

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 any 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:

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

Write down the integral expression for the density of states, $g(E)$, in terms of E , k_x , and dk_x .

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