Moments <r^N>(l,n) in QM and CM

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From QM we know that we can compute the **expectation value of the any power of the observable r** by an integral involving the square of the radial part of the hydrogen wavefunction. The computations can be done analytically with relatively huge effort and the results for some powers, which are listed in *table 1*, can be taken for example from (Weissbluth, 1978).

To compare this with the **classical analogue** it is important to realize that one must look for the time-average of the radius vector in the Kepler problem, not just the semi-major axis, which is usually referred to as the mean radius, which it is in fact if one averages with respect to arc-length.
We know from the treatment of the Kepler problem in classical mechanics (Lifschitz, 1987):

$$U=-\frac{k}{r},\quad \varepsilon=\left(1+\frac{2EL^2}{m_e k^2}\right)^{1/2},\quad a=\frac{k}{2|E|},\quad k_{Coulomb}=\frac{Ze^2}{4\pi\varepsilon_0} \tag{1}$$

Here, of course, the potential is taken to be the electrostatic potential of the nucleus instead of the gravitational potential usually taken in the **Kepler treatment**. The average over time of the distance in the Kepler problem can be computed by the following exact analytic expression involving Gauss's hypergeometric function (Al Lehnen, 2004):

$$\left\langle\left(\frac{r}{a}\right)^N\right\rangle_t={}_2F_1\left(-\frac{N}{2},-\frac{N+1}{2},1,\varepsilon^2\right) \tag{2}$$

$$\boxed{\left\langle r^N\right\rangle_t=\left(\frac{a_0 n^2}{Z}\right)^N {}_2F_1\left(-\frac{N}{2},-\frac{N+1}{2},1,1-\frac{l(l+1)}{n^2}\right)} \tag{3}$$

The results of this formula coincide with the results given in (Classical mnemonic approach for obtaining hydrogenic expectation values of r^P, 1990), $\left\langle r^N\right\rangle=a^N(b/a)^{N+1}P_{|N+3/2|-1/2}(a/b)$, using Legendre Polynomials, after the same corresponding substitutions are carried out.

Here, [3] was obtained by combining [2] with the basic QM results for the hydrogen Energy spectrum, the Bohr radius and the following natural QM treatment of angular momentum (i.e. [4] into [1]):

$$a_0=\frac{\varepsilon_0 h^2}{\pi m_e e^2},\quad E_n=-\frac{Z^2e^2}{8\pi\varepsilon_0 a_0 n^2},\quad L^2=\hbar^2 l(l+1) \tag{4}$$

This semi-classical version of the expectation value of the radius-moments ([3]) is the main result of this paper and will be shown to be in good agreement with QM for large l and n for selected moments (see *figures* and *table 1*), which is of course just as expected from the *Ehrenfest Theorem* (**correspondence principle**) for large quantum numbers.

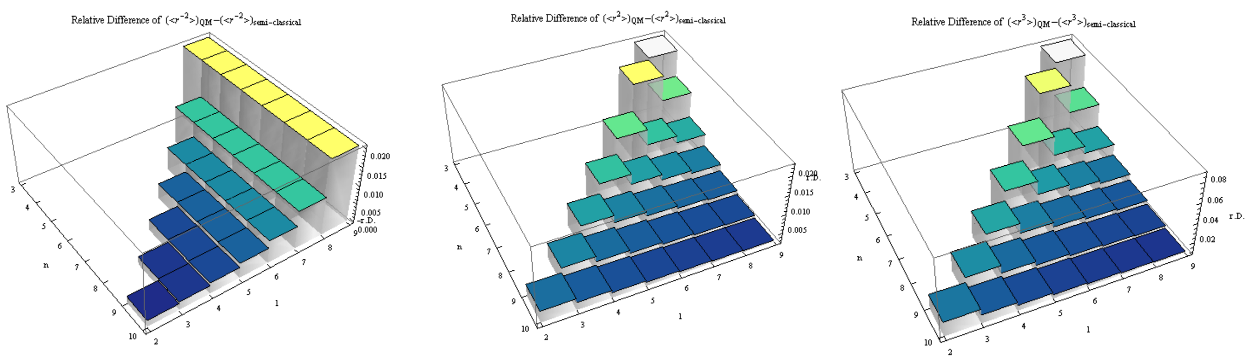
It should also be mentioned, that a rather **complicated exact** closed formulation of QM expectation values has recently been developed, see (Classical mnemonic approach for obtaining hydrogenic expectation values of r^P, 1990), for arbitrary moments by use of a lengthy recursive formula, a form of the cited alternative equation above and selective replacement of the occurring coefficients.

table 1

	QM: $\langle r_{nl}{}^{N}\rangle_{QM}$	Semi-Classical: $\langle r_{nl}{}^{N}\rangle_{t}$	$\left(\langle r^{N}\rangle_{QM}-\langle r^{N}\rangle_{t}\right)/\langle r^{N}\rangle_{QM}$
$\langle r^{4}\rangle$	$\frac{a_0{}^4 n^4}{8Z^4}\left\{\begin{matrix}63n^4-35n^2\left(2l^2+2l-3\right)+\\+5l\left(l+1\right)\left(3l^2+3l-10\right)+12\end{matrix}\right\}$	$\frac{a_0{}^4 n^4}{8Z^4}\left\{\begin{matrix}63n^4+l^2(15-70n^2)\\-70ln^2+15l^4+30l^3\end{matrix}\right\}$	$\frac{105n^2-50l^2-50l+12}{63n^4+15l^4-70l^2n^2+30l^3-70ln^2+105n^2-35l^2-50l+12}$
$\langle r^{3}\rangle$	$\frac{a_0{}^3 n^2}{8Z^3}\left\{\begin{matrix}35n^2\left(n^2-1\right)-30n^2\left(l+2\right)\left(l-1\right)\\+3\left(l+2\right)\left(l+1\right)l\left(l-1\right)\end{matrix}\right\}$	$\frac{a_0{}^3 n^2}{8Z^3}\left\{\begin{matrix}35n^4-l^2(30n^2-3)\\-30ln^2+3l^4+6l^3\end{matrix}\right\}$	$\frac{25n^2-6l^2-6l}{35n^5+3l^4n-30l^2n^3+6l^3n-30ln^3+25n^3-3l^2n-6ln}$
$\langle r^{2}\rangle$	$\frac{a_0{}^2 n^4}{Z^2}\left(\frac{5}{2}-\frac{3l\left(l+1\right)-1}{2n^2}\right)$	$\frac{a_0{}^2 n^4}{Z^2}\left(\frac{5}{2}-\frac{3l\left(l+1\right)}{2n^2}\right)$	$\frac{1}{1-3l\left(l+1\right)-5n^2}$
$\langle r^{1}\rangle$	$\frac{a_0 n^2}{Z}\left(\frac{3}{2}-\frac{l\left(l+1\right)}{2n^2}\right)$	$\frac{a_0 n^2}{Z}\left(\frac{3}{2}-\frac{l\left(l+1\right)}{2n^2}\right)$	0
$\langle r^{-1}\rangle$	$\frac{Z}{a_0 n^2}$	$\frac{Z}{a_0 n^2}$	0
$\langle r^{-2}\rangle$	$\frac{Z^2}{a_0{}^2 n^3\left(l+1/2\right)}$	$\frac{Z^3}{a_0{}^2 n^3\left(l\left(l+1\right)\right)^{1/2}}$	$-\frac{1}{8l^2}+\frac{1}{8l^3}-\frac{15}{128l^4}+\mathrm{O}\left(\frac{1}{l^5}\right)$
$\langle r^{-3}\rangle$	$\frac{Z^3}{a_0{}^3 n^3 l\left(l+1/2\right)\left(l+1\right)}$	$\frac{Z^2}{a_0{}^3 n^3\left(l\left(l+1\right)\right)^{3/2}}$	$-\frac{1}{8l^2}+\frac{1}{8l^3}-\frac{15}{128l^4}+\mathrm{O}\left(\frac{1}{l^5}\right)$
$\langle r^{-4}\rangle$	$\frac{Z^4\left(3n^2-l\left(l+1\right)\right)}{2a_0{}^4 n^5\left(l+\frac{3}{2}\right)\left(l+1\right)\left(l+\frac{1}{2}\right)l\left(l-\frac{1}{2}\right)}$	$\frac{Z^4\left(3n^2-l\left(l+1\right)\right)}{2a_0{}^4\left(l\left(l+1\right)\right)^{5/2}n^5}$	$\frac{5}{8l^2}-\frac{5}{8l^3}+\frac{93}{128l^4}-\mathrm{O}\left(\frac{1}{l^5}\right)$

The agreement found here is within a few percent for all quantum numbers, except for the N=2 case. But again, the **error goes rapidly to zero for large n and l** in all cases. The use for the easy, though not exact, result [3] might be in the domain of Rydberg atoms and computation of their electric multipole moments, or simply as a nice further demonstration of the correspondence principle.

figures: absolute relative differeces



Works Cited

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