# Problem Set 1: Virial Theorem, Hydrogenic Ions and Harmonic Oscillator

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## Exercise 1: Proof of the Virial Theorem

In this exercise we will proof the quantum mechanical version of the so called Virial Theorem. We start with the Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}$$

where the first term in the Hamiltonian is the kinetic energy operator $\hat{T}$ and the second part $\hat{V}$ is the potential. Assuming the generic form of the potential $\hat{V} = \alpha \hat{x}^s$, the Virial Theorem relates the expectation values of the kinetic energy operator $\hat{T}$ and the potential energy operator $\hat{V}$ for a given energy eigenstate $|\psi_\nu\rangle$ with energy $\nu$:

$$\langle \hat{T} \rangle_\nu = \frac{1}{2} s \langle \hat{V} \rangle_\nu \tag{1}$$

*Remark*: This exercise is expected to be solved with pen and paper.

*Hint*: Apply the Ehrenfest theorem $\frac{\mathrm{d}}{\mathrm{d}t}\langle \hat{\Omega} \rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{\Omega}] \rangle$ to the operator $\hat{p}\hat{x}$.

## Exercise 2: Hydrogenic ions

Hydrogenic ions are atoms consisting of one electron bound to a nucleus with $Z > 1$. They are of interest for precision experiments to test quantum electrodynamics or determine the fine structure constant. In this exercise we will explore the similarities with the Hydrogen atom as well as the scaling of several quantities with the nuclear charge $Z$.

*Remark*: This exercise is expected to be solved with pen and paper.

a) Write down the Hamiltonian for a hydrogenic atom. By introducing a change of variable $\rho := \frac{r}{Z}$ show that this Hamiltonian, up to a scaling factor, is the same as for the Hydrogen atom. Therefore, what is the natural length scale for hydrogenic ions compared to Hydrogen?

For the rest of the exercise determine the scaling with the nuclear charge $Z$ of the following quantities:

b) the expectation values of $r$, $1/r$ and $1/r^3$, where $r$ is the distance of the electron to the nucleus.

c) the expectation value of the potential energy $V$.

d) the total Energy $E$.

e) the probability to find the electron at the origin $\left|\psi(r=0)\right|^2$.

f) $\left|\frac{\partial}{\partial r}\psi(r=0)\right|^2$.

g) the fine structure splitting due to the relative movement between nucleus and electron.

*Hints:* (i) Motivated by the semi-classical Bohr model, you can use that from the point-of-view of the electron, the nucleus of charge $Z$ is orbiting around it with a velocity $v \approx Z\alpha c$ with $\alpha$ the fine-structure constant.
(ii) The magnetic field can then be calculated using the formula $B = \left|\frac{\vec{v} \wedge \vec{\epsilon}}{c}\right|$ for the orthogonal component of a magnetic field $B$ originating from a static electric field $\epsilon$ in a reference frame moving with velocity $v$ (in the system of units where $4\pi\epsilon_0 = 1$).

h) the hyperfine energy splitting due to the magnetic dipole moment of the nucleus.

*Hint*: The magnetic field of a dipole falls off as $\frac{1}{r^3}$.

# Exercise 3: Harmonic Oscillator in three dimensions

Consider an isotropic harmonic oscillator in three dimensions with the Hamiltonian

$$H = \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + \frac{m\omega^2}{2}(x^2 + y^2 + z^2). \tag{1}$$

In this exercise we will explore the similarities of this system with the Hydrogen atom.

*Remark*: This exercise is expected to be solved with pen and paper.

a) Using what you know about the harmonic oscillator, what is the energy spectrum of the Hamiltonian (1) and what are the degeneracies?

b) Without calculation, show that $H$ commutes with the operators $l_z$ and $L^2$. What are the implications of this on the eigenfunctions of the Hamiltonian (1).

To continue the exercise we will first state some results.
There are different methods to solve the eigenvalue equation associated with equation (1). In cartesian coordinates, the problem is separable and one can use the solution of the problem in 1 dimension to solve the equation in three dimensions. The corresponding eigenvalues are:

$$E_n = (n + \frac{3}{2})\hbar\omega,$$

where the integer $n$ is given by the sum n = $n_x + n_y + n_z$, where $n_x, n_y, n_z \geq 0$. Therefore the degeneracy $g_n$ of each energy level is:

$$g_n = \frac{1}{2}(n+1)(n+2).$$

The corresponding eigenfunctions can be written as:

$$\psi_{n_x n_y n_z}(x, y, z) = \phi_{n_x}(x)\phi_{n_y}(y)\phi_{n_z}(z)$$

where the functions $\phi_{n_u}(u) = N_{n_u} H_{n_u}(\sqrt{\frac{m\omega}{\hbar}}u)e^{-\frac{m\omega}{2\hbar}u^2}$ are the solutions of the harmonic oscillator in 1 dimension ($u = x, y, z$ respectively). The functions $H_{n_u}(u)$ are Hermite Polynomials and $N_{n_n}$ are the normalization constants satisfying: $N_0 = (\frac{m\omega}{\pi\hbar})^{\frac{1}{4}}$, $N_{n_u} = \frac{N_0}{\sqrt{2^{n_u} n_u!}}$.

Motivated by the isotropy of the problem, one can look at the problem in spherical coordinates. There is a basis of eigenfunctions that are not only eigenfunctions of $H$ but also of the operators $l_z$ and $L^2$.
The structure of the solutions is

$$\psi_{k,l,m}(r, \theta, \phi) = \frac{u_{k,l}(r)}{r} Y_l^m(\theta, \phi)$$

with the spherical harmonics $Y_{lm}(\theta, \phi)$ we already know from the hydrogen atom. The radial part further satisfies:

$$u_{k,l}(r) = \exp\big(-\frac{m\omega}{2\hbar}r^2\big) \cdot r^{l+1} \sum_{q=0}^{+\infty} a_q r^q.$$

For the coefficients $a_q$ one can derive the recursion relation:

$$\forall q \in \mathbb{N}, (q+2)(q+2l+3)a_{q+2} = \Big(\frac{m\omega}{\hbar}(2q+2l+3) - \epsilon_{k,l}\Big)a_q, \tag{2}$$

where $\epsilon_{k,l}$ is related to the eigenenergy $\epsilon_{k,l} := \frac{2m}{\hbar^2}E_{k,l}$. Furthermore the coefficient $a_1$ must be zero ($a_1 = 0$), forcing all odd coefficients to be zero according to relation (2).

c) Consider $u_{k,l}(r)$ given the results above. Which condition must always be satisfied in order for the overall function to represent a physically meaningful eigenfunction? *Hint*: Use that the resulting function must be square-integrable. Consider the case where no even coefficient $a_q$ is equal to zero: can the resulting eigenfunction be square-integrable? Then show that there is one $q$ for which $a_{q+2} = 0$.

d) Write down the energy spectrum, now in terms of the integers $k, l$. What are the degeneracies and how does this compare to the result in (a)? Draw the energy spectrum in the $(l, E)$ plane.

e) For the two lowest energy states write down the relation between the eigenfunctions $\psi_{n_x,n_y,n_z}$

and $\psi_{k,l,m}$.

*Remark*: More details on the derivation of (2) starting from the Schrödinger equation can be found, for example, in *Claude Cohen-Tannoudji, Bernard Diu, Frank Laloe*, **Quantum Mechanics 1**, appendix B$_{VII}$.

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