Entropy-variation with respect to the resistance in quantized RLC circuit derived by generalized Hellmann-Feynman theorem

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By virtue of the generalized Hellmann-Feynman theorem for ensemble average, we obtain internal energy and average energy consumed by the resistance $R$ in a quantized RLC electric circuit. We also calculate entropy-variation with respect to $R$. The relation between entropy and $R$ is also derived. By depicting figures we indeed see that the entropy increases with the increment of $R$.

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\section{I. INTRODUCTION}

In the field of mesoscopic physics Louisell was the first who quantized a mesoscopic L-C (inductance $L$ and capacitance $C$) circuit as a quantum harmonic oscillator \cite{1}. He made it by quantizing electric charge as the coordinate operator $q$, while quantizing electric current $I$ multiplied by $L$ as the momentum operator $p$. Louisell’s work has become more and more popular because mesoscopic L-C circuits may have wide applications in quantum computer. However, Louisell only calculated quantum fluctuation of L-C circuit at zero-temperature. In Ref.\cite{2} Fan and Liang pointed out that since electric current generates Joule thermal effect, one should take thermo effect into account, thus every physical observable should be evaluated in the context of ensemble average. Besides, since entropy increases with the generation of Joule heat, one should consider how the resistance $R$ in RLC electric circuit affects the variation of entropy. We shall use the generalized Hellmann-Feynman theorem (GHFT) for ensemble average to discuss this topic. The usual Hellmann-Feynman (H-F) theorem states \cite{3,4}

\[
\frac{\partial E_n}{\partial \chi} = \langle \psi_n | \frac{\partial H}{\partial \chi} | \psi_n \rangle, \quad (1)
\]

where $H$ (a Hamiltonian which involves parameter $\chi$) possesses the eigenvector $|\psi_n\rangle$, $H |\psi_n\rangle = E_n |\psi_n\rangle$. For many troublesome problems in searching for energy level in quantum mechanics, people can resort to the H-F theorem to make the analytical calculation. However, this formula is only available for the pure state, quantum statistical mechanics is the study of statistical ensembles of quantum mechanics. A statistical ensemble is described by a density matrix $\rho$, which is a non-negative, self-adjoint, trace-class operator of trace 1 on the Hilbert space describing the quantum system. Extending Eq. (1) to the ensemble average case is necessary and has been done in Refs.\cite{3,4,5}.

Our paper is arranged as follows: In Sec. 2 we briefly introduce the GHFT for ensemble average $\langle H (\chi) \rangle_e$, where the subscript $e$ denotes ensemble average. In Sec. 3 based on von Neuman’s quantum entropy definition $S = -k \text{tr} (\rho \ln \rho)$ and using the GHFT we derive the entropy-variation formula for $\frac{\partial S}{\partial \chi}$ and its relation to $\frac{\partial}{\partial \chi} \langle H (\chi) \rangle_e$. In Sec. 4 we use the GHFT to calculate internal energy of the quantized RLC circuit and its fluctuation, as well as the average energy consumed by resistance $R$. In Sec. 5 we employ the GHFT to find the relation between entropy and $R$. By depicting figures we indeed see that the entropy increases with the increment of resistance $R$.

\section{II. BRIEF REVIEW OF THE GENERALIZED HELLMANN-FEYNMAN THEOREM}

For the mixed states in thermal equilibrium described by density operators

\[
\rho = \frac{1}{Z} e^{-\beta H}, \quad \beta = (kT)^{-1},
\]

where $Z = \text{tr}(e^{-\beta H})$ is the partition function ($k$ is Boltzmann constant and $T$ is temperature), we have proposed the GHFT \cite{5}. Thus the ensemble average of the Hamiltonian $H$ (which is dependent of parameter $\chi$) is

\[
\langle H (\chi) \rangle_e = \text{tr} \rho H (\chi) = \frac{1}{Z(\chi)} \sum_j e^{-\beta E_j(\chi)} E_j (\chi) \equiv \bar{E} (\chi),
\]

and $\langle A \rangle_e \equiv \text{tr} (\rho e^{-\beta H})$ for arbitrary operator $A$ of system. Performing the partial differentiation with respect to $\chi$, we have \cite{6}

\[
\frac{\partial \langle H \rangle_e}{\partial \chi} = \frac{1}{Z(\chi)} \left\{ \sum_j e^{-\beta E_j(\chi)} \left[ -\beta E_j (\chi) + \beta \langle H \rangle_e + 1 \frac{\partial E_j (\chi)}{\partial \chi} \right] \right\}. \quad (4)
\]

Then using Eq. (1) we can further write Eq. (4) as

\[
\frac{\partial}{\partial \chi} \langle H \rangle_e = \left\langle (1 + \beta \langle H \rangle_e - \beta H) \frac{\partial H}{\partial \chi} \right\rangle_e. \quad (5)
\]
Noting the relation
\[ \left\langle H \frac{\partial H}{\partial \chi} \right\rangle_e = -\frac{\partial}{\partial \beta} \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e + \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e \langle H \rangle_e, \] (6)
when \( H \) is independent of \( \beta \), we can reform Eq. (4) as
\[ \frac{\partial}{\partial \chi} \langle H \rangle_e = \beta \frac{\partial}{\partial \beta} \left[ \beta \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e \right] = \left( 1 + \beta \frac{\partial}{\partial \beta} \right) \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e. \] (7)
The integration of Eq.(7) yields two forms. One is
\[ \beta \left\langle \frac{\partial H(\chi)}{\partial \chi} \right\rangle_e = \int d\beta \frac{\partial}{\partial \chi} \langle H \rangle_e + K, \] (8)
which deals with integration over \( d\beta \) and \( K \) is an integration constant; and the other is
\[ \langle H \rangle_e = \int_0^\infty \left( 1 + \beta \frac{\partial}{\partial \beta} \right) \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e \, d\chi + \langle H(0) \rangle_e, \] (9)
which tackles integration over \( d\chi \). Note that the fluctuation of \( H \) can be obtained by virtue of
\[ (\Delta H)^2 = \langle H^2 \rangle_e - E^2 = -\frac{\partial \langle H \rangle_e}{\partial \beta}. \] (10)

III. DERIVING ENTROPY-VARIATION \( \frac{\partial S}{\partial \chi} \) AND ITS RELATION TO \( \frac{\partial \langle H \rangle}{\partial \chi} \) FROM

\[ S = -kT \sigma (\rho \ln \rho) \]
Entropy \( S \) in classical statistical mechanics is defined as
\[ F = U - TS, \] (11)
where \( U \) is system’s internal energy or the ensemble average of Hamiltonian \( \langle H \rangle_e \), and \( F \) is Helmholtz free energy,
\[ F = -\frac{1}{\beta} \ln \sum_n e^{-\beta E_n}. \] (12)
According to Eq.(12), the entropy can not be calculated until systems’ energy level \( E_n \) is known. In this work we consider how to derive entropy without knowing \( E_n \) in advance, i.e., we will not diagonalize the Hamiltonian before calculating the entropy, instead, our starting point is using entropy’s quantum-mechanical definition,
\[ S = -k \sigma (\rho \ln \rho). \] (13)
It is von Neumann who extended the classical concept of entropy (put forth by Gibbs) into the quantum domain. Note that, because the trace is actually representation independent, Eq. (13) assigns zero entropy to any pure state. However, in many cases \( \ln \rho \) is unknown until \( \rho \) is diagonalized, so we explore how to use the GHFT to calculate entropy of some complicated systems, which, to our knowledge, has not been calculated in the literature before. Rewriting Eq. (13) as
\[ S = \beta kT (\rho H) + kT (\rho \ln Z) = \frac{1}{T} \langle H \rangle_e + k \ln Z, \] (14)
where \( \langle H \rangle_e \) corresponding to \( U \) in Eq.(11), it then follows
\[ \frac{\partial S}{\partial \chi} = \frac{1}{T} \left( \frac{\partial}{\partial \chi} \langle H \rangle_e - \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e \right), \] (15)
which indicates that the entropy-variation is proportional to the difference between internal energy’s variation and the ensemble average of \( \frac{\partial H}{\partial \chi} \). In particular, when \( \rho \) is a pure state, then \( \frac{\partial}{\partial \chi} \langle H \rangle_e = \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e, \frac{\partial S}{\partial \chi} = 0, \) \( S \) is a constant (zero). Supposing the case is
\[ H = \sum_i \chi_i H_i, \] (16)
then due to \( \left\langle \frac{\partial H}{\partial \chi_i} \right\rangle_e = \langle H_i \rangle_e, \) we also have
\[ \frac{\partial S}{\partial \chi_i} = 0. \] (17)
Eq. (15) also appears in Ref. [6], but it does not mention the von Neuman entropy \( S = -kT \sigma (\rho \ln \rho) \). Substituting Eq. (15) into Eq. (7) yields
\[ T \frac{\partial S}{\partial \chi} = \beta \frac{\partial}{\partial \beta} \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e, \] (18)
this is another form of the entropy-variation formula. It then follows
\[ TS = \langle H \rangle_e - \int \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e \, d\chi + C, \] (19)
where \( C \) is an integration constant of parameters involved in \( H \) other than \( \chi \).

IV. INTERNAL ENERGY AND AVERAGE ENERGY CONSUMED BY RESISTANCE IN THE RLC CIRCUIT

In terms of \( q - p \) quantum variables \( (q,p) = i\hbar \), Louisell’s Hamiltonian for the quantized RLC circuit is
\[ H = \frac{1}{2L} p^2 + \frac{1}{2C} q^2 + \frac{R}{2L} (pq + qp). \] (20)
We now use GHFT to calculate the internal energy \( \langle H \rangle_e \). Substituting Eq.(20) into Eq.(5) and letting \( \chi \) be \( L, C \), and \( R \), respectively, we obtain
\[ -2L^2 \frac{\partial \langle H \rangle_e}{\partial L} = \langle 1 + \beta \langle H \rangle_e - \beta H \rangle (p^2 + R(pq + qp)) \rangle_e, \] (21)
\[ -2C^2 \frac{\partial \langle H \rangle_e}{\partial C} = \langle 1 + \beta \langle H \rangle_e - \beta H \rangle (q^2) \rangle_e, \] (22)
\[ 2L \frac{\partial \langle H \rangle_e}{\partial R} = \langle 1 + \beta \langle H \rangle_e - \beta H \rangle (pq + qp) \rangle_e. \] (23)
Supposing the eigenvector of Hamiltonian is $|\Psi_n\rangle$, $H|\Psi_n\rangle = E_n|\Psi_n\rangle$, $E_n$ is the energy eigenvalue, due to

$$
\langle \Psi_n | [q^2 - p^2, H] | \Psi_n \rangle = 0,
$$

(24)

and

$$
[q^2 - p^2, H] = \left( \frac{i}{L} + \frac{i}{C} \right) (pq + qp) + 2i \frac{R}{L} (p^2 + q^2),
$$

(25)

which leads to the following relation

$$
\langle \Psi_n | \left[ \left( \frac{i}{L} + \frac{i}{C} \right) (pq + qp) + 2i \frac{R}{L} (p^2 + q^2) \right] | \Psi_n \rangle = 0,
$$

(26)

and noticing $\langle 1 + \beta \langle H \rangle_e - \beta H \rangle_e = 0$, thus we can have the ensemble average

$$
\langle (1 + \beta \langle H \rangle_e - \beta H) \rangle_e \times \left[ \left( \frac{i}{L} + \frac{i}{C} \right) (pq + qp) + 2i \frac{R}{L} (p^2 + q^2) \right] = 0.
$$

(27)

Substituting Eqs. (21) - (23) into Eq. (27), we obtain a partial differential equation

$$
L^2 \frac{\partial \langle H \rangle_e}{\partial L} + C^2 \frac{\partial \langle H \rangle_e}{\partial C} + \left( LR - \frac{L^2}{2RC} - \frac{L}{2R} \right) \frac{\partial \langle H \rangle_e}{\partial R} = 0,
$$

(28)

which can be solved by virtue of the method of characteristics \cite{8,9}. According to it we have the equation

$$
\frac{dL}{C^2} = \frac{dC}{LR - \frac{L^2}{2RC} - \frac{L}{2R}},
$$

(29)

it then follows that

$$
\frac{1}{L} - \frac{1}{C} = c_1, \quad \frac{R^2}{L} - \frac{1}{LC} = c_2,
$$

(30)

where $c_1$ and $c_2$ are two arbitrary constants. We can now apply the method above in which the general solution of the partial differential equation \cite{28} is found by writing $\langle H \rangle_e = f[c_1, c_2]$, i.e.,

$$
\langle H \rangle_e = f \left[ \frac{1}{L} - \frac{1}{C}, \frac{R^2}{L} - \frac{1}{LC} \right],
$$

(31)

where $f[x, y]$ is some function of $x, y$. In order to determine the form of this function, we examine the special case when $R = 0$, i.e.

$$
H_0 = \frac{1}{2L} p^2 + \frac{1}{2C} q^2 = \hbar \omega_0 \left( a^+ a + \frac{i}{2} \right),
$$

(32)

where $a = \sqrt{\frac{\hbar \omega_0}{2}} q + i \sqrt{\frac{\hbar \omega_0}{2L}} p$ with $\omega_0 = 1/\sqrt{LC}$. According to the well-known Bose statistics formula $\langle H_0 \rangle_e = \frac{\hbar \omega_0}{2} \coth \frac{\hbar \omega_0}{2}$, then we know

$$
\langle H | R = 0 \rangle_e = f \left[ \frac{1}{L} - \frac{1}{C}, \frac{R}{L} - \frac{1}{LC} \right] = \frac{\hbar \omega_0}{2} \coth \frac{\hbar \omega_0}{2}.
$$

(33)

To determine the form of function $f[x, y]$, let $x = \frac{1}{L} - \frac{1}{C}$, $y = \frac{1}{2L} - \frac{1}{2C}$, then its reverse relations are $L = \frac{x + \sqrt{x^2 - 4y}}{2}$, $C = \frac{-x + \sqrt{x^2 - 4y}}{2y}$, and $\omega_0 = \sqrt{-y}$. This implies that the form of function $f[x, y]$ is

$$
f[x, y] = \frac{\hbar \sqrt{-y}}{2} \coth \frac{\hbar \beta \sqrt{-y}}{2},
$$

(34)

and we obtain the internal energy

$$
\langle H \rangle_e = f \left[ \frac{1}{L} - \frac{1}{C}, \frac{R^2}{L^2} - \frac{1}{LC} \right] = \frac{\hbar \omega}{2} \coth \frac{\hbar \beta}{2},
$$

(35)

where $\omega = \sqrt{\frac{1}{LC} - \frac{4R}{L^2}}$.

Then according to Eq. (10) the fluctuation of $H$ is

$$
(\Delta H)^2 = \frac{\hbar^2 \omega^2}{4} \frac{1}{\sinh^2 \frac{\hbar \omega \beta}{2}}.
$$

(36)

Using Eq. (8) and the following integration formula,

$$
\int \frac{e^{ax}}{x} \, dx = \ln (e^{ax} - 1) - ax,
$$

(37)

we have

$$
\int \frac{\partial H}{\partial R} \, d\beta = \frac{1}{\beta} \int \frac{\partial \langle H \rangle_e}{\partial R} \, d\beta = -\frac{\hbar R}{2 \omega \omega \coth \frac{\hbar \omega \beta}{2}},
$$

(38)

so the average energy consumed by the resistance is

$$
\frac{R}{2L} \langle (pq + qp) \rangle_e = -\frac{\hbar R^2}{2 \omega \omega L^2} \coth \frac{\hbar \omega \beta}{2}, \quad \omega = \omega_0 \sqrt{1 - R^2 C/L},
$$

(39)

where the minus sign implies that the resistance is a kind of energy consuming element.

V. ENTROPY-VARIATION WITH RESPECT TO THE RESISTANCE

In this section, based on the above results we investigate the influence of the resistance on the entropy of RLC electric circuit. By substituting Eqs. (31) and (33) into Eq. (15), it is easily obtained that

$$
\frac{\partial S}{\partial R} = \frac{\beta R^2}{4(T - 1)^2} \exp \left[ \frac{\beta \omega_0}{2} \right] = \frac{\beta R^2}{4(T - 1)^2} \frac{1}{\sinh^2 \frac{\beta \omega_0}{2}}.
$$

(40)

Further, making use of the integral formula

$$
\int \frac{\ln y}{(y - 1)^2} \, dy = \ln (y - 1) - \frac{y \ln y}{y - 1},
$$

(41)
we derive the relation between the entropy and the resistance as follows

\[ S = -k \ln \left[ \exp \left( \frac{\hbar \omega}{\beta} \right) - 1 \right] + \frac{1}{T} \exp \left( \frac{\hbar \omega}{\beta} \right) - 1. \]  \hspace{1cm} (42)

Obviously when \( R = 0 \), the entropy in (42) corresponds to LC electric circuit. Based on the relation in Eq. (42), we in Figure 1 depict the variation of the entropy as a function of resistance in the range of \( [0, \sqrt{L/C}] \). The figure illustrates that the entropy has a monotonically increasing with the resistance \( R \). When \( R \) goes to the limit \( \sqrt{L/C} \), the entropy tends to infinity.

In summary, by virtue of the generalized Hellmann-Feynman theorem for ensemble average, we have obtained internal energy and average energy consumed by the resistance, we have also calculated entropy-variation with respect to the resistance in quantized RLC electric circuit. The relation between entropy and resistance is also derived. By depicting figure we indeed see that the entropy increases with the increment of \( R \).

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FIG. 1: Entropy S as a function of resistance.