

# Dongfang Modified Equations of Molecular Dynamics

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The unitary principle test of the pressure equation of ideal gas gives a negative conclusion, so I systematically revise the basic equation of molecular dynamics. The specific logic and conclusions are as following. The classical molecular dynamics theory established the wrong physical model of uniform motion of molecules under the action of an equivalent constant force, and the classical equations of ideal gas pressure and temperature derived from this model that violates the principle of mechanics is all incorrect. A variety of physical models of molecular interaction in accordance with the mechanical principle is established, and the correct equation of ideal gas pressure is derived consistently. It is proved that the pressure of an ideal gas is equal to the molecular energy per unit volume, and the thermodynamic temperature of an ideal gas is equal to the quotient of molecular average kinetic energy and Boltzmann constant. Various inferences of different models are consistent, so they comply with the unitary principle. Finally, I introduce the problem of the definite solution of the gas molecular rate distribution function that meets the limit condition of the speed of light, and put forward experimental suggestions to verify the theoretical gas temperature correction equation.

**Keywords:** Ideal Gas; Average molecular kinetic energy; Molecular velocity distribution; Basic laws of molecular dynamics; Dongfang formulas.

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## 1 Introduction

Classical molecular kinetic theory<sup>[1,2,5]</sup> holds that the thermodynamic temperature of an ideal gas is directly proportional to the average kinetic energy of a large number of molecules. This qualitative conclusion is true. However, it is not correct for Classical molecular kinetic theory to establish the physical model of uniform motion of molecules under a constant force in the process of deriving quantitative equations. Then, are the basic equations of molecular dynamics such as pressure equation and temperature equation, which are the basic laws of ideal gas derived from the incorrect model, correct?

Revealing mistakes of classical theories will always encounter great resistance, but the wrong theories will inevitably encounter logical difficulties. Different metrics can be selected to describe natural laws. The inference of physical theory must conform to some basic principles, one of which is the Dongfang unitary principle<sup>[3,4]</sup>: *There is a definite transformation relationship between different metrics describing the natural law, and the natural law itself does not change due to the selection of different metrics. When the mathematical expression of natural laws under different metrics is transformed into one metric, the result must be the same as the inherent form*

*under this metric,  $1=1$ , meaning the transformation is unitary.* The unitary principle is a universal principle of logical self consistency test, conforming to the unitary principle is the prerequisite of theory.

It should be pointed out that the theory conforming to the unitary principle may not be correct. But the theory violating the unitary principle must not be correct. The pressure equation of ideal gas is tested by the unitary principle. It is found that the classical molecular kinetic theory only chooses the momentum theorem as one of the metrics for inferring the pressure equation of an ideal gas for calculation, and its quantitative conclusion is not consistent with the calculation result of the kinetic energy theorem which is another metric for inferring the pressure equation of the ideal gas, and does not meet the unitary principle. The reason is that the classical molecular kinetic theory has established an incorrect physical model of uniform motion of molecules under the action of an equivalent constant force. The relationship between the pressure of an ideal gas and the average molecular velocity and the relationship between the temperature of an ideal gas and the thermodynamic temperature need to be corrected.

According to the unitary principle, various physical models that conform to the mechanical principle for the

interaction of ideal gas molecules are studied here, including the equivalent constant force interaction model of the frequent collision between single molecule gas and the container wall and the pressure model of the uniform circular motion of single molecule gas. Under the action of an equivalent constant force, the motion of molecules can only be equivalent to motion with constant acceleration. This is one of the basic principles of mechanics. The pressure equation deduced from different models is consistent, and the conclusion conforms to the unitary principle. The correct form of the ideal gas pressure equation can be determined by using the idea of squeeze theorem, and then the basic molecular dynamics equations such as the temperature and internal energy of the ideal gas can be modified. The results show that the average rate of ideal gas molecules is equal to the maximum probability rate, the pressure of ideal gas is equal to the total kinetic energy of gas molecules in unit volume, and the product of thermodynamic temperature of ideal gas and Boltzmann is equal to the average kinetic energy of molecules. These modified conclusions are called Dongfang formula of basic laws of molecular dynamics. Based on the Dongfang temperature formula, I discussed the constant volume and constant pressure specific heat capacity of gas, and proposed a new equation to explain the experimental measured value of gas specific heat capacity.

In addition, considering that the speed of light is the maximum speed of matter, and the upper limit of temperature depends on the upper limit of the average velocity of molecules, I put forward a definite problem for determining the solution of distribution of molecular speeds with the condition of the light speed limit. However, there are mathematical difficulties in the solution of this definite solution problem. At present, there is no quantitative answer.

## 2 Classical equations of ideal gas violate unitary principle

It is generally accepted that the pressure of a gas is caused by frequent collisions between molecules. The pressure of an ideal gas can be calculated either based on a single molecule model or based on a multi-molecule model. According to the unitary principle, the single molecule model and the multi molecule model are two metrics for calculating the ideal gas pressure, and the conclusions of the two models should be same.

Investigating an ideal gas consisted of the same molecules, in which the mass of the molecule is  $m$ , the average speed is  $\bar{v}$ , and the mean square value of the velocity is  $\overline{v^2}$ . It is assumed that the average distance between gas molecules or the average distance between the gas molecules that is impacting the container wall and the container wall is  $l$ , and  $l$  is just the free path of the molecules. If the whole process of molecular collision

is equivalent to constant force action, the molecule's motion is equivalent to a uniform decrease in velocity from  $\bar{v}$  to 0, whereas it increases uniformly from 0 to  $\bar{v}$  in the opposite direction. That time is a collision periods. The force a molecule marked  $i$  on the container wall and the average reaction force on the molecule are equal, which is denoted by  $F_i$ .

The standard theory selects the multi particle model, first calculates the collision periods  $\Delta t = 2l/\bar{v}_{iz}$  by a component motion of uniform motion, such as the motion in  $oz$  direction. Then it uses the component form of momentum theorem  $\sum (-F_i \Delta t) = \sum (-2m_i \bar{v}_{iz})$  as one of the metrics to calculate the equivalent constant force  $F = \sum F_i$  acting on the collision cross section  $A$ . So  $\sum (-F_i l) = \sum (-m_i \bar{v}_{iz}^2)$ . This result was wrongly written as  $\sum (-F_i l) = \sum (-m_i \overline{v_{iz}^2})$  in the textbook because of the traditional interpretation of the average kinetic energy of the molecules, which actually violates the conclusion of Maxwell's velocity distribution of  $\overline{v^2} \neq \bar{v}^2$ . The average volume of a gas corresponding to a free path is  $V = \sum Al$ , and the pressure is  $p = F/A$ , so  $\sum F_i l = pV$ . As a result, the product of pressure  $p$  and volume  $V$  is  $pV = \sum m \overline{v_{iz}^2}$ . Classical theory makes further energy equipartition hypothesis  $m \overline{v_x^2}/2 = m \overline{v_y^2}/2 = m \overline{v_z^2}/2$ , which gives  $\overline{v_{ix}^2} = \overline{v_{iy}^2} = \overline{v_{iz}^2}$ , so  $\overline{v_{iz}^2} = \overline{v_i^2}/3$ . This also needs to be understood as  $\overline{v_i^2}/3 = \overline{v_{iz}^2}$ , we can get the classic pressure equation  $pV = \sum m \overline{v_i^2}/3$ . This equation is combined with the experimental law  $pV = NkT$ <sup>[6,7]</sup> of ideal gas to give the classical expressions of absolute temperature and average kinetic energy of ideal gas,

$$kT = \frac{1}{3} m \overline{v^2}, \quad \bar{\epsilon}_k = \frac{1}{2} m \overline{v^2} = \frac{3}{2} kT \quad (1)$$

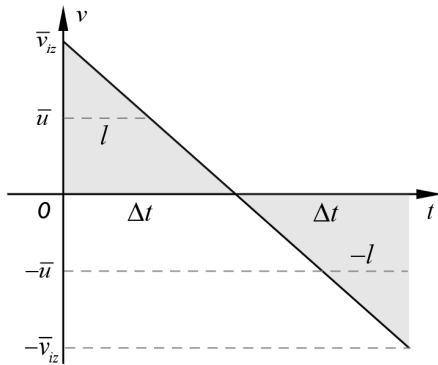
where  $k$  is the Boltzmann constant<sup>[8]</sup>,  $\overline{v^2}$  is the average of the square of the velocity,  $T$  is the thermodynamic temperature of gas, and  $\bar{\epsilon}_k$  is the average translational kinetic energy of molecules.

However, if we use the kinetic energy theorem as another metric to calculate, according to the classical theory, the molecular collision is equivalent to the constant force model, then there is the equation  $\sum \int (-F_i) dl = \sum (0 - m_i \overline{v_{iz}^2}/2)$ . Where  $\sum \int F_i dl = \sum F_i l$ . If the hypothesis of equipartition of energy  $m \overline{v_x^2}/2 = m \overline{v_y^2}/2 = m \overline{v_z^2}/2$  is established, the product of the gas pressure  $p$  and the volume  $V$  should be  $pV = Nm \overline{v^2}/6$ . Combining this formula with ideal gas experimental law of  $pV = NkT$  gives the relationships that are completely different from (1),

$$kT = \frac{1}{6} m \overline{v^2}, \quad \bar{\epsilon}_k = \frac{1}{2} m \overline{v^2} = 3kT \quad (2)$$

Obviously, the two classical corollaries of momentum theorem and kinetic energy theorem based on the assumption of equipartition of energy are contradictory,

that is, the reasoning method of pressure equation and temperature equation of ideal gas in classical thermodynamic theory does not conform to the unitary principle, and the reasoning is naturally incorrect. The momentum theorem and kinetic energy theorem are two parallel inferences of Newton's law of motion, which constitute two metrics of logical self consistency test<sup>[9]</sup>. Their deductions must be consistent. The two conflicting deductions reveal the error of classical theory about concept interpretation and calculation. There are many reasons why the classical derivation of ideal gas pressure equation is wrong and difficult to find. For example, in the calculation process, the classical theory expresses the momentum theorem  $\sum F_i dt = \sum 2m_i v_{iz}$  remove the integral symbol, or use the molecular velocity distribution function  $f(v)$  and the volume microelement  $dV = Adt$  to calculate the molecular number  $N = f(v) dV$ , so the intermolecular collision is equivalent to the constant force, and the molecular motion is misunderstood as the uniform motion, and the error of the collision time  $\Delta t$  is concealed. On the other hand, the unequal relationship  $\bar{v}^2 \neq \overline{v^2}$  between  $\bar{v}^2 = \left( \int_0^N v f(v) dN / N \right)^2 = 8kT/\pi m$  and  $\overline{v^2} = \int_0^N v^2 dN / N = 3kT/m$  of classical theory from Maxwell's velocity distribution theory has not attracted the attention.



**Figure 1** The schematic diagram of the equivalent constant force action of molecular collisions. When the molecular collision is equivalent to the constant force, the whole process of each completion of the collision in the free path can only be equivalent to the motion with constant acceleration, the collision time is not the false inference  $\Delta t = 2l/\bar{v}_{iz}$  of the standard course, but the correct inference  $\Delta t = 2l/\bar{u} = 4l/\bar{v}_{iz}$ , where  $\bar{u} = \bar{v}_{iz}/2$ .

The pressure is the result that the molecular collision is equivalent to the impact of the collision time constant force. Since the interaction of the intermolecular collisions is equivalent to the constant force, the motion of the molecule can only be equivalent to a uniform linear motion. Figure 1 clearly shows that the action time should be  $\Delta t = \int dt = 4l/\bar{v}_{iz}$  instead of  $\Delta t = 2l/\bar{v}_{iz}$  calculated by classical thermodynamic theory. This is because the velocity of a molecule  $i$  de-

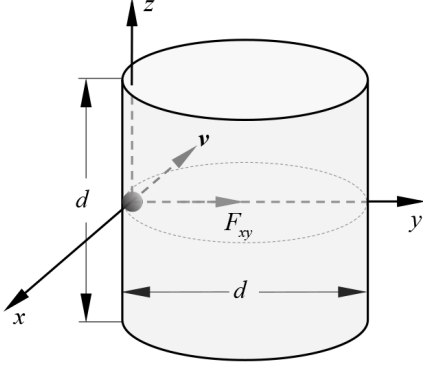
creases from  $\bar{v}_{iz}$  to 0 under the equivalent constant force and increases from 0 to  $\bar{v}_{iz}$ , with an average velocity of  $\bar{u}_{iz} = (\bar{v}_{iz} + 0)/2 = \bar{v}_{iz}/2$ . and the time to return in the free path  $l$  is  $\Delta t = 2l/\bar{u}_{iz} = 4l/\bar{v}_{iz}$ . Using the component form  $\sum (-F_i \Delta t) = \sum (-2m_i \bar{v}_{iz})$  of momentum theorem, the equivalent constant force  $F = \sum F_i = PA$  acting on the collision cross section  $A$  is further calculated, and the result should be  $\sum (-F_i 4l) = \sum (-2m_i \bar{v}_{iz})$ , so  $\sum (-F_i l) = \sum (-m_i \bar{v}_{iz}^2/2)$ . This is the same as the result calculated by the direct kinetic energy theorem, which implies the essential difference that  $\bar{\epsilon} = m_i \bar{v}_{iz}^2/2$  is the expression defined, while  $m_i \bar{v}_{iz}^2/2$  is the result of calculation.  $\sum (-F_i l) = PA l = PV$ . Combing with the so called energy equipartition hypothesis  $m_i \bar{v}_{iz}^2/2 = m_i \bar{v}_i^2/6$  gives the product of the pressure  $p$  and the volume  $V$ , which is also  $pV = Nm \bar{v}_i^2/6$ , and then uses the experimental law of ideal gas  $pV = NkT$  to derive the formula (2). The conclusion that this derivation does not contain incorrect concepts is obviously also deformed, which is due to the use of the energy partition hypothesis which can not be proved.

To sum up, the model of uniform motion under the equivalent constant force is not reasonable, and the calculated collision time is wrong. The deduction process and conclusion of the classical theory are not correct, and the inference of any correct model based on the assumption of the so-called equipartition theorem of kinetic energy can not be accepted. The relationship between temperature and molecular average kinetic energy is one of the basic equations of the theory of thermodynamics. Although it is not very influential in engineering, it has a wide range of influence on the theory. The pressure and temperature equations of ideal gas need to be corrected. We need to find the inference that is consistent with the scientific logic.

### 3 Dongfang pressure formula of ideal gas

Molecules are moving irregularly, so the velocity changes continuously. Since the pressure of the gas generated in collisions between molecules, under equivalent constant force the pressure from a frontal collision or an oblique collision should be same. Why? A molecule bounces-back after the frontal collision and occupy the original channel, blocking other molecules collide with the container. The molecule will fly in the other direction if take an oblique collision, and the other molecules will fill in the original channel to collide with the container again. It is speculated that the frontal collision with low collision frequency will produce a large force, and the oblique collision with high collision frequency will produce a small force. Under the condition of that the same average velocity of the same like molecules, the force per unit area produced by the two collision models should be same. As a matter of fact, a linear motion collision under equivalent constant force can only be equivalent

to a frontal collision. Otherwise, the molecules will describe a curved path in space, and the classical theory on the pressure of an ideal gas is ineffective. Collisions between molecules have an equivalent interaction space. The calculation of the pressure by using the component wise of momentum theorem repeats the equivalent interaction space. So the equation of gas pressure from this algorithm is not accurate.



**Figure 2** Model of single molecule of uniform circular motion

Collisions between gas molecules are complex. If a molecule continuously oblique impact with other molecules, the average effect of this movement can be equivalent to a local uniform circular motion. As shown in Figure 2, it is assumed that a molecule is tied to a cylinder with the same diameter and height. The volume of the average space occupied by the molecule is  $V_0 = \pi r^2 h$ , where  $r = d/2$  and  $h = d$ . This is also the size of the equivalent interaction space. Use  $\bar{v}$  to express the average velocity of the equivalent uniform circular motion of the molecules. Its average centripetal force is  $F_{xy} = m\bar{v}^2/r$ . This force is provided by the equivalent cylinder side wall. According to Newton's third law, the size of the average force on the side of the cylinder is equivalent to this value, and the pressure takes the form  $p_{xy} = F_{xy}/(\pi dh)$ . Consequently, the calculated pressure formula of the ideal gas based on the model of a single molecule in a circular motion is

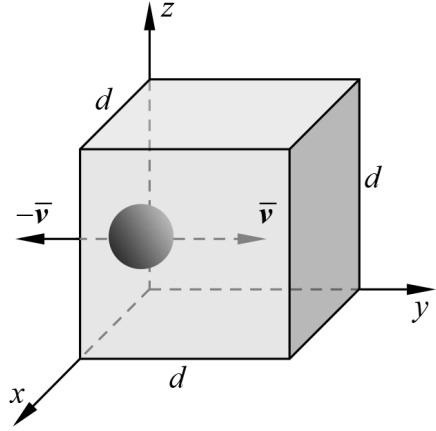
$$p_{xy}V_0 = \frac{1}{2}m\bar{v}^2 \quad (3)$$

The results prompted us to reflect on new conclusions: the average kinetic energy of an ideal gas is described by the square value of the average velocity, and the gas pressure is equal to the average molecular kinetic energy per unit volume rather than three times the average kinetic energy of molecules.

All molecules remain random thermal motion. It usually establishes the elastic collision model to calculate the ideal gas pressure. It is assumed that the average distance between molecules is  $d$ , and each molecule takes up space of average volume  $V_0 = d^3$ . The process of a molecule and other molecules with frontal collision

can be equivalently regarded as that the molecule under the action of the average constant force  $\bar{F}$  does a round straight-line movement with piecewise constant acceleration. On average, in each collision periods it completes a collision between any two molecules or one molecule and the container. In this course, molecular velocity is from  $\bar{v}$  to 0, then reversely from 0 to  $\bar{v}$ . The equivalent beeline path length of the molecular back-and-forth movement is  $2d$ . It is obtained for the equivalent collision time  $\Delta t = 2d/(\bar{v}/2)$ . In the vertical direction of movement, the equivalent constant force  $\bar{F}$  per unit area of the collision cross section is the pressure,  $p = \bar{F}/d^2$ . As shown in Figure 3, the applications of the momentum theorem  $\int_0^{\Delta t} \bar{F} dt = m\bar{v} - (-m\bar{v})$  and the kinetic energy theorem  $\int_0^d -\bar{F} dy = 0 - m\bar{v}^2/2$  give the same conclusion  $\bar{F} = m\bar{v}^2/2d$ . Apparently, the average velocity of a molecule meets the relation  $\bar{v} \cdot \bar{v} = \bar{v}^2$ , and the average molecular kinetic energy should be expressed as  $E_k = m\bar{v}^2/2$  rather than the classical expression  $E_k = m\bar{v}^2/2$ . Consequently, the calculated pressure formula of the ideal gas based on the model of a single molecule in a frontal collision is

$$pV_0 = \frac{1}{2}m\bar{v}^2 \quad (4)$$



**Figure 3** Model of frontal collision of single molecule

More generally, no matter which direction motion of molecules, it has  $\int_0^d \mathbf{F} \cdot d\mathbf{r} = 0 - m\bar{v}^2/2$  in any collision periods. For the equivalent constant force  $\mathbf{F}$ ,  $\int_0^d \mathbf{F} \cdot d\mathbf{r} = -\bar{F}d = -pV_0$ , combining them gives the equation (4), showing that the above correction of the pressure equation of an ideal gas is reliable.

Gas is composed of a large number of molecules in thermal motion. Ideal gas molecules of statistical sense are the identical particles. Thermal motion of the molecule is disorderly, but even if we consider the disordered movement as an orderly movement, the average molecular velocity will not change, so the pressure and temperature of gas also remain unchanged. As shown in



Fgi.3, consider an ideal gas sealed in a cube container, which the total molecular number is  $N$ . It is assumed that in one collision periods there are  $1/6$  molecules make directional collision in the six directions respectively. The molecules of each direction in directional collisions occupy  $1/6$  total volume of space of the gas, so  $NV_0 = V$ . The average collision forces between the molecules are equal, so are the average areas of the collision cross sections. According to the equation (4), It can be written as the following form<sup>[10]</sup>,

$$\begin{aligned} p_{+x} \frac{NV_0}{6} &= \frac{N}{6} \frac{1}{2} m \bar{v}^2, & p_{-x} \frac{NV_0}{6} &= \frac{N}{6} \frac{1}{2} m \bar{v}^2 \\ p_{+y} \frac{NV_0}{6} &= \frac{N}{6} \frac{1}{2} m \bar{v}^2, & p_{-y} \frac{NV_0}{6} &= \frac{N}{6} \frac{1}{2} m \bar{v}^2 \\ p_{+z} \frac{NV_0}{6} &= \frac{N}{6} \frac{1}{2} m \bar{v}^2, & p_{-z} \frac{NV_0}{6} &= \frac{N}{6} \frac{1}{2} m \bar{v}^2 \end{aligned}$$

There are the same gas pressures everywhere,  $p_{+x} = p_{-x} = p$ ,  $p_{+y} = p_{-y} = p$  and  $p_{+z} = p_{-z} = p$ . Combining the six equations gives  $pNV_0 = Nm\bar{v}^2/2$ , and it is easy to obtain  $pNV_0 = Nm\bar{v}^2/2$ . So, the ideal gas pressure calculated by the model of large numbers of molecules with ordered motion in a regular hexahedron container takes the form

$$pV = \frac{1}{2} Nm\bar{v}^2 \quad (5)$$

It is now clear that the pressure of an ideal gas is determined by the average molecular kinetic energy and the average molecular space. Imaging that all molecules in the container are at rest, and their volume is negligible. After adiabatic expansion with an equal pressure, the molecular volume increase from 0 to  $V$ . Gas does work while expanding, and the work in this course is  $W = \int_V p dV = pV$ . On the other hand, according to the theorem of kinetic energy, this work is equal to the total kinetic energy obtained by the gas molecules,  $W = Nm\bar{v}^2/2$ . Combining the above two equations reads the above equation.

By two kinds of single-molecule limit models, using the momentum theorem and the theorem of kinetic energy respectively to calculate the pressure of an ideal gas reads the equations (3) and (4) that are the same, showing the self-consistency of the correction logic, which accords with the unitary principle. Let  $N$  express the total number of total number of molecules of an ideal gas, the gas volume of the ideal gas is  $V = NV_0$ . Use the equation (3) or the (4) can also export the equation (5). Equation (5) is called the Dongfang pressure formula of ideal gas, which shows that the pressure of an ideal gas is equal to the total kinetic energy of molecules in unit volume.

#### 4 Dongfang Temperature formula of ideal gas

The internal energy of the ideal gas is equal to the product of the gas pressure and the gas volume. Since the potential energy between any ideal gas molecules is zero, its total kinetic energy is the product of the total gas molecules number and the kinetic energy of the gas molecules. Therefore, the corrected gas pressure equation (5) of the ideal gas satisfies the law of conservation of energy, it is only another representation of the energy of an ideal gas. Equation (5) combines with the ideal gas law<sup>[11,15]</sup>  $pV = NkT$  to get immediately the temperature equation of ideal gas,

$$kT = \frac{1}{2} m \bar{v}^2 = \bar{\varepsilon}_k \quad (6)$$

The results indicated that the thermodynamic temperature of an ideal gas is equivalent to the quotient of the average translational kinetic energy and Boltzmann constant. Equation (6) is called the Dongfang Temperature formula of ideal gas. Using the equation (6), the relationship between the internal energy of ideal gas and the physical quantities such as the average kinetic energy or thermodynamic temperature of the molecule<sup>[16-19]</sup> is revised to

$$U = \frac{1}{2} Nm\bar{v}^2 = PV = nRT \quad (7)$$

where  $n$  is the number of moles of an ideal gas. These modified consequences satisfy the laws of conservation of momentum and energy. In principle, the relevant theories<sup>[12,20-24]</sup> established on the basis of the classical ideal gas pressure, temperature and internal energy need to be corrected accordingly. We are convinced that the revised conclusion is in good agreement with the experimental observations under the condition that the effects of various objective factors are fully taken into account.

Ideal gas is a simplified model of the actual gas that neglects the potential energy of intermolecular interaction. It is an infinitely thin gas from the macroscopic point of view and follows the ideal gas equation of state. However, from the perspective of energy transformation and conservation, the ideal gas molecules are the single particles with kinetic energy but no binding energy. Even the extremely thin monatomic gas cannot form an ideal gas, because the single atom is a multi particle system composed of nuclear and extra nuclear electrons. In the effective understanding of the microscopic structure of matter, only a large number of neutrons which are stored in a container can form an ideal gas in a real sense, but in fact no such ideal gas exists.

The experimental laws of gas are all derived from the actual gas under certain conditions. The specific heat capacity of the actual gas is related to the law of the temperature of the gas, but it is not the only connection. This is because the heat absorbed by the actual

gas molecules not only increases the total kinetic energy of the molecules, but is also absorbed by atoms or molecules to increase the energy of the atoms in the molecules and molecules. Ignoring the heat absorption of the container wall molecules, the energy relation of the constant volume process is,

$$Q = \sum (\Delta \varepsilon_i + \Delta E_{\text{molecule}} + \Delta E_{\text{atom}}) \quad (8)$$

Among them,  $Q$  is the heat absorbed by the gas with the total number of  $N$ ,  $\sum \varepsilon_i = N\bar{\varepsilon} = NkT$ ,  $E_{\text{molecule}}$  the energy of the molecule, and  $E_{\text{atom}}$  the energy of the atom. The principle formula for calculating the average specific heat capacity  $c_v = \frac{1}{N} \left( \frac{Q}{\Delta T} \right)$  of each molecule in the process of the fixed volume is,

$$c_v = k + \frac{1}{N} \frac{\sum (\Delta E_{\text{molecule}} + \Delta E_{\text{atom}})}{\Delta T} \quad (9)$$

The specific heat capacity of any gas has its own wider distribution range<sup>[25-27]</sup>. The molecules of a diatomic or polyatomic gas will absorb more energy than the single atom. According to the experimental measurements of the constant volume ratio of the gas to the heat, the monatomic gas  $c_v \approx 3k/2$ , the diatomic gas  $c_v \approx 5k/2$ , the polyatomic gas  $c_v \approx 7k/2$ . In the process of constant pressure, the volume of gas expands, the gas is doing work to the outside world, and the surface area of the solid container increases, and the number of solid molecules that absorb heat increases. Ignoring the heat absorption of the container wall molecules, the energy relation of the constant pressure process is,

$$Q = \sum (\Delta \varepsilon_i + \Delta E_{\text{molecule}} + \Delta E_{\text{atom}}) + W \quad (10)$$

Where  $W$  is the work done by the gas in the process of constant pressure. In this way, From this, the principle formula for calculating the average specific heat capacity  $c_p = \frac{1}{N} \left( \frac{Q}{\Delta T} \right)$  of each molecule during constant pressure is,

$$c_p = k + \frac{1}{N} \frac{\sum (\Delta E_{\text{molecule}} + \Delta E_{\text{atom}})}{\Delta T} + \frac{W}{\Delta T} \quad (11)$$

Considering the influence of the container, when the gas molecules absorb heat and thus the temperature changes, the molecules in the container wall absorb energy and the temperature changes synchronously, which is also related to the material of the container. Consider the transition of the atomic energy level, the specific heat capacity  $c_v$  of constant volume and the specific heat capacity  $c_p$  of constant pressure cannot be constant at all times. Therefore, it is very difficult to theoretically derive the precise formula for the specific heat capacity of gas.

However, the experimental law of gases is not directly related to the energy of atoms or molecules. Therefore,

the Dongfang Temperature formula of ideal gas based on the correct physical model and the correct reasoning of the ideal gas is generally applicable to the thin real gas.

## 5 Problem for determining solution of velocity distribution function

The equation (6) is consistent with a conclusion of statistical physics. According to Maxwell velocity distribution law, if the temperature of an ideal gas is  $T$ , the number of molecules with the speed  $v$  makes up percentage  $f(v)$  of the total number of gas molecules<sup>[5]</sup>, where,

$$f(v) = 4\pi \left( \frac{m}{2\pi kT} \right)^{3/2} v^2 e^{-\frac{mv^2}{2kT}} \quad (12)$$

where  $m$  is the particle mass, and  $kT$  is the product of Boltzmann's constant and thermodynamic temperature. The corresponding speed of the extreme point of the above distribution function,  $df(v)/dv|_{v=v_p} = 0$ , is the most probable speed.

$$v_p = \sqrt{\frac{2kT}{m}} \quad (13)$$

This is just the equation (6). It follows that the average molecular speed is equal to the most probable speed. Our modified ideal gas temperature is consistent with the conclusion of statistical physics.

However, Maxwell velocity distribution law predicting the statistical average values conceals a difficulty that the roots of physical quantities with the high orders are different. The corresponding calculations violate the basic mathematical rules of  $\sqrt{|a|^2} = |a|$ . For example,

$$\langle v \rangle = \frac{1}{N} \int_0^N v dN = \int_0^\infty v f(v) dv = \sqrt{\frac{8kT}{\pi m}}$$

and

$$\sqrt{\langle v^2 \rangle} = \left( \int_0^\infty v^2 f(v) dv \right)^{1/2} = \sqrt{\frac{3kT}{m}}$$

It was obvious that  $\sqrt{\langle v^2 \rangle} \neq \langle v \rangle$ , the logic is not self-consistent! Classical theory defined these two calculations, respectively, as the statistically average velocity and root-mean-square speed<sup>[28-30]</sup>, but ignored the nature why the calculations are very different. In fact, these results have no effects of experimental observations, and the physical quantities that have the effect of experimental observation are the average velocity or the most probable speed. A theory based on the relationship  $\sqrt{|a|^2} \neq |a|$  is only a formal theory. An inference of the formal theory is often similar to but deviate from the true law. Investigating the power radiated from a black body in terms of its temperature. According to the Stefan-Boltzmann law<sup>[31-33]</sup>,

$$j^* = \frac{2\pi^5 k^4}{15c^2 h^3} T^4 \propto \bar{v}^8 \quad (14)$$

Where  $j^*$  is the black-body radiant exitance,  $h$  is the Planck's constant,  $k$  is the Boltzmann constant, and  $c$  is the speed of light in a vacuum. Now that the term  $\bar{v}^8$  appears in the Stefan–Boltzmann law, then according to the Maxwell velocity distribution law, we can define the generally statistical averages to compare their roots,

$$\sqrt[n]{\langle v^n \rangle} = \frac{1}{N} \left( \int_0^N v^n dN \right)^{1/n}$$

Apparently, different values of  $n$  lead to the results vary widely. These formal consequences have no physical meaning. But giving them different definitions or assumptions respectively would be representative of the logical difficulties.

Since the molecular speed cannot reach the speed of light, it can only describe roughly the gas molecules velocity distribution by Maxwell speed distribution function of depending on the normalized conditions that the speed limit is infinity<sup>[34–36]</sup>. Formally, using the relativistic energy equation  $E^2 = p^2 c^2 + m_0^2 c^4$  can rewrite the Maxwell velocity distribution functions<sup>[37–41]</sup>, but we cannot strictly prove the result of rewriting. In fact, the relativistic normalization coefficient written in the speed of light<sup>[42]</sup> can not be expressed by the elementary function, so it is difficult to obtain the accurate rate distribution function. It usually considers that a velocity distribution function gives the probability, per unit speed, of finding the particle with a speed near  $v$ . We found a velocity distribution function can also be understood as describing the probability of a molecule reaches the speed  $v$ , and the corresponding results are not affected. An accurate gas molecule velocity distribution function should be determined by the following boundary value problem,

$$\begin{aligned} \psi(v=0) &= 0, \quad \psi(v=c) = 0 \\ \int_0^c \psi(v) dv &= 1, \quad \left. \frac{d\psi(v)}{dv} \right|_{v=\bar{v}} = 0 \\ \bar{v} &= \left( \int_0^c v^n \psi(v) dv \right)^{1/n}, \quad n = 1, 2, \dots \end{aligned} \quad (15)$$

We do not know yet whether this molecular velocity distribution function exists, and whether the iconic factor of relativity is included in the solution. However, it can be sure that the Maxwell velocity distribution function must be an approximation of the solution of this boundary value problem.

## 6 Comments and conclusions

The Dongfang Temperature formula of ideal gas was discovered when studying the com quantum law<sup>[2]</sup> of stellar radiation temperature, which promoted the normalization principle test of the basic equation of molecular

dynamics and found its errors, leading to the generation of systematic modified equations. According to the unitary principle of logical self consistency test, all the problems and conclusions proposed in this paper are easy to understand. In short, establishing various reasonable physical models for calculating the pressure of an ideal gas and modifying the basic equations of pressure and temperature of an ideal gas, the conclusions obtained are consistent and therefore cannot be overturned. The modified equation is named as the Dongfang formula of the basic laws of molecular dynamics to distinguish it from the incorrect equation of classical molecular dynamics.

Computations that violate the common sense of physics in physics standard courses are usually difficult to be discovered directly, and correcting such calculations is not easy to be accepted. The main reason is that some simple but trivial causal relationships have not attracted the attention of researchers, and mainstream physicists' excessive pursuit of personal fame and wealth has led to hegemony and sophistry that have been shrouded in the physical world. Even if wrong inferences and even wrong theories are found, they have been permanently strangled. But we believe that future scientists will distinguish between correct and wrong inferences and make the right choices. Since the average force produced by a gas molecular collision is equivalent to a constant force, the motion of a gas molecule must be equivalent to a motion with constant acceleration; otherwise all the inferences are contrary to the law of conservation of energy. Various equivalent motions in the process of molecular collision constitute a variety of model metrics. Momentum theorem and kinetic energy theorem constitute two kinds of computational metrics, which belong to sub metrics. It is only necessary to investigate the equivalent molecular motion process in one of collision periods, and calculate the pressure, temperature and internal energy of the ideal gas<sup>[28–30]</sup> independently in various metrics. The calculation results of the same physical quantity must be consistent. This is the specific application of the principle of normalization. The physical process and conclusion following the unitary principle are the most reliable.

The ideal gas pressure is equal to the kinetic energy of the molecule in a unit volume, and the product of the thermodynamic temperature of the ideal gas and the Boltzmann constant is equal to the average kinetic energy of the molecule. In the laboratory, the number of molecules, gas pressure and gas temperature of the same kind of gas in an adiabatic sealed container can be measured. If the average speed of the same kind of gas molecules at the same temperature is measured, the Dongfang Temperature formula of ideal gas can be verified experimentally. Therefore, the measurement of the average rate of gas molecules at a certain temperature is a meaningful basic experiment.

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## Guided Reading

For decades, I have systematically and carefully studied the basic theories of physics and found that not all physical inferences are correct. When studying the generalized wave equation and its exact solution, I found

that the classical equation of the ideal gas temperature was wrong, and found the cause of the error. In this paper, the modified equation of the ideal gas temperature is given, and the relevant experimental explanations are



reviewed. It is a very cautious thing to revise the basic theorem of classical theory. The popularization of physics and mathematical logic in this article makes me rack my brains. In the past decade, it has been misread by commentators of academic journals. Ignoring malicious slander and strangulation, of course, I thank all those who read this article. The concise logical structure of this paper is listed here. I hope this article will not cause misunderstanding again.

#### • Calculation errors in standard textbooks

1. The classical molecular kinetic theory establishes the equivalent constant-force model to describe molecular collisions, this is not a problem.
2. The classical molecular kinetic theory does not calculate the collision periods between molecule and container wall in detail, the molecular motion under the equivalent constant force action is treated as a uniform motion, and the collision half period is understood to be  $\Delta t/2 = l/\bar{v}$ . These are all wrong.
3. The classical molecular kinetic theory have use an unfounded hypothesis,  $\bar{v}_x^2 = \bar{v}_y^2 = \bar{v}_z^2$ , which is magnified to the equipartition theorem of energy, and this hypothesis is actually not true;
4. On the basis of the above unreasonable logic, classical molecular dynamic theory uses the momentum theorem, one of the deductions of Newton's law of motion, to derive an incorrect pressure formula  $pV = \sum m\bar{v}_i^2/3$  and an incorrect temperature formula  $kT = m\bar{v}^2/3$ ;
5. However, if the kinetic energy theorem, another deduction of Newton's law of motion, is used, the logical inference of the classical molecular dynamic theory should be  $pV = \sum m\bar{v}_i^2/3$  and  $kT = m\bar{v}^2/3$ .
6. The molecular collision half periods of the equivalent constant force action model is actually  $\Delta t/2 = 2l/v$ , If one would again quote the unfounded hypothesis,  $\bar{v}_x^2 = \bar{v}_y^2 = \bar{v}_z^2$ , the inference of the momentum theorem would also be  $kT = m\bar{v}^2/3$ , this conclusion is obviously not acceptable.

Therefore, even if the so-called the equipartition theorem of energy based on the unfounded hypothesis  $\bar{v}_x^2 = \bar{v}_y^2 = \bar{v}_z^2$  is recognized, the conclusion of the molecular dynamic theory can only be  $kT = m\bar{v}^2/3$  rather than  $kT = m\bar{v}^2/3$ . But the hypothesis of  $\bar{v}_x^2 = \bar{v}_y^2 = \bar{v}_z^2$  is not

reasonable, and the two classical results are not correct. I build a variety of models and calculate them from different angles to get consistent results.

#### • Calculation correction and correct inference

1. In one collision periods, the article considers two extreme models to describe the collision of molecules: uniformly accelerated linear motion and uniform circular motion;
2. For circular motion model, the article uses the centripetal force equation to calculate the ideal gas pressure, the result is  $pV = Nm\bar{v}^2/2$ , where  $N$  is the total number of molecules and  $V$  is the volume of ideal gas. So, the temperature equation is  $kT = m\bar{v}^2/2$ , which called the Dongfang Temperature formula of ideal gas;
3. For the uniform acceleration linear motion model, one can prove that the collision time of a molecule in the free path is  $\Delta t = 4l/\bar{v}$ . The article uses the momentum theorem and the kinetic theorem to calculate the ideal gas pressure respectively, and the results are the same equation,  $pV = Nm\bar{v}^2/2$ , where  $N$  is the total number of molecules. Thinking about it further also reads the ideal gas temperature equation  $kT = m\bar{v}^2/2$ ;
4. Now that the conclusions of the two extreme models are the same, by the squeezing theorem, the temperature of the ideal gas inevitably satisfies the formula  $kT = m\bar{v}^2/2$ . The actual motion of the molecular collisions is between the uniform circular motion and the special model of the uniform velocity linear motion. Therefore, the equation  $kT = m\bar{v}^2/2$  is the correct inference of the relationship between the ideal gas temperature and kinetic energy;
5. The revised calculation explains that the physical quantity which has physical significance is the average velocity  $\bar{v}$  rather than the average square speed  $\bar{v}^2$ . The hypothesis  $\bar{v}_x^2 = \bar{v}_y^2 = \bar{v}_z^2$  of classical textbook is unable to be proven, and it's actually superfluous.

One can also establish a variety of different physical models to prove the correction formulas of basic laws of molecular dynamics, thus realizing that some simple concepts and calculations in physics may be misunderstood, and the errors of the conclusions derived from the incorrect methods have been difficult to be found. Physical computation requires a universal test rule to avoid errors and meaningless arguments.