Exercise: Brute-Force Approach Applied to Harmonic Oscillator Problem and Coulomb Potential in 1D

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1. Small-amplitude vibrations of a diatomic molecule can be studied using as a model of the true molecular vibrational potential the simple harmonic oscillator potential:

$$V(x) = \frac{1}{2} k_f x^2$$

where k_f is the force constant. For a typical diatomic molecule, the force constant is roughly $k_f = 1.0\ (J/m^2)$. The mass is $9.57\, m_0$.

(a) Using the above values, calculate the value of the zero-point vibrational energy of a diatomic molecule (in *eV*)

(b) Calculate the energy spacing (in *eV*) between the ground vibrational state and the first excited vibrational state of the molecule.

(c) Suppose the molecule undergoes a transition from the first excited vibrational state to the ground state, emitting a photon in the process. Calculate the energy, frequency, and the wavelength of the emitted photon. In what range of the electromagnetic spectrum is this photon found?

2. The potential energy of an electron in a hydrogen atom (in MKS units) is

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r},$$

where e is the electron charge and r is the distance of the electron from the proton. The hydrogen atom is, of course, a three-dimensional system, and r is the radial coordinate of a spherical coordinate system with the origin at the proton. However, we can model this system by a simple, continuous one-dimensional potential energy whose TISE we can solve. For this purpose, we can assume that the potential energy term in the 1D TISE is of the form:

$$V(x) = \begin{cases} -\dfrac{e^2}{4\pi\varepsilon_0 x}, & x > 0 \\ \infty, & x \le 0 \end{cases}$$

The bound state energies of an electron in this potential can be determined using the method of power series that was explained on the example of a simple harmonic oscillator (SHO). Let's find the solution step-by-step:

(a) Simplify the TISE for the total energy E by changing the variable of differentiation from x to one that is dimensionless. Define this new variable ξ in terms of the constant:

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} \ ,$$

which represents the Bohr radius of the hydrogen atom. Introduce a dimensionless energy parameter ε defined by:

$$\varepsilon^{-2} = -\frac{2mEa_0^2}{\hbar^2} \ ,$$

and the dimensionless length variable ξ

$$\xi = \frac{2x}{\varepsilon a_0} \ .$$

(b) The equation that you have obtained can not be immediately solved by, for example, inserting into a power series expansion. You need to calculate the asymptotic limit, i.e. the solution $g(\xi)$ for $\xi \to \infty$.

(c) Once you have calculated the asymptotic solution $g(\xi)$, express the wavefunction as $\psi(\xi) = Ag(\xi)f(\xi)$, and find the differential equation for $f(\xi)$.

(d) Solve the differential equation for $f(\xi)$ using a power series expansion, i.e.

$$f(\xi) = \sum_{j=0}^{\infty} c_j \xi^j \ ,$$

in which one must set $c_0 = 0$ (Why?). Derive a recurrence relation for the coefficients c_j in this series.

(e) Give an argument to show that the infinite series for $f(\xi)$ must be truncated at some finite order, and show that doing so leads to the restriction that ε must equal a positive integer number.

(f) From the results from part (*e*), obtain an expression for the allowed bound state energies of this model hydrogen atom. Look up the equation for the bound-state energies of an actual, three-dimensional hydrogen atom and compare your result to this answer. Is the result you obtained accurately describing the energies of this system? Can you think of any important physical effects that have been totally ignored in this model?

(g) Using the recurrence relation of part (*e*), write down the un-normalized spatial functions for the first three bound states of this model potential energy. Plot these functions and discuss their behavior.

3. Using the definition for the momentum probability amplitude, transform the TISE for the simple harmonic oscillator (SHO) into momentum space. Now solve this equation for $\phi_n(k)$ for the SHO.

Remark: The SHO is one of the few systems for which the momentum-space TISE is easily solved.