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Double Wilczek–Zee connection and mixed-state quantum geometric tensor

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The Wilczek–Zee connection (WZC) is a key concept in the study of topology of quantum systems. Here, we introduce the double Wilczek–Zee connection (DWZC) which naturally appears in the pure-state quantum geometric tensor (QGT), another important concept in the field of quantum geometry. The DWZC is Hermitian with respect to the two integer indices, just like the original Hermitian WZC. Based on the symmetric logarithmic derivative operator, we propose a mixed-state quantum geometric tensor. Using the symmetric properties of the DWZC, we find that the real part of the QGT is connected to the real part of the DWZC and the square of eigenvalue differences of the density matrix, whereas the imaginary part can be given in terms of the imaginary part of the DWZC and the cube of the eigenvalue differences. For density matrices with full rank or no full rank, the QGT can be given in terms of real and imaginary parts of the DWZC.

Keywords: quantum geometry, Wilczek–Zee connection, quantum geometric tensor

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1. Introduction

As a generalization of the Berry connection,[1] the Wilczek–Zee connection[2] is an important concept in the field of topological physics. It is defined on a Hilbert space spanned by N normalized orthogonal states $|\psi_k(\boldsymbol{\lambda})\rangle$ $(k=1,\dots,N)$ with the local coordinates $(\lambda_\mu)_{\mu=1}^d$. For two states $|\psi_i\rangle$, $|\psi_j\rangle$, and parameter λ_μ, the WZC is given by[2]

$$\mathcal{A}_{ij}^{\mu}(\boldsymbol{\lambda}) \equiv \mathcal{A}_{ij}^{\lambda_\mu}(\boldsymbol{\lambda}) = \mathrm{i}\langle\psi_i(\boldsymbol{\lambda})|\partial_{\lambda_\mu}|\psi_j(\boldsymbol{\lambda})\rangle. \tag{1}$$

Specifically, it can be used for enabling quantum computation with the computation space being degenerate eigenspace of a family of Hamiltonians and the different adiabatic loops of underlined classical space will give useful quantum gates which can build a universal quantum computer.[3,4]

From the definition of the WZC and the completeness relation $\sum_i |\psi_i(\boldsymbol{\lambda})\rangle\langle\psi_i(\boldsymbol{\lambda})| = \mathbb{1}$, one may find that state $|\psi_j(\boldsymbol{\lambda})\rangle$ satisfies the following equation:

$$\mathrm{i}\partial_{\lambda_\mu}|\psi_j(\boldsymbol{\lambda})\rangle = \sum_i \mathcal{A}_{ij}^{\mu}(\boldsymbol{\lambda})|\psi_i(\boldsymbol{\lambda})\rangle. \tag{2}$$

Using the ortho-normal relations $\langle\psi_i|\psi_j\rangle = \delta_{ij}$, we immediately have the property

$$\langle\psi_i|\partial_\alpha|\psi_j\rangle = -\langle\partial_\alpha\psi_i|\psi_j\rangle = -\langle\psi_j|\partial_\alpha|\psi_i\rangle^*, \tag{3}$$

and from which $\mathcal{A}^\mu(\boldsymbol{\lambda})$ is found to be an $N\times N$ Hermitian matrix with respect to two integer indices i and j, namely

$$\mathcal{A}_{ij}^{\mu} = (\mathcal{A}_{ji}^{\mu})^*. \tag{4}$$

Since the WZC is complex, it can be written as

$$\mathcal{A}_{ij}^{\mu} = \mathcal{R}_{ij}^{\mu} + \mathrm{i}\mathcal{I}_{ij}^{\mu}. \tag{5}$$

Due to the Hermiticity of the WZC, the real and imaginary parts satisfy

$$\mathcal{R}_{ij}^{\mu} = \mathcal{R}_{ji}^{\mu},\ \mathcal{I}_{ij}^{\mu} = -\mathcal{I}_{ji}^{\mu}. \tag{6}$$

We see that the real part displays symmetry, while the imaginary part is anti-symmetric under the exchange of two integer indices.

The QGT[5,6] is another important concept when we study local geometry of a quantum state with many parameters and useful to detect various kinds of quantum phase transitions.[7–13] Its symmetric part is the quantum metric, and the antisymmetric part is the Berry curvature. It also has applications in various physical systems such as superconductor-quantum dot chains[14] and adiabatic quantum thermal machines.[15] Experimentally, the QGT can be extracted in an optical Raman lattice,[16] a superconducting qubit,[17] topological Josephson matter,[18] and crystalline solids.[19]

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The QGT was extended to the non-Abelian[20,21] and non-Hermitian situations,[22] respectively. Most of previous studies of QGT were about pure states, however we often have mixed states such as thermal states at finite temperature in the field of quantum information. Another typical mixed state is the degenerate ground state which is an equal mixture of all ground states at zero temperature. Recently, two mixed-state QGTs were proposed based on Uhlmann approach[23] and the Sjöqvist distance,[24] respectively. Here, we introduce the DWZC, give another mixed-state QGT based on the symmetric logarithmic derivative (SLD) operator, and provide relations between the WZC and QGT. Furthermore, we apply the concept of the DWZC to the field of quantum metrology.

2. Double WZC and pure-state QGT

For pure state $|\psi_i\rangle$, the QGT is defined as

$$\begin{aligned} Q_{\alpha\beta}(\psi_i) &= \langle \partial_\alpha \psi_i | \partial_\beta \psi_i \rangle - \langle \partial_\alpha \psi_i | \psi_i \rangle \langle \psi_i | \partial_\beta \psi_i \rangle. \\ &= \sum_{j=1, j\neq i}^{N} \langle \partial_\alpha \psi_i | \psi_j \rangle \langle \partial_\beta \psi_i | \psi_j \rangle^* \\ &= \sum_{j=1, j\neq i}^{N} \langle \psi_i | \partial_\alpha \psi_j \rangle \langle \psi_i | \partial_\beta \psi_j \rangle^* \\ &= \sum_{j=1, j\neq i}^{N} \mathcal{A}_{ij}^{\alpha} (\mathcal{A}_{ij}^{\beta})^*, \end{aligned} \tag{7}$$

where the completeness relation and the definition of the WZC were used. Thus, it is natural to define the following quantity:

$$\begin{aligned} \mathcal{A}_{ij}^{\alpha\beta} &= \mathcal{A}_{ij}^{\alpha} (\mathcal{A}_{ij}^{\beta})^* \\ &= \langle \psi_i | \partial_\alpha \psi_j \rangle \langle \psi_i | \partial_\beta \psi_j \rangle^* \\ &= \langle \partial_\beta \psi_j | \psi_i \rangle \langle \psi_i | \partial_\alpha \psi_j \rangle \\ &= \langle \partial_\alpha \psi_i | \psi_j \rangle \langle \psi_j | \partial_\beta \psi_i \rangle, \end{aligned} \tag{8}$$

where we have used Eq. (3) in the last line. We denote it the double WZC with two real and two integer indices. Thus, in terms of the DWZC, the QGT can be writen as

$$Q_{\alpha\beta}(\psi_i)) = \sum_{j=1, j\neq i}^{N} \mathcal{A}_{ij}^{\alpha\beta},$$

i.e., it is a sum of $N-1$ DWZCs.

Now we investigate the symmetric properties of the four-index DWZC. From the Hermiticity of WZC and the definition of the DWZC, one finds

$$\mathcal{A}_{ij}^{\alpha\beta} = (\mathcal{A}_{ij}^{\beta\alpha})^*, \quad \mathcal{A}_{ij}^{\alpha\beta} = \mathcal{A}_{ji}^{\beta\alpha}, \tag{9}$$

which leads to the Hermiticity of the DWZC, namely,

$$\mathcal{A}_{ij}^{\alpha\beta} = (\mathcal{A}_{ji}^{\alpha\beta})^*. \tag{10}$$

Exchange of two integer or two real indices of the DWZC results in its complex conjugate and it is invariant if we exchange integer and real indices simultaneously. Since the DWZC is also complex, it is written as

$$\mathcal{A}_{ij}^{\alpha\beta} = \mathcal{R}_{ij}^{\alpha\beta} + \mathrm{i} \ \mathcal{I}_{ij}^{\alpha\beta}. \tag{11}$$

Due to the Hermiticity of the DWZC, the real and imaginary parts satisfy

$$\mathcal{R}_{ij}^{\alpha\beta} = \mathcal{R}_{ji}^{\alpha\beta}, \, \mathcal{I}_{ij}^{\alpha\beta} = -\mathcal{I}_{ji}^{\alpha\beta}. \tag{12}$$

The same as WZC, the real part exhibits symmetry, while the imaginary part is anti-symmetric under the exchange of two integer indices. Next, we first generalize the QGT to the case of mixed states and then study the mixed-state QGT via these symmetric properties of the DWZC.

3. Mixed-state QGT

We start with the SLD operator which is defined by

$$\partial_\alpha \rho = \frac{1}{2}(L_\alpha \rho + \rho L_\alpha), \tag{13}$$

where ρ is a density operator depending on parameter α. We now try to give a new form of the QGT in terms of SLDs. Let us consider a quantum pure state written in terms of a density matrix $\rho = |\psi\rangle\langle\psi|$. It follows from $\rho^2 = \rho$ that

$$\partial_\alpha \rho = \partial_\alpha \rho^2 = (\partial_\alpha \rho)\,\rho + \rho\,(\partial_\alpha \rho), \tag{14}$$

implying that SLD operator can be written as

$$L_\alpha = 2\partial_\alpha \rho, \tag{15}$$

where we have used Eq. (13).

For pure state $\rho = |\psi\rangle\langle\psi|$ depending on two parameters α and β, the corresponding SLDs are

$$L_\alpha = 2(|\partial_\alpha \psi\rangle\langle\psi| + |\psi\rangle\langle\partial_\alpha \psi|), \tag{16}$$

$$L_\beta = 2(|\partial_\beta \psi\rangle\langle\psi| + |\psi\rangle\langle\partial_\beta \psi|). \tag{17}$$

By calculating the expectation value of $L_\alpha L_\beta$, we obtain

$$\mathrm{Tr}(\rho L_\alpha L_\beta) = 4(\langle \partial_\alpha \psi | \partial_\beta \psi \rangle + \langle \psi | \partial_\beta \psi \rangle \langle \psi | \partial_\alpha \psi \rangle). \tag{18}$$

Thus, in terms of two SLDs, the QGT for pure states can be written as

$$Q_{\alpha\beta} = \frac{1}{4} \mathrm{Tr}\left(\rho L_\alpha L_\beta\right). \tag{19}$$

Since the SLD is defined on an arbitrary mixed state described by a density operator, it is natural to generalize the pure-state QGT directly to the case of mixed states as given in the above equation. In other words, the above definition of the QGT is applicable to an arbitrary state.

4. Full-rank density matrix

The spectral decomposition of a density matrix ρ is given by

$$\rho = \sum_{i=1}^{N} p_i |\psi_i\rangle\langle\psi_i|, \tag{20}$$

which is assumed to be a full rank matrix, i.e., all the eigenvalues are larger than zero. The pure state is a rank-one matrix, i.e., one eigenvalue is one and others are zero.

Using the completeness relation, it can be shown that

$$\begin{aligned}\langle L_\alpha L_\beta\rangle = \mathrm{Tr}(\rho L_\alpha L_\beta) &= \sum_{i=1}^{N} p_i \langle\psi_i|L_\alpha L_\beta|\psi_i\rangle \\ &= \sum_{i,j=1}^{N} p_i (L_\alpha)_{ij} (L_\beta)_{ji}.\end{aligned} \tag{21}$$

Therefore, we need to determine the form of the SLDs. From Eq. (20), the left side of Eq. (13) reads

$$\begin{aligned}\partial_\alpha \rho = \sum_k (\partial_\alpha p_k)|\psi_k\rangle\langle\psi_k| \\ + p_k|\partial_\alpha\psi_k\rangle\langle\psi_k| + p_k|\psi_k\rangle\langle\partial_\alpha\psi_k|.\end{aligned} \tag{22}$$

We then find

$$\begin{aligned}(\partial_\alpha\rho)_{ij} &= (\partial_\alpha p_i)\delta_{ij} + (p_j - p_i)\langle\psi_i|\partial_\alpha\psi_j\rangle, \\ &= (\partial_\alpha p_i)\delta_{ij} + \mathrm{i}(p_i - p_j)\mathcal{A}_{ij}^{\alpha}.\end{aligned} \tag{23}$$

Here, the definition of WZC in Eq. (1) was used in the last line. The right hand of Eq. (13) reads

$$\frac{1}{2}\sum_k[(L_\alpha)_{ik}\rho_{kj} + \rho_{ik}(L_\alpha)_{kj}] = \frac{1}{2}(p_i + p_j)(L_\alpha)_{ij}, \tag{24}$$

where we have used

$$\rho_{ij} = p_i\delta_{ij} \tag{25}$$

as the density matrix is diagonal in this representation. Then, from Eqs. (23) and (24), the matrix elements of the SLD operators can be obtained as

$$\begin{aligned}(L_\alpha)_{ij} &= \frac{\partial_\alpha p_i}{p_i}\delta_{ij} + \frac{2\mathrm{i}(p_i - p_j)}{p_i + p_j}\mathcal{A}_{ij}^{\alpha}, \\ (L_\beta)_{ji} &= \frac{\partial_\beta p_i}{p_i}\delta_{ij} - \frac{2\mathrm{i}(p_i - p_j)}{p_i + p_j}(\mathcal{A}_{ij}^{\beta})^*.\end{aligned} \tag{26}$$

Substituting the above two equations into Eq. (21) and using the definition of DWZC in Eq. (8) leads to

$$\langle L_\alpha L_\beta\rangle = \sum_{i=1}^{N}\frac{(\partial_\alpha p_i)(\partial_\beta p_i)}{p_i} + \sum_{i\neq j} p_i \frac{4(p_i - p_j)^2}{(p_i + p_j)^2}\mathcal{A}_{ij}^{\alpha\beta}. \tag{27}$$

There are four terms after the substitution, but only two terms survive as $\delta_{ij}(p_i - p_j) = 0$ for any indices i and j.

Now we investigate the last term on the right hand of Eq. (27) and one finds

$$\begin{aligned}&\sum_{ij} p_i \frac{4(p_i - p_j)^2}{(p_i + p_j)^2}\mathcal{A}_{ij}^{\alpha\beta} \\ &= \sum_{ij}\frac{2(p_i - p_j)^2}{(p_i + p_j)^2}\left(p_i\mathcal{A}_{ij}^{\alpha\beta} + p_j\mathcal{A}_{ji}^{\alpha\beta}\right) \\ &= \sum_{ij}\frac{2(p_i - p_j)^2}{(p_i + p_j)^2}\left[p_i\mathcal{A}_{ij}^{\alpha\beta} + p_j(\mathcal{A}_{ij}^{\alpha\beta})^*\right] \\ &= \sum_{ij}\frac{2(p_i - p_j)^2}{(p_i + p_j)}\mathcal{R}_{ij}^{\alpha\beta} + \mathrm{i}\sum_{ij}\frac{2(p_i - p_j)^3}{(p_i + p_j)^2}\mathcal{I}_{ij}^{\alpha\beta}.\end{aligned} \tag{28}$$

Here, the first equality was obtained by exchanging the two indices, the second followed from Hermiticity of the DWZC, and last was derived from Eq. (11). Finally, the QGT in Eq. (19) can be written as

$$\begin{aligned}Q_{\alpha\beta} = &\frac{1}{4}\sum_{i=1}^{N}\frac{(\partial_\alpha p_i)(\partial_\beta p_i)}{p_i} \\ &+ \frac{1}{2}\sum_{i\neq j}\left[\frac{(p_i - p_j)^2}{(p_i + p_j)}\mathcal{R}_{ij}^{\alpha\beta} + \mathrm{i}\frac{(p_i - p_j)^3}{(p_i + p_j)^2}\mathcal{I}_{ij}^{\alpha\beta}\right].\end{aligned} \tag{29}$$

We find that the real part of the mixed-state QGT is connected to the real part of the DWZC and the square of eigenvalue differences of the density matrix, whereas the imaginary part is written in terms of the imaginary part of the DWZC and the cube of the eigenvalue differences. Note that the QGT only relates to the non-diagonal terms of the DWZC.

5. Density matrix with no full rank

We now study the QGT of a density matrix with no full rank, i.e., the rank M of the density operator is less than the dimension N of the Hilbert space. The density matrix is written as

$$\rho = \sum_{i=1}^{M} p_i|\psi_i\rangle\langle\psi_i|. \tag{30}$$

The expectation value of operator $L_\alpha L_\beta$ on this state is obtained as

$$\begin{aligned}\langle L_\alpha L_\beta\rangle &= \sum_{i=1}^{M}\sum_{j=1}^{N} p_i (L_\alpha)_{ij}(L_\beta)_{ji} \\ &= \sum_{i=1}^{M}\sum_{j=1}^{M} p_i (L_\alpha)_{ij}(L_\beta)_{ji} \\ &\quad + \sum_{i=1}^{M}\sum_{j=M+1}^{N} p_i (L_\alpha)_{ij}(L_\beta)_{ji},\end{aligned} \tag{31}$$

from which we observe that the expectation value is divided into two terms and the first one can be given by Eq. (29) by just replacing N with M. Next, we investigate the second term.

When $i = 1,\ldots,M$ and $j = M+1,\ldots,N$, it follows from Eq. (26) that

$$(L_\alpha)_{ij} = 2\mathrm{i}\mathcal{A}_{ij}^{\alpha}, (L_\beta)_{ji} = -2\mathrm{i}(\mathcal{A}_{ij}^{\beta})^* \tag{32}$$

as $p_j = 0$. Therefore, from the above equation, one finds

$$\sum_{i=1}^{M}\sum_{j=M+1}^{N} p_i (L_\alpha)_{ij}(L_\beta)_{ji}$$

$$
\begin{aligned}
&= \sum_{i=1}^{M} \sum_{j=M+1}^{N} 4 p_i \mathcal{A}_{ij}^{\alpha\beta} \\
&= \sum_{i=1}^{M} \sum_{j=M+1}^{N} 4 p_i \langle \partial_\alpha \psi_i | \psi_j \rangle \langle \psi_j | \partial_\beta \psi_i \rangle \\
&= \sum_{i=1}^{M} 4 p_i \langle \partial_\alpha \psi_i | \left(I - \sum_{j=1}^{M} |\psi_j\rangle\langle\psi_j| \right) |\partial_\beta \psi_i\rangle \\
&= \sum_{i=1}^{M} 4 p_i \langle \partial_\alpha \psi_i | \partial_\beta \psi_i \rangle - 4 \sum_{i=1}^{M} \sum_{j=1}^{M} p_i \mathcal{A}_{ij}^{\alpha\beta}, \qquad (33)
\end{aligned}
$$

where the definition of DWZC was used in the first and second equality and the completeness relation was used again in the third equality. From the above equation, we get

$$
\begin{aligned}
&\sum_{i=1}^{M} \sum_{j=M+1}^{N} p_i (L_\alpha)_{ij} (L_\beta)_{ji} \\
&= \sum_{i=1}^{M} 4 p_i \langle \partial_\alpha \psi_i | \partial_\beta \psi_i \rangle - 2 \sum_{i,j=1}^{M} \left[p_i \mathcal{A}_{ij}^{\alpha\beta} + p_j (\mathcal{A}_{ij}^{\alpha\beta})^* \right] \\
&= \sum_{i=1}^{M} 4 p_i \langle \partial_\alpha \psi_i | \partial_\beta \psi_i \rangle - \sum_{i,j=1}^{M} 2 (p_i + p_j) \mathcal{R}_{ij}^{\alpha\beta} \\
&- \mathrm{i} \sum_{i,j=1}^{M} 2 (p_i - p_j) \mathcal{I}_{ij}^{\alpha\beta} \\
&= \sum_{i=1}^{M} 4 p_i (\langle \partial_\alpha \psi_i | \partial_\beta \psi_i \rangle - \mathcal{R}_{ii}^{\alpha\beta}) - \sum_{i \neq j}^{M} 2 (p_i + p_j) \mathcal{R}_{ij}^{\alpha\beta} \\
&- \mathrm{i} \sum_{i \neq j}^{M} 2 (p_i - p_j) \mathcal{I}_{ij}^{\alpha\beta}. \qquad (34)
\end{aligned}
$$

Finally, from Eqs. (29), (31), and (34), we obtain the QGT as the following form

$$
\begin{aligned}
Q_{\alpha\beta} = &\frac{1}{4} \sum_{i=1}^{M} \frac{(\partial_\alpha p_i)(\partial_\beta p_i)}{p_i} + \sum_{i=1}^{M} p_i (\langle \partial_\alpha \psi_i | \partial_\beta \psi_i \rangle - \mathcal{R}_{ii}^{\alpha\beta}) \\
&- 2 \sum_{i \neq j}^{M} \frac{p_i p_j}{p_i + p_j} \left[\mathcal{R}_{ij}^{\alpha\beta} + \mathrm{i} \frac{p_i - p_j}{p_i + p_j} \mathcal{I}_{ij}^{\alpha\beta} \right]. \qquad (35)
\end{aligned}
$$

We see that the QGT for the non-full rank density matrix relates to both the diagonal and non-diagonal terms of the DWZC.

6. Examples

We now consider two examples and the first one is the full-rank thermal state with non-zero temperature. As the thermal state can be written in an exponential form, using the method given by Ref. [25], one can obtain the SLD with respect to parameters α and β. Then from Eq. (19), we can get the expression of the QGT. Note that all the derivations are based on an assumption, namely, the rank of the state does not vary with changes of parameters.

Next, we investigate the K-fold degenerate ground state which can be written as

$$\rho_{\mathrm{GS}} = \frac{1}{K} \sum_{i=1}^{K} |\Psi_i\rangle\langle\Psi_i|. \qquad (36)$$

Here, $|\Psi_i\rangle$ is i-th ground state of a physical Hamiltonian. The state with no full rank is an equal mixture of all pure ground states. Then, from Eq. (35), one obtains the mixed-state QGT as

$$Q_{\alpha\beta} = \frac{1}{K} \left[\sum_{i=1}^{K} (\langle \partial_\alpha \psi_i | \partial_\beta \psi_i \rangle - \mathcal{R}_{ii}^{\alpha\beta}) - \sum_{i \neq j}^{K} \mathcal{R}_{ij}^{\alpha\beta} \right]. \qquad (37)$$

This simplified form benefits from the fact that all the probabilities are equal to $1/K$. And we find that the QGT only depends on real part of the DWZC.

7. Conclusions

In conclusion, we have generalized the concept of WZC to the DWZC. Both of them are Hermitian with respect to the two integer indices. We also generalize the pure-state QGT to the case of mixed states and find that mixed-state QGT can be represented in terms of real and imaginary parts of the DWZC. Specifically, the imaginary part of QGT can be written in terms of the imaginary part of the DWZC and the cube of the eigenvalue differences. These findings imply that the concept of DWZC plays a key role in the field of quantum geometry and we can further apply them to quantum metrology for estimating useful physical parameters. We also expect that the DWZC will have applications in other field of quantum physics.

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