Physical Chemistry Cume
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1. How would you find in a ***momentum representation*** the form of energy eigenstates for a quantum harmonic oscillator? Show formulas. Which of these eigenstates have broader momentum spectra?

2. Imagine that in a system of many identical quantum particles somebody exchanges two particles. What happens with the wave function of the particles and their probability density? Why?

3. How could an exact solution of the electronic wave function in a He atom (ground state) look like? Which single-electron or two-electron states in this system the two electrons retain forever? How could we approximate the ground state electron wave function? Explain.

4. How would you obtain in a H_2 molecule the energies of all internal states (not nuclei)? Roughly describe the steps by suitable formulas.

Possibly useful formulas:

$$E_n = (n+0.5)\hbar\nu_0, \quad \psi_n(x) = \left[\left(\frac{1}{\pi}\right)^{1/2}\frac{1}{2^n n!}\right]^{1/2} H_n(y)\exp\left[-\frac{y^2}{2}\right], \quad y = \alpha^{1/2}x, \quad \alpha = \frac{(\mu k)^{1/2}}{\hbar},$$

$$H = -\frac{\hbar^2}{2}\sum_\alpha \frac{1}{m_\alpha}\nabla_\alpha^2 - \frac{\hbar^2}{2m_e}\sum_i \nabla_i^2 + \sum_\alpha\sum_{\beta>\alpha}\frac{Z_\alpha Z_\beta e'^2}{r_{\alpha\beta}} - \sum_\alpha\sum_i \frac{Z_\alpha e'^2}{r_{i\alpha}} + \sum_i\sum_{i>j}\frac{e'^2}{r_{ij}},$$

$$H\,\Psi(q_i, q_\alpha) = E_{i,\alpha}\,\Psi(q_i, q_\alpha)$$

$$\left[-\frac{\hbar^2}{2m_\alpha}\nabla_\alpha^2 - \frac{\hbar^2}{2m_\beta}\nabla_\beta^2 + U(R)\right]\psi_N = E\,\psi_N,$$