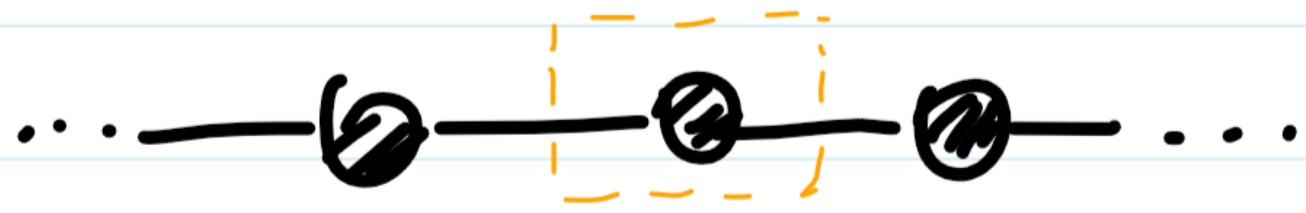
Tight-Binding Notes

Let us consider one unidimensional system like an atomic chain 

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

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

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

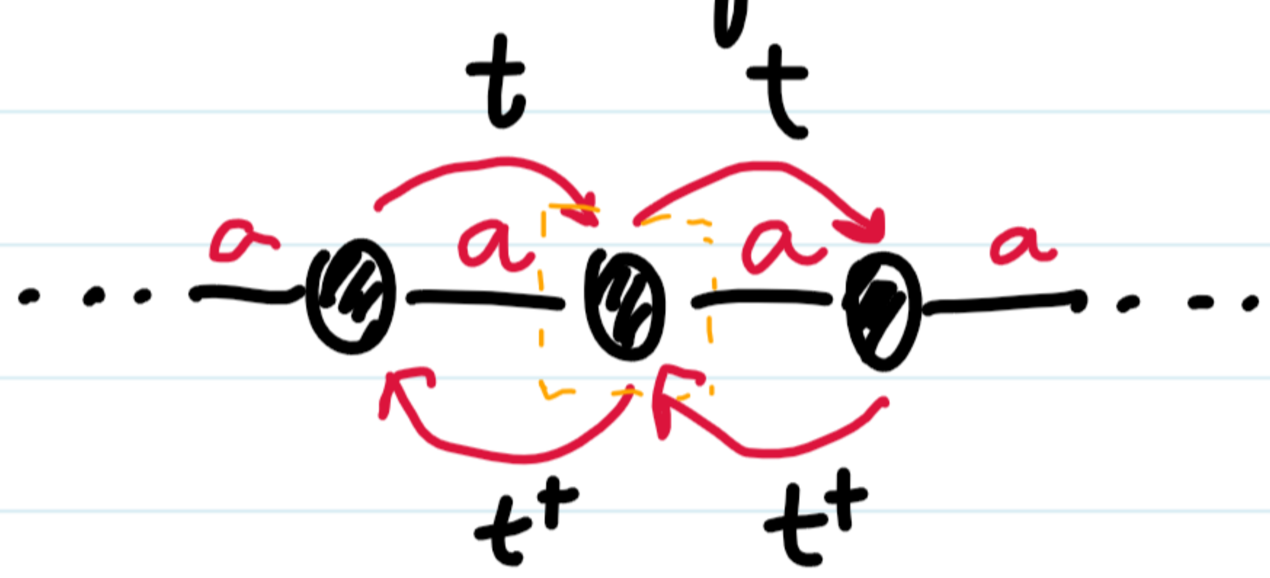
$\vec{R}$: Unit-cell vector.

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.fcs. dictates strongly site-binded electrons.

This aparent paradox is comprehended by defining a simple hamiltonian,

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

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 (anihilation) $c^\dagger$ (c) operators. Turning back to de chain example:



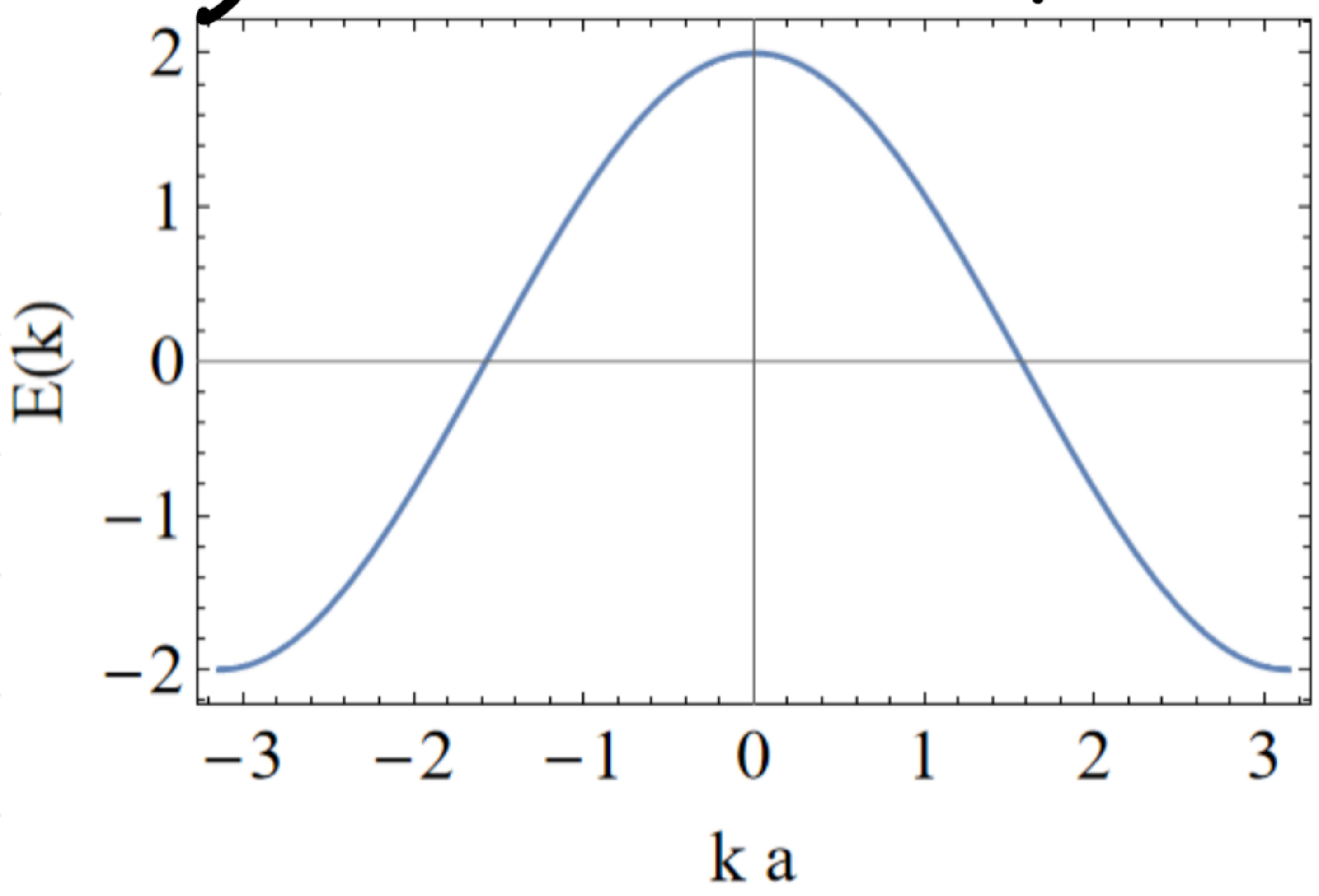
a: Lattice parameter

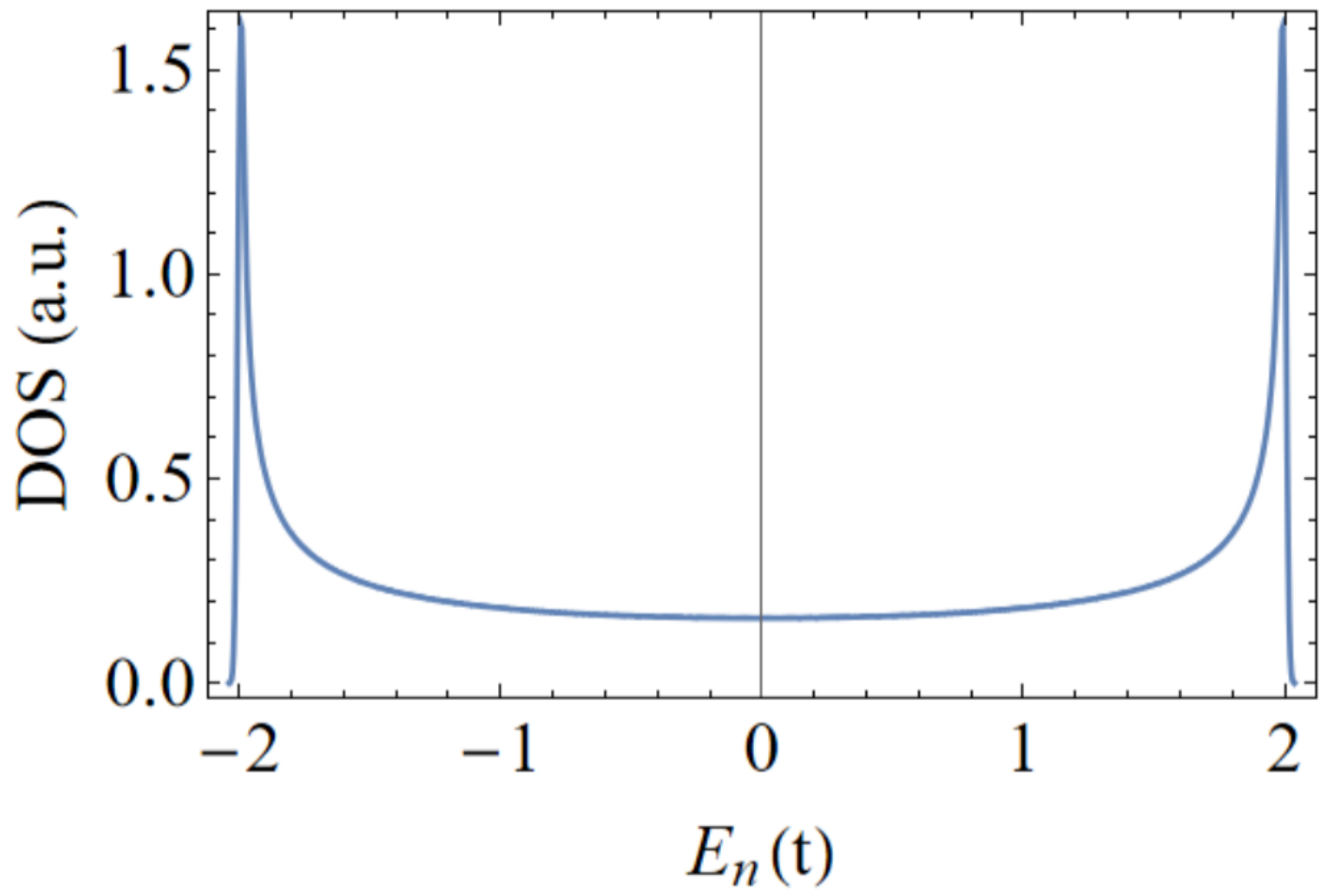
The Schrodinger eingen sol. for this stationary problem gives $E(k) = t(e^{ika} + e^{-ika}) = 2t\cos(ka)$, where we considered $t = t^\dagger$. The energy dispersion is simple a cosine wave with amplitude $2t$.

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

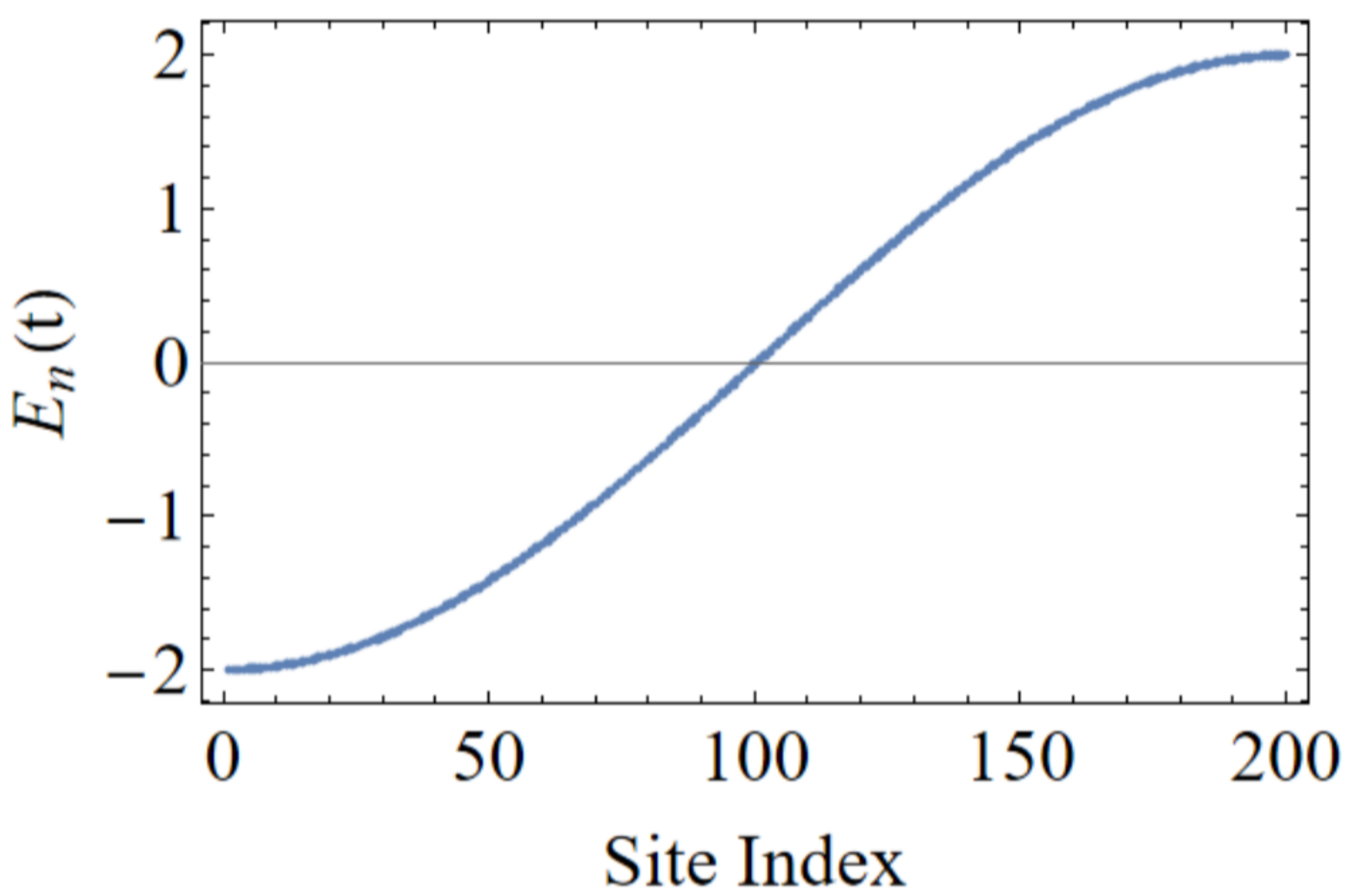
From the codes:

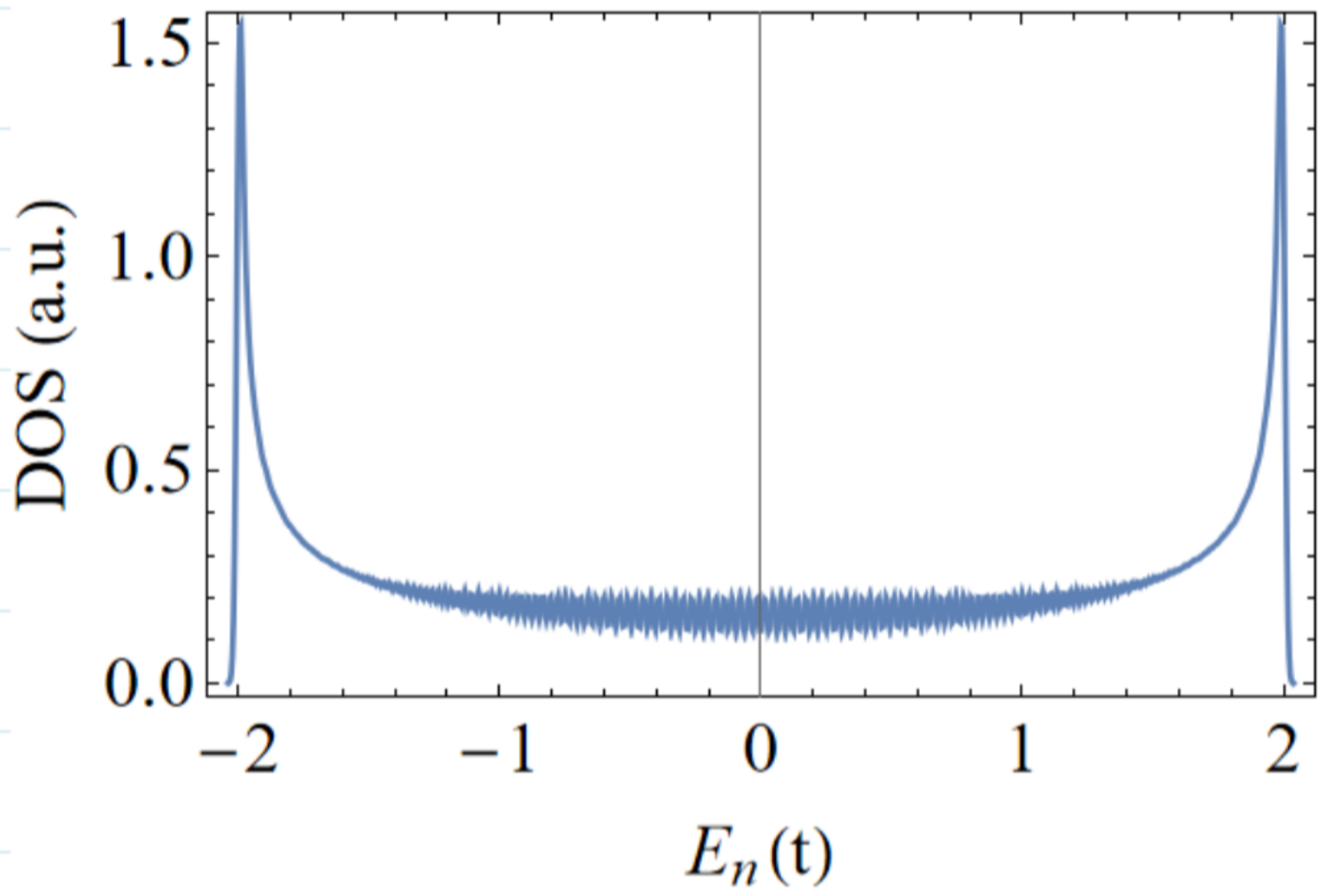
Bloch waves : Periodic Boundary Conditions (PBC)



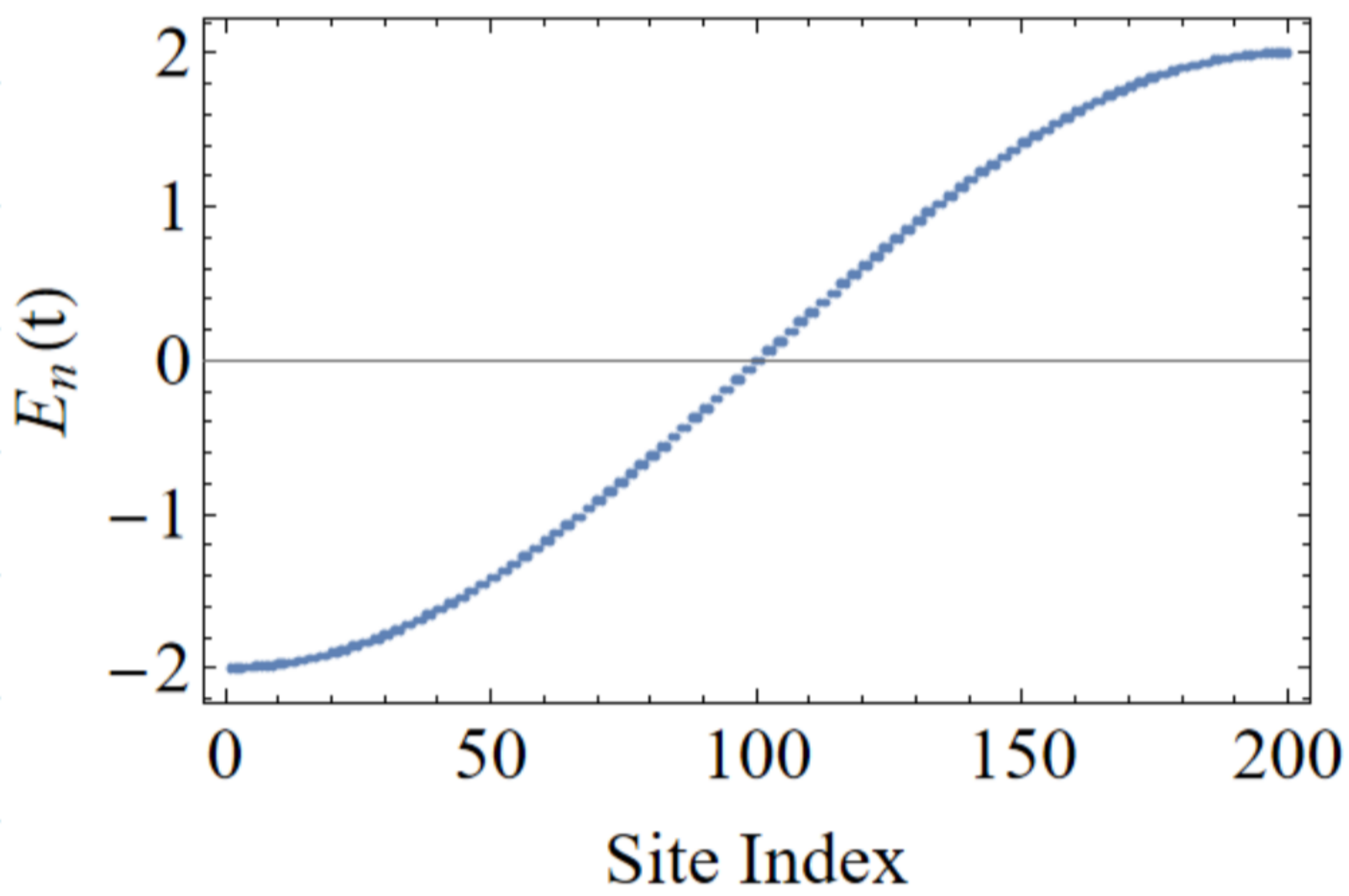


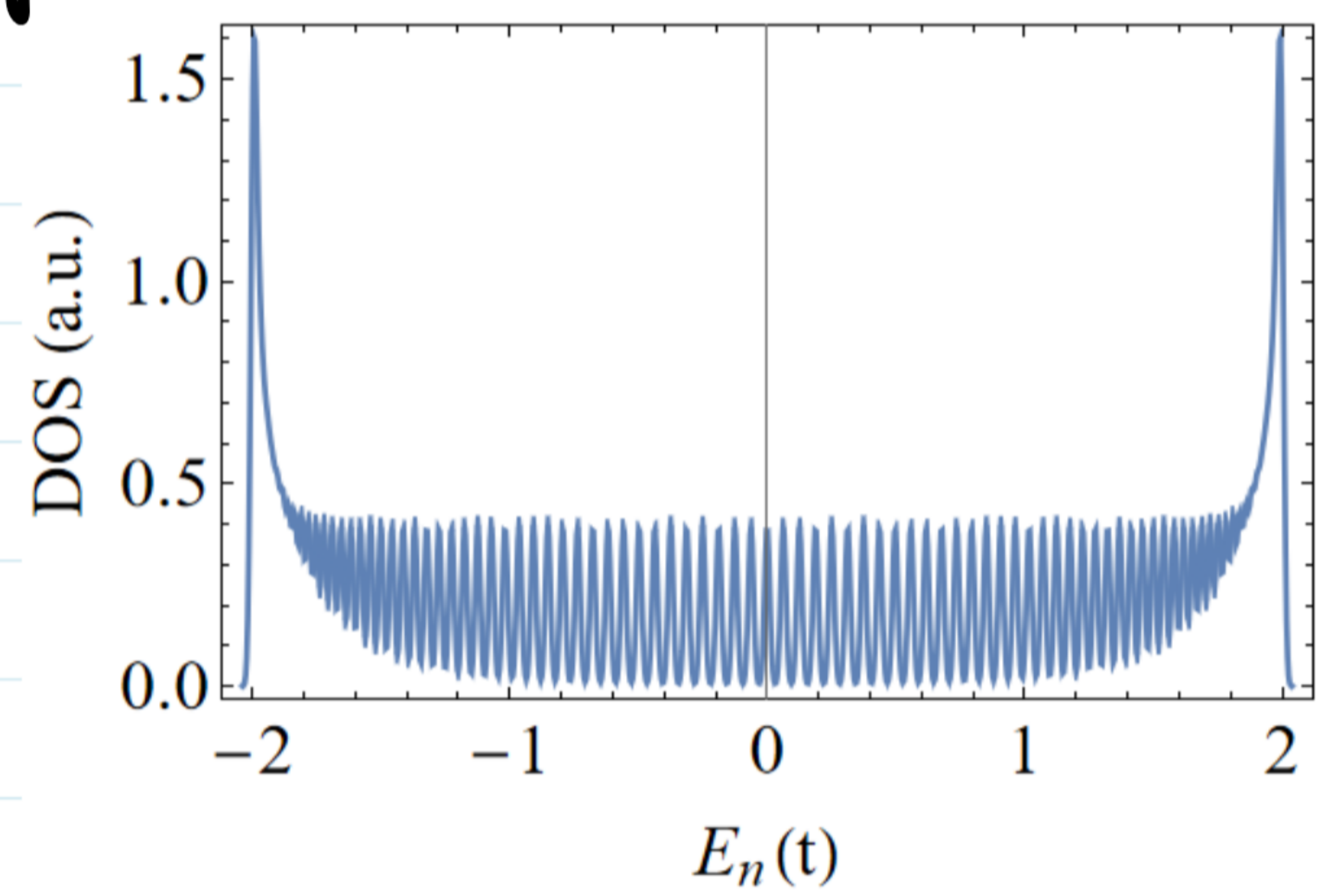
Open Boundary Conditions (OBC)





Closed Boundary Conditions (CBC)





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