Entropy-variation with resistance in a quantized RLC circuit derived by the generalized Hellmann–Feynman theorem*

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

Keywords: entropy, RLC circuit, generalized Hellmann–Feynman theorem
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1. Introduction

In the field of mesoscopic physics Louisell was the first to quantize a mesoscopic inductance–capacitance (L-C) circuit as a quantum harmonic oscillator,[1] specifically 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 computers. However, Louisell calculated only quantum fluctuation in the L-C circuit at zero-temperature. In Ref. [2] Fan and Liang pointed out that the thermal effect should be taken into account, because electric current generates a Joule thermal effect, thus every physical observable should be evaluated in the context of the ensemble average. Besides, since entropy increases with the generation of Joule heat, one should consider how the resistance R in a resistance–inductance–capacitance (RLC) electric circuit affects the variation of entropy. We shall use the generalized Hellmann–Feynmam theorem (GHFT) for the ensemble average to discuss this topic. The usual Hellmann–Feynman (H-F) theorem states[3,4]

$$\frac{\partial E_n}{\partial \chi} = \langle \psi_n | \frac{\partial H}{\partial \chi} | \psi_n \rangle , \tag{1}$$

where H is the Hamiltonian which involves parameter χ, and it possesses the eigenvector $|\psi_n\rangle$: $H|\psi_n\rangle = E_n|\psi_n\rangle$. For many troublesome problems in searching for energy levels in quantum mechanics, one can resort to the H-F theorem to do the analytical calculation. However, this formula is available only for a pure state, and quantum statistical mechanics is for the study of statistical ensembles of quantum mechanics. A statistical ensemble is described by density matrix ρ, 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. [5]–[10].

The rest of the present paper is arranged as follows. In Section 2 we briefly introduce the GHFT for the ensemble average $\langle H(\chi)\rangle_{\rm e}$, where the subscript e denotes ensemble average. In Section 3, based on von Neuman's quantum entropy definition $S = -k\,{\rm tr}(\rho \ln \rho)$ and using the GHFT, we derive the entropy-variation formula for $\partial S/\partial\chi$ and its relation to $\partial \langle H(\chi)\rangle_{\rm e}/\partial\chi$. In Section 4 we use the GHFT to calculate internal energy of the quantized RLC circuit and its fluctuation, as well as the average energy consumed on resistance R. In Section 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 increase of resistance R.

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2. Brief review of the generalized Hellmann–Feynman theorem

We have proposed the GHFT,[5−7] for a mixed state in thermal equilibrium described by density operators

$$\rho = \frac{1}{Z}\,\mathrm{e}^{-\beta H} \quad \text{and} \quad \beta = (kT)^{-1}, \tag{2}$$

where $Z = \mathrm{tr}\left(\mathrm{e}^{-\beta H}\right)$ is the partition function, k is the Boltzmann constant, and T is temperature. Thus the ensemble average of the Hamiltonian H, which is dependent on parameter χ, is

$$\begin{aligned}\langle H(\chi)\rangle_{\mathrm{e}} &= \mathrm{tr}\left[\rho H(\chi)\right] \\ &= \frac{1}{Z(\chi)}\sum_j \mathrm{e}^{-\beta E_j(\chi)} E_j(\chi) \\ &\equiv \bar{E}(\chi), \end{aligned} \tag{3}$$

and $\langle A\rangle_{\mathrm{e}} \equiv \mathrm{tr}\,(\rho A)$ for arbitrary operator A of the system. Performing the partial differentiation with respect to χ, we have[5−7]

$$\begin{aligned}\frac{\partial \langle H\rangle_{\mathrm{e}}}{\partial\chi} &= \frac{1}{Z(\chi)}\Bigg\{\sum_j \mathrm{e}^{-\beta E_j(\chi)}[-\beta E_j(\chi) \\ &\quad + \beta\langle H\rangle_{\mathrm{e}} + 1]\frac{\partial E_j(\chi)}{\partial\chi}\Bigg\}. \end{aligned} \tag{4}$$

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

$$\frac{\partial}{\partial\chi}\langle H\rangle_{\mathrm{e}} = \left\langle\left(1+\beta\langle H\rangle_{\mathrm{e}} - \beta H\right)\frac{\partial H}{\partial\chi}\right\rangle_{\mathrm{e}}. \tag{5}$$

Noting the relation

$$\left\langle H\frac{\partial H}{\partial\chi}\right\rangle_{\mathrm{e}} = -\frac{\partial}{\partial\beta}\left\langle\frac{\partial H}{\partial\chi}\right\rangle_{\mathrm{e}} + \left\langle\frac{\partial H}{\partial\chi}\right\rangle_{\mathrm{e}}\langle H\rangle_{\mathrm{e}}, \tag{6}$$

when H is independent of β, we can reform Eq. (5) as

$$\begin{aligned}\frac{\partial}{\partial\chi}\langle H\rangle_{\mathrm{e}} &= \frac{\partial}{\partial\beta}\left[\beta\left\langle\frac{\partial H}{\partial\chi}\right\rangle_{\mathrm{e}}\right] \\ &= \left(1+\beta\frac{\partial}{\partial\beta}\right)\left\langle\frac{\partial H}{\partial\chi}\right\rangle_{\mathrm{e}}. \end{aligned} \tag{7}$$

The integration of Eq. (7) yields two forms: one is

$$\beta\left\langle\frac{\partial H(\chi)}{\partial\chi}\right\rangle_{\mathrm{e}} = \int \mathrm{d}\beta\frac{\partial}{\partial\chi}\langle H\rangle_{\mathrm{e}} + K, \tag{8}$$

which deals with the integral over $\mathrm{d}\beta$, where K is an integral constant; and the other is

$$\langle H\rangle_{\mathrm{e}} = \int_0^{\chi}\left(1+\beta\frac{\partial}{\partial\beta}\right)\left\langle\frac{\partial H}{\partial\chi}\right\rangle_{\mathrm{e}}\mathrm{d}\chi + \langle H(0)\rangle_{\mathrm{e}}, \tag{9}$$

which tackles the integral over $\mathrm{d}\chi$. Note that the fluctuation of H can be obtained by virtue of

$$(\Delta H)^2 = \left\langle H^2\right\rangle_{\mathrm{e}} - \bar{E}^2 = -\frac{\partial\langle H\rangle_{\mathrm{e}}}{\partial\beta}. \tag{10}$$

3. Deriving entropy-variation $\partial S/\partial\chi$ and its relation to $\partial\langle H\rangle_{\mathrm{e}}/\partial\chi$ from $S = -k\,\mathrm{tr}(\rho\ln\rho)$

Entropy S in classical statistical mechanics is defined as

$$F = U - TS, \tag{11}$$

where U is the internal energy or the ensemble average of the Hamiltonian $\langle H\rangle_{\mathrm{e}}$, and F is the Helmholtz free energy,

$$F = -\frac{1}{\beta}\ln\sum_n \mathrm{e}^{-\beta E_n}. \tag{12}$$

According to Eq. (12) the entropy cannot be calculated until the energy level E_n of the system is known. In this work we consider how to derive the entropy without knowning E_n in advance, i.e., we do not diagonalize the Hamiltonian before calculating the entropy, instead, our starting point is to use the quantum-mechanical definition of entropy,

$$S = -k\,\mathrm{tr}\,(\rho\ln\rho), \tag{13}$$

where ρ is the density operator of the system. It was von Neuman who extended the classical concept of entropy put forth by Gibbs into the quantum domain. Note that because the trace is actually independent of representation, equation (13) assigns zero entropy to any pure state. However, in many cases $\ln\rho$ is unknown until ρ is diagonalized, so we explore how to use the GHFT to calculate the entropies of some complicated systems, which, to our knowledge, have not been calculated in the literature yet. Rewriting Eq. (13) as

$$\begin{aligned}S &= \beta k\,\mathrm{tr}(\rho H) + k\,\mathrm{tr}\,(\rho\ln Z) \\ &= \frac{1}{T}\langle H\rangle_{\mathrm{e}} + k\ln Z, \end{aligned} \tag{14}$$

where $\langle H\rangle_{\mathrm{e}}$ corresponds to U in Eq. (11), yields

$$\frac{\partial S}{\partial\chi} = \frac{1}{T}\left(\frac{\partial}{\partial\chi}\langle H\rangle_{\mathrm{e}} - \left\langle\frac{\partial H}{\partial\chi}\right\rangle_{\mathrm{e}}\right), \tag{15}$$

which indicates that the entropy-variation is proportional to the difference between the internal energy's

variation and the ensemble average of $\partial H/\partial\chi$. In particular, when ρ is in a pure state, then $\partial \langle H\rangle_{\rm e}/\partial\chi = \langle \partial H/\partial\chi\rangle_{\rm e}$, $\partial S/\partial\chi = 0$, so S is a constant (zero). Supposing that

$$H = \sum_i \chi_i H_i, \quad \text{and} \quad \langle H\rangle_{\rm e} = \sum_i \chi_i \langle H_i\rangle_{\rm e}, \tag{16}$$

then due to $\langle \partial H/\partial\chi_i\rangle_{\rm e} = \langle H_i\rangle_{\rm e}$, we also have

$$\frac{\partial S}{\partial \chi_i} = 0. \tag{17}$$

Equation (15) also appears in Ref. [8], where, however, the von Neuman entropy $S = -k\,{\rm tr}\,(\rho\ln\rho)$ was not mentioned. Substituting Eq. (15) into Eq. (7) yields

$$T\frac{\partial S}{\partial\chi} = \beta\frac{\partial}{\partial\beta}\left\langle\frac{\partial H}{\partial\chi}\right\rangle_{\rm e}, \tag{18}$$

which is another form of the entropy-variation formula. It then follows

$$TS = \langle H\rangle_{\rm e} - \int\left\langle\frac{\partial H}{\partial\chi}\right\rangle_{\rm e}{\rm d}\chi + C, \tag{19}$$

where C is an integration constant of a parameter involved in H other than χ.

4. Internal energy and average energy consumed on resistance in the RLC circuit

In terms of q–p quantum variables ($[q,p] = {\rm i}\hbar$), Louisell's Hamiltonian for the quantized RLC circuit is

$$H = \frac{1}{2L}p^2 + \frac{1}{2C}q^2 + \frac{R}{2L}(pq+qp). \tag{20}$$

We now use the GHFT to calculate the internal energy $\langle H\rangle_{\rm e}$. Substituting Eq. (20) into Eq. (5) and letting χ be L, C, and R, respectively, we obtain

$$\begin{aligned} &-2L^2\frac{\partial\langle H\rangle_{\rm e}}{\partial L} \\ &= \left\langle\left(1+\beta\langle H\rangle_{\rm e} - \beta H\right)\left(p^2 + R(pq+qp)\right)\right\rangle_{\rm e}, \end{aligned} \tag{21}$$

$$\begin{aligned} &-2C^2\frac{\partial\langle H\rangle_{\rm e}}{\partial C} \\ &= \left\langle\left(1+\beta\langle H\rangle_{\rm e} - \beta H\right)\left(q^2\right)\right\rangle_{\rm e}, \end{aligned} \tag{22}$$

$$\begin{aligned} &2L\frac{\partial\langle H\rangle_{\rm e}}{\partial R} \\ &= \left\langle\left(1+\beta\langle H\rangle_{\rm e} - \beta H\right)(pq+qp))\right\rangle_{\rm e}. \end{aligned} \tag{23}$$

Supposing that 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

$$\langle\Psi_n|\left[q^2 - p^2, H\right]|\Psi_n\rangle = 0, \tag{24}$$

and

$$\begin{aligned} \left[q^2-p^2, H\right] &= \left(\frac{\rm i}{L} + \frac{\rm i}{C}\right)(pq+qp) \\ &\quad + 2{\rm i}\frac{R}{L}\left(p^2+q^2\right), \end{aligned} \tag{25}$$

which leads to the following relation:

$$\langle\Psi_n|\left[\left(\frac{\rm i}{L}+\frac{\rm i}{C}\right)(pq+qp) + 2{\rm i}\frac{R}{L}\left(p^2+q^2\right)\right]|\Psi_n\rangle = 0, \tag{26}$$

and noticing that $\left\langle\beta\langle H\rangle_{\rm e} - \beta H\right\rangle_{\rm e} = 0$, we can have the ensemble average

$$\begin{aligned} &\left\langle(1+\beta\langle H\rangle_{\rm e} - \beta H)\left[\left(\frac{\rm i}{L}+\frac{\rm i}{C}\right)(pq+qp)\right.\right. \\ &\left.\left. + 2{\rm i}\frac{R}{L}\left(p^2+q^2\right)\right]\right\rangle_{\rm e} = 0. \end{aligned} \tag{27}$$

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

$$\begin{aligned} &L^2\frac{\partial\langle H\rangle_{\rm e}}{\partial L} + C^2\frac{\partial\langle H\rangle_{\rm e}}{\partial C} \\ &+\left(LR - \frac{L^2}{2RC} - \frac{L}{2R}\right)\frac{\partial\langle H\rangle_{\rm e}}{\partial R} = 0, \end{aligned} \tag{28}$$

which can be solved by the method of characteristics.[11,12] Thus we have the equation

$$\frac{{\rm d}L}{L^2} = \frac{{\rm d}C}{C^2} = \frac{{\rm d}R}{LR - L^2/2RC - L/2R}, \tag{29}$$

and that

$$\frac{1}{L} - \frac{1}{C} = c_1, \quad \text{and} \quad \frac{R^2}{L^2} - \frac{1}{LC} = c_2, \tag{30}$$

where c_1 and c_2 are both arbitrary constants. We can now use the method above to obtain the general solution of the partial differential equation (28) by writing $\langle H\rangle_{\rm e} = f\left[c_1, c_2\right]$, i.e.

$$\langle H\rangle_{\rm e} = f\left[\frac{1}{L} - \frac{1}{C}, \frac{R^2}{L^2} - \frac{1}{LC}\right], \tag{31}$$

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

$$H_0 = \frac{1}{2L}p^2 + \frac{1}{2C}q^2 = \hbar\omega_0\left(a^\dagger a + \frac{1}{2}\right), \tag{32}$$

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

$$\langle H|_{R=0}\rangle_{\rm e} = f\left[\frac{1}{L} - \frac{1}{C}, -\frac{1}{LC}\right]$$

$$= \frac{\hbar\omega_0}{2}\coth\frac{\hbar\omega_0\beta}{2}. \tag{33}$$

To determine the form of function $f[x,y]$, let $x = 1/L - 1/C$, $y = -1/LC$, then its reverse relations will be $L = (x+\sqrt{x^2-4y})/2y$, $C = (-x+\sqrt{x^2-4y})/2y$, and $\omega_0 = \sqrt{-y}$. Thus the form of function $f[x,y]$ is

$$f[x,y] = \frac{\hbar\sqrt{-y}}{2}\coth\frac{\hbar\beta\sqrt{-y}}{2}, \tag{34}$$

and the internal energy is obtained to be

$$\begin{aligned}\langle H\rangle_{\mathrm{e}} &= f\left[\frac{1}{L}-\frac{1}{C},\frac{R^2}{L^2}-\frac{1}{LC}\right]\\ &= \frac{\hbar\omega}{2}\coth\frac{\hbar\omega\beta}{2},\end{aligned} \tag{35}$$

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

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

$$(\Delta H)^2 = \frac{\hbar^2\omega^2}{4}\frac{1}{\sinh^2(\beta\hbar\omega/2)}. \tag{36}$$

Using Eq. (8) and the integration formula,

$$\int\frac{1}{\mathrm{e}^{ax}-1}\mathrm{d}x = \frac{1}{a}\left(\ln\left(\mathrm{e}^{ax}-1\right)-ax\right), \tag{37}$$

we have

$$\begin{aligned}&\left\langle\frac{\partial H}{\partial R}\right\rangle_{\mathrm{e}}\\ &= \frac{1}{2L}\langle(pq+qp)\rangle_{\mathrm{e}}\\ &= \frac{1}{\beta}\int\frac{\partial\langle H\rangle_{\mathrm{e}}}{\partial R}\mathrm{d}\beta\\ &= -\frac{\hbar R}{2\omega L^2}\coth\frac{\hbar\omega\beta}{2}.\end{aligned} \tag{38}$$

So the average energy consumed on the resistance is

$$\begin{aligned}&\frac{R}{2L}\langle(pq+qp)\rangle_{\mathrm{e}} = -\frac{\hbar R^2}{2\omega L^2}\coth\frac{\hbar\omega\beta}{2},\\ &\omega = \omega_0\sqrt{1-R^2C/L},\end{aligned} \tag{39}$$

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

5. Entropy-variation with resistance

In this section, based on the above results we investigate the influence of the resistance on the entropy of the RLC electric circuit. By substituting Eqs. (31) and (38) into Eq. (15), it is easily obtained that

$$\begin{aligned}\frac{\partial S}{\partial R} &= \frac{\beta R\hbar^2}{TL^2}\frac{\exp(\hbar\beta\omega)}{(\exp(\hbar\beta\omega)-1)^2}\\ &= \frac{\beta R\hbar^2}{4TL^2}\frac{1}{\sinh^2(\beta\hbar\omega/2)}.\end{aligned} \tag{40}$$

Further, by making use of the integral formula

$$\int\frac{\ln y}{(y-1)^2}\mathrm{d}y = \ln(y-1) - \frac{y\ln y}{y-1}, \tag{41}$$

we derive the relation between the entropy and the resistance as follows:

$$S = -k\ln[\exp(\hbar\beta\omega)-1] + \frac{1}{T}\frac{\hbar\omega\exp(\hbar\beta\omega)}{\exp(\hbar\beta\omega)-1}. \tag{42}$$

Obviously when $R = 0$, entropy S_0 in Eq. (42) corresponds to that of the LC electric circuit. Based on the relation in Eq. (42), we depict the variation of the entropy as a function of resistance in a range of $\left[0,\sqrt{L/C}\right]$ in Fig. 1. This figure illustrates that the entropy monotonically increases with resistance R. When R goes to the limit $\sqrt{L/C}$, the entropy tends to infinity.

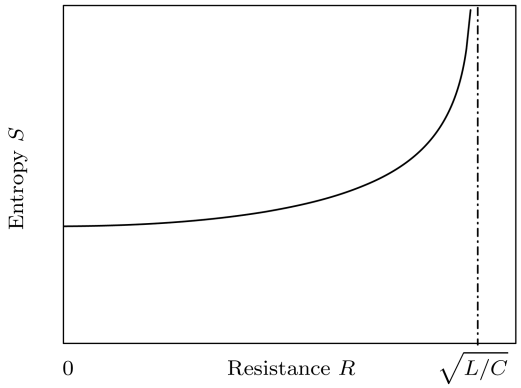


Fig. 1. Entropy S as a function of resistance.

In summary, by virtue of the generalized Hellmann–Feynman theorem for the ensemble average, we have obtained the internal energy and the average energy consumed on the resistance, and we have also calculated entropy-variation with resistance in a quantized RLC electric circuit. The relation between entropy and resistance is also derived. By the use of a figure we indeed see that the entropy increases with the increase of R. For more discussion about RLC flunctation and entropy evolution, readers may refer to Refs. [13] and [14].

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