \hbar\ \frac{\partial}{\partial x}(e^{ikx}u_{n,k}(x)) = e^{ikx}\left(\hbar\ ku_{n,k}(x) - i\ \hbar\ \frac{\partial u_{n,k}(x)}{\partial x}\right) \\
&= e^{ikx}(\hbar\ k + p_x)u_{n,k}(x)
\end{aligned} \tag{51}$$

Acting p_x^2 on $\psi_{n,k}(x)$ gives

$$\begin{aligned}
p_x^2\psi_{n,k}(x) &= p_x\big(e^{ikx}(\hbar\ k+p_x)u_{n,k}(x)\big) \\
&= \hbar\ ke^{ikx}(\hbar\ k+p_x)u_{n,k}(x) + e^{ikx}p_x(\hbar\ k+p_x)u_{n,k}(x) \\
&= e^{ikx}(\hbar\ k+p_x)^2u_{n,k}(x)
\end{aligned} \tag{52}$$

Thus we can see that,

$$
\begin{aligned}
& H\psi_{n,k}(x) = E_{n,k}\psi_{n,k}(x) \\
\implies & \left[\left(-\frac{\hbar^2}{2m}\right)p_x^2 + V(x)\right] e^{ikx}u_{n,k}(x) = E_{n,k}e^{ikx}u_{n,k}(x) \\
\implies & e^{ikx}\left[\left(-\frac{\hbar^2}{2m}\right)(\hbar\ k + p_x)^2 + V(x)\right] u_{n,k}(x) = E_{n,k}e^{ikx}u_{n,k}(x) \\
\implies & h_k u_{n,k}(x) = E_{n,k}u_{n,k}(x)
\end{aligned} \tag{53}
$$

b) We now consider the case when $V(x)$ is a weak perturbing potential. We can write $V(x)$ as

$$V(x) = V_{G_1}e^{iG_1x} + V_{G_1}^* e^{-iG_1x} \tag{54}$$

where $G = 2\frac{\pi}{a}$ is the reciprocal lattice vector. The unperturbed Hamiltonian is just the hamiltonian of a free particle. The energy eigenvalues are given by

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m} \tag{55}$$

The energy levels are doubly degenerate since $\epsilon_0(k) = \epsilon_0(-k)$. The Perturbation $V(x)$ lifts this degeneracy, and introduces a band gap at the boundary of the Brillouin zone $k = \pm\frac{\pi}{a}$. At the boundary of the Brillouin zone, the energy is given by

$$\epsilon_0 = \frac{\hbar^2\pi^2}{2ma^2} \tag{56}$$

Let us consider the states $|\pm k_1\rangle = \left|k = \pm\frac{G_1}{2}\right\rangle$. The diagonal elements are given by

$$\langle \pm k_1|H|\pm k_1\rangle = \epsilon_0 \tag{57}$$

We now need to calculate the off-diagonal elements. Note that the off diagonal elements in the unperturbed hamiltonian are 0. We have

$$
\begin{aligned}
\langle k_1|H|-k_1\rangle &= \langle k_1|V|-k_1\rangle \\
&= \int_0^a \frac{dx}{a} e^{-ik_1x}\left[V_{G_1}e^{iG_1x} + V_{G_1}^* e^{-iG_1x}\right]e^{-ik_1x} \\
&= \int_0^a \frac{dx}{a}\left[V_{G_1}e^{i(G_1-G_1)x} + V_{G_1}^* e^{-i(G_1+G_1)x}\right] = V_{G_1}
\end{aligned} \tag{58}
$$

Similarly,

$$\langle -k_1|H|k_1\rangle = V_{G_1}^* \tag{59}$$

The matrix elements of the Hamiltonian in this block in this basis are given by,

$$H = \begin{pmatrix} \langle k_1|H|k_1\rangle & \langle k_1|H|-k_1\rangle \\ \langle -k_1|H|k_1\rangle & \langle -k_1|H|-k_1\rangle \end{pmatrix} = \begin{pmatrix} \epsilon_0 & V_{G_1} \\ V_{G_1}^* & \epsilon_0 \end{pmatrix} \tag{60}$$

The Energy eigenvalues are,

$$E = \epsilon_0 \pm |V_{G_1}| \tag{61}$$

The Bandgap at the boundary of the Brillouin zone is therefore given by

$$\Delta = 2\ |V_{G_1}| \tag{62}$$

c) We have the periodic Gaussian potential given by

$$V(x) = -V_0 \sum_n e^{-\alpha(x-na)^2} \tag{63}$$

The Fourier components of the potential are given by

$$\begin{aligned} V_G &= \frac{1}{a}\int_0^a V(x) e^{-iGx} dx \\ &= -\frac{V_0}{a}\sum_n \int_0^a e^{-\alpha(x-na)^2} e^{-iGx} dx \\ &= -\frac{V_0}{a}\sum_n e^{-iGna} \int_{a-na}^{na} e^{-\alpha x'^2} e^{-iGx'} dx' \text{ where } x' = x - na \end{aligned} \tag{64}$$

Note that $e^{-iGna} = 1$ since $G = 2\pi\frac{m}{a}$. Also note the integral goes over the interval $(a-na, na)$. If $n \in \mathbb{Z}$, then the sum of all these integrals is equal to the integral from $-\infty$ to ∞. Therefore, we have a gaussian integral,

$$\begin{aligned} V_G &= -\frac{V_0}{a}\int_{-\infty}^{\infty} e^{-\alpha x'^2} e^{-iGx'} dx' \\ &= -\frac{V_0}{a}\sqrt{\frac{\pi}{\alpha}} e^{-\frac{G^2}{4\alpha}} \end{aligned} \tag{65}$$

The bandgap at the boundary of the Brillouin zone for the weak potential approximation is therefore given by

$$\Delta = 2\ |V_{G_1}| = \frac{2V_0}{a}\sqrt{\frac{\pi}{\alpha}} \exp\left(-\frac{\pi^2}{a^2\alpha}\right) \tag{66}$$

d) We allow the Bloch wavevector to be complex, i.e., $k = \frac{G}{2} + i\chi$. The energy for a free particle is given by

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{G^2}{4} - \chi^2 + iG\chi\right) \tag{67}$$

The energy at the boundary of the Brillouin zone is given by

$$\begin{aligned} \varepsilon_0^{\pm} &= \frac{\hbar^2}{2m}\left(\pm\frac{G_1}{2} \pm i\chi\right)^2 = \frac{\hbar^2}{2m}\left(\frac{G_1^2}{4} - \chi^2 \pm iG_1\chi\right) \\ &= \underbrace{\epsilon_0 - \frac{\hbar^2\chi^2}{2m}}_{E} \pm i\underbrace{\frac{\hbar^2 G_1 \chi}{2m}}_{\xi} \\ &= E \pm i\xi \end{aligned} \tag{68}$$

The Hamiltonian matrix in the basis $\{|k_1\rangle, |-k_1\rangle\}$ is given by,

$$H = \begin{pmatrix} E + i\xi & V_{G_1} \\ V_{G_1}^* & E - i\xi \end{pmatrix} \tag{69}$$

The energy eigenvalues are given by

$$E^{\pm} = E \pm \sqrt{|V_{G_1}|^2 - \xi^2} = \epsilon_0 - \frac{\hbar^2\chi^2}{2m} \pm \sqrt{|V_{G_1}|^2 - \left(\frac{\hbar^2 G_1}{2m}\right)^2 \chi^2} \tag{70}$$

For the energy eigenvalues to be real, we need

$$\begin{aligned} |V_{G_1}|^2 - \left(\frac{\hbar^2 G_1}{2m}\right)^2 \chi^2 &\geq 0 \\ \implies |\chi| &\leq \frac{2m\,|V_{G_1}|}{\hbar^2 G_1} \end{aligned} \tag{71}$$

Over the this range of χ, the energy eigenvalues are real. In this range from 0 to $\chi = \pm\frac{2m\,|V_{G_1}|}{\hbar^2 G_1}$, the energy eigenvalues vary from $\epsilon_0 \pm |V_{G_1}|$ to $\epsilon_0 \pm \frac{2m\,|V_{G_1}|^2}{\hbar^2 G_1^2}$. Thus by a suitable choice of complex wavevector, the energies within the bandgap can be obtained.

Problem 6 — Reciprocal Lattice Vectors

a) **Body Centred Cubic Lattice**
The primitive lattice vectors for a body centred cubic lattice are given by

$$\boldsymbol{a_1} = \frac{a}{2}(1,1,-1) \quad ; \quad \boldsymbol{a_2} = \frac{a}{2}(-1,1,1) \quad ; \quad \boldsymbol{a_3} = \frac{a}{2}(1,-1,1) \tag{72}$$

The volume of the primitive cell is given by

$$V_c = \boldsymbol{a_1} \cdot (\boldsymbol{a_2} \times \boldsymbol{a_3}) = \frac{a^3}{2} \tag{73}$$

The reciprocal lattice vectors are given by

$$\begin{aligned} \boldsymbol{b_1} &= 2\pi \frac{\boldsymbol{a_2} \times \boldsymbol{a_3}}{\boldsymbol{a_1} \cdot (\boldsymbol{a_2} \times \boldsymbol{a_3})} = \frac{2\pi}{a}(1,1,0) \\ \boldsymbol{b_2} &= 2\pi \frac{\boldsymbol{a_3} \times \boldsymbol{a_1}}{\boldsymbol{a_2} \cdot (\boldsymbol{a_3} \times \boldsymbol{a_1})} = \frac{2\pi}{a}(0,1,1) \\ \boldsymbol{b_3} &= 2\pi \frac{\boldsymbol{a_1} \times \boldsymbol{a_2}}{\boldsymbol{a_3} \cdot (\boldsymbol{a_1} \times \boldsymbol{a_2})} = \frac{2\pi}{a}(1,0,1) \end{aligned} \tag{74}$$

These correspond to the primitive vectors of an face centred cubic lattice.

b) **Two Dimensional Equilateral Triangular Lattice**
The primitive lattice vectors for a two dimensional equilateral triangular lattice are given by

$$\boldsymbol{a_1} = a(1,0) \quad ; \quad \boldsymbol{a_2} = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right) \tag{75}$$

The area of the primitive cell is given by

$$A_c = |\boldsymbol{a_1} \times \boldsymbol{a_2}| = \frac{\sqrt{3}a^2}{2} \tag{76}$$

The reciprocal lattice vectors are given by

$$\begin{aligned} \boldsymbol{b_1} &= 2\pi \frac{\hat{z} \times \boldsymbol{a_2}}{\boldsymbol{a_1} \cdot (\hat{z} \times \boldsymbol{a_2})} = \frac{2\pi}{a}\left(1, -\frac{1}{\sqrt{3}}\right) \\ \boldsymbol{b_2} &= 2\pi \frac{\hat{z} \times \boldsymbol{a_1}}{\boldsymbol{a_2} \cdot (\hat{z} \times \boldsymbol{a_1})} = \frac{2\pi}{a}\left(0, \frac{2}{\sqrt{3}}\right) \end{aligned} \tag{77}$$

These correspond to the primitive vectors of a two dimensional hexagonal lattice.

Problem 7 — Ultracold atoms

The given periodic potential is

$$V(x) = V_0(\cos^2\left(\frac{\pi x}{a}\right) = \frac{V_0}{2}\left(1 + \cos\left(\frac{2\pi x}{a}\right)\right) \tag{78}$$

We note that the potential has minima at $x = \left(n + \frac{1}{2}\right)a$ where $n \in \mathbb{Z}$. So near each lattice site, we can approximate the potential as a harmonic oscillator potential. Quantifying $\xi_n = (x - x_n)$ to be small displacement. Near the minima, we can expand the potential as,

$$V(x) \approx \frac{\pi^2 V_0}{a^2}\xi_n^2 + O(\xi_n^4) \tag{79}$$

So the total potential can be written as a sum over harmonic oscillator potentials at each lattice site,

$$V(x) \approx \sum_n \left(\frac{\pi^2 V_0}{a^2}(x - x_n)^2\right) \tag{80}$$

with the oscillation frequency given by

$$\omega = \sqrt{\frac{2\pi^2 V_0}{ma^2}} \tag{81}$$

a) The ground state wavefunction of a harmonic oscillator potential is given by

$$\psi_0(\xi_n) = \left(\frac{m\omega}{\pi\ \hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega\xi_n^2}{2\ \hbar}\right) \tag{82}$$

In our case, the ground state wavefunction localized at the n^{th} lattice site is given by

$$w_n(x) = \left(\frac{m\omega}{\pi\ \hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega(x-x_n)^2}{2\ \hbar}\right) = \frac{1}{(\pi s^2)^{\frac{1}{4}}} \exp\left(-\frac{(x-x_n)^2}{2s^2}\right) \text{ where } s = \sqrt{\frac{\hbar}{m\omega}} \quad (83)$$

where $x_n = \left(n + \frac{1}{2}\right)a$ is the position of the n^{th} lattice site. The bloch wavefunction can then be written as a superposition of these localized wavefunctions as

$$\psi_k(x) = \frac{1}{\sqrt{N}} \sum_n e^{ikx_n} w_n(x) \quad (84)$$

b) We also need to find the nearest neighbour hopping amplitude t. The hopping amplitude is given by

$$t = -\int dx w^*_{n+1}(x) \left[-\frac{\hbar^2}{2m}\frac{d^2}{d}x^2 + V(x)\right] w_n(x) \quad (85)$$

For our localized functions with Gaussian tails, the major contribution only arises from the sites n and $n+1$. Therefore, we can approximate the potential $V(x)$ between these two sites as a harmonic oscillator potential averaged over the sites. The potential can be approximated as

$$V(x) \approx \frac{1}{2}m\omega^2(x-x_n)^2 + \frac{1}{2}m\omega^2(x-x_{n+1})^2 \quad (86)$$

Note that $x_{n+1} - x_n = a$.We changing variable to $\xi = x - x_n$. Also note that the Wannier functions are represented in terms of the Harmonic oscillator eigenfunctions $\varphi_0(x)$. This gives us,

$$t = -\int_{-\infty}^{\infty} d\xi \varphi_0(\xi - a) \left[-\frac{\hbar^2}{2m}\frac{d^2}{d}\xi^2 + \frac{1}{2}m\omega^2\xi^2 + \frac{1}{2}m\omega^2(\xi-a)^2\right] \varphi_0(\xi) \quad (87)$$

After completing the algebra, the hopping term comes out to be,

$$t = -\frac{\hbar\ \pi}{2a}\sqrt{\frac{V_0}{m}}\left(\frac{3}{2} + \frac{\pi}{4}\sqrt{\frac{2mV_0a^2}{\hbar^2}}\right) \exp\left(-\frac{\pi^2}{4}\sqrt{V_0 m\frac{a^2}{\hbar^2}}\right) \quad (88)$$