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ON THE LOCAL RIEMANNIAN STRUCTURE OF THE STATE SPACE OF CLASSICAL INFORMATION THERMODYNAMICS.

Dedicated to Professor Akitsugu Kawaguchi on the occasion of his 80th birthday.

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The paper is a continuation of the investigations of the local Riemannian structure of the state-space of thermodynamical systems by one of the authors (R.S.I.). Now the following two cases have been investigated: 1) the space of all statistical states, equilibrium or nonequilibrium, for the classical discrete finite systems (they correspond to the Ising models of finite spin systems), 2) the state space of the so-called control thermodynamics, i.e., information thermodynamics with the usual (1st order) temperature and 2nd order (control) temperature, of an ideal gas (for simplicity only a system of one degree of freedom is considered). The result is that in the case 1) the space is of a constant and positive Riemann curvature, while in the case 2) the Riemann curvature is not constant and not necessarily positive and depends critically on the 2nd order temperature.

§1. Introduction. Some years ago one of the present authors (R.S.I.) started an investigation of differential geometry of thermodynamics, especially of statistical thermodynamics considered as information thermodynamics [1][1], [2]. These investigations have been connected with the geometrical ideas of mathematical statistics (cf. the monographs [3], [4], where the earlier references can be found, and [5]), and the term information geometry has been introduced because of the importance of relative information for the definition of distance in the state space [6]. Actually, the distance is not of the Fréchet type, but in the limit of small distances, i.e., locally it is of the Fréchet type and we obtain then a Riemannian geometry. In [6] the local Riemannian structure of the state space of classical thermodynamics of the ideal gas and of a system of linear and generalized oscillators has been investigated. The result is that all these thermodynamical spaces are flat in the Riemannian sense, so can be considered as locally Euclidean. In the present paper we shall ivestigate some other classical cases, and we shall see that they are essentially non-Euclidean ones.

§2. The complete state space for discrete systems. Let us now consider the space of all possible statistical states for a discrete finite classical system. Such a system has $n=1, 2, \cdots$ pure states and a general mixed state can be written as $p=(p_1, p_2, \cdots, p_n)$, where

$$(1)\qquad p_i \geqslant 0 \qquad (i=1, 2, \cdots, n), \qquad \sum_{i=1}^{n} p_i = 1 .$$

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1) Numbers in brackets refer to the references at the end of the paper.

In such a way we have $n-1$ independent parameters of a state p, e.g., $p_1, \cdots, p_{n-1}$, and

$$p_n = 1 - p_1 - \cdots - p_{n-1}\,. \tag{2}$$

Since $0 \leqslant p_n \leqslant 1$, we have the following conditions for the independent parameters $p_\alpha \geqslant 0$ ($\alpha = 1, 2, \cdots, n-1$), $0 \leqslant p_1 + \cdots + p_{n-1} \leqslant 1$, i.e., they fill the inside and borders of the rectangular triangle (for $n=3$), in general a simplex, (cf. Fig. 1) defined by n equations of sides

$$p_\alpha = 0 \qquad (\alpha = 1, \cdots, n-1)\,, \qquad p_1 + p_2 + \cdots + p_{n-1} = 1 \tag{3}$$

in space $(p_1, \cdots, p_{n-1})$. The "state space" on Fig. 1 is actually

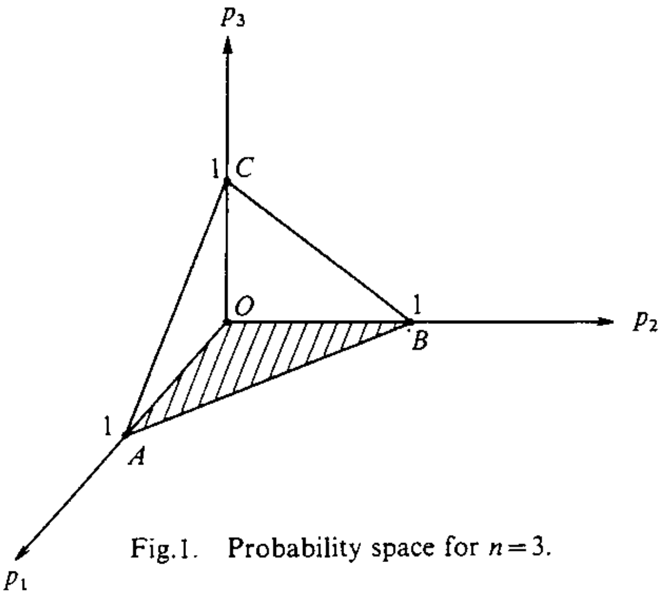

Fig. 1. Probability space for $n=3$.

the triangle ABC with "barycentric" coordinates $p_1, \cdots, p_n$ (by one too numerous, therefore not all independent, but symmetrical), while the space of independent parameters may be taken as ABO or ACO or BCO, etc.

The *information distance* of states p and q (in this order) is now defined by means of the relative information (entropy)

$$\begin{aligned} s^2(q\,|\,p) = S(q\,|\,p) = \sum_{i=1}^{n} p_i(\ln p_i - \ln q_i) = \sum_{\alpha=1}^{n-1} p_\alpha(\ln p_\alpha - \ln q_\alpha) \\ + \left(1 - \sum_{\alpha=1}^{n-1} p_\alpha\right)\left[\ln\left(1 - \sum_{\alpha=1}^{n-1} p_\alpha\right) - \ln\left(1 - \sum_{\alpha=1}^{n-1} q_\alpha\right)\right] \geqslant 0\,. \end{aligned} \tag{4}$$

Taking into account only independent parameters p_α we may write the Taylor expansion (using the Einstein summation convention)

$$ds^2 = S(p\,|\,p+dp) = S(p\,|\,p) + \left.\frac{\partial S}{\partial p_\alpha}\right|_{p=q} dp_\alpha + \frac{1}{2}\left.\frac{\partial^2 S}{\partial p_\alpha \partial p_\beta}\right|_{p=q} dp_\alpha dp_\beta + \cdots,$$

where (cf. (4))

$$S(p\,|\,p) = 0\,, \qquad \left.\frac{\partial S}{\partial p_\alpha}\right|_{p=q} = \left[\ln p_\alpha - \ln q_\alpha - \ln\left(1 - \sum_\alpha p_\alpha\right) + \ln\left(1 - \sum_\alpha q_\alpha\right)\right]_{p=q} = 0\,,$$

$$\left.\frac{\partial^2 S}{\partial p_\alpha \partial p_\beta}\right|_{p=q} = \frac{\delta_{\alpha\beta}}{p_\alpha} + \left(1 - \sum_\alpha p_\alpha\right)^{-1} = \frac{\delta_{\alpha\beta}}{p_\alpha} + \frac{1}{p_n}\,.$$

Finally, in this approximation

(5) $$ds^2 = S(p\,|\,p+dp) = S(p+dp\,|\,p) = g_{\alpha\beta}(p)dp_\alpha dp_\beta \geqslant 0\,,$$

where (without summation!)

(6) $$g_{\alpha\beta}(p) = \frac{1}{2}\left(\frac{\delta_{\alpha\beta}}{p_\alpha} + \left(1 - \sum_\alpha p_\alpha\right)^{-1}\right), \qquad (\alpha, \beta = 1, \cdots, n-1)\,.$$

The same result can be obtained directly from the general formula [2]–[6]

(7) $$g_{\alpha\beta}(u) = \frac{1}{2}\left\langle \frac{\partial \ln p}{\partial u_\alpha}\frac{\partial \ln p}{\partial u_\beta}\right\rangle = \frac{1}{2}\sum_{i=1}^{n} p_i \frac{\partial \ln p_i}{\partial u_\alpha}\frac{\partial \ln p_i}{\partial u_\beta}$$

(we introduce into $g_{\alpha\beta}$ the factor 1/2 otherwise than usually [3]), when we put for parameters $u_\alpha := p_\alpha$ ($\alpha = 1, \cdots, n-1$).

To facilitate the further calculations we transform the parameters in the following way:

$$p_\alpha = \tfrac{1}{2}x_\alpha^2\,, \qquad x_\alpha \geqslant 0 \qquad (\alpha = 1, \cdots, n-1)\,, \qquad \partial p_\alpha/\partial x_\beta = x_\alpha \delta_{\alpha\beta}$$

(in the latter formula no summation!) and we obtain the new variables

$$\tilde{g}_{\alpha\beta}(x) = \frac{\partial p_\gamma}{\partial x_\alpha}\frac{\partial p_\delta}{\partial x_\beta} g_{\gamma\delta}(p(x)) = \delta_{\alpha\beta} + \frac{x_\alpha x_\beta}{\left(\frac{1}{2}\right)^{-1} - \delta_{\gamma\delta}x_\gamma x_\delta}\,.$$

This form of the metric tensor is, however, well-known in the theory of Riemannian spaces (cf. [7], p. 136). Namely, this is a special form of the metric tensor of a Riemannian space of constant Riemannian (for $n=2$ Gaussian) curvature $K = \frac{1}{2}$, which can be imagined as an $(n-1)$-dimensional sphere with the radius $r = \sqrt{2}$ in an n-dimensional Euclidean space E^n. The equation of these sphere in E^n is

(8) $$x_1^2 + x_2^2 + \cdots + x_{n-1}^2 + x_n^2 = 2\,.$$

Going back from x_α to our previous parameters p_α, and putting

(9) $$p_n = \tfrac{1}{2}x_n^2\,, \qquad x_n \geqslant 0\,.$$

we obtain from (8) an equation of a plane (hyperplane) in p-space, $p_1 + \cdots + p_n = 1$, which is just the normalization equation (1) or (2) of our starting point. The construction is thus universal for any point of state space. According to the general formulae of the Riemannian spaces of constant curvature [7] we have for the scalar Riemann curvature $R = n(n-1)K = n(n-1)/2$, and for the full Riemann curvature tensor $R_{\alpha\beta\gamma\delta} = -K(g_{\alpha\gamma}g_{\beta\delta} - g_{\alpha\delta}g_{\beta\gamma}) = -\frac{1}{2}(g_{\alpha\gamma}g_{\beta\delta} - g_{\alpha\delta}g_{\beta\gamma})$. Geodesics and any other geometrical constructions can be easily traced as the constructions on a sphere.

The exact coincidence of (9) with (1) does not mean, however that the information distance is calculated exactly. The exact formula is precisely (4) for any global distances, while (5)–(6) is only a differential or infinitesimal approximation of the second (the first non-vanishing one) and is valid only locally. How big these discrepancies can be for finite distances can be seen from the following example:

$$p = M = (1/n, \cdots, 1/n)\,, \qquad q = A = (1, 0, \cdots, 0)\,,$$

$$S(q\,|\,p) = S(A\,|\,M) = \infty\,, \qquad S(p\,|\,q) = S(M\,|\,A) = \ln n\,,$$

while the Riemann distance is always finite. For $n=3$ $\ln 3=1.0986122\cdots=S(M|A)$ while in the Riemannian (or 2nd) approximation we obtain

$$S_2(M|A)=S_2(A|M)=1.3510217\cdots.$$

The last number has been calculated by observing that the angle between vectors M and A is $54°.73561\cdots$ and is a $6.5770711\cdots$-th part of the circle with radius $\sqrt{2}$ [2)].

The question may be raised why we use an approximation when the exact formula is known. The answer is that the geometry of the general case (the so-called asymmetric Pythagorean geometry [4]) is not yet sufficiently known and therefore it is easier to use the Riemannian one as an approximation. The latter is good enough when we confine ourselves to a small vicinity of some state, e.g., an equilibrium state. When we are interested only in the shape of the curve in the state space and not in the absolute value of the length of the curve, it is sufficient to discuss local geometry since changes of direction of the curve are determined by the latter. (We mean only one direction, e.g., only left or only right, and do not consider topological properties of curves which may be essentially of non-local character.)

§ 3. A system with two temperatures of different order. Let us now consider a classical statistical system with two temperatures of different order [8]. For simplicity we consider only a system with one degree of freedom, cf. [9] (without potential energy and in a one-dimensional "volume" $V=1$; parameter V has no influence on the curvature of the Riemannian space considered here). Further simplification can be made by confining oneself only to the cases when the partition function Z (sum over states) can be exactly calculated by well-known special functions. In one set of these cases a state can be represented by density functions (we denote $x=p(2m)^{-1}$, where p is momentum and m is mass)

$$f(x)=Z^{-1}(\alpha,\beta)\exp(-\alpha x^n-\beta x^{2n}), \quad n=1,2,\cdots, \quad -\infty<\alpha<+\infty, \quad \beta>0, \quad -\infty<x<+\infty.$$

Then we have

$$(10) \qquad Z(\alpha,\beta)=\int_{-\infty}^{+\infty}\exp(-\alpha x^n-\beta x^{2n})dx=\frac{\Gamma(1/n)}{n\beta^{1/2n}}\left[H_{-1/n}\left(\frac{\alpha}{2\sqrt{\beta}}\right)+H_{-1/n}\left(\frac{(-1)^n\alpha}{2\sqrt{\beta}}\right)\right],$$

where $H_\nu(z)$ is a Hermite function connected with the Weber function $D_\nu(z)$ of parabolic cyclinder by

$$H_\nu(z)=2^{-\nu/2}\exp(z^2/2)D_\nu(\sqrt{2}\,z),$$

cf. [10]–[13]. In particular, denoting $Z(\alpha,\beta)=Z_n(\alpha,\beta)$ we obtain

$$Z_1(\alpha,\beta)=\exp(\alpha^2/4\beta)\sqrt{\pi/\beta},$$

$$Z_2(\alpha,\beta)=\frac{\sqrt{\pi}}{(2\beta)^{1/4}}\exp\left(\frac{\alpha^2}{8\beta}\right)D_{-1/2}\left(\frac{\alpha}{2\sqrt{\beta}}\right)=\begin{cases}\frac{1}{2}\sqrt{\alpha/\beta}\exp(\alpha^2/8\beta)K_{1/4}(\alpha^2/8\beta) & \text{for } \alpha>0,\\ \Gamma(1/4)/2\beta^{1/4} & \text{for } \alpha=0,\\ \frac{1}{4}\pi\sqrt{-\alpha/\beta}\exp(\alpha^2/8\beta)\mathscr{I}_{1/4}(\alpha^2/8\beta) & \text{for } \alpha<0,\end{cases}$$

2) This is in accordance with the Bhattacharyya formula $s(p|q)=\sqrt{2}\arccos(\sum_{i=1}^n\sqrt{p_iq_i})$ quoted in [16] equ. (6) (we renormalized this formula by factor $1/\sqrt{2}$ because of the difference in the definition of s).

where $K_\nu(z)$ is the MacDonald (Kelvin) function or modified Bessel function of the 2nd order, while

$$\mathcal{I}_\nu(z)=\{I_{-\nu}(z)+I_\nu(z)\}/\cos\gamma\pi\,,\qquad |\arg z|<\pi\,,$$

where $I_\nu(z)$ is the modified Bessel function of the 1st order (cf. [11], [12]). Denoting

$$U=\langle x^n\rangle=Z^{-1}\int_{-\infty}^{+\infty}x^n f(x)dx\,,\qquad W=\langle x^{2n}\rangle\,,$$

we obtain

$$U=-\frac{1}{Z}\frac{\partial Z}{\partial\alpha}=-\frac{\partial\ln Z}{\partial\alpha},\qquad W=-\frac{1}{Z}\frac{\partial Z}{\partial\beta}=-\frac{\partial\ln Z}{\partial\beta}=\frac{1}{Z}\frac{\partial^2 Z}{\partial\alpha^2}. \tag{11}$$

Since $\partial Z/\partial\beta=-\partial^2 Z/\partial\alpha^2$, we also have

$$W=U^2-\partial U/\partial\alpha\,,\qquad \partial W/\partial\alpha=\partial U/\partial\beta\,. \tag{12}$$

Calculating the components of the metric tensor from the general formula analogous to (7) ([2]–[6]) we get

$$g_{\alpha\alpha}=\tfrac{1}{2}\langle(\partial\ln f/\partial\alpha)^2\rangle=\tfrac{1}{2}(W-U^2)=-\tfrac{1}{2}\partial U/\partial\alpha\,,$$

$$g_{\beta\alpha}=g_{\alpha\beta}=\tfrac{1}{2}\langle\partial\ln f/\partial\alpha,\,\partial\ln f/\partial\beta\rangle=\tfrac{1}{2}(\langle x^{3n}\rangle-WU)=-\tfrac{1}{2}\partial W/\partial\alpha=-\tfrac{1}{2}\partial U/\partial\beta\,,$$

$$g_{\beta\beta}=\tfrac{1}{2}\langle(\partial\ln f/\partial\beta)^2\rangle=\tfrac{1}{2}(\langle x^{4n}\rangle-W^2)=-\tfrac{1}{2}\partial W/\partial\beta\,.$$

This gives $g=\det(g_{\mu\lambda})=\frac{1}{4}\{(\partial U/\partial\alpha)(\partial W/\partial\beta)-(\partial U/\partial\beta)(\partial W/\partial\alpha)\}$ and

$$g^{\alpha\alpha}=g_{\beta\beta}/g=-\tfrac{1}{2}g^{-1}\partial W/\partial\beta\,,\qquad g^{\beta\beta}=g_{\alpha\alpha}/g=-\tfrac{1}{2}g^{-1}\partial U/\partial\alpha\,,$$

$$g^{\alpha\beta}=g^{\beta\alpha}=-g_{\alpha\beta}/g=\tfrac{1}{2}g^{-1}\partial U/\partial\beta=\tfrac{1}{2}g^{-1}\partial W/\partial\alpha\,.$$

Then we calculate the Christoffel symbols

$$\left\{{\alpha\atop\alpha\alpha}\right\}=\frac{1}{8g}\left(\frac{\partial W}{\partial\beta}\frac{\partial^2U}{\partial\alpha^2}-\frac{\partial U}{\partial\beta}\frac{\partial^2W}{\partial\alpha^2}\right),\qquad \left\{{\beta\atop\beta\beta}\right\}=\frac{1}{8g}\left(\frac{\partial U}{\partial\alpha}\frac{\partial^2W}{\partial\beta^2}-\frac{\partial W}{\partial\alpha}\frac{\partial^2U}{\partial\beta^2}\right),$$

$$\left\{{\beta\atop\alpha\alpha}\right\}=\frac{1}{8g}\left(\frac{\partial U}{\partial\alpha}\frac{\partial^2W}{\partial\alpha}-\frac{\partial W}{\partial\alpha}\frac{\partial^2U}{\partial\alpha^2}\right),\qquad \left\{{\alpha\atop\beta\beta}\right\}=\frac{1}{8g}\left(\frac{\partial W}{\partial\beta}\frac{\partial^2U}{\partial\beta^2}-\frac{\partial U}{\partial\beta}\frac{\partial^2W}{\partial\beta^2}\right),$$

$$\left\{{\alpha\atop\alpha\beta}\right\}=\frac{1}{8g}\left(\frac{\partial U}{\partial\beta}\frac{\partial^2W}{\partial\alpha^2}-\frac{\partial W}{\partial\alpha}\frac{\partial^2U}{\partial\beta^2}\right),\qquad \left\{{\beta\atop\alpha\beta}\right\}=\frac{1}{8g}\left(\frac{\partial U}{\partial\alpha}\frac{\partial^2W}{\partial\beta^2}-\frac{\partial U}{\partial\beta}\frac{\partial^2W}{\partial\alpha^2}\right).$$

In the two dimensional case the Riemann curvature tensor has only one independent component

$$R_{\alpha\beta\alpha\beta}=\frac{1}{2}\left(2\frac{\partial^2g_{\alpha\beta}}{\partial\alpha\partial\beta}-\frac{\partial^2g_{\alpha\alpha}}{\partial\beta^2}-\frac{\partial^2g_{\beta\beta}}{\partial\alpha^2}\right)+g_{\alpha\alpha}\left(\left\{{\alpha\atop\alpha\beta}\right\}\left\{{\alpha\atop\alpha\beta}\right\}-\left\{{\alpha\atop\beta\beta}\right\}\left\{{\alpha\atop\alpha\alpha}\right\}\right)$$
$$+g_{\alpha\beta}\left(\left\{{\alpha\atop\alpha\beta}\right\}\left\{{\beta\atop\alpha\beta}\right\}-\left\{{\alpha\atop\beta\beta}\right\}\left\{{\beta\atop\alpha\alpha}\right\}\right)+g_{\beta\alpha}\left(\left\{{\beta\atop\alpha\beta}\right\}\left\{{\alpha\atop\alpha\beta}\right\}-\left\{{\beta\atop\beta\beta}\right\}\left\{{\alpha\atop\alpha\alpha}\right\}\right)+g_{\beta\beta}\left(\left\{{\beta\atop\alpha\beta}\right\}\left\{{\beta\atop\alpha\beta}\right\}-\left\{{\beta\atop\beta\beta}\right\}\left\{{\beta\atop\alpha\alpha}\right\}\right).$$

In our case the sum of the first three terms vanishes because of (12) and after some calculation we finally obtain for the scalar curvature

$$R=\frac{R_{\alpha\beta\alpha\beta}}{g}=\frac{1}{32g}\left\{\frac{\partial W}{\partial\beta}\left[\frac{\partial^2 U}{\partial\beta^2}\frac{\partial^2 U}{\partial\alpha^2}-\left(\frac{\partial^2 W}{\partial\alpha^2}\right)^2\right]+\frac{\partial U}{\partial\alpha}\left[\frac{\partial^2 W}{\partial\beta^2}\frac{\partial^2 W}{\partial\alpha^2}-\left(\frac{\partial^2 U}{\partial\beta^2}\right)^2\right]\right.$$
$$\left.+\frac{\partial U}{\partial\beta}\left[\frac{\partial^2 U}{\partial\beta^2}\frac{\partial^2 W}{\partial\alpha^2}-\frac{\partial^2 W}{\partial\beta^2}\frac{\partial^2 U}{\partial\alpha^2}\right]\right\}. \tag{13}$$

We above said that the introduction of general volume V (not necessarily $=1$) has no influence on the curvature. More specifically, the problem looks as follows. We have $Z\to VZ$, $g_{\alpha\alpha}$, $g_{\alpha\beta}$, $g_{\beta\beta}$ do not change, while the only non-zero new component of the metric tensor is $g_{VV}=1/V^2$. Also all the Christoffel symbols given above do not change, while the only non-zero new symbol is $\{_V{}^V{}_V\}=-1/V$. No new components of the Riemann curvature tensor appear, and there is no change in $R_{\alpha\beta\alpha\beta}$. Therefore, also R is not changed.

To get the explicit expression for R as function of α and β, the function Z (10) has to be put into (11) and then into (13) and the corresponding differentiations have to be performed. The result, however, is so complicated in the general case that is not worth while reproducing it here. The complete discussion is easy to perform only in the case $n=1$ (which is actually known from elsewhere). To get a first orientation for $n=2$ we calculate the curvature in the asymptotic case in the first approximation of the dimensionless parameter β/α^2.

§ 4. The case $n=1$.

In this case we obtain from (11)

$$U=-\alpha/2\beta\,, \qquad W=\alpha^2/4\beta+1/2\beta=U^2+1/2\beta\,,$$

and solving with respect to α and β

$$\alpha=-U/(W-U^2)\,, \qquad \beta=1/2(W-U^2)\,.$$

Physically, the problem can be interpreted as that of "signal plus noise" in the classical case. The quantum analogue of this problem has been discussed in the book of Louisell ([**14**] sections 6.11). The signal is represented by the mean value U and its "temperature" (or "inverse temperature") α, while the noise by the mean value W and its temperature coefficient β (being connected with the usual thermal inverse temperature). In mathematical statistics the case $n=1$ corresponds simply to the general Gauss distribution (normal probability law) with an arbitrary shift $m=-\alpha/2\beta$ and its interpretation is obvious.

Performing all calculations as given in the previous section we finally obtain $R=-1$, i.e., a space of constant negative curvature, as well known in mathematical statistics (cf. e.g. [**5**] where further references are given).

§ 5. The case $n=2$.

In this case U can be interpreted as a mean energy of thermal noise and W as a controlled value of fluctuation of energy. Therefore, α has interpretation as a "thermal inverse temperature" and β as a "control inverse temperature" or "control parameter" (for more thorough discussion cf. [**8**] and [**15**]).

We shall discuss the asymptotic case $\alpha>0$ and $\alpha^2/8\beta\gg1$ or $8\beta/\alpha^2\ll1$. This corresponds to a small control by given thermal temperature (noise). Making all calculations systematically in the linear approximation of the dimensionless parameter $\xi=8\beta/\alpha^2$, we finally obtain

$$Z=\sqrt{\pi/\alpha}\,(1+3\beta/4\alpha^2)\,, \qquad U=1/2\alpha+3\beta/2\alpha^3\,, \qquad W=3/4\alpha^2+6\beta/\alpha^4\,,$$

$$g_{\alpha\alpha}=1/4\alpha^2+9\beta/4\alpha^4\,, \qquad g_{\alpha\beta}=3/4\alpha^3+12\beta/\alpha^5\,, \qquad g_{\beta\beta}=3/\alpha^4+297\beta/4\alpha^6\,.$$

Then we have in this approximation $R_{\alpha\beta\alpha\beta} = 9/8\alpha^6 - 373.25\beta/\alpha^8$, and for the scalar curvature $R = 6 - 2181.3\beta/\alpha^2$. We see that for $\xi = 0$ the scalar curvature is positive, but for $\xi = (8.6)/2181.3 = 0.0220052 \ll 1$, the curvature R vanishes, while for greater ξ it becomes negative. So the control parameter (anyhow in this approximation) can essentially influence the Riemannian curvature of the state space.

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