The information geometric descriptions of denormalized thermodynamic manifolds

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Abstract. In view of information geometry, the state space of thermodynamic parameters $S = \{\rho|\rho = Z^{-1}\exp\{-\sum_{i=1}^{n}\beta_i F_i, \operatorname{Tr}\rho = 1\}$ has been investigated. Here the α-geometric structures of the denormalization of S called $\widetilde{S} = \{\widetilde{\rho}|\widetilde{\rho} = f(\tau)\rho, f(\tau) > 0, \operatorname{Tr}\rho = 1\}$ is investigated. The covariant derivative and the α-curvature tensor is studied. Therefore, the relation of the α-geometric structures between S and $\widetilde{S}$ are obtained. The results were obtained in [8] when $\alpha = 0$ and in [2] when $f(\tau) = 1$.

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1 Introduction

Information geometry ([1]) originated from investigating the geometric structures of the manifold which consists of probability density functions and it has various applications such as in statistical inference and neural networks.

Recently, some authors ([7, 6, 5, 3, 4, 2]) considered the geometric structure of the space of thermodynamic parameters, which forms a manifold called S. This manifold characterizes a given physical system. One of the main results they obtained is to give the Riemannian Gaussian curvature of the manifold S. In the present paper, we firstly define the α-connection and obtain the α-Gaussian curvature which will becomes the Riemannian Gaussian curvature when $\alpha = 0$. Ingarden ([3]), Janyzek ([4]), Zheng Z. [10] and other authors reaching a Riemannian metric by statistical method. For a given equilibrium density operator ([7]) $\rho = Z^{-1}\exp\{-\sum_{i=1}^{n}\beta_i F_i\}$, where $F_1, F_2, \cdots, F_n$ are linear independent operators, $Z = \operatorname{Tr}\exp\{-\sum_{i=1}^{n}\beta_i F_i\}$ is a partition function and $\beta = (\beta_1, \beta_2, \cdots, \beta_n)$ are classical real parameters (statistical temperature, press, magnetic field), which describes the environment of a physical system. The thermodynamic parameters set $S = \{\rho|\operatorname{Tr}\rho = 1\}$ can be regarded as a differential manifold equipped with a Riemannian metric

$$g_{ij} = \operatorname{Tr}[\rho(\partial_i \ln\rho)(\partial_j \ln\rho)]$$

for the case of commuting operators F_i, where Tr denotes the trace of the matrix, and ∂_i means the partial derivative with respect to the parameter β_i.

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In [1], Amari investigated the denormalization of statistical model. Here we consider the denormalization of thermodynamic parameters model, a more general manifold, namely

$$\widetilde{S} = \{\widetilde{\rho} | \widetilde{\rho} = f(\tau)\rho, f(\tau) > 0, \mathrm{Tr}\,\rho = 1\},$$

where $f(\tau)(> 0)$ is an arbitrary-order differentiable function. Then $\widetilde{S}$ is a manifold which contains S as a submanifold with $\dim \widetilde{S} = \dim S + 1$. $\widetilde{S}$ is called the denormalization of S. By calculating the covariant derivative and the α-curvature tensor, we obtain the relation of the α-geometric structures between S and $\widetilde{S}$. At last, we use a example to illustrate our conclusions.

2 The information geometric structures of the manifold $\widetilde{S}$

Parameterizing the elements of $\widetilde{S}$ as $\widetilde{\rho}$ by a coordinate system $[\beta, \tau] = (\beta_1, \cdots, \beta_n, \tau)$ and letting

$$\widetilde{l}^{(\alpha)} := \begin{cases} \dfrac{2}{1-\alpha}\widetilde{\rho}^{\frac{1-\alpha}{2}} & (\alpha \neq 1) \\ \ln \widetilde{\rho} & (\alpha = 1), \end{cases}$$

the components of the α-metric $\widetilde{g}^{(\alpha)}$ and the coefficients of the α-connection $\widetilde{\nabla}^{(\alpha)}$ are represented respectively by

$$\widetilde{g}^{(\alpha)}_{ij} = \mathrm{Tr}(\partial_i \widetilde{l}^{(\alpha)} \partial_j \widetilde{l}^{(-\alpha)}), \tag{2.1}$$

$$\widetilde{\Gamma}^{(\alpha)}_{ijk} = \mathrm{Tr}(\partial_i \partial_j \widetilde{l}^{(\alpha)} \partial_k \widetilde{l}^{(-\alpha)}). \tag{2.2}$$

We denote its natural basis by $\widetilde{\partial}_i = \frac{\partial}{\partial \beta_i}, \widetilde{\partial}_\tau = \frac{\partial}{\partial \tau}$ and use $\mu, \nu, \lambda, \gamma$ to denote the subscripts of the natural basis, that is, $\mu, \nu, \lambda, \gamma \in \{1, \cdots, n, n+1\}$, while $i, j, k, l \in \{1, \cdots, n\}$. For the case of commuting operators F_i, from (2.1), we see that

$$\widetilde{g}_{\mu\nu} = \mathrm{Tr}(\widetilde{\rho}\widetilde{\partial}_\mu \ln \widetilde{\rho}\widetilde{\partial}_\nu \ln \widetilde{\rho}).$$

By a calculation, we get

$$\widetilde{g}_{ij} = f(\tau) g_{ij}, \quad \widetilde{g}_{i\tau} = 0, \quad \widetilde{g}_{\tau\tau} = f(\tau)^{-1}(\partial_\tau f(\tau))^2.$$

The Riemannian metric of $\widetilde{S}$ and its inverse are given by

$$\widetilde{G} = \begin{pmatrix} f(\tau)G & 0 \\ 0 & f(\tau)^{-1}(\partial_\tau f(\tau))^2 \end{pmatrix}, \quad \widetilde{G}^{-1} = \begin{pmatrix} f(\tau)^{-1}G^{-1} & 0 \\ 0 & f(\tau)(\partial_\tau f(\tau))^{-2} \end{pmatrix}. \tag{2.3}$$

The square of the arc length of S defined by $ds^2 = g_{ij} d\beta_i d\beta_j$. Thus, the square of the arc length of $\widetilde{S}$ is given by

$$d\widetilde{s}^2 = f(\tau) ds^2 + f(\tau)^{-1}(\partial_\tau f(\tau))^2 d\tau^2.$$

Note that the volume element of S is given by

$$dV = \sqrt{\det(G)} d\beta_1 \Lambda \cdots \Lambda d\beta_n,$$

we have the relation between the volume elements dV and $d\widetilde{V}$

$$
\begin{aligned}
d\widetilde{V} &= \sqrt{\det(\widetilde{G})}d\beta_1\Lambda\cdots\Lambda d\beta_n\Lambda d\tau \\
&= (f(\tau))^{\frac{n-1}{2}}\partial_\tau f(\tau)\sqrt{\det(G)}d\beta_1\Lambda\cdots\Lambda d\beta_n\Lambda d\tau \\
&= dV(f(\tau))^{\frac{n-1}{2}}df(\tau).
\end{aligned}
$$

Proposition 1. *The α-connection coefficients of $\widetilde{\nabla}^{(\alpha)}$ for $\widetilde{S}$ satisfy*

$$
\begin{aligned}
&\widetilde{\Gamma}^{(\alpha)}_{ij,k} = f(\tau)\Gamma^{(\alpha)}_{ij,k}, \qquad \widetilde{\Gamma}^{(\alpha)}_{ij,\tau} = -\frac{1+\alpha}{2}\partial_\tau f(\tau)g_{ij}, \\
&\widetilde{\Gamma}^{(\alpha)}_{i\tau,k} = \widetilde{\Gamma}^{(\alpha)}_{\tau i,k} = \frac{1-\alpha}{2}\partial_\tau f(\tau)g_{ik}, \quad \widetilde{\Gamma}^{(\alpha)}_{i\tau,\tau} = \widetilde{\Gamma}^{(\alpha)}_{\tau i,\tau} = 0, \quad \widetilde{\Gamma}^{(\alpha)}_{\tau\tau,k} = 0, \\
&\widetilde{\Gamma}^{(\alpha)}_{\tau\tau,\tau} = -\frac{1+\alpha}{2}f(\tau)^{-2}(\partial_\tau f(\tau))^3 + f(\tau)^{-1}\partial_\tau f(\tau)\partial_\tau\partial_\tau f(\tau),
\end{aligned} \tag{2.4}
$$

and

$$
\begin{aligned}
&\widetilde{\Gamma}^{(\alpha)k}_{ij} = f(\tau)\Gamma^{(\alpha)k}_{ij}, \qquad \widetilde{\Gamma}^{(\alpha)\tau}_{ij} = -\frac{1+\alpha}{2}f(\tau)(\partial_\tau f(\tau))^{-1}g_{ij}, \\
&\widetilde{\Gamma}^{(\alpha)k}_{i\tau} = \widetilde{\Gamma}^{(\alpha)k}_{\tau i} = \frac{1-\alpha}{2}f(\tau)^{-1}\partial_\tau f(\tau)\delta^k_i, \quad \widetilde{\Gamma}^{(\alpha)\tau}_{i\tau} = \widetilde{\Gamma}^{(\alpha)\tau}_{\tau i} = 0, \quad \widetilde{\Gamma}^{(\alpha)k}_{\tau\tau} = 0, \\
&\widetilde{\Gamma}^{(\alpha)\tau}_{\tau\tau} = -\frac{1+\alpha}{2}f(\tau)^{-1}\partial_\tau f(\tau) + (\partial_\tau f(\tau))^{-1}\partial_\tau\partial_\tau f(\tau),
\end{aligned} \tag{2.5}
$$

where the α-connection coefficients of $\nabla^{(\alpha)}$ for S satisfies

$$
\Gamma^{(\alpha)}_{ijk}(\beta) = \frac{1-\alpha}{2}\partial_i\partial_j\partial_k \ln Z.
$$

Proof. By (2.2) and notice that

$$
\begin{aligned}
&\widetilde{\partial}_i\widetilde{\partial}_j\widetilde{l}^{(\alpha)} = f(\tau)^{\frac{1-\alpha}{2}}\partial_i\partial_j l^{(\alpha)}, \qquad \widetilde{\partial_\tau}\widetilde{\partial}_i\widetilde{l}^{(\alpha)} = \frac{1-\alpha}{2}f(\tau)\partial_\tau f(\tau)\partial_i l^{(\alpha)}, \\
&\widetilde{\partial_\tau}\widetilde{\partial_\tau}\widetilde{l}^{(\alpha)} = -\frac{1+\alpha}{2}f(\tau)^{-\frac{3+\alpha}{2}}(\partial_\tau f(\tau))^2\rho^{\frac{1-\alpha}{2}} + f(\tau)^{-\frac{1+\alpha}{2}}\partial_\tau\partial_\tau f(\tau)\rho^{\frac{1-\alpha}{2}},
\end{aligned}
$$

we can obtain proposition 1.

These equations enable us to verify that the following relations hold for the covariant derivatives ∇ (on S) and $\widetilde{\nabla}$ (on $\widetilde{S}$), respectively:

$$
\widetilde{\nabla}_{\widetilde{X}}\widetilde{Y} = (\nabla_X Y)^{\sim} - \frac{1+\alpha}{2}(\partial_\tau f(\tau))^{-1} < \widetilde{X},\widetilde{Y} > \widetilde{\partial}_\tau, \tag{2.6}
$$

$$
\widetilde{\nabla}_{\widetilde{X}}\widetilde{\partial}_\tau = \widetilde{\nabla}_{\widetilde{\partial}_\tau}\widetilde{X} = \frac{1-\alpha}{2}f(\tau)^{-1}\partial_\tau f(\tau)\widetilde{X}, \tag{2.7}
$$

$$
\widetilde{\nabla}_{\widetilde{\partial}_\tau}\widetilde{\partial}_\tau = \left[-\frac{1+\alpha}{2}f(\tau)^{-1}\partial_\tau f(\tau) + (\partial_\tau f(\tau))^{-1}\partial_\tau\partial_\tau f(\tau)\right]\widetilde{\partial}_\tau, \tag{2.8}
$$

where X and Y are arbitrary vector fields on S, and $(\cdots)^{\sim}$ denotes $\widetilde{(\cdots)}$.

From proposition 1, we can obtain the following

Theorem 1. *S is (-1)-autoparallel in $\widetilde{S}$.*

Theorem 2. *Let M be a submanifold of S and $\widetilde{M}$ be its denormalization. For every $\alpha \in \mathbb{R}$, the following conditions (i) and (ii) are equivalent.*

(i) M is α-autoparallel in S.

(ii) $\widetilde{M}$ is α-autoparallel in $\widetilde{S}$.

Proof. Let $\widetilde{\nabla}^{(\alpha)}$ and $\nabla^{(\alpha)}$ be the α-connections on $\widetilde{S}$ and S as above. Noting that every vector field on $\widetilde{M}$ can be represented as $h^i\widetilde{X_i} + h^0\widetilde{\partial_\tau}|_{\widetilde{M}}$ by vector fields $\{X_i\}$ on M and functions $\{h^i\}$ and h^0 on M, we see from (2.7) and (2.8) that condition (ii) is equivalent to stating that $\widetilde{\nabla}^{(\alpha)}_{\widetilde{X}}\widetilde{Y} \in T(\widetilde{M})$ for all $X, Y \in T(M)$. On the other hand, we have for all $X, Y \in T(M)$,

$$\widetilde{\nabla}^{(\alpha)}_{\widetilde{X}}\widetilde{Y} \in T(\widetilde{M}) \Leftrightarrow (\nabla^{(\alpha)}_X Y)^{\sim} \in T(\widetilde{M}) \Leftrightarrow \nabla^{(\alpha)}_X Y \in T(M),$$

where the first equivalence follows from (2.6) and the second one is obvious. Therefore, (i) and (ii) are equivalent.

Remark 1. The result is Theorem 2.10 in [1] when $f(\tau) = \tau$.

Proposition 2. *The components of the α-curvature tensor of $\widetilde{S}$ are given by*

$$\begin{aligned}
\widetilde{R}^{(\alpha)}_{ijkl} &= f(\tau)R^{(\alpha)}_{ijkl} - \frac{1-\alpha^2}{4}f(\tau)(g_{il}g_{jk} - g_{jl}g_{ik}),\\
\widetilde{R}^{(\alpha)}_{ijk\tau} &= \widetilde{R}^{(\alpha)}_{i\tau k\tau} = 0,
\end{aligned}$$

where the components of α-curvature tensor of S satisfy

$$R^{(\alpha)}_{ijkl} = \frac{1-\alpha^2}{4}(\partial_k\partial_m\partial_i \ln Z \partial_j\partial_l\partial_n \ln Z - \partial_k\partial_m\partial_j \ln Z \partial_i\partial_l\partial_n \ln Z)g^{mn}.$$

Proof. Since

$$\widetilde{R}^{(\alpha)}_{\beta\gamma\lambda\mu} = (\widetilde{\partial_\gamma}\widetilde{\Gamma}^{(\alpha)\nu}_{\beta\gamma} - \widetilde{\partial_\beta}\widetilde{\Gamma}^{(\alpha)\nu}_{\gamma\lambda})g_{\nu\mu} + (\widetilde{\Gamma}^{(\alpha)}_{\gamma\omega\mu}\widetilde{\Gamma}^{(\alpha)\omega}_{\beta\lambda} - \widetilde{\Gamma}^{(\alpha)}_{\beta\omega\mu}\widetilde{\Gamma}^{(\alpha)\omega}_{\gamma\lambda}),$$

combining (2.3), (2.4) and (2.5), we obtain

$$\begin{aligned}
\widetilde{R}^{(\alpha)}_{ijkl} &= f(\tau)R^{(\alpha)}_{ijkl} + \frac{1-\alpha^2}{4}f(\tau)(g_{il}g_{jk} - g_{jl}g_{ik}), \qquad \widetilde{R}^{(\alpha)}_{i\tau k\tau} = 0,\\
\widetilde{R}^{(\alpha)}_{ijk\tau} &= \frac{1+\alpha}{2}\partial_\tau f(\tau)(\partial_i g_{jk} - \partial_j g_{ik} + \Gamma^{(\alpha)}_{jkl} - \Gamma^{(\alpha)}_{ikj}).
\end{aligned}$$

From (2.2), we get

$$\Gamma^{(\alpha)}_{ijk}(\beta) = \mathrm{Tr}[\rho(\partial_i\partial_j \ln\rho)(\partial_k \ln\rho)] + \frac{1-\alpha}{2}\,\mathrm{Tr}[\rho(\partial_i \ln\rho)(\partial_j \ln\rho)(\partial_k \ln\rho)] = \frac{1-\alpha}{2}\partial_i\partial_j\partial_k \ln Z.$$

On the other hand, from (2.1), we get

$$\begin{aligned}\partial_k g_{ij} &= \partial_k(\mathrm{Tr}[\rho\partial_i \ln\rho\partial_j \ln\rho]) \\ &= \mathrm{Tr}[\rho\partial_k \ln\rho\partial_i \ln\rho\partial_j \ln\rho] + \mathrm{Tr}[\rho\partial_k\partial_i \ln\rho\partial_j \ln\rho] + \mathrm{Tr}[\partial_i \ln\rho\rho\partial_k\partial_j \ln\rho] \\ &= \partial_i\partial_j\partial_k \ln Z.\end{aligned}$$

From above we can get

$$\widetilde{R}^{(\alpha)}_{ijk\tau} = 0$$

and

$$R^{(\alpha)}_{ijkl} = \frac{1-\alpha^2}{4}(\partial_k\partial_m\partial_i \ln Z\partial_j\partial_l\partial_n \ln Z - \partial_k\partial_m\partial_j \ln Z\partial_i\partial_l\partial_n \ln Z)g^{mn}.$$

This finishes the proof of proposition 2.

Remark 2. Clearly manifold S and $\widetilde{S}$ are ± 1-flat manifolds.

By a direct calculation, we obtain the α-sectional curvatures and the α-scalar curvature of $\widetilde{S}$

$$\widetilde{K}^{(\alpha)}_{ijij} = \frac{\widetilde{R}^{(\alpha)}_{ijij}}{\widetilde{g}_{ii}\widetilde{g}_{jj} - \widetilde{g}_{ij}\widetilde{g}_{ji}} = (f(\tau))^{-1}K^{(\alpha)}_{ijij} - \frac{1-\alpha^2}{4}(f(\tau))^{-1}, \tag{2.9}$$

and

$$\widetilde{R}^{(\alpha)} = \widetilde{R}^{(\alpha)}_{\mu\nu\lambda\gamma}\widetilde{g}^{\mu\nu}\widetilde{g}^{\lambda\gamma} = f(\tau)^{-1}R^{(\alpha)} + \frac{1-\alpha^2}{4}f(\tau)^{-1}(n-n^2).$$

When $n = 2$, from (2.9), we see that the α-Gaussian curvature of $\widetilde{S}$ satisfies

$$\widetilde{K}^{(\alpha)} = \frac{f(\tau)^{-1}(1-\alpha^2)}{4\det(G)^2}\begin{vmatrix} \partial_1^2 \ln Z & \partial_1^3 \ln Z & \partial_1^2\partial_2 \ln Z \\ \partial_1\partial_2 \ln Z & \partial_1^2\partial_2 \ln Z & \partial_1\partial_2^2 \ln Z \\ \partial_2^2 \ln Z & \partial_1\partial_2^2 \ln Z & \partial_2^3 \ln Z \end{vmatrix} - \frac{f(\tau)^{-1}(1-\alpha^2)}{4}.$$

Remark 3. The result is the conclusion in [8] when $\alpha = 0$.

Here, we will use an example to verify our conclusion above.

Example 1. Suppose that $S = \{\rho|\rho = Z^{-1}\exp\big[-\sum_{i=1}^2 \beta_i F_i\big]\}$, and the matrices F_i are given by

$$F_1 = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \end{pmatrix}, \quad F_2 = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 0 & 0 \\ -1 & 1 & 0 \end{pmatrix}.$$

Taking $f(\tau) = \tau > 0$, we get

$$\widetilde{S} = \{\widetilde{\rho}|\widetilde{\rho} = \tau Z^{-1}\exp\big[-\sum_{i=1}^{2}\beta_i F_i\big]\}.$$

An equilibrium density $\rho \in S$ can be represented by

$$\rho = \frac{1}{Z}\exp\left[\begin{pmatrix} -\beta_2 & \beta_2 & 0 \\ \beta_1 & -\beta_1 & 0 \\ \beta_1+\beta_2 & -\beta_1-\beta_2 & 0 \end{pmatrix}\right],$$

and the partition functions of ρ is $Z = \exp[-\beta_1]+\exp[-\beta_2]+1$. Under the coordinate system (β_1, β_2), the geometric metrics of S are given by

$$G = (g_{ij}) = (\partial_i \partial_j \ln Z),$$

$$\det(G) = \partial_1^2 \ln Z \partial_2^2 \ln Z - (\partial_1 \partial_2 \ln Z)^2 = \frac{\exp 2(\beta_1 + \beta_2)}{(\exp(\beta_1) + \exp(\beta_2) + \exp(\beta_1 + \beta_2))^3},$$

and

$$\begin{aligned} R^{(\alpha)}_{1212} &= -\frac{1-\alpha^2}{4\det(G)} \begin{vmatrix} \partial_1^2 \ln Z & \partial_1^3 \ln Z & \partial_1^2 \partial_2 \ln Z \\ \partial_1 \partial_2 \ln Z & \partial_1^2 \partial_2 \ln Z & \partial_1 \partial_2^2 \ln Z \\ \partial_2^2 \ln Z & \partial_1 \partial_2^2 \ln Z & \partial_2^3 \ln Z \end{vmatrix} = \\ &= \frac{(1-\alpha^2) \exp 2(\beta_1 + \beta_2)}{4(\exp(\beta_1) + \exp(\beta_2) + \exp(\beta_1 + \beta_2))^3}, \\ K^{(\alpha)}_{1212} &= \frac{R^{(\alpha)}_{1212}}{\det(G)} = \frac{1-\alpha^2}{4}, \qquad R^{(\alpha)} = \frac{2}{\det(G)} R^{(\alpha)}_{1212} = \frac{1-\alpha^2}{2}. \end{aligned}$$

Under the coordinate system (β_1, β_2, τ), we obtain the geometric metrics of $\widetilde{S}$ corresponding to those of S:

$$\widetilde{G} = \begin{pmatrix} -\tau \partial_1^2 \ln Z & -\tau \partial_1 \partial_2 \ln Z & 0 \\ -\tau \partial_1 \partial_2 \ln Z & -\tau \partial_2^2 \ln Z & 0 \\ 0 & 0 & \tau^{-1} \end{pmatrix} = \begin{pmatrix} \tau G & 0 \\ 0 & \tau^{-1} \end{pmatrix},$$

and

$$\begin{aligned} \widetilde{R}^{(\alpha)}_{1212} &= \tau R^{(\alpha)}_{1212} - \frac{1-\alpha^2}{4} \tau \det(G) = 0, \\ \widetilde{R}^{(\alpha)}_{1\tau 1\tau} &= \widetilde{R}^{(\alpha)}_{121\tau} = \widetilde{R}^{(\alpha)}_{212\tau} = \widetilde{R}^{(\alpha)}_{1\tau 2\tau} = \widetilde{R}^{(\alpha)}_{2\tau 2\tau} = 0, \\ \widetilde{K}^{(\alpha)}_{1212} &= \tau^{-1} K^{(\alpha)}_{1212} - \frac{1-\alpha^2}{4} \tau^{-1} = 0. \end{aligned}$$

The scalar curvature of $\widetilde{S}$ satisfies

$$\widetilde{R}^{(\alpha)} = \frac{\tau^{-1}(1-\alpha^2)}{2\det(G)^2} \begin{vmatrix} \partial_1^2 \ln Z & \partial_1^3 \ln Z & \partial_1^2 \partial_2 \ln Z \\ \partial_1 \partial_2 \ln Z & \partial_1^2 \partial_2 \ln Z & \partial_1 \partial_2^2 \ln Z \\ \partial_2^2 \ln Z & \partial_1 \partial_2^2 \ln Z & \partial_2^3 \ln Z \end{vmatrix} - \frac{\tau^{-1}(1-\alpha^2)}{2} = 0.$$

3 The approximation of the equilibrium density

In this section, we firstly define a Kullback-Leibler divergence, which is different from the general distance of two points in the manifold.

Definition 1. Let $\widetilde{\rho}$ and $\widetilde{\sigma}$ be two points in manifold $\widetilde{S}$, the Kullback-Leibler divergence between two states is defined by

$$D(\widetilde{\rho}|\widetilde{\sigma}) = \mathrm{Tr}[\widetilde{\rho}(\ln \widetilde{\rho} - \ln \widetilde{\sigma})]. \tag{3.1}$$

So, we have the relation of the Kullback-Leibler divergences between S and $\widetilde{S}$

$$D(\widetilde{\rho}|\widetilde{\sigma}) = f(\tau) D(\rho|\sigma). \tag{3.2}$$

Definition 2. Let

$$\widetilde{M} = \left\{ \widetilde{\sigma} | \widetilde{\sigma} = f(\tau) Z_\sigma^{-1} \exp\{-\sum_{j=1}^{r} \theta_j E_j\} \right\} \tag{3.3}$$

be an r-dimensional manifold, where $r \leq n$ and E_j is related to F_i. $\widetilde{M}$ is a submanifold of $\widetilde{S}$.

Clearly submanifold $\widetilde{M}$ is a ± 1-flat manifold, where $\theta = (\theta_1, \cdots, \theta_r)$ is the e–affine coordinate system of $\widetilde{M}$.

Definition 3. For $\widetilde{\rho} \in \widetilde{S}$, the projection onto $\widetilde{M}$ is defined by

$$\widetilde{\sigma^*} = \prod \widetilde{\rho} = \arg\min_{\widetilde{\rho} \in \widetilde{S}} D(\widetilde{\rho} | \widetilde{\sigma}). \tag{3.4}$$

So we have the following proposition.

Proposition 3. *Suppose that the projection from a point $\widetilde{\rho}$ in $\widetilde{S}$ onto $\widetilde{M}$ is σ^*. Then σ^* can be considered as a optimal approximation of the equilibrium density $\widetilde{\rho}$ in $\widetilde{M}$, and σ^* is a solution of the following differential equation*

$$-\frac{\partial}{\partial \theta_i} \ln Z_\sigma = \mathrm{Tr}[\rho E_i]. \tag{3.5}$$

Proof. From (3.1) and (3.2) we have

$$\begin{aligned} D(\widetilde{\rho} | \widetilde{\sigma}) &= \mathrm{Tr}[\widetilde{\rho}(\ln \widetilde{\rho} - \ln \widetilde{\sigma})] = f(\tau) D(\rho | \sigma) \\ &= f(\tau) \mathrm{Tr}[\rho(-\sum_{i=1}^{n} \beta_i F_i - \ln Z_\rho + \sum_{j=1}^{r} \theta_j E_j + \ln Z_\sigma)] \\ &= f(\tau) \left\{ -\sum_{i=1}^{n} \beta_i \mathrm{Tr}[\rho F_i] - \ln Z_\rho + \sum_{j=1}^{r} \theta_j \mathrm{Tr}[\rho E_j] + \ln Z_\sigma \right\}. \end{aligned}$$

Since

$$\frac{\partial D(\widetilde{\rho} | \widetilde{\sigma}(\theta, \tau))}{\partial \theta_i} = -f(\tau) \frac{\partial}{\partial \theta_i} \mathrm{Tr}[\rho \ln \sigma] = f(\tau)(\mathrm{Tr}[\rho E_i] + \frac{\partial}{\partial \theta_i} \ln Z_\sigma) = 0,$$

we obtain (3.5). This finishes the proof of Proposition 3.

Example 2. Let S be a 3-dimensional manifold and take

$$\widetilde{S} = \left\{ \widetilde{\rho} = f(\tau) Z_\rho^{-1} \exp - \sum_{i=1}^{3} \beta_i F_i \right\} = \left\{ \widetilde{\rho} = f(\tau) \rho \right\},$$

where $\beta = (\beta_1, \beta_2, \beta_3)$ is the e-affine coordinate system of S, and the matrixes F_i are given by

$$F_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad F_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad F_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Then submanifold $\widetilde{M}$ of $\widetilde{S}$ satisfies

$$\widetilde{M} = \left\{ \widetilde{\sigma} = f(\tau) Z_\sigma^{-1} \exp - \sum_{j=1}^{2} \theta_j E_j \right\} = \left\{ \widetilde{\sigma} = f(\tau)\sigma \right\},$$

where $\theta = (\theta_1, \theta_2)$ is the e-affine coordinate system of M, and the matrixes E_j are given by

$$E_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad E_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

So the equilibrium density $\widetilde{\rho}$ and $\widetilde{\sigma}$ can be written as

$$\widetilde{\rho} = \frac{f(\tau)}{Z_\rho(\beta)} \begin{pmatrix} \exp\{-\beta_1\} & 0 & 0 \\ 0 & \exp\{-\beta_2\} & 0 \\ 0 & 0 & \exp\{-\beta_3\} \end{pmatrix},$$

and

$$\widetilde{\sigma} = \frac{f(\tau)}{Z_\sigma(\theta)} \begin{pmatrix} \exp\{-\theta_1\} & 0 & 0 \\ 0 & \exp\{-\theta_1\} & 0 \\ 0 & 0 & \exp\{-\theta_2\} \end{pmatrix},$$

respectively.

From (3.5), we have

$$\frac{2\exp\{-\theta_1\}}{2\exp\{-\theta_1\} + \exp\{-\theta_2\}} = \frac{\exp\{-\beta_1\} + \exp\{-\beta_2\}}{\exp\{-\beta_1\} + \exp\{-\beta_2\} + \exp\{-\beta_3\}},$$
$$\frac{\exp\{-\theta_2\}}{2\exp\{-\theta_1\} + \exp\{-\theta_2\}} = \frac{\exp\{-\beta_3\}}{\exp\{-\beta_1\} + \exp\{-\beta_2\} + \exp\{-\beta_3\}}.$$

So we obtain the coordinates θ_i of the optimal approximation σ^* of $\widetilde{\rho}$ as

$$\theta_1^* = -\ln \frac{\exp\{-\beta_1\} + \exp\{-\beta_2\}}{2}, \quad \theta_2^* = \beta_3.$$

4 Conclusions

In this paper, we investigate the structures of the state space of the thermodynamic parameters based upon the information geometric approach to the denormalization $\widetilde{S}$ of S. By calculating the covariant derivative and the α-curvature tensor, we obtain the relation of the α-geometric structures between S and $\widetilde{S}$. At last, we study the approximation of the equilibrium density and use two examples to illustrate our conclusions.

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References

[1] S. Amari and H. Nagaoka, *Methods of Information Geometry*, AMS and Oxford University Press, 2000.

[2] L. Cao, H. Sun and L. Wu, *Information geometry of the thermodynamic manifold*, II Nuovo Cimento 123 (2008), 593-598.

[3] R.S. Ingarden, *Differential geometry and physics*, Tensor N.S. 30 (1976), 201-209.

[4] H. Janyszek and R. Mrugala, *Riemannian geometry and the thermodynamics of model magnetic systems*, Phys. Rev. A 39 (1989), 6515-6523.

[5] D.A. Johnston, W. Janke and R. Kenna, *Information geometry, one, two, three.*, Acta Phys. Pol. B 34 (2003), 4923-4937.

[6] M. Portesi, F. Pennini and A. Plastino, *Geometrical aspects of a generalized statistical mechanics*, Phys. A 373 (2007), 273-279.

[7] M. Portesi, A. Plastino and F. Pennini, *Information geometry and phase transitions*, Int. J. of Mod. Phys. B 20 (2006), 5250-5253.

[8] L. Wu, H. Sun and L. Cao, *Geometrical description of denormalized thermodynamic manifold*, Chin. Phys. B 18 (2009), 3790-3794.

[9] Z. Zhang, H. Sun and F. Zhong, *Geometrical structures of certain class of statistical manifolds*, J. of BIT 17 (2008), 368-372.

[10] Z. Zhang, H. Sun and F. Zhong, *Information geometry of the power inverse Gaussian distribution*, Appl. Sci. 9 (2007), 194-203.

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