Energy average formula of photon gas rederived by using the generalised Hermann–Feynman theorem*

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By virtue of the generalised Hermann–Feynmam theorem we re-derive the energy average formula of photon gas. This is another useful application of the theorem.

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1. Introduction

It is common knowledge in the black-body radiation that the expectation value of a Planck oscillator of frequency ϖ_s is (excluding the zero-point energy term)

$$\bar{E}_s = \frac{\hbar\varpi_s}{\mathrm{e}^{\beta\hbar\varpi_s}-1}. \tag{1}$$

Historically, Planck derived this result in 1900 first by using thermodynamics and then by classical statistics.[1] Later in 1924 Bose[2] studied the question about the probability of energy level E_s $(=\hbar\varpi_s)$ occupied by n_s photons at a time, he found that the mean value of n_s is $1/(\mathrm{e}^{\beta\hbar\varpi_s}-1)$. Einstein, after reading Bose's paper, concluded that the basic fact to remember in the process of distributing the various photons over the various energy levels is that the photons are indistinguishable—a fact that had been implicitly taken care of in Bose's treatment (he essentially treated the light quanta as particles of a gas).[3] Planck and Bose–Einstein obtained the same mean photon number and mean energy formulas in different approaches. We then ask: is there any other method with which we can re-derive this formula? If so, then this method is worth paying attention in quantum statistics. The purpose of this work is to re-derive the energy average formula of photon gas by using the generalised Hermann–Feynman theorem (GHFT), a theorem that is about the ensemble average of mixed states. The rest of the present work is arranged as follows. In Section 2 we briefly review the GHFT. In Section 3 we apply the GHFT to the Bose oscillator Hamiltonian and employ the method of characteristics as well as L'Hopital's rule to re-derive Planck's formula.

2. Brief rewiew of GHFT

In quantum mechanics the usual Hermann–Feynman theorem[4,5] is for pure states, which states that

$$\frac{\partial E_j(\chi)}{\partial\chi} = \langle j|\frac{\partial H(\chi)}{\partial x}|j\rangle\ , \quad \langle j|j\rangle = 1\ , \tag{2}$$

where H is the Hamiltonian dependent on parameter χ; E_j and $|j\rangle$ are energy eigenvalues and eigenvectors of H, respectively. This theorem has been widely used in molecular physics, quantum chemistry and quantum statistics. Having noticed that Eq. (1) is just for pure state expectation value, we need a generalised Hellmann-Feynman theorem for mixed state in the sense of ensemble average in quantum statistics. In Ref. [6] the GHFT has been set up as

$$\frac{\partial}{\partial\chi}\langle H\rangle_{\mathrm{ea}} = \left\langle [1+\beta\langle H\rangle_{\mathrm{ea}} - \beta H]\frac{\partial H}{\partial\chi}\right\rangle_{\mathrm{ea}}\ , \tag{3}$$

where subscript ea represents ensemble average, $\beta = (\kappa T)^{-1}$, k is the Boltzmann constant, T denotes temperature, and $\langle A\rangle_{\mathrm{ea}} \equiv \mathrm{Tr}\left(\mathrm{e}^{-\beta H}A\right)/\mathrm{Tr}\left(\mathrm{e}^{-\beta H}\right)$ for arbitrary operator A. When H is β-independent, $\partial H/\partial\beta = 0$, Eq. (3) can be reformed into

$$\frac{\partial}{\partial\chi}\langle H\rangle_{\mathrm{ea}} = \frac{\partial}{\partial\beta}\left[\beta\left\langle\frac{\partial H}{\partial\chi}\right\rangle_{\mathrm{ea}}\right]\ . \tag{4}$$

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3. Re-derivation of formula (1)

Now for Bose oscillator Hamiltonian $H = \hbar\varpi a^+ a$, using (4) we see

$$\begin{aligned}\frac{\partial}{\partial\varpi}\langle H\rangle_{\rm ea} &= \frac{\partial}{\partial\beta}\left[\beta\left\langle\frac{\partial H}{\partial\varpi}\right\rangle_{\rm ea}\right]\\ &= \frac{\partial}{\partial\beta}\left[\beta\left\langle\hbar a^+ a\right\rangle_{\rm ea}\right]\\ &= \frac{\partial}{\varpi\partial\beta}\left[\beta\left\langle\hbar\varpi a^+ a\right\rangle_{\rm ea}\right]\\ &= \frac{\partial}{\varpi\partial\beta}\left[\beta\langle H\rangle_{\rm ea}\right]\\ &= \frac{1}{\varpi}\langle H\rangle_{\rm ea} + \frac{\beta\partial}{\varpi\partial\beta}\left[\langle H\rangle_{\rm ea}\right]\ , \end{aligned}\tag{5}$$

that is

$$\left(\varpi\frac{\partial}{\partial\varpi} - \beta\frac{\partial}{\partial\beta}\right)\langle H\rangle_{\rm ea} = \langle H\rangle_{\rm ea}\,,\tag{6}$$

which can be solved by the method of characteristics.[7] According to Eq. (6) we have the following equation:

$$\frac{{\rm d}\varpi}{\varpi} = -\frac{{\rm d}\beta}{\beta} = \frac{{\rm d}\langle H\rangle_{\rm ea}}{\langle H\rangle_{\rm ea}}\ .\tag{7}$$

It then yields two integration constants

$$\ln\varpi = -\ln\beta + C_1\ ,\quad \ln\langle H\rangle_{\rm ea} - \ln\varpi = C_2\ ,\tag{8}$$

which show that $\langle H\rangle_{\rm ea}$ is of the form

$$\langle H\rangle_{\rm ea} = \varpi F(\beta\varpi)\ ,\tag{9}$$

while the form of F is to be determined. Equation (9) can be confirmed by noting that

$$\varpi\frac{\partial}{\partial\varpi} = \frac{\partial}{\partial\ln\varpi}\ ,\quad \ln\varpi\equiv x\ ,\quad \ln\beta\equiv y\ ,\tag{10}$$

and rewriting Eq. (6) as

$$\left(\frac{\partial}{\partial x} - 1\right)\langle H\rangle_{\rm ea} = \frac{\partial}{\partial y}\left[\langle H\rangle_{\rm ea}\right]\ ,\tag{11}$$

whose solution is

$$\langle H\rangle_{\rm ea} = {\rm e}^x g(x+y) = \varpi F(\beta\varpi)\ .\tag{12}$$

In order to make sure of the concrete form of function F, we introduce $a = \left(X\sqrt{m\varpi/\hbar} + {\rm i}P/\sqrt{m\varpi\hbar}\right)\big/\sqrt{2}$, so up to a zero-point energy term,

$$H = \frac{P^2}{2m} + \frac{1}{2}m\varpi^2 X^2.\tag{13}$$

We see when $\varpi\to 0$, $H\to p^2/2m$ (free particle's Hamiltonian), Eq. (9) reduces to

$$\lim_{\varpi\to 0}\langle H\rangle_{\rm ea} = \lim_{\varpi\to 0}\varpi F(\beta\varpi)\ ,\tag{14}$$

so if $\lim\limits_{\varpi\to 0}\varpi F(\beta\varpi)$ is finite, then

$$\lim_{\varpi\to 0} F(\beta\varpi)\to\infty\ .\tag{15}$$

On the other hand, we recall the Bloch equation for density matrix $\boldsymbol{\rho}$ of a free particle[8]

$$-\frac{\partial\boldsymbol{\rho}(p,\beta)}{\partial\beta} = \frac{p^2}{2m}\boldsymbol{\rho}(p,\beta)\ ,\tag{16}$$

whose normalised solution is

$$\boldsymbol{\rho}(p,\beta) = \sqrt{\frac{\beta}{2m\pi}}\,{\rm e}^{-\beta p^2/(2m)}\ ,\quad {\rm Tr}\boldsymbol{\rho} = 1\ ,\tag{17}$$

so the energy average for $H_f = \dfrac{p^2}{2m}$ is

$$\begin{aligned}\langle H_f\rangle_{\rm ea} &= \left\langle\frac{p^2}{2m}\right\rangle_{\rm ea}\\ &= \sqrt{\frac{\beta}{2m\pi}}\int_{-\infty}^{\infty}\frac{p^2}{2m}\,{\rm e}^{-\beta p^2/(2m)}\,{\rm d}p\\ &= \sqrt{\frac{\beta}{2m\pi}}\left(-\frac{\partial}{\partial\beta}\right)\int_{-\infty}^{\infty}{\rm e}^{-\beta p^2/(2m)}\,{\rm d}p\\ &= \frac{1}{2\beta}\\ &= \frac{\kappa T}{2}\ . \end{aligned}\tag{18}$$

Combining Eqs. (14) and (18) (where there is $1/2\beta$), we see

$$\begin{aligned}\langle H_f\rangle_{\rm ea} &= \lim_{\varpi\to 0}\langle H\rangle_{\rm ea}\\ &= \lim_{\varpi\to 0}\varpi F(\beta\varpi)\\ &= 0\times\infty\\ &= \frac{1}{2\beta}\ , \end{aligned}\tag{19}$$

which implies that the application of L'Hopital's rule can converts an indeterminate form into a determinate form. Obviously,

$$\frac{1}{\beta} = \lim_{\varpi\to 0}\frac{\hbar}{\beta\hbar\,{\rm e}^{\beta\hbar\varpi}}\ .\tag{20}$$

It is known that with L'Hopital's rule one uses derivatives to help evaluate limits involving indeterminate forms (here we deal with $0\times\infty$), the easiest expression in which employing the L'Hopital's rule can approach to $\lim\limits_{\varpi\to 0}(\hbar/\beta\hbar\,{\rm e}^{\beta\hbar\varpi})$ is

$$\hbar\lim_{\varpi\to 0}\varpi\times\frac{1}{{\rm e}^{\beta\hbar\varpi}-1} = \lim_{\varpi\to 0}\frac{\hbar}{\beta\hbar\,{\rm e}^{\beta\hbar\varpi}}\ .\tag{21}$$

Comparing Eq. (21) with Eqs. (19) and (20) and considering Eq. (15) we can determine the form of $F(\beta\varpi)$ as

$$F(\beta\varpi) = \frac{1}{\mathrm{e}^{\beta\hbar\varpi} - 1} , \tag{22}$$

so from Eq. (12) it follows that $\langle H\rangle_{\mathrm{ea}} = \hbar\varpi/(\mathrm{e}^{\beta\hbar\varpi} - 1)$, that is to say, Eq. (1) is re-derived.

Besides, using the GHFT we can also present the following points:

1) average kinetic energy = average potential energy. To prove this, using expression (13) we have

$$[XP\,,\,H] = \mathrm{i}\frac{P^2}{m} - \mathrm{i}m\varpi^2X^2 . \tag{23}$$

Due to

$$\mathrm{Tr}\,(XPH) = \mathrm{Tr}\,(HXP) , \tag{24}$$

and

$$0 = \langle [XP\,,\,H]\rangle_{\mathrm{ea}} = \mathrm{i}\left\langle \frac{P^2}{m}\right\rangle_{\mathrm{ea}} - \mathrm{i}\left\langle m\varpi^2X^2\right\rangle_{\mathrm{ea}} , \tag{25}$$

we have

$$\begin{aligned}\langle H\rangle_{\mathrm{ea}} &= \left\langle \frac{P^2}{2m} + \frac{1}{2}m\varpi^2X^2\right\rangle_{\mathrm{ea}} \\ &= \left\langle \frac{P^2}{m}\right\rangle_{\mathrm{ea}} \\ &= \left\langle m\varpi^2X^2\right\rangle_{\mathrm{ea}} ,\end{aligned} \tag{26}$$

thus the kinetic energy average is equal to potential energy average.

2) Though H involves the mass, $\langle H\rangle_{\mathrm{ea}}$ is m independent. In fact, using Eqs. (2) and (25) we have

$$\begin{aligned}\frac{\partial}{\partial m}\langle H\rangle_{\mathrm{ea}} &= \frac{\partial}{\partial\beta}\left[\beta\left\langle\frac{\partial H}{\partial m}\right\rangle_{\mathrm{ea}}\right] \\ &= \frac{\partial}{\partial\beta}\left\langle\beta\left(\frac{\varpi^2}{2}X^2 - \frac{1}{2m^2}P^2\right)\right\rangle_{\mathrm{ea}} \\ &= 0 .\end{aligned} \tag{27}$$

In summary, we have re-derived the energy average formula of photon gas (Bose distribution) by using the GHFT, a fresh look at the known problem. This is another useful application of the theorem. The other applications can be seen in Refs. [8] and [9].

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