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INFORMATION GEOMETRY OF QUANTUM STATISTICAL SYSTEMS.

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

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The paper is devoted to an investigation of the Riemannian structure of the state (parameter) space of quantum statistical systems. The paper is a continuation of the previous investigations concerning information geometry in the classical case by some of the authors of this work (R.S.I. and H.J.) [4]-[7][2].

A generalization of the Riemannian structure of the parameter space to the case of quantum statistical thermodynamics has been presented. The paper is based on the concept of Umegaki's relative information which is a quantum generalization of the classical Rényi-Kullback information gain used in the previous papers. Three examples illustrating the Riemannian structure of quantum statistical systems have been presented and discussed: 1) the spin 1/2 system in the complete state space, 2) the harmonic oscillator in space of two thermodynamical parameters, 3) the ideal gas in space of two thermodynamical parameters.

§1. Introduction. Few years ago one of the present authors (R.S.I.) began the investigation of the geometric structure of statistical thermodynamics ([4], [5]). This investigation is connected with geometrical ideas of mathematical statistics (cf. the monographs [2], [9], and [10]). The idea of information geometry has been introduced by means of the relative information as an "information distance" (divergence) in parameter space. In general, this "distance" is not a Fréchet distance (does not satisfy the axioms of symmetry and triangle inequality), but in the limit of small distances is a Fréchet distance. in particular, a Riemannian distance. In this paper the local Riemannian structure is investigated for the quantum systems. We have to point out that the quantum case is not a special case of the classical one, but, reversibly, the classical case can be obtained as the limiting case of the quantum theory. Therefore, our theory is from the beginning a more general one than the theories considered in this field before.

§2. Information distance in the state space and its Riemannian structure. *The information gain* (relative entropy) or *information distance* between two statistical states ρ and σ has the following form (Umegaki entropy [11])

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

(1) $$S(\rho\,|\,\sigma)=\mathrm{Tr}\,[\rho(\ln\rho-\ln\sigma)]\geqslant 0\,,$$

where ρ and σ are positive definite trace class linear operators of trace one (density operators) on a separable complex Hilbert space $\mathscr{H}$,

(2) $$\rho,\ \sigma\geqslant 0\,,\qquad \mathrm{Tr}\,\rho=\mathrm{Tr}\,\sigma=1\,.$$

We assume (of course, this assumption is essential only when the Hilbert space $\mathscr{H}$ is infinite-dimensional) that any observable A on $\mathscr{H}$ used to thermodynamical measurement (as energy, etc.) is *thermodynamically regular*, or is *of $\theta(\mathscr{H})$ class* (cf. **[8]**, p. 282), i.e., such that its spectrum is discrete, and at most finitely degenerated,

(3) $$A=\sum_{i=1}^{\dim\mathscr{H}}\lambda_i P_i\,,\qquad \lambda_i\in\boldsymbol{R}\,,\qquad (i,j=1,2,\cdots,\dim\mathscr{H})\,,$$

(4) $$P_i\geqslant 0\,,\qquad P_iP_j=P_i\delta_{ij}\,,\qquad \mathrm{Tr}P_i=1\,,\qquad \sum_{i=1}^{\dim\mathscr{H}}P_i=I\,,$$

(5) $$\exists\beta\in\boldsymbol{R}\,;\qquad \mathrm{Tr}[\exp(-\beta A)]=\sum_{i=1}^{\dim\mathscr{H}}\exp(-\beta\lambda_i)<\infty\,,$$

cf. also (**[13]**, **[15]**). Only the property (5) is essential (the other follow from it, cf. **[13]**). Now a state (2) is said to be *thermodynamically regular*, or *of class $\Delta(\mathscr{H})$*, iff

(6) $$\exists A\in\theta(\mathscr{H}):^{3)}\qquad \bar{A}=\langle A,\rho\rangle=\mathrm{Tr}\,(\rho A)=u<\infty\,.$$

It is easy to see that entropies $S(\rho)=-\mathrm{Tr}\,(\rho\ln\rho)$ and $S(\rho\,|\,\sigma)$ of thermodynamically regular states are always finite, and not only continuous, but even analytic (as in the classical case) (cf. **[3]**, **[12]**, **[13]**). Now we consider the states (being elements of the set of all states on $\mathscr{H}$, $P(\mathscr{H})$)

(7) $$\rho=\rho(x)\,,\qquad \sigma=\rho(y)$$

as values of a function of parameters $\rho: M\to P(\mathscr{H})$ for $x,\ y\in M$, where M is a K-dimensional thermodynamical parameter space assumed as a differentiable manifold of class at least C^3 with local coordinates x^i, y^i (we assume below that $K<\infty$), $i=1,\cdots,K$.

In order to simplify the calculations we symmetrize[4)] the information distance

(8) $$S(x,y)=\tfrac{1}{2}[S(\rho(x)\,|\,\rho(y))+S(\rho(y)\,|\,\rho(x))]\,.$$

We write $\rho(x)$ in the form

(9) $$\rho(x)=Z^{-1}(x)e^{A(x)}\,,$$

where

(10) $$Z(x)=\mathrm{Tr}\,[e^{A(x)}]\,,\qquad A(x)=\ln\rho(x)+\ln Z(x)\,,$$

and we obtain after a short calculation

(11) $$S(x,y)=\tfrac{1}{2}\mathrm{Tr}\,\{[\rho(x)-\rho(y)][A(x)-A(y)]\}\,.$$

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3) If $\dim\mathscr{H}=\infty$, A should be bounded from below and unbounded from above, such as the energy operators.

4) This has no influence on the local metric.

From (11) we see that

(12) $$S(x, x)=0 .$$

Expanding (11) into a power series in the neighbourhood of x ($y=x+dx$) we consider only the terms to the second order in dx (according to the above mentioned restriction to investigate only the local properties of the parameter space). In order to calculate the first and the second order derivatives of S we use the well-known formula (cf. [14])

(13) $$\frac{de^{A(\mu)}}{d\mu}=\int_0^1 d\lambda e^{(1-\lambda)A}\frac{dA}{d\mu}e^{\lambda A}=\int_0^1 d\lambda e^{\lambda A}\frac{dA}{d\mu}e^{(1-\lambda)A} .$$

After a short calculation we obtain

(14) $$\left.\frac{\partial S(x, y)}{\partial x^i}\right|_{y=x}=0 \qquad (i=1, \cdots, K),$$

(15) $$\left.\frac{\partial^2 S(x, y)}{\partial x^i \partial x^j}\right|_{y=x}=\int_0^1 d\lambda\left\langle e^{-\lambda A}\left(\frac{\partial A}{\partial x^i}-\left\langle\frac{\partial A}{\partial x^i}\right\rangle\right)e^{\lambda A}\left(\frac{\partial A}{\partial x^j}-\left\langle\frac{\partial A}{\partial x^j}\right\rangle\right)\right\rangle$$

$$=\int_0^1 d\lambda\left\langle e^{-\lambda A}\frac{\partial \ln \rho}{\partial x^i}e^{\lambda A}\frac{\partial \ln \rho}{\partial x^j}\right\rangle ,$$

where $\langle\cdots\rangle=\mathrm{Tr}\,[\rho(\cdots)]$. This expression can be written in another final form

(16) $$\left.\frac{\partial^2 S(x, y)}{\partial x^i \partial x^j}\right|_{y=x}=\frac{\partial^2 \ln Z}{\partial x^i \partial x^j}-\left\langle\frac{\partial^2 A}{\partial x^i \partial x^j}\right\rangle=-\left\langle\frac{\partial^2 \ln \rho}{\partial x^i \partial x^j}\right\rangle .$$

Thus the local metric has the form

(17) $$dS^2=g_{ij}dx^i dx^j , \qquad g_{ij}(x)=g_{ji}(x)=\frac{1}{2}\left(\frac{\partial^2 \ln Z}{\partial x^i \partial x^j}-\left\langle\frac{\partial^2 A}{\partial x^i \partial x^j}\right\rangle\right)=-\frac{1}{2}\left\langle\frac{\partial^2 \ln \rho}{\partial x^i \partial x^j}\right\rangle ,$$

(since now we adopt the Einstein summation convention). Due to the positivity of $S(\rho|\sigma)$ (1), the symmetric matrix $g_{ij}(x)$ is positive definite. We see that the local structure of the parameter space is Riemannian, as in the classical case. We remark that $g_{ij}(x)$ is essentially different than in the classical case, cf. [9], where

(17)a) $$g_{ij}(x)=\frac{1}{2}\left\langle\frac{\partial \ln \rho}{\partial x^i}\frac{\partial \ln \rho}{\partial x^j}\right\rangle .$$

The (17)a) cannot be generalized to the quantum case because then $\partial \ln \rho/\partial x^i$ does not commute, in general, with $\partial \ln \rho/\partial x^j$.

§ 3. Spin 1/2.

Let us put

(18) $$A=x^i\sigma_i \qquad (i=1, 2, 3) ,$$

where σ_i are the Pauli matrices

(19) $$\sigma_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \qquad \sigma_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \qquad \sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} ,$$

and $x=(x^1, x^2, x^3)\in \boldsymbol{R}^3$. In this case tensor g_{ij} has the simple form

(20) $$g_{ij}(x)=\tfrac{1}{2}\partial^2 \ln Z/\partial x^i \partial x^j .$$

After a simple calculation we obtain

(21) $$Z=\mathrm{Tr}\, e^A=2 \,\mathrm{ch}\, r , \qquad r=|x|=[(x^1)^2+(x^2)^2+(x^3)^2]^{1/2} ,$$

(22) $$g_{ij}=\tfrac{1}{2}r^{-1}(\delta_{ij}-x^i x^j/r)\,\mathrm{th}\, r+x^i x^j/r\, \mathrm{ch}^2 r ,$$

(23) $$\det (g_{ij})=\tfrac{1}{2}\mathrm{th}^2\, r/r^2\, \mathrm{ch}^2\, r>0 ,$$

(24) $$g^{ij}=(2r/\mathrm{th}\, r)\delta^{ij}-(2\alpha r\, \mathrm{ch}^2\, r/\mathrm{th}\, r)x^i x^j , \qquad \alpha=(r-\mathrm{ch}^2 r\, \mathrm{th}\, r)/r^3\, \mathrm{ch}^2\, r .$$

The Christoffel symbols have the form

(25) $$\Gamma^m_{ij}=\alpha r[x^m(1-\alpha\, \mathrm{ch}^2\, r-r^2)\delta_{ij}+x^j\delta^m_i+x^i\delta^m_j+\gamma x^i x^j x^m]/2\, \mathrm{th}\, r ,$$

where

(26) $$\gamma=(\mathrm{sh}^2\, r+r\, \mathrm{th}\, r-2r^2)/r^6 .$$

The Riemann curvature tensor is

(27) $$R_{ikjm}=(\alpha^2 r^2/8\, \mathrm{th}^2\, r)\{(\delta_{kj}\delta_{im}-\delta_{km}\delta_{ij})(\mathrm{sh}^2\, r/r^2)(\mathrm{th}\, r+\alpha r^4)+(x^i x^m\delta_{kj}+x^k x^j\delta_{im} \\ -x^i x^j\delta_{km}-x^k x^m\delta_{ij})(2\, \mathrm{sh}^2\, r/r^2+\gamma\, \mathrm{sh}^2\, r+2\alpha r\, \mathrm{ch}\, r\, \mathrm{sh}\, r+\alpha\gamma r^3\, \mathrm{ch}\, r\, \mathrm{sh}\, r-\mathrm{th}\, r/r)\}.$$

The scalar curvature is

(28) $$R(r)=(r-\mathrm{ch}\, r\, \mathrm{sh}\, r)[4r\, \mathrm{ch}^2\, r-\mathrm{sh}\, r\, \mathrm{ch}\, r-3r]/r^2\, \mathrm{sh}^2\, r .$$

$R(r)$ is negative for $r>0$, $R(0)=0$, and is monotonically decreasing function of (increasing) r,

$$\lim_{r\to\infty} R(r)=-\infty \qquad \text{and} \qquad \left.\frac{dR(r)}{dr}\right|_{r=0}=0 , \quad \text{cf. Fig. 1.}$$

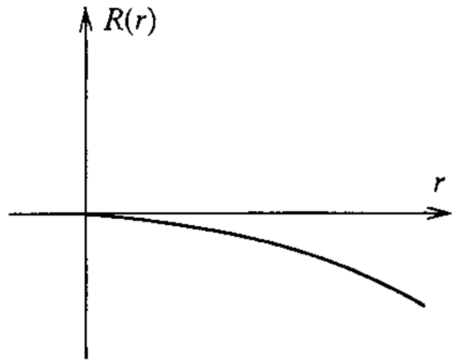

Fig. 1.

§ 4. **Harmonic oscillator.** In this case we take as thermodynamical parameters the inverse temperature $\beta>0$ and the circular frequency $\omega>0$. The hamiltonian for the quantum linear harmonic oscillator and its eigenvalues are

(29) $$H=p^2/2m+\tfrac{1}{2}m\omega^2 q^2 , \qquad E_n=\hbar\omega(n+\tfrac{1}{2}) , \qquad n=0, 1, 2, \cdots .$$

We consider the density operator

(30) $$\rho=Z^{-1}(\beta,\omega)e^{-\beta H}=\sum_{n=0}^{\infty}p_nP_n,\ P_n=|n\rangle\langle n|\,,\ p_n=Z^{-1}(\beta,\omega)\exp\left(-\tfrac{1}{2}\beta\omega\hbar(2n+1)\right),$$

where

(31) $$H|n\rangle=E_n|n\rangle\,,\qquad Z(\beta,\omega)=1/2\,\mathrm{sh}\,\xi\,,\qquad \xi=\tfrac{1}{2}\hbar\omega\beta\,.$$

After a simple calculation we obtain ($A=-\beta H$)

(32) $$\frac{\partial^2\ln Z}{\partial\beta^2}=\frac{\hbar^2\omega^2}{4\,\mathrm{sh}^2\xi}\,,\quad \frac{\partial^2\ln Z}{\partial\omega^2}=\frac{\hbar^2\beta^2}{4\,\mathrm{sh}^2\xi}\,,\quad \frac{\partial^2\ln Z}{\partial\beta\partial\omega}=-\frac{\hbar}{2}\mathrm{cth}\xi+\frac{\hbar^2\omega\beta}{4\,\mathrm{sh}^2\xi}\,,$$

(33) $$\left\langle\frac{\partial^2 A}{\partial\beta^2}\right\rangle=0\,,\quad \left\langle\frac{\partial^2 A}{\partial\omega^2}\right\rangle=-\frac{\hbar\beta}{2\omega}\mathrm{cth}\xi\,,\quad \left\langle\frac{\partial^2 A}{\partial\beta\partial\omega}\right\rangle=-\frac{\hbar}{2}\mathrm{cth}\xi\,.$$

Using the formula (17) we obtain

(34) $$g_{\beta\beta}=\omega^2 a\,,\qquad g_{\omega\omega}=\beta^2 a+(\beta/\omega)b\,,\qquad g_{\beta\omega}=g_{\omega\beta}=\omega\beta a\,,$$

(35) $$\det(g)=\beta\omega ab\,,$$

(36) $$g^{\beta\beta}=\beta/\omega b+1/\omega^2 a\,,\qquad g^{\omega\omega}=\omega/\beta b\,,\qquad g^{\beta\omega}=g^{\omega\beta}=-1/b\,,$$

where

(37) $$a=\tfrac{1}{8}\hbar^2(1/\mathrm{sh}^2\,\xi)\,,\qquad b=\tfrac{1}{4}\hbar\,(1/\mathrm{th}\,\xi)\,.$$

The Christoffel symbols are

(38) $$\Gamma^{\omega}_{\omega\omega}=-\beta a/b\,,\qquad \Gamma^{\beta}_{\beta\beta}=-2\omega b\,,$$

(39) $$\Gamma^{\omega}_{\beta\beta}=0\,,\qquad \Gamma^{\beta}_{\omega\omega}=\beta^2 a/\omega b-2\beta^2 b/\omega-b/2\omega^2 a+\beta/2\omega^2\,,$$

(40) $$\Gamma^{\omega}_{\omega\beta}=1/2\beta-\tfrac{1}{2}\omega a/b\,,\qquad \Gamma^{\beta}_{\omega\beta}=a\beta/2b-2\beta b+1/2\omega\,.$$

The Riemann tensor and the scalar curvature have the form

(41) $$R_{\omega\beta\omega\beta}=-b^2+a/4-ab\omega\beta+\omega\beta a^2/4b+1/4\beta^2\omega^2=f_1(\xi)\,,$$

(42) $$R=2R_{\omega\beta\omega\beta}/\det(g)=-2b/\beta\omega a+1/2\omega\beta b-2+a/2b^2+\tfrac{1}{2}(1/ab\beta^3\omega^3)=f_2(\xi)\,.$$

For the small values of $\xi=\frac{1}{2}\hbar\omega\beta\ll 1$ (the quasi-classical approximation) we obtain

(43) $$a=1/2\omega^2\beta^2\,,\qquad b=1/2\omega\beta\,,\qquad \text{and hence}\quad R_{\omega\beta\omega\beta}=0\,,\qquad R=0\,,$$

as in the classical case [6]. In the limiting case of the large values $\xi\to\infty$ we obtain

(44) $$R_{\omega\beta\omega\beta}=-\hbar^2/16\,,\qquad \text{and}\qquad R=-\infty\,.$$

§5. Quantum perfect gas. Let us consider one particle contained in a one-dimensional box of length L with infinitely high potential walls. The hamiltonian and its eigenvalues are

(45) $$\begin{aligned} H&=p^2/2m &&\text{for}\quad 0<x\leqslant L\,,\\ &=p^2/2m+V\,,\qquad V=\infty\,, &&\text{for}\quad x\leqslant 0\quad\text{and}\quad x>L\,,\end{aligned}$$

(46) $$E_n=\pi^2\hbar^2 n^2/2mL^2\,,\qquad (n=1,2,\cdots)\,.$$

As parameters we take: the inverse temperature $\beta=1/kT$ and the length L. The density operator and its eigenvalues are

$$\rho=Z^{-1}e^{-\beta H}, \qquad p_n=Z^{-1}\exp(-\beta\pi^2\hbar^2n^2/2mL^2), \qquad Z(\beta, L)=\sum_{n=1}^{\infty}\exp(-\beta\gamma n^2). \tag{47}$$

For the sake of simplificity we took the parameter γ instead of L,

$$\gamma=\pi^2\hbar^2/2mL^2. \tag{48}$$

The sum over states Z can be approximated for small values of $\gamma\beta\ll 1$ (the quasi-classical approximation) by the integral [1]

$$Z=\sum_{n=1}^{\infty}e^{-\beta\gamma n^2}\simeq\int_0^{\infty}e^{-\beta\gamma x^2}dx=\tfrac{1}{2}\sqrt{\pi/\beta\gamma}. \tag{49}$$

The metric tensor in this coordinate system takes the form

$$g_{\beta\beta}=1/4\beta^2, \qquad g_{\gamma\gamma}=1/4\gamma^2, \qquad g_{\beta\gamma}=g_{\gamma\beta}=0. \tag{50}$$

After the coordinate transformation

$$u=\tfrac{1}{2}\ln\beta, \qquad v=\tfrac{1}{2}\ln\gamma \qquad \text{or} \qquad \beta=e^{2u}, \qquad \gamma=e^{2v}, \tag{51}$$

we obtain

$$g_{uu}=g_{vv}=1, \qquad g_{uv}=g_{vu}=0, \qquad ds^2=(du)^2+(dv)^2. \tag{52}$$

From the above calculation it is seen that the parameter space is (locally) Euclidean. The generalization of this case to the three-dimensional box and to arbitrary number of particles is trivial. We obtain always a flat space, as in the classical case [6].

§ 6. **Discussion of results.** The results obtained in the quantum-mechanical case give various Riemannian structures of the thermodynamical parameter space. The example of spin 1/2 is a typical quantum-mechanical case without a classical analogy. In this case we obtained the parameter space with negative scalar curvature, except of the point $r=0$ which corresponds to the absolute equilibrium state (i.e., state of the maximal entropy), where $R=0$. In the two other cases the quasi-classical approximation has been performed, and in the both cases the flat space (the Euclidean space) has been obtained as in the classical case (cf. [6]).

For the quantum harmonic oscillator the limiting non-classical case ($\xi\to\infty$) gives negative values of $R\to-\infty$, and it seems that qualitatively the dependence of R on ξ is similar as in Fig. 1. The exact relation $R=f_2(\xi)$ is given in formula (42), but it is not easy for discussion, except in the limiting cases. Thus it seems that the difference between the quantum and classical case is in possibly negative values of the scalar curvature.

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