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Barometric distribution of gas density obeying the Lorentz equation of state

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An exact explicit barometric formula is obtained for a non-ideal gas obeying the Lorentz equation of state. The formula describes the density distribution of such a gas in a homogeneous gravitational field. The formula can be useful, for example, when testing codes of molecular dynamics. An example of the application of the formula in deriving the Einstein-Smoluchowski-type relation for a gas with the Lorentz equation of state in a gravitational field is given..

Keywords: non-ideal gas, gravitational field, barometric formula, Lorentz equation of state.

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Introduction

Barometric law for some gas is itself a dependence of gas concentration $n(x)$ (or its density $\rho(x) = mn(x)$) in the gravitational field $U(x)$ on the height x at some concentration of $n(x = 0) = n_0$ specified in some cross-section and temperature of T . In homogeneous and stationary gravitational fields, the barometric law is expressed as [1,2]:

$$n(x) = n_0 \exp\left(-\frac{mgx}{kT}\right) = n_0 \exp\left(-\frac{x}{\Lambda}\right), \quad (1)$$

where m — mass of gas particles, g — acceleration of free fall (acceleration in the gravitational field), k — the Boltzmann constant, $\Lambda = kT/mg$ — the characteristic length at which the concentration decreases in e times. The formula (1) is valid only for a gas with the equation of state $P = nkT$ at a fixed temperature (isothermal case), where P is the gas pressure. It is widely used to describe various processes of the dynamics of gases, liquids, and plasmas [3–6], as well as in chemistry [7,8], planetary sciences [9,10], and astrophysical sciences [11].

Barometric laws and distributions of concentration and density in the potential field are known for some other gases. For example, in [6,12–14] to describe the non-linear processes in plasma a similar formula is used for the adiabatic and polytropic equations of state of an ideal gas, and in [15,16] the distributions of a model gas of hard spheres in a gravitational field is considered [17] presents a relativistic generalization of the barometric law for a number of equations of state, which is applied to the polytropic equation of state of a gas, the equation of state of a degenerate electron gas in the presence of atomic nuclei, the equation of state of a degenerate

neutron gas, and the equation of state of a photonic gas.

The barometric laws for quantum gases are known. Thus, in [18,19] the barometric distributions of the bosonic gas are derived, and in [20] the exact barometric law for the fermionic gas under partial quantum degeneracy is derived. The barometric law for fermions has been used, for example, in the theories of ion-sound [21,22] and Langmuir waves [23,24] in plasma with quantum degenerate electrons. A barometric formula was also derived for an ultrarelativistic degenerate gas (in which the Fermi energy is much greater than the rest mass of the particles) obeying the Chandrasekhar equation of state [25].

Barometric laws for real (non-ideal) gases are of great practical importance. The analysis of barometric distributions for gases described by Van der Waals and Wohl polynomial equations of state was performed in [26,27], and in recent paper [28] the barometric law for Dieterici transcendental equation of state was derived.

For further development of this direction in the theory of equilibrium and dynamics of gases, it is necessary to replenish the list of accurate barometric formulas for other equations of state of real (non-ideal) gases.

In 1881 H.A. Lorentz suggested the polynomial equation of state [29] (see also [30,31]):

$$\left(P + \frac{a}{V^2}\right)V = RT\left(1 + \frac{b}{V}\right), \quad (2)$$

where P — gas pressure, V — molar volume, R — the universal gas constant, a, b — parameters having the same sense as is in the Van der Waals equation: these

constants take into account the attraction and repulsion of gas particles. Despite the fact that the Lorentz equation of state has been known for a long time and is mathematically simpler than the Van der Waals equation, the barometric law for a gas obeying the equation (2) has so far been unknown. The aim of this work was to mathematically derive an accurate and explicit barometric law for a non-ideal gas from the Lorentz equation of state(2). Note that explicit representations of barometric laws for real Van der Waals gases in [26,27] and Diterici gases in [28] could not be obtained. It is very inconvenient to use implicit formulas in the form of inverse functions from [26–28] in theoretical calculations.

1. Derivation of barometric law

First, rewrite the equation (2) in variables „pressure–concentration“

$$P = nkT(1 + \bar{b}n) - \bar{a}n^2. \quad (3)$$

Here \bar{a} , $[\text{J}\cdot\text{m}^3] = a/N_A^2$ and \bar{b} , $[\text{m}^3] = b/N_A$ — the given parameters of the Lorentz equation of state, N_A — the Avogadro constant. It is evident that in the limit

$$\lim_{\bar{a}, \bar{b} \rightarrow 0} nkT(1 + \bar{b}n) - \bar{a}n^2 = nkT, \quad (4)$$

in other words, the Lorentz equation transforms in this limit into the equation of state of an ideal gas.

There are several ways to derive a barometric law. We will follow the simplest gas-static method, for example, in [25,28,32]. To do this, consider the equation of gas-static equilibrium

$$\frac{dU}{dx} + \frac{1}{n} \frac{dP}{dx} = 0. \quad (5)$$

Let's substitute the transformed equation of state (3) into the equation (5) and we obtain the following ordinary differential equation:

$$\frac{dU}{dx} + \left(\frac{kT}{n} + 2\bar{b}kT - 2\bar{a} \right) \frac{dn}{dx} = 0. \quad (6)$$

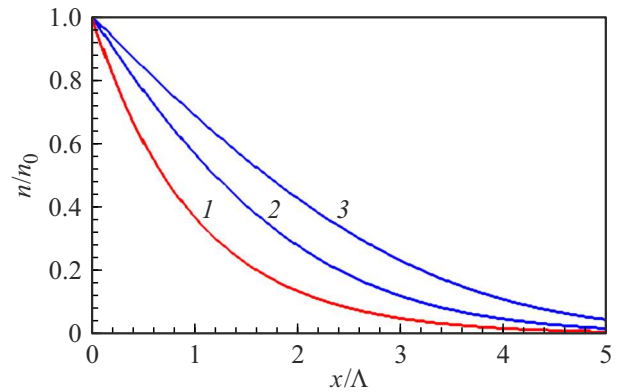
The equation (6) is easily integrated, its general solution with an arbitrary constant C is

$$U + kT \ln n + 2(\bar{b}kT - \bar{a})n = C. \quad (7)$$

Let's find the constant C from the condition $n(U=0) = n_0$. Then, substituting in (7) the expression for the potential energy $U = mgx$ and the expression for C , we obtain

$$mgx + kT \ln \frac{n}{n_0} + 2(\bar{b}kT - \bar{a})(n - n_0) = 0. \quad (8)$$

In fact, the equation (8) is an implicit barometric expression. In it, the second term on the left corresponds to



Barometric dependence (9) at various values of non-ideality parameter G : 1 — at $G = 0$ (ideal gas); 2 — at $G = 1$; 3 — at $G = 2$.

an ideal gas, and the third term corresponds to the Lorentz corrections in the equation of state. Equation (8) can be solved relative to n and the barometric law can be obtained in a more convenient explicit way:

$$n = n_0 \exp \left\{ -W_0 \left[G \exp \left(G - \frac{x}{\Lambda} \right) \right] + \left(G - \frac{x}{\Lambda} \right) \right\}, \quad (9)$$

where the dimensionless parameter was introduced

$$G = \frac{2n_0(\bar{b}kT - \bar{a})}{kT}, \quad (10)$$

which can be called the imperfection parameter of a gas obeying the Lorentz equation of state, and the function $W_0[\dots]$ is the main (positive) branch of the Lambert W function, which is the inverse of the function $x \cdot \exp(x)$ [6,33,34]. It can be easily found that in the limit $G \rightarrow 0$ the obtained barometric law (9) transits to (1).

2. Numerical example

The dependence (9) was calculated for several values of parameter G . The calculation results are presented in the figure.

The figure shows that the barometric dependence for an imperfect gas obeying the Lorentz equation of state, as well as for an ideal gas, is a decreasing function, and with an increase in the imperfection parameter G , the gradient of the function declines.

3. The ratio of diffusion constant to mobility

Derived barometric law (9) can be used, for example, to test molecular dynamics codes in which real gases are modeled in one way or another.

Here is another example of using the resulting formula (9) for analytical calculations. For example, the famous Einstein-Smolukhovsky formula is known, expressing the

ratio of the diffusion constant D to the mobility μ of ideal gas particles in a potential (electric) field [35–38]:

$$\frac{D}{\mu} = kT. \quad (11)$$

It is noteworthy that this ratio does not depend on gas concentration. We can derive the formula for the ratio D/μ , similar to (11), for a gas obeying the Lorentz equation of state. For this, it is required to find

$$\frac{D}{\mu} = -\frac{n(U)}{dn(U)/dU}. \quad (12)$$

Replacing the argument x/Λ in (9) with a new argument U/kT and then calculating (12), we obtain

$$\frac{D}{\mu} = kT \left\{ 1 + W_0 \left[G \exp \left(G - \frac{U}{kT} \right) \right] \right\}. \quad (13)$$

Let's substitute the previously derived expression for $U = mgx$ (8) in (13), and using the definition of the Lambert W function, after simple transformations, we write the following relation

$$\frac{D}{\mu} = kT \left\{ 1 + W_0 \left[G \frac{n}{n_0} \exp \left(\frac{n}{n_0} G \right) \right] \right\} = kT \left(1 + G \frac{n}{n_1} \right), \quad (14)$$

in which the first term — kT — coincides with (11), and the second term follows from the Lorentz corrections to the equation of state. If the second term is positive, then the ratio D/μ in (13) will be greater than for an ideal gas. Note that, unlike in the case of an ideal gas, the ratio D/μ depends on the gas concentration.

4. Conclusion

An exact explicit barometric law is derived for an imperfect gas obeying the Lorentz equation of state. The equation of gas-static equilibrium was used for its mathematical derivation.

The resulting formula describes the density distribution of such a gas in a homogeneous gravitational field. A numerical example is given showing the effect of the non-ideality parameter on the concentration gradient. The formula can be useful, for example, when testing molecular dynamics codes. An example is given for the use of law in derivation of the Einstein-Smoluchowski relation for a gas with Lorentz equation of state in a potential field.

Conflict of interest

The author declares that he has no conflict of interest.

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