Effects of simulated surfaces on Knudsen gases in a homogeneous field and the second law of thermodynamics

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Abstract

It is easy to compute equilibrium properties of Knudsen gases (high and ultra high vacuum) because the molecules in a Knudsen gas are only moving on trajectory parabolas and every trajectory parabola is determined by the initial velocity and the height. So the expectation values in a Knudsen gas in a homogeneous field are only depending on the surface temperature, structure, field strength and the height over the ground. The computations and simulations were made with a) surfaces which consit only of harmonic bound hard spheres and b) surfaces which consits of little, harmonic bound hard spheres and mostly a reflecting plane. The results are that in case a), the ground emits with a direction-independent flux-density, the gas density decreases mono-exponential and that the gas is isothermal. In case b) the ground emits with a direction-independent flux, the gas density decreases more rapid than mono-exponential with height and the gas temperature increases rapidly with height. So, due to the second law of thermodynamics, simulated or calculated surfaces have to emitt with a direction-independent flux-density (cosine-like).

I. Introduction

It is known [1] that in a gas in a homogeneous field with Maxwallian velocity distribution and statisticaly independent places and momenta the gas temperature is independent of the height and the gas density decreases mono-exponentially - in agreement with the second law of thermodynamics. In a Knudsen gas over a ground in a homogeneous field this would mean that the ground emitted the gas molecule flux density direction-independently (second Lambert cosine law).
So I made the calculations with an isotropically emitting ground which emits the gas molecules direction-independent (without a cosine factor). Analog effects are calculated for a thermal photon-gas in a gravitational field.

II. Analytical calculations

For simplicity the Knudsen gas is monoisotopic, monoatomic and in a field with the constant acceleration g. If the gas atoms are not on the ground they are only moving on trajectory parabolas. So if an atom starts with the velocity v_0 at the height h it has the velocity $v = \sqrt{v_0^2 - 2 \cdot g \cdot h}$. This means $v_0 = \sqrt{v^2 + 2 \cdot g \cdot h}$ and the Maxwellian velocity-density-distribution in spherical coordinates is modified to:

$$\varphi_\theta(v,h) = \frac{4}{\sqrt{\pi}} \left(\frac{m}{2 \cdot k \cdot T}\right)^{\frac{3}{2}} \cdot (v^2 + 2 \cdot g \cdot h) \cdot e^{-\frac{(v^2+2\cdot g\cdot h)\cdot m}{2\cdot k\cdot T}} \cdot \Theta\left(v - \sqrt{2 \cdot g \cdot h} \cdot \tan(\theta)\right) \cdot \frac{v}{\sqrt{v^2 + 2 \cdot g \cdot h}} \tag{1}$$

This velocity-density-distribution is normalized only for h=0m. So only

$$\frac{\varphi_\theta(v,h)}{\int_0^{\pi/2}\int_0^{2\cdot\pi}\int_0^{\infty} \varphi_\theta(v,h) \cdot \sin(\theta) dv d\varphi d\theta} \equiv \varphi_\theta(v,h)_N \tag{2}$$

is normalized.

It is important to note that the velocity-density-distribution of the gas flux from an isotropic-like emitting ground is

$$\varphi_N(v,0) \cdot v_0 \tag{3}$$

and that this is the (unnormalized) velocity-density-distribution of the gas that reaches the height h per unit time. The temperature of the gas atoms which are impacting on a thermometer is the average kinetic energy per atom times 1/2k :

$$T = \frac{m \cdot \overline{v^2}}{4 \cdot k} \tag{4}$$

Therefore the temperature of a Knudsen gas with the phase space density $\varphi_\theta(v,h)_N$ is:

$$T(h) = \frac{m \cdot \overline{v^2}}{4 \cdot k} = \frac{m}{4 \cdot k} \int_0^{\pi/2}\int_0^{2\cdot\pi}\int_{\sqrt{2\cdot g\cdot h}\cdot\tan(\theta)}^{\infty} v_0 \cdot v^2 \cdot \varphi_\theta(v,h)_N \cdot \sin(\theta) \cdot dv d\varphi d\theta \tag{5}$$

With the substitution

$$\frac{(v^2 + 2 \cdot g \cdot h)\cos(\theta)^2}{2g} = M \tag{6}$$

the reversion of the integration order the result is:

$$\frac{T}{4} \cdot \frac{3 \cdot \sqrt{m \cdot g \cdot h \cdot k \cdot T \cdot \pi} \cdot erfc\left(\sqrt{\frac{m\cdot g\cdot h}{k\cdot T}}\right) e^{\frac{m\cdot g\cdot h}{k\cdot T}} - 8 \cdot k \cdot T - 2 \cdot m \cdot g \cdot h}{\sqrt{m \cdot g \cdot h \cdot k \cdot T \cdot \pi} \cdot erfc\left(\sqrt{\frac{m\cdot g\cdot h}{k\cdot T}}\right) e^{\frac{m\cdot g\cdot h}{k\cdot T}} - 2 \cdot k \cdot T} - \frac{2 \cdot m \cdot g \cdot h}{4 \cdot k} \tag{7}$$

An example of this temperature distribution in Xenon above a ground with a temperature of 293K is shown in figure 1. The analogous calculation of the relative Knudsen gas density shows that the height formula over an isotropically emitting ground is augmented by a correction term:

$$\varrho(h) = e^{-\frac{m\cdot g\cdot h}{k\cdot T}} - \frac{1}{2} Ei\left(-\frac{m \cdot g \cdot h}{k \cdot T}\right) \tag{8}$$

Ei is the Exponential Integral.

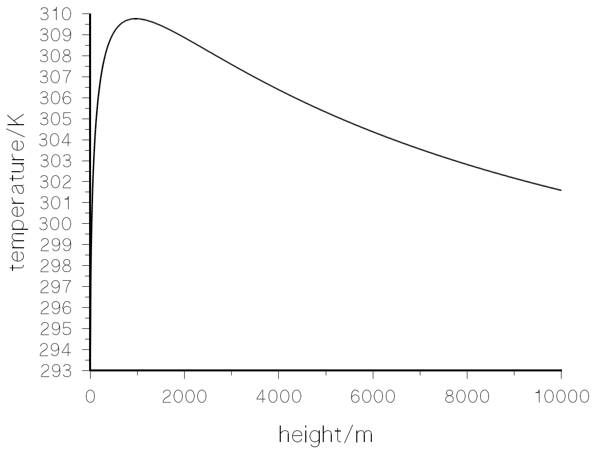

Figure 1: The temperature in K in a Xenon Knudsen gas above an isotropically emitting ground with a temperature of 293K in the gravitational field of the earth.

III. Deterministic simulations with hard spheres

Because Monte Carlo simulations are reproducing the above calculations with the idealisations 3 and 4 the first principles simulations were carried out completely deterministic with atoms as hard spheres.
Due to the system time dependent pseudo random initialisation it is easy to show the reproducebility of the above calculated effects. For simplicity the simulated gas consitits only of one hard sphere and the ground consist of a cubic lattice of hard spheres, which are in thermal motion around their rest positions. The rest positions are located in a plane (surroundig underground lattice) which reflects the gas atom elastically before it moves into the lattice. The system is limited by a ceiling at the height h and consists of the same lattice as the ground lattice. The walls of the system are elastically reflecting because otherwise the gas would diffuse away from the ground atoms and the ceiling atoms at the middle of the ground and ceiling plane.
The simulations were made a) with atoms which are so large that the gas could not reach neither the reflecting ground plane nor ceiling plane and b) with atoms that are so small that in approximately sixty percent of the impacts of the gas atom on the ground or the ceiling the gas atom impacts on the reflecting plane. In the case of the other forty percent the gas atom impacts with one lattice atom.
In case a) the angle probability density of the impacts shows the mutual "shading" of the large lattice atoms. Therefore the angle probability density from the impacts from trajectory parabolas which are longer than two latice constants is nearly cosine-like (see fig. 2). In case b) the angle probability density of the impacts shows, due to the isotropic scattering of hard spheres [2] and the little mutual "shading" of the lattice atoms, that the angle probability density of the impacts from trajectory parabola which are longer than two lattice constants is roughly constant (see fig. 2).

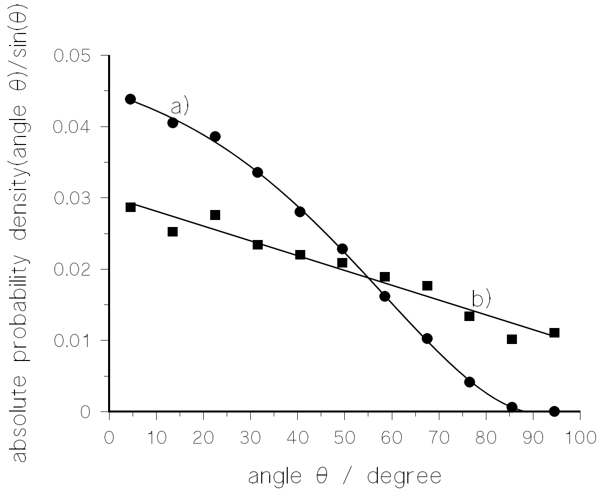

Figure 2: The angle probability density divided by the functional determinant in spherical coordinates above the angle for case a) and b).

So the case a) is approximately the case of parallel surfaces with the second Lambert cosine law which means height independent temperature and height formula and case b) is approximately the case of parallel isotropically emitting surfaces. Therefore, for the case $g = 0m/s^2$ the temperatures of the two lattices (=average energy per degree of freedom times 2/k) are noisy but equal (fig. 3). In the case a) due to the cosine-like

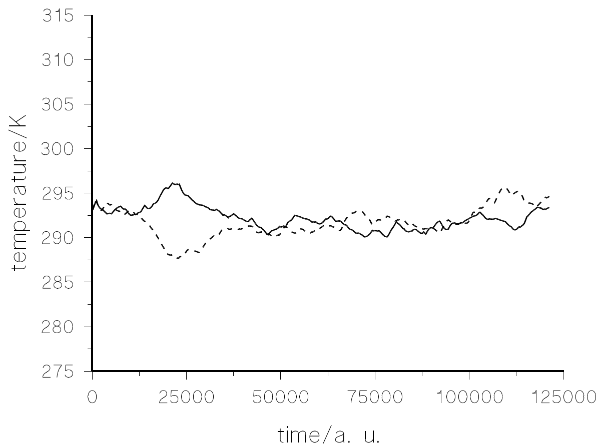

Figure 3: The ground temperature (291.68±3.03)K (dashed) and the ceiling temperature (291.22 ± 1.00)K at h=1m, $g = 0.0\frac{m}{s^2}$.

angle probability density even at high potentials the ground and the ceiling lattice have no significant average temperature difference (fig. 4). In the case b) due to the roughly constant angle probability density the ground and the ceiling lattice have comparably large differences in average temperature (fig. 5). Even if ground and ceiling lattice are initialised with the same starting temperature the temperature difference is reproduceble (fig. 6).

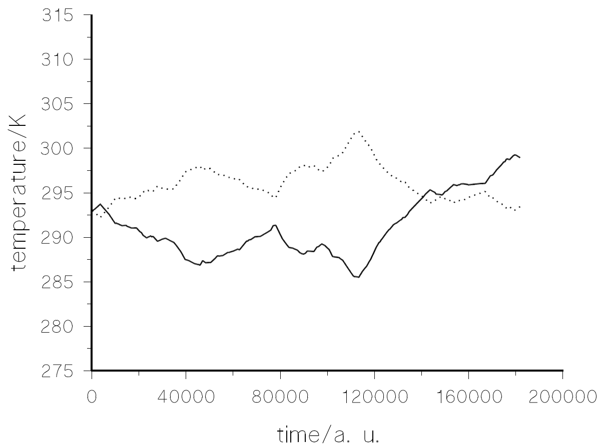

Figure 4: The ground temperature (dashed) and the ceiling temperature with cosine-like emission at h=1m, $g = 10^4 \frac{m}{s^2}$.

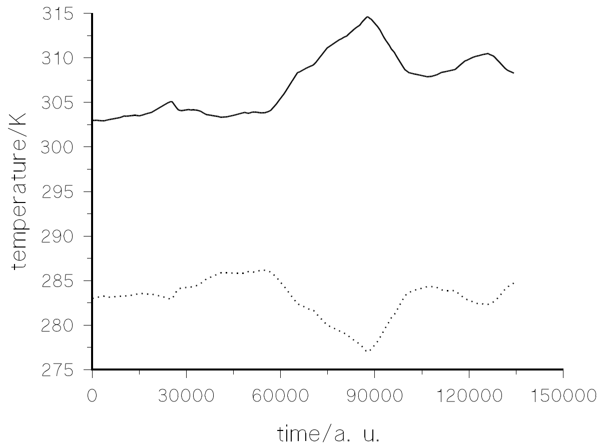

Figure 5: The ground temperature (283.01±5.00)K (dashed) and the ceiling temperature (307.23 ± 11.96)K with constant-like emission at h=1m, $g = 10^4 \frac{m}{s^2}$.

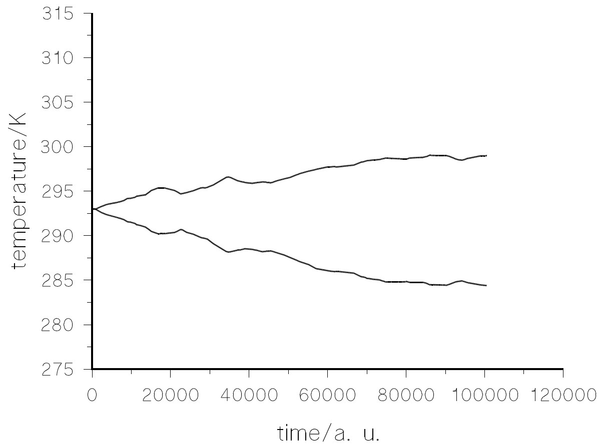

Figure 6: The ground temperature (dashed) and the ceiling temperature with constant-like emission at h=1m, $g = 10^4 \frac{m}{s^2}$.

IV. Discussion and Conclusions

Because the Knudsen gas above a ground in a homogeneous field is determined by the potential gh, the ground temperature and especially the angle probability density of the trajectory parabolas in the Knudsen gas it is simple to make analytical calculations and first principles simulations with, for example, isotropic-like emitting surfaces. Because a Knudsen gas between not cosine-like emitting surfaces in a homogeneous field produces reproduceble significant temperature differences, it would be interesting to find out if every real surface emits on average according to the second Lambert cosine law and therefor satisfies the second law of thermodynamics.

References

[1] Becher, Richard: *Theorie der Wärme*, 3. ed., Berlin, Heidelberg, New York, Tokyo, 1985, page 89 f.

[2] Messiah, Albert: *Quatenmechanik, Volume 1*, Berlin, New York, 2. ed., 1991, page 352