Solid State Theory
Solution 3

Problem 3.1 The Kronig-Penney model

(a) With $ya = x$ and $\varphi(y) = \Psi(x)$ we obtain the Schrödinger equation

$$-\varphi''(y) + v\sum_n \delta(y-n)\varphi(y) = \beta^2\varphi(y). \tag{1}$$

Since $\delta(y \neq 0)$ vanishes we can write the general solution of the Schrödinger equation for $y \in (n, n+1)$ in the form

$$\varphi(y) = Ae^{i\beta y} + Be^{-i\beta y},\ E = \frac{\hbar^2\beta^2}{2ma^2}. \tag{2}$$

Using Bloch's ansatz we find the solution in the interval $y \in (n+1, n+2)$ through $\varphi(y+n) = \exp(i\lambda n)\varphi(y)$. For $y = n$, $\varphi'(y)$ has a jump. To see this, we integrate the Schrödinger equation from $n - \eta$ to $n + \eta$ and then let $\eta \to 0$. Thus, one obtains

$$-\varphi'(n+0^+) + \varphi'(n+0^-) + v\varphi(n) = 0. \tag{3}$$

Thus, the boundary conditions linking an interval $(n, n+1)$ with an interval $(n+1, n+2)$ read

$$\begin{aligned} \tilde{A} + \tilde{B} &= e^{-i\lambda}(\tilde{A}e^{i\beta} + \tilde{B}e^{-i\beta}), & (4)\\ \tilde{A} - \tilde{B} &= e^{-i\lambda}\left(\tilde{A}e^{i\beta} - \tilde{B}e^{-i\beta}\right) + \frac{v}{i\beta}(\tilde{A} + \tilde{B}), & (5) \end{aligned}$$

where we have set $\tilde{A} = Ae^{i\beta n}$ and $\tilde{B} = Be^{-i\beta n}$. We can rewrite this equation in matrix form,

$$\begin{pmatrix} 1 - e^{-i(\lambda-\beta)} & 1 - e^{-i(\lambda+\beta)} \\ 1 - e^{-i(\lambda-\beta)} - \frac{v}{i\beta} & -1 + e^{-i(\lambda+\beta)} - \frac{v}{i\beta} \end{pmatrix} \begin{pmatrix} \tilde{A} \\ \tilde{B} \end{pmatrix} = 0. \tag{6}$$

The determinant vanishes when

$$\cos\lambda = \cos\beta + \frac{v}{2\beta}\sin\beta. \tag{7}$$

This equation determines the dispersion $E = E(k)$ of the electrons in the periodic potential.

The right hand side of Eq. (7) is plotted in Fig. 1. As the left hand side of Eq. (7) takes values only between -1 and 1, there are no solutions for energies where $|\cos\beta + \frac{v}{2\beta}\sin\beta| > 1$.

Remark: Actually, we can solve Eq. (7) also for energies where the right hand side is not between -1 and 1. For such energies, we find an imaginary λ which, in an infinite system, always leads to exponential growth in one direction and thus to unphysical solutions. This is, however, not the case if our system ends at some point. Then, we can have a localized state at the surface, cf. part d.

(b) We can now analyze the dispersion for the two limits $v \ll 1$ and $v \gg 1$.

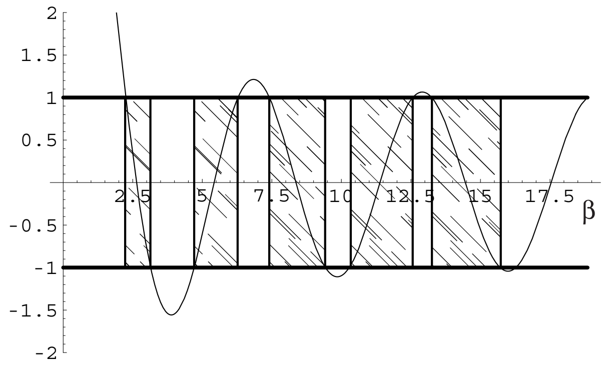

Figure 1: Graphical solution of Eq. (7). Allowed energies are hatched.

- In the limit $v = 0$, Eq. (7) yields the condition

$$\beta = \lambda + (2n\pi) \quad \Rightarrow \quad E = \frac{\hbar^2}{2m}(k+G)^2\,, \tag{8}$$

where $G = 2n\pi/a$ is a reciprocal lattice vector. We therefore obtain the dispersion of free electrons.

For $v \ll 1$ but $v \neq 0$, there are some forbidden regions (band gaps) for β, cf. Fig. 1. The dispersion (8) is modified to

$$\beta = \lambda + 2n\pi + \delta\,, \tag{9}$$

where $\delta \ll 1$. At the boundary of the Brillouin zone, $\lambda = \pi$, we can approximate

$$\cos\beta \approx -\left(1 - \frac{\delta^2}{2}\right)\,, \quad \sin\beta \approx -\delta\,, \quad \text{and} \quad \frac{1}{2\beta} \approx \frac{1}{2\pi(2n+1)}\left(1 - \frac{\delta}{(2n+1)\pi}\right)\,, \tag{10}$$

such that (keeping terms up to second order in δ and v) Eq. (7) is approximated by

$$0 = \frac{\delta^2}{2} - \frac{v\delta}{2\pi(2n+1)} \quad \Rightarrow \quad \delta \in \left\{0, \frac{v}{(2n+1)\pi}\right\}\,. \tag{11}$$

We obtain the energy as

$$E \approx \frac{\hbar^2}{2ma^2}\left((2n+1)^2\pi^2 + 2(2n+1)\pi\delta\right)\,, \tag{12}$$

leading to a band gap of

$$\Delta E \approx 2V_0/a\,. \tag{13}$$

The same calculation can be performed for $\lambda = 0$, in the middle of the Brillouin zone, also leading to an energy splitting of $\Delta E \approx 2V_0/a$.

- In the limit $v \to \infty$, Eq. (7) only has a solution for

$$\sin\beta = 0\,,\ \beta \neq 0 \quad \Rightarrow \quad E = \frac{\hbar^2 n^2 \pi^2}{2ma^2}\,,\ n = 1, 2, \ldots\,, \tag{14}$$

which corresponds to a system of disconnected infinite wells.

For $v \gg 1$ but not in the infinite limit, we approximate β starting from Eq. (14) by

$$\beta = \pi n + \delta\,, \tag{15}$$

with $\delta \ll 1$. This leads to

$$E \propto \beta^2 \approx n^2\pi^2 + 2n\pi\delta\,. \tag{16}$$

Assuming $v \gg 2n\pi$, and approximating

$$\cos\beta \approx (-1)^n\,, \quad \sin\beta \approx (-1)^n\delta\,, \quad \text{and} \quad \frac{1}{2\beta} \approx \frac{1}{2n\pi}\,, \tag{17}$$

Eq. (7) is approximated by

$$\cos\lambda \approx (-1)^n\left(1 + \frac{v}{2n\pi}\delta\right) \quad \Rightarrow \quad \delta \approx (-1)^n\frac{2n\pi}{v}\left(\cos\lambda - 1\right)\,. \tag{18}$$

Inserting this into Eq. (16), we obtain a tight-binding-like dispersion

$$\beta^2 \approx n^2\pi^2\left(1 + \frac{4(-1)^n}{v}\left(\cos\lambda - 1\right)\right)\,, \tag{19}$$

where the hopping matrix element is proportional to n^2 and inversely proportional to v.

(c) For a finite periodic system of length Na there are $dkNa/2\pi$ states in the interval dk. The number of states in the energy interval dE is thus given by

$$2\frac{Na}{2\pi}dk = 2\frac{Na}{2\pi}\left|\frac{dk}{dE}\right|dE. \tag{20}$$

The additional factor of 2 comes from the fact that the bands are symmetric with respect to $k = 0$. We thus find

$$\rho(E) = \frac{Na}{\pi}\left|\frac{dk}{dE}\right| = \frac{N}{\pi}\left|\frac{d\lambda}{d\beta}\frac{d\beta}{dE}\right| = \frac{Nma^2}{\hbar^2\pi\beta}\left|\frac{d\lambda}{d\beta}\right|. \tag{21}$$

From Eq. (7) we find

$$\left|\frac{d\lambda}{d\beta}\right| = \frac{\left|(1 + \frac{v}{2\beta^2})\sin\beta - \frac{v}{2\beta}\cos\beta\right|}{\sqrt{1 - \left(\cos\beta + \frac{v}{2\beta}\sin\beta\right)^2}}. \tag{22}$$

The density of states is shown in Fig. 2. It has square-root singularities at the band boundaries, $\propto |\epsilon - \epsilon_0|^{-1/2}$, where $\epsilon = \beta^2$ and $\epsilon_0 = \beta_0^2$ with β_0 a solution of $|\cos\beta_0 + \frac{v}{2\beta_0}\sin\beta_0| = 1$. To see this we define $\delta\beta = |\beta - \beta_0|$, $f(\beta) = 1 - \left(\cos\beta + \frac{v}{2\beta}\sin\beta\right)^2$ and $s = \mathrm{sign}(\mathrm{f}'(\beta_0))$. It then follows that

$$f(\beta_0 + s\delta\beta) \approx |f'(\beta_0)|\delta\beta \approx \frac{|f'(\beta_0)|}{2\beta_0}\delta\epsilon, \tag{23}$$

where $\delta\epsilon = |\epsilon - \epsilon_0|$. Note that the total number of states (the area under $\rho(E)$) is equal for all bands which is due to the factor β^{-1} in Eq. (21).

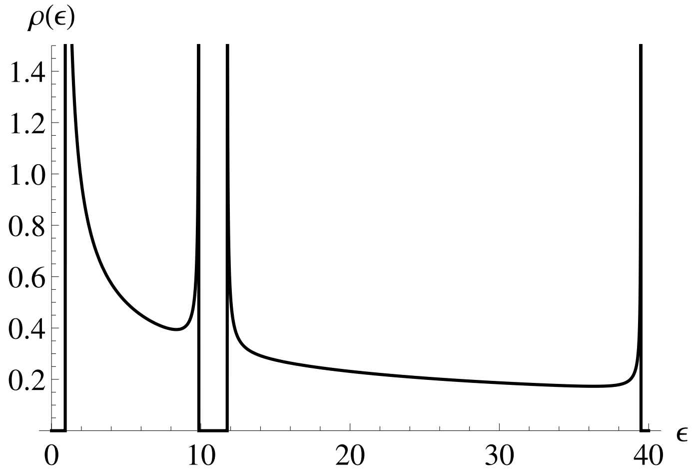

Figure 2: Density of states $\rho(\varepsilon)$ of the Kronig-Penney model with the square root divergences at the boundaries, typical of one-dimensional systems.

(d) We start with the ansatz

$$\varphi(y) = \begin{cases} Ce^{\kappa y} & y \leq 0, \\ Ae^{i\beta y} + Be^{-i\beta y} & y > 0. \end{cases} \tag{24}$$

From the continuity of the wave function and its first derivative at $y = 0$ we find the condition

$$\frac{A}{B} = -\frac{\kappa + i\beta}{\kappa - i\beta}. \tag{25}$$

In addition, the first line of Eq. (6) yields

$$\frac{A}{B} = -\frac{1 - se^{\mu}e^{-i\beta}}{1 - se^{\mu}e^{i\beta}}, \tag{26}$$

where we have used the notation of the exercise sheet. From these equations it follows that

$$se^{-\mu} = \frac{\kappa}{\beta}\sin\beta + \cos\beta. \tag{27}$$

with Eq. (7) in the form

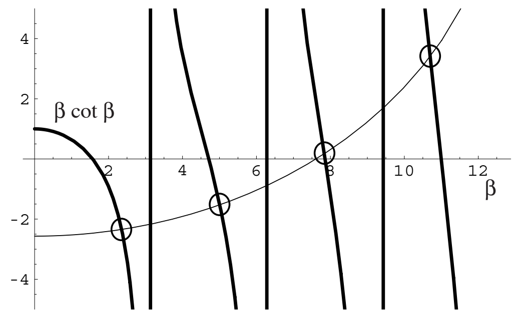

Figure 3: Graphical solution of Eq. (29).

$$s\cosh\mu = \frac{v}{2\beta}\sin\beta + \cos\beta, \tag{28}$$

and some straightforward calculation to eliminate μ, these two equations yield the relation

$$\beta\cot\beta = \frac{u}{v} - \sqrt{u-\beta^2}, \tag{29}$$

defining the energies of the surface states. Since $\cot\beta$ takes all the values between $-\infty$ and ∞ for $\beta \in (n\pi, (n+1)\pi)$, there is exactly one solution in every band gap (except for the first if $u/v - \sqrt{u} > 1$). Fig. 3 shows the graphical solution of Eq. (29).

Appendix A: Solution of part 1(a) in Fourier space.
Because of the periodicity of the system it is natural to solve the Schrödinger equation in the Fourier space. Introducing the Fourier transformations

$$\begin{aligned}\varphi(y) &= \int \frac{dq}{2\pi} \mathrm{e}^{iqy}\tilde{\varphi}(q)\\ V(y) &= \int \frac{dq}{2\pi} \mathrm{e}^{iqy}\tilde{V}(q)\end{aligned}$$

with $q = ka =: \lambda$ and $\tilde{V}(q) = \sum_n \mathrm{e}^{-iqn}$ and Fourier transforming the Schrödinger equation (1) we get

$$q^2\tilde{\varphi}(q) + \frac{v}{2\pi}\int_{-\infty}^{+\infty} dk \sum_{n=-\infty}^{+\infty} \mathrm{e}^{ikn}\tilde{\varphi}(k+q) = \beta^2\tilde{\varphi}(q). \tag{30}$$

From the formula $f(k) = \sum_{n'=-\infty}^{+\infty} \delta(k+2\pi n') = \frac{1}{2\pi}\sum_{n=-\infty}^{+\infty} \mathrm{e}^{ikn}$ (Fourier series decomposition of the 2π-periodic function $f(k)$) one obtains

$$q^2\tilde{\varphi}(q) + v\sum_{n'=-\infty}^{+\infty} \tilde{\varphi}(q-2\pi n') = \beta^2\tilde{\varphi}(q). \tag{31}$$

Performing the substitution $q = \bar{q} + 2\pi n$ and defining $\tilde{\varphi}(\bar{q}+2\pi n) =: \tilde{\varphi}_n(\bar{q})$ we get

$$(\bar{q}+2\pi n)^2\tilde{\varphi}_n(\bar{q}) + v\sum_{n'=-\infty}^{+\infty} \tilde{\varphi}_{n'}(\bar{q}) = \beta^2\tilde{\varphi}_n(\bar{q}). \tag{32}$$

(The second term of the left hand side was found after rearranging the terms of the sum $\sum_{n'}\tilde{\varphi}(q-2\pi n') = \sum_{n'}\tilde{\varphi}(\bar{q}+2\pi n-2\pi n') = \sum_{n'}\tilde{\varphi}(\bar{q}+2\pi n') = \sum_{n'}\tilde{\varphi}_{n'}(\bar{q})$.) We can rewrite the equation as

$$\tilde{\varphi}_n = \frac{v\sum_{n'}\tilde{\varphi}_{n'}}{\beta^2 - (\bar{q}+2\pi n)^2}. \tag{33}$$

Summing over n on both sides we finally find

$$1 = \sum_{n=-\infty}^{+\infty} \frac{v}{\beta^2 - (\lambda+2\pi n)^2}. \tag{34}$$

We can now show that this equation is equivalent to (7): Let us write the above condition as

$$1/v = \sum_{n=-\infty}^{\infty} f(2\pi n) \tag{35}$$

with

$$f(z) = \frac{1}{\beta^2 - (\lambda + z)^2}. \tag{36}$$

To calculate such an infinite sum, often complex analysis can be useful: The function

$$g(z) = \frac{1}{1 - e^{iz}} \tag{37}$$

has poles at $z = 2\pi m$ with residue i. If we now consider the integral

$$\int_\gamma \frac{dz}{2\pi i} f(z) g(z) \tag{38}$$

with γ a circle of radius R with $R \to \infty$, this integral vanishes as $f(z)z \to 0$ for $|z| \to \infty$ while g(z) is finite. Making use of the residue theorem and of the fact that $f(z)$ has poles for $z = \pm\beta - \lambda$, we obtain

$$\begin{aligned} 0 = \int_\gamma \frac{dz}{2\pi i} f(z) g(z) = \sum_n f(2\pi n) \cdot i \\ + \mathrm{Res}_{z=\beta-\lambda} f(z) g(\beta - \lambda) + \mathrm{Res}_{z=-\beta-\lambda} f(z) g(-\beta - \lambda), \end{aligned} \tag{39}$$

where we already used that the Residues of g(z) at the poles is i. This expression can be evaluated and simplified to

$$\frac{1}{v} = \sum_{n=-\infty}^{\infty} f(2\pi n) = \frac{\sin\beta}{2\beta} \frac{1}{\cos\lambda - \cos\beta}, \tag{40}$$

from which Eq.(7) follows directly.

Appendix B: Transfer matrix approach to the KP model.
Both the infinite and the semi-infinite Kronig-Penney model can be solved with the transfer-matrix approach. In fact, while for the infinite Kronig-Penney model the application of the Bloch theorem is justified, this is not the case for the semi-infinite model as there translational invariance of the system is not fulfilled. However, we will see that it leads to the right result as it enforces the right condition on the surface state.

Infinitely extended Kronig-Penney model
Let us start by considering the infinite Kronig-Penney model discussed in Ex.1.1. We use the notation from the exercise and the solution sheet.
We start by considering states with a certain energy E (and corresponding $\beta = a\sqrt{2mE/\hbar^2}$). In between the delta-barriers, the state is given by a superposition of plane wave states. Therefore, the state $\varphi(y)$ is given by a combination of the states in between the delta-functions and we define $\varphi(y)$ as

$$\varphi(n - 1 \leq y \leq n) = \varphi_n(y) \tag{41}$$

where $\varphi_n(y)$ describes the wave function in the region $[n-1, n]$ and is given as

$$\varphi_n(y) = A_n e^{i\beta(y-n+1)} + B_n e^{-i\beta(y-n+1)} \tag{42}$$

with the coefficients A_n and B_n characterizing the state in this region (Note that we splited off a phase $\exp(\pm i\beta(n-1))$ on the purpose of simplification).

Due to the two conditions at every delta-function, i.e.

$$\varphi_{n+1}(n) = \varphi_n(n), \tag{43}$$
$$\varphi'_{n+1}(n) = \varphi'_n(n) + v\varphi_n(n), \tag{44}$$

we get a connection between the coefficients (A_n, B_n) and (A_{n+1}, B_{n+1}) of the form

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = M \begin{pmatrix} A_n \\ B_n \end{pmatrix} \tag{45}$$

with the matrix M given as

$$M = L^{-1}VLT \tag{46}$$

with

$$L = \begin{pmatrix} 1 & 1 \\ i\beta & -i\beta \end{pmatrix}, \tag{47}$$
$$V = \begin{pmatrix} 1 & 0 \\ v & 1 \end{pmatrix}, \tag{48}$$
$$T = \begin{pmatrix} e^{i\beta} & 0 \\ 0 & e^{-i\beta} \end{pmatrix}. \tag{49}$$

The determinant of M is 1 ($\det M = 1$) which means that the product of the eigenvalues of this matrix $\mu_{1/2}$ fulfill $\mu_1 \cdot \mu_2 = 1$ and therefore either $|\mu_1| = |\mu_2| = 1$ or $|\mu_1| < 1 < |\mu_2|$ (where we have assumed μ_2 to be the larger eigenvalue).
The eigenvalues can be calculated and one obtains

$$\mu_{1/2} = \cos(\beta) + \frac{v}{2\beta}\sin(\beta) \mp \sqrt{\left(\cos(\beta) + \frac{v}{2\beta}\sin(\beta)\right)^2 - 1}. \tag{50}$$

We have to distinguish two cases: i) $|\cos(\beta)+\frac{v}{2\beta}\sin(\beta)| < 1$ and ii) $|\cos(\beta)+\frac{v}{2\beta}\sin(\beta)| > 1$. As we will discuss right now, this condition determines if at a certain energy E (at a certain β), a state can exist. We will see, that in the first case i), states exist, whereas the second case ii) leads to unphysical behavior and therefore no states. This leads to the opening of a band gap as discussed on the solution sheet.

Case i): $|\cos(\beta) + \frac{v}{2\beta}\sin(\beta)| < 1$ In this case, we should rewrite the eigenvalues as

$$\mu_{1/2} = \cos(\beta) + \frac{v}{2\beta}\sin(\beta) \mp i\sqrt{1 - \left(\cos(\beta) + \frac{v}{2\beta}\sin(\beta)\right)^2}. \tag{51}$$

The absolute value of this eigenvalues is 1 and therefore, we can write $\mu_{1/2} = e^{\pm i\lambda}$ (with λ having the same meaning as on the exercise sheet) which leads to the dispersion relation

$$\cos(\lambda) = \cos(\beta) + \frac{v}{2\beta}\sin(\beta). \tag{52}$$

There are eigenvectors corresponding to these eigenvalues:

$$\begin{pmatrix} A^{(1/2)} \\ B^{(1/2)} \end{pmatrix} = \begin{pmatrix} e^{-i\beta}\left(-\cos(\beta) + \frac{2\beta}{v}\sin(\beta) \pm \frac{2\beta}{v}\sqrt{1 - \left(\cos(\beta) + \frac{v}{2\beta}\sin(\beta)\right)^2}\right) \\ 1 \end{pmatrix} \tag{53}$$

From these eigenvectors, we can construct eigenstates of the system by plugging in an eigenstate for φ_0 and calculating the continuation from the transfer-matrices.
We have two eigenstates

$$\varphi_n^{(1/2)}(y) = e^{\pm i\lambda n}(A^{(1/2)}e^{i\beta(y-n+1)} + B^{(1/2)}e^{-i\beta(y-n+1)}) \tag{54}$$

such that directly for both states, the Bloch theorem is fulfilled. It is easy to see now that λ introduced above is nothing else but the phase $k \cdot a$ between two points separated by a.
Case ii): $|\cos(\beta) + \frac{v}{2\beta}\sin(\beta)| > 1$ In this case, the eigenvalues are given above as

$$\mu_{1/2} = \cos(\beta) + \frac{v}{2\beta}\sin(\beta) \mp \sqrt{\left(\cos(\beta) + \frac{v}{2\beta}\sin(\beta)\right)^2 - 1}. \tag{55}$$

and the state vectors are

$$\begin{pmatrix} A^{(1/2)} \\ B^{(1/2)} \end{pmatrix} = \begin{pmatrix} e^{-i\beta}\left(-\cos(\beta) + \frac{2\beta}{v}\sin(\beta) \pm i\frac{2\beta}{v}\sqrt{\left(\cos(\beta) + \frac{v}{2\beta}\sin(\beta)\right)^2 - 1}\right). \\ 1 \end{pmatrix} \tag{56}$$

The eigenvalues are now real and we have $\mu_1 = \pm e^{-\rho}$ and $\mu_2 = \pm e^{\rho}$ which would lead to the two eigenstates

$$\varphi_n^{(1/2)}(y) = (\pm 1)^n e^{\mp\rho n}(A^{(1/2)}e^{i\beta(y-n+1)} + B^{(1/2)}e^{-i\beta(y-n+1)}) \tag{57}$$

such that the state $\varphi^{(1)}(y)$ diverges for $y \to -\infty$ (as $\varphi^{(1)}_{n\to-\infty}(y)$ diverges) and $\varphi^{(2)}(y)$ diverges for $y \to \infty$ (as $\varphi^{(2)}_{n\to\infty}(y)$ diverges).
Therefore, there are no states in the band gap for an infinitely extended Kronig-Penney model. However, we will show next, that there are discrete surface states in the case of an semi-infinite Kronig-Penney model.

Semi-infinitely extended Kronig-Penney model

We again consider a state with a given energy $E < U_0$ and make the Ansatz

$$\varphi(y < 0) = Ce^{\kappa y}, \tag{58}$$
$$\varphi(n-1 \le y \le n) = \varphi_n(y). \tag{59}$$

From the boundary at $y = 0$, we obtain the following condition on the coefficients A_1 and B_1:

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = L^{-1}\begin{pmatrix} 1 \\ \kappa \end{pmatrix} C. \tag{60}$$

Due to the transfer-matrix M, all other coefficients A_n and B_n are determined from A_1 and B_1. A state is physical if the coefficients stay finite for all n and do not diverge.
For the states in the energy band, this can be always fulfilled. For the states in the gap, we have to make the following consideration:
The state vector (A_1, B_1) can be written as a linear combination of the eigenstates of M, i.e.

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = c_1\begin{pmatrix} A^{(1)} \\ B^{(1)} \end{pmatrix} + c_2\begin{pmatrix} A^{(2)} \\ B^{(2)} \end{pmatrix}. \tag{61}$$

From our consideration above, we know that

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = c_1 \mu_1^n \begin{pmatrix} A^{(1)} \\ B^{(1)} \end{pmatrix} + c_2 \mu_2^n \begin{pmatrix} A^{(2)} \\ B^{(2)} \end{pmatrix}. \tag{62}$$

As $|\mu_2| > 1$ the state vector diverges if $c_2 \neq 0$. Therefore, to have a state in the gap, the state vector (A_1, B_1) should be proportional to the first eigenvector, i.e.

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = c_1 \begin{pmatrix} A^{(1)} \\ B^{(1)} \end{pmatrix}. \tag{63}$$

This is the condition to find a surface state (as this component is decaying for $n \to \infty$) in the band gap. From this condition, we can derive the condition

$$\frac{A_1}{B_1} = \frac{A^{(1)}}{B^{(1)}}. \tag{64}$$

This equation has a real part and an imaginary part. Plugging both equations into each other in order to eliminate $\sqrt{\left(\cos(\beta) + \frac{v}{2\beta}\sin(\beta)\right)^2 - 1}$ and simplifying the equation, we can obtain

$$\beta \cot(\beta) = \frac{u}{v} - \kappa = \frac{u}{v} - \sqrt{u - \beta^2} \tag{65}$$

which is the condition for a surface state mentioned on the exercise sheet and calculated on the solution sheet using the Bloch Ansatz.

Why does Bloch's Ansatz work?
As you can see above, it is important that the state vector (A_1, B_1) be an eigenvector of the transfer-matrix (corresponding to the smaller eigenvalue). An eigenvector of the transfer-matrix leads to a Bloch state as mentioned above. Therefore, the condition of (A_1, B_1) being an eigenvector of the transfer-matrix and the state being a Bloch state with decaying amplitudes are equivalent and lead to the same result. However, it is not justified to use Bloch's Ansatz without this correspondence or at least it does not guarantee to find all the solution in general.