Convexity inequalities for estimating free energy and relative entropy

Mary Beth Ruskai† and Frank H Stillinger

AT&T Bell Laboratories, Murray Hill, NJ 07974, USA

Abstract. For quantum systems, it is shown that the relative entropy $S(P, Q) = -\text{Tr } P \log P + \text{Tr } P \log Q$ of two positive semi-definite operators P and Q satisfies $\gamma^{-1} \text{Tr}[P - P^{1+\gamma}Q^{-\gamma}] \leq S(P, Q) \leq \gamma^{-1} \text{Tr}[P^{1-\gamma}Q^{\gamma} - P]$ for $0 < \gamma \leq 1$, and that these bounds become exact in the limit $\gamma \to 0$. Analogous inequalities hold, for states in classical statistical mechanics or information theory, with trace replaced by integration or summation. Furthermore, the average of these bounds is, in general, a better approximation to $S(P, Q)$ than either bound alone, and the average is amenable to further improvement via repeated Richardson extrapolation.

If P and Q are Gibbs equilibrium states, then these inequalities can also be used to obtain bounds on the free energy of a perturbed system in terms of the free energy of the unperturbed system and expectations of the perturbation. Several examples are presented which illustrate the salient features of these bounds and estimates in a variety of systems.

A new expression for estimating the error from repeated extrapolation is given in an appendix on Richardson extrapolation.

1. Introduction

Only a few of the many statistical mechanical models of physical interest have been solved explicitly. While the search for more exactly solvable cases continues, the demands of physical science require the introduction and exploitation of approximate solutions. Unfortunately, many of these approximation schemes are uncontrolled, and thus leave unresolved serious questions about the validity and reliability of their implications.

An especially useful class of approximations in classical statistical mechanics stems from an inequality of Gibbs (often referred to as the Gibbs-Bogoliubov inequality) that provides rigorous bounds on both free energies and relative entropy [1]. Many examples can be found in the literature [2, 3]. The corresponding inequality in quantum statistical mechanics, which has been attributed to Bogoliubov [4, 5], can be derived from an inequality of Peierls [6]. Equivalent inequalities can be found in an earlier paper‡ of Delbrück and Moliére [7]. All of these inequalities can be considered as either special cases, or generalisations, of the well known Jensen's inequality for convex functions [8] (which might more appropriately be called the Hölder-Jensen [9, 10]

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† 1988-89 Sabbatical Visitor; on leave from Department of Mathematics, University of Lowell, Lowell, MA 01854, USA (permanent address).
‡ This rather obscure 1936 paper is the earliest reference we know of to inequalities of this type in the quantum case. Section 8 of this remarkable paper also contains proofs of many properties of quantum mechanical entropy including concavity, subadditivity, and the extremal property of Gibbs equilibrium states.

inequality). Useful reviews of these inequalities and related properties of thermodynamic variables have been given by Falk [11], Huber [12], Thirring [13] and Wehrl [14].

This paper is devoted to the examination of convexity inequalities that extend those mentioned above. Specific numerical examples are presented which show that substantially tighter upper and lower bounds can be obtained in some cases. Furthermore, the average of these bounds, in conjunction with the well known technique of Richardson extrapolation [15, 16], can be used to generate further improvements in the estimates of thermodynamic variables. These improvements, which can be extremely accurate, provide estimates, rather than absolute bounds. However, in practice, Richardson error estimation procedures can often be used to establish that a given estimate is actually a bound. We also establish that the estimates converge rapidly with repeated extrapolation; in doing so, we derive a formula, which appears to be new, for estimating the error at the kth extrapolation.

The relevant theory is presented in section 2. Section 3 contains several specific numerical examples, as well as some analytic examples involving subsystems. This section also includes a comparison of our upper bounds to those obtainable from the subadditivity inequality for relative entropy. Finally, to make the paper self-contained, we include a brief appendix on Richardson extrapolation.

Before presenting our results, we review some basic definitions. In the classical statistical mechanics of continuous systems, a state is described by a probability density $\rho(x)$ with respect to a measure μ, i.e. $\rho(x) > 0$ and $\int \rho(x) \, d\mu(x) = 1$. The Gibbs equilibrium state for a system at temperature T whose Hamiltonian is given by the function $H(x) = H[p(x), q(x)]$ is

$$g(x) = \exp(-\beta H(x)) \left(\int \exp(-\beta H(x)) \, d\mu(x) \equiv \exp\{\beta[F - H(x)]\} \right)^{-1}$$

where $\beta = 1/T$, $F = -\beta^{-1} \log \int \exp(-\beta H(x)) \, d\mu(x)$ denotes the Gibbs free energy; and, for simplicity, we have chosen to work in units in which Boltzmann's constant is 1. The entropy of the state ρ can then be defined as

$$S(\rho) = - \int \rho(x) \log \rho(x) \, d\mu(x).$$

In classical discrete (i.e. lattice) systems, a state is defined by a set of discrete probabilities $p_k > 0$ normalised so that $\Sigma_k p_k = 1$. The entropy is defined by

$$S(p) = - \sum_k p_k \log p_k.$$

In quantum statistical mechanics, a state is described by a density matrix P, i.e. a positive semi-definite operator on a Hilbert space $\mathcal{H}$ satisfying $\operatorname{Tr} P = 1$. The Gibbs equilibrium state of a self-adjoint, semi-bounded Hamiltonian operator H is

$$P = \exp(-\beta H) / \operatorname{Tr} \exp(-\beta H) \equiv \exp(\beta[F - H])$$

where β is as above and the free energy satisfies $F = -\beta^{-1} \log \operatorname{Tr} \exp(-\beta H)$. The entropy of P is defined by

$$S(P) = -\operatorname{Tr} P \log P \equiv - \sum_k \lambda_k \log \lambda_k$$

where $\{\lambda_k\}$ denote the eigenvalues of P, and we interpret '$0 \log 0$' as 0.

In the quantum case, the differences between continuous and discrete systems are reflected in the choice of Hilbert space and Hamiltonian. The mathematical formalism,

as described above, is identical in both situations. It is also worth pointing out that the mathematical formalism for the two types of classical systems is identical to that used in information theory (see, e.g., [17-19]). Although we will emphasise applications to statistical mechanics, we anticipate that our results will also be of interest to those who work in information theory, signal analysis, and related areas.

In order to treat simultaneously the three basic types of systems described above, let τ denote integration, summation, or trace respectively, depending on the type of system so that, e.g.

$$S(P) = -\tau(P \log P) \tag{1}$$

denotes the entropy of the state P. Although one could use traces on von Neumann algebras or non-commutative measure theory to justify this [20-23], and even extend our results to general von Neumann algebras [23, 24], we will not require this level of sophistication. We merely regard τ as a notational convenience to emphasise that our techniques can be applied to any of the usual statistical mechanical formalisms, as well as to the corresponding situations in information theory.

With this notation, the relative entropy of the states P and Q can be defined as

$$S(P, Q) \equiv -\tau(P \log P) + \tau(P \log Q). \tag{2}$$

(It should be noted that there is some disagreement in the literature about both the order of the arguments in, and the sign of, $S(P, Q)$.) If

$$P = \exp[\beta(F_0 - H_0)] \qquad \text{and} \qquad Q = \exp\{\beta[F_1 - (H_0 + V)]\} \tag{3}$$

are Gibbs states for which the Hamiltonian corresponding to Q, namely $H = H_0 + V$, is a perturbed version of that for P, then

$$S(P, Q) = \beta[F_1 - F_0 - \tau(PV)]. \tag{4}$$

This identity implies that bounds on $S(P, Q)$ can be used to generate bounds on the free energy of the perturbed system.

Rather than using the exponential form of the Gibbs–Peierls–Bogoliubov inequality, we will use an equivalent logarithmic version known as Klein's inequality[†] [25] (see also [7, 11-14, 21, 26, 27]). This inequality can be stated as

$$S(P, Q) = -\tau(P \log P) + \tau(P \log Q) \leq \tau(Q - P). \tag{5}$$

Since $\tau(Q - P) = 0$ if both states are normalised, it follows immediately that $S(P, Q) \leq 0$ in this case. Furthermore, if P and Q are given by (3), it then follows that

$$F_1 \leq F_0 + \tau(PV). \tag{6}$$

Similarly, by considering $S(Q, P)$, one finds

$$F_1 \geq F_0 + \tau(QV). \tag{7}$$

The upper bound (6) to F_1 uses only information about the unperturbed state, whereas the lower bound (7) also requires an estimate involving the perturbed state.

[†] Several authors [13, 14, 26] use the term Klein's inequality for the more general inequality $\tau[f(A) - f(B) - (A - B)f'(B)] \geq 0$, where f is convex, although only (5) appears in [25].

2. Theory

By letting $x \to x^{\pm \gamma}$ in the elementary inequality

$$\log x \leq x - 1 \qquad \forall x \geq 0$$

one readily concludes that

$$1 - x^{-\gamma} \leq \gamma \log x \leq x^{\gamma} - 1. \tag{8}$$

This observation leads to our main result.

Theorem. If P and Q are states, then

$$\gamma^{-1} \tau [P - P^{1+\gamma} Q^{-\gamma}] \leq S(P, Q) \leq \gamma^{-1} \tau [P^{1-\gamma} Q^{\gamma} - P]. \tag{9}$$

Proof. By first letting $x = a/b$ in (8) and then multiplying by a/γ, one finds

$$\gamma^{-1} [a - a^{1+\gamma} b^{-\gamma}] \leq -a \log a + a \log b \leq \gamma^{-1} [a^{1-\gamma} b^{\gamma} - a] \qquad \forall a, b > 0. \tag{10}$$

This result also holds in a suitable limiting sense when a and b are both zero. The theorem then follows easily for classical systems. For continuous systems it suffices to let $a = p(x)$ and $b = q(x)$ and integrate; whereas for discrete systems, one should choose $a = p_k$, $b = q_k$, and sum over k. Completion of the proof in the quantum case is somewhat more subtle, and follows the strategy given in Ruelle [26] for establishing Klein's inequality. Let $\{a_j\}$ and $\{b_k\}$ denote the eigenvalues of P and Q, and let $\{\alpha_k\}$ and $\{\beta_k\}$ denote the corresponding eigenfunctions. It then follows from (10) that

$$\sum_j \sum_k |\langle \alpha_j, \beta_k \rangle|^2 \{\gamma^{-1} [a_j - a_j^{1+\gamma} b_k^{-\gamma}] + a_j \log a_j - a_j \log b_k\}$$

$$\leq 0 \leq \sum_j \sum_k |\langle \alpha_j, \beta_k \rangle|^2 \{\gamma^{-1} [a_j^{1-\gamma} b_k^{\gamma} - a_j] + a_j \log a_j - a_j \log b_k\}. \tag{11}$$

In each of the double sums the quantities in brackets are all of one sign, so that these sums either converge absolutely or diverge to $\pm \infty$. The desired inequality (9) then follows from standard properties of the trace and the fact that

$$\tau [f(P) G(Q)] = \sum_j \sum_k |\langle \alpha_j, \beta_k \rangle|^2 [f(a_j) g(b_k)] \tag{12}$$

where (12) should be regarded as the definition of $\tau [f(P) g(Q)]$ if $f(P)$ or $g(Q)$ is unbounded. $\qquad \square$

Note that $\gamma = 1$ corresponds to the usual Klein's inequality (5). Because there is a correlation between the magnitude of $S(P, Q)$, and the extent to which $\tau(P^{1-\gamma} Q^{\gamma})$ deviates from $\tau(Q)$, one expects significant improvement in precisely those cases where (5) is very bad. The examples presented in the next section show that this is indeed true.

Although the upper bound will always be finite, the lower bound may diverge to $-\infty$. We will show how to combine these bounds with Richardson extrapolation to obtain very accurate estimates when both are finite. In actual applications, it is often necessary to restrict the system to a finite volume, and then take the thermodynamic limit, in order to insure that intensive thermodynamic variables like the free energy and entropy per degree of freedom are finite. We expect that these cut-off procedures will also suffice to yield finite lower bounds, so that the extrapolation procedure

described below can be widely applied. Before giving the details of our procedure, it will be useful to introduce some notation and to make a few technical remarks.

For a fixed pair of states P and Q let

$$u(\gamma) \equiv u_{PQ}(\gamma) \equiv \begin{cases} \gamma^{-1}\tau[P^{1-\gamma}Q^{\gamma} - P] & \gamma \neq 0 \\ S(P, Q) & \gamma = 0. \end{cases} \tag{13}$$

Then our new bounds can be rewritten in the form

$$u(-\gamma) \leq S(P, Q) \leq u(\gamma) \qquad \forall 0 \leq \gamma \leq 1. \tag{14}$$

With this definition, one expects u to be continuous at $\gamma = 0$ and analytic in a neighbourhood of 0. We now assume that u is analytic in the disk $D_{\Gamma} = \{z: |z| < \Gamma\}$ for some $\Gamma > 0$, and depending on P and Q. The validity of this assumption, which we expect to be satisfied in those situations in which these estimates are computationally useful, is discussed in appendix 2. In particular, in the case of quantum systems, it is shown that $\Gamma_{PQ} = \sup\{|\gamma|: -u_{PQ}(-\gamma) < \infty\}$ when Tr $P = $ Tr Q.

The analyticity of u implies

$$u(\gamma) = S(P, Q) + u'(0)\gamma + O(\gamma^2) \tag{15}$$

so that the error in estimating $S(P, Q)$ by either the upper bound $u(\gamma)$ or lower bound $u(-\gamma)$ is $O(\gamma)$, with the leading linear term identical, except for sign, for the two bounds. Therefore,

$$\begin{aligned} \mathrm{av}(\gamma) &\equiv \tfrac{1}{2}[u(\gamma) + u(-\gamma)] \\ &= (1/2\gamma)\tau(P^{1-\gamma}Q^{\gamma} - P^{1+\gamma}Q^{-\gamma}) \\ &= S(P, Q) + O(\gamma^2). \end{aligned} \tag{16}$$

This suggests that the average of the two bounds will, in general, be a much better approximation than either bound. The results in tables 1–3 show that this is indeed the case, and that the improvement can be quite significant even when the individual bounds are far from optimal.

Moreover, since $\mathrm{av}(\gamma)$ is even and analytic, it can be written in the form

$$\mathrm{av}(\gamma) = S(P, Q) + \sum_{k=1}^{\infty} c_k \gamma^{2k} \tag{17}$$

where the coefficients $\{c_k\}$ depend on P and Q. This implies that $\mathrm{av}(\gamma)$ is amenable to Richardson extrapolation for improving the estimates even further.

Although, in general, $\mathrm{av}(\gamma)$ can be either larger or smaller than the exact value for $S(P, Q)$, heuristic arguments suggest that it will yield a lower bound when $\tau(P) = \tau(Q)$. A simple computation shows that

$$c_1 = -\tfrac{1}{6}\tau[P(\log P - \log Q)^3]. \tag{18}$$

Proceeding as above in the quantum case, it then follows that

$$c_1 = \tfrac{1}{6}\sum_j \sum_k |\langle \alpha_j, \beta_k\rangle|^2 [a_j(-\log a_j + \log b_k)^3].$$

Terms with $a_k > b_k$ will be negative, whereas those with $a_k < b_k$ will be positive. Since terms of both signs are multiplied by a_k, one expects the negative terms (i.e. those with relatively large a_k) to dominate when $\Sigma_k a_k = \Sigma_k b_k$. A similar analysis could be made in the classical cases. In practice, the Richardson error estimate $\tfrac{1}{3}[\mathrm{av}(\gamma) - \mathrm{av}(2\gamma)]$ can be used to determine whether or not the expectation $\mathrm{av}(\gamma) \leq S(P, Q)$ actually holds.

Some additional insights into the nature and potential uses of these estimates can be obtained by rewriting $u(\gamma)$ and $\mathrm{av}(\gamma)$ in the form

$$u(\gamma) = \gamma^{-1}\tau[P \exp(\gamma W) - P] \tag{19}$$

$$\mathrm{av}(\gamma) = \gamma^{-1}\tau[P \sinh(\gamma W)] \tag{20}$$

where

$$W = \gamma^{-1} \log(P^{-\gamma/2} Q^\gamma P^{-\gamma/2}). \tag{21}$$

For simplicity, we first discuss commutative situations, in which case

$$W = \log Q - \log P \qquad \text{and} \qquad S(P, Q) = \tau(PW). \tag{22}$$

Then our estimates can be written as

$$\gamma^{-1}\tau[P(1 - \exp(-\gamma W))] \leq \tau(PW) \leq \gamma^{-1}\tau[P(\exp(\gamma W) - 1)] \tag{23}$$

and

$$\tau(PW) \approx \gamma^{-1}\tau[P \sinh(\gamma W)]. \tag{24}$$

Note that these estimates have the same form as elementary inequalities for the real variable functions $\exp(\gamma x)$ and $\sinh(\gamma x)$. If, furthermore, P and Q denote Gibbs states of the form (3), then

$$W = \beta[F_1 - F_0 - V] = \beta[\Delta F - V] \qquad \text{where } \Delta F = F_1 - F_0$$

so that these relationships can be further rewritten as

$$\tau[\![P\{1 - \exp[\gamma\beta(-\Delta F + V)]\}]\!] \leq \gamma\beta[\Delta F - \tau(PV)] \leq \tau[\![P\{\exp[\gamma\beta(\Delta F - V)] - 1\}]\!] \tag{25}$$

and

$$\gamma\beta[\Delta F - \tau(PV)] \approx \tau\{P \sinh[\gamma\beta(\Delta F - V)]\}. \tag{26}$$

Since $\gamma\beta = \gamma/T$, decreasing γ from 1 toward 0 is equivalent to letting the temperature T increase toward ∞. Thus γ can be regarded as a rescaling of the temperature, but with the entropy and free energy fixed at the equilibrium values determined by the original temperature.

Because ΔF occurs in all terms of (25), these inequalities yield estimates rather than absolute bounds on the free energy. One can obtain such estimates by rewriting (26) in the form

$$\phi - \gamma\beta\tau(PV) \approx \tfrac{1}{2}\{e^\phi\tau[P \exp(-\gamma\beta V)] - e^{-\phi}\tau[P \exp(\gamma\beta V)]\} \tag{27}$$

where $\phi = \gamma\beta\Delta F$. This gives an approximate transcendental equation for ϕ, which can be solved numerically for any fixed value of $\gamma\beta$ to determine the corresponding approximation to ΔF.

If P and Q do not commute, then $W = W(\gamma) = \gamma^{-1} \log(P^{-\gamma/2} Q^\gamma P^{-\gamma/2})$ will depend upon γ. If P and Q are strictly positive matrices on a finite-dimensional Hilbert space $\mathcal{H}$, then (22) can be replaced by

$$\lim_{\gamma \to 0} W(\gamma) = \log Q - \log P \tag{28}$$

$$S(P, Q) = \lim_{\gamma \to 0} \tau[PW(\gamma)]. \tag{29}$$

However, in the general case $W(\gamma)$ will be unbounded so that the existence of these formal limits is much more subtle. It is shown in appendix 2 that (29) holds when

$u(\gamma)$ is analytic. In any case, (23) still holds with W replaced by $W(\gamma)$; similarly, both (23) and (24) remain valid if $\tau(PW)$ is replaced by $S(P, Q)$ as well as W by $W(\gamma)$. The discussion for the Gibbs states is more complicated since, in this case,

$$W = \beta \Delta F + \gamma^{-1} \log\{\exp(\gamma\beta H_0/2) \exp[-\gamma\beta(H_0 + V)] \exp(\gamma\beta H_0/2)\} \equiv \beta[\Delta F - \tilde{V}(\gamma)].$$

Then (25)-(27) must be modified by substituting the effective potential $\tilde{V} = \tilde{V}(\gamma)$ for V; the appropriate transcendental equation for $\phi = \gamma\beta\Delta F$ thus becomes

$$\phi - \gamma\beta\tau(PV) \approx \tfrac{1}{2}\{e^{\phi}\tau[P \exp(-\gamma\beta\tilde{V})] - e^{-\phi}\tau[P \exp(\gamma\beta\tilde{V})]\}. \tag{30}$$

A final curious observation can be made by recalling that, for functions of real variables, $\sinh x \approx x \approx \sin x$ when $x \approx 0$. This suggests that one might also consider the estimates

$$S(P, Q) \approx \gamma^{-1}\tau[P \sin(\gamma W)] \quad \text{and} \quad \gamma\beta[\Delta F - \tau(PV)] \approx \tau\{P \sin[\gamma\beta(\Delta F - \tilde{V})]\}.$$

Although these approximations are also valid, we see no obvious way to exploit this observation in practical computations. The estimates involving $\sinh(\gamma W)$ are easily computed if efficient methods are available to calculate the real roots P^{γ} and Q^{γ}, along with the corresponding integrals or traces. (In fact, an efficient method for computing square roots[†], together with a procedure for evaluating $u(\gamma)$ when γ is a dyadic rational of the form 2^{-k} or $(2^k \pm 1)/2^k$, is all that is required for Richardson extrapolation.) However, we are unaware of any techniques for evaluating $P^{i\gamma}$ and $Q^{i\gamma}$ which are computationally efficacious.

3. Examples

Most of the features of these new bounds and estimates are illustrated by a simple two-level classical discrete example. Let $Q = \{1 - \varepsilon, \varepsilon\}$ and $P = \{\varepsilon, 1 - \varepsilon\}$ where ε is a small, positive real number. Then $S(P, Q) = (1 - 2\varepsilon) \log[\varepsilon/(1 - \varepsilon)] \approx \log \varepsilon \to -\infty$ as $\varepsilon \to 0$. Because P and Q approach 0 on non-overlapping regions of their domains, this simple example effectively illustrates the essential features of the approximations described above when ε is small. For $\varepsilon = 0.05$, $S(P, Q) = -2.649\,995\,0812$. The results of our estimates for this case are summarised in tables 1 and 2.

In table 1(a), the values of the new upper bound, lower bound, and av(γ) are given for decreasing values of γ as indicated. The last two columns give both the actual error $S(P, Q) - \text{av}(\gamma)$ and an estimation of the error using Richardson extrapolation as in (A1.10) with $k = 0$.

In table 1(b), repeated extrapolation is applied to the values of av(γ) from the first five rows (i.e. $\gamma = 2^{-k}$, ($k = 0, 1 \ldots 4$)). Note that (using the notation of appendix 1) the estimate $S(P, Q) \approx R(3, 3) = -2.649\,983\,8891$, which requires only four evaluations of av(γ), is already better than that obtained from av(2^{-10}), which requires almost three times (i.e. 11) as many evaluations of av(γ); and the final estimate $R(4, 4) = -2.649\,995\,0845$ is accurate to nine significant figures.

Table 1(c) lists the ratio of successive error estimates for this example; as explained in appendix 1, this will be close to $4^{\text{col}} = 4^{k+1}$, when the hypotheses of Richardson extrapolation procedure are satisfied. Only the first three rows and columns are relevant

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[†] Higham [28, 29] has discussed efficient methods for computing the square root of a positive definite matrix.

Table 1. (Example 1) Relative entropy for a two-level classical discrete system. For $P = \{0.05, 0.95\}$ and $Q = \{0.95, 0.05\}$, $S(P, Q) = -2.649\,995\,0812\ldots$.

(*a*) Bounds and averages.

k	γ	Upper bound	Lower bound	Average	Error	Error estimate
0	1.0	0	−17.052 631 579	−8.526 315 789	5.876	0
1	0.5	−1.128 220 211	−6.304 849 566	−3.716 534 889	1.067	1.603
2	0.25	−1.762 340 697	−4.029 425 719	−2.895 883 208	0.2459	0.2736
3	0.125	−2.162 229 516	−3.258 233 737	−2.710 231 627	0.6024×10^{-1}	0.6188×10^{-1}
4	0.0625	−2.393 283 678	−2.936 672 178	−2.664 977 928	0.1498×10^{-1}	0.1508×10^{-1}
5	0.03125	−2.518 176 047	−2.789 296 031	−2.653 736 039	0.3741×10^{-2}	0.3747×10^{-2}
6	0.015625	−2.583 185 881	−2.718 674 166	−2.650 930 024	0.9349×10^{-3}	0.9353×10^{-3}
7	0.0078125	−2.616 361 208	−2.684 096 389	−2.650 228 798	0.2337×10^{-3}	0.2337×10^{-3}
8	0.00390625	−2.633 120 274	−2.666 986 745	−2.650 053 509	0.5843×10^{-4}	0.5843×10^{-4}
9	0.001953125	−2.641 543 141	−2.658 476 236	−2.650 009 688	0.1461×10^{-4}	0.1461×10^{-4}
10	0.9766×10^{-3}	−2.645 765 468	−2.654 231 998	−2.649 998 733	0.3652×10^{-5}	0.3652×10^{-5}
11	0.4883×10^{-3}	−2.647 879 363	−2.652 112 626	−2.649 995 994	0.9129×10^{-6}	0.9129×10^{-6}
12	0.2441×10^{-3}	−2.648 936 994	−2.651 053 625	−2.649 995 309	0.2282×10^{-6}	0.2282×10^{-6}
13	0.1221×10^{-3}	−2.649 465 981	−2.650 524 296	−2.649 995 138	0.5706×10^{-7}	0.5706×10^{-7}
14	0.6104×10^{-4}	−2.649 730 517	−2.650 259 674	−2.649 995 096	0.1426×10^{-7}	0.1426×10^{-7}
15	0.3052×10^{-4}	−2.649 862 795	−2.650 127 374	−2.649 995 085	0.3565×10^{-8}	0.3566×10^{-8}
16	0.1526×10^{-4}	−2.649 928 937	−2.650 061 227	−2.649 995 082	0.8896×10^{-9}	0.8919×10^{-9}

(*b*) Richardson extrapolation[†].

j	$k = 0$	$k = 1$	$k = 2$	$k = 3$	$k = 4$
0	−8.526 315 7894				
1	−3.716 534 8887	−2.113 274 5884			
2	−2.895 883 2080	−2.622 332 6478	−2.656 269 8518		
3	−2.710 231 6265	−2.648 347 7660	−2.650 082 1072	−2.649 983 8891	
4	−2.664 977 9278	−2.649 893 3615	−2.649 996 4012	−2.649 995 0408	−2.649 995 0845

(*c*) Error ratios[†].

j	Double precision					Single precision	
	$k = 0$	$k = 1$	$k = 2$	$k = 3$	$k = 4$	$k = 0$	$k = 1$
1	5.86					5.86	
2	4.42	19.57				4.42	19.57
3	4.10	16.83	72.20			4.10	16.83
4	4.03	16.20	65.95	277.15		4.03	15.47
5	4.01	16.05	64.48	261.10	1082.74	4.01	8.55
6	4.00	16.01	64.12	257.95	669.12	4.02	2.23
7	4.00	16.00	64.00	1793.67	2.31	4.24	0.39
ideal value	4	16	64	256	1024	4	16

[†] In these two tables, j and k are as defined in (A1.6) and (A1.12) respectively.

for the extrapolation given in table 1(*b*), for which double precision was used. However, we present additional values, as well as two columns for the corresponding single precision values, in order to illustrate the use of this ratio as a detector of round-off error.

To explore the effect of non-commutativity, consider a similar two-level quantum system where Q is a diagonal matrix with eigenvalues $1 - \varepsilon$ and ε and let $P = P_\theta = U_\theta Q U_\theta$ where

$$U_\theta = \begin{pmatrix} \sin\theta & \cos\theta \\ \cos\theta & -\sin\theta \end{pmatrix}$$

is a real, symmetric, orthogonal matrix corresponding to a pseudo-rotation parameterised by angle θ. When $\theta = 0$, one obtains the previous example; when $\theta = \pm\pi/2$, $P = Q$ and $S(P, Q) = u(\gamma) = 0$. For all values of θ one has

$$u_{P_\theta Q}(\gamma) = \cos^2\theta\, u_{P_0 Q}(\gamma) \qquad S(P_\theta, Q) = \cos^2\theta\, S(P_0, Q).$$

Thus, the only effect of non-commutativity is to multiply the results in tables 1(*a*) and 1(*b*) by $\cos^2\theta$. This suggests that commutativity is not an issue; the essential point is how P and Q compare in a region which one might describe as the 'approximate null space' of Q.

Several interesting examples of a different type can be obtained by considering states involving subsystems. Suppose that ρ_{12} is the state of a system composed of subsystems related by partial traces so that $\rho_1 = \tau_2(\rho_{12})$ and $\rho_2 = \tau_1(\rho_{12})$ describe states of subsystems [13, 14, 21, 23, 26, 30-34]. In the quantum case, the Hilbert space $\mathcal{H}_{12}$ for the total system is a tensor product of those for the subsystems, i.e. $\mathcal{H}_{12} = \mathcal{H}_1 \otimes \mathcal{H}_2$. Similarly, in classical situations, the probability space for the total system will be a product space with a product measure μ_{12} of the form $\mu_{12} = \mu_1 \times \mu_2$. Physically, the subsystems may represent disjoint sets of particles, or disjoint regions of phase space. If $\tau_{12}(\rho_{12}) = 1$, then $\tau_1(\rho_1) = 1$ and $\tau_2(\rho_2) = 1$, but $\tau_{12}(\rho_1) = d_2$ where $d_2 = \tau_2(I_2)$ and I_2 denotes the identity for subspace 2. Thus, the traditional upper bound (5) yields

$$S(\rho_{12}, \rho_1) \leqslant \tau_{12}(\rho_1 - \rho_{12}) = d_2 - 1. \tag{31}$$

We first consider a quantum example in which ρ_1 and ρ_2 are both one-dimensional projections and let $\rho_{12} = \rho_1 \otimes \rho_2$. Then

$$S(\rho_{12}) = S(\rho_1) = S(\rho_2) = 0 \qquad \text{and} \qquad S(\rho_{12}, \rho_1) = S(\rho_{12}, \rho_2) = 0.$$

Since $\rho_{12}^\gamma = \rho_{12}$ and $\rho_1^\gamma = \rho_1 \,\forall\, \gamma > 0$, it is easy to see that the new upper bound (9) implies

$$S(\rho_{12}, \rho_1) \leqslant \gamma^{-1}\tau_{12}(\rho_{12}\rho_1 - \rho_{12}) = 0 \qquad \text{for } 0 < \gamma < 1.$$

Thus, as soon as γ is decreased even slightly from 1, the bound jumps discontinuously to the exact value of zero. Similarly, by taking limits, or using generalised inverses, one can show that the lower bound also gives the exact result.

In the next example ρ_{12} is an arbitrary state of a product system. By applying Hölder's inequality to (9), one can conclude that

$$S(\rho_{12}, \rho_1) \leqslant \gamma^{-1}\{[\tau_{12}(\rho_{12})]^{1-\gamma}[\tau_1(\rho_1)]^\gamma - \tau_{12}(\rho_{12})\}$$

$$\leqslant \gamma^{-1}[d_2^\gamma - 1] \to \log d_2 \qquad \text{when } \gamma \to 0.$$

This is a substantial improvement over the estimate $d_2 - 1$.

However, in both of these examples, one could have used subadditivity [7, 32-34] (see also [11-14, 21, 23, 26])

$$S(\rho_{12}, \rho_1) \leq S(\rho_2) \tag{32}$$

to obtain bounds which are identical to those from our improved estimates. (In the second case, one also needs the fact that $S(\rho_2) \leq \log d_2$.) One might therefore ask whether our new upper bounds ever surpass those obtainable from subadditivity. The following numerical example shows that, in certain cirumstances, our new bounds are much better than those obtainable from subadditivity.

If the subsystems 1 and 2 are both simple discrete two-level systems, then the state ρ_{12} of the corresponding four-level product system has the form $\rho_{12} = \{p_{11}, p_{12}, p_{21}, p_{22}\}$ and $\rho_1 = \{p_{11} + p_{12}, p_{21} + p_{22}\}$. In the next example, the p_{jk} are chosen so that $\rho_{12} = \{a \, a' \, a' \, a\}$ where $a + a' = \frac{1}{2}$. Then $\rho_1 = \rho_2 = \{\frac{1}{2}, \frac{1}{2}\}$ so that $S(\rho_1) = S(\rho_2) = \log 2$, and $S(\rho_{12}, \rho_1) = -2(a \log a + a' \log a') - \log 2$. A summary of our estimates is given in table 2; the upper bound should be compared with the subadditivity bound of $\log 2 = 0.693\,147\,180\,56\ldots$. It should be noted that $\rho_{12} = \rho_1 \otimes \rho_2$ if and only if $a = a'$, and that the deviation of ρ_{12} from a simple tensor product corresponds to the extent to which a deviates from $\frac{1}{4}$. It is also worth pointing out that the average is an upper, rather than a lower, bound in this case. This is not inconsistent with the discussion following (18) because $\tau(Q - P) = \tau(\rho_1 - \rho_{12}) = d_2 - 1 \neq 0$; on the contrary, $b_k = \frac{1}{2} \geq a_j = \{a, a'\} \, \forall j, k$ so that $c_1 \geq 0$.

In order to determine whether subadditivity or the new procedure will yield a better upper bound, one should recall that subadditivity follows from the standard Klein inequality (5) with $P = \rho_{12}$ and $Q = \rho_1 \otimes \rho_2$. Thus we expect the new inequality to be preferable when ρ_{12} is very different from $\rho_1 \otimes \rho_2$. Of course, unless subadditivity is exact, our new procedures will always yield better results if γ is sufficiently small; the relevant issue is which estimate gives a better result for comparable computational effort.

A final example illustrates our procedures for estimating the free energy in the case of a classical continuous system. Specifically, we consider a one-dimensional quartic oscillator on the real line, and its approximation with an appropriately chosen harmonic oscillator. Let

$$P(x) = \exp[\beta(F_0 - ax^2)] \tag{33a}$$

$$Q(x) = \exp[\beta(F_1 - Ax^4)] \tag{33b}$$

where $a, A > 0$ and

$$\beta F_0(\beta) = \tfrac{1}{2} \log(\beta a / \pi) \tag{34a}$$

$$\beta F_1(\beta) = \tfrac{1}{4} \log(16 \beta A / [\Gamma(\tfrac{1}{4})]^4). \tag{34b}$$

Furthermore, one has

$$\tau(QV) = \int_{-x}^{x} \exp[\beta(F_1 - Ax^4)](Ax^4 - ax^2)\,dx$$

$$= \frac{1}{\Gamma(\tfrac{1}{4})} \left(\frac{\Gamma(\tfrac{5}{4})}{\beta} - \frac{a\Gamma(\tfrac{3}{4})}{(\beta A)^{1/2}} \right). \tag{35}$$

Because $u_{PQ}(\gamma)$ is divergent when $\gamma < 0$, we obtain free energy bounds of the form (7) corresponding to $S(Q, P)$, i.e.

$$-u_{QP}(\gamma) \leq \beta[F_1 - F_0 - \tau(QV)] \leq -u_{QP}(-\gamma) \tag{36}$$

Table 2. (Example 2) Relative entropy of a system and subsystem. For $P = \rho_{12} = \{p_{11}, p_{12}, p_{21}, p_{22}\} = \{a\, a'\, a'\, a\}$ with $a + a' = \frac{1}{2}$, $Q = \rho_1 = \rho_2 = \{\frac{1}{2}, \frac{1}{2}\}$ and $S(P, Q) = S(\rho_{12}, \rho_1) = -2(a \log a + a' \log a') - \log 2$. Subadditivity implies $S(\rho_{12}, \rho_1) \leqslant S(\rho_2) = \log 2 = 0.693\,147\,180\,56\ldots$. ($a$) Bounds and averages.

(i) For $a = 0.05$, $a' = 0.45$, $S(P, Q) = 0.325\,082\,973\,391$.

	$\gamma = 1.0$	$\gamma = 0.5$	$\gamma = 0.25$	$\gamma = 0.125$	$\gamma = 0.0625$
Upper bound	1.000 000 00	0.529 822 13	0.407 396 11	0.362 268 78	0.342 788 54
Average	0.590 000 00	0.379 473 32	0.338 023 05	0.328 278 09	0.325 879 28
Lower bound	0.180 000 00	0.229 124 51	0.268 649 98	0.294 287 41	0.308 970 02

(ii) For $a = 0.10$, $a' = 0.40$, $S(P, Q) = 0.500\,402\,423\,538$.

	$\gamma = 1.0$	$\gamma = 0.5$	$\gamma = 0.25$	$\gamma = 0.125$	$\gamma = 0.0625$
Upper bound	1.000 000 00	0.683 281 57	0.579 867 07	0.537 579 08	0.518 399 13
Average	0.660 000 00	0.536 656 31	0.509 250 84	0.502 601 28	0.500 951 31
Lower bound	0.320 000 00	0.390 031 06	0.438 634 61	0.467 623 48	0.483 503 50

(iii) For $a = 0.15$, $a' = 0.35$, $S(P, Q) = 0.610\,864\,302\,055$.

	$\gamma = 1.0$	$\gamma = 0.5$	$\gamma = 0.25$	$\gamma = 0.125$	$\gamma = 0.0625$
Upper bound	1.000 000 00	0.768 765 17	0.682 582 50	0.645 109 10	0.627 604 88
Average	0.710 000 00	0.634 403 80	0.616 673 86	0.612 312 02	0.611 225 94
Lower bound	0.420 000 00	0.500 042 43	0.550 765 22	0.579 514 95	0.594 847 00

(iv) For $a = 0.20$, $a' = 0.30$, $S(P, Q) = 0.673\,011\,667\,009$.

	$\gamma = 1.0$	$\gamma = 0.5$	$\gamma = 0.25$	$\gamma = 0.125$	$\gamma = 0.0625$
Upper bound	1.000 000 00	0.814 104 40	0.738 819 97	0.704 823 23	0.688 654 93
Average	0.740 000 00	0.689 311 99	0.677 059 32	0.674 021 87	0.673 264 11
Lower bound	0.480 000 00	0.564 519 57	0.615 298 67	0.643 220 52	0.657 873 29

(v) For $a = 0.25$, $a' = 0.25$, $S(P, Q) = 0.693\,147\,180\,550$.

	$\gamma = 1.0$	$\gamma = 0.5$	$\gamma = 0.25$	$\gamma = 0.125$	$\gamma = 0.0625$
Upper bound	1.000 000 00	0.828 427 12	0.756 828 46	0.724 061 86	0.708 380 52
Average	0.750 000 00	0.707 106 78	0.696 621 40	0.694 014 76	0.693 364 01
Lower bound	0.500 000 00	0.585 786 44	0.636 414 34	0.663 967 65	0.678 347 51

(b) Richardson extrapolates.

a	$R(1, 1)$	$R(2, 2)$	$R(3, 3)$	$R(4, 4)$
0.05	0.309 297 758 960	0.325 200 190 709	0.325 082 842 854	0.325 082 973 416
0.10	0.495 541 752 800	0.500 420 606 983	0.500 402 413 478	0.500 402 423 539
0.15	0.609 205 064 285	0.610 867 805 621	0.610 864 300 963	0.610 864 302 055
0.20	0.672 415 982 556	0.673 012 366 834	0.673 011 666 885	0.673 011 667 009
0.25	0.692 809 041 582	0.693 147 420 981	0.693 147 180 535	0.693 147 180 560

where

$$u_{QP}(\gamma) = \gamma^{-1}\left(1 - \int_{-\infty}^{x} P^{\gamma}Q^{1-\gamma}\,\mathrm{d}x\right).$$

The quadratic force constant a appearing in $P(x)$ can be chosen to maximise the linear free energy estimate $F_0 + \tau(QV)$, with the result that

$$a = \frac{\Gamma(\frac{1}{4})}{2\Gamma(\frac{3}{4})}\left(\frac{A}{\beta}\right)^{1/2}$$

$$F_0 + \tau(QV) = \frac{1}{4\beta}\log\left[e^{-1}\left(\frac{\Gamma(\frac{1}{4})}{2\pi\Gamma(\frac{3}{4})}\right)^2 \beta A\right]. \tag{37}$$

This choice optimises the tightness of the lower bound in (36).

It is straightforward to show that $u_{QP}(z)$ is analytic for $|z| < 1$; and that for $\gamma < 1$ the integrals appearing in $u_{QP}(\gamma)$ can be readily evaluated [35] in terms of the modified Bessel function $K_{1/4}(z)$. Consequently, numerical values can be obtained for the upper and lower bounds in (36); some values are displayed in table 3. It follows from (34) and (38) that these bounds should be compared to the exact value of

$$\beta[F_1 - F_0 - \tau(QV)] = \tfrac{1}{4}\log\left(\frac{64\pi^2 e[\Gamma(\frac{3}{4})]^2}{[\Gamma(\frac{1}{4})]^6}\right)$$

$$= 0.031\,692\,4024\ldots. \tag{38}$$

Entries in table 3 once again illustrate that both upper and lower bounds improve as γ decreases from the conventional value of 1 toward 0; and furthermore, that the average of the two bounds is a superior estimate.

It should be noted that this model example is presented solely to illustrate the efficacy of the bounds. If one actually wished to estimate F_1 from F_0, or vice-versa, one would need to use a modified version of (27) involving $\tau(QV)$ rather than $\tau(PV)$.

Table 3. (Example 3) Classical one-dimensional oscillators. For $P(x) = \exp[\beta(F_0 - ax^2)]$, and $Q(x) = \exp[\beta(F_1 - Ax^4)]$ with $a = [\Gamma(\frac{1}{4})/2\Gamma(\frac{3}{4})](A/\beta)^{1/2}$, $\beta[F_1 - F_0 - \tau(QV)] = 0.031\,692\,4024\ldots$. Free energy bounds.

Gamma	Lower bound	Upper bound	Average
0.1†	0.028 81	0.033 95	0.031 38
0.2	0.026 81	0.036 50	0.031 65
0.3	0.024 23	0.038 79	0.031 51
0.4	0.021 60	0.041 10	0.031 35
0.5	0.018 84	0.043 41	0.031 12
0.6	0.015 91	0.045 71	0.030 81
0.7	0.012 75	0.048 02	0.030 38
0.8	0.009 25	0.050 32	0.029 78
0.9	0.005 17	0.052 63	0.028 90
1.0	0.000 00	0.054 95	0.027 47

† Entries for this gamma are subject to large relative computational errors.

Acknowledgment

Appendix 1. Richardson extrapolation

Richardson extrapolation [15, 16] is essentially a procedure to combine two approximations so that the leading error term cancels, resulting in an improved estimate. The approximation is assumed to depend upon a parameter λ so that the error can be written in the form

$$\text{err}(\lambda) = x(\lambda) - \text{ap}(\lambda) = c_\nu \lambda^\nu + O(\lambda^{\nu'}) \tag{A1.1}$$

where $\nu' > \nu$, typically $\nu' = \nu + 1$ or $\nu + 2$. It is most convenient, particularly if repeated extrapolation will be used, to assume that successive values of λ differ by a factor of 2. Then one expects that the new approximation,

$$\text{Rich}(\lambda) = \frac{2^\nu \text{ap}(\lambda) - \text{ap}(2\lambda)}{2^\nu - 1} = \text{ap}(\lambda) + \frac{\text{ap}(\lambda) - \text{ap}(2\lambda)}{2^\nu - 1} \tag{A1.2}$$

will have an error $x(\lambda) - \text{Rich}(\lambda) = O(\lambda^{\nu'})$. Instead of using the Richardson extrapolation procedure to produce an improved estimate, one could use it to estimate the error, i.e.

$$\text{errest} \approx \frac{\text{ap}(\lambda) - \text{ap}(2\lambda)}{2^\nu - 1}. \tag{A1.3}$$

In our numerical examples, this estimate always correctly predicted the number of significant figures, even when the estimates themselves were extremely bad. Furthermore, one can examine the ratio of successive estimates to determine whether or not they satisfy the condition

$$\frac{\text{ap}(\lambda) - \text{ap}(2\lambda)}{\text{ap}(\lambda/2) - \text{ap}(\lambda)} \approx 2^\nu. \tag{A1.4}$$

When $\text{err}(\lambda) \approx c_{\nu_1} \lambda^{\nu_1} + c_{\nu_2} \lambda^{\nu_2} + c_{\nu_3} \lambda^{\nu_3} + \dots$ this extrapolation procedure can be repeated until the round-off error becomes excessive provided that one knows the values of ν_k for which c_{ν_k} is non-zero.

In the case of interest here, one expects

$$\text{err}(\gamma) = S(P, Q) - \text{av}(\gamma) = \sum_{m=1}^{\infty} c_m \gamma^{2m}. \tag{A1.5}$$

To use repeated Richardson extrapolation, let

$$R(j, 0) = \text{av}(2^{-j}) \qquad j = 0 \dots n \tag{A1.6a}$$

$$R(j, 1) = \frac{4 \, \mathrm{av}(2^{-j}) - \mathrm{av}(2^{-j+1})}{3}$$

$$= R(j, 0) + \frac{R(j, 0) - R(j-1, k)}{3} \qquad j = 1 \ldots n \qquad (A1.6b)$$

$$R(j, k) = R(j, k-1) + \frac{R(j, k-1) - R(j-1, k-1)}{2^{2k} - 1} \qquad j = k \ldots n. \qquad (A1.6c)$$

This procedure will give a pyramid of values, culminating in $R(n, n)$.

One might expect the error at the kth level to be $O(\gamma^{-2(k+1)})$; however, estimation of the leading error term is more subtle because the extrapolation procedure alters the coefficients in the series, i.e. after k steps one has

$$S(P, Q) = R(n, k) + \sum_{m=k+1}^{\infty} c_m^k \gamma^{2m} \qquad 1 \leqslant k < n$$

where

$$c_m^k = \frac{4^k - 4^m}{4^k - 1} c_m^{k-1} \quad (1 \leqslant k \leqslant m) \qquad \text{and} \qquad c_m^0 = c_m. \qquad (A1.7)$$

Both n and γ should now be regarded as fixed, with γ having the value used in $R(n, 0)$ (i.e. $\gamma = 2^{-n}$). Then (A1.7) implies $c_k^k = 0$, as expected, and the error after k steps is

$$E(n, k) = S(P, Q) - R(n, k) \approx c_{k+1}^k \gamma^{2(k+1)}$$

where

$$c_{k+1}^k = c_{k+1} \prod_{i=1}^{k} \left(\frac{4^i - 4^{k+1}}{4^i - 1} \right)$$

$$= (-1)^k c_{k+1} \prod_{i=1}^{k} 4^i$$

$$= (-1)^k c_{k+1} 4^{k(k+1)/2}$$

$$= (-1)^k c_{k+1} 2^{k(k+1)}. \qquad (A1.8)$$

Thus, with the choice $\gamma = 2^{-n}$, one has

$$E(n, k) \approx \pm c_{k+1} (2^{k(k+1)} \gamma^{2(k+1)}) = \pm c_{k+1} (2^{(k+1)(k-2n)}) \qquad (A1.9)$$

so that, in the absence of significant round-off error, $R(n, n)$ is the best estimate that can be generated from $\mathrm{av}(1) \ldots \mathrm{av}(2^{-n})$ with an error satisfying

$$E(n, n) = S(P, Q) - R(n, n) \approx \pm c_{n+1} 2^{-n(n+1)}. \qquad (A1.10)$$

This suggests $E(n, n) = O(2^{-n(n+1)})$; however, the total error depends on both the behaviour of the coefficients c_k and the round-off error. In view of (20) the coefficients used in this paper satisfy $c_k = \tau[PW^{2k+1}]/(2k+1)!$ so that the error decays exceedingly rapidly with n. This is born out by the very rapid convergence of $R(n, n)$ to $S(P, Q)$ in examples 1 and 2. (In example 1, $c_k = [(1-2\varepsilon)/(2k+1)!]\{\log[(1-\varepsilon)/\varepsilon]\}^{2k+1}$ so that for $\varepsilon = 0.05$ the leading term in $E(n, n)$ has the values 3.89, -4.15×10^{-1}, 5.35×10^{-3}, -1.01×10^{-5}, 3.10×10^{-9} for $n = 0, 1, 2, 3, 4$ respectively.)

The possible intrusion of round-off error can be checked by examining the ratio of successive error estimates to determine how closely they satisfy

$$\text{ratio}(j, k) = \frac{R(j+1, k) - R(j, k)}{R(j, k) - R(j-1, k)} \approx 4^{k+1}. \tag{A1.11}$$

This ratio is shown in table $1(c)$ for the first example. Its reliability in detecting round-off error enhances the utility of the estimation procedure presented in this paper.

Note again that, as above, extrapolation can also be used to estimate the error instead of producing further estimates. Thus, as in (A1.3), the error after $k < n$ steps can be estimated as

$$S(P, Q) - R(j, k) \approx \text{errest} = \frac{R(j, k) - R(j-1, k)}{2^{2(k+1)} - 1}. \tag{A1.12}$$

Appendix 2. Continuity and analyticity

In this appendix, we show that $u(\gamma)$ is analytic in a neighbourhood of 0 under certain conditions. The details are presented only for quantum systems, which automatically include classical discrete systems. A similar analysis, including an appropriately modified version of theorem A2.1, can be presented for the classical continuous case; the details are left to the reader.

In order to study the quantum case, let

$$W_{ab}(\gamma) = \begin{cases} \gamma^{-1} a[(b/a)^\gamma - 1] & 1 \geq |\gamma| \geq 0, \quad b \neq 0 \\ a \log(b/a) & \gamma = 0, \quad b \neq 0 \\ 0 & a = b = 0. \end{cases} \tag{A2.1}$$

If $S(P) < \infty$ and $S(P, Q) < \infty$, define

$$u(\gamma) = u_{PQ}(\gamma) = \sum_j \sum_k |\langle \alpha_j, \beta_k \rangle|^2 W_{a_j b_k}(\gamma) \tag{A2.2}$$

where a_j, b_k, and α_j, β_k are as in (11), and it is understood that the sum is to be taken over those values of j, k for which $\langle \alpha_j, \beta_k \rangle \neq 0$. It follows from standard properties of the trace that this is consistent with (13). (Note that although $W_{a_j b_k}$ is undefined when $b_k = 0$ and $a_j \neq 0$, the finite entropy conditions imply that $\langle \alpha_j, \beta_k \rangle = 0$ in this situation, so that such terms are omitted from the sum.) Because $W_{ab}(\gamma)$ is a monotone increasing function of γ, (10) can be improved to

$$W_{ab}(-\gamma) \leq W_{ab}(0) \leq W_{ab}(\gamma) \leq b - a \qquad \gamma > 0. \tag{A2.3}$$

It is easy to check that $W_{ab}(\gamma)$ can be extended to an entire function $W_{ab}(z)$. It then follows from the maximum modulus principle that

$$\sup\{|W_{ab}(z)|: |z| < \gamma_0\} = \sup\{|W_{ab}(z)|: |z| = \gamma_0\}$$
$$\leq \max\{a\gamma_0^{-1}[1 + (b/a)^{\pm\gamma_0}]\}$$
$$\leq \{a\gamma_0^{-1}[1 + (b/a)^{\gamma_0} + (b/a)^{-\gamma_0}]\} \tag{A2.4}$$

for $a, b \neq 0$. We now show that $u(z)$ is analytic on a suitable region.

Definition. If $S(P) < \infty$ and $S(P, Q) < \infty$, let

$$\Gamma(P, Q) = \sup\{|\gamma| < 1: |u(\pm\gamma)| < \infty\} \tag{A2.5}$$

and $\Gamma(P, Q) = 0$ otherwise.

Note that, if Tr $P = $ Tr Q, then $\Gamma(P, Q) = \sup\{0 \leqslant \gamma < 1: -u(-\gamma) < \infty\}$.

Theorem A2.1. If $\Gamma(P, Q) > 0$, $u(z)$ is analytic on $D_{\Gamma(P,Q)} = \{z: |z| < \Gamma(P, Q)\}$.

Proof. Let $0 < \gamma_0 < \Gamma(P, Q)$ and let

$$m_{jk} = a_j \gamma_0^{-1}[1 + (b_k/a_j)^{\gamma_0} + (b_k/a_j)^{-\gamma_0}].$$

Then it follows from (A2.4) that on $D_{\gamma_0} = \{z: |z| < \gamma_0\}$

$$\sum_j \sum_k |\langle \alpha_j, \beta_k \rangle|^2 |W_{a_j b_k}(z)| \leqslant \sum_j \sum_k |\langle \alpha_j, \beta_k \rangle|^2 m_{jk} \leqslant u(\gamma_0) - u(-\gamma_0) + 3\gamma_0^{-1} \operatorname{Tr}(P) < \infty.$$

Since $W_{a_j b_k}(z)$ is analytic on $D_{\Gamma(P,Q)}$, it follows by repeated application of the Weierstrass M test [36] that $u(z)$ is also. $\qquad\square$

The next theoreom shows that the second limit in (30) holds.

Theorem A2.2. If $\Gamma(P,Q) > 0$, then $S(P,Q) = \lim_{\gamma \to 0} \tau[PW(\gamma)]$.

Proof. Fix P, Q and $\gamma > 0$ and let

$$\int_0^\infty \mu \, \mathrm{d}E(\mu) = P^{-\gamma/2}Q^\gamma P^{-\gamma/2} = \exp(\gamma W(\gamma)) \tag{A2.6}$$

be the spectral decomposition of the indicated unbounded positive semi-definite operator. Then if $\omega(\cdot)$ is the measure defined by $\omega(\cdot) = \tau[PE(\cdot)]$,

$$\gamma^{-1} \int_0^1 (1 - \mu^{-1}) \, \mathrm{d}\omega(\mu) \leqslant \gamma^{-1} \int_0^1 \log \mu \, \mathrm{d}\omega(\mu) \leqslant \gamma^{-1} \int_0^1 (\mu - 1) \, \mathrm{d}\omega(\mu) \tag{A2.7}$$

and similarly for integrals over the interval $(1, \infty)$. Furthermore,

$$0 < \int_0^\infty \mu \, \mathrm{d}\omega(\mu) = \tau(P^{1-\gamma}Q^\gamma) = [\gamma u(\gamma) + \tau(P)] < \infty$$

and

$$0 < \int_0^\infty \mu^{-1} \, \mathrm{d}\omega(\mu) = \tau(P^{1+\gamma}Q^{-\gamma}) = [\tau(P) - \gamma u(-\gamma)] < \infty.$$

Therefore, if $0 < \gamma < \Gamma(P, Q)$, all of the integrals in (A2.7) converge on both the intervals $(0, 1)$ and $(1, \infty)$. It then follows that the corresponding integrals on the interval $(0, \infty)$ converge absolutely and satisfy

$$u(-\gamma) = \gamma^{-1} \int_0^\infty (1 - \mu^{-1}) \, \mathrm{d}\omega(\mu)$$

$$\leqslant \gamma^{-1} \int_0^\infty \log \mu \, \mathrm{d}\omega(\mu)$$

$$\leqslant \gamma^{-1} \int_0^\infty (\mu - 1) \, \mathrm{d}\omega(\mu) = u(\gamma)$$

and

$$\tau[PW(\gamma)] = \gamma^{-1} \int_0^\infty \log \mu \, \mathrm{d}\omega(\mu).$$

Therefore, $\forall\, 0 < \gamma < \Gamma(P, Q)$

$$u(-\gamma) \le \tau[PW(\gamma)] \le u(\gamma).$$

It then follows from the continuity of $u(\gamma)$ at $\gamma = 0$ that

$$\lim_{\gamma \to 0} \tau[PW(\gamma)] = \lim_{\gamma \to 0} u(\gamma) = S(P, Q). \qquad \square$$

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