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Statistical properties of the Hamiltonian generating phase state derived by using the generalized Hellmann–Feynman theorem

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ABSTRACT

We study statistical properties of the Hamiltonian $\left(H = \omega a^{\dagger}a + \kappa a^{\dagger}\sqrt{N+1} + \kappa\sqrt{N+1}a\right)$ generating phase state. Using the generalized Hellmann–Feynman theorem for ensemble average, we derive its mean energy and find the ratio of the mean energies contributed from the term $a^{\dagger}a$ to that from $a^{\dagger}\sqrt{N+1} + \kappa\sqrt{N+1}a$. The relation on the entropy-variation with respect to the dynamic parameters ω and κ is also examined.

1. Introduction

One of the major tasks in quantum statistics is to know the internal energy and energy distribution of a dynamical system. Feynman in his book "Statistical Mechanics" calculated average potential and kinetic energy of a harmonic oscillator [1]. In this work we consider statistical thermodynamics of an anharmonic oscillator whose Hamiltonian can generate phase state

$$H = \omega a^{\dagger}a + \kappa a^{\dagger}\sqrt{N+1} + \kappa\sqrt{N+1}a, \tag{1}$$

where $\left[a, a^{\dagger}\right] = 1$, a and $a^{\dagger}$ are bosonic annihilation and creation operators, respectively, $N = a^{\dagger}a$ is a number operator.

The aim of this paper is to study this Hamiltonian system (1) from the point of view of quantum statistics. We shall derive its mean (internal) energy and entropy-variation (with respect to the parameters ω and κ), we also evaluate the ratio of the mean energy contributed from the number term $a^{\dagger}a$ to that from the $a^{\dagger}\sqrt{N+1} + \kappa\sqrt{N+1}a$. To fulfill our task, we shall adopt a new approach, i.e., employ the generalized Hellmann–Feynman theorem (GHFT) (in the sense of ensemble average) and the method of characteristics.

Our paper is arranged as follows: In Section 2 we briefly review the GHFT for ensemble average $\langle H(\chi)\rangle_e$, where χ is some parameter involved in a Hamiltonian H, and the subscript e denotes ensemble average. The GHFT is the generalization of the Hellmann–Feynman theorem in the sense of pure state expectation. Moreover, based on von Neuman's definition of quantum entropy $S = -k\mathrm{tr}(\rho\ln\rho)$ and using the GHFT we present the entropy-variation formula showing how $\frac{\partial S}{\partial\chi}$ is related to $\frac{\partial}{\partial\chi}\langle H(\chi)\rangle_e$. In Section 3 we mention the anharmonic oscillator generating phase state and its Hamiltonian. In Section 4, we employ the GHFT to study statistical properties for the system described the Hamiltonian in Eq. (1), including internal energy, the average energy distribution and the entropy-variation.

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2. Brief review of the GHFT and the entropy-variation

The usual Hellmann–Feynman (HF) [2,3] theorem regarding to pure state expectation states

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

where H (a Hamiltonian which involves parameter χ) possesses the normalized 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 HF theorem to make the analytical calculation. However, this formula is only available for the pure state, while quantum statistical mechanics is the study of statistical ensemble described by a density matrix ρ, which is a non-negative, self-adjoint, trace-class operator of trace 1. Extending Eq. (2) to the ensemble average is of necessity [4–7].

For the mixed states in thermal equilibrium described by density operators

$$\rho = \frac{1}{Z} e^{-\beta H}, \quad \beta = (kT)^{-1}, \tag{3}$$

where $Z = \mathrm{tr}\left(e^{-\beta H}\right)$ is the partition function (k is the Boltzmann constant and T is the temperature), we have proposed the GHFT. Thus $\langle A\rangle_e \equiv \mathtt{tr}(\rho A)$ is the ensemble average of for arbitrary operator A, the mean energy is given by

$$\langle H(\chi)\rangle_e = \mathrm{tr}[\rho H(\chi)] = \frac{1}{Z(\chi)} \sum_j e^{-\beta E_j(\chi)} E_j(\chi) \equiv \bar{E}(\chi), \tag{4}$$

where the Hamiltonian H is independent of parameter χ. Performing the partial differentiation with respect to χ, we have

$$\frac{\partial \langle H\rangle_e}{\partial \chi} = \frac{1}{Z(\chi)} \left\{ \sum_j e^{-\beta E_j(\chi)} \left[-\beta E_j(\chi) + \beta \langle H\rangle_e + 1\right] \frac{\partial E_j(\chi)}{\partial \chi} \right\}. \tag{5}$$

Then using Eq. (2) we can further rewrite Eq. (5) as

$$\frac{\partial}{\partial \chi} \langle H\rangle_e = \left\langle (1 + \beta \langle H\rangle_e - \beta H) \frac{\partial H}{\partial \chi} \right\rangle_e, \tag{6}$$

which is the GHFT. Noting the relation

$$\left\langle H \frac{\partial H}{\partial \chi} \right\rangle_e = -\frac{\partial}{\partial \beta} \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e + \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e \langle H\rangle_e, \tag{7}$$

when H is independent of β, we can reform the GHFT into another form

$$\frac{\partial}{\partial \chi} \langle H\rangle_e = \frac{\partial}{\partial \beta} \left[\beta \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e\right] = \left(1 + \beta \frac{\partial}{\partial \beta}\right) \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e. \tag{8}$$

Performing the integration in Eq. (8) over $d\beta$ yields

$$\beta \left\langle \frac{\partial H(\chi)}{\partial \chi} \right\rangle_e = \int d\beta \frac{\partial}{\partial \chi} \langle H\rangle_e + K, \tag{9}$$

where K is an integration constant. Another way to perform integration in Eq. (8) is over $d\chi$, we see that

$$\langle H\rangle_e = \int_0^\chi \left(1 + \beta \frac{\partial}{\partial \beta}\right) \left\langle \frac{\partial H}{\partial \chi} \right\rangle_e d\chi + \langle H(0)\rangle_e, \tag{10}$$

Now we turn to the relation between entropy-variation of S with respect to χ. In classical statistical mechanics S is defined as $F = U - TS$, where T is the temperature, U is the system's internal energy or the ensemble average of Hamiltonian $\langle H\rangle_e$, and F is the Helmholtz free energy $F = -\frac{1}{\beta} \ln \sum_n e^{-\beta E_n}$. Then the entropy cannot 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,

$$S = -k\mathtt{tr}(\rho \ln \rho). \tag{11}$$

It is von Neuman 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. (11) assigns zero entropy to any pure state. However, in many