Estado Sólido I
Tarea 6: Estructura de Bandas

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Nombre del Estudiante: _____

Problema 1 *Tight binding model for the linear chain*

Apply the tight-binding model for the linear chain with only one atomic species in the basis. Consider interactions up to first-nearest neighbors and use s and p (p_x, p_y, and p_z) orbitals as expansion basis. In particular, obtain the following:

(a) The complete (non-diagonal) matrix-form Hamiltonian $\hat{H}$.

(b) The diagonal-form of $\hat{H}$, in particular the expressions of each band of the system.

(c) The plot of the band structure (by any software of your preference), using the following numerical values: $\epsilon_s = 4$, $\epsilon_{p_x} = \epsilon_{p_y} = \epsilon_{p_z} = 18$, $V_{ss\sigma} = -1.4$, $V_{sp\sigma} = 1.84$, $V_{pp\sigma} = 3.24$, and $V_{pp\pi} = -0.81$.

Hint: You can use a software to diagonalize the matrix $\hat{H}$.

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Problema 2 *Density of states for a $2D$ system*

For the square lattice ($2D$), with only one atomic species, s-orbitals as expansion basis, and taking into account interactions up to first nearest-neighbors, the following band-structure is obtained:

$$E(\mathbf{k}) = \epsilon_s + 2V_{ss\sigma}\left(\mathrm{Cos}k_x a + \mathrm{Cos}k_y a\right).$$

Write down the integral expression for the density fo states, $g(E)$.

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