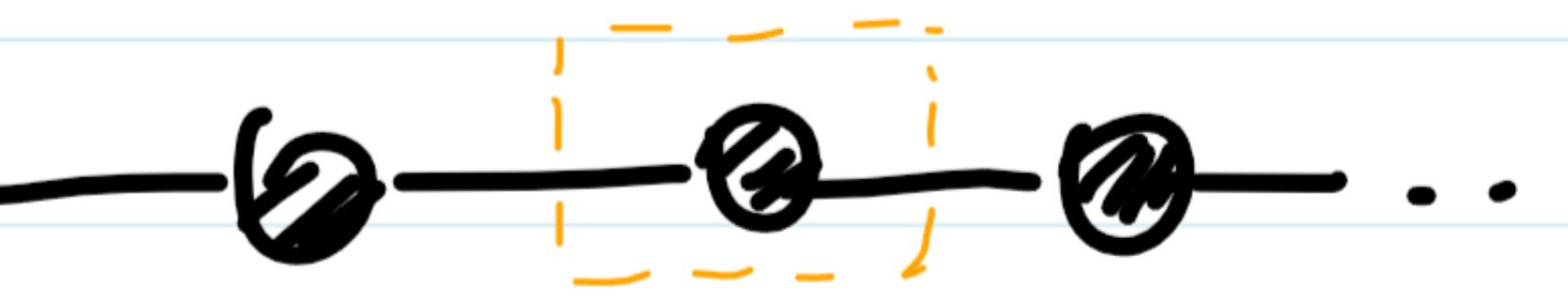


Tight-Binding Notes

Let us consider one unidimensional system like an atomic chain ... 

if the system assumes translational invariance then it can be described by a repeating unit cell. Thus the Bloch theorem can be employed

$$\Psi(\vec{r}) = e^{i\vec{k} \cdot \vec{R}} u(\vec{r}) . \quad (1)$$

$u(\vec{r})$: Periodic spatial site localization function.

\vec{R} : Unit-cell vector.

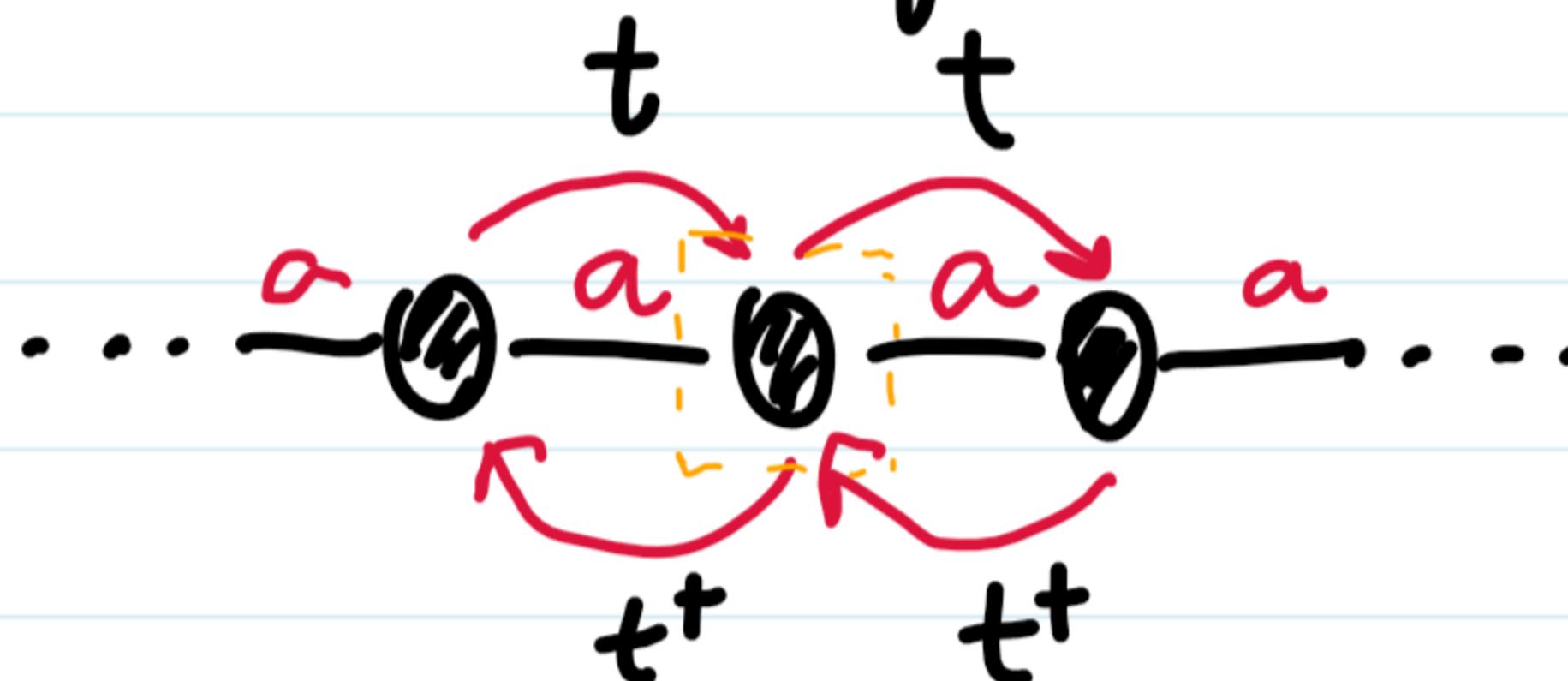
The crystal wave function $\Psi(\vec{r})$ will be given by the product of plane waves by a spatial function that spatially localizes the site positions. Electrons are delocalized in a molecule, ion, or solid metal that are not confined to a single atom or covalent bond, but are instead spread out over several atoms. However the model associated to Bloch W.F.s. dictates strongly site-binded electrons.

This apparent paradox is comprehended by defining a simple hamiltonian,

$$\mathcal{H} = \sum_i \epsilon_i c_i^{\dagger} c_i + \sum_{\langle i,j \rangle} t_{ij} c_i^{\dagger} c_j + h.c. \quad (2)$$

This hamiltonian (2) is the simplest used in tight-binding (TB) approximations. The on-site energy ϵ_i acts as a Coulombian potential, and the electronic dynamics given by a hopping term t_{ij} from site- i to $-j$, both in terms of creation(annihilation) $c^{\dagger}(c)$ operators. Turning back to the chain

example :



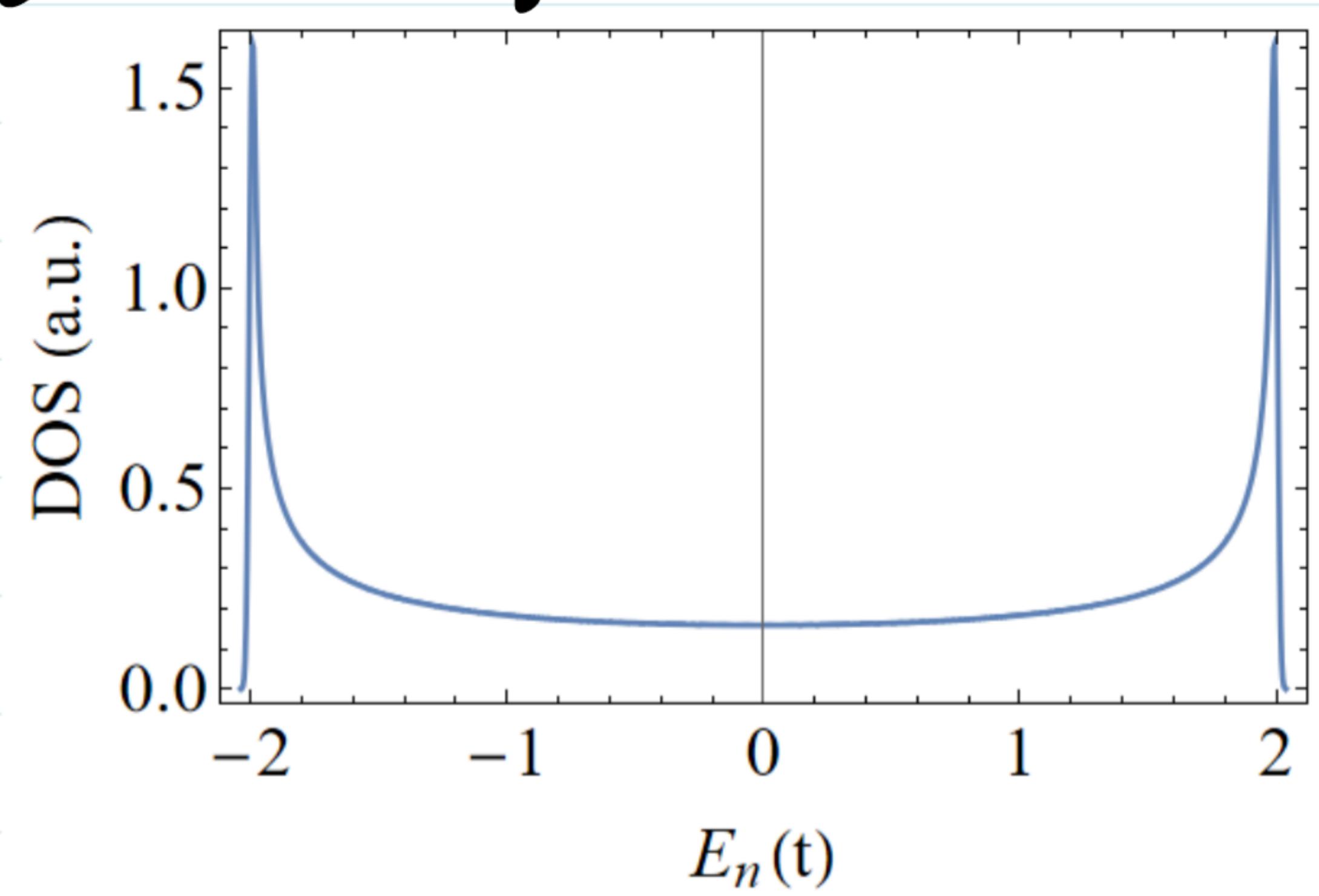
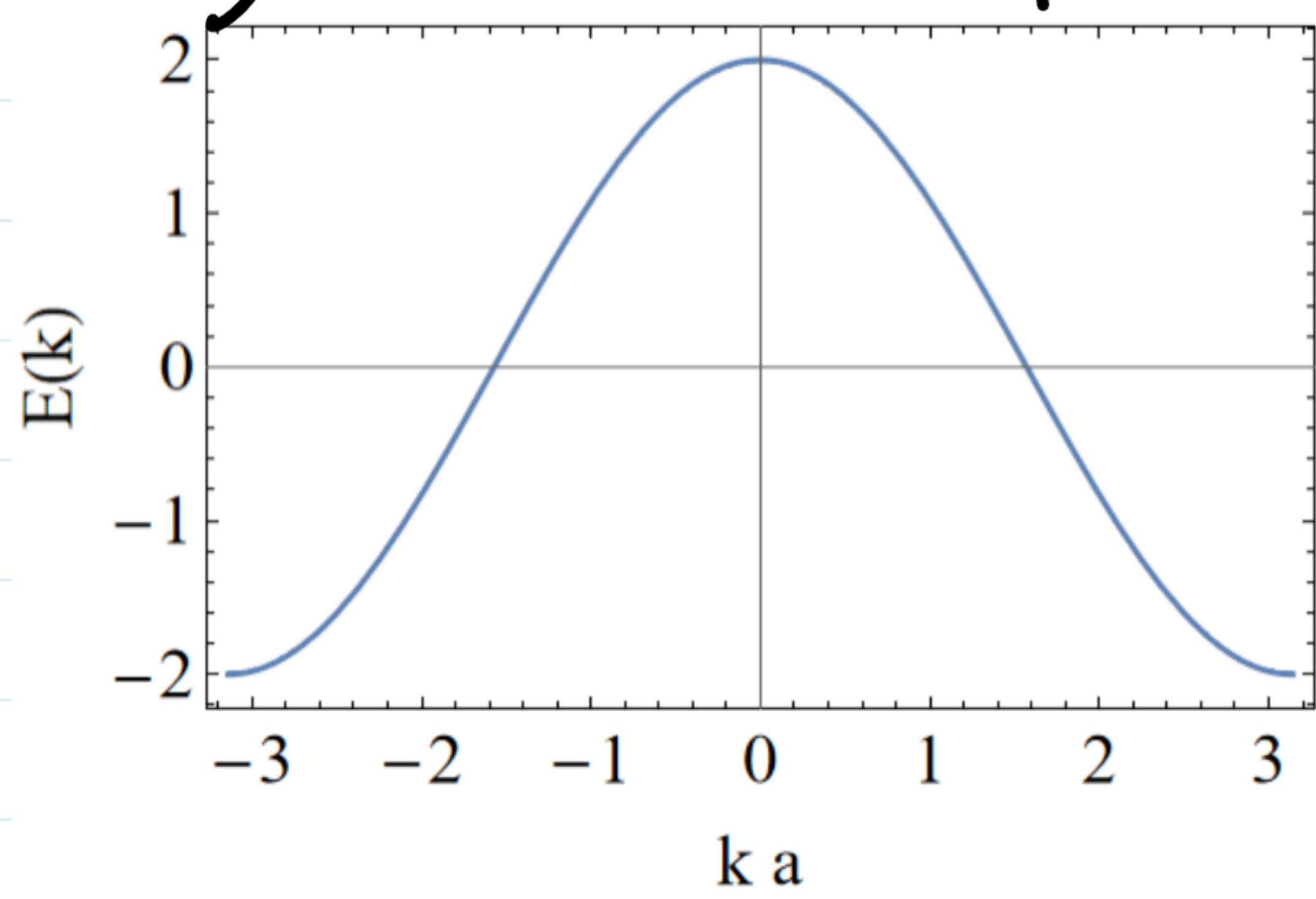
a : lattice parameter

The Schrodinger eigen sol. for this stationary problem gives $E(k) = t(e^{ika} + e^{-ika}) = 2t \cos(Ka)$, where we considered $t=t^*$. The energy dispersion is simple a cosine wave with amplitude $2t$.

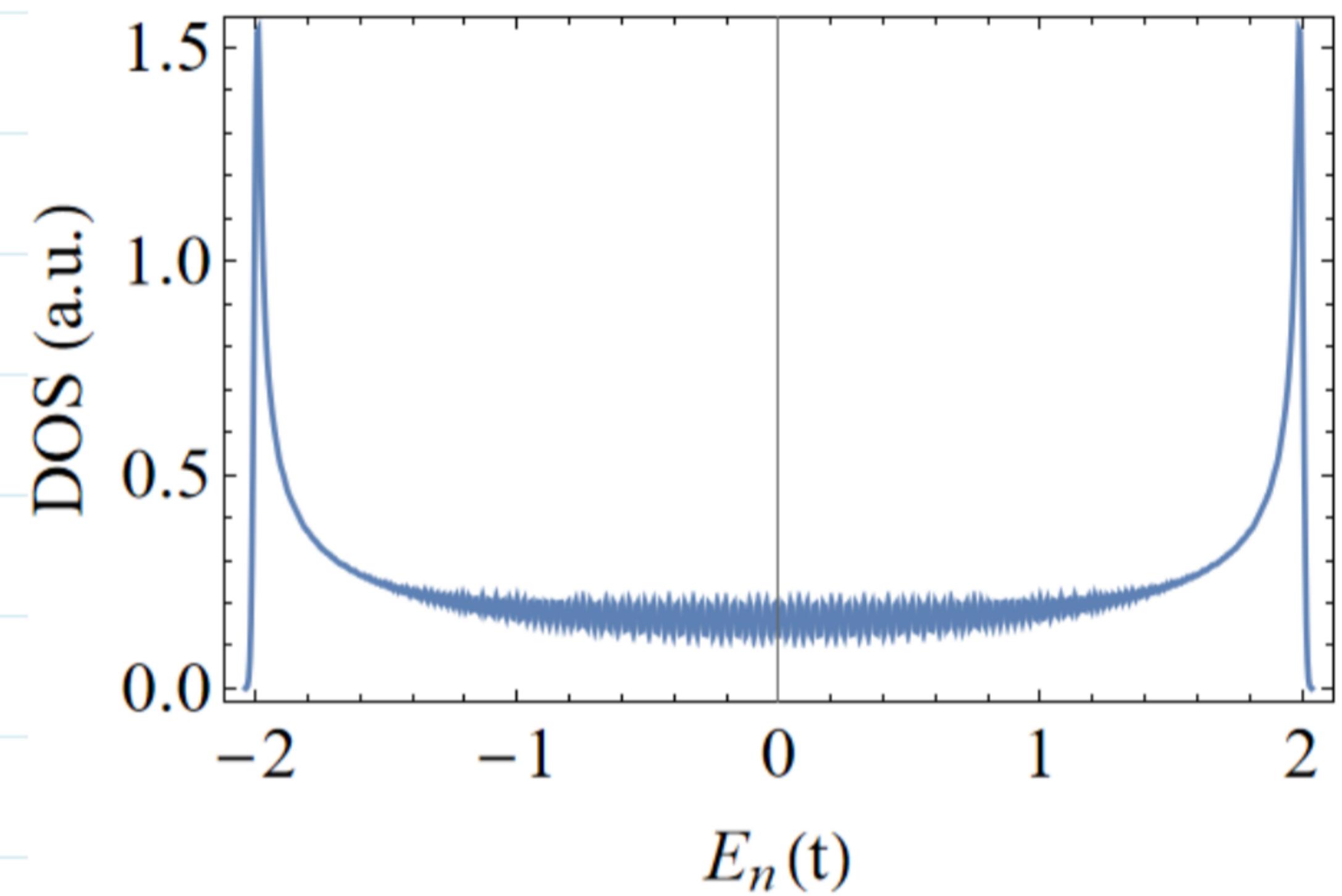
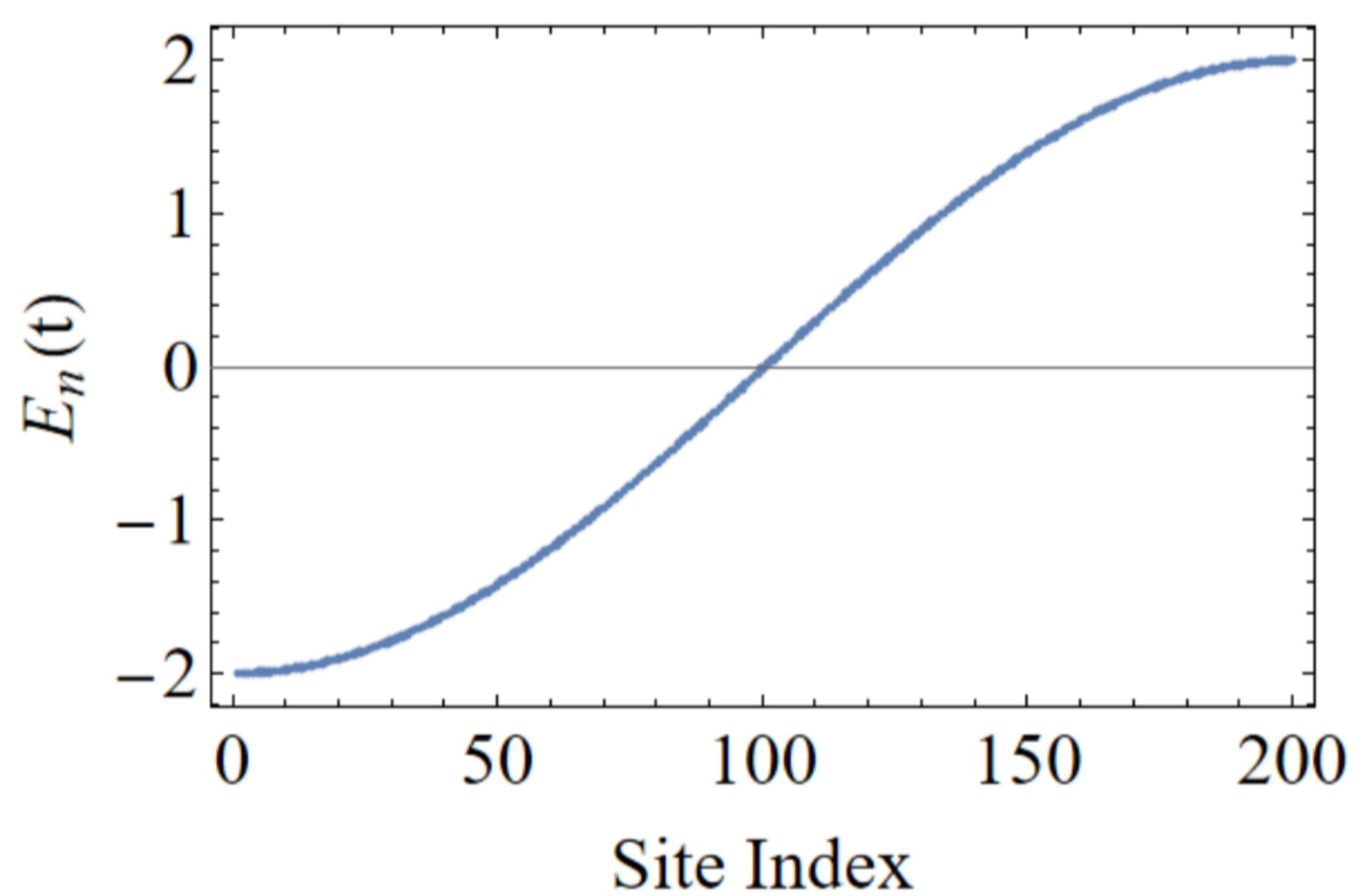
Now let us consider a finite chain with and without the edges sticked. See chain.py code

From the codes:

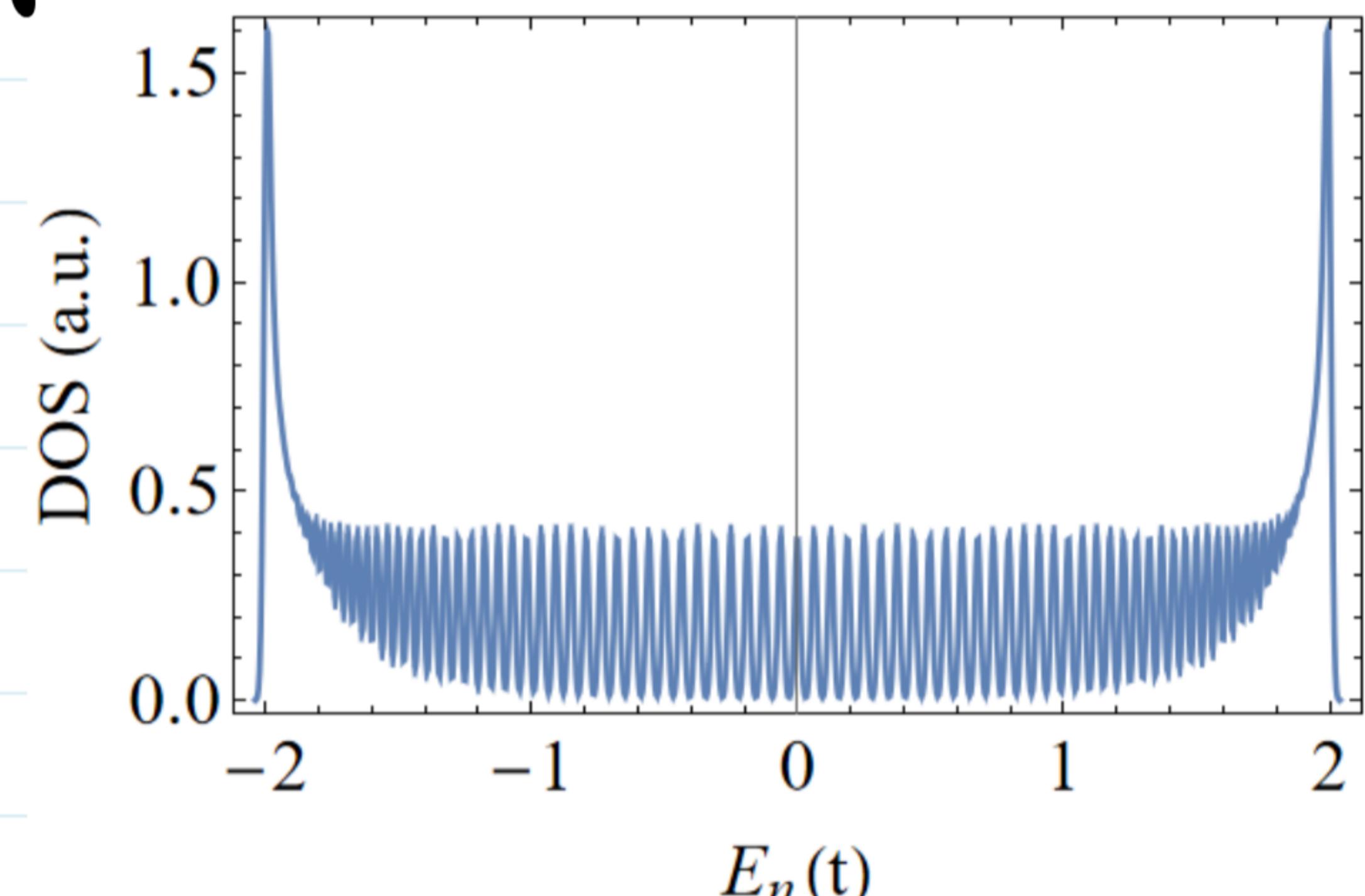
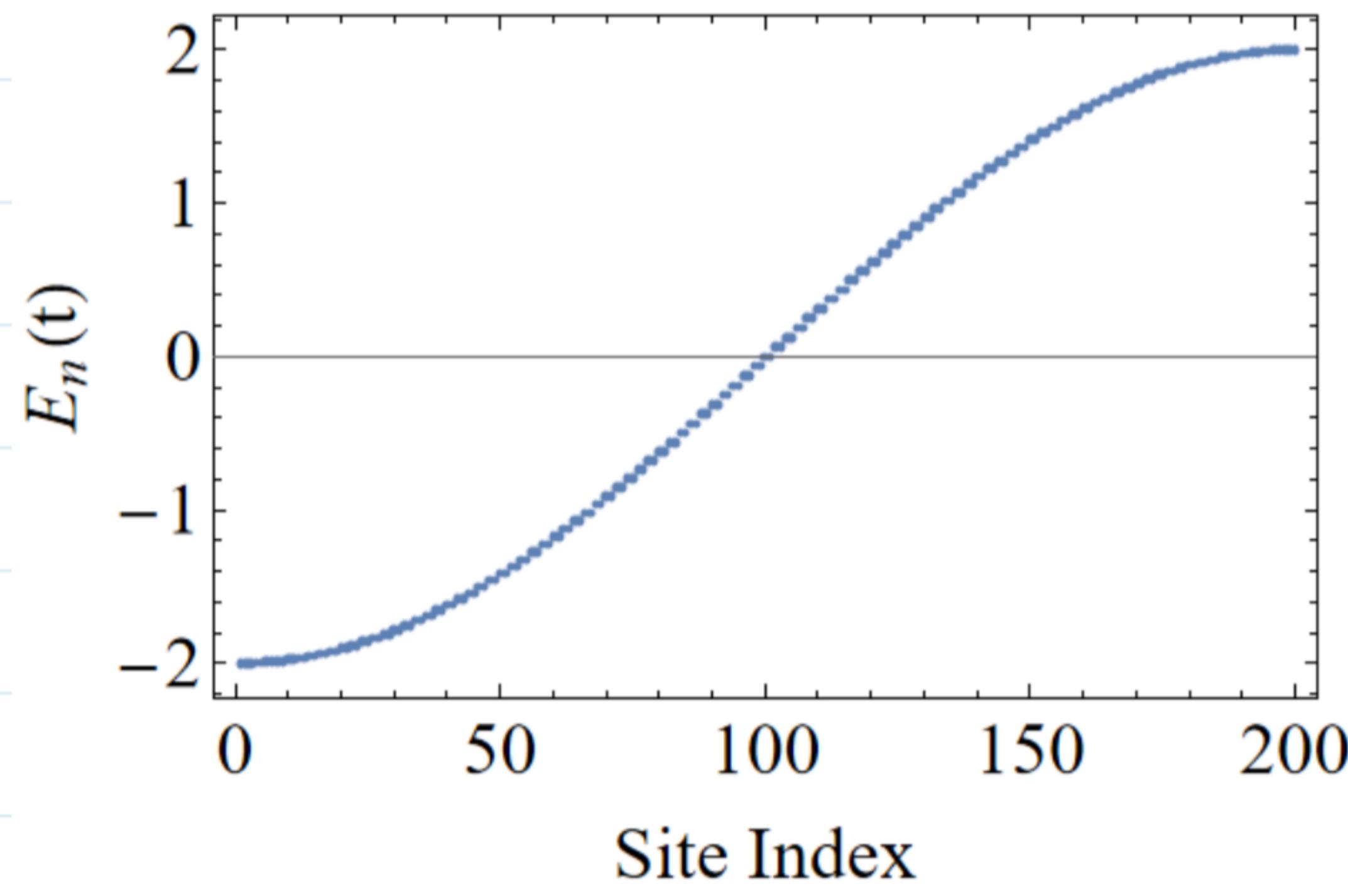
Bloch waves : Periodic Boundary Conditions (PBC)



Open Boundary Conditions (OBC)



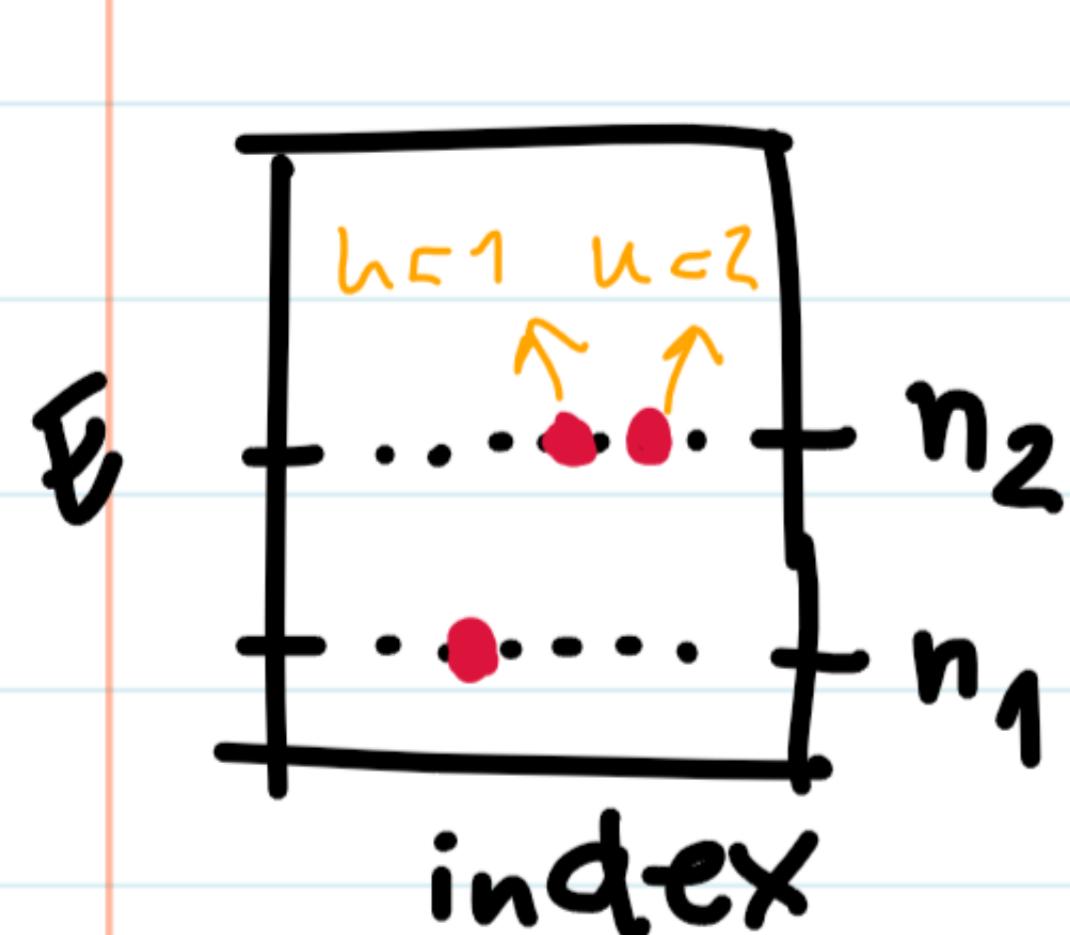
Closed Boundary Conditions (CBC)



We notice that CBC slowly converges to the PBC cases while OBC has only small oscillations near the Fermi level within the Density of States, here simple computed by a smooth histogram function.

We further calculate the local density of states (LDOS) for the OBC with $L=50$

A scheme to understand such calculations

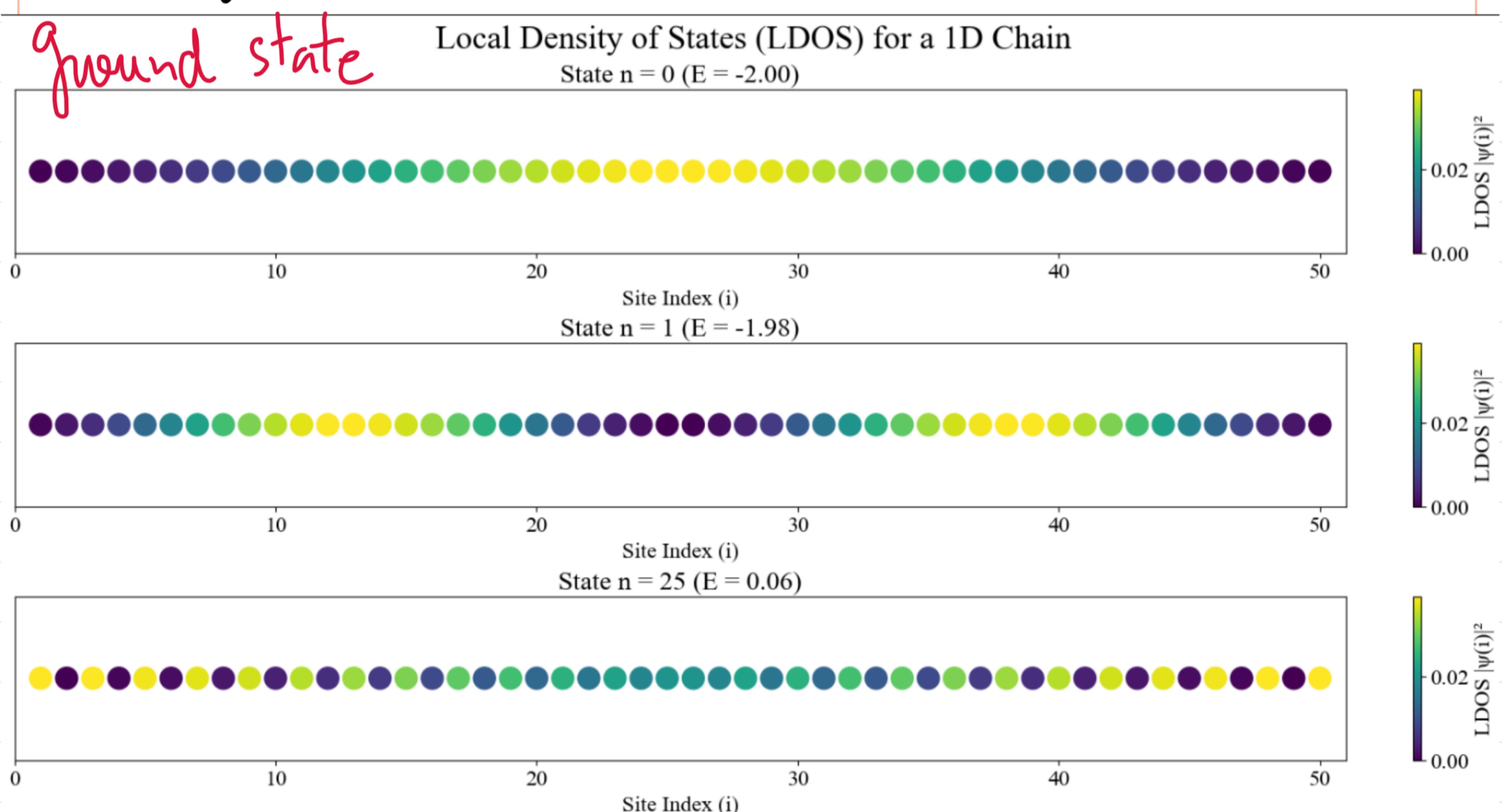


$$E_{n_1} \rightarrow \Psi_{n_1} = (\alpha_1^{n_1}, \alpha_2^{n_1}, \alpha_3^{n_1}, \dots)$$

Ψ_{n_1} is the associated E_{n_1} eigenstate with weights: $\alpha_i^{n_1}$ where $i = 1, \dots, L$

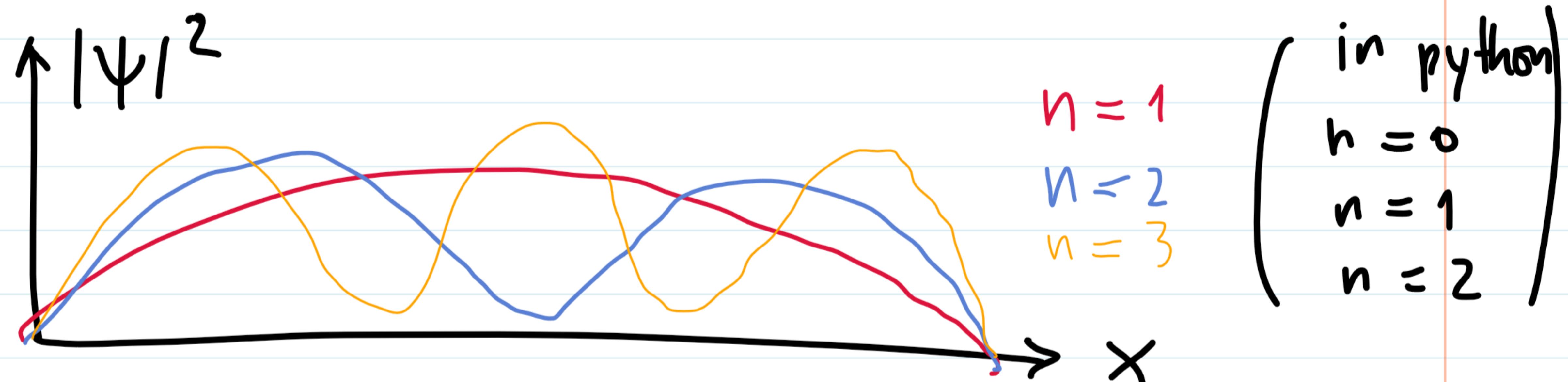
Notice that one energy level is degenerated: E_{n_2} , in this case we must compute $\sum_{h=1}^2 \Psi_{n_2}^h$

Going back to the finite chain LDOS:



As expected the lower energy states shows a stationary wave pattern with n -th lower states showing $\frac{n}{L}$ max. values.

This result is compatible with the solution obtained solving the Schrödinger equation for 1D confined electronic wave, where



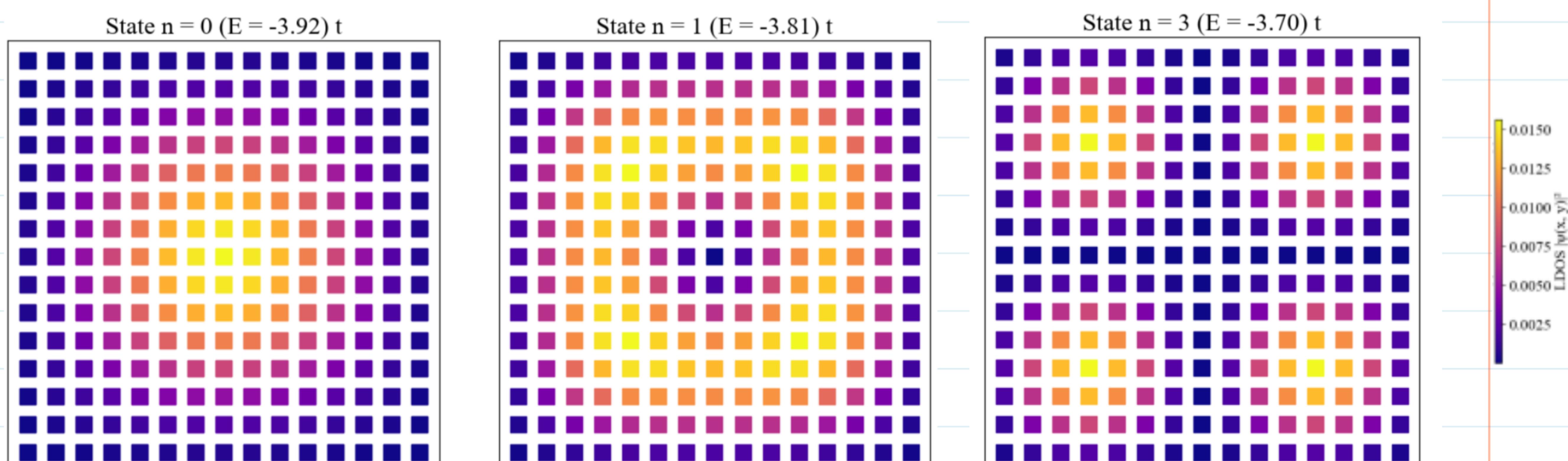
You can convince yourself by plotting further lower eigenstates.

`calculate_and_plot_ldos(0, axes[0])`

↑ change
the index
here

Moreover we can stack the chains and create a finite squared lattice.

The LDOS for this case considering OBC is like the following



Similar solutions to electrons trapped in a 2D box check it in your favorite Q.M. book.

