

Física Atómica y Molecular

Tarea 03: Bases de expansión

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Nombre del Estudiante: _____

Problema 1 *Product of two gaussians*

Show that the product of two gaussians is also a gaussian, given by:

$$e^{-\alpha|\mathbf{r}-\mathbf{R}_A|^2} e^{-\beta|\mathbf{r}-\mathbf{R}_B|^2} = K_{AB} e^{-\gamma|\mathbf{r}-\mathbf{R}_C|^2}$$

where:

$$\gamma = \alpha + \beta, \quad \mathbf{R}_C = \frac{\alpha\mathbf{R}_A + \beta\mathbf{R}_B}{\alpha + \beta},$$
$$K_{AB} = \left[\frac{2\alpha\beta}{\pi(\alpha + \beta)} \right]^{3/4} e^{-\alpha\beta/\gamma|\mathbf{R}_A-\mathbf{R}_B|^2}.$$

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Problema 2 *Tight-binding interactions: s and p orbitals*

Calculate and plot the band structure for a 2D square metal, taking the following considerations:

- 1) Monoatomic basis set.
 - 2) Interactions to first-nearest-neighbors.
 - 3) Basis expansion with s and p orbitals.
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Problema 3 *Linearized function's derivatives*

For the radial Schrödinger equation,

$$\hat{H}\psi_l(\epsilon, \rho) = \epsilon\psi_l(\epsilon, \rho) \quad \forall \quad \hat{H} = -\frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial \rho^2} + \frac{l(l+1)}{\rho^2} + V_s(\rho),$$

demonstrate the following relationships,

$$\begin{aligned} a) \quad & \left(\hat{H} - \epsilon_0 \right) \dot{\psi}_l(\epsilon_0, \rho) = \psi_l(\epsilon_0, \rho), \\ b) \quad & \left(\hat{H} - \epsilon_0 \right) \psi_l^{(n)}(\epsilon_0, \rho) = n \psi_l^{(n-1)}(\epsilon_0, \rho), \end{aligned}$$

where n is the order of the energy-derivative, and:

$$\psi_l(\epsilon, \rho) \approx \psi_l(\epsilon_0, \rho) + (\epsilon - \epsilon_0) \dot{\psi}_l(\epsilon_0, \rho).$$

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Problema 4 *Orthogonality condition*

Demonstrate the orthogonality of the wave-functions,

$$\left\langle \psi_l \left| \dot{\psi}_l \right. \right\rangle = \left\langle \dot{\psi}_l \left| \psi_l \right. \right\rangle = 0,$$

assuming that the ψ_l are orthonormal: $\langle \psi_l | \psi_{l'} \rangle = \delta_{ll'}$.

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