On Quantum Equipartition Theorem for General Systems

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Does the quantum equipartition theorem truly exist for any given system? If so, what is the concrete form of such a theorem? The extension of the equipartition theorem, a fundamental principle in classical statistical physics, to the quantum regime raises these two crucial questions. In the present Letter, we focus on how to answer them for arbitray systems. For this propose, the inverse problem of the quantum equipartition theorem has been successfully solved. This result, termed as the inverse equipartition theorem, toghther with nonnegativity and normalizability of the distribution function $\mathbb{P}(\omega)$ serves as a criterion for determining whether a given system adheres to quantum equipartition theorem. If yes, the concrete form of the theorem can be readily obtained. Fermionic version of them is also discussed. Our results can be viewed as a general solution to the topics of quantum equipartition theorem.

Introduction. — The energy equipartition theorem (EET), 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 19th 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 EET states that, in thermal equilibrium, each degree of freedom contributes equally to the total energy of the system, and this contribution is on average $k_{\mathrm{B}}T/2$, 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, we may recast the classical EET as $[\beta \equiv 1/(k_{\mathrm{B}}T)]$

$$E_i(\beta) = \mathbb{E}_i[\mathcal{E}(\omega,\beta)] \coloneqq \int_0^\infty \mathrm{d}\omega\, \mathbb{P}_i(\omega)\mathcal{E}(\omega,\beta), \tag{1}$$

where E_i, the mean energy contributed by the i-th degree of freedom, is expressed as the expectation ($\mathbb{E}_i[...]$) of the energy density $\mathcal{E}(\omega,\beta)$ with respect to the distribution $\mathbb{P}_i(\omega)$. In classical the 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 the classical EET, $E_i(\beta) = k_{\mathrm{B}}T/2$.

Recently, many researches [13–22] try to extend the classical EET to the quantum regime with several models, such as the electrical circuits [15], the Brownian oscillators [16, 18, 19, 23], dissipative diamagnetism [19, 21]. The quantum EET also acquires the form of Eq. (1), but with the energy density $\mathcal{E}(\omega,\beta)$ generally depends on ω. Though the energy of different degree of freedom i differs from each other, the enenrgy density $\mathcal{E}(\omega,\beta)$ is univeral. This is the energy equipartition in quantum sense. In

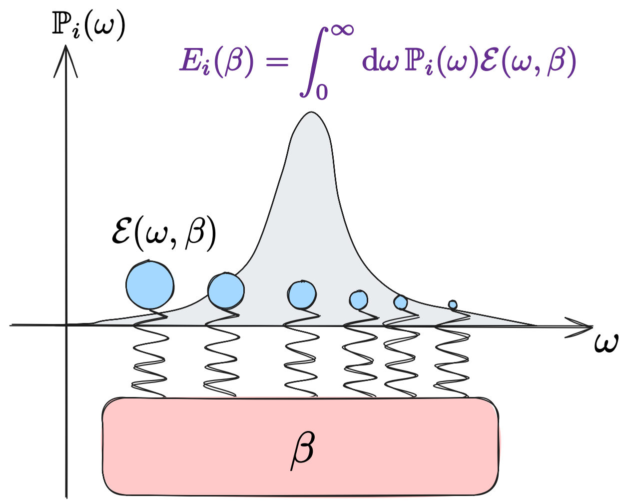

FIG. 1: A illustration for quantum energy partition theorem [cf. Equation (1)], where $\mathbb{P}_i(\omega)$ is the distribution and $\mathcal{E}(\omega,\beta)$ is the energy density.

these researches, the systems are assumed to be quadratic and $\mathcal{E}(\omega,\beta)$ is set to be $(\omega/2)\coth(\beta\omega/2)$, the energy of the quantum harmonic oscillator in equilibrium thermal state. The normalized distribution functions $\mathbb{P}_i(\omega)$ are obtained in these quadratic systems. Besides, the fermionic version of quantum EET theorem is also investigated, which enlarges the applicable range of the quantum EET [24]. They altogether provide novel insights into the application to the quantum EET for the accurate and convenient evaluations of thermodynamic quantities [13, 17, 23]. However, for more general systems beyond above mentioned quadratic models, does the quantum EET still hold? If so, how to obtain the corresponding distribution function $\mathbb{P}_i(\omega)$? The answers to these questions will serve as a promising methodology for studying the quantum thermodynamics. This Letter aims to provide a universal approach, the generalized

EET, to answering these questions. The involved key tool is the Möbius inversion formula. It originates from the number theory [25], and has been used in various inverse problems in physics [26–28]. Based on the Möbius inversion, we give a criterion to determine whether the quantum EET holds for a given quantum system. Furthermore, it tells us how to obtain the distribution $\mathbb{P}_i(\omega)$ in a systematic approach. We implement the proposed formalism to some typical models, including the free photon gas [29, 30], the harmonic oscillator [31], the Riemann gas [32, 33], and the Ising model [29, 34]. It is worth noting that our formalism applies to both the bosonic and fermionic scenarios.

Quantum EET for quadratic systems.— As a prelude, we first briefly review the quantum EET for quadratic systems [13–22], followed by an illustrative example. We will explain the relationship between the quantum EET and its classical counterpart. The quantum EET was discussed in the scenario of open system, whose simplest quadratic model reads

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

with

$$H_{\mathrm{S}} = \frac{\hat{P}^2}{2M} + \frac{1}{2}M\Omega^2\hat{Q}^2. \quad (3)$$

This is the Calderia-Leggett model [35] of an harmonic oscillator $(\hat{Q}, \hat{P})$ coupled to the heat bath $(\{\hat{x}_j, \hat{p}_j\})$. For the system oscillator, the kinetic energy $E_{\mathrm{k}}(\beta) := \langle\hat{P}^2\rangle/(2m)$ while the potential energy $E_{\mathrm{p}}(\beta) := M\Omega^2\langle\hat{Q}^2\rangle/2$. The average is defined over the total Gibbs state. It was shown that [14] both $E_{\mathrm{k}}(\beta)$ and $E_{\mathrm{p}}(\beta)$ can be expressed in the form of Eq. (1), where

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

and

$$\mathbb{P}_{\mathrm{k}}(\omega) = \frac{2M\omega}{\pi}\,\mathrm{Im}\,J(\omega), \quad \mathbb{P}_{\mathrm{p}}(\omega) = \frac{2M\Omega^2}{\pi\omega}\,\mathrm{Im}\,J(\omega). \quad (5)$$

Here, $J(\omega)$ denotes the generalized susceptibility [23]. It was verified that $\mathbb{P}_{\mathrm{p,k}}(\omega)$ satistifies the normalized condition [14, 23]. In the classical limit $\hbar \to 0$, $\mathcal{E}(\omega,\beta) \to 1/(2\beta)$, giving rise to the classical EET.

For the quadratic system [cf. Eq. (2)], the quantum EET exhibits the energy distribution of each degree of freedom with the energy density $\mathcal{E}(\omega,\beta)$. The latter shall be interpreted as the average potential or kinetic energy of a harmonic oscillator with frequency ω in the canonical ensemble. In the no coupling limit [23] [$\forall j, c_j = 0$ in Eq. (2)], $\mathbb{P}_{\mathrm{p,k}}(\omega) \to \delta(\omega - \Omega)$, where only the oscillation frequency Ω contributes. Besides, as explained in Ref. [13, 17], 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.

Inverse Energy Equipartition Theorem (IEET).— To explore the quantum EET 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 here and below. It is shown in this work that for any given energy specturm $E(\beta)$ from theoretical calculation or experimental measurement, if the quantum EET is valid, then

$$\mathbb{P}(\omega) = \frac{2}{\omega}\sum_{n=1}^{\infty}\frac{\mu(n)}{n}\check{E}\left(\frac{\omega}{n}\right). \quad (6)$$

Here, $\check{f}(\omega) \equiv \mathcal{L}^{-1}[f(\beta)]$ denotes the inverse Laplace transform of function $f(\beta)$, and $\mu(n)$ is the celebrated Möbius function [25]. Looking at Eq. (6) from another angle, to ensure the validity of the EET in the such system with the spectrum $E(\beta)$, we first obtain the $\mathbb{P}(\omega)$ from the right-hand-side of Eq. (6), it is the next task to check its non-negativity. Furthermore, normalizability requires $\int_0^\infty \mathrm{d}\omega\,\mathbb{P}(\omega)$ converge to a finite positive number. This global constant, possibly dependent on the the size of the system, shall be absorbed into $\mathbb{P}(\omega)$ [13]. By substituding the normalized $\mathbb{P}(\omega)$ into Eq. (1), we obtain the quantum EET. Otherwise, if the obtained $P(\omega)$ via Equation (6) is without non-negativity and normalizablity, we can claim there is no EET for such a system. In this sense, Eq. (6), termed as the inverse energy equipartition theorem (IEET) in this Letter, supplies a sufficient and necessary condition to ascertain the presence of the EET. If EET holds, IEET also gives the concrete expression of $\mathbb{P}(\omega)$.

Now we give a detailed derivation of the Eq. (6). First notice the following expansion

$$\mathcal{E}(\omega,\beta) = \frac{\omega}{4}\left[2\sum_{n=1}^{\infty}e^{-n\beta\omega} + 1\right], \quad (\omega > 0). \quad (7)$$

Substitute it into Eq. (1) and we obtain

$$E(\beta) = \sum_{n=1}^{\infty}\int_0^\infty \mathrm{d}\omega\,\frac{\omega}{2}\mathbb{P}(\omega)e^{-n\beta\omega} + \frac{1}{4}\int_0^\infty \mathrm{d}\omega\,\omega\mathbb{P}(\omega), \quad (8a)$$

$$\simeq \sum_{n=1}^{\infty}\mathcal{L}[\frac{\omega}{2}\mathbb{P}(\omega)](n\beta). \quad (8b)$$

For the second term on the right-hand-side of Eq. (8a), 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)]. To deal with Eq. (8b), we consult the modified Möbius inversion formula [36], i.e., for two functions $f(x)$ and $g(x)$

$$f(x) = \sum_{n=1}^{\infty}g(nx) \Longleftrightarrow g(x) = \sum_{n=1}^{\infty}\mu(n)f(nx). \quad (9)$$

By noticing the right-hand-side of Eq. (8b) is just a function with argument of $n\beta$, the Möbius inversion gives

$$\mathcal{L}[\frac{\omega}{2}\mathbb{P}(\omega)](\beta)=\sum_{n=1}^{\infty}\mu(n)E(n\beta), \tag{10}$$

or equivalently Equation (6), since $\mathcal{L}^{-1}[E(n\beta)](\omega)=n^{-1}\mathcal{L}^{-1}[E(\beta)](\omega/n)$. Equation (10) is equivalent to

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

Here, the symbol $\mathcal{L}^{-1}$ denotes the inverse Laplace transform and we used $\mathcal{L}^{-1}[E(n\beta)](\omega)\equiv\mathcal{L}^{-1}[E(\beta)](\omega/n)/n$. By introducing a simpler notation $\check{f}(\omega)\equiv\mathcal{L}^{-1}[f(\beta)](\omega)$, we arrive at Eq. (6).

Typical Examples.— Turn to several examples to illustrate the procedures to utilize the IEET. Generally speaking, the asymptotic behavior of the energy spectrum at infinite temperature ($\beta=0$) play crucial roles. Note $\mathcal{E}(\omega,\beta)\sim\beta^{-1}$ and $\mathbb{P}(\omega)$ is normalized, we conclude from Eq. (1) that $E(\beta)\sim\beta^{-1}$ for any degree of freedom and so is the total energy. As a result, quantum EET does *not* hold in such as the Ising model [29, 34] and the Riemann gas [32, 33], whose energy spectrum converges to be finite when $\beta\to0$. The same criterion also rules out the photon gas governed by the well-known Stefan–Boltzmann law in two or three dimensions, whose total energy spectrum diverges as β^{-3} and β^{-4}, respectively.

For generality we set $E^{\text{tot}}(\beta)=\int_0^\infty \mathrm{d}k\,A(k)\beta^{-k}$ with $A(k)$ being the undetermined function, whose inverse Laplace transform reads $\check{E}^{\text{tot}}(\omega)=\int_0^\infty \mathrm{d}k\,A(k)\Gamma(k)\omega^{k-1}$. The distribution function is evaluated to be [cf. Eq. (6)] $\mathbb{P}(\omega)=\int_0^\infty \mathrm{d}k\,A(k)\Gamma(k)\omega^{k-2}/\zeta(k)$. 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 testify whether this distribution function satisfies the nonnegativity and normalizability, which totally depends on the concrete form of $A(k)$. For a simple example we choose $A(k)=C\delta(k-k_0)$ with constant $C\in\mathbb{R}^+$, then $\mathbb{P}(\omega)=C\Gamma(k_0)\omega^{k_0-2}/\zeta(k_0)$, which cannot be normalized for $k_0=3,4$. This conclusion aligns with our previous analysis.

Now we turn to the linear superposition property of IEET. Assume that we have a set of energy spectrums $\{E_i(\beta)\}$, and all of which have quantum equipartition theorem. We denote the corresponding distribution function as $\{\mathbb{P}_i(\omega)\}$. Due to the linear property of inverse Laplace transform and integral, the energy spectrum $E(\beta)=\sum_i\alpha_iE_i(\beta)$ also satisfies the IEET 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 $\mathbb{P}(\omega)=\sum_i\alpha_i\mathbb{P}_i(\omega)/\sum_i\alpha_i$. This is immediately followed the example, where the energy spectrum reads $E_l(\beta)=\omega_0e^{-l\beta\omega_0}/\big(e^{\beta\omega_0}-1\big)$ with ω_0 denoting a positive constant and $l\in\mathbb{N}$. In this case, we have

$$\begin{aligned}\check{E}_l(\omega)&=\omega_0\mathcal{L}^{-1}\left[\frac{e^{-(l+1)\beta\omega_0}}{1-e^{-\beta\omega_0}}\right]=\omega_0\mathcal{L}^{-1}\left[\sum_{n=l+1}^{\infty}e^{-n\beta\omega_0}\right]\\&=\omega_0\sum_{n=l+1}^{\infty}\delta(\omega-n\omega_0).\end{aligned} \tag{12}$$

From Eq. (12) and IEET, we obtain the corresponding distribution function,

$$\begin{aligned}\mathbb{P}_l(\omega)&=\frac{2}{\omega}\sum_{n=l+1}^{\infty}\frac{\mu(n)}{n}\omega_0\sum_{m=1}^{\infty}\delta(\omega/n-m\omega_0)\\&=2\sum_{k=l+1}^{\infty}\sum_{n|k}\frac{\mu(n)}{k}\delta(\omega-k\omega_0)\\&=2\sum_{k=l+1}^{\infty}\frac{\delta_{k,1}}{k}\delta(\omega-k\omega_0).\end{aligned} \tag{13}$$

where $n|k$ means the integer n divide k. To obtain the last equality, we used the identity $\sum_{n|k}\mu(n)=\delta_{k,1}$. For $l\le0$, the distribution function (13) 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

$$E(\beta)=\sum_{l\le0}\alpha_lE_l(\beta) \tag{14}$$

is invertible with the distribution function

$$\mathbb{P}(\omega)=2\sum_{l\le0}\alpha_l\delta(\omega-\omega_0), \tag{15}$$

up to a normalization. Specifically, if we set $\alpha_l=1/4$ for $l=-1,0$ and $\alpha_l=0$ otherwise, Eq. (14) is the spectrum of the quantum harmonic oscillator system:

$$E(\beta)=\frac{1}{4}[E_0(\beta)+E_{-1}(\beta)]=\frac{\omega_0}{4}\coth\frac{\beta\omega_0}{2}, \tag{16}$$

with $\mathbb{P}(\omega)=\delta(\omega-\omega_0)$.

Fermionic IEET.— Here we present the fermionic version of the quantum EET and its inverse via analogy. Note that in bosonic case, the quantum EET can be recast as

$$\begin{aligned}E(\beta)&=\frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\mathbb{P}(\omega)\frac{\omega}{e^{\beta\omega}-1}\\&\equiv\frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\mathbb{P}(\omega)\omega\rho^{\text{B}}(\omega),\end{aligned} \tag{17}$$

with the even extension $\mathbb{P}(-\omega)=\mathbb{P}(\omega)$. The factor $\rho^{\text{B}}\equiv1/(e^{\beta\omega}-1)$ is recognized as the expected number of bosonic particles with the energy ω. In fermionic case, we just replace $\rho^{\text{B}}(\omega)$ by $\rho^{\text{F}}(\omega)=1/(e^{\beta\omega}+1)$. This result is equivalent to that in [24].

To obtain the inverse EET, we follow a similiar procedures as in the bosonic case. Firstly, we substitute the following series expansion,

$$\mathcal{E}^{\mathrm{F}}(\omega,\beta) = -\frac{\omega}{4}\left[2\sum_{n=1}^{\infty}(-1)^n e^{-n\beta\omega}+1\right], \tag{18}$$

into the fermionic EET, obtaining

$$\begin{aligned} E(\beta) = &\sum_{n=1}^{\infty}\int_0^{\infty}\mathrm{d}\omega\,\frac{\omega}{2}\mathbb{P}(\omega)(-1)^{n-1}e^{-n\beta\omega} \\ &-\frac{1}{4}\int_0^{\infty}\mathrm{d}\omega\,\omega\mathbb{P}(\omega). \end{aligned} \tag{19}$$

Since $\lim_{\beta\to\infty}\mathcal{E}^{\mathrm{F}}(\omega,\beta) = -\omega/4$, the second term in Eq. (19) equals $E(\infty)$, which can also be absorbed into $E(\beta)$ to redefine the energy specturm. Applying the modified Möbius inversion formula for alternating series [40],

$$\begin{aligned} g(x) &= \sum_{n=1}^{\infty}(-1)^{n-1}f(nx) \\ \Leftrightarrow f(x) &= \sum_{n=1}^{\infty}\mu(n)\left[\sum_{m=1}^{\infty}2^{m-1}g(2^{m-1}nx)\right], \end{aligned} \tag{20}$$

to Eq. (19), we finally obtain

$$\mathbb{P}(\omega) = \frac{2}{\omega}\sum_{n=1}^{\infty}\frac{\mu(n)}{n}\sum_{m=1}^{\infty}\check{E}(\frac{\omega}{2^{m-1}n}), \tag{21}$$

which is termed as the fermionic inverse EET.

Summary.— In conclusion, we have developed the inverse equipartition theorem to establish the existence of a quantum equipartition theorem and derive the distribution function $\mathbb{P}(\omega)$ for a given system. Our theorem is applied to various systems, and we have extended the bosonic quantum equipartition theorem to fermions. Future work includes exploring additional connections between number theory and statistical physics, investigating nontrivial energy spectra in open quantum systems, and exploring links between the quantum EET and level statistics or random matrix theory [32, 41, 42].

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