Química Cuántica de Sólidos
Tarea 03: Bases de expansión

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Problema 1 *Product of two gsaussians*

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:

$$\gamma = \alpha + \beta, \quad \mathbf{R}_C = \frac{\alpha\mathbf{R}_A + \beta\mathbf{R}_C}{\alpha+\beta},$$

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

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

Calculate and plot the band structure for a $2D$ 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,

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

demonstrate the following relationships,

$$a) \quad \left(\hat{H} - \epsilon_0\right)\dot{\psi}_l(\epsilon_0,\rho) = \psi_l(\epsilon_0,\rho),$$

$$b) \quad \left(\hat{H} - \epsilon_0\right)\psi_l^{(n)}(\epsilon_0,\rho) = n\psi_l^{(n-1)}(\epsilon_0,\rho),$$

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,

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

where we assume that the ψ_l are normalized: $\langle \psi_l | \psi_l \rangle = 1$.

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Problema 5 *LAPW secular equation*

Carry out the manipulations to show that the Hamiltonian and overlap matrix elements can be cast in the linearized energy-independent form of,

$$\begin{aligned}
&\sum_m \left[\left\langle m' \middle| \hat{H} \middle| m \right\rangle_{mt} - \left\langle m' \middle| m \right\rangle_{mt} \epsilon_{i\mathbf{k}} \right] c_{im}(\mathbf{k}) = 0, \\
&\Rightarrow \quad \sum_m \Bigg\{ (\epsilon_0 - \epsilon_{i\mathbf{k}}) \sum_{Ls} [A^*_{Ls}(\mathbf{k}+\mathbf{G}_{m'}) A_{Ls}(\mathbf{k}+\mathbf{G}_m) + \ldots \\
&\ldots + B^*_{Ls}(\mathbf{k}+\mathbf{G}_{m'}) B_{Ls}(\mathbf{k}+\mathbf{G}_m) \left\langle \dot{\psi}_l(\epsilon_0,\rho) \middle| \dot{\psi}_l(\epsilon_0,\rho) \right\rangle \Big] + \ldots \\
&\ldots + \frac{1}{2} \sum_{Ls} [A^*_{Ls}(\mathbf{k}+\mathbf{G}_{m'}) B_{Ls}(\mathbf{k}+\mathbf{G}_m) + A_{Ls}(\mathbf{k}+\mathbf{G}_{m'}) B^*_{Ls}(\mathbf{k}+\mathbf{G}_m)] \Bigg\} c_{im}(\mathbf{k}) = 0.
\end{aligned}$$

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