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Generalized Hellmann-Feynman Theorem for Coupled Anisotropic Two-Mode Boson System

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Abstract We apply the Generalized Hellmann-Feynman theorem (GHFT) to calculate the thermodynamical relations of two-coupled anisotropic boson system by the method of characteristics. Its internal energy, Helmholtz free energy, and entropy in thermodynamics are obtained. It is found that GFHT is a new approach to directly calculate these thermodynamical functions.

Keywords Two-coupled bosonic Hamiltonian model · Method of characteristics · Generalized Hellmann-Feynman theorem

1 Introduction

The dynamics of interacting Boson systems is an important issue not only because of its fundamental theoretical implications but also due to its important experimental applications [1, 2]. Recently study on interacting Boson systems has become a hot topic. For example, there are explosive activities in the study of the entanglement and nonclassical properties of various Boson systems in quantum information theory [3–6]. As a particular example, two-coupled bosonic Hamiltonian model is of great interest and the corresponding Hamiltonian can be expressed as

$$H = \frac{1}{2m}(p_1^2 + p_2^2) + \frac{\Lambda}{2}(x_1 p_2 - x_2 p_1) + \frac{1}{8}m\Lambda_1^2 x_1^2 + \frac{1}{8}m\Lambda_2^2 x_2^2, \tag{1}$$

which describes anisotropic Harmonic oscillator due to $\Lambda_1 \neq \Lambda_2$. The coupling between two Harmonic oscillators is governed by the constant Λ. In fact, this model originates from quantum motion of an electron in a uniform magnetic field, first investigated by Landau [7].

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In the present work, we apply the generalized Hellmann-Feynman theorem (GHFT) for ensemble average to discuss the above model in the domain of quantum statistical mechanics. That is to say, we shall derive internal energy and other system's thermodynamical functions by virtue of the GFHT. To our knowledge, these problems have not been calculated in the literature before. As one can see shortly later, the GFHT provides us with a new approach to directly calculate thermodynamical functions. The work is organized as follows: In Sect. 2, we first review the theory on GFHT. In Sect. 3 we mostly make some transformations of the Hamiltonian of (1) to derive conveniently in the following calculation. We devote Sect. 4 and Sect. 5 to deriving the internal energy and obtaining Helmholtz free energy and entropy by virtue of the GHFT, respectively.

2 Generalized Hellmann-Feynman Theorem

To begin with, we review the theory on GFHT, in which we generalize the statistical mechanical description of Hermann-Feynman theorem developed to quantum systems. As we all know, quantum statistical mechanics is the study of statistical ensembles of quantum mechanics. A statistical ensemble is described by a density matrix ρ, which is a non-negative, self-adjoint, trace-class operator of trace 1 on the Hilbert space describing the quantum system. Here ρ is the density operator, $\rho = e^{-\beta H}/Z$, and $Z = \mathrm{tr}(e^{-\beta H})$ is called the partition function of the system with Hamiltonian H, $\beta = 1/(kT)$, k is Boltzmann constant, T is temperature.

In calculating quantum mechanical expectation values and analyzing the variation of bound state energy with respect to the dynamic parameter involved in the Hamiltonian, the Hellmann-Feynman (HF) theorem [8, 9] is very useful, so HF theorem has been widely applied to molecular physics, quantum chemistry, and quark potential analysis. The HF theorem states that

$$\frac{\partial E_n}{\partial \chi} = \langle \Psi_n | \frac{\partial H}{\partial \chi} | \Psi_n \rangle, \tag{2}$$

where H is dependent on some real parameter χ, E_n and $|\Psi_n\rangle$ are energy eigenvalues and eigenvectors of H, respectively. If one notices that (2) is just for pure state expectation value, one is naturally challenged to explore a theorem for mixed state ensemble average in quantum statistics. At this point, for internal energy $\langle H \rangle_e$, the form of GHFT is first set up in [10] and then reformulated in [11, 12], i.e.,

$$\frac{\partial}{\partial \chi} \langle H \rangle_e = \left\langle (1 + \beta \langle H \rangle_e - \beta H) \frac{\partial H}{\partial \chi} \right\rangle_e, \tag{3}$$

where the subscript e stands for the ensemble average, and $\langle A \rangle_e \equiv \mathrm{Tr}(\rho A)$ for arbitrary operator A. Using the relation

$$\left\langle H \frac{\partial H}{\partial \chi} \right\rangle_e = -\frac{\partial}{\partial \beta} \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e + \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e \langle H \rangle_e, \tag{4}$$

when H is independent on β, we can further simplify (3) as

$$\frac{\partial \langle H \rangle_e}{\partial \chi} = \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e + \beta \frac{\partial}{\partial \beta} \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e = \frac{\partial}{\partial \beta} \left[\beta \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e \right]. \tag{5}$$

As long as we know the internal energy $\langle H\rangle_e$ and $\langle\frac{\partial H}{\partial\chi}\rangle_e$, we can find other thermodynamic functions by virtue of the following formulas. For example, we shall obtain the energy fluctuation by differentiating $\langle H\rangle_e$ with respect to β,

$$(\Delta H)^2 = \langle H^2\rangle_e - \langle H\rangle_e^2 = -\frac{\partial\langle H\rangle_e}{\partial\beta} = -kT^2 C_V, \tag{6}$$

with the heat capacity at constant volume $C_V = (\frac{\partial\langle H\rangle_e}{\partial T})_V$, i.e., by differentiating $\langle H\rangle_e$ with respect to T.

3 Disposal of Two-Coupled Anisotropic Harmonic Oscillators

3.1 Transformation I

In order to study the properties of Hamiltonian system conveniently in (1), we first transform it into another bosonic form. By means of the following transformation

$$\begin{pmatrix} a_1 \\ a_1^\dagger \\ a_2 \\ a_2^\dagger \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} x_1 \\ p_1 \\ x_2 \\ p_2 \end{pmatrix}, \tag{7}$$

then (1) become

$$\begin{aligned} H = {}& \omega_1 a_1^\dagger a_1 + \kappa_1(a_1^2 + a_1^{\dagger 2}) + \omega_2 a_2^\dagger a_2 + \kappa_2(a_2^2 + a_2^{\dagger 2}) \\ & + g(a_1^\dagger a_2 - a_1 a_2^\dagger) + \frac{\omega_1+\omega_2}{2}, \end{aligned} \tag{8}$$

where $g \equiv \frac{\Lambda}{2i}$ is the coupling constant between these fields, a_j and $a_j^\dagger$ $(j = 1, 2)$ are Bose annihilation and creation operators, respectively, satisfying $[a_i, a_j^\dagger] = \delta_{ij}$. The parameters are determined by

$$\begin{aligned} \omega_1 &= 2\left(\frac{1}{16}m\Lambda_1^2 + \frac{1}{4m}\right), \qquad \kappa_1 = \left(\frac{1}{16}m\Lambda_1^2 - \frac{1}{4m}\right), \\ \omega_2 &= 2\left(\frac{1}{16}m\Lambda_2^2 + \frac{1}{4m}\right), \qquad \kappa_2 = \left(\frac{1}{16}m\Lambda_2^2 - \frac{1}{4m}\right). \end{aligned} \tag{9}$$

Substituting (8) into (3) and letting χ_i be ω_1, ω_2, κ_1, κ_2, and g, respectively, one has

$$\left.\begin{aligned} \frac{\partial\langle H\rangle_e}{\partial\omega_1} &= \left\langle(1+\beta\langle H\rangle_e - \beta H)\left(a_1^\dagger a_1 + \frac{1}{2}\right)\right\rangle_e, \\ \frac{\partial\langle H\rangle_e}{\partial\omega_2} &= \left\langle(1+\beta\langle H\rangle_e - \beta H)\left(a_2^\dagger a_2 + \frac{1}{2}\right)\right\rangle_e, \\ \frac{\partial\langle H\rangle_e}{\partial\kappa_1} &= \langle(1+\beta\langle H\rangle_e - \beta H)(a_1^2 + a_1^{\dagger 2})\rangle_e, \\ \frac{\partial\langle H\rangle_e}{\partial\kappa_2} &= \langle(1+\beta\langle H\rangle_e - \beta H)(a_2^2 + a_2^{\dagger 2})\rangle_e, \\ \frac{\partial\langle H\rangle_e}{\partial g} &= \langle(1+\beta\langle H\rangle_e - \beta H)(a_1^\dagger a_2 - a_1 a_2^\dagger)\rangle_e, \end{aligned}\right\}. \tag{10}$$

We also obtain the commutation relation

$$\begin{aligned}&\left[\frac{(\kappa_1+\kappa_2)}{2g}[(a_1^2-a_1^{\dagger 2})-(a_2^2-a_2^{\dagger 2})]+(a_1^\dagger a_2+a_1a_2^\dagger),H\right]\\&=\left(\frac{4\kappa_1(\kappa_1+\kappa_2)}{g}-2\lambda\right)a_1^\dagger a_1+\left(2g-\frac{4\kappa_2(\kappa_1+\kappa_2)}{g}\right)a_2^\dagger a_2\\&\quad+\frac{\omega_1(\kappa_1+\kappa_2)}{g}(a_1^2+a_1^{\dagger 2})-\frac{\omega_2(\kappa_1+\kappa_2)}{g}(a_2^2+a_2^{\dagger 2})\\&\quad+(\omega_1-\omega_2)(a_1^\dagger a_2-a_1a_2^\dagger)+\frac{2}{g}(\kappa_1^2-\kappa_2^2).\end{aligned}\tag{11}$$

According to $H|\Psi_n\rangle=E_n|\Psi_n\rangle$, it is easily obtained that

$$0=\langle\Psi_n|\left[\frac{(\kappa_1+\kappa_2)}{2g}[(a_1^2-a_1^{\dagger 2})-(a_2^2-a_2^{\dagger 2})]+(a_1^\dagger a_2+a_1a_2^\dagger),H\right]|\Psi_n\rangle.\tag{12}$$

Combining (10) with (11) and (12), we lead to a first-order differential equation for $\langle H\rangle_e$,

$$\begin{aligned}0&=\left(\frac{4\kappa_1(\kappa_1+\kappa_2)}{g}-2g\right)\frac{\partial\langle H\rangle_e}{\partial\omega_1}+\left(2g-\frac{4\kappa_2(\kappa_1+\kappa_2)}{g}\right)\frac{\partial\langle H\rangle_e}{\partial\omega_2}\\&\quad+\frac{\omega_1(\kappa_1+\kappa_2)}{g}\frac{\partial\langle H\rangle_e}{\partial\kappa_1}-\frac{\omega_2(\kappa_1+\kappa_2)}{g}\frac{\partial\langle H\rangle_e}{\partial\kappa_2}-(\omega_1-\omega_2)\frac{\partial\langle H\rangle_e}{\partial g},\end{aligned}\tag{13}$$

which can be solved by virtue of the method of characteristics (see Appendix A). The characteristic equations deduced from (13) are

$$\begin{aligned}\frac{d\omega_1}{\frac{4\kappa_1(\kappa_1+\kappa_2)}{g}-2g}&=-\frac{d\omega_2}{\frac{4\kappa_2(\kappa_1+\kappa_2)}{\lambda}-2g}=\frac{gd\kappa_1}{\omega_1(\kappa_1+\kappa_2)}\\&=-\frac{gd\kappa_2}{\omega_2(\kappa_1+\kappa_2)}=-\frac{dg}{\omega_1-\omega_2}=\frac{d\langle H\rangle_e}{0}.\end{aligned}\tag{14}$$

From (14), it is difficult to obtain five constants by using the method of characteristics [13, 14] due to so many parameters. Even if these constants have been found, we still have difficulty to determine the form of characteristics function. So we must find more convenient Hamiltonian to deal with this problem.

3.2 Transformation II

Next, we further dispose (8) by making the following transformation

$$\begin{pmatrix}b_1\\b_1^\dagger\\b_2\\b_2^\dagger\end{pmatrix}=\begin{pmatrix}\lambda_1&\mu_1&0&0\\\mu_1&\lambda_1&0&0\\0&0&\lambda_2&\mu_2\\0&0&\mu_2&\lambda_2\end{pmatrix}\begin{pmatrix}a_1\\a_1^\dagger\\a_2\\a_2^\dagger\end{pmatrix},\tag{15}$$

where boson annihilation operators b_j and creation operators $b_j^\dagger$ $(j=1,2)$ also obeys $[b_i,b_j^\dagger]=\delta_{ij}$, so the parameters satisfy the relations $\lambda_1^2-\mu_1^2=1$ and $\lambda_2^2-\mu_2^2=1$. Therefore (8) can reform as

$$H = \Omega_1\left(b_1^\dagger b_1 + \frac{1}{2}\right) + \Omega_2\left(b_2^\dagger b_2 + \frac{1}{2}\right) + G_1(b_1^\dagger b_2 - b_1 b_2^\dagger) + G_2(b_1^\dagger b_2^\dagger - b_1 b_2), \tag{16}$$

where $G_1 \equiv g(\lambda_1\lambda_2 - \mu_1\mu_2)$ and $G_2 \equiv g(\mu_1\lambda_2 - \lambda_1\mu_2)$ are the coupling constants as well,

$$\begin{aligned} \Omega_1 &= \sqrt{\omega_1^2 - 4\kappa_1^2}, \qquad \Omega_2 = \sqrt{\omega_2^2 - 4\kappa_2^2}, \\ \lambda_1 &= \sqrt{\frac{\omega_1}{2\Omega_1} + \frac{1}{2}}, \qquad \mu_1 = \sqrt{\frac{\omega_1}{2\Omega_1} - \frac{1}{2}}, \\ \lambda_2 &= \sqrt{\frac{\omega_2}{2\Omega_2} + \frac{1}{2}}, \qquad \mu_2 = \sqrt{\frac{\omega_2}{2\Omega_2} - \frac{1}{2}}. \end{aligned} \tag{17}$$

The Hamiltonian system is just the model of two-coupled harmonic oscillators [5, 6].

4 Internal Energy Derived by Virtue of GHFT

Based on the above discussion, we now use GHFT to calculate $\langle H\rangle_e$ for H in (16). Similarly, substituting (16) into (3) and letting χ_i be Ω_1, Ω_2, G_1, G_2, respectively, we obtain

$$\left.\begin{aligned} \frac{\partial\langle H_2\rangle_e}{\partial\Omega_1} &= \left\langle(1+\beta\langle H\rangle_e - \beta H)\left(b_1^\dagger b_1 + \frac{1}{2}\right)\right\rangle_e, \\ \frac{\partial\langle H_2\rangle_e}{\partial\Omega_2} &= \left\langle(1+\beta\langle H\rangle_e - \beta H)\left(b_2^\dagger b_2 + \frac{1}{2}\right)\right\rangle_e, \\ \frac{\partial\langle H_2\rangle_e}{\partial G_1} &= \langle(1+\beta\langle H\rangle_e - \beta H)(b_1^\dagger b_2 - b_1 b_2^\dagger)\rangle_e, \\ \frac{\partial\langle H_2\rangle_e}{\partial G_2} &= \langle(1+\beta\langle H\rangle_e - \beta H)(b_1^\dagger b_2^\dagger - b_1 b_2)\rangle_e. \end{aligned}\right\}. \tag{18}$$

Due to

$$0 = \langle\Psi_n|\left[(b_1b_2 + b_1^\dagger b_2^\dagger) - \left[\left(\frac{G_1}{2\Omega_1}b_1^{\dagger 2} - \frac{G_1}{2\Omega_2}b_2^{\dagger 2}\right) - \left(\frac{G_1}{2\Omega_1}b_1^2 - \frac{G_1}{2\Omega_2}b_2^2\right)\right], H\right]|\Psi_n\rangle \tag{19}$$

and noticing

$$\begin{aligned} &\left[(b_1b_2 + b_1^\dagger b_2^\dagger) - \left[\left(\frac{G_1}{2\Omega_1}b_1^{\dagger 2} - \frac{G_1}{2\Omega_2}b_2^{\dagger 2}\right) - \left(\frac{G_1}{2\Omega_1}b_1^2 - \frac{G_1}{2\Omega_2}b_2^2\right)\right], H\right] \\ &= 2G_2(b_1b_1^\dagger + b_2^\dagger b_2) - \left(\frac{G_1G_2}{\Omega_1} + \frac{G_1G_2}{\Omega_2}\right)(b_1^\dagger b_2 - b_1 b_2^\dagger) \\ &\quad - \left(\Omega_1 + \Omega_2 + \frac{G_1^2}{\Omega_1} + \frac{G_1^2}{\Omega_2}\right)(b_1^\dagger b_2^\dagger - b_1 b_2), \end{aligned} \tag{20}$$

we construct the following equation

$$0=\left\langle(1+\beta\langle H\rangle_e-\beta H)\left\{2G_2(b_1b_1^\dagger+b_2^\dagger b_2)-\left(\frac{G_1G_2}{\Omega_1}+\frac{G_1G_2}{\Omega_2}\right)(b_1^\dagger b_2-b_1b_2^\dagger)\right.\right.$$
$$\left.\left.-\left(\Omega_1+\Omega_2+\frac{G_1^2}{\Omega_1}+\frac{G_1^2}{\Omega_2}\right)(b_1^\dagger b_2^\dagger-b_1b_2)\right\}\right\rangle_e. \tag{21}$$

Combining (18) with (21), we obtain a first-order partial differential equation for $\langle H\rangle_e$,

$$0=2G_2\left(\frac{\partial\langle H\rangle_e}{\partial\Omega_1}+\frac{\partial\langle H\rangle_e}{\partial\Omega_2}\right)-\left(\frac{G_1G_2}{\Omega_1}+\frac{G_1G_2}{\Omega_2}\right)\frac{\partial\langle H\rangle_e}{\partial G_1}$$
$$-\left(\Omega_1+\Omega_2+\frac{G_1^2}{\Omega_1}+\frac{G_1^2}{\Omega_2}\right)\frac{\partial\langle H\rangle_e}{\partial G_2}, \tag{22}$$

which can be solved via the method of characteristics (see Appendix A). On a characteristic curve, we have

$$\frac{d\Omega_1}{2G_2}=\frac{d\Omega_2}{2G_2}=-\frac{dG_1}{\frac{G_1G_2}{\Omega_1}+\frac{G_1G_2}{\Omega_2}}$$
$$=-\frac{dG_2}{\Omega_1+\Omega_2+\frac{G_1^2}{\Omega_1}+\frac{G_1^2}{\Omega_2}}. \tag{23}$$

Carrying out the integrations in (23), we find some arbitrary constants as follows

$$\begin{aligned}-G_1\sqrt{\Omega_1\Omega_2}&=c_1,\\ -\Omega_1+\Omega_2&=c_2,\\ \frac{G_2^2-G_1^2+\Omega_1\Omega_2}{2}&=c_3.\end{aligned} \tag{24}$$

Then the general solution of (22) can be written as

$$\langle H\rangle_e=f\left[(-G_1\sqrt{\Omega_1\Omega_2}),(-\Omega_1+\Omega_2),\left(\frac{G_2^2-G_1^2+\Omega_1\Omega_2}{2}\right)\right]. \tag{25}$$

To determine the form of f, we consider the limiting case by $G_2=0$. Noticing the conclusion in the Appendix B, we see that f in (25) becomes

$$f\left[(-G_1\sqrt{\Omega_1\Omega_2}),(-\Omega_1+\Omega_2),\left(\frac{-G_1^2+\Omega_1\Omega_2}{2}\right)\right]$$
$$=\frac{\frac{(\Omega_1+\Omega_2)+\sqrt{(\Omega_1-\Omega_2)^2-4G_1^2}}{2}}{\exp(\beta\frac{(\Omega_1+\Omega_2)+\sqrt{(\Omega_1-\Omega_2)^2-4G_1^2}}{2})-1}+\frac{\Omega_1}{2}$$
$$+\frac{\frac{(\Omega_1+\Omega_2)-\sqrt{(\Omega_1-\Omega_2)^2-4G_1^2}}{2}}{\exp(\beta\frac{(\Omega_1+\Omega_2)-\sqrt{(\Omega_1-\Omega_2)^2-4G_1^2}}{2})-1}+\frac{\Omega_2}{2}. \tag{26}$$

Assuming $x=-G_1\sqrt{\Omega_1\Omega_2}$, $y=-\Omega_1+\Omega_2$, $z=\frac{-G_1^2+\Omega_1\Omega_2}{2}$, their reverse relations are $\Omega_1=\frac{1}{2}(-y-\sqrt{y^2+4z-4\sqrt{x^2+z^2}})$, $\Omega_2=\frac{1}{2}(y-\sqrt{y^2+4z-4\sqrt{x^2+z^2}})$, and $G_1=-\sqrt{-z-\sqrt{x^2+z^2}}$, then the form of function f is determined as follows

$$\begin{aligned} f[x,y,z] &= \frac{\mathcal{A}}{e^{\beta\mathcal{A}}-1}+\frac{\mathcal{B}}{e^{\beta\mathcal{B}}-1}+\frac{\mathcal{A}+\mathcal{B}}{2} \\ &= \frac{\mathcal{A}}{2}\coth\left(\beta\frac{\mathcal{A}}{2}\right)+\frac{\mathcal{B}}{2}\coth\left(\beta\frac{\mathcal{B}}{2}\right), \end{aligned} \tag{27}$$

where

$$\begin{aligned} \mathcal{A} &\equiv \frac{\sqrt{4z+4\sqrt{x^2+z^2}+y^2}-\sqrt{4z-4\sqrt{x^2+z^2}+y^2}}{2}, \\ \mathcal{B} &\equiv -\frac{\sqrt{4z-4\sqrt{x^2+z^2}+y^2}+\sqrt{4z+4\sqrt{x^2+z^2}+y^2}}{2}. \end{aligned} \tag{28}$$

According to the function f, we finally obtain the internal energy for H,

$$\begin{aligned} \langle H\rangle_e &= \frac{A}{e^{\beta A}-1}+\frac{B}{e^{\beta B}-1}+\frac{A}{2}+\frac{B}{2} \\ &= \frac{A}{2}\coth\left(\beta\frac{A}{2}\right)+\frac{B}{2}\coth\left(\beta\frac{B}{2}\right), \end{aligned} \tag{29}$$

where

$$A\equiv\frac{\sqrt{S+R}-\sqrt{S-R}}{2},\qquad B\equiv-\frac{\sqrt{S+R}+\sqrt{S-R}}{2} \tag{30}$$

with

$$R\equiv 4\sqrt{\Omega_1\Omega_2G_1^2+\left(\frac{G_2^2-G_1^2+\Omega_1\Omega_2}{2}\right)^2},\qquad S\equiv 2G_2^2-2G_1^2+\Omega_1^2+\Omega_2^2. \tag{31}$$

By differentiating $\langle H\rangle_e$ with respect to β, the energy fluctuation is

$$(\Delta H)^2=\frac{A^2}{4\sinh^2(\beta\frac{A}{2})}+\frac{B^2}{4\sinh^2(\beta\frac{B}{2})}. \tag{32}$$

In fact, thermal fluctuations are expected to attenuate the entanglement [5].

5 Helmholtz Free Energy and Entropy of System

It is well-known that entropy S in classical statistical mechanics is defined as $F=U-TS$, and U is system's internal energy or the ensemble average of Hamiltonian; F is Helmholtz free energy, $F=-\frac{1}{\beta}\ln\sum_n e^{-\beta E_n}$. Thus entropy can not be calculated until systems' energy level E_n is known. Here 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,

$$S = -k\,\mathrm{tr}(\rho \ln \rho). \tag{33}$$

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, (33) assigns zero entropy to any pure state. However, in many cases $\ln\rho$ is hardly dealt with, so we shall employ the GHFT to calculate entropy of some coupled oscillators. Equation (33) is reexpressed as

$$S = -k\,\mathrm{tr}(\rho \ln \rho) = \frac{1}{T}\langle H\rangle_e + k \ln Z, \tag{34}$$

where $\langle H\rangle_e$ correspond to U. It then follows

$$\frac{\partial S}{\partial \chi} = \frac{1}{T}\left(\frac{\partial}{\partial \chi}\langle H\rangle_e - \left\langle \frac{\partial H}{\partial \chi}\right\rangle_e\right), \tag{35}$$

which states that the entropy-variation is proportional to the difference between internal energy's variation and the ensemble average of $\frac{\partial H}{\partial \chi}$. The relation (35) was also obtained in [11], but in the different way. Substituting (5) into (35) yields

$$T\frac{\partial S}{\partial \chi} = \beta \frac{\partial}{\partial \beta}\left\langle \frac{\partial H}{\partial \chi}\right\rangle_e, \tag{36}$$

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

$$TS = \langle H\rangle_e - \int \left\langle \frac{\partial H}{\partial \chi}\right\rangle_e d\chi + C, \tag{37}$$

where C is an integration constant of parameters involved in H other than χ. From $F = U - TS$ and $\langle H\rangle_e = U$, we see the Helmholtz free energy is given by

$$F = \int \left\langle \frac{\partial H}{\partial \chi}\right\rangle_e d\chi - C. \tag{38}$$

Reforming (5) as

$$\left\langle \frac{\partial H}{\partial \chi}\right\rangle_e = \frac{1}{\beta}\int \frac{\partial \langle H\rangle_e}{\partial \chi} d\beta, \tag{39}$$

and using the integration formula

$$\int \frac{1}{e^{ax}-1}dx = \frac{1}{a}[\ln(e^{ax}-1) - ax], \tag{40}$$

we can find the first term $(b_1^\dagger b_1 + \frac{1}{2})$'s contribution

$$\begin{aligned}&\left\langle \left(b_1^\dagger b_1 + \frac{1}{2}\right)\right\rangle_e \\ &\quad = \left\langle \frac{\partial H}{\partial \Omega_1}\right\rangle_e = \frac{1}{\beta}\int d\beta \frac{\partial \langle H\rangle_e}{\partial \Omega_1}\end{aligned}$$

$$
\begin{aligned}
&= \left(-\frac{\Omega_1 \frac{R}{2} + \Omega_1 \Omega_2^2 + \Omega_2 G_1^2 + \Omega_2 G_2^2}{R\sqrt{S+R}} - \frac{-\Omega_1 \frac{R}{2} + \Omega_1 \Omega_2^2 + \Omega_2 G_1^2 + \Omega_2 G_2^2}{R\sqrt{S-R}}\right) \\
&\quad \times \frac{\exp(\beta A)}{1-\exp(\beta A)} \\
&\quad + \left(\frac{\Omega_1 \frac{R}{2} + \Omega_1 \Omega_2^2 + \Omega_2 G_1^2 + \Omega_2 G_2^2}{R\sqrt{S+R}} + \frac{\Omega_1 \frac{R}{2} - \Omega_1 \Omega_2^2 - \Omega_2 G_1^2 - \Omega_2 G_2^2}{R\sqrt{S-R}}\right) \\
&\quad \times \frac{\exp(\beta B)}{1-\exp(\beta B)} \\
&\quad - \frac{\Omega_1 \Omega_2^2 + \Omega_2 G_1^2 + \Omega_2 G_2^2 - \frac{1}{2} R\Omega_1}{R\sqrt{S-R}}. \qquad (41)
\end{aligned}
$$

Substituting (41) into (38) and letting χ be Ω_1, we finally derive the Helmholtz free energy of system

$$
\begin{aligned}
F &= \int \left\langle \frac{\partial H}{\partial \Omega_1} \right\rangle_e d\Omega_1 \\
&= -\frac{1}{\beta} \int \left(\frac{1}{1-x}\right) dx \bigg|_{x=\exp(\beta A)} - \frac{1}{\beta} \int \left(\frac{1}{1-y}\right) dy \bigg|_{y=\exp(\beta B)} + \int \frac{dz}{2} \bigg|_{z=\sqrt{S-R}} \\
&= \frac{1}{\beta} \ln(x-1) \bigg|_{x=\exp(\beta A)} + \frac{1}{\beta} \ln(y-1) \bigg|_{y=\exp(\beta B)} + \int \frac{dz}{2} \bigg|_{z=\sqrt{S-R}} \\
&= \frac{1}{\beta} \ln[(\exp(\beta A)-1)(\exp(\beta B)-1)] + \frac{\sqrt{S-R}}{2} \\
&= \frac{1}{\beta} \ln[(\exp(\beta A)-1)(\exp(\beta B)-1)] - \frac{A+B}{2}. \qquad (42)
\end{aligned}
$$

Further, the entropy is related to the internal energy by (37). Combinating (29) and (41) with (37), we have

$$
\begin{aligned}
S &= \frac{1}{T} \langle H \rangle_e - \frac{1}{T} \int \left\langle \frac{\partial H}{\partial \Omega_1} \right\rangle_e d\Omega_1 \\
&= -k \ln[(\exp(\beta A)-1)(\exp(\beta B)-1)] + \frac{1}{T} \frac{A e^{\beta A}}{e^{\beta A}-1} + \frac{1}{T} \frac{B e^{\beta B}}{e^{\beta B}-1}. \qquad (43)
\end{aligned}
$$

In summary, by virtue of the GHFT and the method of characteristics we have calculated some thermodynamic functions for the considered coupled anisotropic two-mode boson systems such as internal energy, Helmholtz free energy, and entropy in thermodynamics, which implies that GFHT is a new approach to directly calculate these thermodynamical functions. In addition, it is shown from [15] that using the GHFT the energy ensemble average of the mesoscopic LC circuits is derived as well.

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Appendix A: The Method of Characteristics

We will discuss in this appendix the method of characteristics [13, 14] as applied to first-order partial differential equations. Consider a function $u(x_1, x_2, \dots, x_n)$ of n independent variables $x_1, x_2, \dots, x_N$ and

$$P_1\frac{\partial u}{\partial x_1} + P_2\frac{\partial u}{\partial x_2} + \cdots + P_n\frac{\partial u}{\partial x_n} = R(x_1, x_2, \dots, x_n, u) \tag{A.1}$$

where $P_1, P_2, \dots, P_n$ are functions of $x_1, x_2, \dots, x_n$, then we have n ordinary differential equations

$$\frac{dx_1}{P_1} = \frac{dx_2}{P_2} = \cdots = \frac{dx_n}{P_n} = \frac{du}{R} \tag{A.2}$$

defining the characteristics. These can, in principle, be integrated and the general solution of (A.1) is found by making one of the n constants of integration an arbitrary function of the others.

Appendix B: Calculation of $\langle H|_{G_2=0}\rangle_e$

In order to calculate internal energy for Hamilton H, whose form is (16), in this appendix we firstly discuss its simple cases $G_2 = 0$ for the Hamiltonian

$$H = \Omega_1 b_1^\dagger b_1 + \Omega_2 b_2^\dagger b_2 + G_1(b_1^\dagger b_2 - b_1 b_2^\dagger), \tag{B.1}$$

where G_1 is a pure imaginary number. Substituting (B.1) into (3) and letting χ_i be Ω_1, Ω_1, G_1 respectively, we obtain

$$\left.\begin{aligned}
\frac{\partial\langle H\rangle_e}{\partial\Omega_1} &= \langle(1+\beta\langle H\rangle_e - \beta H)(b_1^\dagger b_1)\rangle_e,\\
\frac{\partial\langle H\rangle_e}{\partial\Omega_2} &= \langle(1+\beta\langle H\rangle_e - \beta H)(b_2^\dagger b_2)\rangle_e,\\
\frac{\partial\langle H\rangle_e}{\partial G_1} &= \langle(1+\beta\langle H\rangle_e - \beta H)(b_1^\dagger b_2 - b_1 b_2^\dagger)\rangle_e.
\end{aligned}\right\} \tag{B.2}$$

Let the eigenvector of H be $|\Psi_n\rangle$, $H|\Psi_n\rangle = E_n|\Psi_n\rangle$, with eigenvalue E_n, due to

$$\langle\Psi_n|[b_1^\dagger b_2 + b_1 b_2^\dagger, H]|\Psi_n\rangle = 0 \tag{B.3}$$

and

$$[b_1^\dagger b_2 + b_1 b_2^\dagger, H] = -(\Omega_1 - \Omega_2)(b_1^\dagger b_2 - b_1 b_2^\dagger) - 2G_1(b_1^\dagger b_1 - b_2^\dagger b_2), \tag{B.4}$$

as well as

$$\langle\Psi_n|[2G_1(b_1^\dagger b_1 - b_2^\dagger b_2) + (\Omega_1 - \Omega_2)(b_1^\dagger b_2 - b_1 b_2^\dagger)]|\Psi_n\rangle = 0, \tag{B.5}$$

we have

$$\langle(1+\beta\langle H\rangle_e - \beta H)[2G_1(b_1^\dagger b_1 - b_2^\dagger b_2) + (\Omega_1 - \Omega_2)(b_1^\dagger b_2 - b_1 b_2^\dagger)]\rangle_e = 0. \tag{B.6}$$

Combining (B.2) with (B.6), we obtain a partial differential equation for $\langle H\rangle_e$,

$$2G_1\left(\frac{\partial\langle H\rangle_e}{\partial\Omega_1}-\frac{\partial\langle H\rangle_e}{\partial\Omega_2}\right)+(\Omega_1-\Omega_2)\frac{\partial\langle H\rangle_e}{\partial G_1}=0 \tag{B.7}$$

on a characteristic curve, we therefore have, following (A.2)

$$\frac{d\Omega_1}{2G_1}=-\frac{d\Omega_2}{2G_1}=\frac{dG_1}{\Omega_1-\Omega_2}. \tag{B.8}$$

From the above equalities and carrying out the integrations we obtain two arbitrary constants as follows

$$\Omega_1+\Omega_2=C_1,\qquad \frac{G_1^2+\Omega_1\Omega_2}{2}=C_2. \tag{B.9}$$

We can apply the method of characteristics described above in which the general solution of (B.7) is found by writing $\langle H\rangle_e=f[C_1,C_2]$, that is

$$\langle H\rangle_e=f\left[(\Omega_1+\Omega_2),\frac{G_1^2+\Omega_1\Omega_2}{2}\right], \tag{B.10}$$

where the form f is to determined by considering the limiting case $G_1\to 0$, in this case H reduces to two independent oscillators, so

$$\begin{aligned}\langle H|_{G_1=0}\rangle_e&=f_2\left[(\Omega_1+\Omega_2),\frac{\Omega_1\Omega_2}{2}\right]\\&=\frac{\Omega_1}{e^{\beta\Omega_1}-1}+\frac{\Omega_2}{e^{\beta\Omega_2}-1}.\end{aligned} \tag{B.11}$$

Assuming $x=\Omega_1+\Omega_2$, $y=\frac{\Omega_1\Omega_2}{2}$, its reverse relation is $\Omega_1=\frac{x+\sqrt{x^2-8y}}{2}$, $\Omega_2=\frac{x-\sqrt{x^2-8y}}{2}$, then (B.11) becomes

$$f[x,y]=\frac{\frac{x+\sqrt{x^2-8y}}{2}}{\exp(\beta\frac{x+\sqrt{x^2-8y}}{2})-1}+\frac{\frac{x-\sqrt{x^2-8y}}{2}}{\exp(\beta\frac{x-\sqrt{x^2-8y}}{2})-1} \tag{B.12}$$

so the form of f is determined. Substituting (B.10) into this functional form (B.12) and identifying $x\to(\Omega_1+\Omega_2)$, $y\to\frac{G_1^2+\Omega_1\Omega_2}{2}$, $x^2-8y\to(\Omega_1-\Omega_2)^2-4G_1^2$, we find that the internal energy of Hamiltonian (B.1) is

$$\langle H\rangle_e=\frac{\tilde{A}}{e^{\beta\tilde{A}}-1}+\frac{\tilde{B}}{e^{\beta\tilde{B}}-1}, \tag{B.13}$$

where

$$\begin{aligned}\tilde{A}&=\frac{(\Omega_1+\Omega_2)+\sqrt{(\Omega_1-\Omega_2)^2-4G_1^2}}{2},\\ \tilde{B}&=\frac{(\Omega_1+\Omega_2)-\sqrt{(\Omega_1-\Omega_2)^2-4G_1^2}}{2}.\end{aligned} \tag{B.14}$$

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