Folding of Brillouin Zone

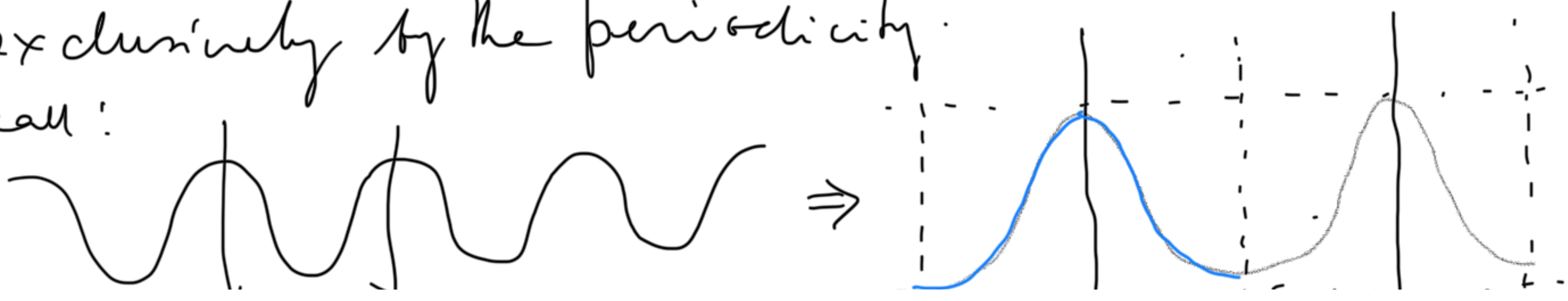
We have already seen that in presence of a periodic potential $v(x) = v(x + la)$; $l = \pm 1, \pm 2, \pm 3, \ldots$

Then the choice of unique q collapses within an interval of $\frac{2\pi}{a}$ in q space where the interval can be arbitrarily chosen.

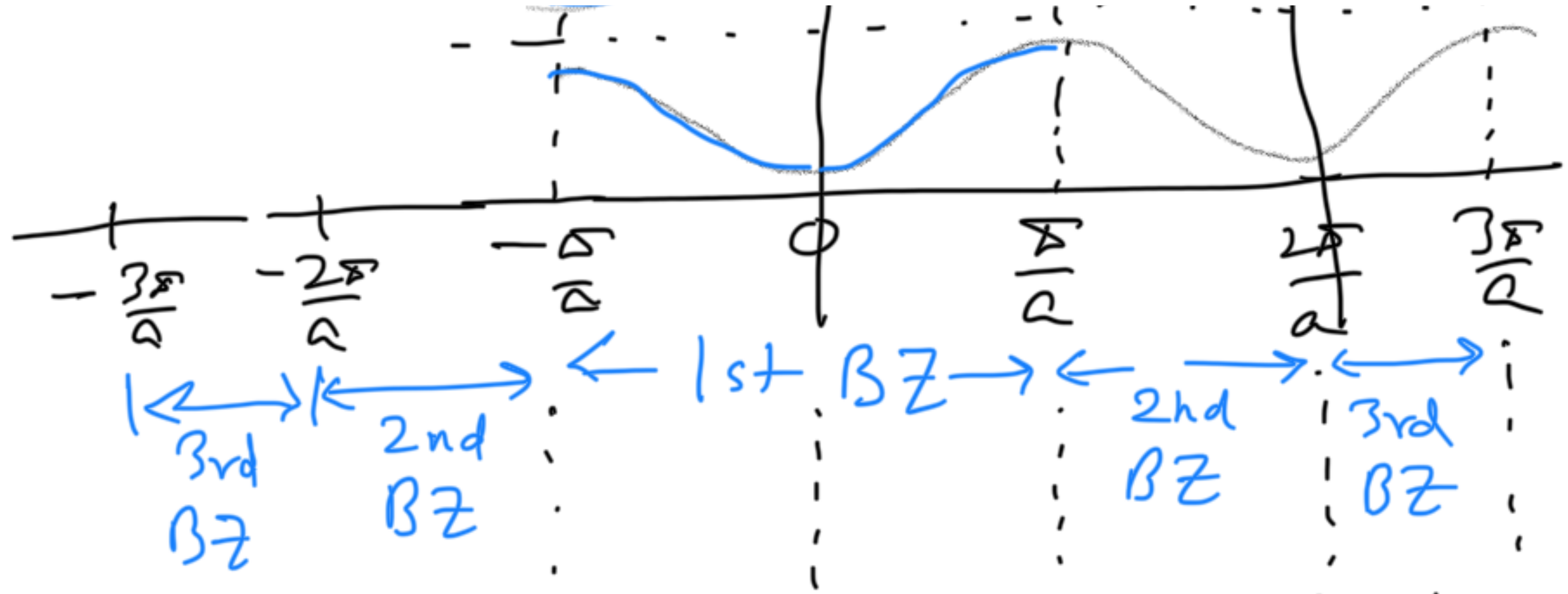
We call it traditionally Brillouin Zone (BZ) arrived from some other context.

Thus the length of BZ in q space is determined exclusively by the periodicity.

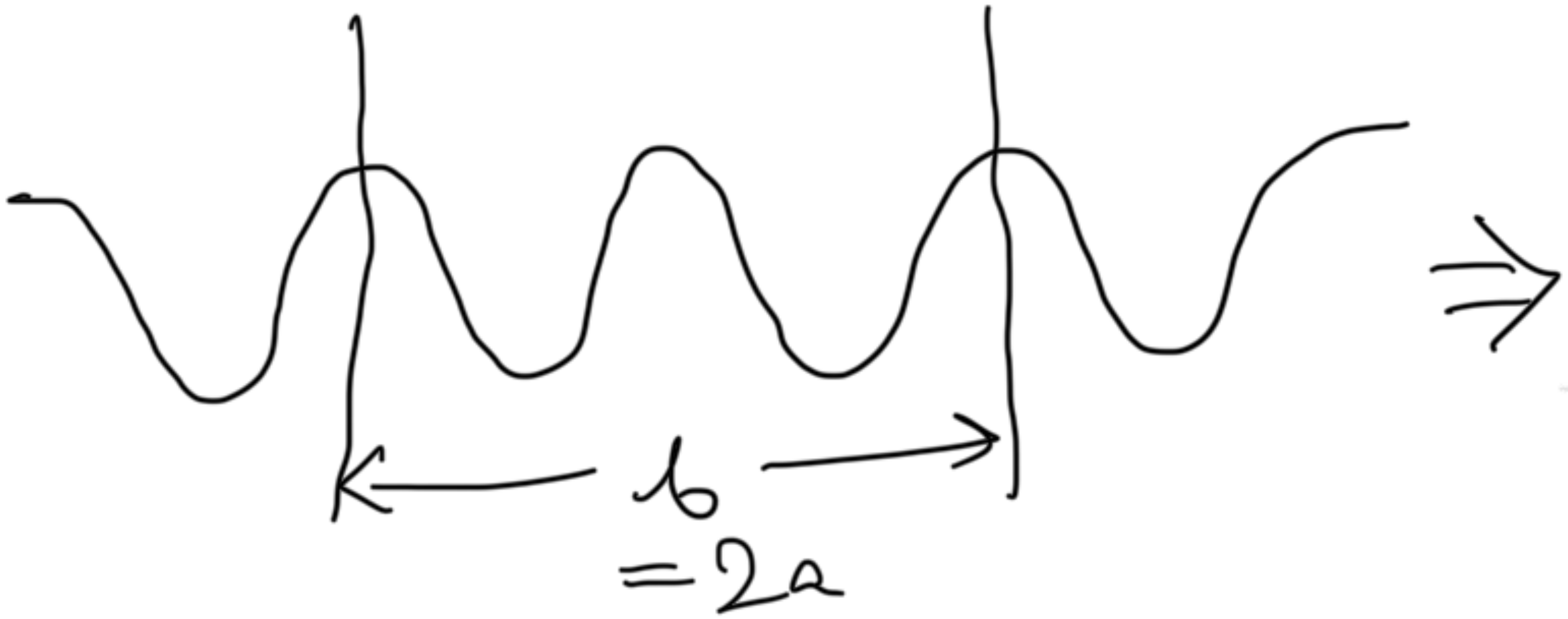
Recall:

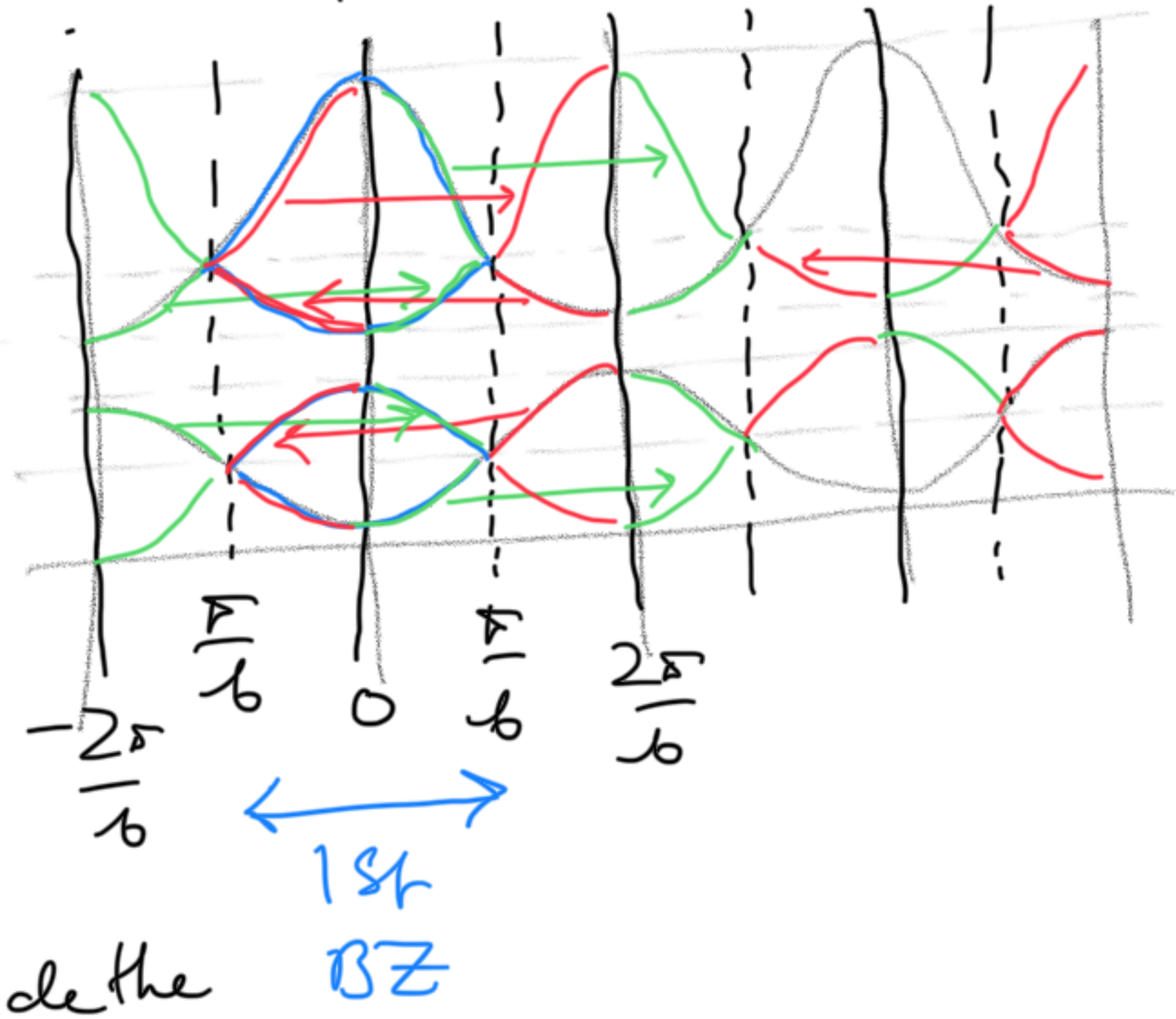


length of BZ $= \frac{2\pi}{a}$



Doubling of unit cell





length of BZ $= \frac{2\pi}{b} = \frac{\pi}{a}$

Note how the red and green segments are getting folded inside the 1st BZ.

The folding happens because $\boxed{E_{q+G} = E_q}$ which is a consequence of $\psi_{q+G} = \psi_q$ since $E_{q+G} = \langle \psi_{q+G} | H | \psi_{q+G} \rangle$

Note $G_1^b = \frac{2\pi}{b} = \frac{2\pi}{2a} = \frac{G_1^a}{2}$

For $0 < q < G_1^b$: $E_q = E_{q+G_1^b} = E_{q+\frac{G_1^a}{2}} = E_{q+\frac{\pi}{a}}$

$\therefore$ $\boxed{\begin{array}{lcl} \text{Doubling of unit cell:} & a & \longrightarrow 2a \\ \text{Periodicity of band structure in } q \text{ space:} & E_q = E_{q+l\frac{2\pi}{a}} & \longrightarrow E_q = E_{q+l\frac{\pi}{a}} \\ & & l = \pm 1, \pm 2, \ldots \end{array}}$

Note that states and energies remain exactly same.
They are simply getting re-labelled.
Shrinking of BZ by half $\rightarrow$ doubling of number of bands.

Note that "half filled band" will now become a "fully filled band" but it will be still be a metal since no gap between 1st and 2nd bands at the edge of the 1st BZ

The gap due to $V_{G_{\pm 1}^a}$ has shifted to the centre of the BZ

... in class)

Think why? (I briefly mentioned [illegible]