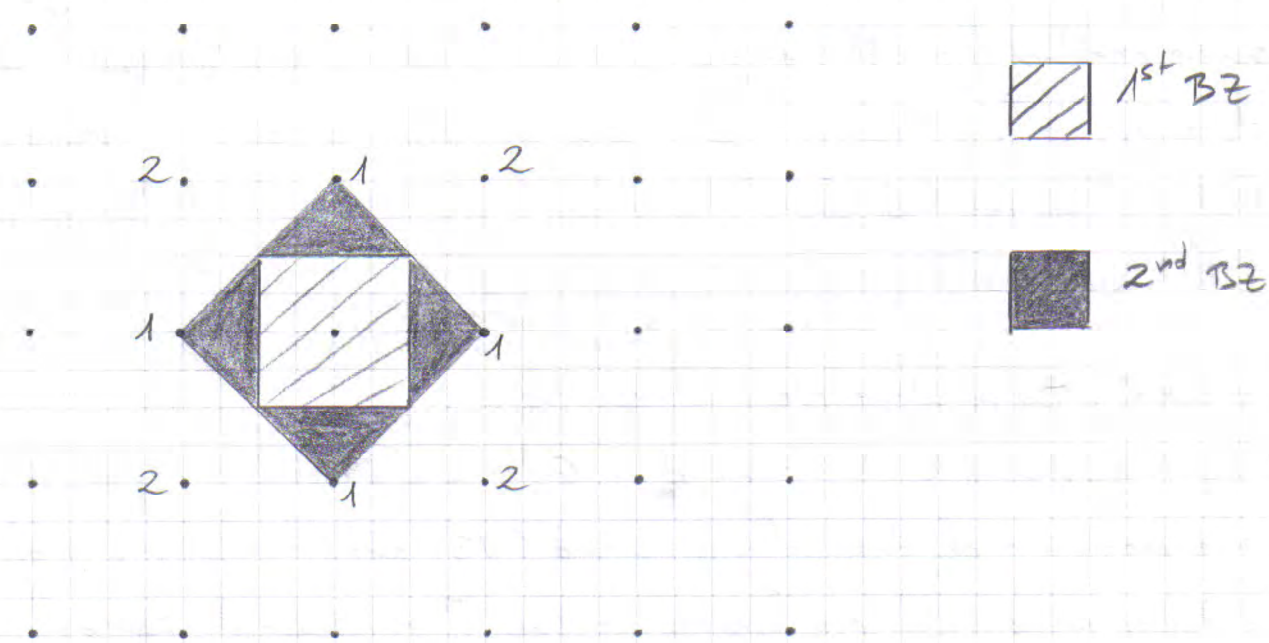
Series - Electronic and optical semiconductor devices

Series 2 - Brillouin zone, band structure (introduction), periodic potentials in one dimension (Kronig-Penney model)

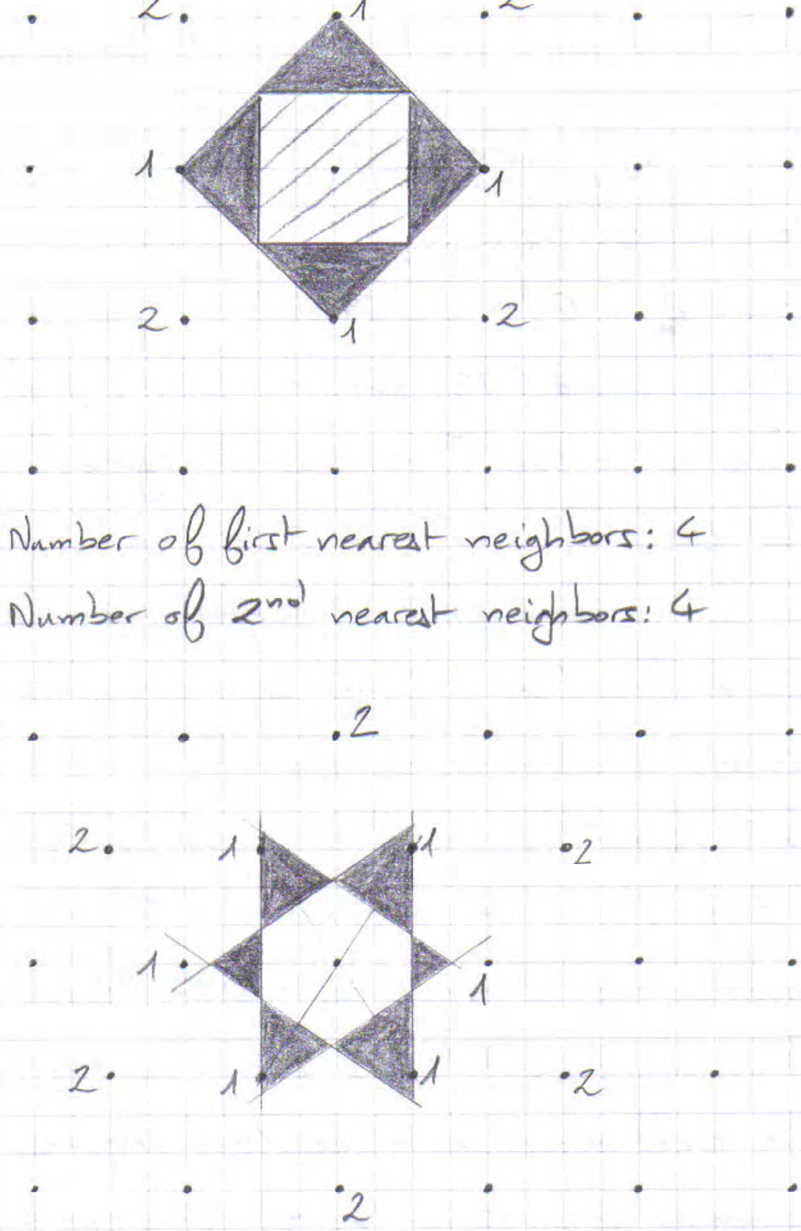
Exercise 1: Introduction to Brillouin zones

1-



2- Number of first nearest neighbors: 4
Number of 2nd nearest neighbors: 4

3-



Number of 1st nearest neighbors: 6
Number of 2nd nearest neighbors: 6

Note that the surface of Brillouin zones (BZ) in reciprocal space is identical: $S_{BZ_1}^{square} = S_{BZ_2}^{square} = S_{BZ_i}^{square}$ (the same remark applies to the hexagonal lattice). This is also true in the 3D case ($V_{BZ_1} = V_{BZ_2} = V_{BZ_i}$)

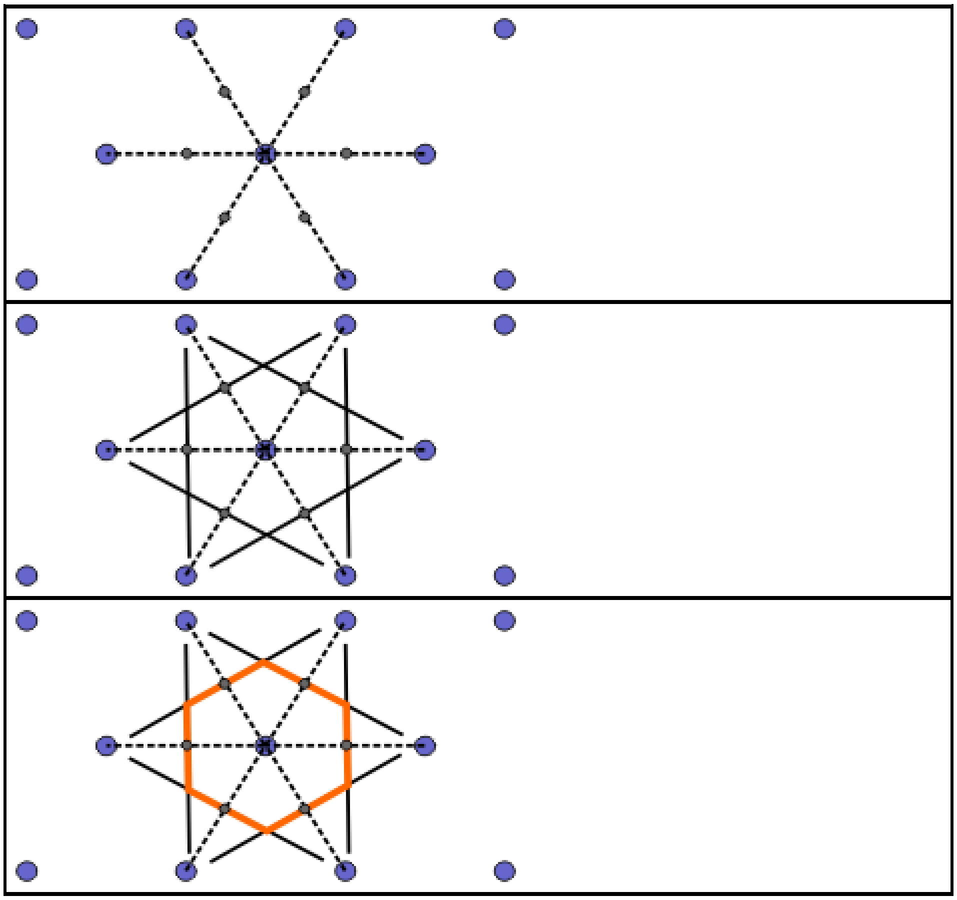
Some more details on BZ: Let $\vec{G}$ be a vector of the reciprocal lattice such that $e^{-i\vec{G}.\vec{r}}$ is a periodic function of the crystal lattice. Then, the

1st BZ is defined as the primitive Wigner-Seitz cell of the reciprocal lattice, i.e. the ensemble of points located closer to $\vec{G} = \vec{0}$ than to any other point of the reciprocal lattice. Since Bragg planes are the bisecting planes of the lines connecting the origin to the points of the reciprocal lattice, the 1st BZ can also be defined as the ensemble of points that can be reached from the origin without crossing any Bragg plane.

More generally, the n^{th} BZ can be defined as the ensemble of points that can be reached from the origin by crossing $(n-1)$ Bragg planes (but not less).

Series 2, exercise 1 : Supplementary information

1st and 2nd Brillouin zones in the case of a two-dimensional hexagonal lattice (case of graphene)



Exercise 3: Periodic potentials in one dimension (Kronig-Penney model)

1- We consider equations (7) and (8) at the position $x = -a/2$. We get:

$$\psi(a/2) = e^{iGa}\,\psi(-a/2) \quad (a)$$

$$\psi'(a/2) = e^{iGa}\,\psi'(-a/2) \quad (b)$$

$$(a) \Rightarrow A\psi_l(a/2) + B\psi_r(a/2) = e^{iGa}\left[A\psi_l(-a/2) + B\psi_r(-a/2)\right]$$

i.e. $$A t e^{ik\frac{a}{2}} + B e^{-ika/2} + B r e^{ika/2} = A e^{i(G-k/2)a} + A r e^{i(G+k/2)a} + B t e^{i(G+k/2)a}$$

then $[te^{ika/2} - e^{i(G-k/2)a} - re^{i(G+k/2)a}]A + [e^{-ika/2} + re^{ika/2} - te^{i(G+k/2)a}]B = 0$ (c)

$\psi'(x) = A\psi_l'(x) + B\psi_r'(x) \Rightarrow$ 2 possible cases can occur.

Case 1 $\quad x \leqslant -a/2$

$$\psi'(x) = A(ike^{ikx} - ikre^{-ikx}) - Btike^{-ikx} \quad (d)$$

Case 2 $\quad x \geqslant a/2$

$$\psi'(x) = Atike^{ikx} + B(rike^{ikx} - ike^{-ikx}) \quad (e)$$

(b)+(d)+(e)

↳ $ik[Ate^{ika/2} + Bre^{ika/2} - Be^{-ika/2}] =$
$ik[Ae^{i(G-k/2)a} - Are^{i(G+k/2)a} - Bte^{i(G+k/2)a}]$

i.e. $[te^{ika/2} - e^{i(G-k/2)a} + re^{i(G+k/2)a}]A + [re^{ika/2} - e^{-ika/2} + te^{i(G+k/2)a}]B = 0$

↳ (f)

(c)+(f) $\Rightarrow$
$$\Delta = \begin{vmatrix} te^{ika/2} - e^{i(G-k/2)a} - re^{i(G+k/2)a} & e^{-ika/2} + re^{ika/2} - te^{i(G+k/2)a} \\ te^{ika/2} - e^{i(G-k/2)a} + re^{i(G+k/2)a} & re^{ika/2} - e^{-ika/2} + te^{i(G+k/2)a} \end{vmatrix}$$
$$= 0 \quad (g)$$

(g) $\Rightarrow (te^{ika/2} - e^{i(G-k/2)a} - re^{i(G+k/2)a})(re^{ika/2} - e^{-ika/2} + te^{i(G+k/2)a})$
$- (te^{ika/2} - e^{i(G-k/2)a} + re^{i(G+k/2)a})(e^{-ika/2} + re^{ika/2} - te^{i(G+k/2)a}) = 0$

$\Delta = \Delta_1 - \Delta_2 = 0$

$\Delta_1 = \cancel{rte^{ika}} - t + t^2e^{i(G+k)a} - \cancel{re^{iGa}} + e^{i(G-k)a} - te^{i2Ga} - r^2e^{i(G+k)a}$
$+ \cancel{re^{iGa}} - \cancel{rte^{i(2G+k)a}}$

$\Delta_2 = t + \cancel{rte^{ika}} - t^2e^{i(G+k)a} - e^{i(G-k)a} - \cancel{re^{iGa}} + te^{i2Ga} + \cancel{re^{iGa}}$
$+ r^2e^{i(G+k)a} - \cancel{rte^{i(2G+k)a}}$

We then get $-2t + 2t^2e^{i(G+k)a} - 2te^{i2Ga} - 2r^2e^{i(G+k)a} + 2e^{i(G-k)a} = 0$ (h)

i.e. $(t^2 - r^2)e^{i(G+k)a} - t(1 + e^{i2Ga}) + e^{i(G-k)a} = 0 \quad \times \frac{e^{-iGa}}{2t}$

$$\frac{(t^2 - r^2)}{2t}e^{ika} - \underbrace{\frac{(e^{-iGa} + e^{iGa})}{2}}_{\cos Ga} + \frac{1}{2t}e^{-ika} = 0$$

$$\Rightarrow \boxed{\cos Ga = \frac{t^2 - r^2}{2t} e^{ika} + \frac{1}{2t} e^{-ika}} \qquad (9)$$

Free electron case

$v = 0 \Rightarrow t = 1$ and $r = 0$

$(9) \Rightarrow \quad \cos Ga = \frac{1}{2} e^{ika} + \frac{1}{2} e^{-ika}$

i.e. $\cos Ga = \cos ka \Rightarrow k = G + 2n\pi/a$ with $n \in \mathbb{Z}$

For $n = 0$ the situation is that of a plane wave.

$\psi(x) = A(e^{ikx} + e^{-ikx})$. The term $2n\pi/a$ is a reminiscence of the periodic space introduced in the problem!

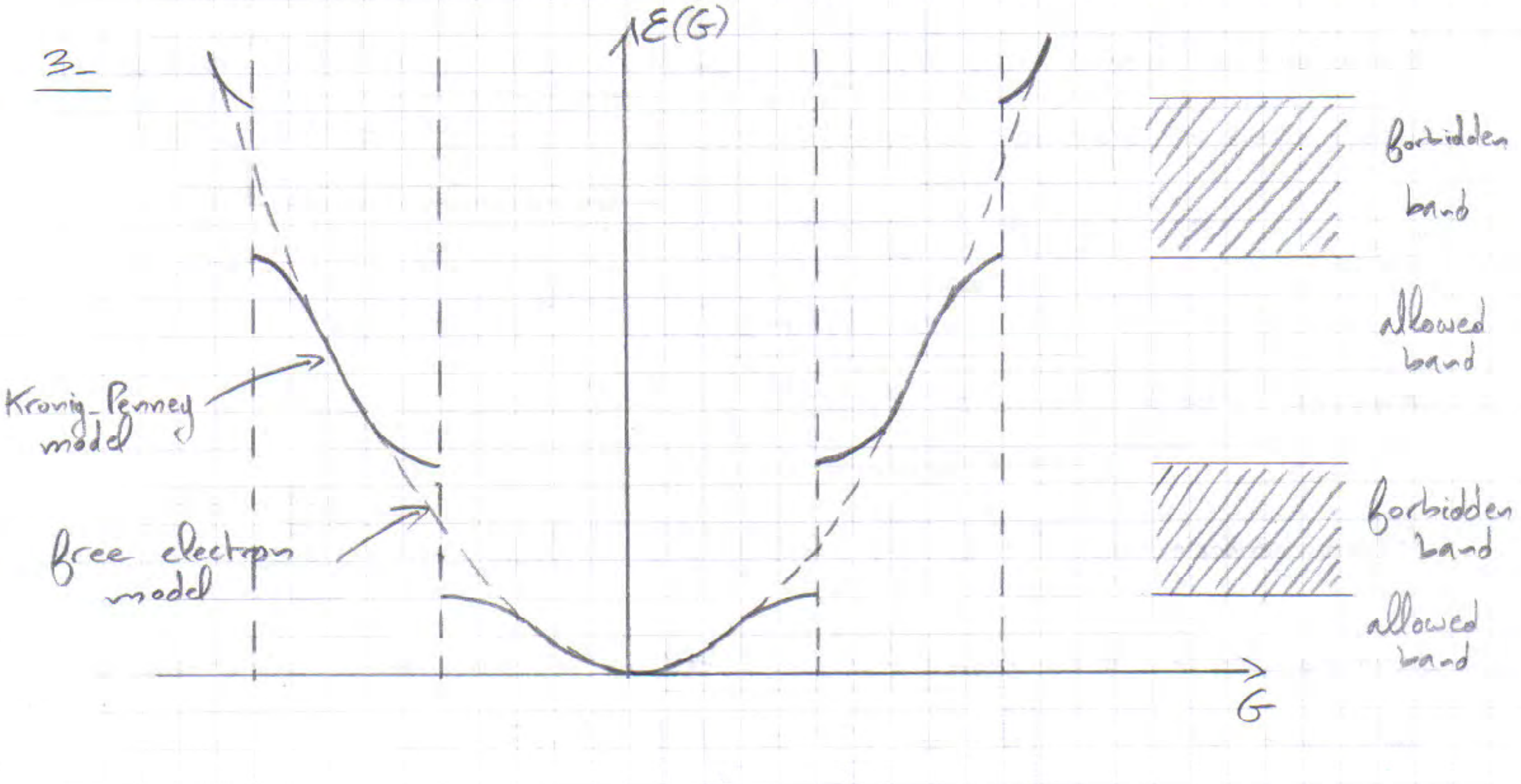
2- $r^2 = -|r|^2 e^{i2\delta} \qquad t^2 = |t|^2 e^{i2\delta}$

$(9) \Rightarrow \frac{|t|^2 + |r|^2}{2|t|e^{i\delta}} e^{i2\delta} e^{ika} + \frac{1}{2|t|e^{i\delta}} e^{-ika} = \cos Ga$

Then $\frac{1}{2|t|} e^{i(ka+\delta)} + \frac{1}{2|t|} e^{-i(ka+\delta)} = \cos Ga$

i.e. $$\boxed{\frac{\cos(ka+\delta)}{|t|} = \cos Ga} \qquad (13)$$

3-



Note here that k is a continuous variable which is not related to the reciprocal lattice. However, the dispersion curves will follow the relationship $E(G)=\frac{\hbar^2 k^2}{2m}$ where G is a vector of the reciprocal lattice.

Equation (13) shown in Fig. (5) indicates there are k values such that forbidden energy bands (band gaps) will be present. The periodic potential will thus induce a deviation to the free electron model. Far from the gaps, the free electron approximation is fully satisfactory. However, close to these gaps, a flattening of the dispersions is observed. Once again it is important not to mix between G (vector of the reciprocal lattice) and k. The dispersion curves will be reported in the E-G space. As a consequence, there will be energy gaps but not gap in G!

Supplementary information on the Kronig-Penney model can be found in "States of Matter" by David L. Goodstein (Dover).

4- Consider equation (14): $ka+\delta = n\pi$. We can then write $\boxed{k=\frac{n\pi}{a}-\frac{\delta}{a}}$ (4.1)

It corresponds to k values in the vicinity of $k=\frac{n\pi}{a}$ ($\delta \simeq 0$).

Now, if we consider equation (13) in the vicinity of the straight line $\cos Ga = 1$, we get: $\cos(ka+\delta) = |t|$

i.e. $\cos ka \cos\delta - \sin ka \sin\delta = |t|$

In addition, $\delta \simeq 0$ and $k \simeq \frac{n\pi}{a}$ so that we obtain: $(-1)^n \cos\delta \approx |t|$

which can be farther simplified to: $\boxed{(-1)^n\left(1-\frac{\delta^2}{2}\right) \approx |t|}$. (4.2)

Moreover, $|t|^2+|r|^2 = 1$ then $|t|^2 = 1-|r|^2$

i.e. $|t| = \pm(1-|r|^2)^{1/2}$

and as $|r| \simeq 0$, $\boxed{|t| \approx \pm\left(1-\frac{|r|^2}{2}\right)}$ (4.3)

When comparing (4.2) and (4.3), we deduce that $\boxed{\delta^2 \approx |r|^2}$ (4.4)

Coming back to equation (4.1) and taking into account equation (4.4), we can write: $\boxed{k_\pm = \frac{n\pi}{a} \pm \frac{|r|}{a}}$ (4.5)

The width of the band gap is then defined by the relationship:

$$\mathcal{E}_{gap} = \frac{\hbar^2}{2m}(k_+^2 - k_-^2)$$

i.e. $$\mathcal{E}_{gap} = \frac{\hbar^2}{2m}\left(k_+^2 - \left(k_+ - \frac{2|r|}{a}\right)^2\right)$$

$$\Rightarrow \mathcal{E}_{gap} = \frac{\hbar^2}{2m}\left(4k_+\frac{|r|}{a} - \frac{4|r|^2}{a^2}\right)$$

$$\Rightarrow \mathcal{E}_{gap} = \frac{\hbar^2}{2m}\left(\frac{4n\pi|r|}{a^2} + \cancel{\frac{4|r|^2}{|a|^2}} - \cancel{\frac{4|r|^2}{|a|^2}}\right)$$

and finally $$\boxed{\mathcal{E}_{gap} = 2n\pi\frac{\hbar^2}{ma^2}|r|} \qquad (4.6)$$

In that specific case, it is seen that the forbidden bands are very narrow (in energy).

5- The situation is the reverse to the previous question, i.e. $|t| \simeq 0$ and $|r| \simeq 1$. The allowed bands of energies will then satisfy the following relationships: $\cos Ga = 1$, position linked to $\mathcal{E}_{min}$

$\cos Ga = -1$, position linked to $\mathcal{E}_{max}$

As for the previous question, we must determine the wave vectors linked to $\mathcal{E}_{max}$ and $\mathcal{E}_{min}$. We can thus write:

$$\frac{\cos(k_{min}a + \delta)}{|t|} = 1 \quad \text{and} \quad \frac{\cos(k_{max}a + \delta)}{|t|} = -1$$

from which we get the following equations:

$$k_{min}a + \delta = \arccos|t| + 2n\pi$$

i.e $$\boxed{k_{min} = \frac{1}{a}[\arccos|t| + 2n\pi - \delta]} \qquad (5.1)$$

and $k_{max}a + \delta + \pi = \arccos|t| + 2n'\pi$ with $n' = n+1$ (Note here that n and n' values are successive integers as we consider extrema of a band (change from n to $n+1$ once crossing the inflection point.))

so that $$\boxed{k_{max} = k_{min} + \frac{\pi}{a}} \qquad (5.2)$$

In addition, $\arcsin x + \arccos x = \frac{\pi}{2}$ and $\arcsin x \approx x$ when $x \to 0$

so that $\arccos |t| \approx \frac{\pi}{2} - |t|$

and $$\boxed{k_{min} = \frac{1}{a}\left[\frac{\pi}{2} - |t| + 2n\pi - \delta\right]} \qquad (5.3)$$

From (5.2), we obtain: $k^2_{max} - k^2_{min} = \frac{\pi^2}{a^2} + \frac{2\pi}{a} k_{min}$

i.e. $$k^2_{max} - k^2_{min} = \frac{\pi^2}{a^2} + \frac{\pi^2}{a^2} - \frac{2\pi|t|}{a^2} - \frac{2\pi\delta}{a^2} + \frac{4n\pi^2}{a^2}$$

$$\Rightarrow \quad \mathcal{E}_{max} - \mathcal{E}_{min} = \frac{\pi\hbar^2}{ma^2}\left[(2n+1)\pi - (|t|+\delta)\right]$$

Boundary conditions also imply that for the infinite barrier potential are $\mathcal{E}_{max} - \mathcal{E}_{min} = 0$, i.e. for $n=0$, $\delta = \pi$ so that

$$\mathcal{E}_{max} - \mathcal{E}_{min} = \frac{\pi\hbar^2}{ma^2} \times -|t|$$

Energy bands are indeed very narrow and verify $\mathcal{E}_{max} - \mathcal{E}_{min} = o(|t|)$