Geometric phase and modulus relations for SU(n) matrix elements in the defining representation

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A set of relations between the modulus and phase is derived for amplitudes of the form $\langle \psi_f | \hat{U}(x) | \psi_i \rangle$ where $\hat{U}(x) \in SU(n)$ in the fundamental representation and $x$ denotes the coordinates on the group manifold. An illustration is given for the case $n = 2$ as well as a brief discussion of phase singularities and superoscillatory phase behavior for such amplitudes. The present results complement results obtained previously [1] for amplitudes valued on the ray space $\mathcal{R} = \mathbb{C}P^n$. The connection between the two is discussed.

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I. INTRODUCTION

In a previous paper, [1] a number of relations have been obtained for the interdependence between the phase and modulo of amplitudes of the form \( \langle \psi_f | \psi(x) \rangle \), where \( |\psi_f\rangle \) is some fixed state and \( |\psi(x)\rangle \) is parameterized on a complex parameter subspace \( \mathcal{M} \) of the ray space \( \mathcal{R} \), with general curvilinear real coordinates \( \{x\} \). In particular, it has been shown that the phase \( \eta(x) = \arg \langle \psi_f | \psi(x) \rangle \) and modulus \( \sqrt{p(x)} = |\langle \psi_f | \psi \rangle| \) are intimately connected functions on \( \mathcal{M} \) through the relation

\[
\nabla \log \sqrt{p} = \Omega (\nabla \eta - A) \tag{1.1}
\]

where \( \Omega \) is the Kähler 2-form on \( \mathcal{M} \) and \( A \) is the Berry-Simon [2, 3] connection \( A = -i \langle \psi(x) | \nabla \psi(x) \rangle \). Such conditions constitute a generalization of ordinary Cauchy-Riemann conditions, and reflect the locally holomorphic nature of such spaces. A number of interesting results follow when \( |\psi(x)\rangle \) sweeps the whole space of quantum states, i.e., the full ray space \( \mathcal{R} \). Using relations (1.1) and the relation between transition probabilities and geodesic distances as measured with the Fubini-Study metric [6], it then becomes possible to show that

\[
q |\nabla \eta - A|^2 = \frac{1}{p} - 1 \tag{1.2a}
\]
\[
q |\nabla \log \sqrt{p}|^2 = \frac{1}{p} - 1 \tag{1.2b}
\]
\[
\nabla p \cdot (\nabla \eta - A) = 0, \tag{1.2c}
\]

where \( q \) is an arbitrary overall scale parameter in the definition of the metric. In particular, it follows from (1.2a) that

\[
\langle \psi_f | \psi(x) \rangle = \frac{e^{i\eta(x)}}{\sqrt{1 + q |\nabla \eta - A|^2}}, \tag{1.3}
\]

implying that the transition amplitude can be expressed entirely in terms of its phase dependence.

In this paper we present a similar set of relations for amplitudes of the form \( \langle \psi_f | U(x) | \psi_i \rangle \) where \( U(x) \) is an element of \( SU(n) \) in the defining \((n\text{-dimensional})\) representation, \( x \) are now coordinates on the group manifold, and \( |\psi_i\rangle \) and \( |\psi_f\rangle \) are any two fixed normalized vectors acting on an \( n \)-dimensional Hilbert space:
Let $p(x)$ and $\eta(x)$ be defined respectively as the modulus squared and phase angle of $\langle \psi_f | \hat{U}(x) | \psi_i \rangle$. It then becomes possible to show that

$$|\nabla \eta|^2 = \frac{1}{p} + \left(1 - \frac{2}{n}\right),$$

(1.4a)

$$|\nabla \log \sqrt{p}|^2 = \frac{1}{p} - 1,$$

(1.4b)

$$\nabla p \cdot \nabla \eta = 0,$$

(1.4c)

where the inner product is now taken with respect to the Cartan-Killing metric on the group manifold, expressible as

$$g_{\mu\nu} = \frac{1}{2} \text{Tr}(\partial_\mu \hat{U} \partial_\nu \hat{U}^\dagger).$$

(1.5)

In particular, (1.4a) implies that the amplitude can be parameterized entirely in terms of its phase according to

$$\langle \psi_f | \hat{U}(x) | \psi_i \rangle = e^{i \eta(x)} \sqrt{|\nabla \eta|^2 - (n - 2)/n},$$

(1.6)

in a similar fashion to (1.3).

That there should exist a connection between relations (1.2) and (1.4) may be inferred from the fact that $SU(n)$ is a principal $U(n-1)$-bundle over the coset space $SU(n)/U(n-1)$, in which the $U(n-1)$ corresponds to the isotropy group leaving a fixed ray in Hilbert space invariant. Relations (1.2) may then be viewed as the set of gauge-invariant relations obtained from (1.4) after “modding out” the subgroup of $SU(n)$ not affecting the angle between rays, in other words, the transition probability. Relations (1.3) will be proved in the next section and in the final section the connection between (1.2) and (1.4) will be established.

Before proceeding with the proofs, however, an illustration of relation (1.6) and some of its consequences may be useful. In the case of $SU(2)$, (1.6) takes the particularly simple form

$$\langle \psi_f | \hat{U}(x) | \psi_i \rangle = e^{i \eta(x)} \frac{1}{|\nabla \eta|}.$$

(1.7)

Thus, let the initial and final states be $|i\rangle = |+\rangle$ and $|f\rangle = |\rangle$ in standard spin-1/2 notation. Since the group manifold for $SU(2)$ is $S^3$, it becomes convenient to introduce a standard polar coordinate chart on the three-sphere $x = (\chi, \theta, \phi)$, where $\chi, \theta \in (0, \pi)$ and $\phi \in [0, 2\pi)$. In terms of these coordinates, a natural parameterization of an $SU(2)$ group element is then
\[ \hat{U}(x) = \cos \chi \mathbb{1} + i \sin \chi \bar{\sigma} \cdot \hat{n} (\theta, \phi), \] (1.8)

with a corresponding metric element on \( S^3 \)

\[ g_{\mu \nu} dx^\mu dx^\nu = d\chi^2 + \sin^2 \chi (d\theta^2 + \sin^2 \theta \, d\phi^2). \] (1.9)

Note that \( \hat{U}(x) \) corresponds, in the language of angular momentum, to a spacial rotation by an angle \( 2\chi \) around the axis \( \hat{n}(\theta, \phi) \) (the unit vector on the two-sphere). A simple calculation then shows that

\[ \langle -|\hat{U}(x)|+ \rangle = i \sin \chi \sin \theta e^{i\phi}, \] (1.10)

from which we identify

\[ \eta(x) = \phi + \pi/2, \quad p(x) = \sin^2 \chi \sin^2 \theta. \] (1.11)

Noting that the inverse metric components are \( g^{\chi \chi} = 1, g^{\theta \theta} = 1/\sin^2 \chi, g^{\phi \phi} = 1/\sin^2 \chi \sin^2 \theta, \)
and all others vanishing, we therefore see that

\[ |\nabla \eta|^2 = g^{\phi \phi} (\partial_\phi \eta)^2 = \frac{1}{\sin^2 \chi \sin^2 \theta} = 1/p(x), \] (1.12)

in consistency with Eq. (1.7).

Two interesting consequences also emerge from equation (1.6): First, we see that as \( x \) approaches a value \( x_o \) such that \( \langle \psi_f |\hat{U}(x_o)|\psi_i \rangle = 0 \), the phase gradient must diverge. The previous illustration shows that in the case of \( SU(2) \), this divergence shows vortex behavior about a string singularity (for the above initial and final states the singular string corresponds to the \( S^3 \) meridians at \( \theta = 0 \) and \( \pi \) running from \( \chi = 0 \) to \( \chi = \pi \)).

The other interesting consequence is that since the modulus may never exceed unity, the phase gradient is bounded from below and is therefore never allowed to vanish. In other words, the phase factor cannot be stationary on the \( SU(n) \) manifold. It is amusing to note that the lower bound on the gradient

\[ |\nabla \eta|_{\min} = \sqrt{2(n-1)/n} \] (1.13)

in fact corresponds to an upper bound on the magnitude of the eigenvalues of any generator \( \hat{l} \) of \( SU(n) \) normalized such that \( Tr(\hat{l}^2) = 2 \). To see the implications of this, note that a single parameter transformation \( \hat{U}(t) = \exp(i\hat{l} t) \) generates a curve on \( SU(n) \) in which the
curve length with respect to the Cartan-Killing metric is \( ds = dt \). If \( \hat{\lambda} \) is now chosen in the
direction of the phase gradient evaluated at the identity (\( \hat{\mathbf{U}} = 1 \)), then the local angular
frequency of the phase oscillation \( \omega(t) \), defined as
\[
\omega(t) = \frac{d}{dt} \arg\langle \psi_f | \exp(i\hat{\lambda}t) | \psi_i \rangle
\] (1.14)
corresponds, at \( t = 0 \) to the phase gradient \( |\nabla \eta| \) evaluated at the identity element, and
must therefore satisfy \( \omega(0) \geq \sqrt{2(n-1)/n} \). On the other hand, \( \langle \psi_f | \exp(i\hat{\lambda}t) | \psi_i \rangle \) has a Fourier
expansion of the form
\[
\langle \psi_f | \exp(i\hat{\lambda}t) | \psi_i \rangle = \sum_k C_k e^{il_k t} \] (1.15)
where \( l_k \) are the eigenvalues of \( \hat{\lambda} \), none of which may exceed in magnitude the value \( \sqrt{2(n-1)/n} \).
Thus, for any two given states \( |\psi_i \rangle \) and \( |\psi_f \rangle \) there always exists a generator \( \hat{\lambda} \) such that around
\( t = 0 \) the function \( \langle \psi_f | \exp(it\hat{\lambda}) | \psi_i \rangle \) exhibits so-called super-oscillatory behavior \( \text{[4, 5]} \): local
phase oscillations which are at least as fast as those of the fastest Fourier component.

II. PROOF OF RELATIONS (1.4)

Let \( \{ \hat{\lambda}_a | a = 1, \ldots, n^2-1 \} \) be a set of linearly-independent, traceless matrix generators for
\( SU(n) \) in the fundamental \( (n\text{-dimensional}) \) representation, chosen so that they satisfy the
matrix inner product \( \text{Tr}(\hat{\lambda}_a \hat{\lambda}_b) = 2\delta_{ab} \). A euclidean inner product is naturally induced on
the Lie algebra, with the metric form
\[
\eta_{ab} = \frac{1}{2} \text{Tr}(\hat{\lambda}_a \hat{\lambda}_b) \quad (= \delta_{ab}) ,
\] (2.1)
coinciding with the so-called Cartan-Killing form \( \text{[7]} \). Now consider an open covering of
\( SU(n) \), parameterized by the matrix \( \hat{\mathbf{U}}(x) \in SU(n) \), where \( x \) stands for \( n^2-1 \) coordinates
\( \{ x^\mu : \mu = 1, \ldots, n^2-1 \} \). A set of left-invariant one-forms \( \{ \omega^a \} \) is defined by the expansion of
the Lie-algebra valued 1-form \( \hat{\mathbf{U}}^\dagger \mathbf{d}\hat{\mathbf{U}} \) as a linear combination of the \( \hat{\lambda} \)-matrices
\[
\hat{\mathbf{U}}^\dagger \mathbf{d}\hat{\mathbf{U}} = i \omega^a \hat{\lambda}_a . \] (2.2)
An invariant metric tensor on the group manifold is then naturally inherited from the Cartan-
Killing according to
\[
g = \eta_{ab} \omega^a \otimes \omega^b = \frac{1}{2} \text{Tr}(\mathbf{d}\hat{\mathbf{U}} \otimes \mathbf{d}\hat{\mathbf{U}}^\dagger) . \] (2.3)
where the left-invariant forms play the role of a *vielbein*. Similarly, the inverse metric tensor

\[ g^{-1} = \eta^{ab} e_a \otimes e_b \]  

is defined from the set of vector fields \( \{ e_a \} \) dual to the left invariant forms, i.e., satisfying \( \omega^a(e_b) = \delta^a_b \).

Now turn to matrix elements of the form \( \langle \psi_f \rvert \hat{U} \lvert \psi_i \rangle \). For simplicity, let us represent this quantity either in terms of its two real polar components \( \sqrt{p} \) and \( \eta \), or in terms of a complex phase \( \chi \):

\[ \langle \psi_f \rvert \hat{U} \lvert \psi_i \rangle = \sqrt{p} e^{i\eta} = e^{i\chi} \]  

(2.5)

Using (2.2), it is then easy to show that

\[ d\chi = d\eta - i d \log \sqrt{p} = \omega^a \langle \psi_f \rvert \hat{U} \hat{\lambda}_a \lvert \psi_i \rangle \]  

\[ \langle \psi_f \rvert \hat{U} \lvert \psi_i \rangle \]  

(2.6)

Thus, using the definition of the Cartan-Killing metric we can then show that \( \nabla \chi \cdot \nabla \chi^* = g^{-1}(d\chi, d\chi^*) \) and \( \nabla \chi \cdot \nabla \chi = g^{-1}(d\chi, d\chi) \) can be expressed as

\[ \nabla \chi \cdot \nabla \chi^* = \eta^{ab} \frac{\langle \psi_f \rvert \hat{U} \hat{\lambda}_a \lvert \psi_i \rangle \langle \psi_i \rvert \hat{\lambda}_b \hat{U}^\dagger \rvert \psi_f \rangle}{\langle \psi_f \rvert \hat{U} \lvert \psi_i \rangle \langle \psi_i \rvert \hat{\lambda}_b \hat{U}^\dagger \rvert \psi_f \rangle} \]

\[ \nabla \chi \cdot \nabla \chi = \eta^{ab} \frac{\langle \psi_f \rvert \hat{U} \hat{\lambda}_a \lvert \psi_i \rangle \langle \psi_i \rvert \hat{\lambda}_b \hat{U} \rvert \psi_i \rangle}{\langle \psi_f \rvert \hat{U} \lvert \psi_i \rangle \langle \psi_i \rvert \hat{\lambda}_b \hat{U} \rvert \psi_i \rangle} \]  

(2.7)

The right-hand sides of these two equations can be computed by using the following identity on the fundamental representation of \( SU(n) \) (See e.g., [8])

\[ \frac{1}{2} \eta^{ab} \text{Tr}(X \hat{\lambda}_a \hat{Y} \hat{\lambda}_b) = \text{Tr}(X) \text{Tr}(Y) - \frac{1}{n} \text{Tr}(X \hat{Y}) \]  

(2.8)

where for the first one we use \( \hat{X} = \hat{U}^\dagger \langle \psi_f \rvert \hat{U} \rvert \psi_i \rangle \) and \( \hat{Y} = \langle \psi_i \rvert \hat{U} \rvert \psi_i \rangle \), and for the second one \( \hat{X} = \hat{Y} = \langle \psi_i \rvert \hat{U} \rvert \psi_i \rangle \). Thus we find that

\[ \nabla \chi \cdot \nabla \chi^* = 2 \left( \frac{1}{p} - \frac{1}{n} \right) \]

\[ \nabla \chi \cdot \nabla \chi = 2 \left( 1 - \frac{1}{n} \right) \]  

(2.9)

Re-expressing the gradient 1-form \( d\chi \) in terms of \( \eta \) and \( p \), and taking real and imaginary parts, one obtains (1.4a-1.4c).
III. CONNECTION BETWEEN RELATIONS (1.4) AND RELATIONS (1.2)

To connect (1.4) and (1.2), we implement the so-called Cartan decomposition of the Lie algebra $\mathcal{L}(SU(n))$ [7]. Let $\{\hat{\lambda}_i\}$, with $i$ ranging from 0 to $(n-1)^2 - 1 = n^2 - 2n$ span the Lie algebra of an isotropy group $U(n-1) = SU(n-1) \times U(1)$, a subgroup of $SU(n)$ in which the $SU(n-1)$ generated by $\hat{\lambda}_i$ acts on the orthogonal subspace to $|\psi_1\rangle$ and the $U(1)$ generated by $\hat{\lambda}_0$ implements a phase transformation on $|\psi_1\rangle$ and commutes with the $SU(n-1)$. The remaining $n^2 - 1 - (n^2 - 2n + 1) = 2(n-1)$ generators of $SU(n)$, denoted by $\{\hat{\lambda}_A\}$, span an orthogonal complement in $\mathcal{L}(SU(n))$ to the Lie algebra of the $U(n-1)$, in the sense of the Cartan-Killing form (CK). For our purposes, it suffices to give $\hat{\lambda}_0$ and the $\hat{\lambda}_A$ explicitly. Given the tracelessness condition plus the normalization condition $\text{Tr}(\hat{\lambda}_0^2) = 2$, the form of $\hat{\lambda}_0$ is determined up to a sign, and we choose

$$\hat{\lambda}_0 = \sqrt{\frac{2}{n(n-1)}} \sum_{k=1}^{n-1} 1 - \sqrt{\frac{2n}{n-1}} |\psi_i\rangle\langle\psi_i|.$$  \hspace{1cm} (3.1)

For the orthogonal generators $\{\hat{\lambda}_A\}$ we choose matrices of the form

$$\hat{X}_k = |\psi_i\rangle\langle k| + |k\rangle\langle\psi_i| \text{ or } \hat{Y}_k = i|\psi_i\rangle\langle k| - i |k\rangle\langle\psi_i|$$ \hspace{1cm} (3.2)

for all $k$ where $\{|k\rangle | k = 1,..,n-1\}$ are a set of vectors orthogonal to $|\psi_i\rangle$.

Similarly, we introduce a local chart on $SU(n)$ such that the coordinates are split into a set of coordinates $\xi^\alpha : 0,..,n^2 - 2n$ for the isotropy subgroup and coordinates $y^\alpha$ ( $\alpha = 1 \ldots, 2(n-1)$) for the coset space $SU(n)/U(n-1)$. This we do in order to decompose $\hat{U} \in SU(n)$ as

$$\hat{U} = \hat{K}(y)\hat{H}(\xi) = \hat{K}(y)\hat{H}_S(\xi_1, \ldots, \xi_{n^2-2n}) e^{i\hat{\lambda}_0}\xi^\alpha$$ \hspace{1cm} (3.3)

where $H_s \in SU(n-1)$ and $\hat{K}(y)$ is a coset representative (for instance $\hat{K} = \exp[i y^A\hat{\lambda}_A]$). A section of states in Hilbert space is then generated by the action of $\hat{K}$ on $|\psi_1\rangle$, i.e.,

$$|\psi(y)\rangle \equiv \hat{K}(y)|\psi_1\rangle.$$ \hspace{1cm} (3.4)

Since $\hat{H}_s|\psi_i\rangle = |\psi_i\rangle$ and $\hat{\lambda}_0|\psi_i\rangle = -\sqrt{\frac{2(n-1)}{n}}|\psi_i\rangle$, it then follows from the decomposition (3.3) that the amplitude $\langle\psi_f|\hat{U}|\psi_i\rangle$ may be expressed in terms of the coset space amplitude $\langle\psi_f|\psi(y)\rangle$ according to

$$\langle\psi_f|\hat{U}|\psi_i\rangle = e^{-i\sqrt{\frac{2(n-1)}{n}}\xi^\alpha} \langle\psi_f|\psi(y)\rangle.$$ \hspace{1cm} (3.5)
We proceed with the left invariant forms and the definition of the Fubini-Study (FS) metric. For this we note that $\hat{H}^\dagger d\hat{H}$ involves only the $\hat{\lambda}_i$, but $\hat{K}^\dagger d\hat{K}$, not being a subgroup of $SU(n)$ expands as a linear combination of all the group generators. We therefore expand $\hat{U}^\dagger d\hat{U}$ as

$$\hat{U}^\dagger d\hat{U} \equiv i\hat{H}^\dagger \left[ \tau^A \hat{\lambda}_A + a^i \hat{\lambda}_i + \omega^i \hat{\lambda}_i \right] \hat{H},$$

(3.6)

where

$$\tau^A \equiv \frac{1}{2i} \text{Tr}(\hat{\lambda}_A \hat{K}^\dagger d_\parallel \hat{K})$$

(3.7)

$$\alpha^i \equiv \frac{1}{2i} \text{Tr}(\hat{\lambda}_i \hat{K}^\dagger d_\parallel \hat{K})$$

(3.8)

$$\omega^i \equiv \frac{1}{2i} \text{Tr}(\hat{H}^\dagger \hat{\lambda}_i d_\perp \hat{H})$$

(3.9)

and $d_\parallel$ and $d_\perp$ denote external differentiation with respect to the coset space ($y^A$) and subgroup ($\xi^i$) coordinates respectively. Note that the vielbein $\omega^i$ is defined in terms of right-invariant forms and therefore differs from a corresponding left-invariant form by an $\text{Ad}_{\hat{H}}$ transformation which nonetheless leaves the $H$-Cartan-Killing metric $\eta_{ij} \omega^i \otimes \omega^j$ invariant.

The Fubini-Study metric and its inverse are defined by considering the forms $\tau_A$ as vielbeins on the coset space

$$g_{FS} = \eta_{AB} \tau^A \otimes \tau^B, \quad g_{FS}^{-1} = \eta^{AB} t_A \otimes t_B$$

(3.10)

where the vector fields $t_A$ are dual to the $\tau^A$, i.e., such that $\tau^A(t_B) = \delta^A_B$. Using (3.4), it is then a matter of some algebra to show that the F.S. metric can be expressed as

$$g_{FS} = \langle d\psi| \otimes |d\psi\rangle_S - \langle d\psi|\psi\rangle \otimes \langle \psi|d\psi\rangle.$$  

(3.11)

where $S$ stands for symmetrized. A similar calculation shows that since the Berry-Simon connection $A$ is $-i\langle \psi_i | \hat{K}^\dagger d_\parallel \hat{K} | \psi_i \rangle$, it is related to $\alpha^0$ through

$$\alpha^0 = \frac{1}{2i} \text{Tr}(\hat{\lambda}_0 \hat{K}^\dagger d_\parallel \hat{K}) = \sqrt{\frac{n}{2(n-1)}} A.$$  

(3.12)

Now, using $g_{CK} = \frac{1}{2} \text{Tr}(dU \otimes dU^\dagger)$, one can then show that the Cartan-Killing metric may be written as

$$g_{CK} = g_{FS} + \eta_{ij}(\alpha^i + \omega^i) \otimes (\alpha^i + \omega^i)$$

(3.13)
(note therefore that the the $t_A$ are only orthonormal with respect to the FS metric). We shall also need the inverse CK metric, which is easily computed and is given by:

$$g_{CK}^{-1} = \eta^{AB} (t_A - a^i_A e_j) \otimes (t_A - a^i_A e_j) + \eta^{ij} e_i \otimes e_j$$

(3.14)

where $a^i_A \equiv \alpha^i(t_A)$.

Now, For any function $f(y, \xi)$ on the group manifold, we can therefore write

$$g_{CK}^{-1}(df, df) = g_{FS}^{-1}(D \parallel f, D \parallel f) + \eta^{ij} \nabla_i f \nabla_j f$$

(3.15)

where

$$D \parallel f = df - \alpha^i \nabla_i f$$

(3.16)

and where $\nabla_i f = d \perp f(e_i)$. In particular, we look at the function

$$\langle \psi_f | U | \psi_i \rangle = \sqrt{p(y)} e^{i\eta(y, \xi_0)}$$

(3.17)

from (3.3), and where

$$\eta(y, \xi^0) = \tilde{\eta}(y, \xi^0 = 0) - \sqrt{\frac{2(n-1)}{n}} \xi^0.$$  

Noting that $\hat{\lambda}_o$ commutes with $H_S$, we find that

$$\omega^0 = \frac{1}{2i} \text{Tr}(\hat{\lambda}_o e^{-i\xi^0 \lambda^0} d \perp e^{\xi^0 \lambda^0}) = d \xi^0.$$  

(3.18)

Thus, it follows that $\nabla_o \eta = \sqrt{\frac{2(n-1)}{n}}$, and from (3.12) that

$$D \parallel \eta = d \parallel \eta + \sqrt{\frac{2(n-1)}{n}} \alpha^o = d \parallel \eta + A.$$  

(3.19)

Similarly, we find that $D \parallel p = d \parallel p$. In this way, relations (1.2) can be obtained from (1.4) by letting $\xi^o = 0$ and using and

$$g_{CK}^{-1}(d\eta, d\eta) = g_{FS}^{-1}(D \parallel \eta, D \parallel \eta) + 2 \left( \frac{n-1}{n} \right)$$

(3.20)

$$g_{CK}^{-1}(d\eta, dp) = g_{FS}^{-1}(D \parallel \eta, d \parallel p)$$

(3.21)

$$g_{CK}^{-1}(dp, dp) = g_{FS}^{-1}(d \parallel p, d \parallel p),$$

(3.22)

respectively. This corresponds to the choice $q = 1$ in the definition of the FS metric.
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