Another possible description of fluctuations

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We show that the developed quantization procedure in the field theory of thermodynamics (especially heat conduction), which handles the thermodynamic variables as operators, is suitable to express the magnitude of energy fluctuation in the case of heat conduction. We can examine a nonequilibrium process and we point out that our formulation of fluctuations is not in contradiction with the statistical mechanics. We can discuss in our treatment whether it would be possible to measure the temperature around the absolute zero temperature. [S1063-651X(96)11410-0]

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I. INTRODUCTION

The solution of a differential equation of a physical process describes an exact path of the phenomenon in space and time. However, we know from experience that if we measure a physical variable, we have information about the average of this quantity because of the random differences around this value [1–4]. We can express the deviation of the field quantity $F(x,t)$ as

$$\Delta F = \sqrt{\overline{F^2} - \overline{F}^2},$$ (1)

where $\overline{F}$ is the average of F, and $\overline{F^2}$ is the average of F^2. It is usual to calculate this kind of deviation using the concepts of statistical mechanics supposing different ensembles and the condition of equilibrium [5–8]. The system, in which nonequilibrium processes take place, can be characterized by different distribution functions of physical variables.

There were several successful attempts to construct a Hamiltonian variational principle to exploit the mathematical background to reach deeper insight into the physical process [9–16]. On the other hand, there are some efforts to put discrete quantities into the theory of thermodynamics [17,18].

We start from the continuum description of the system. We quantize the field, as is usual in quantum theories [19,20], and eventually all we can handle the system as a space of a lot of quanta. We obtain discrete levels of the quantities as the eigenvalue of the introduced operators [21], which operate on nonequilibrium irreversible field variables. (A similar idea introducing of operators can be found in [22]). We summarize the states and we have to take into account an exponential factor. Because of the higher levels for quanta, the probability to fill these is decreased. In this manner we calculate the fluctuation of the variables. In the present paper we show the energy density fluctuation in Fourier heat conduction. This is one of the simplest examples and there is no doubt about the existence of quanta in the present phenomenon; these are quanta of energy. We can speak about energy density fluctuation in the case of a heat conduction (purely dissipative), but we emphasize that this is a kind of irreversible process.

II. TEMPERATURE OPERATOR AND ITS EIGENVALUES

We are dealing with source-free heat conduction [16,21] in the infinite field to calculate the temperature deviation in arbitrary time and coordinate of space. The relevant differential equation, Fourier heat conduction is

$$\dot{T} - \frac{\lambda}{c_v} \Delta T = 0,$$ (2)

which is a parabolic differential equation. We define [16,21] a new physical space φ which generates the measurable quantity T in this way,

$$T = -\dot{\varphi} - \frac{\lambda}{c_v} \Delta \varphi.$$ (3)

The Lagrangian density can be given in the following form:

$$L = \frac{1}{2}\dot{\varphi}^2 + \frac{1}{2}\frac{\lambda^2}{c_v^2}(\Delta\varphi)^2.$$ (4)

This Lagrangian pertains to a purely dissipative process, and of course, it contains the irreversibility of the process itself. We just mention here that those kinetic models, which are based on the Hamilton-Lagrangian formalism, admit reversible terms in the heat transmission. This fact shows an essential difference between the theories.

We obtain the Euler-Lagrange equation for the φ,

$$-\ddot{\varphi} + \frac{\lambda^2}{c_v^2}\Delta\Delta\varphi = 0.$$ (5)

It is easy to see that this equation is equivalent with that equation which can be obtained by substituting Eq. (3) into Eq. (2). We can restrict the domain of potential function $\varphi(x,t)$ to an arbitrarily large but finite cubical box of volume $V = l^3$ centered at the origin, at the walls of which the function obeys periodic boundary conditions. The Fourier series of φ [21] reads

$$\varphi = \sum_k \sqrt{\frac{2}{V}} \ (C_k \cos kx + S_k \sin kx),$$ (6)

where the coefficients C_k and S_k are the function of time, and $k=(k_1,k_2,k_3)$ is not an arbitrary vector. The components are restricted to the values $k_1=2\pi n_1/l$; $k_2=2\pi n_2/l$; $k_3=2\pi n_3/l$, where n_1,n_2,n_3 are positive or negative integers or zero. It is always assumed that the limit $l\rightarrow\infty$ is taken at the end of calculation. The temperature space can be given by these coefficients using Eqs. (3) and (6),

$$T=-\sum_k \sqrt{\frac{2}{V}}(\dot{C}_k\cos kx+\dot{S}_k\sin kx)$$

$$+\sum_k \sqrt{\frac{2}{V}}\frac{\lambda k^2}{c_v}(C_k\cos kx+S_k\sin kx). \quad (7)$$

If we integrate over the volume, we can calculate the Lagrangian of the system

$$L=\int L dV=\frac{1}{2}\sum_k \left[(\dot{C}_k^2+\dot{S}_k^2)+\frac{\lambda^2}{c_v^2}k^4(C_k^2+S_k^2)\right]. \quad (8)$$

We got the Lagrangian expressed by the normal coordinates C_k and S_k. The next step is to introduce the canonically conjugated quantities to C_k and S_k, which are the first derivative of these,

$$P_k^{(C)}=\dot{C}_k, \quad (9)$$

$$P_k^{(S)}=\dot{S}_k, \quad (10)$$

by which the Hamiltonian of the heat conduction process is

$$H=\sum_k \left(\frac{1}{2}P_k^{(C)2}-\frac{\lambda^2}{c_v^2}k^4C_k^2\right)+\sum_k \left(\frac{1}{2}P_k^{(S)2}-\frac{\lambda^2}{c_v^2}k^4S_k^2\right). \quad (11)$$

After these, let $P_k^{(C)}$, C_k, $P_k^{(S)}$, and S_k be operators that obey the following commutation rules:

$$[P_k^{(C)},C_l]=h\delta_{kl}, \quad (12)$$

$$[P_k^{(S)},S_l]=h\delta_{kl}. \quad (13)$$

We introduce new coefficients C_k^+, C_k^-, S_k^+, and S_k^- for the theory,

$$C^{\mp}=\frac{P_k^{(C)}}{\sqrt{2}}\mp\frac{\lambda k^2}{\sqrt{2}c_v}C_k, \quad (14)$$

$$S^{\mp}=\frac{P_k^{(S)}}{\sqrt{2}}\mp\frac{\lambda k^2}{\sqrt{2}c_v}S_k, \quad (15)$$

where we used the sign $\mp$ to reduce the number of equations. It is useful to choose $C^{\mp},S^{\mp}$ as new normal coordinates. We handle these as operators and we can derive the following commutation rules from the Eqs. (12) and (13):

$$C_k^-C_l^+-C_l^+C_k^-=\frac{\lambda}{c_v}k^2h\delta_{kl}, \quad (16)$$

$$S_k^-S_l^+-S_l^+S_k^-=\frac{\lambda}{c_v}k^2h\delta_{kl}. \quad (17)$$

We can obtain the Hamiltonian operator if we take into account Eqs. (12)–(15),

$$\mathcal{H}=\sum_k (C_k^+C_k^-+S_k^+S_k^-). \quad (18)$$

We would like to introduce the temperature operator $\mathcal{T}$. Since,

$$C_k=\frac{c_v}{\sqrt{2}\lambda k^2}(C_k^+-C_k^-), \quad (19)$$

$$S_k=\frac{c_v}{\sqrt{2}\lambda k^2}(S_k^+-S_k^-). \quad (20)$$

We substitute these into the formula of temperature, Eq. (7),

$$\mathcal{T}=-\sum_k \sqrt{\frac{1}{V}}\frac{c_v}{\lambda k^2}[(\dot{C}_k^+-\dot{C}_k^-)\cos kx+(\dot{S}_k^+-\dot{S}_k^-)\sin kx]$$

$$+\sum_k \sqrt{\frac{1}{V}}[(C_k^+-C_k^-)\cos kx+(S_k^+-S_k^-)\sin kx], \quad (21)$$

and now we can speak about temperature operator because of the coefficients which are operators. This equation contains the first time derivatives of C_k^+, C_k^-, S_k^+, and S_k^-. The Poisson bracket expression of a certain quantity and Hamiltonian operator give the time derivative of it, e.g., for C_k^+ and C_k^-,

$$\dot{C}_k^+=\frac{1}{h}[C_k^+,\mathcal{H}]=-\frac{\lambda}{c_v}k^2C_k^+, \quad (22)$$

$$\dot{C}_k^-=\frac{1}{h}[C_k^-,\mathcal{H}]=\frac{\lambda}{c_v}k^2C_k^-. \quad (23)$$

Similar equations are valid for S_k^+ and S_k^-. We substitute all of these into Eq. (21) and we can write the temperature operator in a short form,

$$\mathcal{T}=\sum_k 2\sqrt{\frac{1}{V}}(C_k^+\cos kx+S_k^+\sin kx). \quad (24)$$

This operator contains the creation operators [21] C_k^+ and S_k^+ (they produce the same quanta), so we take $\mathcal{T}$ as a creation operator, which is the combination of these. In this way we can calculate the eigenvalues of the operator $\mathcal{H}$. Let us suppose the α is an eigenvalue of the operator $\mathcal{H}$ with the eigenfunction Ψ,

$$\mathcal{H}\Psi=\alpha\Psi. \quad (25)$$

It can be proved that $\mathcal{T}\Psi$ is an eigenfunction of $\mathcal{H}$,

$$\mathcal{H}\mathcal{T}\Psi=\left(\alpha+\frac{\lambda}{c_v}k^2h\right)\mathcal{T}\Psi, \quad (26)$$

and we can read the new eigenvalue of $\mathcal{H}$ with the eigenfunction $\mathcal{T}\Psi$. The difference in the eigenvalues

$$\frac{\lambda}{c_v}k^2h \qquad (27)$$

can be considered as the ''quanta of temperature.''

III. ENERGY FLUCTUATION

For the calculation of the number of quanta as a function of k in a finite volume, which obeys the periodic boundary conditions, we express the number k as

$$k=\frac{2\pi n}{l}, \qquad (28)$$

where n may be an integer and l is the edge of a cube in which the process is going. The specific heat capacity c_v can be defined with the internal energy density $u(x,t)$ and the temperature $T(x,t)$, which shows that the system is in local equilibrium,

$$\frac{\partial u}{\partial T}=c_v. \qquad (29)$$

Equation (2) is valid when

$$u=c_vT \qquad (30)$$

linear connection holds, i.e., c_v is independent of the temperature T. That is why we can speak about temperature or energy fluctuation at the same time in the following. It is more usual to summarize over energy states, so we follow this. The possible energy states are

$$\varepsilon(k)=\lambda hk^2, \qquad (31)$$

which can be written with the n_1, n_2, and n_3,

$$\varepsilon_{n_1n_2n_3}=\lambda h\frac{4\pi^2}{l^2}(n_1^2+n_2^2+n_3^2). \qquad (32)$$

The three different series of n belong to the three different space directions. We imagine a one-eighth sphere with a radius k. The numbers n are within this part of space,

$$k\geqslant\frac{2\pi}{l}\sqrt{n_1^2+n_2^2+n_3^2}, \qquad (33)$$

and we can give the number of the possible states $N(k)$ if we calculate the volume of it,

$$N(k)=\frac{1}{8}\frac{4\pi}{3}\left(\frac{lk}{2\pi}\right)^3=\frac{1}{48}\frac{l^3k^3}{\pi^2}. \qquad (34)$$

If we derive this with respect to k,

$$dN(k)=\frac{l^3}{16\pi^2}k^2dk, \qquad (35)$$

we will know how many possible states exist within the dk interval in the total space. If we devide it by the volume of coordinate space l^3, we receive the density of these states,

$$dn(k)=\frac{1}{16\pi^2}k^2dk. \qquad (36)$$

We obtain the average energy per one quantum $\bar{\epsilon}_1$ if we integrate over all of the energy states weighted by the number of states and divided by the number of these,

$$\bar{\epsilon}_1=\frac{\displaystyle\int_0^\infty\varepsilon(k)dn(k)}{\displaystyle\int_0^\infty dn(k)}=\frac{\displaystyle\int_0^\infty\lambda hk^2\frac{1}{16\pi^2}k^2dk}{\displaystyle\int_0^\infty\frac{1}{16\pi^2}k^2dk}\to\infty. \qquad (37)$$

We are not surprised at this result at all, because there is no limit in k. This integration supposes an infinite radius k of sphere and this means that an infinite number of quanta exist. That is the reason why the average enregy per one quantum is infinite. We can assume that the lower energy states are more possible and we are allowed to introduce a function

$$\sim e^{-\alpha k^2}, \qquad (38)$$

which can decrease the number of states exponentially. We multiply the integrand of Eq. (36) by this factor and the average energy per one quantum can be obtained as an infinite integral over all of the k,

$$\bar{\epsilon}_1=\frac{\displaystyle\int_0^\infty\frac{\lambda hk^4}{16\pi^2}e^{-\alpha k^2}dk}{\displaystyle\int_0^\infty\frac{k^2}{16\pi^2}e^{-\alpha k^2}dk}. \qquad (39)$$

We use the well-known infinite integral

$$\int_0^\infty x^ne^{-\alpha x^2}=\frac{\Gamma\left(\dfrac{n+1}{2}\right)}{2\alpha^{(n+1)/2}} \qquad (40)$$

to calculate $\bar{\epsilon}_1$,

$$\bar{\epsilon}_1=\frac{\dfrac{\lambda h}{2\pi^2}\dfrac{\Gamma\left(\dfrac{5}{2}\right)}{2\alpha^{5/2}}}{\dfrac{1}{2\pi^2}\dfrac{\Gamma\left(\dfrac{3}{2}\right)}{2\alpha^{3/2}}}=\frac{3}{2}\lambda h\frac{1}{\alpha}. \qquad (41)$$

If the whole space contains N number of quanta, the energy of this space can be calculated,

$$\bar{\epsilon}=N\bar{\epsilon}_1=\frac{3}{2}\lambda hN\frac{1}{\alpha}. \tag{42}$$

The heat capacity C_V of the whole system is defined as

$$C_V=\frac{\partial\bar{\epsilon}}{\partial T}. \tag{43}$$

We can calculate C_V using this formula,

$$C_V=\frac{3}{2}\lambda hN\frac{\partial\frac{1}{\alpha}}{\partial T}. \tag{44}$$

If we suppose that C_V is a constant quantity, i.e., when the whole system is close to the equilibrium, we obtain for α

$$\alpha=\frac{3\lambda hN}{2C_V}\frac{1}{T}. \tag{45}$$

In this case we are allowed to assume that C_V is independent of the temperature T, so $\bar{\epsilon}=C_VT$. Now, we make a comparison with the statistical mechanics. If we take into account the result of the statistical mechanics, namely, $C_V=\frac{1}{2}fk_BN$, where f is the degrees of freedom and k_B is the Boltzmann constant, we get for the $\bar{\epsilon}_1$ (41)

$$\bar{\epsilon}_1=\frac{1}{2}fk_BT. \tag{46}$$

This result shows that our description of the physical problem is in line with the results of statistical physics. Namely, our method gives back these results as an extreme case of it.

To obtain the energy fluctuation we have to express the average of ϵ_1 square, which can be calculated as

$$\overline{\epsilon_1^2}=\frac{\int_0^\infty\frac{\lambda^2h^2}{16\pi^2}k^6e^{-\alpha k^2}dk}{\int_0^\infty\frac{1}{16\pi^2}k^2e^{-\alpha k^2}dk}. \tag{47}$$

After a short calculation we get that

$$\overline{\epsilon_1^2}=\frac{15}{4}\lambda^2h^2\frac{1}{\alpha^2}. \tag{48}$$

The described procedure allows us to derive the magnitude of energy fluctuation in the sense of Eq. (1). The square of magnitude of deviation of $\Delta\epsilon_1$ can be read if we use the equation

$$(\Delta\epsilon_1)^2=\overline{\epsilon_1^2}-\overline{\epsilon_1}^2. \tag{49}$$

The energy fluctuation of the system can be obtained in the case of N quanta,

$$(\Delta\epsilon)^2=N(\Delta\epsilon_1)^2, \tag{50}$$

which means that

$$(\Delta\epsilon)^2=\frac{3}{2}\lambda^2h^2N\frac{1}{\alpha^2} \tag{51}$$

in our case.

Now, we can compare our result with the result of statistical mechanics again if we use the form of α (45),

$$(\Delta\epsilon)^2=\frac{1}{6}f^2k_B^2NT^2 \tag{52}$$

or

$$(\Delta\epsilon)=\sqrt{\frac{1}{6}}fk_B\sqrt{N}T. \tag{53}$$

The good agreements with the statistical mechanics calm us, and we believe that we can check our results and ideas in a continuous comparison in this way.

Now, we are dealing with Eqs. (42) and (51). These equations contain the parameter α, which is not known in general and it is in the exponential of expression (38). We can calculate the relative fluctuation, which is

$$\frac{\Delta\epsilon}{\bar{\epsilon}}=\sqrt{\frac{2}{3}}\frac{1}{\sqrt{N}}. \tag{54}$$

On the one hand, it can be seen that the result is independent of α. On the other hand, we are not restricted to choosing the number N as too great a number. That is why the interesting thing is when

$$\Delta\epsilon\sim\epsilon, \tag{55}$$

i.e., the fluctuation is comparable with the energy. This is valid when the number of quanta N is not a great number, practically a few hundred or less. We think this means that we cannot measure the temperature exactly, because the amplitude of fluctuations will be comparable with the energy independently of the temperature. When we tend to the zero temperature, we can assume that the number of quanta decrease, consequently the relative fluctuation increases. Maybe this is the reason why we cannot measure around the absolute zero temperature exactly, when we cool the body with heat conduction. We can measure the average of energy and temperature but we are not sure what the exact energy and temperature is when we have a small number of quanta.

IV. CONCLUSION

The fluctuation theory of physical processes is based on the concepts of statistical mechanics. This theory of physics takes into account the physical system as the certain en-

semble of the physical variables. We reverse the way of thinking. We start from the continuum description of fields, we quantize this, and there will be discrete characteristics of it in this way. We showed how to use the quantized field of heat conduction to discuss the energy fluctuation. We think that this method shows more possibilities to describe the fluctuations and to find deeper connection with the statistical mechanics. There may be a chance that we can discuss processes in solid state physics. These works will be great challenges for us in the future.

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