Química Cuántica de Sólidos
Tarea 01: Fundamentos de teoría cuántica

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Nombre del Estudiante: ____

Problema 1 *Four-order potential*

Consider a particle in a one-dimensional potential:

$$V(x) = \lambda x^4.$$

Using the variational method, find an approximate value for the energy of the ground state. Compare it to the exact value,

$$E_0 = 1.06 \frac{\hbar^2}{2m} k^{1/3} \;\; \forall \;\; k = \frac{2m\lambda}{\hbar^2}.$$

Choose as a trial function,

$$\psi = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2}.$$

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Problema 2 *Harmonic oscillator*

Estimate the ground-state energy of a one-dimensional simple harmonic oscillator using as trial function:

(a) $\psi_a(x) = \text{Cos}\alpha x$ for $|\alpha x| < \pi/2$, zero elsewhere.

(b) $\psi_b(x) = \alpha^2 - x^2$ for $|x| < \alpha$, zero elsewhere.

(c) $\psi_c(x) = C\exp(-\alpha x^2)$.

In each case, α is the variational parameter. Don't forget the normalization. Sketch the wavefunctions and compare them with the actual ground-state wavefunction.
Hint: You may use the following results,

$$\int_{-\infty}^{\infty} \exp(-\alpha x^2)dx = \sqrt{\frac{\pi}{2}}, \quad \int_{-\pi/2\alpha}^{\pi/2\alpha} x^2 \text{Cos}^2 \alpha x dx = \pi(\pi^2 - 6)/24\alpha^3.$$

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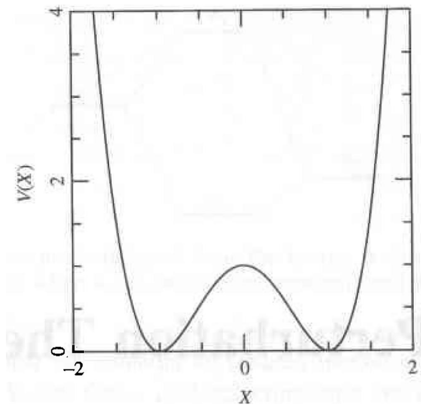
Problema 3 *Linear combination of orbitals*

Consider the following one-dimensional potential,



given by,

$$V(x) = (x^2 - 1)^2.$$

Using the linear variation method, find the ground-state energy and wavefunction using the following basis functions $\{\chi_j\}$,

$$\chi_1(x) = e^{-(x-1)^2}, \quad \chi_2(x) = e^{-(x+1)^2}, \quad \chi_3(x) = (x-1)e^{-(x-1)^2}, \quad \chi_4(x) = (x+1)e^{-(x+1)^2}.$$

Compare your results (plot the wavefunctions) with the ones using: $\{\chi_1(x)\}$ and $\{\chi_1(x), \chi_2(x)\}$.

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Problema 4 *Perturbation theory up to second order*

From the general expresion of the Schrödinger equation in terms of perturbation parameter series,

$$\left[c_l^{(0)} + \lambda c_l^{(1)} + \lambda^2 c_l^{(2)} + \ldots\right] E_l^{(0)} + \lambda \sum_i \left[c_i^{(0)} + \lambda c_i^{(1)} + \lambda^2 c_i^{(2)} + \ldots\right] \left\langle \psi_l^{(0)} \middle| \hat{H}_1 \middle| \psi_i^{(0)} \right\rangle = \ldots$$

$$\ldots = \left[E_k^{(0)} + \lambda E_k^{(1)} + \lambda^2 E_k^{(2)} + \ldots\right] \left[c_l^{(0)} + \lambda c_l^{(1)} + \lambda^2 c_l^{(2)} + \ldots\right],$$

find the contribution to the energy and wavefunction up to second order on the perturbation, that is:

$$\text{from: } E_k = E_k^{(0)} + \lambda E_k^{(1)} + \lambda^2 E_k^{(2)} + \ldots, \quad \text{then } E_k^{(2)},$$

$$\text{from: } \psi_k = \sum_i \left[c_i^{(0)} + \lambda c_i^{(1)} + \lambda^2 c_i^{(2)} + \ldots\right] \psi_i^{(0)} \quad \text{then } \sum_i c_i^{(2)} \psi_i^{(0)}.$$

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