Letter

Quantum counterpart of equipartition theorem: A Möbius inversion approach

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The equipartition theorem is crucial in classical statistical physics, and recent studies have revealed its quantum counterpart for specific systems. This raises the question: does a quantum counterpart of the equipartition theorem exist for any given system, and if so, what is its concrete form? In this Letter, we employ the Möbius inversion approach to address these questions, providing a criterion to determine whether a system adheres to the quantum counterpart of the equipartition theorem. If it does, the corresponding distribution function can be readily derived. Furthermore, we construct the fermionic version of the criterion in a manner analogous to the bosonic case.

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Introduction. The equipartition theorem, a fundamental law in classical statistical physics, plays a crucial role in understanding the distribution of energy among the different degrees of freedom of a system in thermal equilibrium. Proposed in the late nineteenth century, the theorem provides a statistical basis for predicting the average energy associated with each degree of freedom in a classical system [1,2]. It forms a cornerstone in the bridge between the microscopic world of particles and the macroscopic observables of thermodynamics [3]. The equipartition theorem states that, in thermal equilibrium, the energy for the each degree of freedom is simply

$$E_i(T) = k_{\mathrm{B}}T/2, \tag{1}$$

where k_{B} is the Boltzmann constant and T the temperature. This theorem proves invaluable in understanding the behavior of gases, solids, and other classical systems, forming a foundation for the development of statistical mechanics [4–12].

Formally, by setting $\beta \equiv 1/(k_{\mathrm{B}}T)$, the inverse temperature, we may recast the classical equipartition theorem Eq. (1) as

$$E_i(\beta) = \mathbb{E}_i[\mathcal{E}(\omega, \beta)] := \int_0^\infty \mathrm{d}\omega\, \mathbb{P}_i(\omega)\mathcal{E}(\omega, \beta), \tag{2}$$

where E_i, the mean energy contributed by the ith degree of freedom, is expressed as the expectation ($\mathbb{E}_i[\bullet]$) of the energy density $\mathcal{E}(\omega, \beta)$ with respect to the distribution $\mathbb{P}_i(\omega)$. In the classical scenario, $\mathcal{E}(\omega, \beta) = 1/(2\beta)$, which is independent of ω. This together with the normalization condition, $\int_0^\infty \mathrm{d}\omega\, \mathbb{P}_i(\omega) = 1$, recovers Eq. (1).

Recently, many researchers [13–22] have tried to extend the classical equipartition theorem to the quantum regime with several models, such as electrical circuits [20], Brownian oscillators [13,14,23,24], dissipative diamagnetism [14,15], and considering kinetic energy for a more general setup [25]. The quantum counterpart of the equipartition theorem also acquires the form of Eq. (2), but now the energy density $\mathcal{E}(\omega, \beta)$ generally depends on ω. Though the energies of different degrees of freedom i differ from each other, the energy density $\mathcal{E}(\omega, \beta)$ is universal for all the degrees of freedom, representing the "equipartition" in the quantum sense [22]. In these researches, the systems are assumed to be quadratic and $\mathcal{E}(\omega, \beta)$ is set to be $(\hbar\omega/4)\coth(\hbar\beta\omega/2)$, which is the energy of the quantum harmonic oscillator in the equilibrium thermal state. This $\mathcal{E}$ can be reduced to the classical case Eq. (1) since $\lim_{\hbar\to 0}(\hbar\omega/4)\coth(\hbar\beta\omega/2) = 1/(2\beta)$, as explained below Eq. (2). The normalized distribution functions $\mathbb{P}_i(\omega)$ are also explicitly obtained in these quadratic systems [16,22]. Moreover, for the fermionic system, the quantum counterpart of the equipartition theorem is also investigated [17]. They altogether provide novel insights for the accurate and convenient evaluations of thermodynamic quantities [19,22,23].

For more general systems beyond the above-mentioned quadratic models, does the quantum counterpart of the equipartition theorem still hold? If so, how does one obtain the corresponding distribution function $\mathbb{P}_i(\omega)$? Answers to these questions will serve as a promising methodology for studying the quantum thermodynamics. This Letter aims to use a universal approach, the Möbius inversion, to answer these questions. It originates from the number theory [26] and has been used in various inverse problems in physics [27–29]. Based on the Möbius inversion, we give a criterion to determine whether the quantum counterpart of the equipartition theorem holds for a given system. Furthermore, it tells us how to obtain the distribution $P_{(\omega)}$ with this systematic approach. We refer the readers to the an intuitive figure (see Fig. 1) to have an overview of the idea presented in this Letter. We implement the proposed formulas to some typical models,

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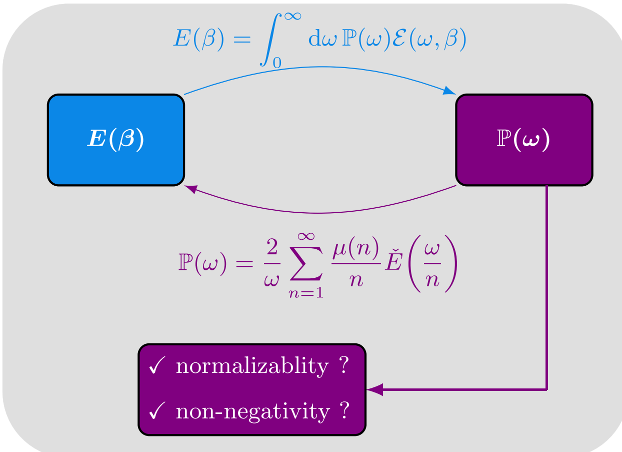

FIG. 1. An illustration for the interplay between energy spectrum $E(\beta)$ and distribution function $\mathbb{P}(\omega)$ with the help of Eqs. (2) and (7). The normalizability and non-negativity should also be checked for $\mathbb{P}(\omega)$.

including the free photon gas [30,31], the harmonic oscillator [32], the Riemann gas [33,34], and the Ising model [30,35]. It is worth noting that this method applies to both bosonic and fermionic scenarios.

Quantum counterpart of equipartition theorem for quadratic systems. As a prelude, we first briefly illustrate the quantum counterpart of the equipartition theorem with an example of a harmonic oscillator [13–16,18–24]. The quantum counterpart of the equipartition theorem was discussed in the scenario of open systems, whose simplest quadratic model reads

$$H_{\mathrm{T}} = H_{\mathrm{S}} + \sum_j \left[\frac{\hat{p}_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2\left(\hat{x}_j - \frac{c_j\hat{Q}}{m_j\omega_j^2}\right)^2\right] \tag{3}$$

with

$$H_{\mathrm{S}} = \frac{\hat{P}^2}{2M} + \frac{1}{2}M\Omega^2\hat{Q}^2. \tag{4}$$

This is the Calderia-Leggett model [36] describing a harmonic oscillator $(\hat{Q}, \hat{P})$ of mass M coupled to the heat bath $(\{\hat{x}_j, \hat{p}_j\})$. For the system oscillator, the kinetic energy and the potential energy are $E_{\mathrm{k}}(\beta) = \langle\hat{P}^2\rangle/(2M)$ and $E_{\mathrm{p}}(\beta) = M\Omega^2\langle\hat{Q}^2\rangle/2$, respectively. The average is defined over the total Gibbs state, i.e., $\langle\bullet\rangle := \mathrm{tr}[\bullet e^{-\beta H_{\mathrm{T}}}]/\,\mathrm{tr}\, e^{-\beta H_{\mathrm{T}}}$. For brevity, we set $\hbar = 1$ hereafter. It was shown [16,23] that both $E_{\mathrm{k}}(\beta)$ and $E_{\mathrm{p}}(\beta)$ can be expressed in the form of Eq. (2) with

$$\mathcal{E}(\omega,\beta) = \frac{\omega}{4}\coth\left(\frac{\beta\omega}{2}\right) \tag{5}$$

and

$$\mathbb{P}_{\mathrm{k}}(\omega) = \frac{2M\omega}{\pi}\,\mathrm{Im}\,J(\omega), \quad \mathbb{P}_{\mathrm{p}}(\omega) = \frac{2M\Omega^2}{\pi\omega}\,\mathrm{Im}\,J(\omega). \tag{6}$$

Here, $J(\omega)$ denotes the generalized susceptibility [23]. It was verified that $\mathbb{P}_{\mathrm{p,k}}(\omega)$ satisfies the normalized and non-negative condition [16,23]. In the classical limit $\hbar \to 0$, we have $\mathcal{E}(\omega,\beta) \to 1/(2\beta)$, which gives rise to the classical equipartition theorem Eq. (1). In the weak-coupling limit [23], $c_j \to 0$ for all j in Eq. (3), resulting in $\mathbb{P}_{\mathrm{p,k}}(\omega) \to \delta(\omega - \Omega)$. Besides, as explained in Refs. [19,22], the free energy $F(\beta)$ is expressed in the same form by simply switching $\mathcal{E}(\omega,\beta)$ into $\mathcal{F}(\omega,\beta) = \ln[2\sinh(\beta\omega/2)]/\beta$, which is the average free energy of the oscillator in the canonical ensemble. For more detailed discussions of general quadratic systems, we refer the readers to Ref. [22].

Möbius inversion approach. To explore the quantum counterpart of equipartition theorem for general systems, it is our task to find a non-negative and normalizable $\mathbb{P}(\omega)$ for each degree of freedom, given the energy spectrum $E(\beta)$. For brevity, we omit the label of degree of freedom hereafter. It will be shown below that for any given energy spectrum $E(\beta)$ from theoretical calculation or experimental measurement, if the quantum counterpart of the equipartition theorem is valid, then we have

$$\mathbb{P}(\omega) = \frac{2}{\omega}\sum_{n=1}^{\infty}\frac{\mu(n)}{n}\check{E}\left(\frac{\omega}{n}\right). \tag{7}$$

Here, $\check{f}(\omega) := \mathcal{L}^{-1}[f(\beta)]$ denotes the inverse Laplace transform of the function $f(\beta)$, and $\mu(n)$ is the celebrated Möbius function [26].

Let us look at Eq. (7) from another angle. To ensure the validity of the equipartition in the system with the spectrum $E(\beta)$, we first obtain $\mathbb{P}(\omega)$ from the right-hand side of Eq. (7). It is the next task to check its non-negativity. Furthermore, the normalizability requires that $\int_0^\infty \mathrm{d}\omega\,\mathbb{P}(\omega)$ converge to a finite positive number. This global constant, possibly dependent on the the size of the system, shall be absorbed into $\mathbb{P}(\omega)$ [22]. By substituting the normalized $\mathbb{P}(\omega)$ into Eq. (1), we obtain the quantum counterpart of the equipartition theorem. On the other hand, if the obtained $P(\omega)$ via Eq. (7) is without non-negativity and normalizability, we claim that there is no such quantum counterpart. In this sense, Eq. (7) supplies a sufficient and necessary condition to ascertain the presence of the quantum counterpart of the equipartition theorem. If the equipartition holds, Eqs. (2) and (7) further give a concrete expression of $\mathbb{P}(\omega)$.

Now we give a detailed derivation of the Eq. (7). First notice the following expansion:

$$\mathcal{E}(\omega,\beta) = \frac{\omega}{4}\left(2\sum_{n=1}^{\infty}e^{-n\beta\omega} + 1\right) \quad \text{for } \omega > 0. \tag{8}$$

By substituting it into Eq. (1), we obtain

$$E(\beta) = \sum_{n=1}^{\infty}\int_0^\infty \mathrm{d}\omega\,\frac{\omega}{2}\mathbb{P}(\omega)e^{-n\beta\omega} + \frac{1}{4}\int_0^\infty \mathrm{d}\omega\,\omega\mathbb{P}(\omega) \tag{9a}$$

$$= \sum_{n=1}^{\infty}\mathcal{L}\left[\frac{\omega}{2}\mathbb{P}(\omega)\right](n\beta). \tag{9b}$$

For the second term on the right-hand side of Eq. (9a), we note that $\lim_{\beta\to\infty}\mathcal{E}(\omega,\beta) = \omega/4$ and $E(\infty) = \int_0^\infty \mathrm{d}\omega\,\omega\mathbb{P}(\omega)/4$ [cf. Eq. (1)]. Therefore, one may absorb this term into the left-hand side of Eq. (9a) to redefine the energy spectrum as $E(\beta) - E(\infty)$ [cf. Eq. (9b)]. To proceed, we consult the modified Möbius inversion formula [27]: for two functions $f(x)$ and $g(x)$, we have

$$f(x)=\sum_{n=1}^{\infty}g(nx)\Longleftrightarrow g(x)=\sum_{n=1}^{\infty}\mu(n)f(nx). \tag{10}$$

By noticing that the right-hand side of Eq. (9b) is just a function with respect to $n\beta$, the Möbius inversion gives

$$\mathcal{L}\Big[\frac{\omega}{2}\mathbb{P}(\omega)\Big](\beta)=\sum_{n=1}^{\infty}\mu(n)E(n\beta), \tag{11}$$

which is equivalent to

$$\mathbb{P}(\omega)=\frac{2}{\omega}\sum_{n=1}^{\infty}\frac{\mu(n)}{n}\mathcal{L}^{-1}[E(\beta)]\Big(\frac{\omega}{n}\Big). \tag{12}$$

Here, we have used $\mathcal{L}^{-1}[E(n\beta)](\omega)=\mathcal{L}^{-1}[E(\beta)](\omega/n)/n$. Then we arrive at Eq. (7).

Typical examples. Let us turn to several examples to illustrate the procedure. Generally speaking, the asymptotic behavior of the energy spectrum at infinite temperature ($\beta=0$) plays a crucial role. Noting that $\mathcal{E}(\omega,\beta)\sim\beta^{-1}$ and $\mathbb{P}(\omega)$ is normalized, we thereby conclude from Eq. (1) that $E(\beta)\sim\beta^{-1}$ for any degree of freedom and so is the total energy. As a result, the quantum counterpart of the equipartition theorem does not hold in such as the Ising model [30,35] and the Riemann gas [33,34], whose energy spectrums converge to a finite real number when $\beta\to 0$. The same criterion also rules out the photon gas governed by the well-known Stefan-Boltzmann law in two and three dimensions, whose total energy spectrums asymptotically behave as β^{-3} and β^{-4}, respectively.

For generality, we set $E^{\rm tot}(\beta)=\int_0^\infty \mathrm{d}k\,A(k)\beta^{-k}$ with $A(k)$ being an undetermined function. The inverse Laplace transform of $E^{\rm tot}(\beta)$ reads $\check{E}^{\rm tot}(\omega)=\int_0^\infty \mathrm{d}k\,A(k)\Gamma(k)\omega^{k-1}$. The distribution function is evaluated to be $\mathbb{P}(\omega)=\int_0^\infty \mathrm{d}k\,A(k)\Gamma(k)\omega^{k-2}/\zeta(k)$ [cf. Eq. (7)]. Here, we used the property of the Möbius function [37], $\sum_{n=1}^\infty\mu(n)/n^s=1/\zeta(s)$ for $\mathrm{Re}\,s>1$, where $\zeta(s)$ is the Riemann zeta function. Therefore, the key point is to examine whether this distribution function satisfies the non-negativity and normalizability, which solely depends on the concrete form of $A(k)$. As a simple example, we choose $A(k)=C\delta(k-k_0)$ with a constant $C\in\mathbb{R}^+$. The resulting distribution function is $\mathbb{P}(\omega)=C\Gamma(k_0)\omega^{k_0-2}/\zeta(k_0)$, which cannot be normalized for $k_0=3,4$. This conclusion aligns with our previous analysis of photon gas.

We should emphasize here that the absence of the quantum counterpart of the equipartition theorem does not show any violation to the fundamental principles of quantum mechanics or statistical physics. One of the prerequisites is the energy spectrum behaving asymptotically as β^{-1} at high temperature, as discussed at the beginning of this paragraph. Therefore, not all real equilibrium necessarily should adhere to the quantum counterpart of the equipartition theorem.

Now turn to the linear superposition property. Assume that we have a set of energy spectrums $\{E_i(\beta)\}$, all of which follow the quantum counterpart of the equipartition theorem. We denote the corresponding distribution function as $\{\mathbb{P}_i(\omega)\}$. Due to the linear property of the inverse Laplace transform, the energy spectrum $E(\beta)=\sum_i\alpha_iE_i(\beta)$ also satisfies the quantum counterpart of the equipartition theorem with the distribution function $\mathbb{P}(\omega)=\sum_i\alpha_i\mathbb{P}_i(\omega)$, as long as all the coefficients $\{\alpha_i\}$ are non-negative. This distribution function shall be further normalized as $\mathbb{P}(\omega)=\sum_i\alpha_i\mathbb{P}_i(\omega)/\sum_i\alpha_i$. The present results are immediately followed by an example in which the energy spectrums are set to be $\{E_l(\beta)=\omega_0e^{-l\beta\omega_0}/(e^{\beta\omega_0}-1)\}$ with ω_0 a positive constant and l an integer. In this case, we have

$$\begin{aligned}\check{E}_l(\omega)&=\omega_0\mathcal{L}^{-1}\Bigg[\frac{e^{-(l+1)\beta\omega_0}}{1-e^{-\beta\omega_0}}\Bigg]=\omega_0\mathcal{L}^{-1}\Bigg[\sum_{n=l+1}^{\infty}e^{-n\beta\omega_0}\Bigg]\\&=\omega_0\sum_{n=l+1}^{\infty}\delta(\omega-n\omega_0).\end{aligned} \tag{13}$$

From Eq. (13) and Möbius inversion, we obtain the corresponding distribution function,

$$\begin{aligned}\mathbb{P}_l(\omega)&=\frac{2}{\omega}\sum_{n=l+1}^{\infty}\frac{\mu(n)}{n}\omega_0\sum_{m=1}^{\infty}\delta(\omega/n-m\omega_0)\\&=2\sum_{k=l+1}^{\infty}\sum_{n|k}\frac{\mu(n)}{k}\delta(\omega-k\omega_0)\\&=2\sum_{k=l+1}^{\infty}\frac{\delta_{k,1}}{k}\delta(\omega-k\omega_0),\end{aligned} \tag{14}$$

where $n|k$ means the integer n divides k. To obtain the last equality, we have used the identity $\sum_{n|k}\mu(n)=\delta_{k,1}$. For $l\leqslant 0$, the distribution function (14) directly reduces to $2\delta(\omega-\omega_0)$. For $l>0$, we have $\mathbb{P}_l(\omega)=0$. Due to the linear superposition property, we know that the spectrum

$$E(\beta)=\sum_{l\leqslant 0}\alpha_lE_l(\beta) \tag{15}$$

adheres to the quantum counterpart of the equipartition theorem with the distribution function

$$\mathbb{P}(\omega)=2\sum_{l\leqslant 0}\alpha_l\delta(\omega-\omega_0) \tag{16}$$

up to a normalization. Specifically, if we set $\alpha_l=1/4$ for $l=-1,0$ and $\alpha_l=0$ otherwise, Eq. (15) reduces to the spectrum of the quantum harmonic oscillator system:

$$E(\beta)=\frac{1}{4}[E_0(\beta)+E_{-1}(\beta)]=\frac{\omega_0}{4}\coth\frac{\beta\omega_0}{2} \tag{17}$$

with $\mathbb{P}(\omega)=\delta(\omega-\omega_0)$. This result also aligns with our expectation, since for the quantum harmonic oscillator we have from Eq. (2) that $(\omega_0/4)\coth(\beta\omega_0/2)=\int_0^\infty \mathrm{d}\omega\,\mathcal{E}(\omega,\beta)\delta(\omega-\omega_0)$.

Fermionic version. Here, we present the fermionic version of the quantum counterpart of the equipartition theorem and its Möbius inverse by analogy. Note that in the bosonic case, Eq. (2) can be recast as

$$\begin{aligned}E(\beta)&=\frac{1}{4}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\mathbb{P}(\omega)\frac{\omega}{e^{\beta\omega}-1}\\&=\frac{1}{4}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\mathbb{P}(\omega)\omega\rho^{\rm B}(\omega)\end{aligned} \tag{18}$$

with the even extension $\mathbb{P}(-\omega) = \mathbb{P}(\omega)$ for $\omega \geqslant 0$. The factor $\rho^{\mathrm{B}}(\omega) := 1/(e^{\beta\omega} - 1)$ is recognized as the expected number of bosonic particles with the energy ω. In the fermionic case, we just replace $\rho^{\mathrm{B}}(\omega)$ by $\rho^{\mathrm{F}}(\omega) = 1/(e^{\beta\omega} + 1)$ and obtain

$$[b]E^{\mathrm{F}}(\beta) = \frac{1}{4}\int_{-\infty}^{\infty} \mathrm{d}\omega\, \mathbb{P}^{\mathrm{F}}(\omega)\omega\rho^{\mathrm{F}}(\omega) = \int_{0}^{\infty} \mathrm{d}\omega\, \mathcal{E}^{\mathrm{F}}(\omega, \beta)\mathbb{P}^{\mathrm{F}}(\omega). \tag{19}$$

In the second equality, we have defined $\mathcal{E}^{\mathrm{F}}(\omega, \beta) := -(\omega/4)\tanh(\beta\omega/2)$ and set $\mathbb{P}^{\mathrm{F}}(-\omega) = \mathbb{P}^{\mathrm{F}}(\omega)$. This result is equivalent to that in [17].

To utilize the Möbius inversion, we follow a similar procedure to that in the bosonic case. First, we substitute the following series expansion,

$$\mathcal{E}^{\mathrm{F}}(\omega, \beta) = -\frac{\omega}{4}\left[2\sum_{n=1}^{\infty}(-1)^n e^{-n\beta\omega} + 1\right], \tag{20}$$

into the fermionic version Eq. (19), obtaining

$$E(\beta) = \sum_{n=1}^{\infty}\int_{0}^{\infty} \mathrm{d}\omega\, \frac{\omega}{2}\mathbb{P}(\omega)(-1)^{n-1}e^{-n\beta\omega} - \frac{1}{4}\int_{0}^{\infty} \mathrm{d}\omega\, \omega\mathbb{P}(\omega). \tag{21}$$

Since $\lim_{\beta\to\infty} \mathcal{E}^{\mathrm{F}}(\omega, \beta) = -\omega/4$, the second term in Eq. (21) is equal to $E(\infty)$, which can also be absorbed into $E(\beta)$ to redefine the energy spectrum. We have the following modified Möbius inversion formula for alternating series [38]:

$$g(x) = \sum_{n=1}^{\infty}(-1)^{n-1}f(nx) \Leftrightarrow f(x) = \sum_{n=1}^{\infty}\mu(n)\left[\sum_{m=1}^{\infty}2^{m-1}g(2^{m-1}nx)\right]. \tag{22}$$

Applying Eq. (22) to Eq. (21), we finally arrive at

$$\mathbb{P}(\omega) = \frac{2}{\omega}\sum_{n=1}^{\infty}\frac{\mu(n)}{n}\sum_{m=1}^{\infty}\check{E}\left(\frac{\omega}{2^{m-1}n}\right), \tag{23}$$

which is the desired fermionic version of the Möbius inversion.

Summary. In conclusion, we introduced the Möbius inversion to study the existence of a quantum counterpart to the equipartition theorem and derived the distribution function $\mathbb{P}(\omega)$ for a given system. Our approach has been applied to various systems, extending the analysis from bosons to fermions. Future work will explore additional connections between number theory and statistical physics, investigate nontrivial energy spectra in open quantum systems, and examine links between the quantum counterpart of the equipartition theorem and level statistics or random matrix theory [33,39,40].

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