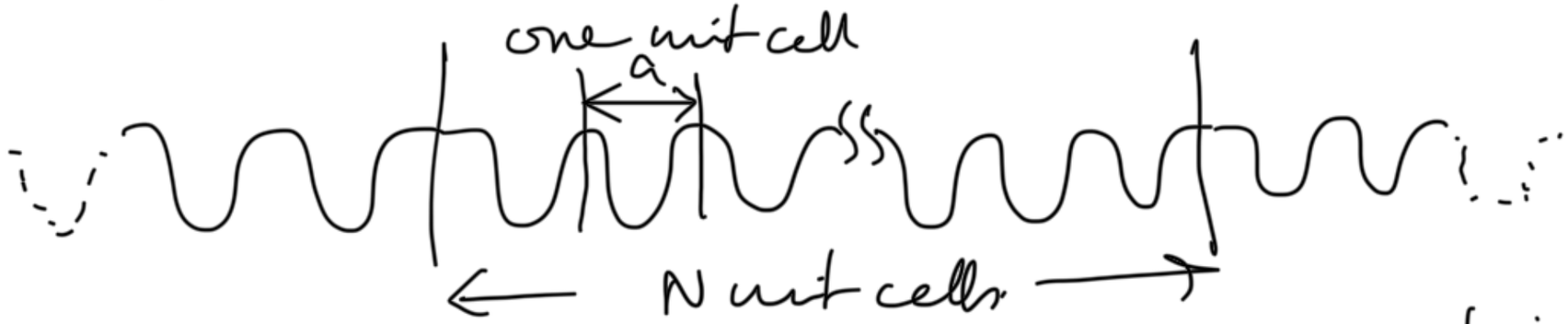
Band filling (at $T = 0°K$)

Recall that we are solving for the BVK cell which contains N number of unit cells.



Setting $N \to \infty$ imply that we are solving for the entire crystal which we ideally would like to do, but would settle for a "large" finite N typically.

Each unit cell represents a repeating unit made for one or more atoms contributing electrons to the crystal.

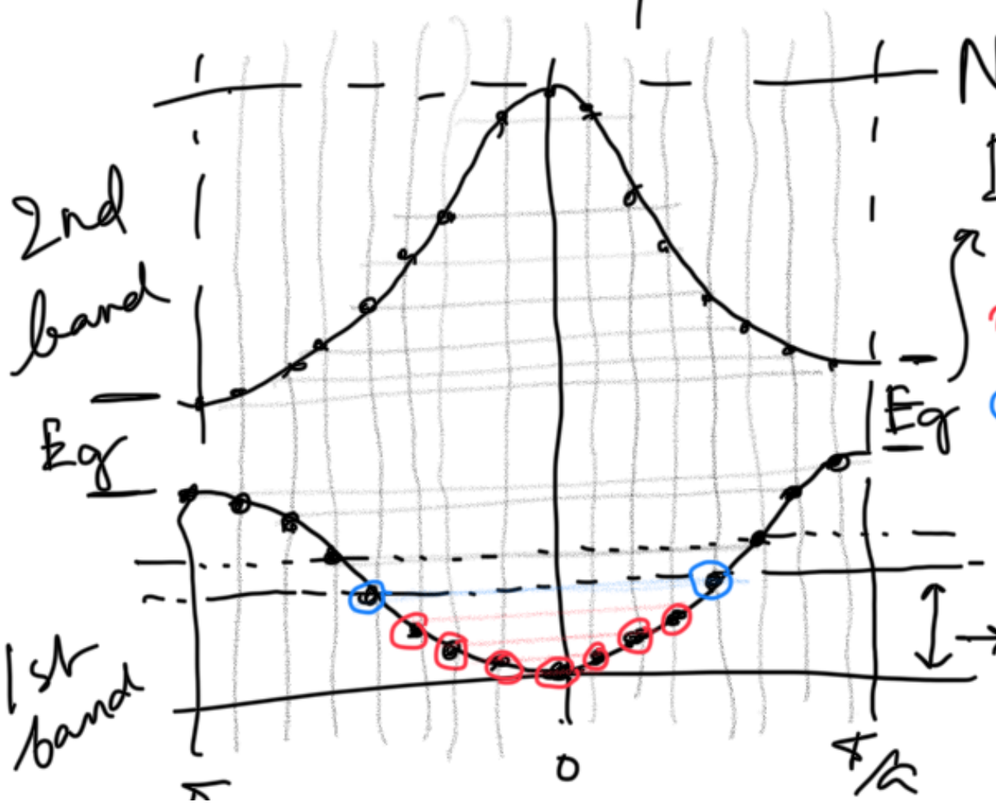
Let each cell contributes 1 electron.

$\Rightarrow$ N electrons in the BVK cell.

$\Rightarrow$ We need N number of states to house them.

Considering spin degeneracy each ψ_{qn} state implies two states: $\psi_{qn\sigma}$ $\psi_{qn\sigma'}$ where σ and σ' on two different spins: $\sigma \equiv \uparrow, \sigma' \equiv \downarrow$ or $\sigma \equiv \downarrow, \sigma' \equiv \uparrow$.

Let us now fill up states from the bottom.

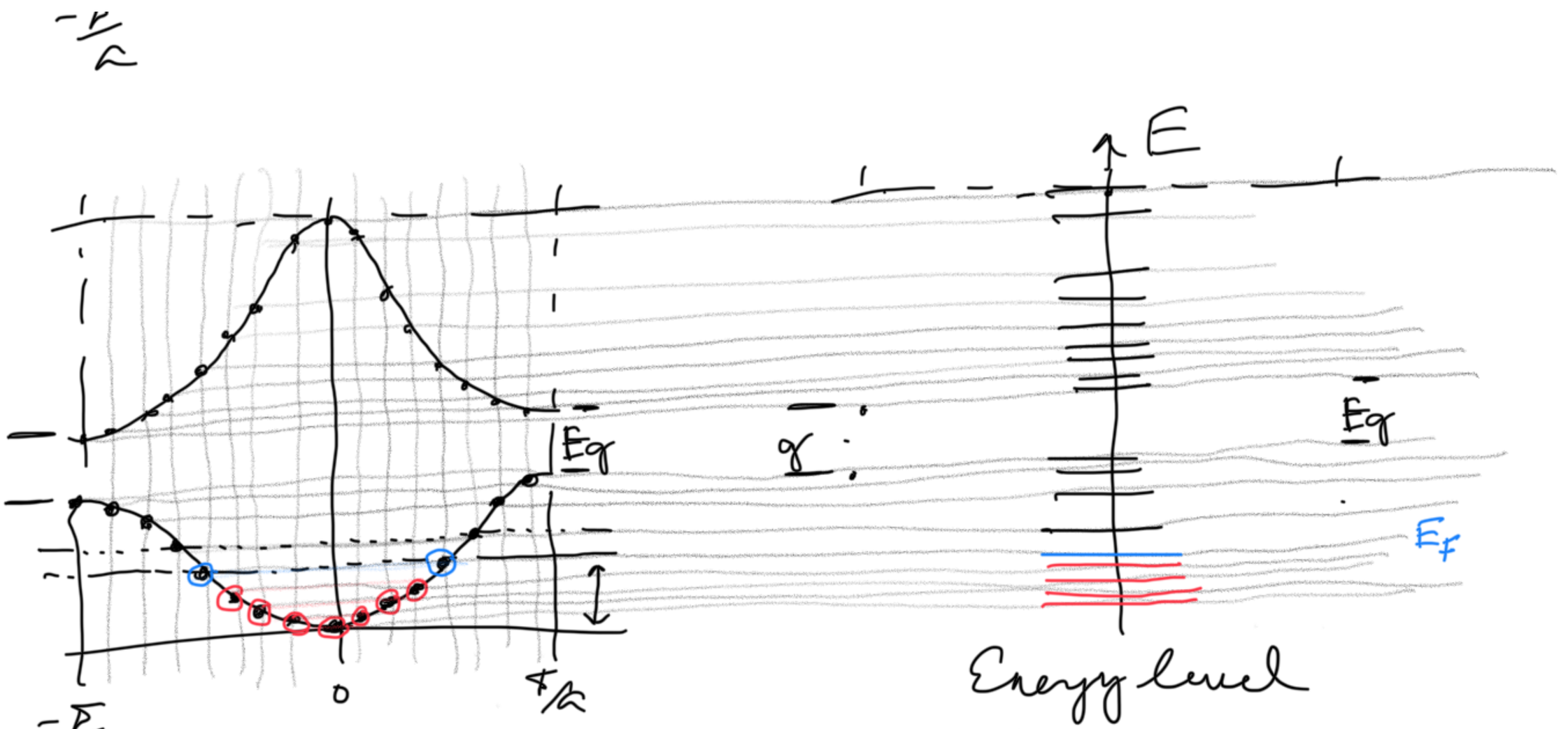


$E_g \rightarrow$ band gap.

- Sites occupied by two electrons, one $\uparrow$, one $\downarrow$
- " " " 1 " , 0.5 $\uparrow$, 0.5 $\downarrow$
- unoccupied states

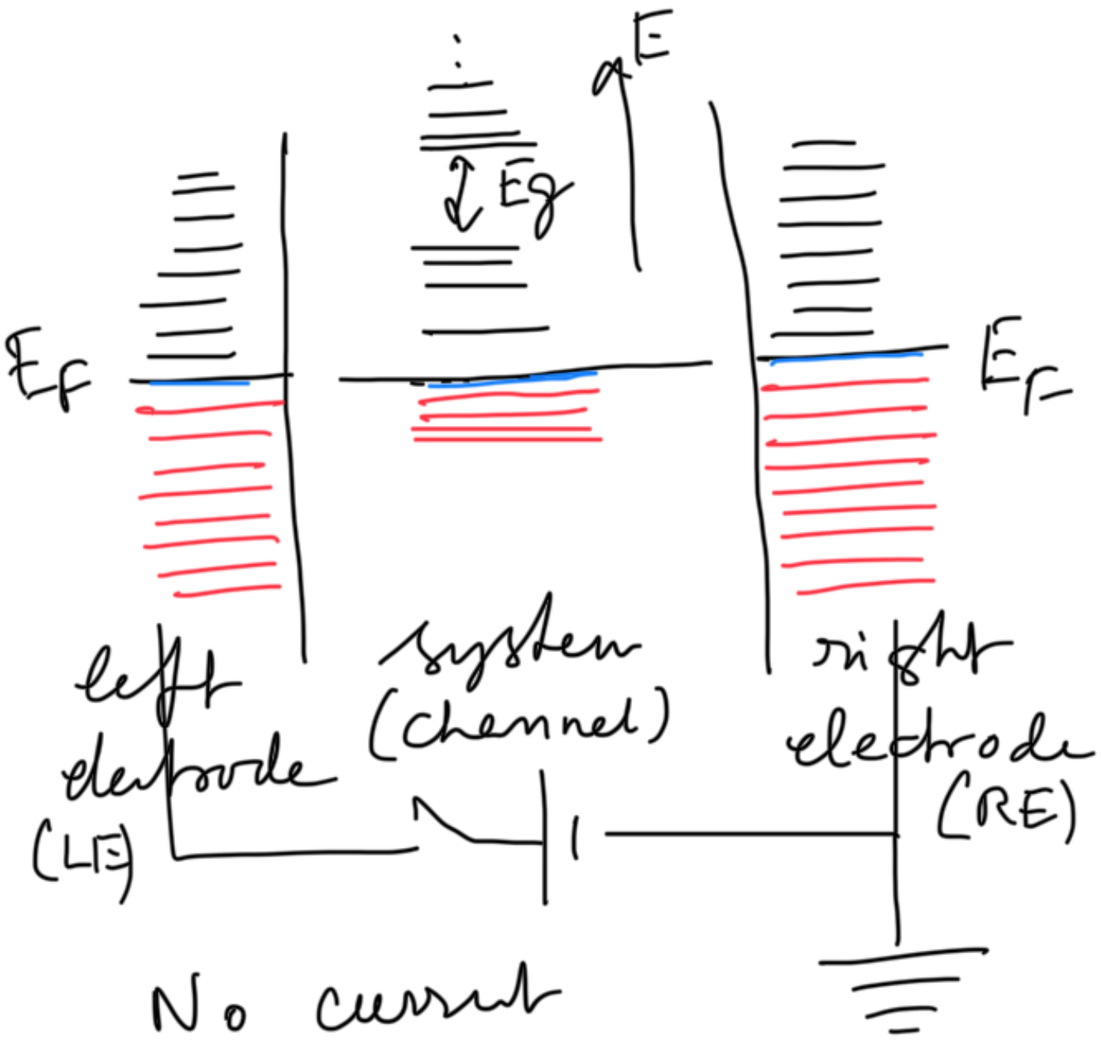
$\rightarrow$ infinitesimally small ΔE as $N \rightarrow \infty$

$\rightarrow$ Half-filled band

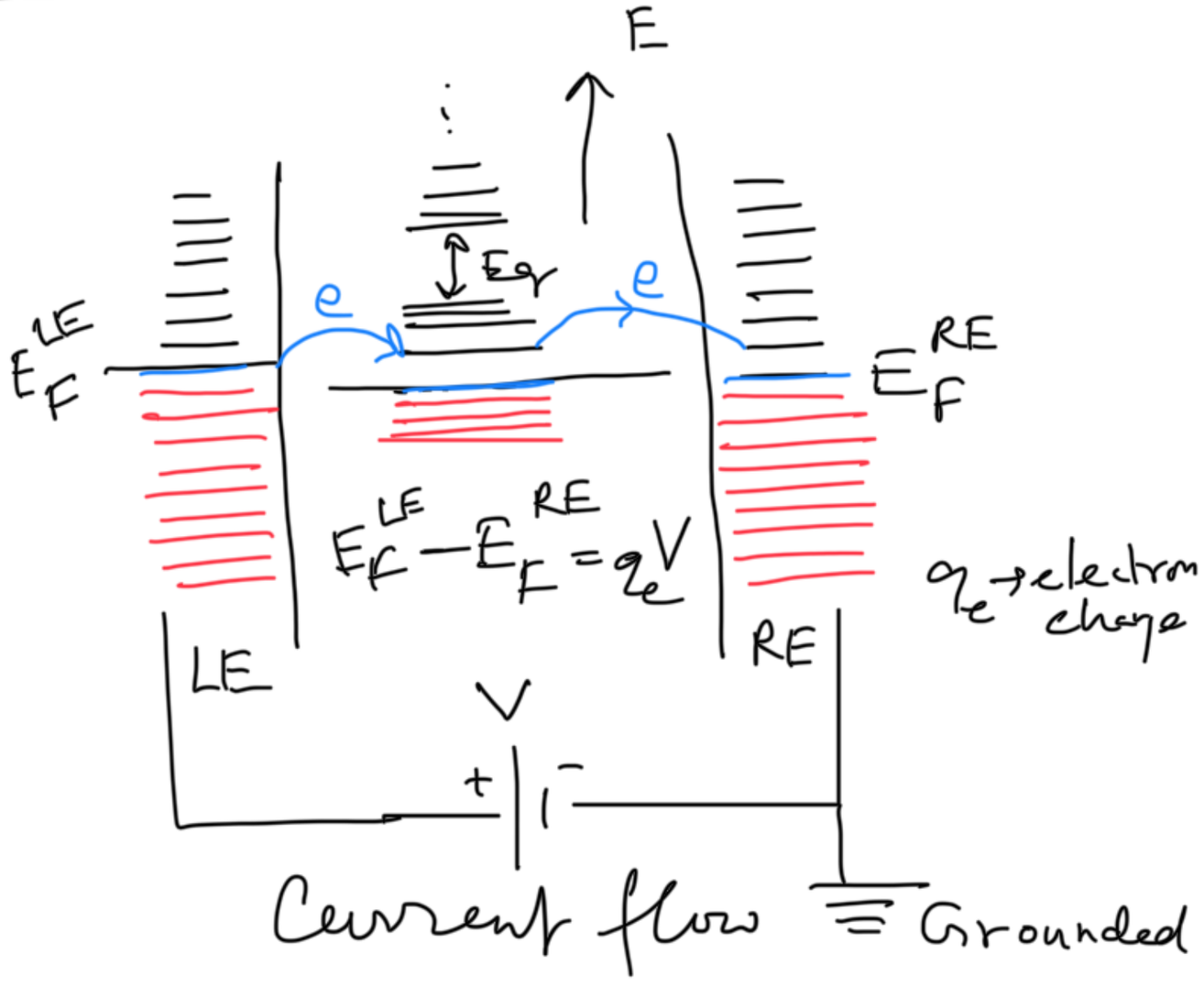


Now let us put the crystal (big chunk) between electrodes.
(We will still assume the crystal to be infinite)
Assume electrodes to be infinitely vast reservoirs of free electrons following Sommerfeld model.

Energy level diagram of device



No current



Current flow ⏚ Grounded

Note that you need available empty states at the channel (system) for current to flow.

(since $N \to \infty$)

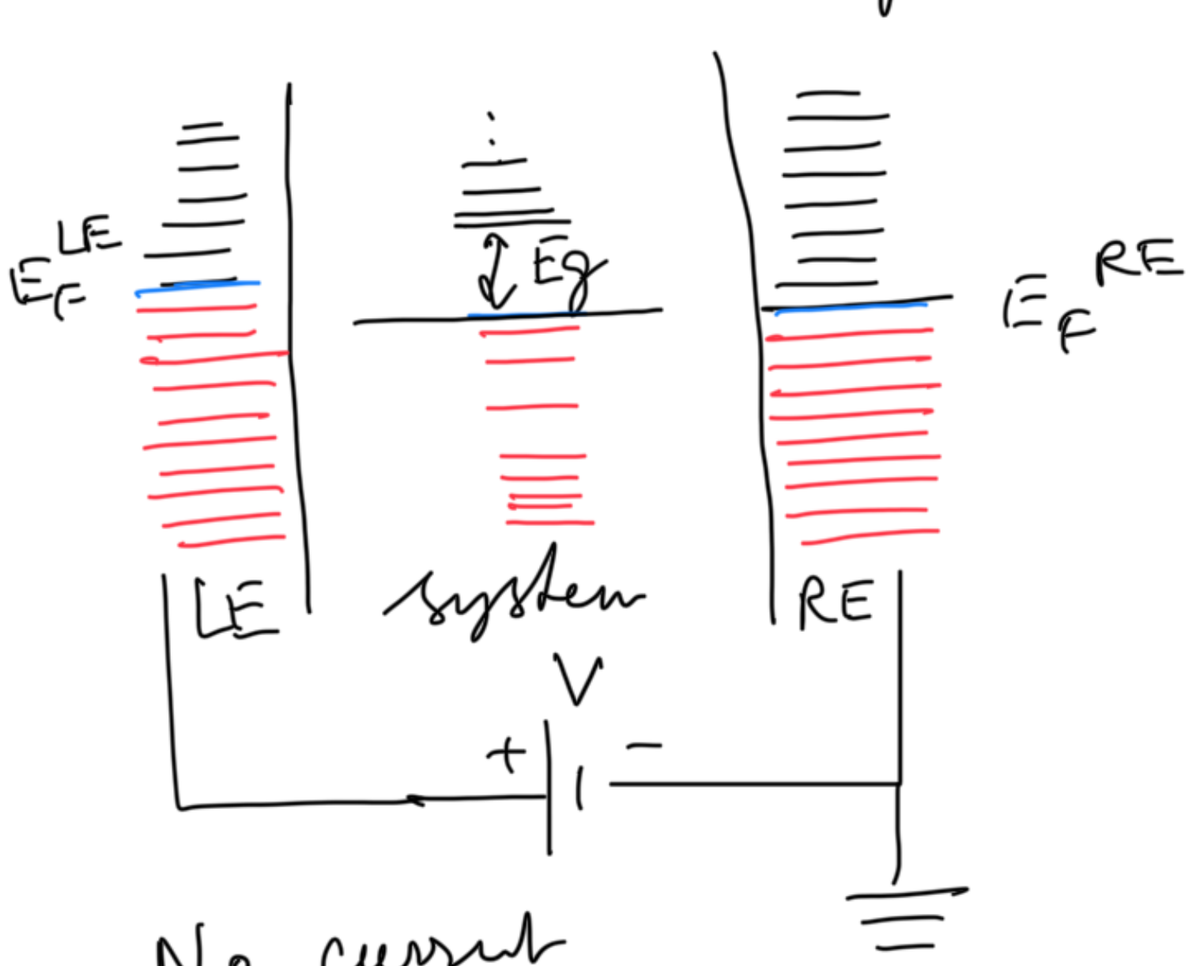
Energy levels are infinitely close in reality except at the band gap E_g.

∴ Infinitesimally small V is sufficient for current to flow.

⇒ Metal!

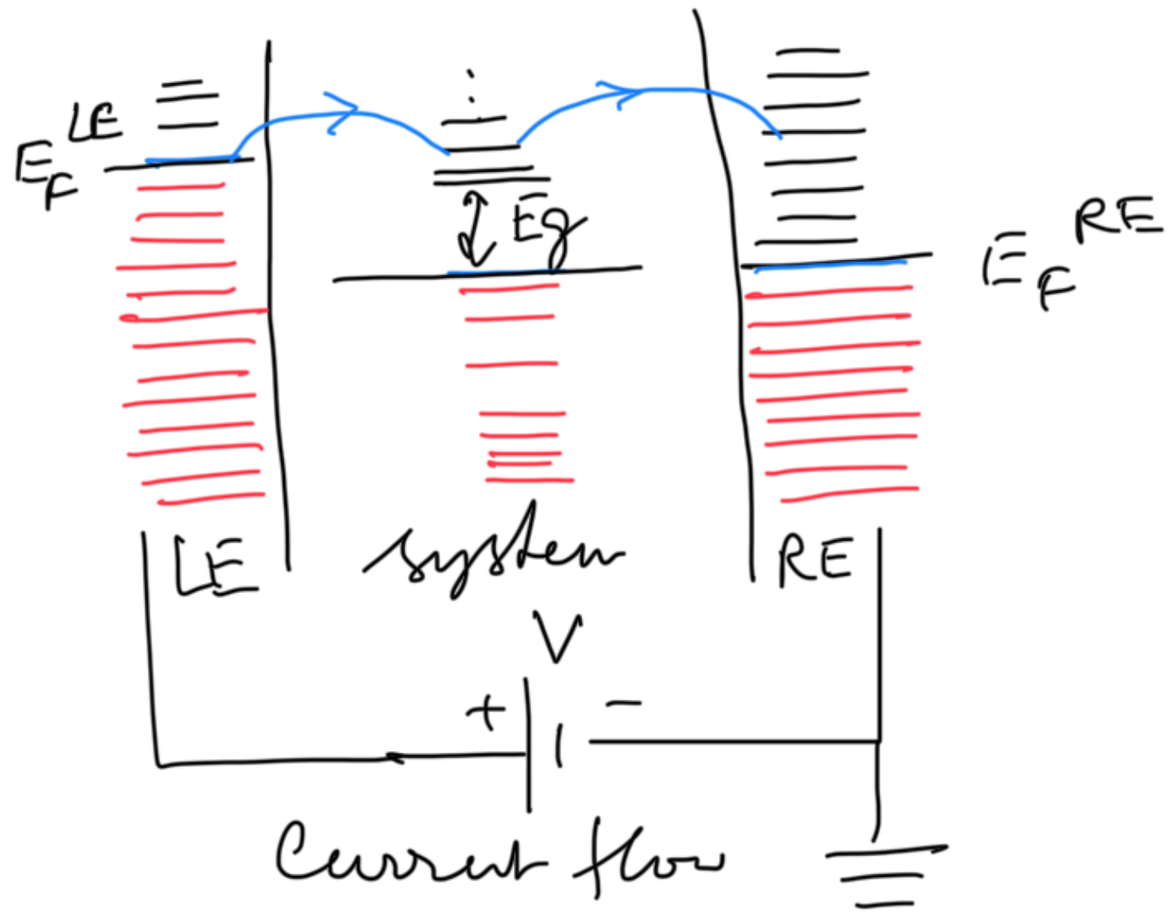
Now if each cell contribute two electron then we need the entire first band to house $2N$ electrons.
In the above picture all 16 q-states of 1st band will be doubly occupied. (Note that $\psi_{-\frac{\pi}{a}} = \psi_{-\frac{\pi}{a}+G_1} = \psi_{\frac{\pi}{a}}$

$\therefore$ filling $q = -\frac{\pi}{a}$ would also imply $q = \frac{\pi}{a}$ is filled.)



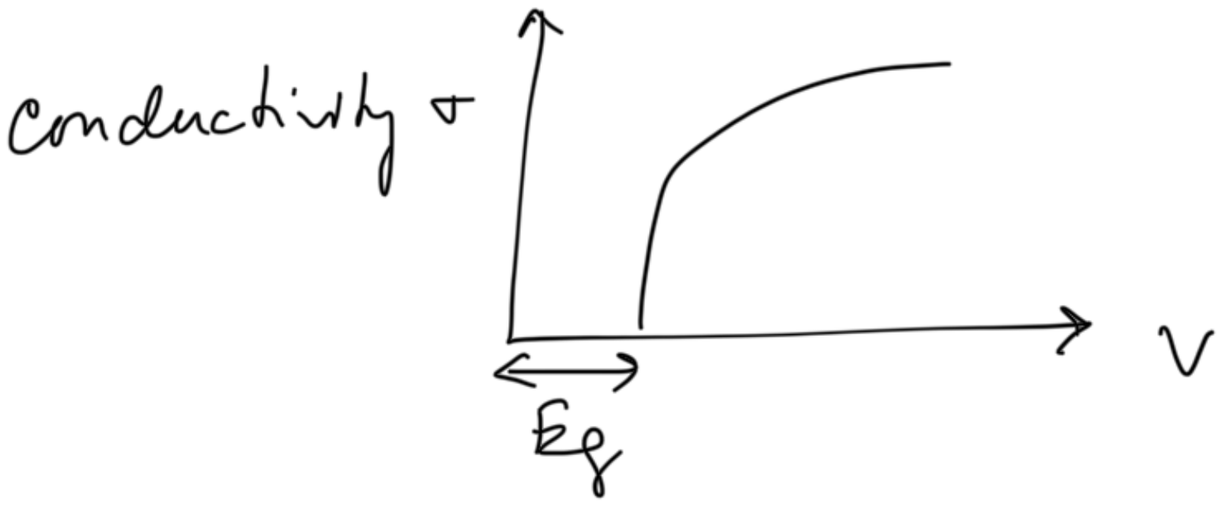
No current

$E_F^{LE} - E_F^{RE} = V q_e < E_g$



$E_F^{LE} - E_F^{RE} = V q_e > E_g$.

Insulator / Semiconductor



∴ 1D chain made of "equispaced" basis each contributing odd number of electron to the crystal will always have the top most populated band half filled and hence a metal.

(basis : one or more atoms decorating a lattice point)