

Generalized Hamilton-Jacobi equation for simple dissipative processes

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Following the method of classical mechanics, we calculate the action for Fourier heat conduction from the classical Hamilton-Jacobi equation. We can write a Schrödinger-type equation and we obtain its solution, the kernel by which we may introduce a kind of wave function. Mathematically, we follow Bohm's method introduced to quantum mechanics. The generalized Hamilton-Jacobi equation—which may be handled as a quantum-thermodynamical form—can be calculated. Irreversibility and dissipation are included in a natural way in the field theory of nonequilibrium thermodynamics, so in this way we obtain a quantum-thermodynamical approach of simple dissipative processes.

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I. INTRODUCTION

The motion of the classical ensemble can be derived from the Lagrangian L_C defined by the following expression: [1–7]

$$L_C = \int p \left[\frac{\partial S}{\partial t} + \frac{1}{2m} (\nabla S)^2 + V \right] d^3x, \quad (1)$$

where the variable $S(x, t)$ is the classical action, the variable $p(x, t)$ is the probability density to find the particle at the space coordinate x at time t . (The probability must be normalized: $\int p d^3x = 1$), $V(x, t)$ is the classical (mechanical) potential, m is the mass of particle, and ∇ is the gradient operator. For the real path of motion the integral

$$\int L_C dt, \quad (2)$$

is extremal, i.e., using the calculus of variations

$$\delta \int L_C dt = 0, \quad (3)$$

is valid. After the variation—with respect to the variables S and p —we obtain two equations as Euler-Lagrange equations

$$\frac{\partial S}{\partial t} + \frac{1}{2m} (\nabla S)^2 + V = 0, \quad (4)$$

which is the classical Hamilton-Jacobi equation, and

$$\frac{\partial p}{\partial t} + \nabla \cdot \left(p \frac{1}{m} \nabla S \right) = 0, \quad (5)$$

which is a continuity equation for the probability density. Following Hall and Reginatto's work [7,8], a modified Lagrangian L_{QM} can be obtained as a consequence of the momentum fluctuations

$$L_{QM} = \int p \left[\frac{\partial S}{\partial t} + \frac{1}{2m} (\nabla S)^2 + \frac{\hbar^2}{8m} \frac{(\nabla p)^2}{p^2} + V \right] d^3x, \quad (6)$$

where \hbar is the Planck constant per 2π . After the calculation of variation, we get two Euler-Lagrange equations, the quantum Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + \frac{1}{2m} (\nabla S)^2 + \frac{\hbar^2}{8m} \left[\frac{(\nabla p)^2}{p^2} - \frac{2\Delta p}{p} \right] + V = 0, \quad (7)$$

where Δ is the Laplace operator, and the continuity equation for the probability density p is

$$\frac{\partial p}{\partial t} + \nabla \cdot \left(p \frac{1}{m} \nabla S \right) = 0. \quad (8)$$

Bohm [1,2] deduced these equations from the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \Delta \Psi + V \Psi, \quad (9)$$

where i is the complex unit, Ψ is a complex function, which can be expressed as

$$\Psi = R \exp\left(i \frac{S}{\hbar}\right). \quad (10)$$

Now R and S are real, and

$$p = R^2. \quad (11)$$

It is readily verified that the quantum Hamilton-Jacobi equation [Eq. (7)] and the continuity equation [Eq. (8)] can be obtained. After these, we make a step towards the study of a

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dissipative process, the linear (Fourier) heat conduction, for which we apply Bohm's method. Several equations of motion of field theories can be calculated from the least action principle. It means not only that these equations are derived for the relevant simple interactions, but the interaction of different fields can be taken into account, i.e., the coupling of fields appears in the field equations. This can be achieved by choosing additional terms in the Lagrangian. This is a possible way to describe the interaction of different processes. The equation of heat conduction is also a field equation; this can describe a dissipative process, but it cannot be connected easily to other fields within the Lagrangian formalism. This was the reason why there were several efforts to construct the Hamiltonian structure of those transport processes, such as heat conduction, diffusion, etc. These processes are treated mostly within the framework of nonequilibrium thermodynamics. This means that the concept of irreversibility and dissipation also can be introduced to those field theories in which these concepts do not exist from the viewpoint of thermodynamics. Advanced results for Lagrangian, Hamiltonian approach using the canonical equations and Hamilton-Jacobi equation to study macroscopic dissipative processes including the fluctuation theory can be found in Sieniutycz *et al.* [9–12] and Bertini *et al.* [13,14].

The developed theory of nonequilibrium thermodynamics includes the Hamiltonian formulation of those dissipative processes [15] which can be given linear parabolic and hyperbolic differential equations (e.g., Fourier heat conduction and telegrapher equation) [16,17]. The completed Poisson-bracket formalism is worked out for these processes; moreover, successful steps were taken towards the description of behavior of quantum [18,19] and stochastic phenomena [20] within dissipative systems. We could discuss the theory [21] from the viewpoint of the extreme physical information principle introduced by Frieden [22–24]. In the present work we calculate the Hamilton-Jacobi equation for Fourier heat conduction, the action, the kernel, and a wave function. We apply Bohm's idea [1,2], by which method we can obtain the quantum-thermodynamical Hamilton-Jacobi equation and the quantum-thermodynamical potential. Here, we will see that the Fisher information [25–27] appears in the thermodynamical theory, and we suppose that this description should have a connection to the extreme physical information, too.

We admit that sometimes the physical interpretation is not easy or sufficient. We can trust in the elegant mathematical formulation and the hope that the basic concepts (Lagrange-Hamilton formalism, canonical formalism, Poisson brackets, dissipation, irreversibility, quantization, etc.) can be generalized; these have a general validity regardless of the examined physical process, and can be summarized in a unified theory.

II. HAMILTONIAN DESCRIPTION OF HEAT CONDUCTION

The mathematical calculus of Hamiltonian formalism is the starting point which was originally developed and applied to describe reversible, nondissipative physical processes [28]. However, we have shown that this mathematical method can be modified and applied to dissipative processes

[15,18–20], e.g., for Fourier heat conduction. (This equation is a parabolic differential equation, i.e., where a not-self-adjoint operator stands in the case of time derivative.) In this section we briefly summarize the description of a thermal field, where we apply the methods of field theory.

A physical process can be described by the Lagrangian, i.e., all information of evolution of a physical process is involved in this scalar function. The time integration of the Lagrangian yields the classical action $S[b, a]$

$$S[b, a] = \int_{t_a}^{t_b} L(\dot{q}, q, t) dt, \quad (12)$$

where a belongs to the initial state at time t_a ; b is the final one at t_b . The classical Lagrangian L of the physical problem may depend on q and its time derivatives (here, just \dot{q}) and the time t . The Hamilton's principle states that the variation of action is zero for the real physical processes

$$\delta S = 0. \quad (13)$$

This principle is generalized for those cases when the Lagrangian depends on the field quantity φ and its derivatives $\partial\varphi/\partial t$, $\partial\varphi/\partial x$, $\Delta\varphi$, etc. Then, L is the Lagrange density function; the action is

$$S = \int L d^3x dt; \quad (14)$$

we must integrate over the volume, where the process is going. The Hamilton's principle—the action has an extremum for the real physical processes—remains the same. The field equation of the source-free Fourier heat conduction is

$$\frac{\partial T}{\partial t} - \frac{\lambda}{c_v} \Delta T = 0, \quad (15)$$

where $T(x, t)$ is the temperature, λ is the heat conductivity, and c_v is the specific heat capacity. This differential equation contains a first-order derivative (time derivative) which is not a self-adjoint operator. This means that no Lagrangian can be written with the original variable(s) (here the temperature) unless we introduce additional variables. The situation is similar to the electrodynamics, where the Maxwell equations can be deduced from the Hamilton's principle using the vector and scalar potentials. There, the operators of the time derivative and the divergence are not self-adjoint. (If the field equation contains just self-adjoint operators, such as second-order time and space derivatives, the Lagrangian can be simply constructed with the original variables.) This is the reason why we have to introduce a scalar, differentiable (potential) field $\varphi(x, t)$ [15]

$$T = -\frac{\partial\varphi}{\partial t} - \frac{\lambda}{c_v} \Delta\varphi, \quad (16)$$

which is connected to the measurable field T in this equation. The Lagrange density function of the physical problem expressed by the φ is

$$L = \frac{1}{2} \left(\frac{\partial \varphi}{\partial t} \right)^2 + \frac{1}{2} \frac{\lambda^2}{c_v^2} (\Delta \varphi)^2, \quad (17)$$

from which we can obtain the field equation of φ as Euler-Lagrange equation

$$0 = \frac{\partial^2 \varphi}{\partial t^2} - \frac{\lambda^2}{c_v^2} \Delta \Delta \varphi. \quad (18)$$

If we substitute the equation of definition of φ we obtain the field equation of Fourier heat conduction [15]. In the field theories the field variables are written in Fourier series, where the Fourier coefficients depend only on the time, and, e.g., the quantization procedure is prepared by these coefficients. These will be the generalized coordinates of the system. Here, we follow this idea [18,19], i.e., let φ be

$$\varphi(x,t) = \sum_{k>0} \sqrt{\frac{2}{V}} (C_k \cos kx + S_k \sin kx), \quad (19)$$

where C_k and S_k are the function of time, and these can be handled as the generalized coordinates of the system; \tilde{V} is the volume in the coordinate space. The Lagrangian of the field can be calculated if we substitute the Fourier series of φ into Eq. (17) and we integrate over the volume (d^3x). We get the Lagrangian of the space, which depends only on the generalized coordinates and the first-order derivatives of these with respect to time

$$L = \frac{1}{2} \sum_{k>0} \left[(\dot{C}_k + \dot{S}_k)^2 + \frac{\lambda^2}{c_v^2} k^4 (C_k^2 + S_k^2) \right]. \quad (20)$$

In its form we find an expression

$$V(C_k, S_k) = - \sum_k \frac{1}{2} \frac{\lambda^2}{c_v^2} k^4 (C_k^2 + S_k^2), \quad (21)$$

which is very similar to the classical quadratic potentials. (We have seen that this potential term—pertaining to a repulsive interaction—appeared in the quantization procedure, and its negative sign caused serious mathematical difficulties [18,19].) So, the Lagrangian can be divided into two parts, a “kinetical” term (K) and a “potential” term (V), by which expressions the usual form $L=K-V$ can be written.

The canonically conjugated quantities are the generalized momenta $P_K^{(C)}$ and $P_K^{(S)}$, i.e.,

$$P_K^{(C)} = \frac{\partial L}{\partial C_k} = \dot{C}_k, \quad (22)$$

and

$$P_K^{(S)} = \frac{\partial L}{\partial S_k} = \dot{S}_k. \quad (23)$$

Now, we can express the Hamiltonian of the system ($H=K+V$) [18,19] by these momenta

$$H = \sum_k \left(\frac{1}{2} P_k^{(C)2} - \frac{1}{2} \frac{\lambda^2}{c_v^2} k^4 C_k^2 \right) + \sum_k \left(\frac{1}{2} P_k^{(S)2} - \frac{1}{2} \frac{\lambda^2}{c_v^2} k^4 S_k^2 \right). \quad (24)$$

III. HAMILTON-JACOBI EQUATION, THE ACTION, THE KERNEL, AND A WAVE FUNCTION

The classical Hamilton-Jacobi equation can be written in general

$$\frac{\partial S}{\partial t} + H \left(q_1, \dots, q_f, \frac{\partial S}{\partial q_1}, \dots, \frac{\partial S}{\partial q_f} \right) = 0, \quad (25)$$

where the q_i 's are the generalized coordinates; the $\partial S / \partial q_i$'s are the momenta P_i 's ($i=1, \dots, f$). In our special case, using Eq. (24) we can express the Hamilton-Jacobi equation of heat conduction by the Fourier coefficients as generalized coordinates

$$\frac{\partial S}{\partial t} + \sum_k \left(\frac{1}{2} \left(\frac{\partial S}{\partial C_k} \right)^2 + \frac{1}{2} \left(\frac{\partial S}{\partial S_k} \right)^2 \right) - \sum_k \frac{1}{2} \frac{\lambda^2}{c_v^2} k^4 (C_k^2 + S_k^2) = 0. \quad (26)$$

This equation can be obtained from the variation of integral over time and space of generalized coordinates

$$0 = \delta \int P \left[\frac{\partial S}{\partial t} + \sum_k \left(\frac{1}{2} \left(\frac{\partial S}{\partial C_k} \right)^2 + \frac{1}{2} \left(\frac{\partial S}{\partial S_k} \right)^2 \right) + V \right] dt d\Omega, \quad (27)$$

where P is the probability density to find the system in the state described by the set of generalized coordinates C_k and S_k ; i.e., $P(C_k, S_k)$; $d\Omega = \dots dC_i \dots dS_j \dots$ is the volume element in the space of generalized coordinates. Here, the classical Lagrangian L_{CL} can be written in the following form:

$$L_{CL} = \int P \left[\frac{\partial S}{\partial t} + \sum_k \left(\frac{1}{2} \left(\frac{\partial S}{\partial C_k} \right)^2 + \frac{1}{2} \left(\frac{\partial S}{\partial S_k} \right)^2 \right) + V \right] d\Omega. \quad (28)$$

After the variation a second equation appears

$$\frac{\partial P}{\partial t} + \nabla (P \nabla S) = 0, \quad (29)$$

which is a continuity equation for the probability density, and here ∇ denotes the vector operator ($\dots \partial / \partial C_i, \dots, \partial / \partial S_j \dots$). The system is developing from the state a at time t_a to the state b at time t_b , and we suppose $t_b > t_a$. Solving this partial differential equation, taking into account the initial and final states, the calculated action for this process is

$$S[b, a] = \sum_{k>0} \frac{\frac{\lambda}{c_v} k^2}{2 \sinh \left(\frac{\lambda}{c_v} k^2 (t_b - t_a) \right)} \times \left[(C_{ka}^2 + C_{kb}^2 + S_{ka}^2 + S_{kb}^2) \cosh \left(\frac{\lambda}{c_v} k^2 (t_b - t_a) \right) - 2C_{ka}C_{kb} - 2S_{ka}S_{kb} \right], \quad (30)$$

which is the solution of the Hamilton-Jacobi equation. In general, the kernel of a quadratic action can be written [29] (or can be calculated by the path integral method [30–32])

$$\begin{aligned}
 K_F(b,a) = & \prod_{k>0} \frac{\frac{\lambda}{c_v} k^2}{2\pi i \hbar^* \sinh\left(\frac{\lambda}{c_v} k^2 t\right)} \\
 & \times \exp\left(\frac{\frac{\lambda}{c_v} k^2 i}{2\hbar^* \sinh\left(\frac{\lambda}{c_v} k^2 t\right)} \left[(C_{ka}^2 + C_{kb}^2 + S_{ka}^2 \right. \right. \\
 & \left. \left. + S_{kb}^2) \cosh\left(\frac{\lambda}{c_v} k^2 t\right) - 2C_{ka}C_{kb} - 2S_{ka}S_{kb} \right] \right), \tag{31}
 \end{aligned}$$

where we denote $t=t_b-t_a$. This propagator might be called the WKB propagator, which is exact for all those Lagrangians which can be expressed by quadratic terms. It can be simply proved that this propagator is the solution of the following generalized Schrödinger-type equation:

$$\begin{aligned}
 -\frac{\hbar^*}{i} \frac{\partial K_F}{\partial t} = & -\sum_k \frac{\hbar^{*2}}{2} \frac{\partial^2 K_F}{\partial C_k^2} - \sum_k \frac{\hbar^{*2}}{2} \frac{\partial^2 K_F}{\partial S_k^2} \\
 & - \sum_k \frac{\lambda^2 k^4}{2c_v^2} (C_k^2 + S_k^2) K_F, \tag{32}
 \end{aligned}$$

which shows the correctness of the propagator from another viewpoint. Here, \hbar^* denotes the unit of dissipative action S : $\hbar^* = 2\hbar/k_B$, where \hbar is the Planck constant per 2π ; k_B is the Boltzmann constant. Moreover, if we take C_k , $P_k^{(C)}$, S_k , and $P_k^{(S)}$ operators, they are obeying the commutation rules $[P_k^{(C)}, C_l] = \hbar^* \delta_{kl}$ and $[P_k^{(S)}, S_l] = \hbar^* \delta_{kl}$; the canonical quantization procedure is based on these requirements [19]. The applicability of Feynman path integral method shows and carries the construction of wave function Ψ which is related to the propagator K_F . These facts may indicate the possibility of particle-wave duality in the present case. The Schrödinger-type equation for the wave function can be read

$$\begin{aligned}
 -\frac{\hbar^*}{i} \frac{\partial \Psi}{\partial t} = & -\sum_k \frac{\hbar^{*2}}{2} \frac{\partial^2 \Psi}{\partial C_k^2} - \sum_k \frac{\hbar^{*2}}{2} \frac{\partial^2 \Psi}{\partial S_k^2} \\
 & - \sum_k \frac{\lambda^2 k^4}{2c_v^2} (C_k^2 + S_k^2) \Psi. \tag{33}
 \end{aligned}$$

This equation should describe the whole system at the same time, and this points out that a kind of quantum behavior appears in the heat process. However, the physical meaning of this equation is not clear at all. It is obvious that the classical Hamilton-Jacobi equation of heat conduction [Eq. (26)] cannot give this equation; we have to find another equation which includes the quantum behavior. We follow

Bohm's idea [1] to obtain the quantum Hamilton-Jacobi equation of the problem. The wave function can be expressed

$$\Psi = R \exp\left(i \frac{S}{\hbar^*}\right), \tag{34}$$

where $R(C_k, S_k)$ is real and

$$\Psi^* \Psi = R^2 = P. \tag{35}$$

We substitute Eq. (34) into Eq. (33); then, we can separate a real and an imaginary part of the resulting equation. So, we obtain a continuity equation

$$\frac{\partial P}{\partial t} + \nabla (P \nabla S) = 0, \tag{36}$$

and the quantum-thermodynamical Hamilton-Jacobi equation

$$\begin{aligned}
 \frac{\partial S}{\partial t} + \sum_k \left(\frac{1}{2} \left(\frac{\partial S}{\partial C_k} \right)^2 + \frac{1}{2} \left(\frac{\partial S}{\partial S_k} \right)^2 \right) - \sum_k \frac{1}{2} \frac{\lambda^2}{c_v^2} k^4 (C_k^2 + S_k^2) \\
 - \frac{\hbar^{*2}}{2R} \sum_k \left(\frac{\partial^2 R}{\partial C_k^2} + \frac{\partial^2 R}{\partial S_k^2} \right) = 0. \tag{37}
 \end{aligned}$$

The third term is the classical potential, similar to the term in Eq. (21); the last term

$$U(C_k, S_k) = -\frac{\hbar^{*2}}{2R} \sum_k \left(\frac{\partial^2 R}{\partial C_k^2} + \frac{\partial^2 R}{\partial S_k^2} \right), \tag{38}$$

is also a potential. This vanishes when $\hbar^* = 0$, so this pertains to a quantum physical behavior of the process. This may be called quantum-thermodynamical potential. We may express this $U(C_k, S_k)$ potential by the probability density $P(C_k, S_k)$ introduced by Eq. (35)

$$\begin{aligned}
 U(C_k, S_k) = & -\frac{\hbar^{*2}}{4} \sum_k \left[\frac{1}{P} \frac{\partial^2 P}{\partial C_k^2} - \frac{1}{2P^2} \left(\frac{\partial P}{\partial C_k} \right)^2 + \frac{1}{P} \frac{\partial^2 P}{\partial S_k^2} \right. \\
 & \left. - \frac{1}{2P^2} \left(\frac{\partial P}{\partial S_k} \right)^2 \right]. \tag{39}
 \end{aligned}$$

IV. ON THE THERMODYNAMICAL POTENTIALS: CLASSICAL $[V(C_k, S_k)]$ AND QUANTUM-THERMODYNAMICAL $[U(C_k, S_k)]$

We discuss the two potentials which appeared in the above sections, but we restrict our examination to the stationary case, i.e., when the time derivative equals zero. Then, the temperature $T(x)$ is simply written as

$$T(x) = -\frac{\lambda}{c_v} \Delta \varphi. \tag{40}$$

Using the Fourier series of φ [see Eq. (19)], we obtain

$$T(x) = \frac{\lambda}{c_v} \sum_{k>0} \sqrt{\frac{2}{V}} k^2 (C_k \cos kx + S_k \sin kx). \quad (41)$$

If we calculate the square of both sides and integrate over the coordinate space x , we get

$$\int T^2(x) d^3x = \frac{\lambda^2}{c_v^2} \sum_{k>0} k^4 (C_k^2 + S_k^2). \quad (42)$$

So, it is easy to verify that in the stationary case the classical (thermodynamical) potential can be written

$$V = -\frac{1}{2} \int T^2(x) d^3x, \quad (43)$$

i.e., a repulsive interaction proportional to the temperature square is working during the heat conduction.

Now, we examine the quantum potential. First, we calculate the probability P . For this, we express the stationary action from Eq. (30)

$$S = \sum_k \frac{1}{2} \frac{\lambda}{c_v} k^2 (C_k^2 + S_k^2 + C_{ka}^2 + S_{ka}^2), \quad (44)$$

and we take into account the stationary version of the continuity equation [Eq. (36)]

$$\nabla(P \nabla S) = 0. \quad (45)$$

Finding the solution, one can verify that the probability density is

$$P = \left(\prod_k C_k S_k \right)^{-1}. \quad (46)$$

We can express the quantum-thermodynamical potential [see Eq. (39)] by the generalized coordinates using the above form of the probability density

$$U(C_k, S_k) = -\frac{3\hbar^*{}^2}{8} \sum_k \left(\frac{1}{C_k^2} + \frac{1}{S_k^2} \right). \quad (47)$$

In order to write this potential in measurable parameters, we give the C_k and S_k using the form of steady-state (stationary) temperature by Eq. (40) and the form of φ by Eq. (19). After the Fourier transformation we obtain

$$C_k = \frac{c_v}{\lambda k^2} \int T(x) \cos kx d^3x, \quad (48)$$

and

$$S_k = \frac{c_v}{\lambda k^2} \int T(x) \sin kx d^3x. \quad (49)$$

We substitute these coefficients into Eq. (47) to get the quantum potential expressed by the temperature $T(x)$

$$U = -\frac{3\hbar^*{}^2 \lambda^2}{8c_v^2} \sum_k k^4 \left(\frac{1}{(\int T(x) \cos kx d^3x)^2} + \frac{1}{(\int T(x) \sin kx d^3x)^2} \right). \quad (50)$$

We mention again that this formula is valid for steady-state

thermal processes. As it can be seen, the smaller temperature is the higher repulsive interaction (U). This means that it plays a significant role when the temperature is close to the absolute zero temperature. When the temperature is high, this potential (U) can be neglected comparing the classical potential (V) given by Eq. (43). This is in line with our expectations.

Finally, we substitute the expression of quantum-thermodynamical potential into the expression of quantum Hamilton-Jacobi equation [Eq. (37)]. Now, we look for the Lagrangian which can give the Hamilton-Jacobi equation and the continuity equation for P . It can be seen that the Lagrangian L_{QT} is

$$L_{QT} = \int P \left[\left(\frac{\partial S}{\partial t} + \frac{1}{2} (\nabla S)^2 + V \right) + \frac{\hbar^*{}^2 (\nabla P)^2}{2P^2} \right] d\Omega, \quad (51)$$

i.e.,

$$L_{QT} = L_{CL} + \frac{\hbar^*{}^2}{2} \int \frac{(\nabla P)^2}{P} d\Omega. \quad (52)$$

The last term of the integral is proportional to the so-called Fisher information written in the generalized coordinate space

$$I_F = \int \frac{(\nabla P)^2}{P} d\Omega, \quad (53)$$

which may play an interesting role in the description of quantized thermodynamical system.

V. SUMMARY

We have showed that the Hamilton-Jacobi equation for some simple dissipative processes (described by linear parabolic differential equation) can be given in a suitable introduced generalized coordinate space. We calculated the action for the Fourier heat conduction, and applying Bohm's method we could obtain the generalized Hamilton-Jacobi equation, which contains the quantum properties. Two repulsive potentials appeared in the thermodynamical theory. We have expressed these potentials by the measurable temperature, but we restricted our examination and calculations to the stationary temperature field. The classical repulsive potential V is proportional to the temperature square integrated over the coordinate space. The quantum-thermodynamical potential U is a function given by the reciprocal of temperature square. When the temperature is large enough, the quantum processes can be neglected; when the temperature is small (very close to the absolute zero temperature), the quantum effects will be more important. We pointed out that the Fisher information plays a central role in the description of the thermal processes and irreversibility.

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