Orbitals of the Bohr and Sommerfeld atoms with quantized x theory

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3 Computation and discussion

The first graph (Fig. 1) shows the Bohr circular orbits for $n = 1$ to $n = 4$ in atomic units:

$$\alpha_f = 0.0072973525, \quad c = \frac{1}{\alpha_f}, \quad \hbar = m = k = 1. \tag{75}$$

Then Eq.(5) simply reads

$$r_B = n^2. \tag{76}$$

The corresponding Bohr energy levels (Eq.(17)) are

$$E_B = \frac{1}{2\,n^2} \tag{77}$$

in Hartree units. The Sommerfeld energy is given by Eq.(69). The Bohr and Sommerfeld energies are shown in Table 1, together with the γ factors, for quantum numbers n. The differences in energy are small and the γ factors deviate from unity by less than 10^{-4}. The deviations become even smaller for growing n.

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n	E_{Bohr}	E_{Somm}	γ
1	-0.5000000	-0.4999800	1.0001065
2	-0.1250000	-0.1249988	1.0000266
3	-0.0555556	-0.0555553	1.0000118
4	-0.0312500	-0.0312499	1.0000067

Table 1: Bohr and Sommerfeld energy levels (in Hartree units) and γ factor for quantum numbers n.

The precession factor of the Sommerfeld theory x^2 is related to the half-right latitude α of the precessing ellipse by Eqs.(64) and (67). x^2 depends on the quantum number n via the Bohr radius (75) and the velocity (35) appearing in the γ factor (37). The dependence $x^2(\alpha)$ has been graphed in Fig. 2 as a function of the argument $\alpha \cdot n^2$ so that all Bohr radii are shifted to $\alpha = 1$ and can be compared directly. There is a sharp pole at $\alpha \approx r_B$ or, more precisely, $\alpha = \gamma r_B$. This pole becomes even sharper for increasing n. Therefore there is only a very small range around the Bohr radii where the Sommerfeld ellipses are defined, namely in the region with $x^2 \approx 1$. We see that the Bohr quantization of orbits is relaxed slightly in Sommerfeld theory but essentially remains valid.

The inverse relation $\alpha(x)$ is graphed in Fig 4. the α values have been normalized by r_B or n^2, respectively, so that the y scale is comparable. We see a very small variation of the α range which gets even smaller for rising x, in accordance with Fig. 3.

The ellipticity ϵ of Sommerfeld theory can be expressed by means of Eqs.(20) and (21) by

$$\epsilon = \sqrt{1 + 2\frac{E\,\alpha}{k}} \tag{78}$$

(see Eq.(70)) with α given by Eq.(67) and E given by Eq.(69). Thus, ϵ depends on x and n. Fig. 4 shows that ϵ is undefined for $x < 0.8$ since the square root argument is negative there. For growing x, the ellipticity is bound by an asymptote for each value of n. The small magnitude of ϵ shows again that Sommerfeld ellipses are extremely close to circles.

The effect of the Bohr velocity (35) has been investigated by artificially doubling this term. then $\epsilon(x)$ only starts at 1.6 (Fig. 5). This is unphysical because $x = 1$ must be included in the range of ϵ. The results are sensitive to the value of v.

The last part of this section investigates the Eckardt quantization. Inserting Eq.(74) into the equation for the precessing ellipse (50) gives

$$r = \frac{r_0}{(n-1)\,\epsilon\cos(n\theta)}. \tag{79}$$

These orbits are shown in Fig. 6. For $n = 1$ where r diverges a circular orbit has been assumed and a constant $\epsilon = 0.3$ has been used for all graphs. It can be seen that Eckardt quantization gives closed orbits (standing circular waves) with n being the number of maxima.

From Sommerfeld theory we know that the ellipticity is a function of energy, therefore we try to derive a corresponding expression for Eckardt quantization. Since the orbits in Eckardt quantization are highly elliptic, we have to use both components of the velocity. According to earlier papers we have

$$v_r = \frac{\epsilon\,L}{\alpha\,m}\sin(n\,\theta), \tag{80}$$

$$v_\theta = \frac{L}{m\,r}. \tag{81}$$

By means of

$$\cos(n\,\theta) = \frac{1}{\epsilon}\left(\frac{\alpha}{r} - 1\right), \tag{82}$$

$$\sin(n\,\theta) = \sqrt{1 - \cos^2(n\,\theta)} \tag{83}$$

we obtain for the squared modulus of velocity after some arithmetics

$$v^2 = \frac{\left(\left(\epsilon^2 - 1\right)\, r + 2\,\alpha\right)\, L^2}{\alpha^2\, m^2\, r}. \tag{84}$$

The total energy is

$$E = \frac{1}{2} m v^2 - \frac{k}{r} \tag{85}$$

$$= \frac{1}{r}\left(\frac{L^2}{\alpha\, m} - k\right) + \left(\epsilon^2 - 1\right) \frac{L^2}{2\,\alpha^2\, m}. \tag{86}$$

This expression must be constant, therefore the r dependence must vanish. This is ensured by setting

$$L^2 = k\,\alpha\, m \tag{87}$$

which relates the angular momentum with a certain half-right latitude. Then the energy becomes

$$E = \frac{\left(\epsilon^2 - 1\right)\, k}{2\,\alpha} \tag{88}$$

from which follows

$$\epsilon^2 = 1 + \frac{2\,E\,\alpha}{k}. \tag{89}$$

Astonishingly this is the same expression as Eq.(70) or (78) derived from Sommerfeld theory. However, the energy is not quantized, α is quantized according to Eq.(74):

$$\alpha = \frac{r_0}{n-1}, \quad n \neq 1. \tag{90}$$

Therefore the orbits look different to Sommerfeld theory, and ϵ is not small for $n > 1$. The first five orbits are graphed in Fig. 7 and the corresponding ϵ values are shown there. Compared to Fig. 6, the orbits do not shrink with n but keep their maximum radius.

The energy could be quantized by inseting the quantized α into Eq.(88) but then E depends on n instead of $1/n^2$ as in Bohr and Sommerfeld theory. A correct behaviour of $E(n)$ would require additional quantization constraints for ϵ.

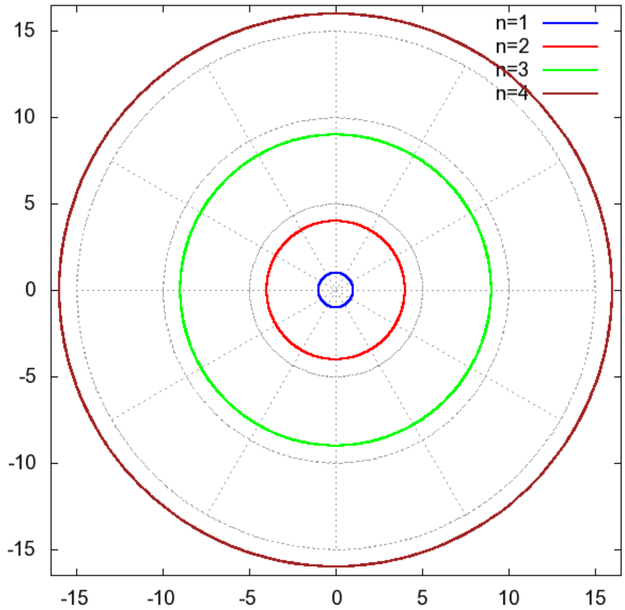

Figure 1: Bohr radii $r_B = n^2$ for quantum numbers n.

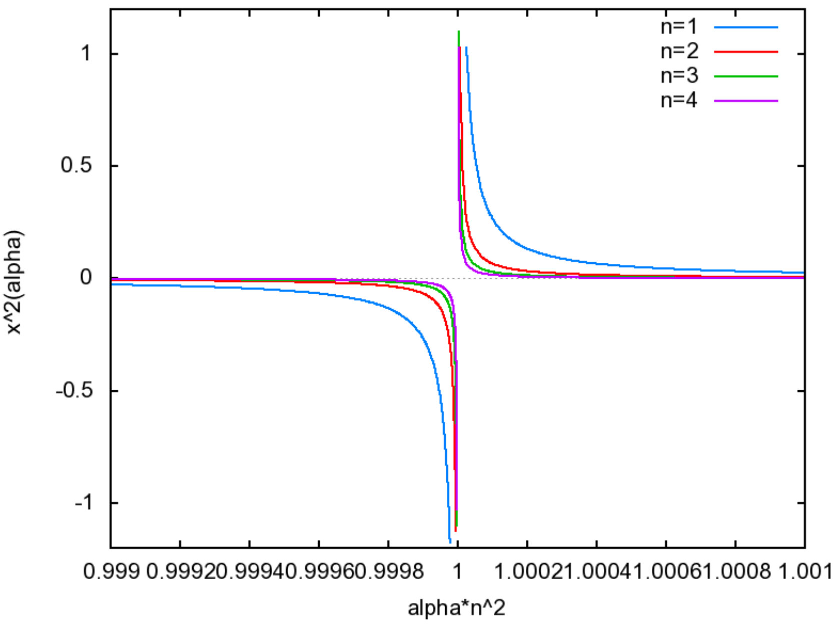

Figure 2: Sommerfeld precession factor $x^2(\alpha \cdot n^2)$ for quantum numbers n.

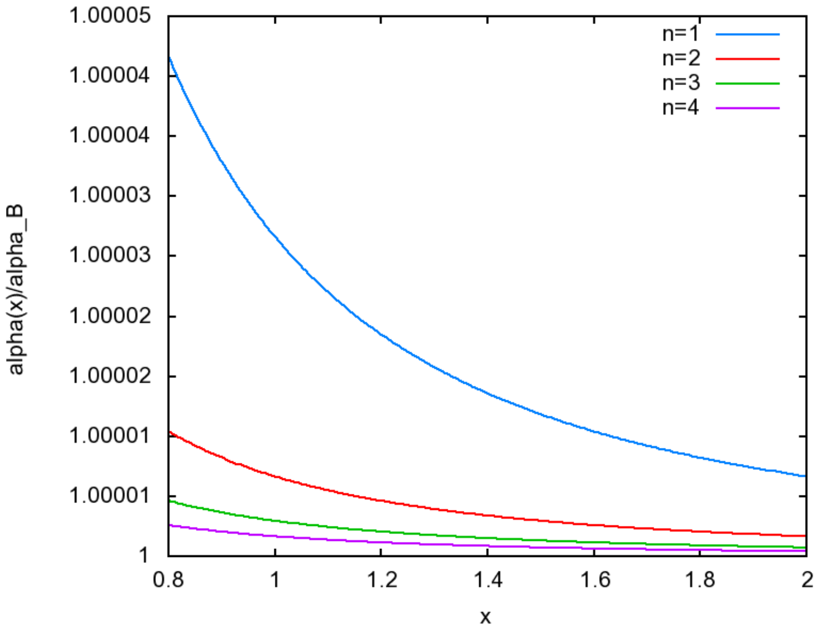

Figure 3: Normalized half-right latitude $\alpha(x)/n^2$ for Sommerfeld ellipses.

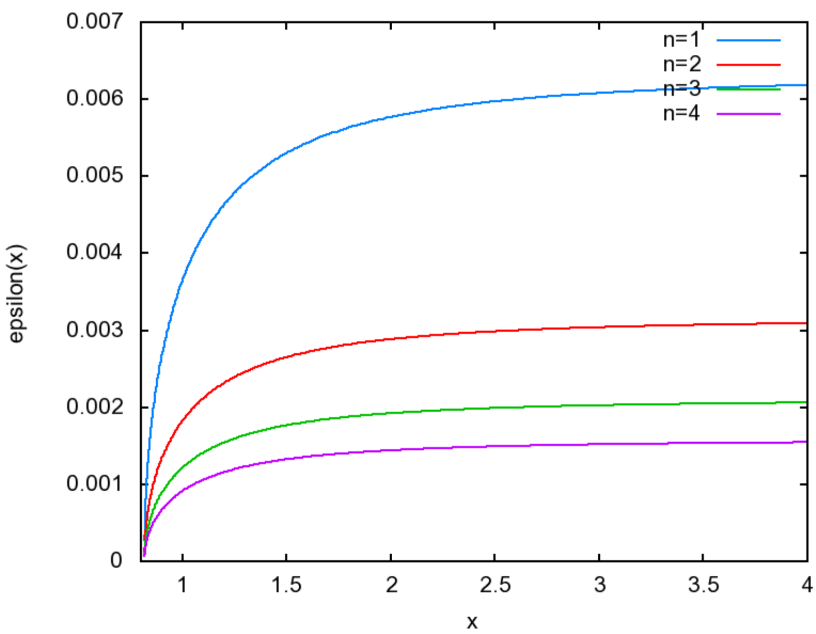

Figure 4: Ellipticity $\epsilon(x)$ for Sommerfeld ellipses.

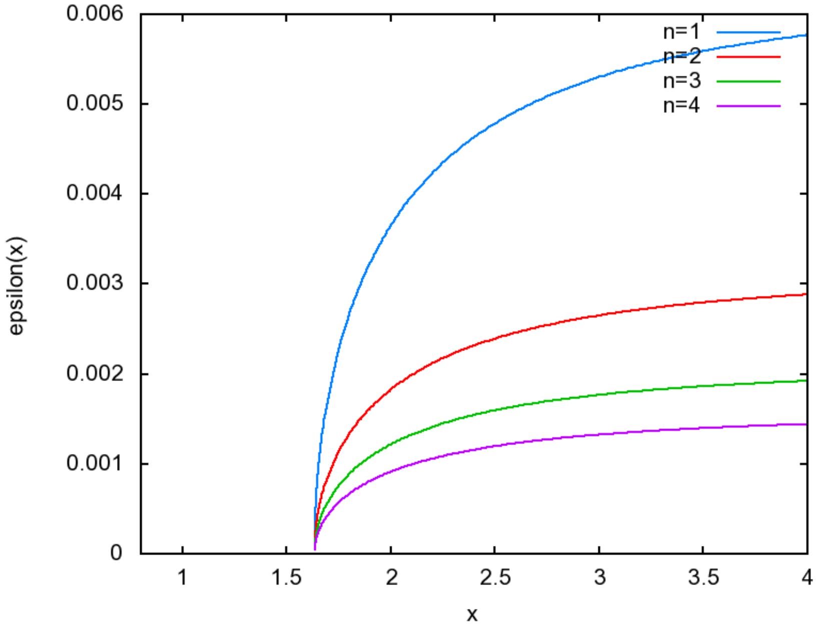

Figure 5: Ellipticity $\epsilon(x)$ for Sommerfeld ellipses with artificially enhanced orbital velocity $v \to 2v$.

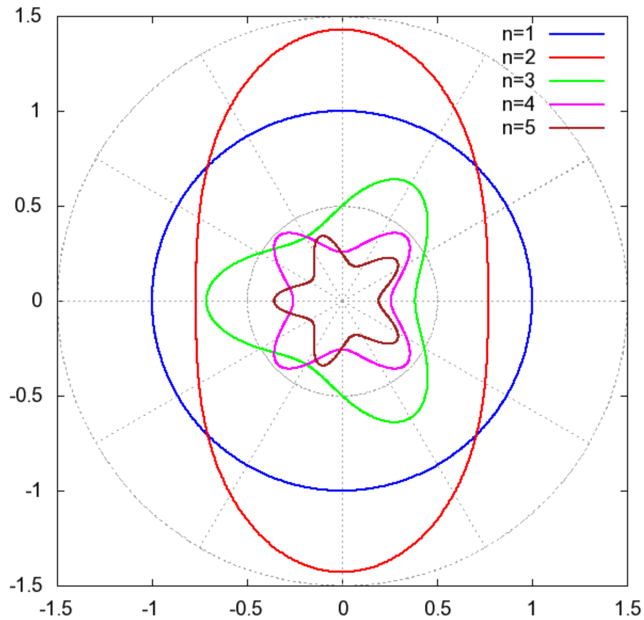

Figure 6: Orbitals of Eckardt quantization with $\epsilon = 0.3$, $r_0 = 1$.

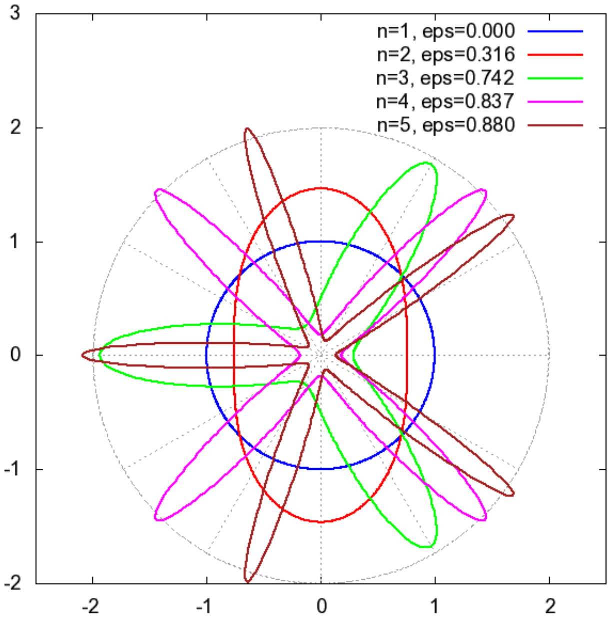

Figure 7: Orbitals of Eckardt quantization with variable ϵ with $r_0 = 1$, $E = -0.45$.