

New Quantum Theory and New Meaning of Specific Heat of an Ideal Gas

By

Yoshifumi ITO and Md Sharif UDDIN

*Department of Mathematical and Natural Sciences, Faculty of Integrated
Arts and Sciences, the University of Tokushima, Tokushima 770-8502,*

*Japan
and*

*Department of Mathematics, Jahangirnagar University, Savar, Dhaka-1342,
Bangladesh*

*E-mail : y-ito@ias.tokushima-u.ac.jp
msharifju@yahoo.com*

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Abstract

In this article, we consider the specific heat of an ideal gas composed of monatomic molecules in the view point of the new quantum theory. Thereby we can clarify a new meaning of specific heat of an ideal gas.

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Introduction

In this article, we consider the molar heat and the specific heat of constant volume of an ideal gas composed of monatomic molecules in the view point of the new quantum theory. We get a reasonable explanation of them. It gives a new true explanation of the results known until now. We use here the framework of the new quantum theory mentioned in chapter 1 of Ito and Uddin [9]. The new quantum theory was originated by Y. Ito [2]-[4] at 1998-2000. As for the new quantum theory, we refer the papers [1]-[9] of the references.

1. Physical setting of the system and the problem

We consider an ideal gas composed of monatomic molecules spreaded infinitely. There are N molecules in the region of volume V . The ideal gas is so

rarefied that there is no mutual interaction among molecules. They only move freely and no forces act on them. Every molecule moves under the Newtonian equation of motion:

$$m \frac{d^2 x}{dt^2} = 0$$

Here m denotes the mass of one molecule.

We wish to consider the specific heat C_V of constant volume and the molar heat C_M of this ideal gas.

Then we have the relation $C_V = nC_M$ where $N = nN_A$ and N_A denotes the Avogadro number.

2. Setting of the mathematical model

We use the notation in chapter 1 of Ito and Uddin [9]. We consider axiom I and axiom III in chapter 1 of Ito and Uddin [9]. Let $\Omega = \Omega(\mathbf{B}, P)$ be the probability space which represents the quantum system considered here. An elementary event ρ of Ω is a monatomic molecule which moves freely in the 3-dimensional Euclidean space \mathbf{R}^3 . Here we consider one degree of freedom of the 3-dimensional free motion. Then we denote the position variable of a monatomic molecule ρ by $x = x(\rho)$, and the momentum variable of ρ by $p = p(\rho)$. Here we put $n = dM = 1$ because the space dimension is $d = 1$, the number of monatomic molecules which compose an elementary event ρ is $M = 1$. The variable x changes in the space \mathbf{R}^1 and the variable p changes in its dual space \mathbf{R}_1 .

Here we need the new axiom for the generalized quantum state.

Axiom II' (generalized quantum state).

We consider the generalized quantum state of the quantum system $\Omega = \Omega(\mathbf{B}, P)$ as the state of the generalized quantum probability distribution of the position variable $x = x(\rho)$ and the momentum variable $p = p(\rho)$ of monatomic molecules ρ composing the quantum system. Here we consider the orthogonal coordinate system of 1-dimensional Euclidean space \mathbf{R}^1 and its dual space \mathbf{R}_1 .

The generalized quantum state is determined as follows:

(II₁') The generalized quantum distribution state of the position variable $x = x(\rho)$ is determined by L^2_{loc} -function ψ .

(II₂') The generalized quantum distribution state of the momentum variable $p = p(\rho)$ is determined by $\hat{\psi}$. Here $\hat{\psi}$ is the function determined as local Fourier transforms of ψ .

Namely

$$\begin{aligned} \hat{\psi}_S(p) &= (2\pi\hbar)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \psi_S(x) e^{-ipx/\hbar} dx, \\ \psi_S(x) &= (2\pi\hbar)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \hat{\psi}_S(p) e^{ipx/\hbar} dp \end{aligned}$$

where S is an arbitrary compact set in \mathbf{R}^1 and, when we denote the characteristic function of S as

$$\chi_S(x) = \begin{cases} 1, & (x \in S), \\ 0, & (x \notin S), \end{cases}$$

we define ψ_S to be the function $\psi_S(x) = \psi(x)\chi_S(x)$. Namely ψ_S is the cut off function of ψ on S . We put $\hbar = \frac{h}{2\pi}$, here h being the Planck constant. In the above we use the classical Fourier transformation.

(II'₃) For a Lebesgue measurable set A in \mathbf{R}^1 , we assume

$$P(\{\rho \in \Omega; x(\rho) \in A \cap S\}) = \frac{\int_{A \cap S} |\psi_S(x)|^2 dx}{\int_S |\psi_S(x)|^2 dx} = \mu_S(A)$$

This gives the probability that the position variable $x(\rho)$ of a monatomic molecule ρ moving in the region S belongs to $A \cap S$. Thereby we have the relative probability space $(S, \mathcal{M}_1 \cap S, \mu_S)$ corresponding to ψ_S . Here \mathcal{M}_1 is the family of Lebesgue measurable sets in \mathbf{R}^1 .

(II'₄) For a Lebesgue measurable set B in \mathbf{R}_1 , we assume

$$P(\{\rho \in \Omega; x(\rho) \in S, p(\rho) \in B\}) = \frac{\int_B |\hat{\psi}_S(p)|^2 dp}{\int_{-\infty}^{\infty} |\hat{\psi}_S(p)|^2 dp} = \nu_S(B)$$

This gives the probability that the momentum variable $p(\rho)$ of the monatomic molecule ρ moving in the region S belongs to B . Thereby, we have the relative probability space $(\mathbf{R}_1, \mathcal{N}_1, \nu_S)$ corresponding to $\hat{\psi}_S$. Here \mathcal{N}_1 is the family of Lebesgue measurable sets in \mathbf{R}_1 .

Then by the axiom II', the L_{loc}^2 -density $\psi(x)$ determines the generalized quantum distribution law of the position variable x and its local Fourier transform $\hat{\psi}_S(p)$ determines the generalized quantum probability distribution law of the momentum variable p . The total energy of each monatomic molecule ρ is determined by the classical mechanics. Its value is $\frac{1}{2m}p(\rho)^2$. Here m is the mass of the monatomic molecule.

This energy variable is considered as a generalized quantum random variable defined on the probability space Ω which represents the quantum system. The evaluation of the local expectation value of this energy variable, namely the local energy expectation value, is carried out by using the axiom II'.

Namely we use the relation

$$P(\{\rho \in \Omega; x(\rho) \in A \cap S\}) = \frac{\int_{A \cap S} |\psi_S(x)|^2 dx}{\int_S |\psi_S(x)|^2 dx},$$

$$P(\{\rho \in \Omega; x(\rho) \in S, p(\rho) \in B\}) = \frac{\int_B |\hat{\psi}_S(p)|^2 dp}{\int_{-\infty}^{\infty} |\hat{\psi}_S(p)|^2 dp},$$

for every compact set S in \mathbf{R}^1 and a subset A in \mathbf{R}^1 and a subset B in \mathbf{R}_1 . Then we have the local energy expectation value \bar{E}_S :

$$\bar{E}_S = E_S \left[\frac{1}{2m} p(\rho)^2 \right] = \frac{\int_{-\infty}^{\infty} \frac{1}{2m} p^2 |\hat{\psi}_S(p)|^2 dp}{\int_{-\infty}^{\infty} |\hat{\psi}_S(p)|^2 dp} = \frac{\int_S \frac{\hbar^2}{2m} \left| \frac{d\psi_S(x)}{dx} \right|^2 dx}{\int_S |\psi_S(x)|^2 dx}.$$

Here we use the Plancherel formula for Fourier transformation. Here we denote this local energy expectation value by

$$J_S[\psi_S] = \frac{\int_S \frac{\hbar^2}{2m} \left| \frac{d\psi_S(x)}{dx} \right|^2 dx}{\int_S |\psi_S(x)|^2 dx}.$$

We call $J_S[\psi_S]$ the local energy functional.

Here we assert the following principle.

Principle II (local variational principle).

In the case of continuous spectrum of the Hamiltonian operator of a quantum system, the stationary state are realized as the state where the energy expectation of the quantum system considered locally takes the stationary value under some conditions.

From this principle, we can choose the true L_{loc}^2 -density for this quantum system. So that we consider the following problem I and problem II :

Problem I.

Let $\{r_n\}$ be a certain increasing sequence of positive numbers: $r_1 \leq r_2 \leq \dots \leq r_n \leq \dots$.

Let $\{K_n\}$ be an exhausting increasing sequence of non-empty compact sets of \mathbf{R}^1 . Namely it satisfy the following conditions (i) and (ii):

(i) $\emptyset \neq K_1 \subset K_2 \subset \dots \subset K_n \subset \dots \subset \mathbf{R}^1$,

(ii) $\bigcup_{j=1}^{\infty} K_j = \mathbf{R}^1$.

For an arbitrary positive number $\mathcal{E} > 0$, determine the locally square integrable function $\psi^{(\mathcal{E})}(x)$ such that the following conditions (1)~(5) are satisfied:

(1) $\psi^{(\mathcal{E})}|_{K_n} = \psi_n$.

(2) $\psi_{n+1}|_{K_n} = \psi_n$.

(3) $\int_{K_n} |\psi_n(x)|^2 dx = r_n > 0$, ($n = 1, 2, \dots$).

(4) $\int_{-\infty}^{\infty} \psi^{(\mathcal{E}')} (x) \ast \psi^{(\mathcal{E})} (x) dx = \delta(\mathcal{E}' - \mathcal{E})$, ($\mathcal{E}, \mathcal{E}' > 0$).

Here $\delta(\mathcal{E})$ denote the delta function.

(5) The functional

$$J_n[\psi_n] = \frac{\int_{K_n} \left(\frac{\hbar^2}{2m} \left| \frac{d\psi_n(x)}{dx} \right|^2 \right) dx}{\int_{K_n} |\psi_n(x)|^2 dx}$$

takes its stationary value under the conditions (2) and (3).

Problem II.

Find out the L_{loc}^2 -density for which the local energy expectation value $J_n[\psi_n]$ takes its stationary value under the condition that $\int_{K_n} |\psi_n(x)|^2 dx$ is equal to a given constant r_n .

3. Mathematical analysis

Solving the problems I and II in chapter 2, we have the Schrödinger equations

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_n(x)}{dx^2} = \mathcal{E} \psi_n(x), \quad x \in K_n (n = 1, 2, \dots)$$

as the Euler equations. Here \mathcal{E} is the Lagrange's unknown constant. By the conditions (1), (2) and (3) of problem I in chapter 2, we have the L_{loc}^2 -function $\psi^{(\mathcal{E})}(x)$ such that it satisfies, for some constant $\mathcal{E} > 0$,

$$\psi^{(\mathcal{E})}(x) = \psi_n(x), \quad x \in K_n (n = 1, 2, \dots).$$

Then $\psi^{(\mathcal{E})}(x)$ satisfies the Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi^{(\mathcal{E})}(x)}{dx^2} = \mathcal{E} \psi^{(\mathcal{E})}(x), \quad x \in \mathbf{R}^1.$$

As solutions of the above generalized eigenvalue problem, we have the generalized eigenfunction $\psi^{(\mathcal{E})}(x)$ corresponding to the eigenvalue $\mathcal{E} > 0$. Namely we have, for every $\mathcal{E} > 0$,

$$\psi_{\pm}^{(\mathcal{E})}(x) = c(\mathcal{E}) \exp\left(\pm \frac{i}{\hbar} x \sqrt{2m\mathcal{E}}\right).$$

For every $\mathcal{E} > 0$, there exist two independent generalized eigenfunctions. Therefore every spectrum \mathcal{E} is degenerated. If we normalize the generalized eigenfunctions in the scale of \mathcal{E} , we have

$$\psi_{\pm}^{(\mathcal{E})}(x) = \left(\frac{m}{2\hbar^2\mathcal{E}}\right)^{\frac{1}{4}} \exp\left(\pm\frac{i}{\hbar}x\sqrt{2m\mathcal{E}}\right).$$

Then we have the relations, for $\mathcal{E} > 0$ and $\mathcal{E}' > 0$,

$$\int_{-\infty}^{\infty} \psi_{+}^{(\mathcal{E}')} (x)^* \psi_{+}^{(\mathcal{E})} (x) dx = \delta(\mathcal{E}' - \mathcal{E}),$$

$$\int_{-\infty}^{\infty} \psi_{-}^{(\mathcal{E}')} (x)^* \psi_{-}^{(\mathcal{E})} (x) dx = \delta(\mathcal{E}' - \mathcal{E})$$

and

$$\int_{-\infty}^{\infty} \psi_{-}^{(\mathcal{E}')} (x)^* \psi_{-}^{(\mathcal{E})} (x) dx = 0.$$

Here c^* denotes the complex conjugate of a complex number c . If we put $k^2 = \frac{2m\mathcal{E}}{\hbar^2}$, for $\mathcal{E} \geq 0$, we have, for $-\infty < k < \infty$,

$$\psi^{(k)}(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

which is normalized in the scale of k :

$$\int_{-\infty}^{\infty} \psi^{(k')} (x)^* \psi^{(k)} (x) dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-k')x} dx = \delta(k' - k), \quad -\infty < k, k' < \infty.$$

Then we have

$$-\frac{\hbar^2}{2m} \frac{d^2\psi^{(k)}(x)}{dx^2} = \mathcal{E}\psi^{(k)}(x), \quad x \in \mathbf{R}^1.$$

If we put $\psi^{(k)}|_{K_n} = \psi_n$, ($n = 1, 2, \dots$), we have

$$J_n[\psi_n] = \frac{\mathcal{E}}{2\pi} \frac{\int_{K_n} 1 dx}{\int_{K_n} 1 dx} = \mathcal{E}, \quad (n = 1, 2, \dots).$$

Thus $\psi^{(k)}(x)$ satisfies all the conditions of problem I. Thus we have the solution of problem I. If we put $p = \hbar k$ and we write

$$\psi^{(p)}(x) = \frac{1}{\sqrt{\hbar}} \psi^{(k)}(x)$$

for $p = \hbar k$. Then we have

$$\psi^{(p)}(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}, \quad \left(\mathcal{E} = \frac{p^2}{2m} \right)$$

which is normalized in the scale of p :

$$\int_{-\infty}^{\infty} \psi^{(p')}(x)^* \psi^{(p)}(x) dx = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{i(p-p')x/\hbar} dx = \delta(p' - p), \quad p, p' \in \mathbf{R}_1.$$

Then we have

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi^{(p)}(x)}{dx^2} = \mathcal{E} \psi^{(p)}(x), \quad x \in \mathbf{R}^1.$$

If we put $\psi^{(p)}|_{K_n} = \psi_n$, ($n = 1, 2, \dots$), we have

$$J_n[\psi_n] = \frac{\frac{\mathcal{E}}{2\pi\hbar} \int_{K_n} 1 dx}{\frac{1}{2\pi\hbar} \int_{K_n} 1 dx} = \mathcal{E}, \quad (n = 1, 2, \dots).$$

This $\psi^{(p)}(x)$ satisfies all the conditions of problem I. Thus we have the solution of problem I. In the above, the L^2_{loc} -densities $\psi^{(\mathcal{E})}(x)$, $\psi^{(k)}(x)$ and $\psi^{(p)}(x)$ are the different representations of the solutions of problem I which differ only in the scale of the normalization.

By virtue of the theory of Fourier transformation, for any $\psi \in L^2(\mathbf{R}^1)$, there exists $c \in L^2(\mathbf{R}_1)$ such that we have

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} c(p) e^{ipx/\hbar} dp$$

and

$$c(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} dx.$$

If the true physical state of the total quantum system Ω is determined by some L^2 -density $\psi(x)$ at the initial time point, then we have the generalized eigenfunction expansion of $\psi(x)$ by $\psi^{(p)}(x)$ as follows:

$$\psi(x) = \int_{-\infty}^{\infty} c(p) \psi^{(p)}(x) dp,$$

$$c(p) = \int_{-\infty}^{\infty} \psi^{(p)}(x)^* \psi(x) dx.$$

Then we have the energy expectation value

$$\overline{E} = J[\psi] = \int_{-\infty}^{\infty} \frac{p^2}{2m} |\hat{\psi}(p)|^2 dp = \int_{-\infty}^{\infty} \frac{p^2}{2m} |c(p)|^2 dp.$$

Further, since the function $\psi(x)$ satisfies the normalization condition

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1,$$

we have

$$\int_{-\infty}^{\infty} |c(p)|^2 dp = 1.$$

Since we have $\frac{p^2}{2m} = \mathcal{E}$, we have

$$\begin{aligned} \bar{E} = J[\psi] &= \int_{-\infty}^0 \frac{p^2}{2m} |c(p)|^2 dp + \int_0^{\infty} \frac{p^2}{2m} |c(p)|^2 dp. \\ &= \frac{1}{2} \int_0^{\infty} \mathcal{E} \sqrt{\frac{2m}{\mathcal{E}}} |c(-\sqrt{2m\mathcal{E}})|^2 d\mathcal{E} + \frac{1}{2} \int_0^{\infty} \mathcal{E} \sqrt{\frac{2m}{\mathcal{E}}} |c(\sqrt{2m\mathcal{E}})|^2 d\mathcal{E}. \\ &= \frac{1}{2} \int_0^{\infty} \mathcal{E} \sqrt{\frac{2m}{\mathcal{E}}} (|c(-\sqrt{2m\mathcal{E}})|^2 + |c(\sqrt{2m\mathcal{E}})|^2) d\mathcal{E}. \end{aligned}$$

If we put

$$I(\mathcal{E}) = \frac{1}{2} \sqrt{\frac{2m}{\mathcal{E}}} (|c(-\sqrt{2m\mathcal{E}})|^2 + |c(\sqrt{2m\mathcal{E}})|^2), \quad \mathcal{E} > 0,$$

we have

$$\int_0^{\infty} I(\mathcal{E}) d\mathcal{E} = \int_{-\infty}^{\infty} |c(p)|^2 dp = 1.$$

So that we have

$$\bar{E} = J[\psi] = \int_0^{\infty} \mathcal{E} I(\mathcal{E}) d\mathcal{E}.$$

If we assume

$$I(\mathcal{E}) = \frac{2}{k_B T} \exp\left(-\frac{2\mathcal{E}}{k_B T}\right),$$

where T denotes the absolute temperature and k_B denotes the Boltzman constant, we have

$$\bar{E} = \frac{1}{2} k_B T.$$

Because the degree of freedom of the 3-dimensional free motion is equal to 3, the energy expectation value of the total quantum system Ω in the 3-dimensional case is equal to

$$\bar{E} = \frac{3}{2} k_B T.$$

Further the L^2 -density $\psi(x)$ of the total quantum system Ω at the state of thermal equilibrium at the temperature T can be represented as follows:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} c(p)e^{ipx/\hbar} dp$$

and

$$c(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x)e^{-ipx/\hbar} dx.$$

Here we follow the reverse order of the method of separation of variables. At first we consider the function

$$\psi^{(p)}(x, t) = \psi^{(p)}(x) \exp\left(-i\frac{\mathcal{E}}{\hbar}t\right).$$

Differentiating this function with respect to the time variable t , we have

$$i\hbar \frac{\partial \psi^{(p)}(x, t)}{\partial t} = \mathcal{E} \psi^{(p)}(x) \exp\left(-i\frac{\mathcal{E}}{\hbar}t\right).$$

Here we denote the Hamiltonian operator of the Schrödinger equation of stationary state as follows:

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}.$$

Then we have

$$H\psi^{(p)}(x) = \mathcal{E}\psi^{(p)}(x), \quad \mathcal{E} = \frac{p^2}{2m}.$$

Hence we have

$$i\hbar \frac{\partial \psi^{(p)}(x, t)}{\partial t} = \{H\psi^{(p)}(x)\} \exp\left(-i\frac{\mathcal{E}}{\hbar}t\right) = H\psi^{(p)}(x, t).$$

Therefore, if we put

$$\psi(x, t) = \int_{-\infty}^{\infty} c(p)\psi^{(p)}(x, t) dp,$$

we have

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = H\psi(x, t). \quad (3.1)$$

This is the Schrödinger equation of time evolution of the total quantum system Ω . Here, using the condition of completeness, we have

$$\int_{-\infty}^{\infty} |\psi(x, t)|^2 dx = \int_{-\infty}^{\infty} |c(p)|^2 dp = 1.$$

By virtue of the conservation law of probability, we can see that the Schrödinger equation of time evolution is nothing else but the equation (3.1) in order that the L^2 -density satisfies this normalization condition.

4. Consideration and conclusion

We can consider that the quantum system (Ω, \mathcal{B}, P) of the 1-dimensional ideal gas composed of monatomic molecules has the following structure at the stationary state. Namely Ω is decomposed into the direct sum

$$\begin{aligned}\Omega &= \bigcup_{-\infty < p < \infty} \Omega_p, \text{ (direct sum),} & (4.1) \\ \Omega_p &= \{\rho \in \Omega; p(\rho) = p\}, \quad (-\infty < p < \infty), \\ P(\Omega_p) &= |c(p)|^2, \quad (-\infty < p < \infty).\end{aligned}$$

Then, we have, for any $A \in \mathcal{B}$,

$$P(A) = \int_{-\infty}^{\infty} P(A|p)|c(p)|^2 dp, \quad (4.2)$$

where $P(A|p)$ denotes the conditional probability. Then for $p : -\infty < p < \infty$, we call the probability space $(\Omega_p, \mathcal{B} \cap \Omega_p, P(\cdot|p))$ as the generalized characteristic quantum system. Considering the equations (4.1) and (4.2) and the results of calculation until now, we put the following assumptions. Now for $p : -\infty < p < \infty$, we assume that $c(p)$ satisfies the following conditions:

$$\begin{aligned}I(\mathcal{E}) &= \frac{1}{2} \left(\sqrt{\frac{2m}{\mathcal{E}}} (|c(-\sqrt{2m\mathcal{E}})|^2) + |c(\sqrt{2m\mathcal{E}})|^2 \right), \\ \int_0^{\infty} I(\mathcal{E}) d\mathcal{E} &= 1, \quad p^2 = 2m\mathcal{E}.\end{aligned}$$

If we use the notation of the axiom Π' , we have

$$\begin{aligned}P(\Omega_p|p) &= 1, \\ P(\{\rho \in \Omega_p; x(\rho) \in A \cap S\}|p) &= \frac{\int_{A \cap S} |\psi_S^{(p)}(x)|^2 dx}{\int_S |\psi_S^{(p)}(x)|^2 dx}, \\ P(\{\rho \in \Omega_p; x(\rho) \in S, p(\rho) \in B\}|p) &= \frac{\int_B |\hat{\psi}_S^{(p)}(p)|^2 dp}{\int_{-\infty}^{\infty} |\hat{\psi}_S^{(p)}(p)|^2 dp}.\end{aligned}$$

Therefore, the conditional energy expectation value \bar{E}_p of the generalized characteristic quantum system Ω_p is equal to

$$\bar{E}_p = \lim_{n \rightarrow \infty} J_{K_n}[\psi_{K_n}^{(p)}] = \mathcal{E} = \frac{p^2}{2m}.$$

By the relation of the total quantum system and the generalized characteristic quantum systems, we have

$$\begin{aligned}\bar{E} &= E \left[\frac{1}{2m} p(\rho)^2 \right] = \int_{-\infty}^{\infty} \bar{E}_p |c(p)|^2 dp \\ &= \int_{-\infty}^{\infty} \frac{p^2}{2m} |c(p)|^2 dp = \int_0^{\infty} \mathcal{E} I(\mathcal{E}) d\mathcal{E}, \quad (p^2 = 2m\mathcal{E}).\end{aligned}$$

If we assume that $I(\mathcal{E})$ is equal to

$$I(\mathcal{E}) = \frac{2}{k_B T} \exp\left(-\frac{2\mathcal{E}}{k_B T}\right),$$

we have

$$\bar{E} = \frac{1}{2} k_B T.$$

Because the degree of freedom of the 3-dimensional free motion is equal to 3, the energy expectation value of the total quantum system Ω in the 3-dimensional case is equal to

$$\bar{E} = \frac{3}{2} k_B T.$$

\bar{E} denotes the energy expectation value for one molecule. Now we consider the ideal gas such as there are N molecules in the region of volume V . So that we have the specific heat C_V of constant volume and the molar heat C_M of this ideal gas as follows:

$$C_V = N \frac{d\bar{E}}{dT} \quad \text{and} \quad C_M = N_A \frac{d\bar{E}}{dT}$$

Namely,

$$C_V = \frac{3}{2} N k_B$$

and

$$C_M = \frac{3}{2} N_A k_B.$$

Here N_A denotes the Avogadro number. If we put $N = nN_A$, we have the relation

$$C_V = nC_M.$$

These results were considered as the specific heats of the ideal gas composed of monatomic molecules. These facts are confirmed in the view point of the new quantum theory. But our results can be derived reasonably in the view point of the new quantum theory. The new and old results are different at the standing points.

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