Microcanonical distributions for quantum systems

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Abstract. The standard assumption for the equilibrium microcanonical state in quantum mechanics, that the system must be in one of the energy eigenstates, is weakened so as to allow superpositions of states. The weakened form of the microcanonical postulate thus asserts that all quantum states giving rise to the same energy expectation value must be realised with equal probability. The consequences that follow from this assertion are investigated. In particular, a closed-form expression for the density of states associated with any system having a nondegenerate energy spectrum is obtained. The result is applied to a variety of examples, for which the behaviour of the state density, as well as the relation between energy and temperature, are determined. Numerical studies indicate that the density of states converges to a distribution when the number of energy levels approaches infinity. (16 December 2013)

1. Introduction

It is sometimes argued that the quantum-mechanical description of the microcanonical distribution is simpler than the corresponding classical counterpart [13]. This is because the standard quantum microcanonical postulate asserts that if the energy of the system lies in the range E to $E + \Delta E$, then all of the energy eigenstates with energy $E_n \in [E, E + \Delta E]$ are realised with equal probability [8]. While such a postulate does indeed provide an elementary statistical description of the quantum system in terms of a uniform probability distribution, it is not clear how this postulate ties in with other fundamental ideas in quantum mechanics.

For example, in quantum mechanics the state of the system can be represented by a general superposition of energy eigenstates, whereas according to the standard quantum microcanonical postulate, superpositions of energy eigenstates with distinct eigenvalues are excluded. Also, if an energy eigenvalue that lies in the interval $[E, E + \Delta E]$ is nondegenerate, then the standard postulate implies that the system can only be in a single eigenstate corresponding to that eigenvalue. These observations suggest that the standard postulate is perhaps too stringent to give rise to a satisfactory statistical description of a quantum system in isolation.

The purpose of the present paper is to study the consequences of a relaxation of the standard quantum microcanonical postulate. Specifically, we consider the following generalisation of the microcanonical postulate: namely, that every quantum state possessing the same energy expectation value must be realised with an equal probability. According to this 'weaker' postulate various superpositions of energy eigenstates with distinct energies are no longer excluded; likewise, a microcanonical state will never correspond to a single eigenstate (except in the case of the smallest and the largest energy levels if these are nondegenerate).

The idea that we investigate here is similar to the classical case, although there is a subtle difference. Classically, the uncertainty in energy is fully characterised by a statistical distribution over the phase space, and for a classical microcanonical distribution having support on a level surface of the Hamiltonian the energy variance vanishes. Quantum mechanically, the contribution to the energy variance from the statistical distribution over the phase space also vanishes. However, if the specified energy level is not the largest or smallest energy eigenvalue, then there is an additional contribution to the energy variance that arises from the intrinsic quantum uncertainty. Therefore, according to our quantum microcanonical postulate the energy variance of a system described by a quantum microcanonical ensemble need not vanish, even though the system is in isolation.

The paper is organised as follows. In §2 we review briefly the formulation of standard quantum theory in terms of the geometry of the space of pure states, as described, e.g., in [1, 2, 3, 5, 9, 10] and references cited therein. When the trajectory of a wave function is projected from Hilbert space $\mathcal{H}$ to the space $\mathcal{P}$ of pure states (rays through the origin of $\mathcal{H}$), the Schrödinger equation on $\mathcal{H}$ reduces to Hamilton's equation on $\mathcal{P}$. More precisely, the space of pure states $\mathcal{P}$ has a natural symplectic structure; and the Schrödinger trajectories, when projected onto $\mathcal{P}$, are the integral curves of the Hamiltonian vector field obtained by taking the symplectic gradient of the function on $\mathcal{P}$ defined by the expectation of the Hamiltonian operator. As a consequence, the formulation of quantum mechanics on $\mathcal{P}$ provides a natural environment in which one can study important issues arising in the context of Hamiltonian mechanics, such as ergodicity conditions or the construction of equilibrium ensembles. For example, the dynamical approach to microcanonical equilibrium introduced by Rugh [12] for classical systems can be seen to apply in the quantum regime.

In §3 we introduce the microcanonical density of states that follows from our weakened microcanonical postulate, together with the associated microcanonical density matrix. In §4 we derive a general integral representation for the density of states, expressed in terms of the energy eigenvalues. We then perform the integration explicitly in §5 in the case for which the energy spectrum is nondegenerate. As an illustration, the properties of a system having an equally spaced energy spectrum are studied in detail in §6. In this example we study the relation between the energy and the temperature in some detail, which we plot for a number of different situations. In particular, a simple procedure for rescaling the energy shows that as the dimensionality of the Hilbert

space increases the system becomes more and more likely to take the intermediate energy value $\frac{1}{2}(E_{\max} + E_{\min})$, where $E_{\max}$ and $E_{\min}$ are, respectively, the largest and the smallest energy eigenvalues. To study the convergence of the distribution numerically, we compute in §7 the Hellinger distance between the density of states associated with an n-level system and an $(n+1)$-level system for $n = 2, 3, \ldots$. The result shows that the logarithmic plot of the relative distances of the distributions against the Hilbert space dimensionality lies on a straight line with gradient -2. Finally in §8 we study the properties of systems having other nondegenerate spectra. In particular, we show numerically that there is an approximate symmetry relation that holds between a system having the spectrum $E_n \sim n^k$ and a system having the spectrum $E_n \sim n^{1/k}$, where k is a constant.

2. Quantum phase space

In order to investigate properties of a closed, isolated quantum system in equilibrium it will be useful first to recall the Hamiltonian formulation of standard quantum mechanics. This has the advantage of allowing us to apply concepts arising in the corresponding classical theory of equilibria as outlined, for example, in Ref. [6].

Physical states in quantum mechanics are represented by elements of a complex Hilbert space $\mathcal{H}$, which we assume to be $(n+1)$-dimensional. Let us denote by Z^α a typical element of $\mathcal{H}$, so that the index α runs over the range $\alpha = 0, 1, \ldots, n$. The Hamiltonian, which acts on elements of $\mathcal{H}$, can thus be denoted H^α_β, and the expectation value of H^α_β in the state Z^α is given by the expression

$$\langle H \rangle = \frac{\bar{Z}_\alpha H^\alpha_\beta Z^\beta}{\bar{Z}_\gamma Z^\gamma}, \tag{1}$$

where $\bar{Z}_\alpha$ is the complex conjugate of Z^α. The Hilbert space $\mathcal{H}$ carries an essentially irrelevant complex degree of freedom given by the overall scale of the state vector. This follows from the fact that the expectation value of a physical observable is invariant under the complex scale transformation $Z^\alpha \to \lambda Z^\alpha$, where $\lambda \in \mathbb{C} - \{0\}$. It is useful in some applications to eliminate this extra degree of freedom by considering the space of equivalence classes under the relation $\lambda Z^\alpha \sim Z^\alpha$ for $\lambda \in \mathbb{C} - \{0\}$. This is the space of rays through the origin of $\mathcal{H}$, otherwise known as the projective Hilbert space $\mathcal{P}$ of complex dimension n. It is well known that quantum theory, when formulated on the projective space $\mathcal{P}$, admits a representation in terms of the standard mathematical structure of Hamiltonian mechanics. This can be seen as follows.

We find it convenient for our purposes to regard the projective space $\mathcal{P}$ as a real manifold Γ of dimension $2n$, letting x^a ($a = 1, 2, \ldots, 2n$) denote a typical point in Γ. Therefore, each point $x^a \in \Gamma$ represents a ray in the Hilbert space $\mathcal{H}$. In this way we can regard the expectation (1) as determining a real-valued function $H(x)$ on Γ.

The space of pure states, when regarded as the real even-dimensional space Γ, is endowed with a symplectic structure, given by a nondegenerate, antisymmetric two-form ω_{ab}. The dynamical laws governing the trajectories of quantum states, given by

the Schrödinger equation on $\mathcal{H}$, can then be represented on Γ in Hamiltonian form as follows:

$$\tfrac{1}{2}\hbar\omega_{ab}\frac{\mathrm{d}x^b}{\mathrm{d}t} = \nabla_a H(x). \tag{2}$$

In other words, the space Γ is a symplectic manifold upon which the evolution of a quantum state is governed by Hamilton's equations, which in the language of symplectic geometry take the form (2). Therefore, we can regard Γ as the quantum analogue of a classical phase space. As a consequence we can also formulate our investigation of equilibrium states on Γ.

3. The microcanonical ensemble

We begin this section by considering the foliation of the quantum phase space Γ by level surfaces of the Hamiltonian function $H(x)$. This is given by a family of hypersurfaces $\{\mathcal{E}_E\}$, $E \in [E_{\min}, E_{\max}]$, determined by level values $H(x) = E$ of the Hamiltonian function. The structure of the typical energy surface in quantum mechanics is quite intricate, even for a system described by low-dimensional Hilbert space. In particular, as E varies in the given range $[E_{\min}, E_{\max}]$ both the dimensionality and the topology of the associated energy surfaces can change. An example can be found in Ref. [3], in which the structures of the energy surfaces for a three-level system are investigated in detail.

Now given this foliation, the 'number' of quantum mechanical microscopic configurations (pure states) with expected energy in the small range E and $E + \Delta E$ is $\Omega(E)\Delta E$, where the state density $\Omega(E)$ for energy E is given by an expression of the form

$$\Omega(E) = \int_{\mathcal{E}_E} \frac{\nabla_a H \mathrm{d}\sigma^a}{\nabla_b H \nabla^b H} \ . \tag{3}$$

Here the natural vector-valued $(2n - 1)$-form $\mathrm{d}\sigma^a$ on Γ is defined by

$$\mathrm{d}\sigma^a = g^{ab}\epsilon_{bc\cdots d}\,\mathrm{d}x^c \cdots \mathrm{d}x^d, \tag{4}$$

where $\epsilon_{bc\cdots d}$ denotes the totally skew tensor with n indices, and g^{ab} is the inverse of the natural Riemannian metric g_{ab} on Γ. The metric g_{ab} is compatible with the symplectic structure ω_{ab} in the sense that $\nabla_a\omega_{bc} = 0$, where ∇_a is the unique torsion-free covariant derivative operator on Γ satisfying $\nabla_a g_{bc} = 0$. It is a remarkable feature of the quantum phase space Γ that it has both a natural Riemannian metric and a compatible symplectic structure. These elements can be regarded as part of the natural geometry of any quantum system.

In the case of an isolated quantum mechanical system with energy in the small range E to $E + \Delta E$, we can adopt the notion of the microcanonical ensemble in classical statistical mechanics (cf. [13]), and identify the entropy of the system by use of the Boltzmann relation

$$S(E) = k\ln(\Omega(E)\Delta E). \tag{5}$$

Here we are implicitly assuming what might be called the *quantum microcanonical postulate*, which asserts that *for an isolated system in equilibrium all states on a given energy surface in the quantum phase space are equally probable.* As a consequence, the temperature T of such a system is determined by the relation

$$\beta = \frac{\mathrm{d}S(E)}{\mathrm{d}E},\tag{6}$$

where $\beta = 1/kT$ and k is Boltzmann's constant. Thus for an isolated quantum system with expected energy E, we assume that the equilibrium configuration is given by a uniform distribution on the energy surface $\mathcal{E}_E$, with entropy $S(E)$ and inverse temperature $\beta(E)$, as given above. The corresponding probability density on Γ, which we call the microcanonical Γ-distribution, is

$$\mu_E(x) \;=\; \frac{1}{\Omega(E)}\,\delta(H(x) - E),\tag{7}$$

where

$$\Omega(E) = \int_\Gamma \delta(H(x) - E)\mathrm{d}V.\tag{8}$$

Here $\mathrm{d}V$ is the volume element on Γ.

It is a straightforward exercise to show that starting from the definition (8) of the density of states $\Omega(E)$ we can deduce the integral formula (3). This can be seen as follows (cf. [11]).

First we note that at each point $x \in \Gamma$ such that $\nabla_a H(x) \neq 0$ the volume element on Γ can be written as a product

$$\mathrm{d}V = \mathrm{d}N\mathrm{d}\sigma,\tag{9}$$

where the $(n-1)$-form $\mathrm{d}\sigma$ defined by

$$\mathrm{d}\sigma = \frac{\nabla^a H \epsilon_{ab\cdots c}\mathrm{d}x^b \cdots \mathrm{d}x^c}{\sqrt{\nabla_d H \nabla^d H}}\tag{10}$$

is the volume element on the energy surface passing through x, and

$$\mathrm{d}N = \frac{\nabla_a H \mathrm{d}x^a}{\sqrt{\nabla_b H \nabla^b H}}.\tag{11}$$

On the other hand, as a consequence of the relation

$$\mathrm{d}H = \nabla_a H \mathrm{d}x^a\tag{12}$$

we observe that

$$\mathrm{d}N = \frac{\mathrm{d}H}{\sqrt{\nabla_a H \nabla^b H}}.\tag{13}$$

Substituting this expression into (8) we obtain

$$\Omega(E) = \int_\Gamma \delta(H(x) - E)\mathrm{d}V$$

$$= \int_\Gamma \delta(H(x) - E)\frac{\mathrm{d}\sigma\mathrm{d}H}{\sqrt{\nabla_a H \nabla^b H}}$$

$$= \int_{\mathcal{E}_E} \frac{\mathrm{d}\sigma}{\sqrt{\nabla_b H \nabla^b H}}$$

$$= \int_{\mathcal{E}_E} \frac{\nabla^a H \epsilon_{ab\cdots c} \mathrm{d}x^b \cdots \mathrm{d}x^c}{\nabla_d H \nabla^d H}, \tag{14}$$

which agrees with expression (3).

A general measurable function $F(x)$ on Γ represents a nonlinear observable in the sense of Kibble [10] and Weinberg [14]. The usual 'linear' observable of standard quantum mechanics then corresponds to the situation for which $F(x)$ can be represented as the expectation of a Hermitian operator. In either case, for each value of x we interpret $F(x)$ as the conditional expectation $\langle F \rangle_x$ of the observable F in the pure state x. The unconditional expectation of F in the microcanonical Γ-ensemble is then given by

$$\langle F \rangle_E = \int_\Gamma F(x) \mu_E(x) \mathrm{d}V. \tag{15}$$

In the case of a linear observable we have

$$F(x) = F_\alpha^\beta \Pi_\beta^\alpha(x), \tag{16}$$

where

$$\Pi_\beta^\alpha(x) = \frac{\bar{Z}_\beta Z^\alpha}{\bar{Z}_\gamma Z^\gamma} \tag{17}$$

is the projection operator onto the state vector $Z^\alpha(x)$ corresponding to the pure state $x \in \Gamma$. Then the unconditional expectation in the state $\mu_E(x)$ is

$$\langle F \rangle_E = F_\alpha^\beta \mu_\beta^\alpha(E), \tag{18}$$

where the quantum microcanonical density matrix $\mu_\beta^\alpha(E)$, parameterised by E, is defined by

$$\mu_\beta^\alpha(E) = \int_\Gamma \Pi_\beta^\alpha(x) \mu_E(x) \mathrm{d}V. \tag{19}$$

Providing we only consider linear observables, i.e. as in standard quantum mechanics, the state of the system is then fully characterised by the density matrix $\mu_\beta^\alpha(E)$.

Now suppose $W(E)$ denotes the total phase space volume for states such that $H(x) \leq E$. Then the density matrix $\mu_\beta^\alpha(E)$ can be calculated explicitly by use of a 'variation-of-parameters' formula given by

$$\mu_\beta^\alpha(E) = -\left(\frac{\mathrm{d}W(E)}{\mathrm{d}E}\right)^{-1} \frac{\partial W(E)}{\partial H_\alpha^\beta}. \tag{20}$$

This representation can be verified as follows. From the definition of $W(E)$ we can write

$$W(E) = \int_{-\infty}^E \int_\Gamma \delta\left(H_\alpha^\beta \Pi_\beta^\alpha(x) - u\right) \mathrm{d}V \mathrm{d}u, \tag{21}$$

and hence

$$\frac{\partial W(E)}{\partial H_\alpha^\beta} = \int_{-\infty}^E \int_\Gamma \Pi_\beta^\alpha(x) \delta'\left(H_\alpha^\beta \Pi_\beta^\alpha(x) - u\right) \mathrm{d}V \mathrm{d}u$$

$$= \int_{\Gamma} \Pi_{\beta}^{\alpha}(x) \left(\int_{-\infty}^{E} \delta' \left(H_{\alpha}^{\beta} \Pi_{\beta}^{\alpha}(x) - u \right) \mathrm{d}u \right) \mathrm{d}V$$

$$= - \int_{\Gamma} \Pi_{\beta}^{\alpha}(x) \, \delta \left(H_{\alpha}^{\beta} \Pi_{\beta}^{\alpha}(x) - E \right) \mathrm{d}V$$

$$= - \Omega(E) \int_{\Gamma} \Pi_{\beta}^{\alpha}(x) \mu_E(x) \mathrm{d}V$$

$$= - \Omega(E) \mu_{\beta}^{\alpha}(E). \tag{22}$$

On the other hand, clearly $\mathrm{d}W(E)/\mathrm{d}E = \Omega(E)$, and thus we obtain (20).

4. Calculating the density of states

As defined in equation (8) above, the density of states is given by the volume integral over Γ of a delta-function having a support on the energy surface $\mathcal{E}_E$. Our objective now is to perform the relevant integration explicitly for a generic Hamiltonian, and obtain a representation for $\Omega(E)$ in terms of the energy eigenvalues.

We find it convenient to pursue the calculation by lifting the integration from the phase space Γ to the Hilbert space $\mathcal{H}$, imposing the constraint that the norm of the Hilbert space vector Z^{α} is unity. Therefore, we write the expression (8) in the following form:

$$\Omega(E) = \frac{1}{\pi} \int_{\mathbb{C}^{n+1}} \delta(\bar{Z}_{\alpha} Z^{\alpha} - 1) \, \delta \left(\frac{\bar{Z}_{\alpha} H_{\beta}^{\alpha} Z^{\beta}}{\bar{Z}_{\gamma} Z^{\gamma}} - E \right) \mathrm{d}^{n+1} \bar{Z} \, \mathrm{d}^{n+1} Z. \tag{23}$$

The additional factor of π arises here from the superfluous phase integration in (23). By use twice of the standard integral representation

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\lambda x} \mathrm{d}\lambda \tag{24}$$

we thus deduce that

$$\Omega(E) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}\nu}{2\pi} \mathrm{e}^{\mathrm{i}(\lambda + \nu E)}$$

$$\times \int_{\mathbb{C}^{n+1}} \exp \left[\left(-\mathrm{i} \left(\lambda \bar{Z}_{\alpha} Z^{\alpha} + \nu H_{\beta}^{\alpha} \bar{Z}_{\alpha} Z^{\beta} \right) \right] \mathrm{d}^{n+1} \bar{Z} \, \mathrm{d}^{n+1} Z. \tag{25}$$

We now observe that we can diagonalise the Hamiltonian by unitary transformation without affecting any of the terms in (25) on account of the fact that every 'ket' vector Z^{α} is coupled to a corresponding 'bra' vector $\bar{Z}_{\alpha}$. Therefore, the density of states can be written in the form

$$\Omega(E) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}\nu}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda}{2\pi} \mathrm{e}^{\mathrm{i}(\lambda + \nu E)} \int_{\mathbb{C}^{n+1}} \mathrm{d}^{n+1} \bar{Z} \, \mathrm{d}^{n+1} Z \exp \left(-\mathrm{i} \sum_{l=0}^{n} (\lambda + \nu E_l) \bar{Z}_l Z^l \right), \tag{26}$$

where $\{E_l\}_{l=0,1,\ldots,n}$ are the energy eigenstates.

This is of course a formal expression; the integration can nevertheless be carried out if we regard (26) as the limit of a similar integral in which λ and ν are displaced into

the complex along the negative imaginary axis. The integration over $\mathbb{C}^{n+1}$ then reduces to a $(2n-2)$-dimensional Gaussian integral, which is readily performed to yield

$$\Omega(E) = (-\mathrm{i})^{n+1}\pi^n \int_{-\infty}^{\infty} \frac{\mathrm{d}\nu}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda}{2\pi} \mathrm{e}^{\mathrm{i}(\lambda+\nu E)} \prod_{l=0}^{n} \frac{1}{(\lambda + \nu E_l)}. \tag{27}$$

This is the desired integral representation for the density of states, expressed in terms of the energy eigenvalues.

5. Density of states for a nondegenerate energy spectrum

We proceed further by evaluating the integration in (27) in the case where the Hamiltonian has no degenerate eigenvalues. Let us consider the integration in the λ variable first. We observe that there are $n+1$ first order poles on the real λ-axis. An application of Cauchy's theorem thus gives us

$$\frac{1}{2\pi\mathrm{i}} \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}(\lambda+\nu E)} \prod_{l=0}^{n} \frac{1}{(\lambda + \nu E_l)}\mathrm{d}\lambda = \sum_{k=0}^{n} \mathrm{e}^{\mathrm{i}\nu(E-E_k)} \prod_{l=0,\neq k}^{n} \frac{1}{\nu(E_l - E_k)}, \tag{28}$$

from which it follows that

$$\Omega(E) = \pi^n \sum_{k=0}^{n} \int_{-\infty}^{\infty} \frac{\mathrm{d}\nu}{2\pi} \frac{\mathrm{e}^{-\mathrm{i}\nu(E_k-E)}}{(\mathrm{i}\nu)^n} \prod_{l=0,\neq k}^{n} \frac{1}{(E_l - E_k)}. \tag{29}$$

We now recognise the ν-integration formally as the n-fold repeated integral of the δ-function, defined by the truncated polynomial

$$\delta^{(-n)}(x) = \begin{cases} 0 & (x < 0) \\ \frac{1}{(n-1)!} x^{n-1} & (x \geq 0). \end{cases} \tag{30}$$

As a consequence, the density of states associated with a quantum system having a nondegenerate energy spectrum can be seen to be given by an expression of the form given by

$$\Omega(E) = (-1)^n \pi^n \sum_{k=0}^{n} \delta^{(-n)}(E_k - E) \prod_{l=0,\neq k}^{n} \frac{1}{E_l - E_k}. \tag{31}$$

In addition to the function $\Omega(E)$ we find it useful for some purposes to introduce the related normalised density of states $\mu(E)$ defined by

$$\mu(E) = \frac{\int_\Gamma \delta(H(x) - E)\mathrm{d}V}{\int_\Gamma \mathrm{d}V}. \tag{32}$$

The function $\mu(E)$ thus satisfies the property that

$$\int_{-\infty}^{\infty} \mu(E)\mathrm{d}E = 1. \tag{33}$$

To calculate the normalisation factor we need to determine the total volume V_Γ of the quantum phase space. This is given by

$$V_\Gamma = \frac{1}{\pi} \int_{\mathbb{C}^{n+1}} \delta(Z^\alpha \bar{Z}_\alpha - 1)\mathrm{d}^{n+1}Z\mathrm{d}^{n+1}\bar{Z}, \tag{34}$$

where again the factor of π in the denominator refers to the removal of the superfluous overall phase of the wave function. Thus, making use of the integral representation of the delta-function, we have

$$
\begin{aligned}
V_\Gamma &= \frac{1}{\pi} \int_{\mathbb{C}^{n+1}} \mathrm{d}^{n+1} Z \mathrm{d}^{n+1} \bar{Z} \int_{-\infty}^{\infty} \frac{1}{2\pi} \mathrm{e}^{\mathrm{i}\lambda(Z^\alpha \bar{Z}_\alpha - 1)} \mathrm{d}\lambda \\
&= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda}{2\pi} \mathrm{e}^{-\mathrm{i}\lambda} \int_{\mathbb{C}^{n+1}} \mathrm{e}^{\mathrm{i}\lambda Z^\alpha \bar{Z}_\alpha} \mathrm{d}^{n+1} Z \mathrm{d}^{n+1} \bar{Z} \\
&= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}\lambda}{2\pi} \mathrm{e}^{-\mathrm{i}\lambda} \left(-\frac{\mathrm{i}\pi}{\lambda} \right)^{n+1} \\
&= \frac{\pi^n}{n!},
\end{aligned} \tag{35}
$$

where in the last step we have used the identity

$$
\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}\lambda}}{\lambda^n} \mathrm{d}\lambda = \frac{\mathrm{i}^n}{(n-1)!}. \tag{36}
$$

This is in agreement, e.g., with the result obtained in Ref. [7] by use of different methods. In particular, we note that in the case $n = 1$ (a two-dimensional Hilbert space) the space of pure states Γ is isomorphic to the geometry of a round two-sphere with radius one-half.

6. Equally spaced energy spectrum

We now specialise the analysis further by considering a quantum system whose energy eigenvalues are equally spaced. There are many elementary systems, such as noninteracting particles with spin, having a spectrum of this kind. To fix the units of energy we set

$$
E_k = \hbar\omega k, \qquad (k = 0, 1, \ldots, n). \tag{37}
$$

Substituting this in (31) we obtain

$$
\Omega(E) = \frac{(-1)^n \pi^n}{(n-1)!} (\hbar\omega)^{n-1} \sum_{k \geq [E]} \left(k - \frac{E}{\hbar\omega} \right)^{n-1} \prod_{l=0, \neq k}^{n} \frac{1}{\hbar\omega(l-k)}. \tag{38}
$$

This expression can be simplified further by writing

$$
\prod_{l=0, \neq k}^{n} \frac{1}{\hbar\omega(l-k)} = \frac{1}{(\hbar\omega)^n (-1)^k k! (n-k)!}, \tag{39}
$$

and hence the microcanonical density of states associated with a system having equally spaced energy spectrum is given by

$$
\Omega(E) = \frac{(-1)^n}{(n-1)!} \pi^n \frac{1}{\hbar\omega} \sum_{k \geq [E]}^{n} \frac{(-1)^k (k - E/\hbar\omega)^{n-1}}{k!(n-k)!}. \tag{40}
$$

Finally, dividing this expression by the normalisation factor (35) we obtain the following formula for the normalised density of states:

$$
\mu(E) = \frac{(-1)^n n}{\hbar\omega} \sum_{k \geq [E]}^{n} \frac{(-1)^k (k - E/\hbar\omega)^{n-1}}{k!(n-k)!}. \tag{41}
$$

It will be useful now to indicate what this function looks like in various situations. In Figure 1 we plot $\mu(E)$ for two, three, and four dimensional Hilbert spaces.
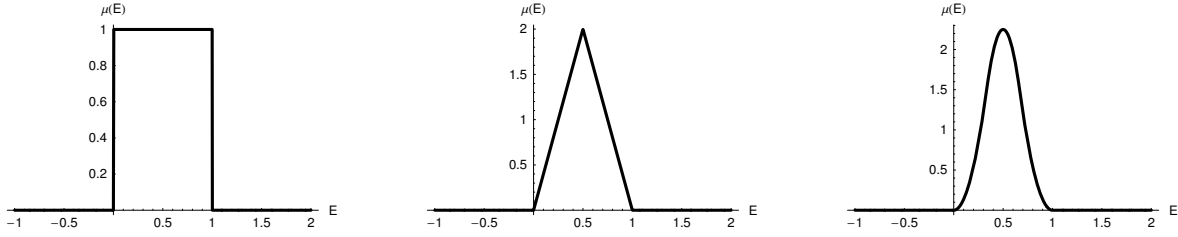
Figure 1. Density of states as a function of energy E for systems with two, three, and four nondegenerate energy eigenstates. The functions are evaluated piecewise. For example, in the case of the four-dimensional system with $E_n/\hbar\omega = 0, 1, 2, 3$, the normalised density of states $\mu(E)$ is zero for $E \leq 0$ and $E > 3$, and is given by three distinct quadratic functions in the intervals $(0, 1]$, $(1, 2]$, and $(2, 3]$. In general, for an n-dimensional system, $\mu(E)$ is given by a combination of polynomials of degree $n - 1$, and is at least $n - 3$ times differentiable for all values of E. In all cases the area under the function integrates to unity.
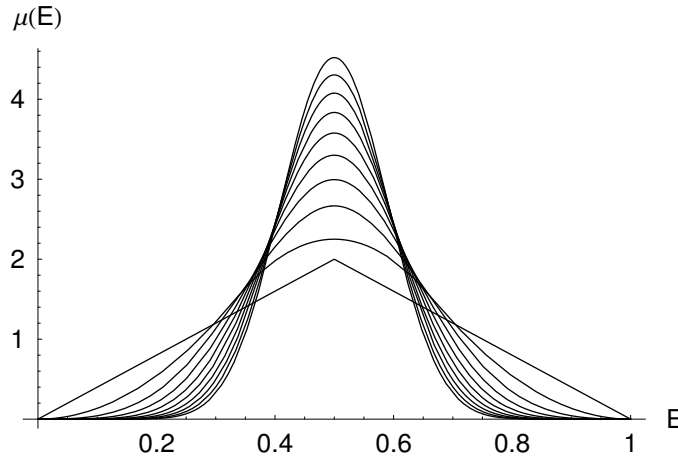
Figure 2. Rescaled normalised density of states $\mu(E)$ as a function of energy E. As we increase the density of energy levels in the interval $[0, 1]$, the corresponding density of states becomes more sharply distributed around the centre $E = \frac{1}{2}$. For these numerical plots we have set $\hbar\omega = 1$. The plots correspond to systems for which the number of energy levels ranges from 3 to 12, and the value of the rescaled energy varies over the unit interval.

We would like now to study the behaviour of the density of states as we increase the number of energy levels. For this purpose we find it convenient to rescale the energy spectrum so that the range of energy is over a fixed interval $[0, 1]$. After the application of a suitable such rescaling, the density of states reduces to

$$\mu(E) = \frac{(-1)^n n^2}{\hbar\omega} \sum_{k \geq [E]}^{n} \frac{(-1)^k (k - nE/\hbar\omega)^{n-1}}{k!(n-k)!}. \tag{42}$$

In Figure 2 we plot this rescaled density of states for a variety of systems with different numbers of energy levels.

Expression (42) for the density of states also allows us to study the relation between energy E and temperature T, by use of the relation (6). In Figure 3 we plot the system energy $E(T)$ as a function of temperature by numerically inverting the relation

$$T = \left(\frac{\mathrm{d}\Omega}{\mathrm{d}E}\right)^{-1}\Omega(E). \tag{43}$$

As the temperature increases from zero, the corresponding energy increases monotonically, and asymptotically approaches the value $E = \frac{1}{2}$ (in the rescaled units). The function $E(T)$ is multi-valued at $T = 0$, where the energy takes the values $E = 0, 1$. In the region $E \in (\frac{1}{2}, 1]$ the density of states $\mu(E)$ is a decreasing function of E, and thus the corresponding 'temperature' is negative. To put the matter differently, this is the region that is not accessible in an equilibrium.
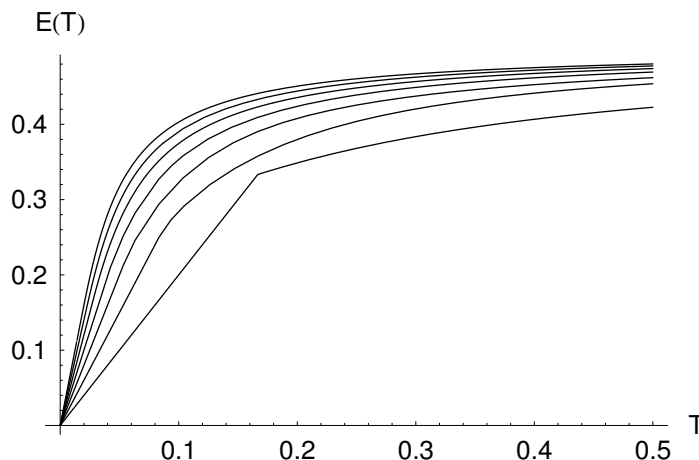
Figure 3. Energy $E(T)$ as a function of temperature T. The linear curve with lowest energy corresponds to a four-level system, and we have plotted $E(T)$ up to the ten-level system with an interval of 1. Although not shown in the plot, the second root for $E(0)$ is given by $E(0) = 1$, where the function is multi-valued. As T is reduced from zero, $E(T)$ reduces monotonically, and approaches $E = \frac{1}{2}$ as $T \to -\infty$. This is the region inaccessible in equilibrium.

7. Convergence in the infinite energy-level limit

In statistical mechanics it is often presumed that the various different distributions used to describe equilibrium states (e.g., microcanonical, canonical, grandcanonical, and pressure-temperature distributions) should in some respects be equivalent in the infinite volume or thermodynamic limit. Now the system that we have studied in the previous section corresponds to a system of noninteracting quantum particles. As a consequence, we would not expect any nontrivial behaviour exhibited by the system in the thermodynamic limit. Nevertheless it would be of interest to study how the

density of states behaves in this limit so that the result might be compared with the corresponding canonical formulation outlined in Ref. [4].

Now the results shown in Figure 2 indicate that as we increase the number of energy levels the density of states becomes more and more peaked at the intermediate energy $E = \frac{1}{2}$. Therefore, in this section we consider the separation of a pair of normalised state densities associated with k-level and $(k+1)$-level systems for a range of values for k, and study whether the separation decreases as we increase k. If so, then the result will indicate that the density function is converging, possibly to a delta-function centred at $E = \frac{1}{2}$.

There are various standard measures that one can use to study the separation of a pair of density functions, such as the relative entropy or the Bhattacharyya distance. Here we shall consider a closely related measure given by

$$D(\mu_m, \mu_n) = \sqrt{2 - 2 \int_0^1 \sqrt{\mu_n(E)} \sqrt{\mu_m(E)} \mathrm{d}E}, \tag{44}$$

known as the Hellinger distance. For clarity we let $\mu_k(E)$ denote the density of states associated with a k-level system. Note that the Hellinger distance is simply the L^2-norm

$$D(\mu_m, \mu_n) = \left\| \sqrt{\mu_n(E)} - \sqrt{\mu_m(E)} \right\| \tag{45}$$

of the difference between the two square-root density functions.
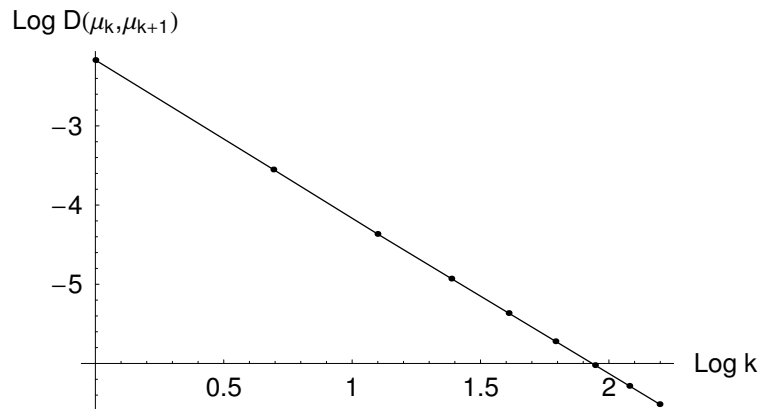
Figure 4. The Hellinger distance $D(\mu_k, \mu_{k+1})$ between two 'consecutive' rescaled state densities is plotted for $k = 2, 3, \ldots, 10$. The plot is presented on a logarithmic scale. We find that the logarithms of the distances lie almost perfectly on a straight line with gradient of -2, indicating that the separation of the densities decays quadratically with an increasing number of energy levels.

The result of the numerical analysis of (44) is shown in Figure 4, which indicates that the relative separation of $\mu_k(E)$ and $\mu_{k+1}(E)$ is decreasing quadratically in k. Therefore, we conclude that the density of states is likely to be converging in the sense of L^2.

8. Other spectral structures

In the example considered in §6 and §7 above we analysed a linear spectral structure of the form $E_k \propto k$, and found that the density of states is centred at an intermediate energy value. In this section we investigate nondegenerate systems having other kinds of energy growths. We start with the case of a system whose energy grows quadratically so that $E_k = \hbar\omega k^2$. In this case we make use of the relation

$$\prod_{l=0, \neq k}^{n} \frac{1}{l^2 - k^2} = \prod_{l=0, \neq k}^{n} \frac{1}{(l+k)(1-k)} = \frac{2(-1)^k}{(n+k)!(n-k)!}, \tag{46}$$

and substitute this in formula (31) to obtain

$$\mu(E) = \frac{2n(-1)^n}{\hbar\omega} \sum_{k \geq [E]}^{n} \frac{(-1)^k \left(k^2 - \frac{E}{\hbar\omega}\right)^{n-1}}{(n+k)!(n-k)!}. \tag{47}$$

As one might have expected, the functions given by (47) have similar characteristics to those of the previous example. For each value of n we obtain a curve $\mu(E)$ which is specified by $n+2$ polynominals of degree $n-1$. The function is continuous and its differentiability is of order $n-2$. The first three examples are plotted in Figure 5. As the plots indicate, the microcanonical density functions in the current examples are no longer symmetric around the intermediate energy $\frac{1}{2}(E_{\min} + E_{\max})$, in contrast to the case of linear energy growth.
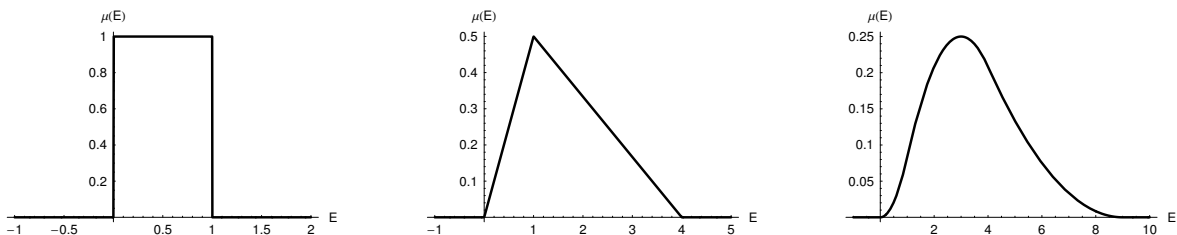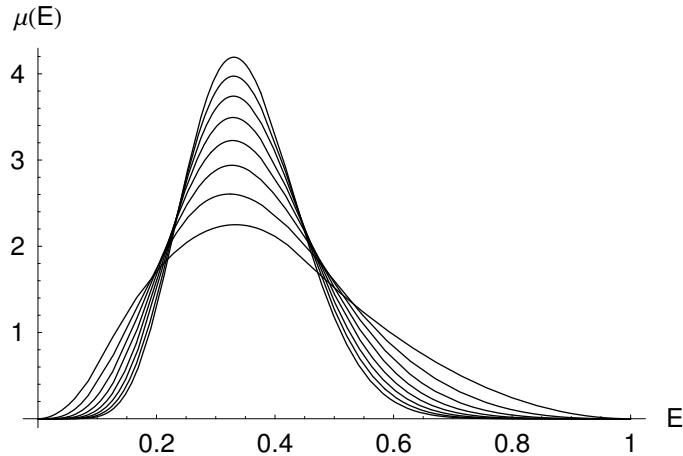

Figure 5. The density of states $\mu_k(E)$ for k-level systems with $k = 2, 3, 4$, in the case of a system with a quadratically growing energy spectrum. For the plot we have set $\hbar\omega = 1$. Unlike the example with a linear, equally-spaced spectrum, the density of states is not symmetric.

As in the previous example, in the present case we can rescale the energy spectrum in such a way that we can directly compare the behaviour of the density of states as we increase the number of energy levels. The result is shown in Figure 6. We observe that the density of states becomes more peaked as we increase the number of energy levels. However, the location of the peak is no longer at $E = \frac{1}{2}$, but rather closer to $E = \frac{1}{3}$.

As a consequence of the skewed form of the distribution, the range of energy for which the derivative of $\mu(E)$ with respect to E remains positive is somewhat reduced. This implies that the range of energy associated with positive temperature is reduced from the previous example of linear energy spectrum. Some examples are illustrated in Figure 7 where we plot the temperature dependence of the energy. As the temperature is

increased, the energy grows monotonically and reaches a value around $\frac{1}{3}$. The remaining values of the energy are associated with negative temperatures that are inaccessible in equilibrium.

Figure 6. The density of states $\mu(E)$ associated with a system having the spectrum $E_k = k^2/(N-1)^2$, where N denotes total number of energy levels. The value of k thus ranges over $k = 0, 1, \ldots, N-1$. Here we plot $\mu(E)$ for $N = 4, 5, \ldots, 11$. Numerical studies show that the peaks of the distributions are located at approximately $E = \frac{1}{3}$.

We have examined systems having a linear energy growth and a quadratic energy growth. In the linear case the microcanonical distribution is symmetric around its centre, while in the quadratic case the peaks of the distributions have shifted to the left with smaller energies. This leads to the question of what happens to the density of states associated with systems having other spectral structures.
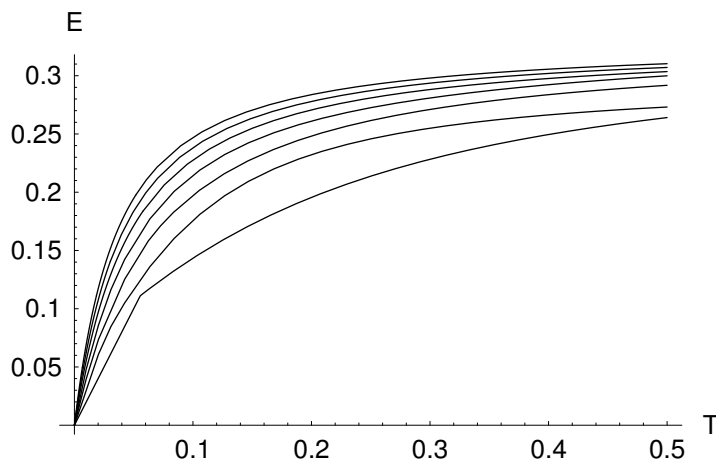

Figure 7. System energy $E(T)$ as a function of temperature T in the case of a system having a quadratic energy spectrum. The plots correspond to a set of k-level systems with $k = 5, 6, \ldots, 11$. Although not shown in the plot, the energy is multi-valued at $T = 0$ so that $E(T) \to 0$ as $T \to 0^+$ and $E(T) \to 1$ as $T \to 0^-$. The range of energy accessible in equilibrium is thus given by $0 \le E \lesssim \frac{1}{3}$.

In the case of a system with an infinite number of degrees of freedom (and thus an infinite number of energy levels), the energy spectrum cannot grow more rapidly than quadratically in the number of energy levels. However, for a finite system there is in principle no limitation on how fast the system energy can grow. Therefore, we would like to study the behaviour of the density of states associated with systems having the following two spectral structures:

$$E_n = n^k \qquad \text{and} \qquad E_n = n^{1/k}, \tag{48}$$

for $k = 1, 2, 3, \ldots$. Thus in one case the growth of the energy is enhanced as k is increased, while in the other case the growth of the energy is suppressed. Various densities of states associated with systems having spectra of the form (48) are computed numerically and plotted in Figure 8. The result shows that as the rate of growth is increased, the location of the peak of $\mu(E)$ becomes smaller, whereas when the rate of energy growth is suppressed, the peak of $\mu(E)$ increases. In particular, the peak of $\mu(E)$ for the system with energy $E_n = n^k$ is located approximately around $E \sim (k+1)^{-1}$, while the peak of $\mu(E)$ for the system with energy $E_n = n^{1/k}$ is located approximately around $E \sim 1 - (k+1)^{-1}$. Therefore, when $k \ll 1$, the values of energy that are accessible in equilibrium becomes negligible when $E_n = n^k$, whereas if $E_n = n^{\frac{1}{k}}$ then virtually all values of $E \in [0, 1]$ are accessible.
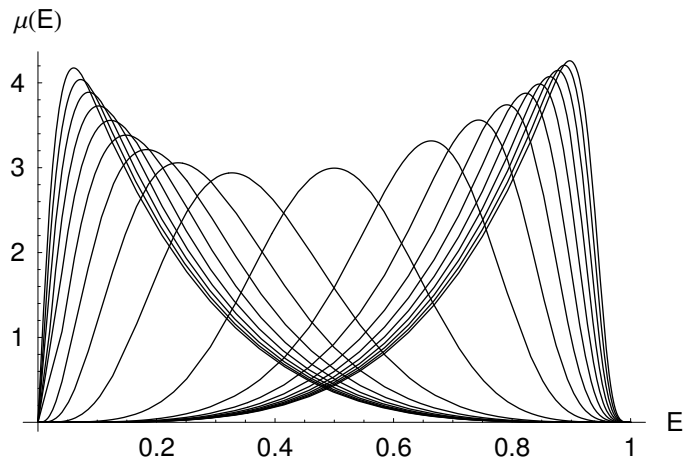
Figure 8. The density of states $\mu(E)$ associated with systems having the spectra $E_n = n^k$ and $E_n = n^{\frac{1}{k}}$, for $k = 1, 2, \ldots, 10$. In the former case the peak of $\mu(E)$ shifts to the left, while in the latter case the peak shifts to the right. The cases $E_n = n^k$ and $E_n = n^{\frac{1}{k}}$ are close to but not exactly symmetric to one another around $E = \frac{1}{2}$. In all examples the number of energy levels is set to six.

In conclusion, we note that the analysis we have pursued here is based on a generalised microcanonical postulate, which relaxes the somewhat more stringent assumptions made in the standard quantum microcanonical postulate as outlined in, e.g., Ref. [8]. To determine whether the assumption made in this paper reflects the actual equilibrium distribution of an isolated quantum system it will be desirable to examine the properties of interacting systems. In the case of a general interacting

system, some of the energy levels are typically highly degenerate, and thus we must return to the integral representation (27) with a view to deriving an efficient way to carry out the integration in the cases when there are higher-order poles. This is an intriguing open problem that we hope to investigate elsewhere.

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