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Asymptotic formulae for the quantum Rényi entropies of position: application to the infinite well

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Abstract. General asymptotic formulae are derived by means of the WKB approximation for the continuous and discrete Rényi entropies of position of one-dimensional quantum systems in energy eigenstates, in terms of the corresponding entropies for a microcanonical ensemble of analogous classical systems. These results are checked in the simplest particular case of the infinite potential well, where the asymptotic formula for continuous entropies holds as an exact identity. For the discrete entropies, analytical expressions are obtained from which the asymptotic formulae given for the limiting cases of large and small measurement resolution can both be verified.

1. Introduction

For a continuous probability distribution with density function $P(x)$, the Boltzmann–Shannon information entropy is defined as

$$S = -\int P(x)\ln P(x)\,\mathrm{d}x = \langle -\ln P(x)\rangle. \tag{1}$$

When $P(x)$ is the quantum probability density of position of a system described by the wavefunction $\psi(x)$, $P_{\mathrm{Q}}(x) = |\psi(x)|^2$, the Boltzmann–Shannon entropy measures the uncertainty in the localization of the particle in position space. The quantum entropy $S_{\mathrm{Q}} = \langle -\ln P_{\mathrm{Q}}(x)\rangle$ and its counterpart in momentum space have been used in recent years to discuss a wide range of quantum mechanical problems, such as, e.g., the mathematical formulation of the position–momentum uncertainty principle [1]. Accordingly, there has been a growing interest in the calculation of S_{Q} for physically interesting quantum states. However, the exact calculation of S_{Q} is a very difficult mathematical problem, even for simple systems as the harmonic oscillator and hydrogen atom [2], which has attracted interest to its approximate calculation, specially for very excited or Rydberg stationary states [3, 4].

In a recent paper [5], the following asymptotic formula was obtained:

$$S_{\mathrm{Q}} \sim S_{\mathrm{C}} - 1 + \ln 2 \tag{2}$$

where S_{Q} is the quantum entropy of position in the nth energy eigenstate of a one-dimensional system with an infinite discrete spectrum $\{E_n\}$, and S_{C} is the entropy of the probability density $P_{\mathrm{C}}(x)$ corresponding to a microcanonical ensemble of analogous classical systems with energy $E = E_n$. This equation, which provides a useful approximation to S_{Q} for large n without requiring previous knowledge of the quantum eigenfunctions, holds for any Hamiltonian of the form

$$H = \frac{p^2}{2m} + V(x) \tag{3}$$

where, at least for large n, there are two classical turning points for $E = E_n$. That is, the motion of a classical particle with (constant) energy E_n is periodic between the turning points x_- and x_+ ($x_- < x_+$), where the speed $v = p/m$ of the particle reduces to zero,

$$V(x_-) = V(x_+) = E_n$$

and there exists a non-vanishing force $-V'(x)$ that causes the particle to move towards the right at $x = x_-$, and towards the left at $x = x_+$,

$$V'(x_-) < 0 \qquad V'(x_+) > 0.$$

Equation (2) follows from the semiclassical (WKB) approximation to quantum mechanics [6], and has an appealing physical interpretation as a manifestation of the so-called configuration form of Bohr's correspondence principle [7], which states that for large n the expected value of any observable $F(x)$ in the nth eigenstate approaches the corresponding average for the analogous classical system having the same energy:

$$\langle F(x)\rangle_{\mathrm{Q}} \sim \langle F(x)\rangle_{\mathrm{C}} \tag{4}$$

with the correction term $-1 + \ln 2$ arising due to the explicit dependence of $F(x) = -\ln P(x)$ on the probability density $P(x)$ [5]. The validity of equation (2) has been checked by numerical and analytical calculations of the involved entropies for several simple systems, namely the particle in a box (infinite potential well), where the asymptotic formula holds as an exact identity, the linear potential and the harmonic oscillator [5].

The differential entropy S defined by (1) is a measure of the uncertainty associated with the continuous random variable whose probability density function is $P(x)$. However, actual physical measurements of any continuous observable such as position are always performed by means of measuring devices that have finite resolution. This means that the continuous spectrum of the position observable is partitioned into a countable set of intervals (or 'bins', in the terminology of [8]) of length $\Delta x > 0$ (for the sake of simplicity, we assume the resolution of the measuring device to be uniform). The probability $P_k^{(\Delta x)}$ of finding the outcome of the position measurement to have a value in the kth interval, $(\Delta x)_k$, is the integral of $P(x)\,\mathrm{d}x$ over this interval,

$$P_k^{(\Delta x)} = \int_{(\Delta x)_k} P(x)\,\mathrm{d}x \tag{5}$$

and the entropy $S^{(\Delta x)}$ corresponding to the discrete probability distribution $\{P_k^{(\Delta x)}\}$ is [8, 9]

$$S^{(\Delta x)} = -\sum_k P_k^{(\Delta x)} \ln P_k^{(\Delta x)}. \tag{6}$$

Unlike the continuous or differential entropy S, the discrete entropy $S^{(\Delta x)}$ is always a non-negative quantity, $S^{(\Delta x)} \geqslant 0$, and also satisfies the inequality [9]

$$S^{(\Delta x)} \geqslant S - \ln(\Delta x)$$

which becomes an equality in the limit $\Delta x \to 0$,

$$S^{(\Delta x)} + \ln(\Delta x) \to S \qquad \Delta x \to 0. \tag{7}$$

The latter equation can be proved by noting that, in the limit $\Delta x \to 0$,

$$P_k^{(\Delta x)} = P(x_k)\Delta x \qquad x_k \in (\Delta x)_k \qquad \sum_k P(x_k) = \frac{1}{\Delta x} \tag{8}$$

so that

$$S^{(\Delta x)} = -\sum_k [P(x_k)\Delta x] \ln[P(x_k)\Delta x]$$
$$= -\sum_k P(x_k) \ln[P(x_k)]\Delta x - \ln(\Delta x)$$

while, on the other hand, assuming that $P(x) \ln P(x)$ is Riemann integrable,

$$S = -\sum_k \int_{(\Delta x)_k} P(x) \ln P(x)\, \mathrm{d}x = -\sum_k P(x_k) \ln[P(x_k)]\Delta x.$$

It follows from (7) that in the limit $\Delta x \to 0$ the difference between the discrete entropies of any two probability densities coincides with the difference between the corresponding differential entropies, i.e., $S_2^{(\Delta x)} - S_1^{(\Delta x)} = S_2 - S_1$. In particular, the asymptotic formula (2) is also valid for the discrete entropies $S^{(\Delta x)}$,

$$S_{\mathrm{Q}}^{(\Delta x)} \sim S_{\mathrm{C}}^{(\Delta x)} - 1 + \ln 2 \qquad \Delta x \to 0. \tag{9}$$

More precisely, it can be shown [5] that:

$$S_{\mathrm{Q}}^{(\Delta x)} \sim S_{\mathrm{C}}^{(\Delta x)} - 1 + \ln 2 \qquad \Delta x \ll \frac{x_+ - x_-}{n} \tag{10}$$

while in the opposite case the asymptotic behaviour of the discrete quantum entropy is given by (4),

$$S_{\mathrm{Q}}^{(\Delta x)} \sim S_{\mathrm{C}}^{(\Delta x)} \qquad \Delta x \gg \frac{x_+ - x_-}{n}. \tag{11}$$

In the framework of Shannon's information theory [10], the entropy defined by equations (1) and (6) is proved to be the only rigorous mathematical measure of the lack of knowledge or uncertainty associated to a continuous or discrete random variable, respectively. However, if one somewhat relaxes the requirements that are axiomatically imposed on the uncertainty measure, a number of other similar quantities can be defined. The most important of these generalized entropies is the order-q Rényi entropy [11, 12], which for a continuous probability density $P(x)$ is defined as

$$S(q) = \frac{1}{1-q} \ln \int [P(x)]^q\, \mathrm{d}x = \frac{1}{1-q} \ln\langle [P(x)]^{q-1}\rangle \qquad q > 0 \tag{12}$$

while for the discrete probability distribution $\{P_k^{(\Delta x)}\}$ the corresponding expression is

$$S^{(\Delta x)}(q) = \frac{1}{1-q} \ln \sum_{k=1}^{N} (P_k^{(\Delta x)})^q \qquad q > 0. \tag{13}$$

It can be shown [11] that, for a fixed probability distribution, the Rényi entropy is a continuous, non-increasing and convex function of the parameter q. Another important generalization of Shannon's entropy is the order-q Tsallis entropy $\tilde{S}(q)$ [12, 13], which is related to the Rényi entropy of the same order by

$$\begin{aligned} \tilde{S}(q) &= \frac{1}{1-q}\{\exp[(1-q)S(q)] - 1\} \\ \tilde{S}^{(\Delta x)}(q) &= \frac{1}{1-q}\{\exp[(1-q)S^{(\Delta x)}(q)] - 1\} \end{aligned} \tag{14}$$

in the continuous and discrete cases, respectively. The Rényi and Tsallis families of generalized entropies both include Shannon's entropy as the particular case $q = 1$, as may be seen by taking the limit $q \to 1$ in the above definitions.

In recent years, the Rényi and Tsallis entropies corresponding to the quantum probability densities of position and momentum have also been applied to the mathematical formulation of the uncertainty principle [14], and their approximate calculation for Rydberg states of physically interesting systems has been the subject of active research [4]. The aims of this paper are (i) to find the generalization of equations (2), (10) and (11) to the whole set of Rényi entropies, and (ii) to check these generalized asymptotic formulae in the simplest particular case of the infinite potential well, where, as we shall see, this can be done in a fully analytical way. The derivation of the asymptotic formulae relating quantum and classical Rényi entropies of position, both continuous and discrete, is carried out in section 2. In section 3, the discrete Rényi entropies are calculated for the eigenstates of the infinite well; although the general expression of the quantum entropies turns out to be rather cumbersome, it is shown to reduce to a simple form in two important particular cases. Using these results, in section 4 we are able to verify analytically the validity of equations (10) and (11), as well as their generalizations to Rényi entropies. Finally, in section 5, some concluding remarks are given and several open problems are pointed out.

2. Generalization of the asymptotic formulae to Rényi entropies

To obtain the generalization of equation (2) to Rényi entropies, we begin by recalling that, under the assumptions of section 1, a classical particle with Hamiltonian (3) and (constant) energy $E = E_n$ undergoes periodic motion between the turning points x_- and x_+, so that $P_C(x) = 0$ outside the interval $[x_-, x_+]$. The probability $P_C(x)\,\mathrm{d}x$ of finding the particle in the region between x and $x + \mathrm{d}x$ is proportional to the amount of time, $\mathrm{d}t$, the particle spends in that region during one traversal of the potential well (from, say, x_- to x_+), which in turn is inversely proportional to the speed $v = \mathrm{d}x/\mathrm{d}t$ at the point x (or, equivalently, to the momentum $p = mv$) [6, 7, 15, 16]. Using equation (3), it can be shown [16] that the normalized classical probability density for the position of the particle is given by

$$P_C(x) = \frac{1}{T}\sqrt{\frac{2m}{E - V(x)}}$$

within the classically allowed region $x_- \leqslant x \leqslant x_+$, where T is the period of the motion.

On the other hand, in the limit of large quantum numbers the quantum probability density $P_Q(x)$ also vanishes outside the classically allowed region, while inside this region the WKB approximation [6] yields [5]

$$P_Q(x) \sim 2P_C(x)\cos^2\phi(x) \qquad \phi(x) = \left(n + \frac{1}{2}\right)u(x) - \frac{\pi}{4} \tag{15}$$

where $u(x)$ is a monotonically increasing function with $u(x_-) = 0$ and $u(x_+) = \pi$. This relation leads to the asymptotic formula

$$\begin{aligned}\int_{-\infty}^{\infty}[P_Q(x)]^q\,\mathrm{d}x &\sim 2^q\int_{x_-}^{x_+}[P_C(x)]^q\cos^{2q}\phi(x)\,\mathrm{d}x\\ &\sim \frac{2^q\Gamma(q+\frac{1}{2})}{\sqrt{\pi}\,\Gamma(q+1)}\int_{x_-}^{x_+}[P_C(x)]^q\,\mathrm{d}x\end{aligned} \tag{16}$$

where in the last step we have taken into account that, for large n, $\cos^{2q}\phi(x)$ is a very rapidly oscillating function and can be replaced in the integral by its average value over a period,

$$\frac{1}{\pi}\int_0^{\pi}\cos^{2q}x\,\mathrm{d}x = \frac{\Gamma(q+\frac{1}{2})}{\sqrt{\pi}\,\Gamma(q+1)}.$$

A rigorous proof of this statement can be achieved by making the change of variable $u(x) = \theta$ and applying, with $g(\theta) = \cos^{2q}\theta$, the following theorem (lemma 2.1 in [4]),

$$\int_0^\pi g(n\theta + \gamma(\theta)) f(\theta)\,\mathrm{d}\theta \sim \frac{1}{\pi}\int_0^\pi g(\theta)\,\mathrm{d}\theta \int_0^\pi f(\theta)\,\mathrm{d}\theta$$

where g is a continuous function such that $g(\theta + \pi) = g(\theta)$, $f \in L^1([0, \pi])$, and γ is a measurable and almost everywhere finite on $[0, \pi]$ function.

Combining equations (12) and (16), we obtain the asymptotic formula relating quantum and classical Rényi entropies,

$$S_{\mathrm{Q}}(q) \sim S_{\mathrm{C}}(q) + \frac{1}{1-q} \ln \frac{2^q\Gamma(q+\frac{1}{2})}{\sqrt{\pi}\,\Gamma(q+1)} \equiv S_{\mathrm{C}}(q) + f(q) \tag{17}$$

which holds for every positive value of q such that the integrals in both sides do exist. The asymptotic difference $f(q)$ between quantum and classical Rényi entropies is a monotonically decreasing function of q for $q \geqslant 0$ (see figure 1), with $f(0) = 0$ and $f(q) \to -\ln 2$ in the limit $q \to \infty$, as may be readily shown by applying the Stirling approximation [17],

$$\Gamma(z) \sim \sqrt{2\pi}\, z^{z-1/2}\mathrm{e}^{-z}$$

to the gamma functions in (17). In the limit $q \to 1$, using L'Hôpital's rule and taking into account that, if n is a non-negative integer,

$$\psi(n+1) = -\gamma + \sum_{k=1}^{n}\frac{1}{k} \qquad \psi\left(n+\frac{1}{2}\right) = -\gamma - 2\ln 2 + \sum_{k=1}^{n}\frac{1}{k-\frac{1}{2}} \tag{18}$$

where $\psi(z) = \Gamma'(z)/\Gamma(z)$ is the logarithmic derivative of the gamma function and γ is Euler's constant [17,18], we readily find that $f(1) = -1 + \ln 2$, thus recovering the asymptotic formula for the quantum Shannon entropy (2).

For the discrete probability distribution $\{P_k^{(\Delta x)}\}$, the q-order Rényi entropy is given by (13). Equation (7) remains valid for Rényi entropies of arbitrary order, since in the limit $\Delta x \to 0$ (8) yields

$$\begin{aligned}
S^{(\Delta x)}(q) &= \frac{1}{1-q}\ln\left\{\sum_k [P(x_k)\Delta x]^q\right\} \\
&= \frac{1}{1-q}\ln\left\{(\Delta x)^{q-1}\sum_k [P(x_k)]^q\,\Delta x\right\} \\
&= -\ln(\Delta x) + \frac{1}{1-q}\ln\left\{\sum_k [P(x_k)]^q\,\Delta x\right\}
\end{aligned}$$

while we also have

$$S(q) = \frac{1}{1-q}\ln\left\{\sum_k \int_{(\Delta x)_k} [P(x)]^q\,\mathrm{d}x\right\} = \frac{1}{1-q}\ln\left\{\sum_k [P(x_k)]^q\,\Delta x\right\}.$$

Therefore, recalling equation (17), we find that

$$S_{\mathrm{Q}}^{(\Delta x)}(q) \sim S_{\mathrm{C}}^{(\Delta x)}(q) + \frac{1}{1-q}\ln\frac{2^q\Gamma(q+\frac{1}{2})}{\sqrt{\pi}\,\Gamma(q+1)} = S_{\mathrm{C}}^{(\Delta x)}(q) + f(q) \qquad \Delta x \to 0 \tag{19}$$

which is the generalization of (9) to Rényi entropies.

The previous statement can be made more precise as in the Shannon entropy case [5] by noting that the function $\cos^2\phi(x)$ in (15) has n zeros, which are located at the points x_k satisfying the condition

$$u(x_k) = \left(\frac{k+\frac{3}{4}}{n+\frac{1}{2}}\right)\pi \qquad k = 0, 1, \ldots, n-1.$$

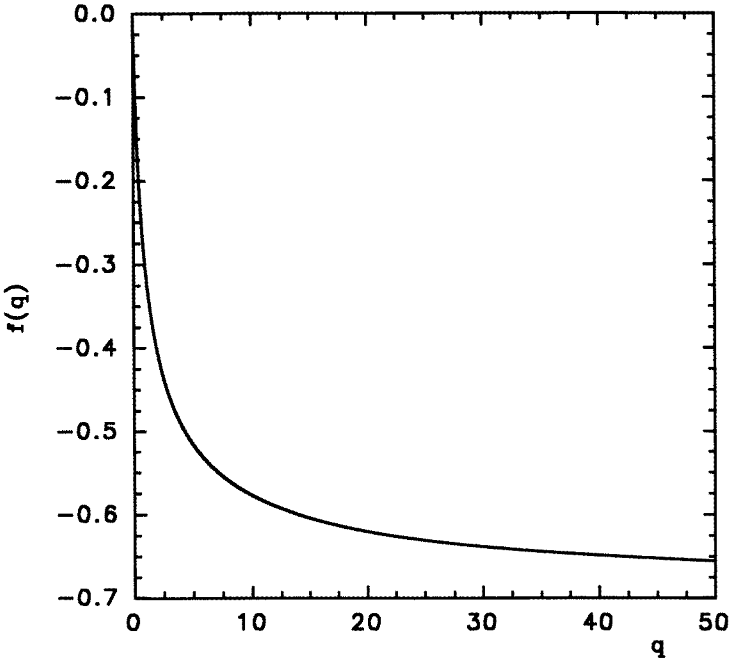

Figure 1. Asymptotic value of the difference between quantum and classical Rényi entropies of position, $S_{\mathrm{Q}}(q) - S_{\mathrm{C}}(q) \equiv f(q)$.

Therefore, the average distance between two consecutive zeros of $\cos^2\phi(x)$ is approximately equal to $(x_+ - x_-)/n$ for large n. If this distance is much less than Δx, the function $\cos^2\phi(x)$ oscillates very rapidly over each interval $(\Delta x)_k$, so that it can be replaced by the average value $\frac{1}{2}$ in the calculation of $P_k^{(\Delta x)}$ using equation (5) together with the WKB quantum probability density (15). We thus find that

$$S_{\mathrm{Q}}^{(\Delta x)}(q) \sim S_{\mathrm{C}}^{(\Delta x)}(q) \qquad \Delta x \gg \frac{x_+ - x_-}{n} \tag{20}$$

while in the opposite case we can make use of (19), which may be written more precisely as

$$S_{\mathrm{Q}}^{(\Delta x)}(q) \sim S_{\mathrm{C}}^{(\Delta x)}(q) + \frac{1}{1-q}\ln\frac{2^q\Gamma(q+\frac{1}{2})}{\sqrt{\pi}\,\Gamma(q+1)} \qquad \Delta x \ll \frac{x_+ - x_-}{n}. \tag{21}$$

These two equations are the generalizations to Rényi entropies of (11) and (10), respectively.

For the nth stationary state of the quantum particle in a box (infinite potential well) of length L, the classical and quantum probability densities are given by [6]

$$P_{\mathrm{C}}(x) = \frac{1}{L} \qquad P_{\mathrm{Q}}(x) = \frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right) \qquad 0 \leqslant x \leqslant L. \tag{22}$$

Using (12), the corresponding Rényi entropies are found to be

$$S_{\mathrm{C}}(q) = \ln L \qquad S_{\mathrm{Q}}(q) = \ln L + \frac{1}{1-q}\ln\frac{2^q\Gamma(q+\frac{1}{2})}{\sqrt{\pi}\,\Gamma(q+1)} = \ln L + f(q)$$

so that in this case the asymptotic formula (17) holds as an exact equality, in the same way as (2). Next, we shall address the more difficult problem of verifying in the same system the validity of the asymptotic formulae for discrete entropies.

3. Calculation of the discrete entropies for the infinite well eigenstates

Let us assume that the interval $[0, L]$ is divided into N bins of length $\Delta x = L/N$, and let $P_k^{(\Delta x)}$ denote the probability of obtaining a value x such that $(k-1)\Delta x \leqslant x \leqslant k\Delta x$ $(k = 1, 2, \ldots, N)$ for the position of the particle when it is measured with a device of resolution Δx. The probabilities $P_k^{(\Delta x)}$ and the corresponding Rényi entropies for the classical density $P_{\mathrm{C}}(x)$ are easily computed from the first equation in (22) using (5) and (6),

$$P_k^{(\Delta x)} = \frac{1}{N} \qquad S_{\mathrm{C}}^{(\Delta x)}(q) = \ln N. \tag{23}$$

On the other hand, for the quantum density $P_{\mathrm{Q}}(x)$ given by the second equation in (22), the discrete probabilities are

$$\begin{aligned} P_k^{(\Delta x)} &= \frac{1}{N} - \frac{1}{2n\pi}\left[\sin\left(\frac{2n\pi k}{N}\right) - \sin\left(\frac{2n\pi(k-1)}{N}\right)\right] \\ &= \frac{1}{N}\left[1 - \nu\cos\left(\frac{n\pi(2k-1)}{N}\right)\right] \end{aligned} \tag{24}$$

where in the second expression we have introduced the convenient notation

$$\nu = \frac{N}{n\pi}\sin\left(\frac{n\pi}{N}\right). \tag{25}$$

The calculation of the quantum discrete entropies thus reduces to that of the sums

$$\sigma(q) \equiv \sum_{k=1}^{N} (P_k^{(\Delta x)})^q \tag{26}$$

where $P_k^{(\Delta x)}$ is given by (24). At first sight, there is only one case for which the expression of $\sigma(q)$, and hence that of $S_{\mathrm{Q}}^{(\Delta x)}(q) = (1-q)^{-1}\ln\sigma(q)$, has a simple form:

Case 1. If $2n$ is a multiple of N, which we denote as $2n = \dot{N}$, then

$$\sigma(q) = N^{1-q} \qquad S_{\mathrm{Q}}^{(\Delta x)}(q) = \ln N. \tag{27}$$

This result follows immediately from the fact that $P_k^{(\Delta x)} = 1/N$ for $2n = \dot{N}$, as can be easily shown from the first line of (24). Thus we see that in this case the asymptotic formula (20) holds as an exact identity.

Using the binomial expansion

$$(1+z)^q = \sum_{l=0}^{\infty} \binom{q}{l} z^l \qquad |z| \leqslant 1$$

where for arbitrary (i.e. not necessarily integer) values of q the binomial coefficient is defined as

$$\binom{q}{l} = \frac{\Gamma(1+q)}{\Gamma(1+q-l)l!} \tag{28}$$

the second expression for $P_k^{(\Delta x)}$ in (24) leads to

$$\sigma(q) = \frac{1}{N^q}\sum_{l=0}^{\infty}\binom{q}{l}(-\nu)^l \sum_{k=1}^{N}\cos^l\left(\frac{n\pi(2k-1)}{N}\right). \tag{29}$$

Taking into account the result

$$\sum_{k=1}^{N}\cos\left(\frac{M\pi(2k-1)}{N}\right) = \begin{cases} (-1)^{M/N}N & \text{if} \quad M = \dot{N} \\ 0 & \text{if} \quad M \neq \dot{N} \end{cases} \tag{30}$$

the second part of which follows from the summation formula [18]

$$\sum_{k=1}^{N} \cos(2k-1)x = \frac{\sin 2Nx}{2\sin x}$$

we see that the $l = 1$ term in equation (29) is identically zero, since $\nu = 0$ if $n = \dot{N}$ and otherwise the summation over k equals zero. Therefore, (29) can be written as

$$\sigma(q) = \frac{1}{N^q}\Bigg[\sum_{m=0}^{\infty}\binom{q}{2m}\nu^{2m}\sum_{k=1}^{N}\cos^{2m}\left(\frac{n\pi(2k-1)}{N}\right) - \sum_{m=2}^{\infty}\binom{q}{2m-1}\nu^{2m-1}\sum_{k=1}^{N}\cos^{2m-1}\left(\frac{n\pi(2k-1)}{N}\right)\Bigg]. \tag{31}$$

Using the trigonometric identities [18]

$$\cos^{2m-1} A = \frac{1}{2^{2m-2}}\sum_{j=0}^{m-1}\binom{2m-1}{j}\cos[(2m-2j-1)A]$$

$$\cos^{2m} A = \frac{1}{2^{2m}}\binom{2m}{m} + \frac{1}{2^{2m-1}}\sum_{j=0}^{m-1}\binom{2m}{j}\cos[(2m-2j)A]$$

with $A = n\pi(2k-1)/N$, (31) reads

$$\begin{aligned}\sigma(q) = \frac{1}{N^{q-1}}\Bigg[&\sum_{m=0}^{\infty}\binom{q}{2m}\binom{2m}{m}\left(\frac{\nu}{2}\right)^{2m} + \frac{2}{N}\sum_{m=1}^{\infty}\binom{q}{2m}\left(\frac{\nu}{2}\right)^{2m}\sum_{j=0}^{m-1}\binom{2m}{j}\\ &\times\sum_{k=1}^{N}\cos\left(\frac{(2m-2j)n\pi(2k-1)}{N}\right)\\ &-\frac{2}{N}\sum_{m=2}^{\infty}\binom{q}{2m-1}\left(\frac{\nu}{2}\right)^{2m-1}\sum_{j=0}^{m-2}\binom{2m-1}{j}\\ &\times\sum_{k=1}^{N}\cos\left(\frac{(2m-2j-1)n\pi(2k-1)}{N}\right)\Bigg]\end{aligned} \tag{32}$$

where: (i) in the second term the lower bound zero in the summation over m has been replaced by one since the summation over j is empty for $m = 0$, and (ii) in the last term the upper bound $m-1$ in the summation over j has been replaced by $m-2$ by noting that the $j = m-1$ term vanishes because of equation (30). It is worth noting that, recalling the definition of the Pochhammer symbol $(z)_k$,

$$(z)_k = \frac{\Gamma(z+k)}{\Gamma(z)} = (-1)^k\frac{\Gamma(1-z)}{\Gamma(1-z-k)} \tag{33}$$

and taking advantage of the duplication formula for the gamma function [17, 18],

$$\Gamma(2z) = \frac{2^{2z-1}}{\sqrt{\pi}}\Gamma(z)\Gamma\left(z+\frac{1}{2}\right) \tag{34}$$

the first term in the right-hand side of (32) can be written as a Gauss hypergeometric function $F(a, b; c; z) = {}_2F_1(a, b; c; z)$,

$$\begin{aligned}\sum_{m=0}^{\infty}\binom{q}{2m}\binom{2m}{m}\left(\frac{\nu}{2}\right)^{2m} &= \sum_{m=0}^{\infty}\frac{(-q/2)_m((1-q)/2)_m}{(1)_m}\frac{\nu^{2m}}{m!}\\ &= F\left(-\frac{q}{2}, \frac{1-q}{2}; 1; \nu^2\right).\end{aligned} \tag{35}$$

In general, the alternative expression for $\sigma(q)$ that we have just obtained is rather cumbersome, and hence less useful than the original one for practical calculations. However, from it we can single out a second particular case where the expressions of $\sigma(q)$ and $S_{\mathrm{Q}}^{(\Delta x)}(q)$ have a remarkably simple form:

Case 2. If $q \geqslant 2$ is an integer, and, either $n = \dot{N}$, or $kn \neq \dot{N}$ for any integer k such that $2 \leqslant k \leqslant q$, then

$$\begin{aligned} \sigma(q) &= N^{1-q} F\left(-\frac{q}{2}, \frac{1-q}{2}; 1; \nu^2\right) \\ S_{\mathrm{Q}}^{(\Delta x)}(q) &= \ln N + \frac{1}{1-q} \ln F\left(-\frac{q}{2}, \frac{1-q}{2}; 1; \nu^2\right). \end{aligned} \tag{36}$$

In the case when $n = \dot{N}$, this result is simply a particular instance of case 1, since then $\nu = 0$ and the value of the hypergeometric function in (36) is unity. On the other hand, under the second condition, equation (30) implies that every summation over j in (32) equals zero. Therefore, the only non-vanishing term in the right-hand side of this equation is the first one, and (35) then leads to the result stated above. It is interesting to note that, for integer values of q, equation (36) holds whenever $N > qn$.

As an immediate application of the theorems constituting cases 1 and 2, we can write down the complete analytical expression of $\sigma(2)$,

$$\sigma(2) = \begin{cases} N^{-1} & \text{if} \quad 2n = \dot{N} \\ N^{-1} F(-1, -\frac{1}{2}; 1; \nu^2) = N^{-1}(1 + \frac{1}{2}\nu^2) & \text{if} \quad 2n \neq \dot{N} \end{cases}.$$

The values of the difference between the quantum Rényi entropy of order 2, $S_{\mathrm{Q}}^{(\Delta x)}(2) = -\ln \sigma(2)$, and its classical counterpart, $S_{\mathrm{C}}^{(\Delta x)}(2) = \ln N$, are displayed in figure 2 for $n = 10$, $1 \leqslant N \leqslant 50$. Expressions of the same kind can be written for any integer value of q, although they become increasingly cumbersome as q increases because of the large number of particular cases that need to be considered. On the other hand, if q is not an integer, then the expansion of $\sigma(q)$ in (32) is actually an infinite series, and (leaving aside the case $n = \dot{N}$) equation (36) only would hold provided that $kn \neq \dot{N}$ for every integer $k \geqslant 2$; however, this assumption cannot be fulfilled, since $kn = \dot{N}$, at least, whenever $k = \dot{N}$.

Differentiating equation (28) with respect to q, we obtain

$$\frac{\partial}{\partial q} \binom{q}{l}\bigg|_{q=1} = \frac{\psi(2) - \psi(2-l)}{\Gamma(2-l) l!}.$$

If p is a non-negative integer, both $\Gamma(z)$ and $\psi(z)$ have simple poles for $z = -p$, with residues $(-1)^p/p!$ and -1 respectively [17]. Therefore, for $l \geqslant 2$ the previous formula simplifies to

$$\frac{\partial}{\partial q} \binom{q}{l}\bigg|_{q=1} = \frac{(-1)^l}{l(l-1)} \qquad l \geqslant 2.$$

Using this result, the Boltzmann–Shannon entropy can be evaluated from (32) as

$$\begin{aligned} S_{\mathrm{Q}}^{(\Delta x)} = -\left.\frac{\partial \sigma(q)}{\partial q}\right|_{q=1} &= \ln N - \sum_{m=1}^{\infty} \frac{(2m-2)!}{(m!)^2} \left(\frac{\nu}{2}\right)^{2m} \\ &\quad - \frac{2}{N} \sum_{m=1}^{\infty} \frac{1}{2m(2m-1)} \left(\frac{\nu}{2}\right)^{2m} \sum_{j=0}^{m-1} \binom{2m}{j} \sum_{k=1}^{N} \cos\left(\frac{(2m-2j)n\pi(2k-1)}{N}\right) \\ &\quad - \frac{2}{N} \sum_{m=2}^{\infty} \frac{1}{(2m-1)(2m-2)} \left(\frac{\nu}{2}\right)^{2m-1} \sum_{j=0}^{m-2} \binom{2m-1}{j} \end{aligned}$$

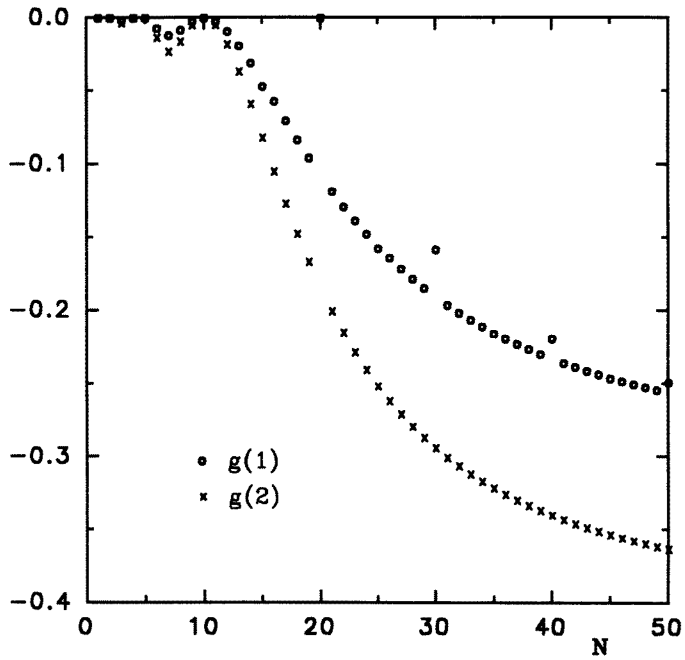

Figure 2. Difference $g(q) \equiv S_{\mathrm{Q}}^{(\Delta x)}(q) - S_{\mathrm{C}}^{(\Delta x)}(q) = S_{\mathrm{Q}}^{(\Delta x)}(q) - \ln N$ between the quantum and classical discrete entropies of position in the tenth eigenstate of the infinite potential well, for $1 \leqslant N \leqslant 50$.

$$\times \sum_{k=1}^{N} \cos\left(\frac{(2m-2j-1)n\pi(2k-1)}{N}\right). \tag{37}$$

Shifting the summation index to $p = m - 1$, and again using equations (33) and (34), we can express the first term in the right-hand side of (37) in terms of a ${}_3F_2$ hypergeometric function,

$$\begin{aligned} \sum_{m=1}^{\infty} \frac{(2m-2)!}{(m!)^2} \left(\frac{\nu}{2}\right)^{2m} &= \frac{\nu^2}{4} \sum_{p=0}^{\infty} \frac{(\frac{1}{2})_p (1)_p}{[(2)_p]^2} \nu^{2p} \\ &= \frac{\nu^2}{4}\, {}_3F_2\left(\frac{1}{2}, 1, 1; 2, 2; \nu^2\right). \end{aligned} \tag{38}$$

As happens for $S_{\mathrm{Q}}^{(\Delta x)}(q)$ when q is not an integer, no compact expression can be found for $S_{\mathrm{Q}}^{(\Delta x)}$ unless the condition of case 1 holds. From the numerical values displayed in figure 2 for $n = 10$, $1 \leqslant N \leqslant 50$, we see that the behaviour of the discrete Shannon entropy is qualitatively similar to that of the order-two Rényi entropy, excepting the case when $N = \dot{n}$, $N > 2n$. We also verify the inequality $S_{\mathrm{Q}}^{(\Delta x)} = S_{\mathrm{Q}}^{(\Delta x)}(1) \geqslant S_{\mathrm{Q}}^{(\Delta x)}(2)$, which illustrates the fact that for a fixed probability distribution the Rényi entropy is a non-increasing function of the parameter q [11, 12].

4. Limiting cases

For the infinite well, where $x_+ - x_- = L$, the conditions $\Delta x \gg (x_+ - x_-)/n$ and $\Delta x \ll (x_+ - x_-)/n$ are equivalent to $N \ll n$ and $N \gg n$, respectively. In the following, we shall show that, in the limits $N/n \to 0$ and $N/n \to \infty$, $S_{\mathrm{Q}}^{(\Delta x)}(q)$ is approximately given by equations (27) and (36), respectively, and, as a consequence, the asymptotic formulae (20) and (21) are verified.

From equation (25), we readily see that the $N/n \to 0$ limit corresponds to $\nu \to 0$. Therefore, according to (24), in this limit the quantum value of $P_k^{(\Delta x)}$ tends to the classical one, which already suffices to verify the validity of (20). More precisely, writing

$$\sum_{k=1}^{N} \cos^l \left(\frac{n\pi(2k-1)}{N} \right) = N \cos\alpha_l$$

(in particular, $\cos\alpha_0 = 1$), equation (31) yields

$$\sigma(q) = N^{1-q}[1 + \mathrm{O}(\nu^2)] \qquad S_{\mathrm{Q}}^{(\Delta x)}(q) = \ln N + \mathrm{O}(\nu^2) \tag{39}$$

so that $S_{\mathrm{Q}}^{(\Delta x)}(q) \to \ln N = S_{\mathrm{C}}^{(\Delta x)}(q)$ as $N/n \to 0$.

Next we consider the limit $N/n \to \infty$. From equation (30) we see that, in the right-hand side of (32), the mth terms in the second and third summations over m do both vanish if $N > 2mn$. Therefore, only the values of m satisfying the inequality $m > N/(2n)$ can give a non-zero contribution to these two series, whose convergence then implies that they must tend to zero as $N/n \to \infty$. We thus conclude that in this limit the only non-vanishing term in the right-hand side of (32) is the first one, so that, recalling equation (35), $\sigma(q)$ and $S_{\mathrm{Q}}^{(\Delta x)}(q)$ are approximately given by (36),

$$\begin{aligned} &\sigma(q) \to N^{1-q} F\left(-\frac{q}{2}, \frac{1-q}{2}; 1; \nu^2\right) \\ &S_{\mathrm{Q}}^{(\Delta x)}(q) \to \ln N + \frac{1}{1-q} \ln F\left(-\frac{q}{2}, \frac{1-q}{2}; 1; \nu^2\right) \qquad N/n \to \infty. \end{aligned} \tag{40}$$

Furthermore, from equation (25) we see that $\nu \to 1$ as $N/n \to \infty$, so that we have

$$S_{\mathrm{Q}}^{(\Delta x)}(q) \to \ln N + \frac{1}{1-q} \ln F\left(-\frac{q}{2}, \frac{1-q}{2}; 1; 1\right) \qquad N/n \to \infty. \tag{41}$$

Finally, taking advantage of the well known Gauss formula [17]

$$F(a, b; c; 1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} \qquad \mathrm{Re}\,(c-a-b) > 0 \qquad c \neq 0, -1, -2, \ldots$$

equation (41) simplifies to

$$S_{\mathrm{Q}}^{(\Delta x)}(q) \to \ln N + \frac{1}{1-q} \ln \frac{\Gamma(q+\frac{1}{2})}{\Gamma(q/2+1)\Gamma(q/2+\frac{1}{2})} \qquad N/n \to \infty. \tag{42}$$

Using (34), the right-hand side of the previous equation is readily shown to be equivalent to that of (21).

In the case $q = 1$, using equations (37) and (38) a similar reasoning shows that

$$S_{\mathrm{Q}}^{(\Delta x)} \to \ln N - \frac{\nu^2}{4}\, {}_3F_2\left(\frac{1}{2}, 1, 1; 2, 2; \nu^2\right) \qquad N/n \to \infty. \tag{43}$$

From figure 2 we see that, if $N > n$ and $N \neq \dot{n}$, the right-hand side of (43) provides a good approximation to $S_{\mathrm{Q}}^{(\Delta x)}$ even when N/n is not very large. Taking the limit $\nu \to 1$, we find

$$S_{\mathrm{Q}}^{(\Delta x)} \to \ln N - \tfrac{1}{4}\, {}_3F_2(\tfrac{1}{2}, 1, 1; 2, 2; 1) \qquad N/n \to \infty \tag{44}$$

and, using the result [17]

$$\begin{aligned} &{}_3F_2(a+1, 1, 1; b+1, 2; 1) = \frac{b}{a}[\psi(b) - \psi(b-a)] \\ &a \neq 0 \qquad b \neq 0, -1, -2, \ldots \qquad \mathrm{Re}\,(b-a) > 0 \end{aligned}$$

together with equation (18), (44) simplifies to

$$S_{\mathrm{Q}}^{(\Delta x)} \to \ln N - 1 + \ln 2 \qquad N/n \to \infty. \tag{45}$$

We thus verify the validity of the asymptotic formula (10) for the discrete Shannon entropy of position.

5. Conclusions and open problems

To summarize, we have derived general asymptotic formulae for the continuous and discrete Rényi entropies of position of one-dimensional quantum systems in energy eigenstates, which are given in terms of the corresponding classical entropies (i.e., the entropies computed from the position probability distribution for a microcanonical ensemble of analogous classical systems with the same energy), and these results have been analytically checked for the particle in a box (infinite potential well).

The asymptotic formula (17) for the continuous entropies defined by (12) follows directly from the semiclassical (WKB) approximation to quantum mechanics, and is valid whenever the Hamiltonian of the system satisfies some very general conditions (see section 1). In turn, from (17) the asymptotic formulae (20) and (21) are obtained for the discrete entropies defined by (13) in the limiting cases when the resolution length Δx of the position measurements is very large or very small, respectively, in comparison with the average distance between the zeros of the wavefunction.

Equations (17), (20) and (21) include as particular cases, respectively, the asymptotic formulae (2), (11) and (10) for the quantum Boltzmann–Shannon entropies of position first derived in reference [5]. As has already been pointed out in relation to (2), the existence of a non-zero asymptotic difference between classical and quantum entropies in equations (17) and (21) can be interpreted in terms of the so-called configuration form of Bohr's correspondence principle (4), with the correction term $f(q)$ arising from the fact that Rényi entropies can be written as the expected value of a quantity that depends explicitly on the probability distribution itself (see equation (12)). It is also worth noting that all the results given in this paper for Rényi entropies may be written in terms of Tsallis entropies using (14), although then they take a more cumbersome and hence less appealing form.

In the particular case of the infinite potential well, the asymptotic formula for continuous entropies (17) becomes an exact identity. To check the validity of the asymptotic formulae for discrete entropies is a more difficult problem, since the explicit expressions of these entropies are, in general, rather cumbersome. However, we have seen that they reduce to remarkably simple forms in two important particular cases, which enable us to verify in a purely analytic way the validity of the limiting asymptotic relations (20) and (21). The transition between the regions of validity of these two approximations as the resolution length Δx of the position measurements decreases is depicted graphically in figure 2.

When equation (17) is used to evaluate the quantum entropy $S_{\mathrm{Q}}(q)$ for large n, it is important to know the rate of convergence of the actual values of $S_{\mathrm{Q}}(q)$ to the asymptotical value in the right-hand side. That is, to know the next term in the asymptotic expansion of $S_{\mathrm{Q}}(q)$ for $n \gg 1$, whose leading term is given by (17). Numerical and analytical studies carried out for some particular systems [3, 5] suggest that (17) may be improved to

$$S_{\mathrm{Q}}(q) \sim S_{\mathrm{C}}(q) + \frac{1}{1-q} \ln \frac{2^q \Gamma(q+\frac{1}{2})}{\sqrt{\pi}\,\Gamma(q+1)} + k(q) n^{-\epsilon} + \mathrm{o}(n^{-\epsilon}) \qquad \epsilon > 0$$

so that when (17) is used the error in the estimation of the quantum entropies falls off according to a power law (the function $k(q)$ and the constant ϵ depend on the considered system).

However, to prove (or disprove) that the previous formula holds indeed in the general case is a very difficult problem, whose solution would require the use of a higher-order WKB approximation and a stronger version of the key theorem used in section 2 (lemma 2.1 in [4]), and, up to now, we have not been able to obtain any result of this kind.

The generalization of the asymptotic formulae obtained in this paper to the D-dimensional case is straightforward for systems whose Hamiltonian is completely separable in Cartesian coordinates [5],

$$H = \sum_{i=1}^{D} H_i(x_i, p_i).$$

Both the quantum and classical probability densities for position are then products of D one-dimensional densities. Since the entropy $S(q)$ is now defined by the D-dimensional generalization of equation (12), $S_Q(q)$ and $S_C(q)$ are sums of D one-dimensional entropies. Therefore, if every one-dimensional Hamiltonian H_i has the form (3), so that equation (17) is valid for each coordinate, in the limit $n_i \gg 1$, $i = 1, \ldots, D$, we have the asymptotic formula

$$S_Q(q) \sim S_C(q) + \frac{D}{1-q} \ln \frac{2^q \Gamma(q+\frac{1}{2})}{\sqrt{\pi}\,\Gamma(q+1)} = S_C(q) + Df(q)$$

which becomes an exact equality for the D-dimensional infinite potential well. The asymptotic formulae for discrete entropies (20) and (21) can be generalized likewise. However, the problem of finding the asymptotic relation between quantum and classical entropies of position for D-dimensional systems whose Hamiltonian is not of the above form remains to be solved. Interesting open problems are also the calculation of the discrete entropies of position for the stationary states of other physically relevant quantum systems, and the derivation of general asymptotic formulae for the quantum entropies in momentum space.

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