Solvable model of quantum microcanonical states

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Abstract. This letter examines the consequences of a recently proposed modification of the postulate of equal *a priori* probability in quantum statistical mechanics. This modification, called the *quantum microcanonical postulate* (QMP), asserts that for a system in microcanonical equilibrium all pure quantum states having the same energy expectation value are realised with equal probability. A simple model of a quantum system that obeys the QMP and that has a nondegenerate spectrum with equally spaced energy eigenvalues is studied. This model admits a closed-form expression for the density of states in terms of the energy eigenvalues. It is shown that in the limit as the number of energy levels approaches infinity, the expression for the density of states converges to a δ function centred at the intermediate value $(E_{\rm max}+E_{\rm min})/2$ of the energy. Determining this limit requires an elaborate asymptotic study of an infinite sum whose terms alternate in sign.

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1. Introduction

This letter investigates a generalization of the usual definition of a quantum system in microcanonical equilibrium. If the Hamiltonian H that describes a system has a nondegenerate spectrum, then according to the standard definition of quantum microcanonical equilibrium the system must be in one of the eigenstates of H. This requirement is known as the *postulate of equal a priori probabilities* [1]. We emphasize that according to the definition of microcanonical equilibrium in Ref. [1] the state of such a system cannot be a linear combination of eigenstates of H. However, if H has a degenerate spectrum, then the density matrix that describes a system of energy E in microcanonical equilibrium contains all states $|E,k\rangle$ of the degenerate energy E with equal weight: $\frac{1}{n}\sum_{k=1}^{n}|E,k\rangle\langle E,k|$, where n is the number of states having energy E.

Because the standard definition of quantum microcanonical equilibrium only allows the system to have energies that are eigenvalues of H, an alternative, less restrictive definition has recently been introduced [2]. By this latter definition, called the *quantum microcanonical postulate* (QMP), a state of a system in microcanonical equilibrium can have an energy that is *not* an eigenvalue of H. The discussion in Ref. [2] of quantum systems obeying the QMP is qualitative. Here, we give a quantitative analysis of a quantum system described by a Hamiltonian having a nondegenerate, equally spaced spectrum. Assuming that the system is in microcanonical equilibrium and that it obeys the QMP, we study the behaviour of the density of states $\mu(E)$ as the number of energy levels becomes large.

This letter is organised as follows: In Sec. 2 we review the representation for the density of states $\mu(E)$ in terms of the energy eigenvalues as outlined in Ref. [2]. We then define the model investigated in this letter in which the energy spectrum is taken to be nondegenerate and to grow linearly: $E_k \propto k$. In the next two sections we investigate the behaviour of $\mu(E)$ as the number of states of H becomes infinite. In Sec. 3 we show that $\mu(E)$ integrates to unity. Section 4 presents an asymptotic study of $\mu(E)$ as the number of states becomes infinite. On the basis of the analysis given in Secs. 3 and 4, we conclude that $\mu(E)$ approaches $\delta[E-(E_{\rm max}+E_{\rm min})/2]$.

2. Definition of the model

Let us review briefly the general mathematical framework proposed in Ref. [2] for describing the density matrix of a mixed state of a quantum system in microcanonical equilibrium. Consider a quantum system defined on an $(n+1)$-dimensional Hilbert space $\mathcal{H}$. Let Z^α $(\alpha=0,1,2,\ldots,n)$ be a typical element of $\mathcal{H}$ and let H^α_β denote the Hamiltonian with eigenvalues E_i $(i=0,1,2,\ldots,n)$. Then, the expectation value of the Hamiltonian in the state Z^α is $\langle H\rangle = \bar{Z}_\alpha H^\alpha_\beta Z^\beta/\bar{Z}_\gamma Z^\gamma$. Assume that in microcanonical equilibrium all states Z^α satisfying the condition $\langle H\rangle = E$ are realised with equal probability. Then, the corresponding unnormalised density of states $\Omega(E)$ is

$$\Omega(E)=\frac{1}{\pi}\int_{\mathcal{H}} {\rm d}^{n+1}\bar{Z}\,{\rm d}^{n+1}Z\,\delta(\bar{Z}_\alpha Z^\alpha-1)\,\delta\left(\frac{\bar{Z}_\alpha H^\alpha_\beta Z^\beta}{\bar{Z}_\gamma Z^\gamma}-E\right). \tag{1}$$

The constraint $\delta(\bar{Z}_\alpha Z^\alpha-1)$ in (1) arises because one is only interested in the unit normalised states, and the factor of π reflects the additional redundant overall phase of the state. It is convenient to use the standard integral representation $\delta(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}{\rm d}\lambda\, e^{-{\rm i}\lambda x}$ for each of the δ functions appearing in (1). The Hilbert-space integration then becomes Gaussian in the Z variables leaving the expression

$$\Omega(E)=\frac{1}{\pi}(-{\rm i}\pi)^{n+1}\int_{-\infty}^{\infty}\frac{{\rm d}\nu}{2\pi}\int_{-\infty}^{\infty}\frac{{\rm d}\lambda}{2\pi}\,e^{{\rm i}(\lambda+\nu E)}\prod_{l=0}^{n}\frac{1}{\lambda+\nu E_l}. \tag{2}$$

Assuming that the energy spectrum is nondegenerate, one can perform the λ integration to obtain

$$\Omega(E)=\pi^n\sum_{k=0}^{n}\int_{-\infty}^{\infty}\frac{{\rm d}\nu}{2\pi}\frac{e^{-{\rm i}\nu(E_k-E)}}{({\rm i}\nu)^n}\prod_{l=0,\neq k}^{n}\frac{1}{E_l-E_k}. \tag{3}$$

The remaining ν integration can now be performed explicitly to give

$$\Omega(E)=(-\pi)^n\sum_{k=0}^{n}\delta^{(-n)}(E_k-E)\prod_{l=0,\neq k}^{n}\frac{1}{E_l-E_k}, \tag{4}$$

where $\delta^{(-n)}(x)$ denotes the nth integral of the δ function:

$$\delta^{(-n)}(x) = \begin{cases} 0 & (x < 0), \\ \frac{1}{(n-1)!}\, x^{n-1} & (x \geq 0). \end{cases} \tag{5}$$

The density of states $\Omega(E)$ as defined in (1) is normalised by dividing it by the volume of the subspace of $\mathcal{H}$ spanned by states having unit length: $\bar{Z}_\alpha Z^\alpha = 1$. This gives the normalised microcanonical state density function $\mu(E)$. The volume is given by $\pi^n/n!$ (see, for example, Ref. [3]). Thus, $\mu(E) = n!\,\pi^{-n}\,\Omega(E)$ gives the density of states that satisfies the normalisation condition $\int_{-\infty}^{\infty} \mathrm{d}E\,\mu(E) = 1$.

In this letter we propose a particular QMP model in which the energy spectrum rises linearly and is given by $E_k = k$. Our objective is to study the behaviour of $\mu(E)$ as the number of energy levels becomes infinite. With this linear choice of spectrum the normalised density of states becomes

$$\mu(E) = (-1)^n n \sum_{k>[E]}^{n} \frac{(-1)^k\,(k-E)^{n-1}}{k!(n-k)!}, \tag{6}$$

where the notation $[E]$ indicates the largest integer less than or equal to E.

It is now convenient to rescale the energy spectrum so that the range of the energy lies in the interval $[0,1]$ for each n. Upon rescaling, (6) transforms to

$$\mu(E) = (-1)^{n+1} n^2 \sum_{k=0}^{[nE]} \frac{(-1)^k (k-nE)^{n-1}}{k!(n-k)!}, \tag{7}$$

where $E \in [0,1]$ for all n. To derive this result we have used the fact that the sum in (6) vanishes when the summation range is taken from $k=0$ to $k=n$.

In Fig. 1 we plot the density of states $\mu(E)$ in (7) for $n = 3$, 6, and 9. This graph suggests that $\mu(E)$ converges to a δ function centred at $E = 1/2$ as n, the number of energy levels, increases. We show analytically that the density of states $\mu(E)$ associated with a quantum system having the spectrum $E_k \propto k$ does indeed approach $\delta(E-1/2)$ in the limit $n \to \infty$. Our analysis is of interest because it involves an asymptotic study of an infinite sum whose terms alternate in sign. To overcome the difficulties associated with this alternating series, we convert the series to a double contour integration whose asymptotic behaviour is obtained using the method of steepest descent. This work also provides a new limit identity for the Dirac δ function.

3. Analysis of the model

To verify that $\mu(E)$ approaches $\delta(E-1/2)$ as the number of states n approaches infinity, we must establish two properties of $\mu(E)$. First, we must show that $\int_{-\infty}^{\infty} \mathrm{d}E\,\mu(E) = 1$. Second, we must show that the limiting value of $\mu(E)$ is zero except at $E = 1/2$ where it tends to infinity. In this section we show that the normalisation condition satisfied by $\mu(E)$ in (7) is valid. Let us define I by $I = \int_0^1 \mathrm{d}E\,\mu(E)$. The summation in (7) must be evaluated piecewise because of the dependence of the summation range on E. Thus,

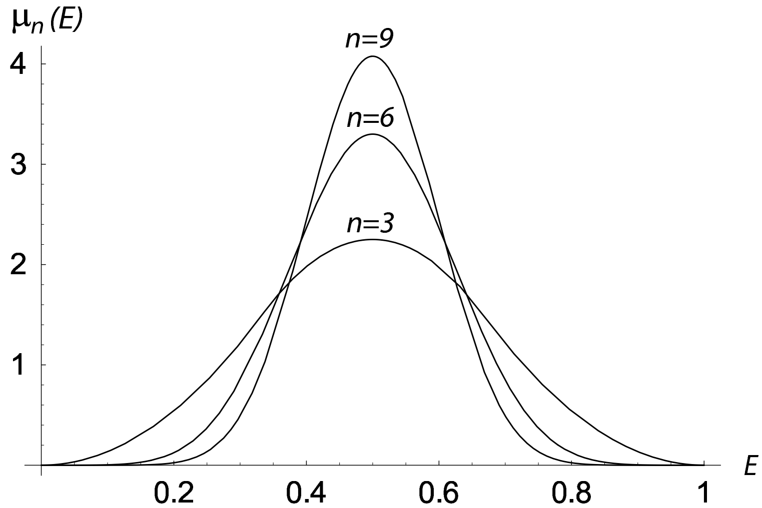

Figure 1. The density of states $\mu_n(E)$ associated with a quantum system having a linear energy spectrum $E_k = k$, where the range of the energy is suitably rescaled so that E lies in the range $[0, 1]$ for all n. Plots of $\mu_n(E)$ are given for 4-, 7-, and 10-state ($n = 3$, 6, and 9) systems. Observe that as the number of energy levels increases, the distribution becomes more peaked at the centre $E = 1/2$, suggesting that as the number of energy levels approaches infinity, the distribution approaches $\delta(E - 1/2)$. The analysis in Secs. 3 and 4 verifies that this is indeed the case.

it is convenient to decompose the integration range of I into n intervals and to write

$$I = (-1)^{n+1} n^2 \sum_{j=1}^{n} \int_{(j-1)/n}^{j/n} \mathrm{d}E \sum_{k=0}^{[nE]} \frac{(-1)^k (k - nE)^{n-1}}{k!(n-k)!}. \tag{8}$$

To perform the integration over E we rewrite the summation in the integrand so that it is independent of E. Given that j ranges from 1 to n and that k ranges from 0 to $n - 1$ with $k \leq j - 1$, we have

$$\begin{aligned} I &= (-1)^{n+1} n^2 \sum_{j=1}^{n} \sum_{k=0}^{j-1} \int_{(j-1)/n}^{j/n} \mathrm{d}E \frac{(-1)^k (k - nE)^{n-1}}{k!(n-k)!} \\ &= (-1)^{n+1} n^2 \sum_{j=1}^{n} \sum_{k=0}^{j-1} \frac{(-1)^k}{k!(n-k)!} \left. \frac{(k - nE)^n}{n(-n)} \right|_{E=(j-1)/n}^{j/n}. \end{aligned} \tag{9}$$

We now interchange the order of summation according to $\sum_{j=1}^{n} \sum_{k=0}^{j-1} = \sum_{k=0}^{n} \sum_{j=k+1}^{n}$:

$$I = \sum_{k=0}^{n-1} \frac{(-1)^k}{k!(n-k)!} \sum_{j=k+1}^{n} \left[(j-k)^n - (j-k-1)^n \right]. \tag{10}$$

Performing the sum over j, we obtain

$$I = \sum_{k=0}^{n} \frac{(-1)^k}{k!(n-k)!} (n-k)^n = \frac{(-1)^n}{n!} \sum_{k=0}^{n} (-1)^k \binom{n}{k} (k-n)^n. \tag{11}$$

Observe that the summation in (11) is the nth discrete difference of k^n. Recall that for the polynomial $f(k) = k^n +$ lower powers, the first discrete difference is

$\mathcal{D}f(k) = f(k) - f(k-1) = nk^{n-1} +$ lower powers. The second discrete difference is $\mathcal{D}^2 f(k) = f(k) - 2f(k-1) + f(k-2) = n(n-1)k^{n-2} +$ lower powers, and so on. The nth discrete difference is especially simple because there are no remaining lower powers: $\mathcal{D}^n f(k) = n!$. This observation allows us to evaluate the sum in (11) :

$$\sum_{k=0}^{n} \binom{n}{k} (-1)^k k^n = (-1)^n n!. \tag{12}$$

We have thus verified the normalization condition $I = 1$.

4. Asymptotic behaviour of (7) for large n

We now examine the behaviour of $\mu(E)$ in the limit as $n \to \infty$. We have already shown in Sec. 3 that the integral of $\mu(E)$ is unity. To show that $\mu(E)$ approaches a delta function as $n \to \infty$ we must establish that $\mu(E)$ becomes singular at the central value $E = \frac{1}{2}(E_{\rm max} + E_{\rm min})$ and that it vanishes at all other points in this limit. Note that by the scaling used in (7) the central value is at $E = 1/2$.

The representation of $\mu(E)$ in (7) for finite values of n is symmetric about the point $E = 1/2$. To verify this symmetry we make the transformation $E \to 1 - E$ and replace the summation variable k by $n - k$. Thus, we need only study the behaviour of $\mu(E)$ for $E = 1/\alpha$, where $\alpha \geq 2$. Without loss of generality, we set $n = \alpha J$, where J is a large integer, and let $\omega_J(\alpha)$ be the value of $\mu(E)$ at $E = 1/\alpha$:

$$\omega_J(\alpha) = \alpha^2 J^2 \sum_{k=0}^{J} \frac{(-1)^k (J-k)^{\alpha J - 1}}{k!(\alpha J - k)!}. \tag{13}$$

It is straightforward to find the behaviour of $\omega_J(\alpha)$ for large J when $\alpha > e$. Using Stirling's formula for the asymptotic behaviour of the factorial function, we observe that each term in the sum in (13) is exponentially small; that is, it has the form e^{-AJ} $(J \to \infty)$, where A is a positive constant. The number of terms in the sum grows linearly with J. Thus, the sum vanishes as $J \to \infty$.

However, when $2 \leq \alpha \leq e$, the terms in the sum (13) are exponentially large. In this case, the factor of $(-1)^k$ in the summand gives rise to a deep global cancellation among all the terms in the sum. When $\alpha > 2$, this cancellation causes $\omega_J(\alpha)$ to vanish exponentially for large J. The case $\alpha = 2$ is special because the sum does not vanish exponentially. We have performed the sum on the right side of (13) numerically for large values of J when $\alpha = 2$ using Richardson extrapolation [4]. We find that

$$\omega_J(2) \sim (1.9544100476\ldots)\sqrt{J} \quad (J \to \infty). \tag{14}$$

Establishing these asymptotic results analytically is difficult. Laplace's method for sums cannot be used to evaluate $\omega_J(\alpha)$ because Laplace's method involves local analysis and this method is inadequate when terms in the sum alternate in sign.

To overcome this difficulty we convert the sum in (13) to a double complex contour integral. We begin by substituting $k = J - p$:

$$\omega_J(\alpha) = \alpha^2 J^2 \sum_{p=1}^{J} \frac{(-1)^{J+p} p^{\alpha J - 1}}{\Gamma(J-p+1)\Gamma[(\alpha-1)J+p+1]}. \tag{15}$$

We then use the identity $\frac{1}{\Gamma(z)} = \frac{1}{2\pi \mathrm{i}} \oint_C \mathrm{d}t\, e^t t^{-z}$ to represent the Γ functions in (15). The contour C is infinite and encloses the negative real-t axis; C can be taken to be a circle around the origin when α is an integer. Rescaling the integration variable t gives

$$\omega_J(\alpha) = (-1)^J \frac{\alpha^2 J^2}{(2\pi \mathrm{i})^2} \oint_C \oint_{C'} \mathrm{d}r\, \mathrm{d}s\, r^{-(\alpha-1)J-1} s^{-J-1} \sum_{p=1}^{J} \frac{1}{p} \left(-\frac{s}{r} e^{r+s}\right)^p, \tag{16}$$

where we have interchanged orders of integration and summation.

Integrating (16) by parts with respect to r, we obtain

$$\omega_J(\alpha) = (-1)^J \frac{\alpha^2 J}{(2\pi \mathrm{i})^2} \oint_C \oint_{C'} \frac{\mathrm{d}r}{r} \frac{\mathrm{d}s}{s} r^{-(\alpha-1)J} s^{-J} \frac{r-1}{\alpha-1} \sum_{p=1}^{J} \left(-\frac{s}{r} e^{r+s}\right)^p. \tag{17}$$

We also integrate (16) by parts with respect to s:

$$\omega_J(\alpha) = (-1)^J \frac{\alpha^2 J}{(2\pi \mathrm{i})^2} \oint_C \oint_{C'} \frac{\mathrm{d}r}{r} \frac{\mathrm{d}s}{s} r^{-(\alpha-1)J} s^{-J} (s+1) \sum_{p=1}^{J} \left(-\frac{s}{r} e^{r+s}\right)^p. \tag{18}$$

We then evaluate the finite geometric sums in (17) and (18) using the identity $\sum_{p=1}^{J} a^p = (a^{J+1} - a)/(a-1)$, where $a = -e^r e^s s/r$. The representation for $\omega_J(\alpha)$ simplifies when we combine the right side of (17) multiplied by $(\alpha-1)/\alpha$ and the right side of (18) multiplied by $1/\alpha$, and then replace s by $-s$:

$$\omega_J(\alpha) = \frac{\alpha J}{(2\pi \mathrm{i})^2} \oint_C \oint_{C'} \mathrm{d}r\, \mathrm{d}s\, (s-r) r^{-\alpha J - 1} e^r \frac{e^{J(r-s)} - r^J s^{-J}}{s e^r - r e^s}. \tag{19}$$

The term proportional to $e^{J(r-s)}$ in the integrand of (19) is analytic in s along the real-s axis for $s \leq 0$. Hence, by shrinking the contour to a small circle about the origin in the complex-s plane, we find that the integrand does not contribute to the asymptotic behaviour of (19) for large J. We have thus reduced the expression for $\omega_J(\alpha)$ to

$$\omega_J(\alpha) = \frac{\alpha J}{(2\pi \mathrm{i})^2} \oint_C \mathrm{d}r\, r^{-(\alpha-1)J-1} \oint_{C'} \mathrm{d}s\, s^{-J} \frac{(r-s)e^r}{s e^r - r e^s}. \tag{20}$$

Also, because the integral $\oint \mathrm{d}s\, s^{-J}$ vanishes for integer $J > 1$, we may simplify (20) further by adding s^{-J} to the integrand of the s integral:

$$\omega_J(\alpha) = \frac{\alpha J}{(2\pi \mathrm{i})^2} \oint_C \mathrm{d}r\, r^{-(\alpha-1)J} \oint_{C'} \mathrm{d}s\, s^{-J} \frac{e^r - e^s}{s e^r - r e^s}. \tag{21}$$

Note that the integrand of (21) is singular if

$$s e^r - r e^s = 0, \tag{22}$$

as long as $e^r - e^s$ does not vanish. Clearly, (22) is satisfied when $r = s$, but the numerator of the integrand in (21) also vanishes when $r = s$. Thus, it may appear at first that there is no singularity at $r = s$. However, for the special point $r = s = 1$ the denominator has a higher-order zero than the numerator and thus the integrand is singular there. To find the asymptotic behaviour of (21) we must perform a steepest-descent analysis. However, if we look for a saddle-point of the double integral, we find that it is located near the singular point $r = 1$ and $s = 1$, which complicates the asymptotic analysis enormously. Instead, we will evaluate the s integral in closed but implicit form and evaluate the remaining single integral in r asymptotically.

It is remarkable that the transcendental equation (22) has other solutions for which $r \neq s$. These solutions cannot be expressed in closed form. However, we have discovered an explicit parametric solution to (22) for which $r \neq s$:

$$r = \lambda\, e^{-\lambda}/\sinh\lambda \quad \text{and} \quad s = \lambda\, e^{\lambda}/\sinh\lambda, \tag{23}$$

where λ is any complex number [5].

To evaluate the s integral in closed form we must take the asymmetric solutions (23) into account. We treat the C' contour as a circle about the origin in the complex-s plane, but rather than considering the singularities inside this circle, we include instead the contributions of the singularities *outside* this circle because the integrand vanishes at $|s| = \infty$ in all directions. We now solve (22) for s as a function of r and denote the solution as $s = S(r)$. We then use residue calculus to evaluate the integral (21) at the simple pole located at $s = S(r)$. The result is

$$\omega_J(\alpha) = -\frac{\alpha J}{2\pi\mathrm{i}} \oint_C \mathrm{d}r\, r^{-(\alpha-1)J-1} [S(r)]^{-J} \frac{r - S(r)}{1 - S(r)}, \tag{24}$$

where we have simplified the integrand by using the algebraic relation in (22).

To prepare for the asymptotic evaluation of the integral in (24) we rewrite it in standard Laplace form in terms of the parametric variable λ in (23):

$$\omega_J(\alpha) = \oint \mathrm{d}\lambda\, g(\lambda) e^{-Jf(\lambda)}, \tag{25}$$

where $f(\lambda) = \log\left(\lambda e^{\lambda}/\sinh\lambda\right) + (\alpha-1)\log\left(\lambda e^{-\lambda}/\sinh\lambda\right)$ and $g(\lambda) = \alpha J \sinh\lambda(1 - \lambda - \lambda/\tanh\lambda)/[\mathrm{i}\pi(\sinh\lambda - \lambda e^{\lambda})]$.

Following standard steepest-descent techniques [4], we identify the saddle point as the solution λ_0 to $f'(\lambda) = 0$, where $f'(\lambda) = 2 - \alpha + \alpha(1/\lambda - 1/\tanh\lambda)$. It is easy to verify that $f(\lambda_0) > 0$ when $\alpha > 2$. This implies that $\omega_J(\alpha)$ vanishes exponentially rapidly like $\omega_J(\alpha) \sim e^{-f(\lambda_0)J}$ as $J \to \infty$ for $\alpha > 2$. However, when $\alpha = 2$, $\lambda_0 = 0$ and $f(\lambda_0) = 0$. In this case $\omega_J(\alpha)$ behaves algebraically for large J. To find this behaviour we calculate $f''(\lambda_0) = -2/3$. Also, $g(\lambda_0) = -2\mathrm{i}J/\pi$. Thus, the leading steepest-descent calculation shows that $\omega_J(2)$ diverges as $J \to \infty$:

$$\omega_J(2) \sim -\frac{2\mathrm{i}J}{\pi} \int \mathrm{d}\lambda\, e^{2J\lambda^2/3} \sim \frac{2\sqrt{3}}{\sqrt{\pi}}\sqrt{J} \quad (J \to \infty). \tag{26}$$

This reproduces the result of the Richardson extrapolation in (14) and we identify $\frac{2\sqrt{3}}{\sqrt{\pi}} = 1.9544100476\ldots$.

In summary, we have shown that as the number of energy levels increases, the normalised density of states $\mu(E)$ approaches zero when $E \neq 1/2$ and diverges when

$E = 1/2$. From this result and the normalisation condition satisfied by $\mu(E)$, we conclude that in this limit $\mu(E) \to \delta(E - 1/2)$. Thus, according to the postulate that every quantum state associated with a given energy E must be realised with equal probability in microcanonical equilibrium, the density of states associated with a system having a nondegenerate linear energy spectrum approaches a delta function in the thermodynamic limit. It follows that in this limit the energy of the system can assume only one value. Whether an analogous result holds for an interacting system having a degenerate spectrum is an interesting open question.

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