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High-temperature expansions of Bures and Fisher information priors

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For certain infinite and finite-dimensional thermal systems, we obtain—incorporating quantum-theoretic considerations into Bayesian thermostatistical investigations of Lavenda—high-temperature expansions over inverse temperature β induced by volume elements (quantum Jeffreys' priors) of Bures metrics. Similarly to Lavenda's results based on volume elements (Jeffreys' priors) of (classical) *Fisher information* metrics, we find that in the limit $\beta \rightarrow 0$ the quantum-theoretic priors either conform to Jeffreys' rule for variables over $[0,\infty]$, by being proportional to $1/\beta$, or to the Bayes-Laplace principle of insufficient reason, by being constant. Whether a system adheres to one rule or to the other appears to depend upon its number of degrees of freedom.

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In this paper—initially motivated by the investigation ''Bayesian Approach to Thermostatistics'' [1] of Lavenda (cf. Refs. [2–4])—we examine certain prior distributions $\omega(\beta)$ over the inverse temperature parameter β that have recently been presented in the literature [5–8]. These distributions are derived from ''quantum Jeffreys' priors,'' that is, the volume elements dV_{Bures} of the Bures/minimal monotone metric [9–12], for various finite and infinite-dimensional convex sets of density matrices. We find that some, but not all, of these derived priors satisfy—in the high-temperature limit, $\beta \rightarrow 0$—Jeffreys' choice of ''$\omega(\beta) \propto 1/\beta$, which is invariant to transformations of the form $\zeta = \beta^n$, since $d\beta/\beta$ and $d\beta^n/\beta^n$ are always proportional. This would not be true if the uniform distribution were used. Jeffreys cited the measurement of the charge of an electron, where some methods give e while others e^2, and certainly de and de^2 are not proportional'' [1]. (Along these lines, let us emphasize for the purposes of this study the obvious assertion that $\beta^{-1} \propto T$, where T is the temperature.)

Lavenda (Ref. [1] Sec. 4) analyzed three models in particular: (i) an ideal monatomic gas having the logarithm of its partition function $\propto -\frac{3}{2} \ln \beta$; (ii) the harmonic oscillator with frequency ν; and (iii) a Fermi oscillator with two levels. He determined that in the high-temperature limit the first two of these yielded priors $\omega(\beta)$ proportional to $1/\beta$, while the third gave a constant prior. Quite similarly to this set of findings of Lavenda, all the prior distributions that we will examine below are either proportional in the high-temperature limit to $1/\beta$ or to a constant. It is interesting to observe that one of the infinite-dimensional systems we study—the displaced thermal states [7]—has the same prior distribution, based on the quantum Jeffreys' prior, as that obtained for the Fermi oscillator by Lavenda [1], in his different analytical (classical) framework. Also, when we attempt to apply the procedure of Lavenda to these states, as well as to the displaced squeezed thermal states [8,13], we find different high-temperature behavior (that is, of the $1/\beta$ type) than when we rely upon the quantum Jeffreys' priors. But, for the squeezed thermal states [14], the behavior using the two different (quantum and classical) approaches near $\beta=0$ is $1/\beta$ in nature.

The term ''quantum Jeffrey prior'' was first employed in Ref. [6]. There, relying upon the innovative study of Twamley [14]—the first to explicitly determine the Bures metric in an *infinite*-dimensional setting—a simple product (independence) form

$$dV_{Bures} = \upsilon(r)\omega(\beta) dr d\beta d\theta, \tag{1}$$

was obtained for the squeezed thermal states

$$\rho(\beta,r,\theta) = S(r,\theta)T(\beta)S^{\dagger}(r,\theta)/Z(\beta). \tag{2}$$

Here, $S(r,\theta)$ is the one-photon squeeze operator, and

$$Z(\beta) = \left(2 \sinh \frac{\beta}{4}\right)^{-1} \tag{3}$$

is a normalization factor (partition function) chosen so that $\mathrm{Tr}\,\rho = 1$. In the form (1) (which we note is independent of the unitary parameter θ), $\upsilon(r) = \sinh 2r$, and of more immediate interest to the investigation here,

$$\omega(\beta) = \frac{\cosh \frac{\beta}{4} \coth \frac{\beta}{4} \,\mathrm{sech}\, \frac{\beta}{2}}{8}. \tag{4}$$

A series expansion in the vicinity of $\beta=0$ yields

$$\omega(\beta) = \frac{1}{2\beta} - \frac{7\beta}{192} + \frac{667\beta^3}{184\,320} + O([\beta]^5). \tag{5}$$

Near $\beta=0$, the first term predominates, so we discern that in the high-temperature limit the β-dependent part (5) of the

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quantum Jeffreys' prior (1), in fact, satisfies the Jeffreys/Lavenda desideratum for a prior distribution over $\beta \in [0,\infty]$ of being proportional to $1/\beta$.

Subsequent to Ref. [6], Paraoanu and Scutaru [7] studied the case of the displaced thermal states. They found the quantum Jeffreys' prior to be of the simple form

$$dV_{Bures} = \frac{\operatorname{sech}\frac{\beta}{2} dp\, dq\, d\beta}{8}, \tag{6}$$

where the variables p and q denote the displacements in momentum and position. Now, it is of interest to note that unlike Eq. (5), this volume element can be normalized over the full infinite range $\beta \in [0,\infty]$ to a *proper* prior probability distribution function, $\omega(\beta) = \operatorname{sech}(\beta/2)/\pi$. (The mean of β for this distribution is the product of Catalan's constant, which is approximately 0.959 66, and $8/\pi$, while the second moment of β is π^2.) Now, expanding around $\beta = 0$, we have

$$\omega(\beta) = \frac{\operatorname{sech}\frac{\beta}{2}}{\pi} = \frac{1}{\pi} - \frac{\beta^2}{8\pi} + \frac{5\beta^4}{384\pi} + O([\beta]^6). \tag{7}$$

So, near $\beta = 0$, the prior behaves as a uniform distribution, *not* fulfilling the Jeffreys/Lavenda desideratum. (''This, however, is precisely the Bayes-Laplace rule, which Jeffreys considers as an unacceptable representation of the ignorance concerning the value of the parameter'' [1].) The thermostatistical characteristics of this model for displaced thermal states [7] is essentially fully equivalent to those found by Lavenda [1] for a Fermi oscillator with two levels: 0 and ϵ_0 [cf. Ref. [15], Eq. (3.5.11)]. (''As we have seen, the [Jeffreys'] invariance property also holds for Bose particles in the high-temperature limit. However, the same is not true for Fermi particles'' [1]. We have determined that this latter behavior also holds generically—in the classical framework of Lavenda—for the $SU_q(2)$ *fermion* model, relying upon its grand partition function [Ref. [16], Eq. (23)].

Kwek, Oh, and Wang [8]—making use of the Baker-Campbell-Hausdorff formula for quadratic operators [17,13]—then, extended these studies [6,7] to the displaced squeezed thermal states. They obtained the volume element [Ref. [8], Eq. (15)],

$$\begin{aligned} dV_{Bures} &= \left(\frac{1}{2}\cosh^2\frac{\beta}{4}\operatorname{sech}^{3/2}\frac{\beta}{2}\right) \\ &\quad \times \sqrt{4\cosh^2(2r) - \sin^2(2r)}\, dp\, dq\, dr\, d\beta \\ &\equiv \upsilon(r)\,\omega(\beta)\, dp\, dq\, dr\, d\beta. \end{aligned} \tag{8}$$

Now,

$$\omega(\beta) = \frac{1}{2}\cosh^2\frac{\beta}{4}\operatorname{sech}^{3/2}\frac{\beta}{2} = \frac{1}{2} - \frac{\beta^2}{16} + \frac{23\beta^4}{3072} + O([\beta]^6). \tag{9}$$

So, similarly to Eq. (7) and unlike Eq. (5), this univariate prior behaves *uniformly* in the immediate vicinity of $\beta = 0$. [The difference between Eqs. (5) and (9), in this respect, is easily evident in Fig. 2 of Ref. [8].] Kwek, Oh, and Wang noted that ''whereas the marginal probability distribution for the undisplaced squeezed state diverges as $\beta \to 0$ or at high temperature, in the case of the displaced squeezed state, the marginal probability distribution goes to a finite value. The result is reminiscent of a similar situation in chi-square distribution curves in which the probability density function diverges at one degree of freedom, but not with higher degrees of freedom. This analogy seems to indicate that the change in the marginal probability density function in terms of inverse temperature stems from an increased degree of freedom associated with the displacement of the squeezed states'' (Ref. [8], p. 6617). This line of argument suggests that perhaps a relation can be established between the degrees of freedom of a system (in particular, the three instances analyzed above) and whether or not the associated prior $\omega(\beta)$ fulfills in the limit $\beta \to 0$ the Jeffreys/Lavenda desideratum or the Bayes-Laplace rule (or conceivably neither).

The three scenarios—squeezed thermal states, displaced thermal states, and displaced squeezed thermal states—examined above all pertain to infinite-dimensional (continuous variable) quantum systems. We now turn our attention to the cases of spin-$\frac{1}{2}$ and spin-1 (that is, two- and three-level) systems. Here, the quantum Jeffreys' priors, that is, the volume elements of the associated Bures metrics, are not typically parameterized in terms of inverse temperature parameters. So we can not immediately study the high-temperature limit but must have recourse to a somewhat more indirect, but quite standard argument. That is, we compute the one-dimensional (univariate) marginal distributions of the (multivariate) quantum Jeffreys' priors [18], which we interpret as densities-of-state or structure functions, $\Omega(\epsilon)$. Then, applying Boltzmann factors and normalizing by the resulting partition functions $Z(\beta)$, we determine the corresponding canonical Gibbs distributions, $\Omega^*(\epsilon|\beta) = \exp[-\beta\epsilon - \ln Z(\beta)]\Omega(\epsilon)$. (We also note that Lavenda [Ref. [1], Eq. (29a)] considers, as well, the different ''structure function'' $\Omega(\beta) = \omega(\beta)/Z(\beta)$, and the possibility of taking its Laplace transform to obtain a moment-generating function, $Y(\epsilon)$.) We use the contention of Lavenda [1] (relying upon the asymptotic equivalence between the maximum-likelihood estimate of β and its average value) that the implied prior (Bayes) distribution over β should be taken to be

$$\omega(\beta) \propto \sqrt{\operatorname{var}(\epsilon)} = \sqrt{\frac{\partial^2}{\partial\beta^2}\ln Z(\beta)}, \tag{10}$$

where $\operatorname{var}(\epsilon)$ is the variance of the energy—that is, $\langle(\epsilon - \langle\epsilon\rangle)^2\rangle$. This is nothing other than the application to the canonical distribution of the Bayesian/Jeffreys procedure for constructing reparameterization-invariant priors. This consists of taking the prior to be proportional to the volume element of the (classical) Fisher information metric [19].

For spin-$\frac{1}{2}$ systems, relying upon the Bures/minimal monotone metric, one finds that [Ref. [20], Eq. (12)]

$$Z(\beta) = \frac{2I_1(\beta)}{\beta}, \tag{11}$$

where $I_n(\beta)$ denotes the modified (hyperbolic) Bessel function of the first kind. Now, in this case,

$$\omega(\beta)=\sqrt{\frac{\partial^2 \ln Z(\beta)}{\partial\beta^2}}=\frac{1}{2}-\frac{\beta^2}{32}+\frac{7\beta^4}{3072}+O([\beta]^6), \tag{12}$$

so, again, the Jeffreys/Lavenda desideratum of being proportional to $1/\beta$ is not satisfied, but rather the prior behaves uniformly in the vicinity of $\beta=0$. {''One method very common in statistical mechanics is the use of a high-temperature expansion: as $T\rightarrow\infty$ one tries to expand the partition function as a series in powers of some parameter $\kappa(T)$ such that $\kappa(T)\rightarrow 0$ as $T\rightarrow\infty$'' (Ref. [21], p. 8). In these studies, we expand not the partition function *per se*, but the square root of the second derivative with respect to β of its logarithm.}

Use of the *maximal* monotone metric (which is based on the *left* logarithmic derivative [12]), in this case, rather than the Bures/minimal one (based on the *symmetric* logarithmic derivative), yields [Ref. [5], Eq. (24)]

$$Z(\beta)=\left(\frac{\pi}{2\beta}\right)^{1/2} I_{1/2}(\beta)=\frac{\sinh\beta}{\beta}, \tag{13}$$

leading to the arguably theoretically preferable Langevin function [22–26],

$$\frac{\partial \ln Z(\beta)}{\partial\beta}=-\langle\epsilon\rangle=\coth\beta-\frac{1}{\beta}. \tag{14}$$

Nevertheless, the high-temperature behavior of the implied prior $\omega(\beta)$—again based on the relation (10)—remains that of a constant near the origin, that is,

$$\omega(\beta)\propto\frac{1}{\sqrt{3}}-\frac{\beta^2}{10\sqrt{3}}+\frac{137\beta^4}{12\,600\sqrt{3}}+O([\beta]^6). \tag{15}$$

In Ref. [27], we studied certain *three*-level systems of the form

$$\rho=\frac{1}{2}\begin{pmatrix} v+z & 0 & x-iy\\ 0 & 2-2v & 0\\ x+iy & 0 & v-z\end{pmatrix}, \tag{16}$$

which are one-parameter (v) extensions, in which the middle level has become accessible, of the two-level systems,

$$\rho=\frac{1}{2}\begin{pmatrix} 1+z & x-iy\\ x+iy & 1-z\end{pmatrix}. \tag{17}$$

(We note that the full convex set of spin-1 density matrices is *eight* dimensional in character [28].) The univariate marginal probability distribution over v, obtained by integrating over the variables *x*, *y*, and *z* in the normalized quadrivariate Bures volume element

$$p(v,x,y,z)=\frac{3}{4\pi^2 v(1-v)^{1/2}(v^2-x^2-y^2-z^2)^{1/2}} \tag{18}$$

is [Ref. [27], Eq. (19)]

$$\tilde{p}(v)=\frac{3v}{4\sqrt{1-v}}, \quad 0\leqslant v\leqslant 1. \tag{19}$$

We interpreted Eq. (19) as a density-of-states or structure function. We then determined {Ref. [5], Eq. (42)} the associated partition function

$$Z(\beta)=\frac{3e^{-\beta}[(1+2\beta)\sqrt{\pi}\,\mathrm{erfi}(\sqrt{\beta})-2\sqrt{\beta}e^{\beta}]}{8\beta^{3/2}} \tag{20}$$

[here erfi(z) represents the imaginary error function, that is $\mathrm{erf}(iz)/i$] by applying the Boltzmann factor $e^{-\beta v}=e^{-\beta\langle H\rangle}$ to Eq. (19), where

$$H=\frac{1}{2}\begin{pmatrix} 1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 1\end{pmatrix}. \tag{21}$$

This leads—*via* the argument of Lavenda [1] again, based on the relation (10)—to

$$\omega(\beta)\propto\frac{1}{\beta}-\frac{119\beta}{40}+\frac{1891\beta^2}{140}+O([\beta]^3), \tag{22}$$

thus, satisfying the Jeffreys/Lavenda desideratum. Since spin-$\frac{1}{2}$ particles are fermions and spin-1 particles are bosons, these results conform to Lavenda's assertion [1] that priors associated with bosons satisfy the Jeffreys' rule, while fermions do not. We also note, somewhat in line with the discussion of Kwek, Oh, and Wang [8], quoted above, that our spin-$\frac{1}{2}$ example has an underlying three degrees of freedom, while the spin-1 case has one more.

For the spin-$\frac{1}{2}$ systems (17), the trivariate (normalized) quantum Jeffreys' prior is

$$p(x,y,z)=\frac{1}{\pi^2(1-x^2-y^2-z^2)^{1/2}}. \tag{23}$$

The univariate marginal probability distributions are of the form

$$\tilde{p}(z)=\frac{2(1-z^2)^{1/2}}{\pi}. \tag{24}$$

Interpreting Eq. (24) as a density-of-states function, and using as the Hamiltonian,

$$H=\begin{pmatrix} 1 & 0\\ 0 & -1\end{pmatrix}, \tag{25}$$

one arrives at the partition function (11).

Now, let us seek to apply the method for generating priors over β of Lavenda directly to the three infinite-dimensional scenarios (squeezed thermal states, displaced thermal states, and displaced squeezed thermal states) first considered above, by taking for the partition function $Z(\beta)$ in Eq. (10), the normalization factor that renders the trace unity, so that one obtains a (properly normalized) density matrix. For the squeezed thermal states, substituting Eq. (3) into Eq. (10), we have

$$\omega(\beta)=\frac{1}{\beta}-\frac{\beta}{96}+\frac{7\beta^2}{92\,160}+O([\beta]^4) \tag{26}$$

thus conforming to Jeffreys' rule—under which $\ln\beta$, not β itself, is distributed uniformly. For the other two types of infinite-dimensional thermal states considered above, the result must be the same as well, because $Z(\beta)$ takes the same form in them as Eq. (3), since the displacement and squeeze operators are unitary (Ref. [13] p. 4187). Contrastingly, based on the volume elements (quantum Jeffreys' priors) of the associated Bures metrics, as we have noted in the first part of this paper, the prior Eq. (4) over β for the squeezed thermal states does conform to the Jeffreys/Lavenda desideratum in the high-temperature limit, but the priors for the other two, Eqs. (6) and (9), follow the Bayes-Laplace principle of insufficient reason. [One might then be puzzled by why, despite the unitarity of the squeeze and displacement operators, these three priors take different forms (cf. Ref. [29]).]

It would, of course, be of interest to study invariance properties of prior distributions over the inverse temperature parameter β for additional physical scenarios, both in relation to quantum Jeffreys' priors and the (Fisher information) scheme of Lavenda for obtaining such distributions, and to elucidate further any underlying governing principles.

Let us note the assertion of Frieden and his associates that many physical laws have a Fisher information-theoretic basis [30]. In particular, Frieden, Plastino, Plastino, and Soffer have ''shown that the Legendre-transform structure of thermodynamics can be replicated without any changes if one replaces the entropy S by Fisher's information measure I'' [31]. Also, Grover's quantum search algorithm has been demonstrated to be determined by a condition for minimizing Fisher information [32]. In influential work, Voiculescu [33] has developed analogues of the entropy and Fisher information measure for random variables in the context of *free* probability theory. (Three different models of free probability theory are provided by convolution operators on free groups, creation and annihilation operators on the Fock space of Boltzmann statistics, and random matrices in the large-N limit.)

In concluding, let us observe that Braunstein and Caves [11] derived the Bures distance between two density operators by optimizing the Fisher information distance (obtained using the Cramér-Rao bound on the variance of any estimator) over arbitrary generalized quantum measurements, not just ones described by one-dimensional orthogonal projectors. Of course, the *volume elements* (Jeffreys' priors and quantum Jeffreys' priors) of the Fisher information and Bures metrics have been the basis for the thermostatistical investigation here.

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