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Invertibility conditions for field transformations with derivatives: Toward extensions of disformal transformation with higher derivatives

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We discuss a field transformation from fields ψ_a to other fields ϕ_i that involves derivatives, $\phi_i = \bar{\phi}_i(\psi_a, \partial_\alpha \psi_a, \ldots; x^\mu)$, and derive conditions for this transformation to be invertible, primarily focusing on the simplest case that the transformation maps between a pair of fields and involves up to their first derivatives. General field transformation of this type changes the number of degrees of freedom; hence, for the transformation to be invertible, it must satisfy certain degeneracy conditions so that additional degrees of freedom do not appear. Our derivation of necessary and sufficient conditions for invertible transformation is based on the method of characteristics, which is used to count the number of independent solutions of a given differential equation. As applications of the invertibility conditions, we show some non-trivial examples of the invertible field transformations with derivatives, and also give a rigorous proof that a simple extension of the disformal transformation involving a second derivative of the scalar field is not invertible.

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1. Introduction

Field transformations are ubiquitous in every field of physics and mathematics. The reason is that by using suitable fields (variables), one can often get a better and more intuitive insight into physical phenomena, find a different form of equations of motion which may allow solutions to be obtained more easily, and so on. For these purposes, the (local) invertibility of a field transformation is essential because, otherwise, physics would not be the same after the field transformation. If a field transformation does not involve derivatives, its local invertibility can be judged by the well-known inverse function theorem. On the other hand, when a field transformation does involve derivatives, it is clear that the invertibility conditions become much more complicated. If one regards such a field transformation as differential equations for old variables (fields), one can naively expect the presence of integration constants associated with the derivatives, which breaks the one-to-one correspondence between the old and new variables. Thus, apparently, one might arrive at the conclusion that no invertible transformation with derivatives exists. But, of course, this is not true in general. If one assumes specific degeneracy

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of the derivative terms in a field transformation which prohibits the appearance of associated integration constants, one can have an invertible field transformation with the derivatives. Indeed, in Ref. [1] we gave explicit necessary and sufficient conditions for the invertibility of a field transformation involving two fields and first derivatives.[1]

The purpose of this paper is twofold. First, we give a full and complete proof of necessary and sufficient conditions for the invertibility of field transformations with derivatives. Here, we fill some gaps in the proof that that were present in Ref. [1]. More importantly, we provide a full proof for the sufficient condition, while we previously gave it only within the perturbative regime. The second goal of this paper is to prove the no-go theorem of disformal transformation of the metric that involves second derivatives of a scalar field. We were strongly motivated by pursuing extensions of conformal and disformal transformations, which are often used in gravity, cosmology, and many other fields (see, e.g., Ref. [3] for a classification of new theories generated from a simpler theory [4] using disformal transformations). A disformal transformation involving the first derivative of a scalar field is a natural extension of a conformal transformation [5]. The next natural question is whether one can further extend a disformal transformation to one involving the second derivatives of a field, or even its higher derivatives. As a useful application of our invertibility conditions, we explicitly prove that there is no invertible disformal transformation involving the second derivatives given by $\tilde{g} = C(\chi, X)g + D(\chi, X)\nabla\chi\nabla\chi + E(\chi, X)\nabla\nabla\chi$ ($X \equiv (\nabla\chi)^2$) with $E \neq 0$. To the best of our knowledge, this is the first rigorous proof of the absence of such a transformation.

The organization of this paper is as follows. In Sect. 2, we give a complete derivation of the necessary conditions. The results in Sect. 2.1 apply to field transformations involving an arbitrary number of fields and their first derivatives. To show the explicit form of the invertibility conditions, in Sects. 2.2 and 2.3 we focus on the field transformation between two fields and their first derivatives. In Sect. 3, the complete proof of the sufficient conditions is given. As an application of our result, in Sect. 4 we construct some examples of invertible field transformation by solving the invertibility conditions. As another application, in Sect. 5 the no-go theorem for a class of disformal transformations of the metric with second derivatives is proven. Section 6 is devoted to conclusions and discussion. In Appendix A we examine a field transformation that changes the number of fields, and show that it cannot be invertible in our sense. In Appendices B and C, we show details of some of the calculations in Sect. 2. Appendix D shows that transformations between single fields and their derivatives can never be invertible, which implies that the two-field case we focus on is the simplest non-trivial case. In Appendix E, the necessity for nonlinear analysis in the inverse function theorem is explained. Appendix F gives some technical details of the derivation in Sect. 4, and Appendix G discusses an extension of the results given in Sect. 5.

1.1 *Notation*

Here we summarize the convention for indices used in this work:

$$\partial_{\mu_1\mu_2\cdots\mu_n} := \partial_{\mu_1}\partial_{\mu_2}\cdots\partial_{\mu_n}, \tag{1}$$

$$C^{(\mu_1\mu_2)} = \tfrac{1}{2}\left(C^{\mu_1\mu_2} + C^{\mu_2\mu_1}\right), \tag{2}$$

[1] See, e.g., Ref. [2] for earlier discussions on invertibility conditions of field transformations.

$$C^{[\mu_1\mu_2]} = \frac{1}{2}\left(C^{\mu_1\mu_2} - C^{\mu_2\mu_1}\right). \tag{3}$$

$C^{(\mu_1\mu_2\cdots\mu_n)}$ and $C^{[\mu_1\mu_2\cdots\mu_n]}$ are defined similarly by permutation (with a factor $(n!)^{-1}$). We introduce the Levi-Civita symbol $\epsilon^{i_1\cdots i_n i_{n+1}\cdots i_N}$, which satisfies the following identities:

$$\begin{aligned}
&\epsilon^{i_1\cdots i_n i_{n+1}\cdots i_N}\epsilon_{j_1\cdots j_n j_{n+1}\cdots j_N} M_{i_1}{}^{j_1}\cdots M_{i_n}{}^{j_n} M_{i_{n+1}}{}^{k} \\
&= \epsilon^{i_1\cdots i_N}\epsilon_{j_1\cdots j_N}\delta^{j_1}_{[l_1}\cdots\delta^{j_n}_{l_n}\delta^{k}_{l_{n+1}]} M_{i_1}{}^{l_1}\cdots M_{i_{n+1}}{}^{l_{n+1}} \\
&= \frac{1}{(n+1)!(N-n-1)!}\epsilon^{i_1\cdots i_N}\epsilon_{j_1\cdots j_N}\epsilon^{j_1\cdots j_n k l_{n+2}\cdots l_N}\epsilon_{l_1\cdots l_N} M_{i_1}{}^{l_1}\cdots M_{i_{n+1}}{}^{l_{n+1}} \\
&= \frac{n!(N-n)!}{(n+1)!(N-n-1)!}\epsilon^{i_1\cdots i_N}\epsilon_{l_1\cdots l_N} M_{i_1}{}^{l_1}\cdots M_{i_{n+1}}{}^{l_{n+1}}\delta^{k}_{[j_{n+1}}\delta^{l_{n+2}}_{j_{n+2}}\cdots\delta^{l_N}_{j_N]} \\
&= \frac{N-n}{n+1}\epsilon^{i_1\cdots i_N}\epsilon_{l_1\cdots l_N} M_{i_1}{}^{l_1}\cdots M_{i_{n+1}}{}^{l_{n+1}}\delta^{k}_{[j_{n+1}}\delta^{l_{n+2}}_{j_{n+2}}\cdots\delta^{l_N}_{j_N]}\,.
\end{aligned} \tag{4}$$

Throughout this work, we do not distinguish the lower and upper indices for the field space indices $a, b, \ldots$ and $i, j, \ldots$, while in some parts upper/lower indices are used for clarity of the notation.

2. Derivation of the necessary conditions

In this section we present a complete derivation of the necessary conditions for the invertibility of the transformation $\phi_i = \bar{\phi}_i(\psi_a, \partial_\alpha\psi_a, x^\mu)$ that transforms fields ϕ_i into fields ψ_a.[2] We divide the derivation of the invertibility conditions into two parts. In Sect. 2.1, we derive necessary conditions for invertibility. An invertible transformation preserves the number of degrees of freedom, while a transformation with field derivatives typically generates additional degrees of freedom. To formulate such an idea mathematically, we employ the method of characteristics for a differential equation to count the number of propagating modes [6].

In Sect. 2.1.1 we explain our approach to deriving the necessary conditions for invertibility based on the method of characteristics. In this approach, the transformation equation in Eq. (5) is converted to a set of differential equations that relates old variables to new ones, and the number of independent solutions for these equations is related to the number of degrees of freedom. To establish invertibility, the transformation must satisfy certain degeneracy conditions to remove unnecessary additional modes originating from the derivatives in the transformation equation. Such degeneracy conditions must be imposed at each order of the aforementioned differential equations, as summarized in Sects. 2.1.2 and 2.1.3. This procedure should be applied iteratively until the number of independent solutions is reduced appropriately, and then we may impose the non-degeneracy conditions to ensure the number of degrees of freedom is not changed by the transformation. We summarize this procedure in Sect. 2.1.4.

The procedure in Sect. 2.1 applies to field transformations for a general number of fields. To illustrate our method, we focus on the transformation between two fields in Sects. 2.2 and 2.3. The necessary conditions for invertibility in the two-field case are derived in Sect. 2.2 based on the general method introduced in the previous sections. The expressions for these conditions are rather complicated, and actually they can be simplified by solving part of the conditions

[2] Here, we concentrate on the case with first-order derivatives. However, our idea of using characteristics and degeneracy applies to the case with arbitrary-order derivatives (and an arbitrary number of fields) in the same way.

explicitly. Based on such an idea, the expressions of the necessary conditions are simplified in Sects. 2.3.1, 2.3.2, and 2.3.3. After simplification, the necessary conditions for the invertibility of two-field transformations are summarized in Eqs. (50), (68), and (73).

After deriving the necessary conditions in this section, in Sect. 3 we show that these conditions are actually sufficient to guarantee invertibility.

2.1 *Method of characteristics as the key to deriving the necessary conditions*

2.1.1 *Invertibility and the number of degeneracies.* Let us consider a field transformation from ψ_a to ϕ_i given by

$$\phi_i = \bar{\phi}_i(\psi_a, \partial_\alpha \psi_a, x^\mu), \tag{5}$$

where $\bar{\phi}_i$ is a function of ψ_a, $\partial_\alpha \psi_a$, and x^μ. We suppose that the numbers of the fields before and after the transformation are the same; that is, we assume that both a and i run from 1 to N, where N is the number of field ψ_a.[3]

If the transformation in Eq. (5) is invertible, it does not change physical properties of theories before and after the transformation, and particularly the causal structure should be invariant. If the transformation changes the number of characteristic hypersurfaces, the causal structure is changed correspondingly. Therefore, for invertibility, the transformation should not change the number of characteristic hypersurfaces. This gives the necessary conditions for invertibility.

To examine whether the transformation in Eq. (5) changes the number of characteristic hypersurfaces, we employ the method of characteristics for partial differential equations. This method can be applied only to quasi-linear differential equations, while the transformation equation in Eq. (5) is nonlinear in $\partial_\alpha \psi_i$ in general. To convert Eq. (5) to a quasi-linear partial differential equation, we act a differential operator $K_{bi}^{(\mu_1\cdots\mu_n)}\partial_{\mu_1\cdots\mu_n}$ on it to obtain

$$\begin{aligned}
&K_{bi}^{(\mu_1\cdots\mu_n)}\partial_{\mu_1\cdots\mu_n}\phi_i \\
&\quad= K_{bi}^{(\mu_1\cdots\mu_n)} A_{ia}^{\mu_{n+1}}\partial_{\mu_1\cdots\mu_{n+1}}\psi_a \\
&\qquad+ \left(K_{bi}^{(\mu_1\cdots\mu_n)} B_{ia} + n\, K_{bi}^{(\alpha\mu_1\cdots\mu_{n-1})}\partial_\alpha A_{ia}^{\mu_n}\right)\partial_{\mu_1\cdots\mu_n}\psi_a \\
&\qquad+ \left(n\, K_{bi}^{(\alpha\mu_1\cdots\mu_{n-1})}\partial_\alpha B_{ia} + \frac{n(n-1)}{2} K_{bi}^{(\alpha_1\alpha_2\mu_1\cdots\mu_{n-2})}\partial_{\alpha_1\alpha_2} A_{ia}^{\mu_{n-1}}\right)\partial_{\mu_1\cdots\mu_{n-1}}\psi_a + \cdots \\
&\qquad+ \left(\binom{n}{k} K_{bi}^{(\alpha_1\cdots\alpha_k\mu_1\cdots\mu_{n-k})}\partial_{\alpha_1\cdots\alpha_k} B_{ia}\right. \\
&\qquad+ \left.\binom{n}{k+1} K_{bi}^{(\alpha_1\cdots\alpha_{k+1}\mu_1\cdots\mu_{n-k-1})}\partial_{\alpha_1\cdots\alpha_{k+1}} A_{ia}^{\mu_{n-k}}\right)\partial_{\mu_1\cdots\mu_{n-k}}\psi_a \\
&\qquad+ \cdots + \mathcal{O}\left(\partial^{\lfloor\frac{n}{2}\rfloor+1}\psi_a, \partial^{\lfloor\frac{n}{2}\rfloor}\psi_a, \ldots\right),
\end{aligned} \tag{6}$$

where A_{ia}^{α} and B_{ia} are $N \times N$ matrices defined by

$$A_{ia}^{\alpha} := \frac{\partial \bar{\phi}_i}{\partial(\partial_\alpha \psi_a)}, \qquad B_{ia} := \frac{\partial \bar{\phi}_i}{\partial \psi_a}, \tag{7}$$

[3]For a field transformation that involves two fields and its first derivatives, it can be explicitly shown that a transformation that changes the number of fields can never be invertible. See Appendix A for details.

and $\binom{n}{k}$ is the binomial coefficient for $k \le n - \lfloor \frac{n}{2} \rfloor - 2$. In this expression, $\partial^{\lfloor \frac{n}{2} \rfloor + 2}\psi_a$ and higher derivatives of ψ_a appear linearly, while the $\mathcal{O}\left(\partial^{\lfloor \frac{n}{2} \rfloor + 1}\psi_a, \partial^{\lfloor \frac{n}{2} \rfloor}\psi_a, \ldots\right)$ part is a nonlinear function of lower-order derivatives of ψ_a. We show the derivation of Eq. (6) in Appendix B.

The operation of the differential operator $K_{bi}^{(\mu_1 \cdots \mu_n)}\partial_{\mu_1 \cdots \mu_n}$ introduces additional characteristic hypersurfaces to those of Eq. (5). Hence, the characteristics of ψ_a, determined by the right-hand side of Eq. (6), are comprised of the original ones inherent to the field transformation equation in Eq. (5) and the additional ones generated by the operation of $K_{bi}^{(\mu_1 \cdots \mu_n)}\partial_{\mu_1 \cdots \mu_n}$.

Now we can analyze the characteristics of the quasi-linear differential equation in Eq. (6), regarding this equation as a partial differential equation in ψ_a. We have N differential equations with $(n+1)$th-order derivatives of ψ_a. Therefore, they generically give $N \times (n+1)$ integration constants in a solution ψ_a, which corresponds to $N \times (n+1)$ characteristics. However, if the field transformation in Eq. (5) is invertible, there are no characteristics inherent to Eq. (5), which implies that Eq. (6) has only the additional characteristics generated by the operation of $K_{bi}^{(\mu_1 \cdots \mu_n)}\partial_{\mu_1 \cdots \mu_n}$. The number of these additional characteristics is $N \times n$, and hence there is a mismatch between the number of derivatives in the equations, $N \times (n+1)$, and the number of characteristics required by the invertibility, $N \times n$.

Such a mismatch can be resolved if the structure of the highest-order derivative part is degenerate. Since the difference between them is N, invertibility requires N degrees of degeneracies. We derive the conditions giving such N degeneracies below.

2.1.2 *Degeneracy condition at leading order.* The characteristic equation for Eq. (6) is given by

$$\det\left(K_{bi}^{(\mu_1 \cdots \mu_n)} A_{ia}^{\mu_{n+1}} \xi_{\mu_1} \cdots \xi_{\mu_{n+1}}\right) = \det\left(K_{bi}^{(\mu_1 \cdots \mu_n)} \xi_{\mu_1} \cdots \xi_{\mu_n}\right) \det\left(A_{ia}^{\mu_{n+1}} \xi_{\mu_{n+1}}\right) = 0, \tag{8}$$

where ξ_μ is a vector which is not tangent to would-be characteristics hypersurfaces. If $\det\left(A_{ia}^{\mu}\xi_\mu\right)$ does not vanish identically for any ξ_μ, the characteristic equation in Eq. (8) implies that there are $N \times (n+1)$ characteristics, and then the transformation in Eq. (5) is not invertible, as explained above. Hence, for invertibility, $A_{ia}^{\mu}\xi_\mu$ must be degenerate for any ξ_μ, that is,

$$\det\left(A_{ia}^{\mu}\xi_\mu\right) = 0 \qquad \text{for any } \xi_\mu. \tag{9}$$

This condition is equivalent to

$$\sum_{a \in S_n} \mathrm{sgn}(a) A_{1a_1}^{(\alpha_1} \cdots A_{Na_N}^{\alpha_N)} = \frac{1}{N!}\epsilon^{i_1 \cdots i_N}\epsilon^{a_1 \cdots a_N} A_{i_1 a_1}^{\alpha_1} \cdots A_{i_N a_N}^{\alpha_N} = 0, \tag{10}$$

where N is the number of fields, and the sum is computed over the set S_n of all permutations $a = \{a_1, \ldots, a_N\}$ of $\{1, \ldots, N\}$. Here, sgn(a) denotes the signature of a permutation a, which is $+1$ whenever the reordering a can be achieved by successively interchanging two entries an even number of times, and -1 whenever it can be achieved by an odd number of such interchanges.

2.1.3 *Degeneracy condition at subleading order.* The condition in Eq. (10) indicates the degeneracy of the highest-order derivatives of Eq. (6). If the degeneracy number is N (i.e. the dimension of the kernel $A_{ia}^{\mu}\xi_\mu$ is N), it implies that $A_{ia}^{\mu} = 0$, and thus the transformation is independent of $\partial_\mu\psi_a$. This is a trivial case; we can directly use the implicit function theorem for Eq. (5). Therefore, we consider non-trivial cases where the number of degeneracy of Eq. (10)

is less than N. Here, we discuss the case where the degeneracy number of Eq. (10) is 1 for simplicity. Generic cases may be discussed in a similar manner.

For later use, we introduce the adjugate matrix of A^{μ}_{ia}, which is the transposed cofactor matrix, as

$$\bar{A}^{\alpha_1\cdots\alpha_{N-1}}_{ai} := {}^t\bar{A}^{\alpha_1\cdots\alpha_{N-1}}_{ia} = (-1)^{i+a}\sum_{\bar{a}\in\bar{S}_n}\mathrm{sgn}(\bar{a})A^{(\alpha_1}_{\bar{i}_1\bar{a}_1}\cdots A^{\alpha_{N-1})}_{\bar{i}_{N-1}\bar{a}_{N-1}}$$
$$= \frac{1}{(N-1)!}\epsilon_i{}^{i_1\cdots i_{N-1}}\epsilon_a{}^{a_1\cdots a_{N-1}}A^{\alpha_1}_{i_1a_1}\cdots A^{\alpha_{N-1}}_{i_{N-1}a_{N-1}}, \quad (11)$$

where $\{\bar{i}_1, \ldots, \bar{i}_{N-1}\} = \{1, \ldots, i-1, i+1, \ldots, N\}$, and the sum is computed over the set $\bar{S}_n$ of all permutations $\bar{a} = \{\bar{a}_1, \ldots, \bar{a}_{N-1}\}$ of $\{1, \ldots, a-1, a+1, \ldots, N\}$. This adjugate matrix satisfies

$$\bar{A}^{(\alpha_1\cdots\alpha_{N-1}}_{ai}A^{\alpha_N)}_{ib} = 0, \qquad A^{(\alpha_1}_{ia}\bar{A}^{\alpha_2\cdots\alpha_N)}_{aj} = 0. \quad (12)$$

As commented above, we suppose that the dimension of the kernel of $A^{\mu}_{ia}\xi_\mu$ is 1 for any ξ_μ. Then the adjugate matrix is a rank-1 matrix.

The fact that the highest derivative part of Eq. (6) is degenerate in one dimension implies that Eq. (6) contains one equation that involves only lower-order derivatives of ψ_a. This does not necessarily imply that one of the equations in Eq. (6) contains only lower-derivative terms; instead, generically, by combining equations in Eq. (6) one should be able to find one lower-derivative equation. Let us extract this subleading equation. First, setting the operator $K^{(\mu_1\cdots\mu_n)}_{bi}\partial_{\mu_1\cdots\mu_n}$ in Eq. (6) to $\tilde{K}^{(\mu_1\cdots\mu_m)}_{b}\bar{A}^{\alpha_1\cdots\alpha_{N-1}}_{bi}\partial_{\mu_1\cdots\mu_m\alpha_1\cdots\alpha_{N-1}}$ with $m = n - N + 1$, Eq. (6) yields

$$\tilde{K}^{(\mu_1\cdots\mu_m)}_{b}\bar{A}^{\alpha_1\cdots\alpha_{N-1}}_{bi}\partial_{\mu_1\cdots\mu_m\alpha_1\cdots\alpha_{N-1}}\phi_i$$
$$= \tilde{K}^{(\mu_1\cdots\mu_m)}_{b}\bar{A}^{(\alpha_1\cdots\alpha_{N-1}}_{bi}A^{\alpha_N)}_{ia}\partial_{\mu_1\cdots\mu_m\alpha_1\cdots\alpha_N}\psi_a$$
$$+ \tilde{K}^{(\mu_1\cdots\mu_m)}_{b}\left[\bar{A}^{\alpha_1\cdots\alpha_{N-1}}_{bi}B_{ia} + (N-1)\bar{A}^{\beta\alpha_1\cdots\alpha_{N-2}}_{bi}\left(\partial_\beta A^{\alpha_{N-1}}_{ia}\right)\right]\partial_{\mu_1\cdots\mu_m\alpha_1\cdots\alpha_{N-1}}\psi_a$$
$$+ m\tilde{K}^{(\beta\mu_1\cdots\mu_{m-1})}_{b}\bar{A}^{\alpha_1\cdots\alpha_{N-1}}_{bi}\left(\partial_\beta A^{\mu_m}_{ia}\right)\partial_{\mu_1\cdots\mu_m\alpha_1\cdots\alpha_{N-1}}\psi_a + \mathcal{O}\left(\partial^{m+N-2}\psi\right). \quad (13)$$

The first term on the right-hand side vanishes because of Eq. (12). Moreover, Eq. (12) gives

$$\bar{A}^{(\alpha_1\cdots\alpha_{N-1}}_{bi}\left(\partial_\beta A^{\alpha_N)}_{ia}\right) = -\left(\partial_\beta\bar{A}^{(\alpha_1\cdots\alpha_{N-1}}_{bi}\right)A^{\alpha_N)}_{ia}. \quad (14)$$

This equation shows that the last term on the right-hand side of Eq. (13) is written as

$$m\tilde{K}^{(\beta\mu_1\cdots\mu_{m-1})}_{b}\bar{A}^{\alpha_1\cdots\alpha_{N-1}}_{bi}\left(\partial_\beta A^{\mu_m}_{ia}\right)\partial_{\mu_1\cdots\mu_m\alpha_1\cdots\alpha_{N-1}}\psi_a$$
$$= -m\tilde{K}^{(\beta\mu_1\cdots\mu_{m-1})}_{b}\left(\partial_\beta\bar{A}^{\alpha_1\cdots\alpha_{N-1}}_{bi}\right)A^{\mu_m}_{ia}\partial_{\mu_1\cdots\mu_m\alpha_1\cdots\alpha_{N-1}}\psi_a. \quad (15)$$

Next, Eq. (6) with $K^{(\mu_1\cdots\mu_n)}_{bi}\partial_{\mu_1\cdots\mu_n}$ replaced by $m\tilde{K}^{(\beta\mu_1\cdots\mu_{m-1})}_{b}\left(\partial_\beta\bar{A}^{\alpha_1\cdots\alpha_{N-1}}_{bi}\right)\partial_{\mu_1\cdots\mu_{m-1}\alpha_1\cdots\alpha_{N-1}}$ gives

$$m\tilde{K}^{(\beta\mu_1\cdots\mu_{m-1})}_{b}\left(\partial_\beta\bar{A}^{\alpha_1\cdots\alpha_{N-1}}_{bi}\right)\partial_{\mu_1\cdots\mu_{m-1}\alpha_1\cdots\alpha_{N-1}}\phi_i$$
$$= m\tilde{K}^{(\beta\mu_1\cdots\mu_{m-1})}_{b}\left(\partial_\beta\bar{A}^{\alpha_1\cdots\alpha_{N-1}}_{bi}\right)A^{\mu_m}_{ia}\partial_{\mu_1\cdots\mu_m\alpha_1\cdots\alpha_{N-1}}\psi_a + \mathcal{O}\left(\partial^{m+N-2}\psi\right). \quad (16)$$

Then, the last term on the right-hand side of Eq. (13) can be replaced with the derivatives of ϕ_i and $\mathcal{O}\left(\partial^{m+N-2}\psi\right)$ terms. Expanding Eq. (13) up to $\partial^{m+N-2}\psi$ and eliminating some $\partial^{m+N-1}\psi$ and $\partial^{m+N-2}\psi$ terms in favor of $\partial^{m+N-2}\phi$ and $\partial^{m+N-3}\phi$ terms, as we did above, we finally obtain

$$\begin{aligned}
&\tilde{K}_b^{(\mu_1\cdots\mu_m)}\bar{A}_{bi}^{\alpha_1\cdots\alpha_{N-1}}\partial_{\mu_1\cdots\mu_m\alpha_1\cdots\alpha_{N-1}}\phi_i + m\tilde{K}_b^{(\beta\mu_1\cdots\mu_{m-1})}\left(\partial_\beta\bar{A}_{bi}^{\alpha_1\cdots\alpha_{N-1}}\right)\partial_{\mu_1\cdots\mu_{m-1}\alpha_1\cdots\alpha_{N-1}}\phi_i \\
&\quad + \binom{m}{2}\tilde{K}_b^{(\beta\gamma\mu_1\cdots\mu_{m-2})}\left(\partial_{\beta\gamma}\bar{A}_{bi}^{\alpha_1\cdots\alpha_{N-1}}\right)\partial_{\mu_1\cdots\mu_{m-2}\alpha_1\cdots\alpha_{N-1}}\phi_i \\
&= \tilde{K}_b^{(\mu_1\cdots\mu_m)}\mathcal{A}_{2,ba}^{\alpha_1\cdots\alpha_{N-1}}\partial_{\mu_1\cdots\mu_m\alpha_1\cdots\alpha_{N-1}}\psi_a \\
&\quad + \left[\tilde{K}_b^{(\mu_1\cdots\mu_m)}\mathcal{B}_{2,ba}^{\alpha_1\cdots\alpha_{N-2}} + m\tilde{K}_b^{(\beta\mu_1\cdots\mu_{m-1})}\left(\partial_\beta\mathcal{A}_{2,ba}^{\mu_m\alpha_1\cdots\alpha_{N-2}}\right)\right]\partial_{\mu_1\cdots\mu_m\alpha_1\cdots\alpha_{N-2}}\psi_a \\
&\quad + \mathcal{O}\left(\partial^{m+N-3}\psi\right),
\end{aligned} \tag{17}$$

where

$$\mathcal{A}_{2,ba}^{\alpha_1\cdots\alpha_{N-1}} := \bar{A}_{bi}^{\alpha_1\cdots\alpha_{N-1}}B_{ia} + (N-1)\bar{A}_{bi}^{\beta(\alpha_1\cdots\alpha_{N-2}}\left(\partial_\beta A_{ia}^{\alpha_{N-1})}\right), \tag{18}$$

$$\mathcal{B}_{2,ba}^{\alpha_1\cdots\alpha_{N-2}} := (N-1)\left[\bar{A}_{bi}^{\beta\alpha_1\cdots\alpha_{N-2}}\left(\partial_\beta B_{ia}\right) + \frac{N-2}{2}\bar{A}_{bi}^{\beta\gamma(\alpha_1\cdots\alpha_{N-3}}\left(\partial_{\beta\gamma}A_{ia}^{\alpha_{N-2})}\right)\right]. \tag{19}$$

The right-hand side of Eq. (17) has one less derivative compared to that of Eq. (6); that is, it is the subleading equation. The combination of the non-degenerate part of Eq. (6), which has $N - 1$ equations, and Eq. (17) gives the structure of the characteristics in the subleading order.

So farm we have established the presence of one degeneracy. To ensure invertibility, there must be N degeneracies. Hence, the characteristics at this subleading order should be degenerate too. By assumption, the matrix $A^\mu_{ia}\xi_\mu$ has one degeneracy; that is, there exists only one eigenvector with a zero eigenvalue, which is denoted $\psi^\perp_a(\xi)$. The other components of ψ_a are collectively defined as $\psi^\parallel_a(\xi)$. (Hereinafter, we omit (ξ) from $\psi^\perp_a(\xi)$ and $\psi^\parallel_a(\xi)$ for brevity.) The characteristic matrix for the highest-derivative part of Eq. (17) and the non-degenerate part of Eq. (6) is written as

$$\begin{array}{rc} & \begin{array}{cc}\psi^\parallel & \psi^\perp\end{array} \\ \begin{array}{r}\text{non-degenerate part of Eq. (6)} \\ \text{Eq. (17)}\end{array} & \begin{pmatrix} {}^{(\mathrm{nd})}A^\mu_{ia}\xi_\mu & 0 \\ K_a & K \end{pmatrix}, \end{array} \tag{20}$$

where $(K_a, K) = \tilde{K}_b^{(\mu_1\cdots\mu_m)}\mathcal{A}_{2,ba}^{\alpha_1\cdots\alpha_{N-1}}\xi_{\mu_1}\cdots\xi_{\mu_m}\xi_{\alpha_1}\cdots\xi_{\alpha_{N-1}}$,[4] and ${}^{(\mathrm{nd})}A^\mu_{ia}\xi_\mu$ is an $(N-1)\times(N-1)$ matrix indicating only the non-degenerate components of $A^\mu_{ia}\xi_\mu$, that is, $\det\left({}^{(\mathrm{nd})}A^\mu_{ia}\xi_\mu\right) \neq 0$. This matrix determines the subleading characteristics, and it should be degenerate for invertibility. Since ${}^{(\mathrm{nd})}A^\mu_{ia}\xi_\mu$ is regular, the requirement of degeneracy gives the condition that $K = 0$ for any $\tilde{K}_b^{(\mu_1\cdots\mu_m)}$, i.e. $\mathcal{A}_{2,ba}^{\alpha_1\cdots\alpha_{N-1}}\xi_{\alpha_1}\cdots\xi_{\alpha_{N-1}}\psi^\perp_a$ vanishes for any ξ.

In order to show the condition explicitly, we express $\psi^\perp$ in terms of A^μ_{ia}. This can be done with the adjugate matrix $\bar{A}_{ai}^{\mu_1\cdots\mu_{N-1}}\xi_{\mu_1}\cdots\xi_{\mu_{N-1}}$. Equation (12) shows that $\bar{A}_{ai}^{\mu_1\cdots\mu_{N-1}}\xi_{\mu_1}\cdots\xi_{\mu_{N-1}}$ is the projection matrix to the kernel of $A^\mu_{ia}\xi_\mu$, in which $\psi^\perp$ lives by definition. Therefore, the subleading degeneracy condition is written as

$$\mathcal{A}_{2,ba}^{(\alpha_1\cdots\alpha_{N-1}}\bar{A}_{ai}^{\mu_1\cdots\mu_{N-1})} = 0. \tag{21}$$

[4]Using the projection tensor $E_{N-1,ab}$ onto the $\psi^\parallel$ space defined by Eq. (26), the components of the vector (K_a, K) may be expressed more precisely as

$$K_a \propto \tilde{K}_b^{(\mu_1\cdots\mu_m)}\mathcal{A}_{2,bc}^{\alpha_1\cdots\alpha_{N-1}}E_{N-1,cb}\xi_{\mu_1}\cdots\xi_{\mu_m}\xi_{\alpha_1}\cdots\xi_{\alpha_{N-1}},$$

$$K \propto \tilde{K}_b^{(\mu_1\cdots\mu_m)}\mathcal{A}_{2,bc}^{\alpha_1\cdots\alpha_{N-1}}\bar{A}_{ci}^{\nu_1\cdots\mu_{N-1}}\bar{A}_{ai}^{\nu_N\cdots\nu_{2N-2}}\xi_{\mu_1}\cdots\xi_{\mu_m}\xi_{\alpha_1}\cdots\xi_{\alpha_{N-1}}\xi_{\nu_1}\cdots\xi_{\nu_{2N-2}}.$$

See Sect. 2.1.4 for more details on this decomposition.

2.1.4 *Degeneracy and non-degeneracy conditions at lower orders.* So far, two degeneracies were realized by imposing the degeneracy conditions in Eqs. (10) and (21). The condition in Eq. (21) makes the matrix in Eq. (20) degenerate, and then the highest-order derivative of the component parallel to $\psi^{\perp}$ appears in a lower-order equation, that is, the subsubleading-order equation. The characteristic matrix is composed of the leading-order equation for the $\psi^{\parallel}$ components and the subsubleading-order equation for the $\psi^{\perp}$ component. Now we have two degeneracies, and thus for $N > 2$ this subsubleading characteristic matrix must give an additional degeneracy for invertibility. Then, similar to the analysis of the subleading order, the degeneracy implies that the highest-order derivative for the $\psi^{\perp}$ component in the subsubleading equation should vanish. This procedure is done iteratively until N degeneracies are established. After that, we impose the condition that the next-order characteristic matrix is *not* degenerate, in order for the transformation to be invertible. The last condition corresponds to that of the inverse function theorem (without derivatives).

In order to implement the procedure described above, it is useful to introduce a projection matrix $E_{N-1,\,ij}(\xi)$ to the $(N-1)$-dimensional field space of $\psi^{\parallel}$; that is, $E_{N-1,\,ij}(\xi)$ is the identity matrix for the $(N-1)$-dimensional field space and zero for the one-dimensional field space parallel to $\psi^{\perp}$. Let us express $E_{N-1,\,ij}(\xi)$ in terms of $A^{\mu}_{ia}\xi_{\mu}$. We consider the matrix

$$\tilde{A}^{\mu_1\cdots\mu_{2N-3}}_{ai} = \frac{1}{(N-1)!}\epsilon_i{}^{i_1\cdots i_{N-1}}\epsilon_a{}^{a_1\cdots a_{N-1}}\bar{A}^{(\mu_1\cdots\mu_{N-1}}_{a_1 i_1} A^{\mu_N}_{i_2 a_2}\cdots A^{\mu_{2N-3})}_{i_{N-1}a_{N-1}}. \tag{22}$$

This matrix satisfies

$$\begin{aligned}(N-1)&\tilde{A}^{\mu_1\cdots\mu_{2N-3}}_{ai} A^{\mu_{2N-2}}_{ib}\xi_{\mu_1}\cdots\xi_{\mu_{2N-2}} \\ &= \left(\bar{A}^{2,\mu_1\ldots\mu_{2N-2}}\delta_{ab} - \bar{A}^{\mu_1\ldots\mu_{N-1}}_{ai}\bar{A}^{\mu_N\cdots\mu_{2N-2}}_{bi}\right)\xi_{\mu_1}\cdots\xi_{\mu_{2N-2}} \\ &= E_{N-1,ab}(\xi)\bar{A}^{2,\mu_1\cdots\mu_{2N-2}}\xi_{\mu_1}\cdots\xi_{\mu_{2N-2}},\end{aligned} \tag{23}$$

where

$$\bar{A}^{2,\mu_1\cdots\mu_{2N-2}} := \bar{A}^{(\mu_1\cdots\mu_{N-1}}_{ai}\bar{A}^{\mu_N\cdots\mu_{2N-2})}_{ai} = \tilde{A}^{(\mu_1\cdots\mu_{2N-3}}_{ai}A^{\mu_{2N-2})}_{ia}. \tag{24}$$

In the calculation in Eq. (23), we use the fact that $\bar{A}^{\mu_1\cdots\mu_{N-1}}_{ai}\xi_{\mu_1}\cdots\xi_{\mu_{N-1}}$ is rank-1 matrix, and then the components of $\bar{A}^{\mu_1\cdots\mu_{N-1}}_{ai}\bar{A}^{\mu_N\cdots\mu_{2N-2}}_{bi}\xi_{\mu_1}\cdots\xi_{\mu_{2N-2}}$ are zero except for the $\psi^{\perp}$–$\psi^{\perp}$ component. The value of this nonzero component is shown to be $\bar{A}^{2,\mu_1\cdots\mu_{2N-2}}\xi_{\mu_1}\cdots\xi_{\mu_{2N-2}}$ by direct calculations. Equation (23) divided by $\bar{A}^{2,\mu_1\cdots\mu_{2N-2}}\xi_{\mu_1}\cdots\xi_{\mu_{2N-2}}$ gives $E_{N-1,\,ab}(\xi)$, which can be regarded as a projector to the $(N-1)$-dimensional space of $\psi^{\parallel}$. Since Eq. (23) holds for any ξ^{μ}, it can be expressed equivalently as

$$\bar{A}^{(\mu_1\cdots\mu_{N-1}}_{ai}\bar{A}^{\mu_N\cdots\mu_{2N-2})}_{bi} + (N-1)\tilde{A}^{(\mu_1\cdots\mu_{2N-3}}_{ai}A^{\mu_{2N-2})}_{ib} = \bar{A}^{2,(\mu_1\cdots\mu_{2N-2})}\delta_{ab}. \tag{25}$$

Let us demonstrate how to obtain the lower-order equations iteratively with the projection tensor of Eq. (23). On the right-hand side of Eq. (17), the leading term is the first term proportional to $\partial^{m+N-1}\psi_a$. The degeneracy condition for the subleading-order Eq. (21) implies that the first term does not have the $\psi^{\perp}$ component, i.e. it can be written as

$$\begin{aligned}&\tilde{K}^{(\mu_1\cdots\mu_m)}_b\mathcal{A}^{\alpha_1\cdots\alpha_{N-1}}_{2,ba}\partial_{\mu_1\cdots\mu_m\alpha_1\cdots\alpha_{N-1}}\psi_a \\ &\quad= \tilde{K}^{(\mu_1\cdots\mu_m)}_b\mathcal{A}^{\alpha_1\cdots\alpha_{N-1}}_{2,bc}E_{N-1,cd}(\partial)\partial_{\mu_1\cdots\mu_m\alpha_1\cdots\alpha_{N-1}}\psi_d.\end{aligned} \tag{26}$$

Considering the case with $\tilde{K}_b^{\mu_1\cdots\mu_m} = \tilde{\tilde{K}}_b^{\mu_1\cdots\mu_{m'}}\bar{A}^{2,\gamma_1\cdots\gamma_{2N-2}}$, we can rewrite Eq. (26) as

$$\begin{aligned}&\tilde{\tilde{K}}_b^{\mu_1\cdots\mu_{m'}}\bar{A}^{2,\gamma_1\cdots\gamma_{2N-2}}\mathcal{A}_{2,bc}^{\alpha_1\cdots\alpha_{N-1}}E_{N-1,ca}(\partial)\partial_{\mu_1\cdots\mu_{m'}\gamma_1\cdots\gamma_{2N-2}\alpha_1\cdots\alpha_{N-1}}\psi_k\\ &\quad=(N-1)\tilde{\tilde{K}}_b^{\mu_1\cdots\mu_{m'}}\mathcal{A}_{2,bc}^{\alpha_1\cdots\alpha_{N-1}}\tilde{A}_{ci}^{\gamma_1\cdots\gamma_{2N-3}}A_{ia}^{\gamma_{2N-2}}\partial_{\mu_1\cdots\mu_{m'}\alpha_1\cdots\alpha_{N-1}\gamma_1\cdots\gamma_{2N-2}}\psi_k,\end{aligned} \tag{27}$$

where we used Eq. (23). Then, by subtracting Eq. (17) from Eq. (6) with its coefficient set to $K_{bi}^{\mu_1\cdots\mu_m} = (N-1)\tilde{\tilde{K}}_b^{\mu_1\cdots\mu_{m'}}\mathcal{A}_{2,bc}^{\alpha_1\cdots\alpha_{N-1}}\tilde{A}_{ci}^{\gamma_1\cdots\gamma_{2N-3}}$, the subleading $(\partial^{m'+3N-3}\psi)$ term is canceled out and the subsubleading-order equation is obtained as a result.

The degeneracy condition can be obtained applying the procedure explained around Eq. (20) to the subsubleading equation, and the condition will be similar to the condition in Eq. (21) for the subleading-order equation. Then, using the projector $E_{N-1,ab}$ again, we can construct the lower-order equation. Applying this procedure iteratively, we can derive N degeneracy conditions and the final non-degeneracy condition, which constitute the necessary conditions for invertibility.

2.2 *Necessary conditions in the two-field case*

Although we have already derived the leading and subleading degeneracy conditions in the previous subsection using the general procedure, it is instructive to follow a concrete example to understand the method. For this purpose, based on the discussion in the previous section, we demonstrate how to derive the necessary conditions for the invertibility of a field transformation of two fields involving up to the first derivative.[5] That is, we consider the case where $N = 2$, $i = 1, 2$, and $a = 1, 2$. In this section we complete the iterations to derive all the degeneracies and the final non-degeneracy conditions. The conditions obtained will be simplified in Sect. 2.3.

We apply the procedure explained in Sect. 2.1 to the two-field case. In this case, $\bar{A}_{ai}^{\mu}$, $\mathcal{A}_{2,ab}^{\mu}$, and $\mathcal{B}_{2,ab}$ that appeared in the previous section are written as

$$\bar{A}_{ai}^{\mu} = \epsilon_i{}^{i_1}\epsilon_a{}^{a_1}A_{i_1a_1}^{\mu}, \qquad \mathcal{A}_{2,ab}^{\mu} := \bar{A}_{ai}^{\mu}B_{ib} + \bar{A}_{ai}^{\beta}\partial_\beta A_{ib}^{\mu}, \qquad \mathcal{B}_{2,ab} := \bar{A}_{ai}^{\beta}\partial_\beta B_{ib}, \tag{28}$$

and $\tilde{A}_{ai}^{\mu}$ is simplified as

$$\tilde{A}_{ai}^{\mu} = \epsilon_i{}^{i_1}\epsilon_a{}^{a_1}\bar{A}_{a_1i_1}^{\mu} = \epsilon_i{}^{i_1}\epsilon_a{}^{a_1}\epsilon_{i_1}{}^{i_2}\epsilon_{a_1}{}^{a_2}A_{i_2a_2}^{\mu} = A_{ia}^{\mu}. \tag{29}$$

Then, the identity in Eq. (25) becomes

$$\bar{A}_{ai}^{(\mu_1}\bar{A}_{bi}^{\mu_2)} + \tilde{A}_{ai}^{(\mu_1}A_{ib}^{\mu_2)} = \bar{A}_{ai}^{(\mu_1}\bar{A}_{bi}^{\mu_2)} + A_{ia}^{(\mu_1}A_{ib}^{\mu_2)} = \bar{A}^{2,\mu_1\mu_2}\delta_{ab}. \tag{30}$$

We operate $K^{(\mu_1\cdots\mu_n)}\partial_{\mu_1\cdots\mu_n}$ on the field transformation equation, Eq. (5), to obtain

$$K^{(\mu_1\cdots\mu_n)}\partial_{\mu_1\cdots\mu_n}\phi_i = K^{(\mu_1\cdots\mu_n)}A_{ia}^{\mu_{n+1}}\partial_{\mu_1\cdots\mu_{n+1}}\psi_a + \mathcal{O}(\partial^n\psi). \tag{31}$$

For Eq. (5) to be invertible, the coefficient of the highest-order derivative on the right-hand side of Eq. (31) must be degenerate, which implies

$$\text{for all } \xi_\mu, \qquad \det(A_{ia}^{\mu}\xi_\mu) = 0 \quad \Leftrightarrow \quad \epsilon^{i_1i_2}\epsilon^{a_1a_2}A_{i_1a_1}^{(\alpha_1}A_{i_2a_2}^{\alpha_2)} = 0. \tag{32}$$

Following the previous section, we assume that the matrix $A_{ia}^{\mu}\xi_\mu$ is degenerate only in one dimension. Then the kernel of $A_{ia}^{\mu}\xi_\mu$ parallel to $\psi_a^{\perp}$ and the field space in the other direction parallel to $\psi_a^{\parallel}$ are one dimension each.

[5] As will be explicitly shown in Appendix D, there is no invertible field transformation of one field involving first derivatives. Hence, among (possibly invertible) transformations with up to first derivatives, the two-field case is the simplest.

The degeneracy condition at the subleading order is obtained following the procedure in Sect. 2.1.3. To construct the subleading equation from Eq. (5), we have to pick up the component of this equation corresponding to the kernel of the coefficient of the highest-order derivative, A^{μ}_{ia}. This can be done by operating $\tilde{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{\mu_{n+1}}_{bi}\partial_{\mu_1\cdots\mu_{n+1}}$ on the transformation equation in Eq. (5) as

$$\begin{aligned}
&\tilde{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{\mu_{n+1}}_{bi}\partial_{\mu_1\cdots\mu_{n+1}}\phi_i \\
&\quad = \tilde{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{\mu_{n+1}}_{bi}A^{\nu}_{ia}\partial_{\mu_1\cdots\mu_{n+1}\nu}\psi_a \\
&\qquad + \left(\tilde{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{\mu_{n+1}}_{bi}B_{ia} + n\,\tilde{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\bar{A}^{\mu_n}_{bi}\partial_\alpha A^{\mu_{n+1}}_{ia} + \tilde{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{\alpha}_{bi}\partial_\alpha A^{\mu_{n+1}}_{ia}\right)\partial_{\mu_1\cdots\mu_{n+1}}\psi_a \\
&\qquad + \mathcal{O}\left(\partial^n\psi\right). \qquad (33)
\end{aligned}$$

The first term on the right-hand side vanishes thanks to Eq. (32). As shown in Sect. 2.1.3, the second term in the brackets proportional to n can be canceled by adding $n\tilde{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\left(\partial_\alpha\bar{A}^{\mu_n}_{bi}\right)\partial_{\mu_1\cdots\mu_n}\phi_i$ to Eq. (33). Nevertheless, without such a cancellation, we can directly obtain the same subleading condition from Eq. (33) by rewriting it as

$$\begin{aligned}
&\tilde{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{\mu_{n+1}}_{bi}\partial_{\mu_1\cdots\mu_{n+1}}\phi_i \\
&\quad = \left(\tilde{K}^{(\mu_1\cdots\mu_n)}\mathcal{A}^{\mu_{n+1}}_{2,ba} + n\,\tilde{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\bar{A}^{\mu_n}_{bi}\partial_\alpha A^{\mu_{n+1}}_{ia}\right)\partial_{\mu_1\cdots\mu_{n+1}}\psi_a + \mathcal{O}\left(\partial^n\psi\right). \qquad (34)
\end{aligned}$$

The subleading degeneracy condition is given by demanding that the coefficient of the highest-order derivative for $\psi^\perp$ vanishes. Noting that $\bar{A}^{\nu}_{ai}\xi_\nu$ works as a projector onto the $\psi^\perp$ space, this condition is written as

$$\left(\tilde{K}^{(\mu_1\cdots\mu_n)}\mathcal{A}^{\mu_{n+1}}_{2,ba} + n\,\tilde{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\bar{A}^{\mu_n}_{bi}\partial_\alpha A^{\mu_{n+1}}_{ia}\right)\bar{A}^{\nu}_{aj}\xi_{\mu_1}\cdots\xi_{\mu_{n+1}}\xi_\nu = 0. \qquad (35)$$

The second term vanishes, which is shown by using Eqs. (12) and (14) as

$$\begin{aligned}
&\tilde{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\bar{A}^{\mu_n}_{bi}\left(\partial_\alpha A^{\mu_{n+1}}_{ia}\right)\bar{A}^{\nu}_{aj}\xi_{\mu_1}\cdots\xi_{\mu_{n+1}}\xi_\nu \\
&\quad = -\tilde{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\left(\partial_\alpha\bar{A}^{\mu_n}_{bi}\right)A^{\mu_{n+1}}_{ia}\bar{A}^{\nu}_{aj}\xi_{\mu_1}\cdots\xi_{\mu_{n+1}}\xi_\nu = 0. \qquad (36)
\end{aligned}$$

Since $\tilde{K}^{(\mu_1\cdots\mu_n)}$ is arbitrary, the subleading condition is

$$\text{for all } \xi_\mu,\quad \mathcal{A}^{\mu}_{2,ba}\bar{A}^{\nu}_{aj}\xi_\mu\xi_\nu = 0 \quad\Leftrightarrow\quad \mathcal{A}^{(\mu}_{2,ba}\bar{A}^{\nu)}_{aj} = \bar{A}^{(\mu}_{bi}B_{ia}\bar{A}^{\nu)}_{aj} + \bar{A}^{\beta}_{bi}\left(\partial_\beta A^{(\mu}_{ia}\right)\bar{A}^{\nu)}_{aj} = 0. \qquad (37)$$

The non-degeneracy condition at the subsubleading order can be constructed following the procedure in Sect. 2.1.4. In this procedure we need to see the structure of the coefficient of the highest-order derivative term in Eq. (33) decomposing the variables into the $\psi^\perp$ and $\psi^\parallel$ space. For this purpose we use Eq. (30). Operating $\tilde{\tilde{K}}^{(\mu_1\cdots\mu_n)}\bar{A}^{\mu_{n+1}}_{bi}\bar{A}^{2,\mu_{n+2}\mu_{n+3}}\partial_{\mu_1\cdots\mu_{n+3}}$ on Eq. (5), we have

$$\begin{aligned}
&\tilde{\tilde{K}}^{(\mu_1\cdots\mu_n)}\bar{A}^{\mu_{n+1}}_{bi}\bar{A}^{2,\mu_{n+2}\mu_{n+3}}\partial_{\mu_1\cdots\mu_{n+3}}\phi_i \\
&\quad = \Bigg(\tilde{\tilde{K}}^{(\mu_1\cdots\mu_n)}\mathcal{A}^{\mu_{n+1}}_{2,ba}\bar{A}^{2,\mu_{n+2}\mu_{n+3}} + n\,\tilde{\tilde{K}}^{(\alpha\mu_1\cdots\mu_{n-1})}\bar{A}^{2,\mu_n\mu_{n+1}}\bar{A}^{\mu_{n+2}}_{bi}\partial_\alpha A^{\mu_{n+3}}_{ia} \\
&\qquad + 2\,\tilde{\tilde{K}}^{(\mu_1\cdots\mu_n)}\bar{A}^{2,\mu_{n+1}\alpha}\bar{A}^{\mu_{n+2}}_{bi}\partial_\alpha A^{\mu_{n+3}}_{ia}\Bigg)\partial_{\mu_1\cdots\mu_{n+3}}\psi_a + \mathcal{O}\left(\partial^{n+2}\psi\right). \qquad (38)
\end{aligned}$$

Using Eq. (30) for the first term in brackets and Eq. (14) for the other two, we have

$$\begin{aligned}
&\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{\mu_{n+1}}_{bi}\bar{A}^{2,\mu_{n+2}\mu_{n+3}}\partial_{\mu_1\cdots\mu_{n+3}}\phi_i\\
&\quad=\left(\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\mathcal{A}^{\mu_{n+1}}_{2,bc}\tilde{A}^{\mu_{n+2}}_{ci}-n\,\overset{\approx}{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\bar{A}^{2,\mu_n\mu_{n+1}}\partial_\alpha\bar{A}^{\mu_{n+2}}_{bi}\right.\\
&\qquad\left.-2\,\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{2,\mu_{n+1}\alpha}\partial_\alpha\bar{A}^{\mu_{n+2}}_{bi}\right)A^{\mu_{n+3}}_{ia}\partial_{\mu_1\cdots\mu_{n+3}}\psi_a+\mathcal{O}\left(\partial^{n+2}\psi\right).
\end{aligned}\tag{39}$$

The $\partial^{n+3}\psi$ term on the right-hand side can be reproduced by applying the operator

$$\left[\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\mathcal{A}^{\mu_{n+1}}_{2,bc}\tilde{A}^{\mu_{n+2}}_{ci}-\left(n\,\overset{\approx}{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\bar{A}^{2,\mu_n\mu_{n+1}}+2\,\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{2,\mu_{n+1}\alpha}\right)\partial_\alpha\bar{A}^{\mu_{n+2}}_{bi}\right]\partial_{\mu_1\cdots\mu_{n+2}}$$

to Eq. (5). Hence, by subtracting it from Eq. (39), we obtain the subsubleading-order equation involving terms only up to $\partial^{n+2}\psi$. Expanding Eqs. (6) and (39) up to the $\partial^{n+2}\psi$ terms, we find (see Appendix C for details)

$$\begin{aligned}
&\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{\mu_{n+1}}_{bi}\bar{A}^{2,\mu_{n+2}\mu_{n+3}}\partial_{\mu_1\cdots\mu_{n+3}}\phi_i-\left[\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\mathcal{A}^{\mu_{n+1}}_{2,bc}\tilde{A}^{\mu_{n+2}}_{ci}\right.\\
&\quad\left.-\left(n\,\overset{\approx}{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\bar{A}^{2,\mu_n\mu_{n+1}}+2\,\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{2,\mu_{n+1}\alpha}\right)\partial_\alpha\bar{A}^{\mu_{n+2}}_{bi}\right]\partial_{\mu_1\cdots\mu_{n+2}}\phi_i\\
&=\left\{-\frac{n(n-1)}{2}\,\overset{\approx}{K}^{(\alpha_1\alpha_2\mu_1\cdots\mu_{n-2})}\bar{A}^{2,\mu_{n-1}\mu_n}\left(\partial_{\alpha_1\alpha_2}\bar{A}^{\mu_{n+1}}_{bi}\right)A^{\mu_{n+2}}_{ia}\right.\\
&\quad+n\,\overset{\approx}{K}^{(\alpha_1\mu_1\cdots\mu_{n-1})}\left[-2\bar{A}^{2,\mu_n\alpha_2}\left(\partial_{\alpha_1\alpha_2}\bar{A}^{\mu_{n+1}}_{bi}\right)A^{\mu_{n+2}}_{ia}-\mathcal{A}^{\mu_n}_{2,bc}\tilde{A}^{\mu_{n+1}}_{ci}\partial_{\alpha_1}A^{\mu_{n+2}}_{ia}\right.\\
&\quad\left.+\bar{A}^{2,\mu_n\mu_{n+1}}\partial_{\alpha_1}\mathcal{A}^{\mu_{n+2}}_{ba}\right]\\
&\quad+\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\left[-\bar{A}^{2,\alpha_1\alpha_2}\left(\partial_{\alpha_1\alpha_2}\bar{A}^{\mu_{n+1}}_{bi}\right)A^{\mu_{n+2}}_{ia}+2\bar{A}^{2,\mu_{n+1}\alpha}\partial_\alpha\mathcal{A}^{\mu_{n+2}}_{2,ba}+\bar{A}^{2,\mu_{n+1}\mu_{n+2}}\bar{A}^{\alpha}_{bi}\partial_\alpha B_{ia}\right.\\
&\quad\left.\left.-2\mathcal{A}^{(\alpha}_{2,bc}\tilde{A}^{\mu_{n+1})}_{ci}\partial_\alpha A^{\mu_{n+2}}_{ia}-\mathcal{A}^{\mu_{n+1}}_{2,bc}\tilde{A}^{\mu_{n+2}}_{ci}B_{ia}\right]\right\}\partial_{\mu_1\cdots\mu_{n+2}}\psi_a+\mathcal{O}\left(\partial^{n+1}\psi_a\right).
\end{aligned}\tag{40}$$

The coefficient of the $\psi^\perp$ component of the highest-order derivative term $\partial^{n+2}\psi$ on the right-hand side of Eq. (40) determines the (non-)degeneracy of the characteristics in the subsubleading order. This coefficient is obtained by contracting $\bar{A}^{\mu_{n+3}}_{ai}$ with the coefficient of $\partial^{n+2}\psi_a$ in Eq. (40). We can show that the terms proportional to $\overset{\approx}{K}^{(\alpha_1\alpha_2\mu_1\cdots\mu_{n-2})}$ and $\overset{\approx}{K}^{(\alpha_1\mu_1\cdots\mu_{n-1})}$ become zero (see Appendix C). Among the terms proportional to $\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}$, the first one, $\partial_{\alpha_1\alpha_2}\bar{A}^{\mu_{n+1}}_{bi}$, vanishes by acting $\bar{A}^{\mu_{n+3}}_{ai}$, and the remaining term must not vanish for the $\psi^\perp$ component to be non-degenerate in this order. Hence, the non-degeneracy condition is given by

$$\left(\bar{A}^{2,\mu_1\mu_2}\mathcal{B}_{2,ab}-\mathcal{A}^{\mu_1}_{2,ac}\tilde{A}^{\mu_2}_{cj}B_{jb}+2\bar{A}^{2,\alpha\mu_1}\partial_\alpha\mathcal{A}^{\mu_2}_{2,ab}-2\mathcal{A}^{(\alpha}_{2,ac}\tilde{A}^{\mu_1)}_{cj}\partial_\alpha A^{\mu_2}_{jb}\right)\bar{A}^{\mu_3}_{bi}\xi_{\mu_1}\xi_{\mu_2}\xi_{\mu_3}\neq 0\tag{41}$$

for any ξ. Using Eq. (30), this can also be written as

$$\begin{aligned}
&\left(\bar{A}^{2,\mu_1\mu_2}\mathcal{B}_{2,ab}\bar{A}^{\mu_3}_{bi}-\mathcal{A}^{\mu_1}_{2,ab}\tilde{A}^{\mu_2}_{bj}B_{jc}\bar{A}^{\mu_3}_{ci}+2\mathcal{A}^{[\alpha|}_{2,ab}\tilde{A}^{\mu_1}_{bj}A^{|\mu_2]}_{jc}\partial_\alpha\bar{A}^{\mu_3}_{ci}\right.\\
&\quad\left.-\mathcal{A}^{\mu_1}_{2,ab}\bar{A}^{\alpha}_{bj}\tilde{A}^{\mu_2}_{cj}\partial_\alpha\bar{A}^{\mu_3}_{ci}\right)\xi_{\mu_1}\xi_{\mu_2}\xi_{\mu_3}\neq 0.
\end{aligned}\tag{42}$$

To summarize, the necessary conditions for invertibility are given by Eqs. (32), (37), and (42).

2.3 *Simplification of the necessary conditions*

Above, we derived the necessary conditions for invertibility, Eqs. (32), (37), and (42), in the two-field case with first-order derivative. We present a simpler form of these expressions in this section. The simplified form of the necessary conditions will be helpful in the proof that these conditions are also sufficient in the next section. In addition, we will use these expressions for building examples of invertible transformations.

2.3.1 *Simplification of Eq. (32).* First of all, we simplify the condition in Eq. (32), which implies that the rank of $A^\mu_{ia}\xi_\mu$ is less than two. Since we have assumed that $A^\mu_{ia}\xi_\mu$ has only one eigenvector with a zero eigenvalue, the rank of $A^\mu_{ia}\xi_\mu$ has to be unity for any ξ, i.e.

$$\xi_0 A^0_{ia} + \xi_1 A^1_{ia} + \cdots + \xi_D A^D_{ia} \tag{43}$$

is a rank-1 matrix for any $\xi_\mu = \{\xi_0, \xi_1, \ldots, \xi_D\}$, where D is the spacetime dimension. Then, by setting $\xi_\mu = \delta_{\mu\nu}$ for each $1 \le \nu \le D$, we find that A^ν_{ia} is a rank-1 matrix for any ν. Any rank-1 2 $\times$ 2 matrix can be written as a product of vectors, i.e. the matrices $A^0_{ia}, A^1_{ia}, \ldots, A^D_{ia}$ are written as

$$A^0_{ia} = V^0_i U^0_a, \qquad A^1_{ia} = V^1_i U^1_a, \qquad \ldots, \qquad A^D_{ia} = V^D_i U^D_a. \tag{44}$$

Below, we show by the induction that, if the rank of Eq. (43) is 1 for any ξ, A^μ_{ia} can be written as

$$A^\mu_{ia} = V_i U^\mu_a \qquad \text{or} \qquad A^\mu_{ia} = V^\mu_i U_a. \tag{45}$$

For $\mu \le 0$ (that is, $\mu = 0$), A^0_{ia} is written as $V^0_i U^0_a$, and thus, regarding (V^0_i, U^0_a) as (V_i, U^μ_a) or (V^μ_i, U_a) for $\mu = 0$, Eq. (45) is satisfied. Then, what we need to show is that, for any integer k, Eq. (45) is satisfied for $\mu \le k+1$ if it is satisfied for $\mu \le k$. Since the two choices of Eq. (45) are symmetric with respect to U_a and V_i, without loss of generality we assume the former ($A^\mu_{ia} = V_i U^\mu_a$) is satisfied for $\mu \le k$. If $A^{k+1}_{ia} = 0$, $A^\mu_{ia} = V_i U^\mu_a$ for $\mu \le k+1$ is trivially satisfied. Therefore, we consider the case where $A^{k+1}_{ia} = V^{k+1}_i U^{k+1}_a \neq 0$. If V^{k+1}_i is parallel to V_i, by rescaling $V^{k+1}_i \to cV^{k+1}_i = V_i$, $U^{k+1}_a \to U^{k+1}_a/c$ with a constant c, we can satisfy $A^\mu_{ia} = V_i U^\mu_a$ for $\mu \le k+1$.

We show that if V^{k+1}_i is not parallel to V_i, all the U^μ_a for $\mu \le k+1$ become parallel, and thus A^μ_{ia} can be written as $V^\mu_i U_a$. We consider a vector $\xi_\mu = (\xi_0, \xi_1, \ldots, \xi_{k+1}, 0, 0, \ldots)$, where the ξ_μ ($\mu \le k+1$) are arbitrary. Since $A^\mu_{ia}\xi_\mu$ should have an eigenvector $e^a(\xi_\mu)$ with zero eigenvalue, we have

$$0 = A^\mu_{ia}\xi_\mu e^a = V_i \sum_{\mu=0}^{k} U^\mu_a e^a \xi_\mu + V^{k+1}_i U^{k+1}_a e^a \xi_{k+1}. \tag{46}$$

If V^{k+1}_i is not parallel to V_i, the above equation gives

$$\sum_{\mu=0}^{k} U^\mu_a \xi_\mu e^a = 0, \qquad U^{k+1}_a \xi_{k+1} e^a = 0. \tag{47}$$

Now suppose that $\xi_{k+1} \neq 0$. In this case, the latter of these equations uniquely fixes e^a because the field space dimension is two. Then, because e^a is independent of ξ_μ ($\mu \le k$), and also the ξ^μ for $\mu \le k$ are arbitrary, Eq. (47) implies

$$U^\mu_a e^a = 0 \qquad \big(\mu \le k+1\big). \tag{48}$$

This implies that all the U_a^μ $(\mu \le k+1)$ are normal to e^a. Since e^a is non-zero and the space of index a is two-dimensional, all the U_a^μ $(\mu \le k+1)$ are parallel to each other. Therefore, by rescaling U_a, A_{ia}^μ can be expressed in terms of the common U_a as

$$A_{ia}^\mu = C^\mu V_i U_a \quad (\mu \le k), \qquad A_{ia}^{k+1} = V_i^{k+1} U_a, \tag{49}$$

where C^μ is a normalization factor. Therefore, by redefining $\{C^\mu V_i^\mu, V_i^{k+1}\}$ $(\mu \le k)$ as $\{V_i, V_i^{k+1}\}$, A_{ia}^μ is written as $V_i^\mu U_a$ for $\mu \le k+1$.

2.3.2 *Further decomposition of* A_{ia}^μ. We have seen that one of the invertibility conditions, Eq. (32), implies that A_{ia}^μ is decomposed as Eq. (45). Using the other conditions, we show that A_{ia}^μ can be decomposed further as

$$A_{ia}^\mu = a^\mu V_i U_a. \tag{50}$$

Let us show the proof in each case of Eq. (45).

2.3.2.1 $A_{ia}^\mu = V_i U_a^\mu$

In this case, if we can show $U_a^\mu = a^\mu U_a$, A_{ia}^μ is expressed as $a^\mu V_i U_a$. We define a vector n_i normal to V_j as

$$n_j := \epsilon_{ij} V_j. \tag{51}$$

We also define a vector m_a^μ with spacetime index μ as

$$m_a^\mu := \epsilon_{ab} U_b^\mu. \tag{52}$$

Then, $\bar{A}_{ia}^\mu$ and $\tilde{A}_{ia}^\mu$ are written as

$$\bar{A}_{ai}^\mu = m_a^\mu n_i, \qquad \tilde{A}_{ai} = U_a^\mu V_i, \tag{53}$$

and the condition in Eq. (37) becomes

$$n_i B_{ia} m_a^\mu = 0 \qquad (\text{for any } \mu). \tag{54}$$

Now we show that U_a^μ has to be written as $a^\mu U_a$. This can be proven by contradiction: the assumption that two of the U_a^μ are not parallel to each other (for instance, U_a^0 is not parallel to U_a^1) leads to a contradiction. Under this assumption, two of the m_a^μ are correspondingly not parallel. Since the space spanned by index a is two-dimensional, Eq. (54) implies that

$$n_i B_{ia} = 0. \tag{55}$$

Then, the left-hand side of Eq. (42) becomes

$$\begin{aligned}
&\Big[V_j^2 U_c^{\mu_1} U_c^{\mu_2} m_a^\beta n_k \left(\partial_\beta B_{kb}\right) m_b^{\mu_3} n_i - m_a^\beta U_b^{\mu_1} n_k \left(\partial_\beta V_k\right) U_b^{\mu_2} V_j B_{jc} m_c^{\mu_3} n_i \\
&\quad - m_a^\beta U_b^{\mu_1} n_k \left(\partial_\beta V_k\right) m_b^\alpha n_j m_c^{\mu_2} n_j \partial_\alpha \left(m_c^{\mu_3} n_i\right) + m_a^\beta U_b^\alpha n_k \left(\partial_\beta V_k\right) U_b^{\mu_1} V_j U_c^{\mu_2} V_j \partial_\alpha \left(m_c^{\mu_3} n_i\right) \\
&\quad - m_a^\beta U_b^{\mu_1} n_k \left(\partial_\beta V_k\right) U_b^{\mu_2} V_j U_c^\alpha V_j \partial_\alpha \left(m_c^{\mu_3} n_i\right)\Big] \xi_{\mu_1}\xi_{\mu_2}\xi_{\mu_3} \\
&= \Big\{V_j^2 U_c^{\mu_1} U_c^{\mu_2} m_a^\beta m_b^{\mu_3} n_i \left[n_k \left(\partial_\beta B_{kb}\right) + \left(\partial_\beta n_k\right) B_{kb}\right] \\
&\quad - V_j^2 m_a^\beta n_k \left(\partial_\beta V_k\right) U_b^{\mu_1} U_b^{\mu_2} \left(U_c^{\mu_3} m_c^\alpha + U_c^\alpha m_c^{\mu_3}\right) \left(\partial_\alpha n_i\right) \\
&\quad - V_j^2 m_a^\beta n_k \left(\partial_\beta V_k\right) \left(U_b^{\mu_1} m_b^\alpha m_c^{\mu_2} - U_b^\alpha U_b^{\mu_1} U_c^{\mu_2} + U_b^{\mu_1} U_b^{\mu_2} U_c^\alpha\right) \left(\partial_\alpha m_c^{\mu_3}\right) n_i \Big\} \xi_{\mu_1}\xi_{\mu_2}\xi_{\mu_3} \\
&= 0.
\end{aligned} \tag{56}$$

Here, we used Eq. (55) and

$$\begin{aligned}
&\mathcal{A}^{\mu}_{2,ab} = m^{\beta}_{a} U^{\mu}_{b} n_k \left(\partial_\beta V_k\right), \qquad \mathcal{B}_{2,ab} = m^{\beta}_{a} n_i \partial_\beta B_{ib}, \qquad \bar{A}^{2,\mu_1\mu_2} = U^{\mu_1}_{a} U^{\mu_2}_{a} V_i V_i, \\
&m^{\mu}_{a} m^{\nu}_{a} = U^{\mu}_{a} U^{\nu}_{a}, \qquad U^{(\mu_1}_{c} m^{\mu_2)}_{c} = 0, \qquad V_k V_j + n_k n_j = V_i^2 \delta_{kj}, \\
&m^{(\mu_1}_{b} m^{\mu_2)}_{c} + U^{(\mu_1}_{b} U^{\mu_2)}_{c} = U^{\mu_1}_{a} U^{\mu_2}_{a} \delta_{bc}, \\
&n_k \left(\partial_\beta V_k\right) V_j B_{jc} = -\left(\partial_\beta n_k\right) V_k V_j B_{jc} = -\left(\partial_\beta n_k\right)\left(V_k V_j + n_k n_j\right) B_{jc} = -V_k^2 \left(\partial_\beta n_j\right) B_{jc}, \\
&n_k \left(\partial_\beta B_{kb}\right) + \left(\partial_\beta n_k\right) B_{kb} = \partial_\beta \left(n_k B_{kb}\right) = 0, \\
&U^{(\mu_1|}_{b} m^{\alpha}_{b} m^{|\mu_2)}_{c} - U^{\alpha}_{b} U^{(\mu_1}_{b} U^{\mu_2)}_{c} + U^{(\mu_1}_{b} U^{\mu_2)}_{b} U^{\alpha}_{c} \\
&\quad = -U^{\alpha}_{b}\left(m^{(\mu_1}_{b} m^{\mu_2)}_{c} + U^{\mu_1}_{b} U^{\mu_2}_{c}\right) + U^{\mu_1}_{b} U^{\mu_2}_{b} U^{\alpha}_{c} = 0.
\end{aligned} \tag{57}$$

Equation (56) is inconsistent with the non-degeneracy condition in Eq. (42), and thus all the U^{μ}_{a} are parallel. Hence, U^{μ}_{a} can be written as $a^{\mu} U_a$.

2.3.2.2 $A^{\mu}_{ia} = V^{\mu}_{i} U_a$

The proof in this case is parallel to that for the case $A^{\mu}_{ia} = V_i U^{\mu}_{a}$ shown above. Defining m_a and n^{μ}_{i} similarly as

$$m_a := \epsilon_{ij} U_a, \qquad n^{\mu}_{i} := \epsilon_{ij} V^{\mu}_{j}, \tag{58}$$

the condition in Eq. (37) becomes

$$n^{\mu}_{i} \left(B_{ia} - V^{\beta}_{i} \partial_\beta U_a\right) m_a = 0 \qquad \text{(for any } \mu\text{)}, \tag{59}$$

where we used

$$n^{\beta}_{i} V^{\mu}_{i} = \epsilon_{ij} V^{\beta}_{j} V^{\mu}_{i} = -V^{\beta}_{i} n^{\mu}_{i}. \tag{60}$$

As we have $A^{\mu}_{ia} = V_i U^{\mu}_{a}$, we show that $V^{\mu}_{i} = a^{\mu} V_i$ by contradiction: we assume that two of the V^{μ}_{i} are not parallel to each other. Then, two of the n^{μ}_{i} are not parallel to each other, which gives the condition

$$\left(B_{ia} - V^{\beta}_{i} \partial_\beta U_a\right) m_a = 0. \tag{61}$$

However, we can show that this is inconsistent with the non-degeneracy condition in Eq. (42). The left-hand side of Eq. (42) is calculated as

$$\begin{aligned}
&\left\{U_c^2 V_k^{\mu_1} V_k^{\mu_2} m_a n_j^\beta \left(\partial_\beta B_{jb}\right) m_b n_i^{\mu_3} - m_a \left[n_j^{\mu_1} B_{jb} + n_j^\beta \partial_\beta \left(V_j^{\mu_1} U_b\right)\right] U_b V_k^{\mu_2} B_{kc} m_c n_i^{\mu_3}\right.\\
&\quad \left. + 2 m_a \left[n_j^{[\alpha|} B_{jb} + n_j^\beta \partial_\beta \left(V_j^{[\alpha|} U_b\right)\right] U_b V_k^{\mu_1} V_k^{|\mu_2]} U_c \partial_\alpha \left(m_c n_i^{\mu_3}\right)\right\} \xi_{\mu_1}\xi_{\mu_2}\xi_{\mu_3}\\
&= \left\{m_a V_k^{\mu_1} V_k^{\mu_2} n_j^\beta \left[\left(\partial_\beta B_{jc}\right) U_b^2 m_c + B_{jb} U_b U_c \partial_\beta m_c + \partial_\beta \left(V_j^\alpha U_b\right) U_b U_c \partial_\alpha m_c\right] n_i^{\mu_3}\right.\\
&\quad \left. - m_a \left[n_j^{\mu_1} B_{jb} + n_j^\beta \partial_\beta \left(V_j^{\mu_1} U_b\right)\right] U_b V_k^{\mu_2} \left(B_{kc} - V_k^\alpha \partial_\alpha U_c\right) m_c n_i^{\mu_3}\right\} \xi_{\mu_1}\xi_{\mu_2}\xi_{\mu_3}\\
&= m_a V_k^{\mu_1} V_k^{\mu_2} n_j^\beta \left[\partial_\beta \left(B_{jc} m_c\right) U_b^2 - B_{jb} m_b m_c \partial_\beta m_c + \partial_\beta \left(V_j^\alpha U_b\right) U_b U_c \partial_\alpha m_c\right] n_i^{\mu_3} \xi_{\mu_1}\xi_{\mu_2}\xi_{\mu_3}\\
&= m_a V_k^{\mu_1} V_k^{\mu_2} n_j^\beta \left\{\partial_\beta \left[V_j^\alpha \left(\partial_\alpha U_c\right) m_c\right] U_b^2 - V_j^\alpha \left(\partial_\alpha U_b\right) m_b m_c \partial_\beta m_c\right.\\
&\quad \left. + \left(\partial_\beta V_j^\alpha\right) U_b^2 U_c \partial_\alpha m_c + V_j^\alpha \left(\partial_\beta U_b\right) U_b U_c \partial_\alpha m_c\right\} n_i^{\mu_3} \xi_{\mu_1}\xi_{\mu_2}\xi_{\mu_3}\\
&= m_a V_k^{\mu_1} V_k^{\mu_2} n_j^\beta \left\{U_b^2 \left[\left(\partial_\beta V_j^\alpha\right) \left(\partial_\alpha U_c\right) m_c + V_j^\alpha \left(\partial_\alpha U_c\right) \partial_\beta m_c + \left(\partial_\beta V_j^\alpha\right) U_c \partial_\alpha m_c\right]\right.\\
&\quad \left. - V_j^\alpha \left(\partial_\alpha U_b\right) \left(U_b U_c + m_b m_c\right) \partial_\beta m_c\right\} n_i^{\mu_3} \xi_{\mu_1}\xi_{\mu_2}\xi_{\mu_3}\\
&= 0,
\end{aligned} \tag{62}$$

where we used Eqs. (60) and (61), and

$$\begin{aligned}
&\mathcal{A}_{2,ab}^\mu = m_a \left[n_i^\mu B_{ib} + n_i^\beta \partial_\beta \left(V_i^\mu U_b\right)\right], \quad \mathcal{B}_{2,ab} = m_a n_i^\beta \partial_\beta B_{ib}, \quad \bar{A}^{2,\mu_1\mu_2} = U_a U_a V_i^{\mu_1} V_i^{\mu_2},\\
&\mathcal{A}_{2,ab}^\mu m_b = 0, \qquad U_c \partial_\alpha m_c = -\left(\partial_\alpha U_c\right) m_c, \qquad V_j^\alpha n_j^\beta \partial_{\alpha\beta} U_c = 0,\\
&U_a U_b + m_a m_b = U_c^2 \delta_{ab}, \qquad n_j^\beta V_j^\alpha \left(\partial_\beta U_b\right) U_b U_c \left(\partial_\alpha m_c\right) = -n_j^\beta V_j^\alpha \left(\partial_\alpha U_b\right) U_b U_c \left(\partial_\beta m_c\right).
\end{aligned} \tag{63}$$

This is inconsistent with the non-degeneracy condition in Eq. (42), and thus all the n_i^μ are parallel. This implies that V_i^μ can be written as

$$V_j^\mu = a^\mu V_i. \tag{64}$$

2.3.3 *Further simplification of Eqs. (37) and (42).* We have shown that, for the invertibility conditions to be satisfied, A_{ia}^μ should be written as

$$A_{ia}^\mu = a^\mu V_i U_a. \tag{65}$$

Without loss of generality, we can normalize V_i and U_a as $V_i V_i = 1 = U_a U_a$. We define unit vectors n_i and m_a that are normal to V_i and U_a respectively as

$$n_i := \epsilon_{ij} V_j, \qquad m_a := \epsilon_{ab} U_b. \tag{66}$$

Since A_{ia}^μ is written with a^μ, V_i, and U_a, the matrices $\bar{A}_{ai}^\mu$, $\tilde{A}_{ai}^\mu$, $\bar{A}^{2,\mu\nu}$, $\mathcal{A}_{2,ab}^\mu$, and $\mathcal{B}_{2,ab}$ are written as

$$\begin{aligned}
&\bar{A}_{ai}^\mu = a^\mu m_a n_i, \qquad \tilde{A}_{ai}^\mu = a^\mu U_a V_i, \qquad \bar{A}^{2,\mu\nu} = a^\mu a^\nu,\\
&\mathcal{A}_{2,ab}^\mu = a^\mu m_a n_i \left[B_{ib} + a^\beta \left(\partial_\beta V_i\right) U_b\right], \qquad \mathcal{B}_{2,ab} = m_a n_i a^\beta \partial_\beta B_{ib}.
\end{aligned} \tag{67}$$

Substituting the above equations into Eq. (37) we have

$$n_i B_{ia} m_a = 0. \tag{68}$$

The non-degeneracy condition in Eq. (42) becomes

$$n_i a^\beta \left(\partial_\beta B_{ia}\right) m_a - n_i B_{ia} U_a V_j B_{jb} m_b - n_i a^\beta \left(\partial_\beta V_i\right) V_j B_{ja} m_a \neq 0. \tag{69}$$

The first term on the left-hand side can be transformed as

$$\begin{aligned} n_i a^\beta \left(\partial_\beta B_{ia}\right) m_a &= -a^\beta \left(\partial_\beta n_i\right) B_{ia} m_a - n_i B_{ia} a^\beta \partial_\beta m_a \\ &= -a^\beta \left(\partial_\beta n_i\right) B_{ia} m_a - n_i B_{ia} U_a U_b a^\beta \partial_\beta m_b \\ &= -a^\beta \left(\partial_\beta n_i\right) B_{ia} m_a + n_i B_{ia} U_a a^\beta \left(\partial_\beta U_b\right) m_b, \end{aligned} \tag{70}$$

where we use the fact that $U_a U_b + m_a m_b = \delta_{ab}$ and Eq. (68). The last term of Eq. (69) can be transformed as

$$-n_i a^\beta \left(\partial_\beta V_i\right) V_j B_{ja} m_a = a^\beta \left(\partial_\beta n_i\right) B_{ia} m_a, \tag{71}$$

where we use the fact that $V_i V_j + n_i n_j = \delta_{ij}$ and Eq. (68). Then, Eq. (69) can be written as

$$n_i B_{ia} U_a \left(V_j B_{jb} - a^\beta \partial_\beta U_b\right) m_b \neq 0. \tag{72}$$

This means that both of

$$n_i B_{ia} U_a \neq 0, \qquad \left(V_j B_{jb} - a^\beta \partial_\beta U_b\right) m_b \neq 0 \tag{73}$$

should be satisfied. As a result, the invertibility conditions in Eqs. (32), (37), and (42) are equivalent to the simplified conditions in Eqs. (50), (68), and (73).

3. Sufficiency of the invertibility conditions

In the previous section we derived the necessary conditions, Eqs. (50), (68), and (73), for invertibility of a field transformation involving two fields and up to their first-order derivatives. In this section we show that these conditions are also sufficient conditions, i.e. Eqs. (50), (68), and (73) are the necessary and sufficient conditions for invertibility in the two-field case. As a preliminary step, in Sect. 3.1 we introduce the notion of "partial invertibility" for a field transformation whose inverse transformation is uniquely determined for part of the variables. Then, we show in Sect. 3.2 with the partial invertibility that Eqs. (50), (68), and (73) are the necessary and sufficient conditions for invertibility.[6]

3.1 *Partial invertibility*

We consider the invertibility of a transformation $\psi_a \to \phi_i$. Suppose that the transformation can be described by

$$F_I(\psi_a, \partial_\mu \psi_a, \partial_\mu \partial_\nu \psi_a, \ldots; \phi_i, \partial_\mu \phi_i, \partial_\mu \partial_\nu \phi_i, \ldots; x^\mu) = 0, \tag{74}$$

where I runs from 1 to a constant $\mathcal{N}$. If $\mathcal{N}$ is equal to the number of all the degrees of freedom in ψ_a, $\partial_\mu \psi_a$, $\partial_\mu \partial_\nu \psi_a$, ...,[7] which is denoted by $\mathcal{N}_\psi$, we can use the implicit function theorem by regarding ψ_a, $\partial_\mu \psi_a$, $\partial_\mu \partial_\nu \psi_a$, ... as independent variables at a point in spacetime. However, we may not need to have $\mathcal{N}_\psi$ equations of the form of Eq. (74) to fix ψ_a uniquely in terms of

[6] See Appendix E for the difference between the standard approach based on the inverse function theorem on functional spaces and our approach based on the implicit function theorem on finite-dimensional subspaces associated with the functional space.

[7] For instance, if F_I depends on up to the second-order derivative of ψ_a, the number of all the degrees of freedom of $(\psi_a, \partial_\mu \psi_a, \partial_\mu \partial_\nu \psi_a)$ is $N + N \times D + N \times D(D+1)/2$, where N and D are the number of ψ_a fields and the dimension of spacetime, respectively.

ϕ_a; indeed, even if we have less than $\mathcal{N}_\psi$ equations, i.e. $\mathcal{N} < \mathcal{N}_\psi$, it may be possible to prove the uniqueness of ψ_a if the equations have a special structure. Once ψ_a is fixed in this manner, its derivatives $\partial_\mu\psi_a$, $\partial_\mu\partial_\nu\psi_a$, ... are uniquely fixed by differentiating ψ_a repeatedly.

To illustrate the procedure explained above, we first discuss a generic case where the equations are for functions of variables x_a, y_b, z_c, and w_d,

$$F_I(x_a, y_b, z_c; w_d) = 0, \tag{75}$$

where x_a corresponds to ψ_a, while y_b and z_c correspond to some combinations of the derivatives $\partial_\mu\psi_a$, $\partial_\mu\partial_\nu\psi_a$, ...[8] The difference between y_b and z_c is explained later. w_d corresponds to the other variables ϕ_i and their derivatives $\partial_\mu\phi_i$, $\partial_\mu\partial_\nu\phi_i$, ... If the number of equations is the same as the sum of those of x_a, y_b, and z_c, we can use the implicit function theorem for them, i.e. x_a, y_b, and z_c can be fixed uniquely in terms of w_d, provided that the conditions for the implicit function theorem are satisfied. However, even if the number of equations is less than the sum of those of x_a, y_b, and z_c, it may be possible to fix x_a in terms w_d uniquely if Eq. (75) have a certain structure, as explained below. Some of y_b and z_c may not be fixed uniquely in this process, but the uniqueness of x_a can be shown independently.

The variables x_a are fixed by stepwise application of the inverse function theorem provided that the function F_I has a structure given by Eq. (77), which will be introduced shortly. Suppose that we have $N + M$ equations of the form of Eq. (75), i.e. I runs from 1 to $N + M(= \mathcal{N})$, where N denotes the number of the fields x_a and M is a positive integer. The variation of Eq. (75) is

$$\begin{aligned}\delta F_I(x_a, y_b, z_c; w_d) = {}& \frac{\partial F_I}{\partial x_a}(x_a, y_b, z_c; w_d)\delta x_a + \frac{\partial F_I}{\partial y_b}(x_a, y_b, z_c; w_d)\delta y_b \\ & + \frac{\partial F_I}{\partial z_c}(x_a, y_b, z_c; w_d)\delta z_c + \frac{\partial F_I}{\partial w_d}(x_a, y_b, z_c; w_d)\delta w_d.\end{aligned} \tag{76}$$

Here, we assume that δy_b and δz_c appear only as M independent combinations in any δF_I, i.e. δF_I is expressed as

$$\begin{aligned}\delta F_I(x_a, y_b, z_c; w_d) = {}& \frac{\partial F_I}{\partial x_a}(x_a, y_b, z_c; w_d)\delta x_a + \frac{\partial F_I}{\partial w_d}(x_a, y_b, z_c; w_d)\delta w_d \\ & + \sum_{b=1}^{M} B_{Ib}(x_a, y_b, z_c; w_d)\big(\delta y_b + \tilde{B}_{bc}(x_a, y_b, z_c; w_d)\delta z_c\big).\end{aligned} \tag{77}$$

Without loss of generality, the principal components of M independent combinations are set to be y_b, which means that the rank of B_{Ib} is M. This makes the difference between y_b and z_c. It also fixes the number of y_b to be M. Then, picking up M equations from the F_I such that y_b is fixed uniquely, we use the implicit function theorem to fix only y_b. Without loss of generality, we assume that these equations are given by F_I with $N + 1 \leq I \leq N + M$; that is, the square matrix B_{Ib} with $I = N + 1, \ldots, N + M$ and $b = 1, \ldots, M$ is regular. Since the numbers of these equations and of y_b are the same, we can apply the implicit function theorem for y_b, and then y_b is uniquely expressed in terms of x_a, z_c, and w_d.

[8]For our purpose of proving the invertibility for the two-field case with first-order derivatives given by Eq. (5), x_a corresponds to ψ_a, y_b is a component of $\partial_\mu\psi_a$, and the z_c correspond to the other components of the derivative $\partial_\mu\psi_a$ and $\partial_\mu\partial_\nu\psi_a$.

Now, the y_b are uniquely written as functions of x_a, z_c, and w_d. Substituting $y_b(x_a, z_c, w_d)$ into Eq. (75) for $N+1 \le I \le N+M$, the derivative of Eq. (75) with respect to z_c is given by

$$\sum_{b=1}^{M} B_{Ib}(x_a, y_b, z_c; w_d)\left(\frac{\partial y_b}{\partial z_c} + \tilde{B}_{bc}\right) = 0. \tag{78}$$

Since B_{Ib} is assumed to be regular, this equation implies that

$$\frac{\partial y_b}{\partial z_c} + \tilde{B}_{bc} = 0. \tag{79}$$

This equation fixes the z_c dependence of $y_b(x_a, z_c, w_d)$. Now the remaining equations can be written purely in terms of x_a, z_c, and w_d as

$$F_I\big(x_a, y_b(x_a, z_c, w_d), z_c; w_d\big) = 0, \tag{80}$$

where I runs from 1 to N. Their variation is given by

$$\delta F_I\big(x_a, y_b(x_a, z_c, w_d), z_c; w_d\big) = \Bigg[\frac{\partial F_I}{\partial x_a}(x_a, y_b, z_c; w_d)\delta x_a + \frac{\partial F_I}{\partial w_d}(x_a, y_b, z_c; w_d)\delta w_d + \sum_{b=1}^{M} B_{Ib}(x_a, y_b, z_c; w_d)\left(\frac{\partial y_b}{\partial x_a}\delta x_a + \frac{\partial y_b}{\partial w_d}\delta w_d\right)\Bigg]_{y_b = y_b(x_a, z_c, w_d)} \tag{81}$$

The δz_c term is canceled here because of Eq. (79). This implies that the F_I for $I = 1, \ldots, N$ are independent of z_c, i.e. they are functions of only x_a and w_d. Since the number of equations is the same as that of x_a, we can use the implicit function theorem; if

$$\det\left[\frac{\partial F_I}{\partial x_a}(x_a, y_b, z_c; w_d) + \sum_{b=1}^{M} B_{Ib}(x_a, y_b, z_c; w_d)\frac{\partial y_b}{\partial x_a}\right]_{y_b = y_b(x_a, z_c, w_d)} \neq 0 \tag{82}$$

is satisfied, x_a has a unique solution locally and it is written in terms of only w_d.

In the next section we will see that the transformation in Eq. (5) in the two-field case behaves as Eq. (77) once the invertibility conditions in Eqs. (50), (68), and (73) are imposed, and then ψ_i is fixed in terms of ϕ_a uniquely as a consequence.

3.2 *Sufficient conditions for the invertibility of our transformation*

The transformation in Eq. (5) can be rewritten in terms of a function of ψ_a, $\partial_\mu \psi_a$, and ϕ_i as

$$F_i(\psi_a, \partial_\mu \psi_a; \phi_i; x^\mu) := \bar{\phi}_i(\psi_a, \partial_\mu \psi_a; x^\mu) - \phi_i = 0. \tag{83}$$

We analyze this equation in the two-field case imposing the necessary conditions for invertibility, Eqs. (50), (68), and (73). Operating $n_i \partial_\mu$ on Eq. (83), we have

$$G_\mu(\psi_a, \partial_\mu \psi_a; \phi_i, \partial_\mu \phi_i; x^\mu) := n_i \partial_\mu F_i = n_i B_{ib} U_b U_a \partial_\mu \psi_a - n_i C_{i\mu} - n_i \partial_\mu \phi_i = 0, \tag{84}$$

where B_{ib}, n_i, and U_a are defined in Sect. 2.3 and $C_{i\mu} := \partial \bar{\phi}_i / \partial x^\mu$. The variation of F_i becomes

$$n_i \delta F_i = (n_i B_{ib} U_b) U_a \delta \psi_a, \tag{85}$$

$$V_i \delta F_i = (V_i B_{ib} U_b) U_a \delta \psi_a + (V_i B_{ib} m_b) m_a \delta \psi_a + a^\mu U_a \delta(\partial_\mu \psi_a), \tag{86}$$

where we omit the variation with respect to ϕ_i because it is irrelevant to the condition for the implicit function theorem.

Now let us evaluate the variation of $a^\mu G_\mu$, which is given as

$$\begin{aligned}
\delta\left(a^\mu G_\mu\right) &= a^\mu n_i \delta\left(\partial_\mu F_i\right) = n_i \delta\left(\partial_\mu \bar{\phi}_i\right) \\
&= a^\mu n_i \delta\left(\frac{\partial \bar{\phi}_i}{\partial\left(\partial_\alpha \psi_a\right)} \partial_\mu \partial_\alpha \psi_a + \frac{\partial \bar{\phi}_i}{\partial \psi_a} \partial_\mu \psi_a + \frac{\partial \bar{\phi}_i}{\partial x^\mu}\right) \\
&= a^\mu n_i \Bigg[\left(\frac{\partial^2 \bar{\phi}_i}{\partial\left(\partial_\alpha \psi_a\right) \partial\left(\partial_\beta \psi_b\right)} \partial_\mu \partial_\alpha \psi_a + \frac{\partial^2 \bar{\phi}_i}{\partial \psi_a \partial\left(\partial_\beta \psi_b\right)} \partial_\mu \psi_a + \frac{\partial^2 \bar{\phi}_i}{\partial x^\mu \partial\left(\partial_\beta \psi_b\right)}\right) \delta\left(\partial_\beta \psi_b\right) \\
&\qquad + \left(\frac{\partial^2 \bar{\phi}_i}{\partial\left(\partial_\alpha \psi_a\right) \partial \psi_b} \partial_\mu \partial_\alpha \psi_a + \frac{\partial^2 \bar{\phi}_i}{\partial \psi_a \partial \psi_b} \partial_\mu \psi_a + \frac{\partial^2 \bar{\phi}_i}{\partial x^\mu \partial \psi_b}\right) \delta \psi_b + B_{ia} \delta\left(\partial_\mu \psi_a\right)\Bigg] \\
&= a^\mu n_i (\partial_\mu B_{ib}) U_b U_a \delta \psi_a + a^\mu n_i (\partial_\mu B_{ib}) m_b m_a \delta \psi_a \\
&\qquad + n_i (a^\mu \partial_\mu V_i + B_{ib} U_b) a^\nu U_a \delta(\partial_\nu \psi_a),
\end{aligned} \tag{87}$$

where we used $\partial_\mu F_i = 0$ at the first equality, and some formulae from Sect. 2.3.3 such as the degeneracy conditions $n_i \frac{\partial \bar{\phi}_i}{\partial(\partial_\alpha \psi_a)} = n_i A^\alpha_{ia} = 0$ and $n_i B_{ia} m_a = 0$ at the fourth equality. The key point is that, in Eqs. (85), (86), and (87), $\delta(\partial_\mu \psi_a)$ appears only in a linear combination $a^\mu U_a \delta(\partial_\mu \psi_a)$. The last term proportional to $a^\mu U_a \delta(\partial_\mu \psi_a)$ in Eq. (87) corresponds to the last line of Eq. (77) for $M = 1$. This allows us to use the result of Sect. 3.1 by regarding ψ_a, $\partial_\mu \psi_a$, and $\partial_\mu \partial_\nu \psi_a$ as independent variables and also identifying x_a, y_b, and z_c as ψ_a, a component of $\partial_\mu \psi_a$, and the other components of $(\partial_\mu \psi_a, \partial_\mu \partial_\nu \psi_a)$, respectively. Then, the condition for invertibility is

$$\begin{aligned}
0 &\neq \det \left(\begin{array}{cc|c}
V_i \dfrac{\partial F_i}{\partial \psi_a} U_a & V_i \dfrac{\partial F_i}{\partial \psi_a} m_a & V_i \dfrac{\partial F_i}{\partial\left(\partial_\nu \psi_a\right)} U_a \\
n_i \dfrac{\partial F_i}{\partial \psi_a} U_a & n_i \dfrac{\partial F_i}{\partial \psi_a} m_a & n_i \dfrac{\partial F_i}{\partial\left(\partial_\nu \psi_a\right)} U_a \\
\hline
\dfrac{\partial\left(a^\mu G_\mu\right)}{\partial \psi_a} U_a & \dfrac{\partial\left(a^\mu G_\mu\right)}{\partial \psi_a} m_a & \dfrac{\partial\left(a^\mu G_\mu\right)}{\partial\left(\partial_\nu \psi_a\right)} U_a
\end{array}\right) \\
&= \det \left(\begin{array}{cc|c}
V_i B_{ia} U_a & V_i B_{ia} m_a & a^\nu \\
n_i B_{ia} U_a & 0 & 0 \\
\hline
a^\mu n_i\left(\partial_\mu B_{ia}\right) U_a & a^\mu n_i\left(\partial_\mu B_{ia}\right) m_a & n_i\left(a^\mu \partial_\mu V_i + B_{ia} U_a\right) a^\nu
\end{array}\right) \\
&= -a^\nu (n_i B_{ia} U_a)^2 (V_j B_{jb} - a^\mu \partial_\mu U_b) m_b,
\end{aligned} \tag{88}$$

where the components of the matrix are expressed with respect to the bases (V_i, n_i) and (U_a, m_a), and also the degenerate row and column whose components are completely zero are removed. Equation (88) is satisfied if $n_i B_{ia} U_a \neq 0$ and $(V_j B_{jb} - a^\mu \partial_\mu U_b) m_b \neq 0$. Therefore, the necessary conditions for invertibility, Eqs. (50), (68), and (73), are also sufficient conditions.

4. Examples of invertible transformations

Invertibility conditions for transformations $\phi_i = \phi_i(\psi_a, \partial \psi_a)$ have been established in the previous sections. In this section we propose some non-trivial examples of field transformations that satisfy the invertibility conditions. In principle, the most general invertible transformation could be constructed by finding the general solution of the invertibility conditions. Unfortunately this is not an easy task,[9] so we proceed by introducing the following field transformation ansatze:

(i) $\phi_i = b\left(\psi_a, Y_\mu\right) V_i(\psi_a) + \tilde{V}_i(\psi_a) \qquad \left(Y_\mu \equiv U_a(\psi_a) \partial_\mu \psi_a\right);$

[9] See Ref. [1] for a previous attempt at constructing examples of invertible transformations.

(ii) $\phi_i = b\,(\psi_a, Y_a)\, V_i(\psi_a) + \tilde{V}_i(\psi_a)$ $\quad\big(Y_a \equiv \tilde{a}^\mu(\psi_a)\partial_\mu\psi_a\big)$;
(iii) $\phi_i = \phi_i\,(\psi_a, Y)$ $\quad\big(Y \equiv \tilde{a}^\mu(\psi_a)U_a(\psi_a)\partial_\mu\psi_a\big)$.

These ansatze are chosen so that the first degeneracy condition, Eq. (50), among the invertibility conditions is automatically satisfied. The second degeneracy condition, Eq. (68), and the non-degeneracy conditions, Eq. (73), are then used to constrain the form of the transformations. Although these transformations may not span the most general transformation satisfying the invertibility conditions, they give a good starting point for investigating the most general invertible field transformation.

In the derivation below, we use the fact that the vector U_a can be set to a constant vector (0,1) if it depends only on ψ_a. We explain this method in Appendix F.

4.1 *Ansatz 1:* $\phi_i = b\left(\psi_a, U_a(\psi_a)\partial_\mu\psi_a\right) V_i(\psi_a) + \tilde{V}_i(\psi_a)$

We first consider the following ansatz for a field transformation:

$$\phi_i = b\left(\psi_a, Y_\mu\right) V_i(\psi_a) + \tilde{V}_i(\psi_a) \qquad \left(Y_\mu \equiv U_a(\psi_a)\partial_\mu\psi_a\right), \tag{89}$$

where V_i is normalized as $V_iV_i = 1$. In this transformation, U_a can be set to $U_a = (0, 1)$ without loss of generality. It then follows that

$$U_a = (0, 1), \qquad m_a = (1, 0), \qquad n_i = \epsilon_{ij}V_j. \tag{90}$$

For Eq. (89), the first degeneracy condition, Eq. (50), is given by

$$A^\mu_{ia} = \frac{\partial\phi_i}{\partial\left(\partial_\mu\psi_a\right)} = \frac{\partial b}{\partial Y_\mu}U_aV_i \equiv a^\mu U_aV_i. \tag{91}$$

The second degeneracy condition, Eq. (68), is evaluated as follows:

$$B_{ia} = \frac{\partial\phi_i}{\partial\psi_a} = \frac{\partial b}{\partial\psi_a}V_i + b\frac{\partial V_i}{\partial\psi_a} + \frac{\partial\tilde{V}_i}{\partial\psi_a}, \tag{92}$$

$$n_iB_{ia}m_a = b\left(\psi_a, Y_\mu\right) n_i\frac{\partial V_i}{\partial\psi_1} + n_i\frac{\partial\tilde{V}_i}{\partial\psi_1}. \tag{93}$$

In Eq. (93), only b depends on Y_μ while the other terms depend only on ψ_a. Because Eq. (93) should be satisfied identically for any ψ_a and Y_μ, it implies that

$$b\,n_i\frac{\partial V_i}{\partial\psi_1} = 0, \tag{94}$$

$$n_i\frac{\partial\tilde{V}_i}{\partial\psi_1} = 0. \tag{95}$$

Equation (94) implies either $n_i\frac{\partial V_i}{\partial\psi_1} = 0$ or $b = 0$. $n_i\frac{\partial V_i}{\partial\psi_1} = 0$ implies $V_i = V_i(\psi_2)$ thanks to the normalization $V_iV_i = 1$, while $b = 0$ gives a transformation without derivatives, $\phi_i = \phi_i(\psi_a)$. Below, we focus on the case $n_i\frac{\partial V_i}{\partial\psi_1} = 0$, in which the transformation depends on derivatives $\phi_i = \phi_i(\psi_a, \partial\psi_a)$. In this case, Eq. (95) implies that $\partial\tilde{V}_i/\partial\psi_1$ is parallel to V_i, i.e.

$$\frac{\partial\tilde{V}_i}{\partial\psi_1} = \tilde{c}(\psi_a)V_i(\psi_2) \quad\Rightarrow\quad \tilde{V}_i = c(\psi_a)V_i(\psi_2) + \hat{V}_i(\psi_2) \tag{96}$$

for some functions $\tilde{c}(\psi_a)$, $c(\psi_1) = \int\tilde{c}(\psi_a)d\psi_1$, and $\hat{V}_i(\psi_2)$. The $c\,V_i$ term can be absorbed into the $b\,V_i$ term in the ansatz of Eq. (89), and the remainder $\hat{V}_i(\psi_2)$ depends only on ψ_2. This implies that, once Eq. (90) is imposed, we may set $\tilde{V}_i = \tilde{V}_i(\psi_2)$ in the ansatz of Eq. (89) without loss of generality by absorbing the $c\,V_i$ term. Below we continue the derivation under this assumption.

The non-degeneracy conditions, Eq. (73), are given by

$$0 \neq n_i B_{ia} U_a = b\, n_i \frac{\partial V_i}{\partial \psi_2} + n_i \frac{\partial \tilde{V}_i}{\partial \psi_2}, \tag{97}$$

$$0 \neq \left(V_i B_{ia} - a^\mu \partial_\mu U_a\right) m_a = \left(\frac{\partial b}{\partial \psi_a} + \frac{\partial b}{\partial Y_\mu}\partial_\mu \psi_b \frac{\partial U_b}{\partial \psi_a} + V_i \frac{\partial \tilde{V}_i}{\partial \psi_a} - a^\mu \partial_\mu U_a\right) m_a = \frac{\partial b}{\partial \psi_1}, \tag{98}$$

which can be regarded as constraints on b, V_i, and $\tilde{V}_i$.

To summarize, a transformation given by

$$\phi_i = b\left(\psi_a, Y_\mu\right) V_i(\psi_2) + \tilde{V}_i(\psi_2) \qquad \left(Y_\mu \equiv \partial_\mu \psi_2\right) \tag{99}$$

is invertible if Eqs. (97) and (98) are satisfied. One may further apply an invertible transformation $\psi_a = \psi_a(\tilde{\psi}_b)$ such that $\det(\partial \psi_a / \partial \tilde{\psi}_b) \neq 0$ on Eq. (99) to reintroduce non-trivial $U_a(\tilde{\psi}_a)$ and construct a transformation of the form of Eq. (89).

4.2 *Ansatz 2:* $\phi_i = b\left(\psi_a, \tilde{a}^\mu(\psi_a)\partial_\mu \psi_a\right) V_i(\psi_a) + \tilde{V}_i(\psi_a)$

The next ansatz is given by

$$\phi_i = b\left(\psi_a, Y_a\right) V_i(\psi_a) + \tilde{V}_i(\psi_a) \qquad \left(Y_a \equiv \tilde{a}^\mu(\psi_a)\partial_\mu \psi_a\right). \tag{100}$$

The first degeneracy condition, Eq. (50), is automatically satisfied for this ansatz:

$$A^\mu_{ia} = \tilde{a}^\mu \frac{\partial b}{\partial Y_a} V_i \equiv a^\mu(\psi_a, Y_a) U_a(\psi_a, Y_a) V_i(\psi_a). \tag{101}$$

The second degeneracy condition, Eq. (68), is given as

$$B_{ia} = \frac{\partial b}{\partial \psi_a} V_i + b \frac{\partial V_i}{\partial \psi_a} + \frac{\partial \tilde{V}_i}{\partial \psi_a}, \tag{102}$$

$$\therefore \quad n_i B_{ia} m_a = n_i \left(b \frac{\partial V_i}{\partial \psi_a} + \frac{\partial \tilde{V}_i}{\partial \psi_a}\right) m_a \propto n_i \left(b \frac{\partial V_i}{\partial \psi_a} + \frac{\partial \tilde{V}_i}{\partial \psi_a}\right) \epsilon_{ab} \frac{\partial b}{\partial Y_b} = 0. \tag{103}$$

Equation (103) is equivalent to

$$\frac{n_i \left(b \frac{\partial V_i}{\partial \psi_1} + \frac{\partial \tilde{V}_i}{\partial \psi_1}\right)}{n_i \left(b \frac{\partial V_i}{\partial \psi_2} + \frac{\partial \tilde{V}_i}{\partial \psi_2}\right)} = \frac{\frac{\partial b}{\partial Y_1}}{\frac{\partial b}{\partial Y_2}} \equiv -c\left(\psi_a, Y_a\right) \tag{104}$$

$$\Longleftrightarrow n_i \left(b \frac{\partial V_i}{\partial \psi_1} + \frac{\partial \tilde{V}_i}{\partial \psi_1}\right) + c\left(\psi_a, Y_a\right) n_i \left(b \frac{\partial V_i}{\partial \psi_2} + \frac{\partial \tilde{V}_i}{\partial \psi_2}\right) = 0,$$

$$\frac{\partial b}{\partial Y_1} + c(\psi_a, Y_a) \frac{\partial b}{\partial Y_2} = 0. \tag{105}$$

Equation (105) may be solved for $\tilde{V}_i(\psi_a)$ and $b(\psi_a, Y_a)$ once $V_i(\psi_a)$ and $c(\psi_a, Y_a)$ are freely specified, and each solution gives an invertible transformation as long as it satisfies the non-degeneracy conditions of Eq. (73).

In a special case where the function $c(\psi_a, Y_a)$ depends only on ψ_a but not on Y_a, one can construct invertible transformations more explicitly as follows. When $c = c(\psi_a)$, we may apply an invertible transformation $\psi_a = \psi_a(\tilde{\psi}_a)$ on Eq. (105) to eliminate $c(\psi_a)$; that is, Eq. (105)

transforms under $\psi_a = \psi_a(\tilde{\psi}_a)$ as

$$0 = \frac{\partial\tilde{\psi}_a}{\partial\psi_1} n_i \left(b\frac{\partial V_i}{\partial\tilde{\psi}_a} + \frac{\partial\tilde{V}_i}{\partial\tilde{\psi}_a} \right) + c(\psi_a) n_i \frac{\partial\tilde{\psi}_a}{\partial\psi_2}(\psi_a, Y_a) \left(b\frac{\partial V_i}{\partial\tilde{\psi}_a} + \frac{\partial\tilde{V}_i}{\partial\tilde{\psi}_a} \right)$$
$$= \left(\frac{\partial\tilde{\psi}_1}{\partial\psi_1} + c(\psi_a)\frac{\partial\tilde{\psi}_1}{\partial\psi_2} \right) n_i \left(b\frac{\partial V_i}{\partial\tilde{\psi}_1} + \frac{\partial\tilde{V}_i}{\partial\tilde{\psi}_1} \right) + \left(\frac{\partial\tilde{\psi}_2}{\partial\psi_1} + c(\psi_a)\frac{\partial\tilde{\psi}_2}{\partial\psi_2} \right) n_i \left(b\frac{\partial V_i}{\partial\tilde{\psi}_2} + \frac{\partial\tilde{V}_i}{\partial\tilde{\psi}_2} \right), \tag{106}$$

and then the function $\tilde{\psi}_a = \tilde{\psi}_a(\psi_a)$ may be chosen (at least locally) so that

$$\frac{\partial\tilde{\psi}_2}{\partial\psi_1} + c(\psi_a)\frac{\partial\tilde{\psi}_2}{\partial\psi_2} = 0, \tag{107}$$

with which Eq. (106) reduces to

$$n_i \left(b\frac{\partial V_i}{\partial\tilde{\psi}_1} + \frac{\partial\tilde{V}_i}{\partial\tilde{\psi}_1} \right) = 0. \tag{108}$$

This is equivalent to setting $c(\psi_a) = 0$ in Eq. (105) by means of a transformation in ψ_a space.

When $c(\psi_a) = 0$, Eq. (104) implies that

$$n_i(\psi_a) \left(b(\psi_a, Y_a)\frac{\partial V_i(\psi_a)}{\partial\psi_1} + \frac{\partial\tilde{V}_i(\psi_a)}{\partial\psi_1} \right) = 0, \qquad \frac{\partial b}{\partial Y_1} = 0. \tag{109}$$

The second equation implies that $b = b(\psi_a, Y_2)$, which gives $U_a = (0, 1)$ and $m_a = (1, 0)$. In the first equation, the first term involving $b(\psi_a, Y_2)$ depends on Y_2 while the second term is independent of Y_a; it then follows that

$$b(\psi_a, Y_2) n_i(\psi_a)\frac{\partial V_i(\psi_a)}{\partial\psi_1} = 0, \tag{110}$$

$$n_i(\psi_a)\frac{\partial\tilde{V}_i(\psi_a)}{\partial\psi_1} = 0. \tag{111}$$

Equation (110) implies either $V_i = V_i(\psi_2)$ or $b = 0$, for the latter of which the transformation in Eq. (100) does not involve $\partial\psi_a$. Below, we focus on the former case, which gives a transformation with derivatives. In this case we can show that $\tilde{V}_i = f(\psi_a)V_i(\psi_2) + \hat{V}_i(\psi_2)$ for some function $f(\psi_a)$ and $\hat{V}_i(\psi_2)$ using Eq. (111) as we did around Eq. (96) for the previous ansatz. Then, setting $U_a = (0, 1)$, by absorbing the $c\,V_i$ term into the $b\,V_i$ term we may set $\tilde{V}_i = \tilde{V}_i(\psi_2)$ without loss of generality.

To summarize the results above, a transformation

$$\phi_i = b(\psi_a, Y_2)V_i(\psi_2) + \tilde{V}_i(\psi_2) \qquad \left(Y_a \equiv \tilde{a}^\mu(\psi_a)\partial_\mu\psi_a \right) \tag{112}$$

may be invertible if Eq. (111) is satisfied. Adding to that, the non-degeneracy conditions in Eq. (73) must be satisfied for invertibility, and also an invertible transformation $\psi_a = \psi_a(\tilde{\psi}_b)$ may be applied to construct a transformation with non-trivial $U_a(\psi_a)$. Actually, this transformation is a special case of the transformation in Eq. (99) examined in the previous section, although we have started from a different ansatz. This result follows from the assumption $c = c(\psi_a)$ imposed at Eq. (106), and more general transformations are obtained if we solve Eq. (105) for $c = c(\psi_a, Y_a)$.

4.3 *Ansatz 3:* $\phi_i = \phi_i\left(\psi_a, \tilde{a}^\mu(\psi_a)U_a(\psi_a)\partial_\mu\psi_a\right)$

The third ansatz we consider is

$$\phi_i = \phi_i(\psi_a, Y) \qquad \left(Y \equiv \tilde{a}^\mu(\psi_a)U_a(\psi_a)\partial_\mu\psi_a \right), \tag{113}$$

for which the first degeneracy condition, Eq. (50), is satisfied automatically as

$$A^{\mu}_{ia} = \tilde{a}^{\mu}(\psi_a)U_a(\psi_a)\frac{\partial\phi_i}{\partial Y}(\psi_a, Y) \equiv a^{\mu}(\psi_a, Y)U_a(\psi_a)V_i(\psi_a, Y). \tag{114}$$

In this expression, V_i is normalized as $V_iV_i = 1$, i.e.

$$V_i \equiv \frac{1}{v(\psi_a, Y)}\frac{\partial\phi_i}{\partial Y}(\psi_a, Y), \qquad a^{\mu}(\psi_a, Y) \equiv v(\psi_a, Y)\tilde{a}^{\mu}(\psi_a), \qquad V_iV_i = 1, \tag{115}$$

where $v(\psi_a, Y)$ is a normalization factor. For simplicity, we assume $v \neq 0$ in the following.

Following the procedure explained in Appendix F, we set $U_a = (0, 1)$ and $m_a = (1, 0)$ without loss of generality. Then, using $n_i = v^{-1}\epsilon_{ij}\partial\phi_j/\partial Y$, the second degeneracy condition, Eq. (68), is evaluated as

$$B_{ia} = \frac{\partial\phi_i}{\partial\psi_a} + \frac{\partial\phi_i}{\partial Y}\frac{\partial\tilde{a}^{\mu}}{\partial\psi_a}\partial_{\mu}\psi_2 = \frac{\partial\phi_i}{\partial\psi_a} + v\,V_i\frac{\partial\tilde{a}^{\mu}}{\partial\psi_a}\partial_{\mu}\psi_2, \tag{116}$$

$$n_iB_{ia}m_a = v^{-1}\epsilon_{ij}\frac{\partial\phi_i}{\partial\psi_1}\frac{\partial\phi_j}{\partial Y} = 0. \tag{117}$$

Equation (117) implies that, provided $v \neq 0$,

$$\frac{\frac{\partial\phi_1}{\partial\psi_1}}{\frac{\partial\phi_1}{\partial Y}} = \frac{\frac{\partial\phi_2}{\partial\psi_1}}{\frac{\partial\phi_2}{\partial Y}}; \tag{118}$$

that is, the gradient vectors $\left(\frac{\partial\phi_1}{\partial\psi_1}, \frac{\partial\phi_1}{\partial Y}\right)$ and $\left(\frac{\partial\phi_2}{\partial\psi_1}, \frac{\partial\phi_2}{\partial Y}\right)$ are parallel to each other in the (ψ_1, Y) space. It then follows that

$$\phi_2 = F\left(\psi_2, \phi_1(\psi_a, Y)\right), \tag{119}$$

where $F(\psi_2, \phi_1)$ is an arbitrary function of ϕ_1 and ψ_2.[10]

Let us examine the non-degeneracy conditions of Eq. (73). One of them is given by

$$\begin{aligned} 0 \neq n_iB_{ia}U_a = n_iB_{i2} &= v^{-1}\epsilon_{ij}\frac{\partial\phi_i}{\partial\psi_2}\frac{\partial\phi_j}{\partial Y} = v^{-1}\left(\frac{\partial\phi_1}{\partial\psi_2}\frac{\partial\phi_2}{\partial Y} - \frac{\partial\phi_2}{\partial\psi_2}\frac{\partial\phi_1}{\partial Y}\right) \\ &= v^{-1}\left[\frac{\partial\phi_1}{\partial\psi_2}\frac{\partial F}{\partial\phi_1}\frac{\partial\phi_1}{\partial Y} - \left(\frac{\partial F}{\partial\psi_2} + \frac{\partial F}{\partial\phi_1}\frac{\partial\phi_1}{\partial\phi_2}\right)\frac{\partial\phi_1}{\partial Y}\right] = -v^{-1}\frac{\partial F}{\partial\phi_1}\frac{\partial\phi_1}{\partial Y}. \end{aligned} \tag{120}$$

This equation implies that v, $\partial F/\partial\phi_1$, and $\partial\phi_1/\partial Y$ must not vanish. The other non-degeneracy condition is given by

$$0 \neq \left(V_iB_{ia} - a^{\mu}\partial_{\mu}U_a\right)m_a = V_i\left(\tfrac{\partial\phi_i}{\partial\psi_1} + v\,V_i\tfrac{\partial\tilde{a}^{\mu}}{\partial\psi_1}\partial_{\mu}\psi_2\right) = V_i\tfrac{\partial\phi_i}{\partial\psi_1} + v\tfrac{\partial\tilde{a}^{\mu}}{\partial\psi_1}\partial_{\mu}\psi_2. \tag{121}$$

To summarize, a transformation as in Eq. (113) is invertible if ϕ_2 is given by Eq. (119) and Eqs. (120) and (121) are satisfied.

5. No-go for disformal transformation of the metric with higher derivatives

Here we apply our approach to disformal metric transformation. The disformal transformations involving only one derivative of the scalar field χ,

$$\tilde{g}_{\mu\nu} = C(\chi, X)g_{\mu\nu} + D(\chi, X)\nabla_{\mu}\chi\nabla_{\nu}\chi, \tag{122}$$

where $X = \partial_{\mu}\chi\partial^{\mu}\chi$, are invertible, provided that $C\left(C - \frac{dC}{dX}X - \frac{dD}{dX}X^2\right) \neq 0$; see, e.g., Refs. [7,8]. This follows from the fact that from the above expression one can straightforwardly express the metric $g_{\mu\nu}$ in terms of $\tilde{g}_{\mu\nu}$, χ, and $\nabla_{\mu}\chi$. Thus, the transformation in Eq. (122) is a one-to-one

[10] When the (ψ_1, Y) space is separated into connected sets by borders on which the gradient vector $\left(\frac{\partial\phi_1}{\partial\psi_1}, \frac{\partial\phi_1}{\partial Y}\right)$ vanishes, the function form of $F(\psi_2, \phi_1(\psi_a, Y))$ may be different on each connected set on the (ψ_1, Y) space. The non-degeneracy conditions, however, imply that $\partial\phi_1/\partial Y \neq 0$, and this guarantees that $F(\psi_2, \phi_1)$ is given uniquely on the entire (ψ_1, Y) space.

change of variables $(\chi, g_{\mu\nu}) \leftrightarrow (\chi, \tilde{g}_{\mu\nu})$ as long as the above condition is satisfied. It is useful to check that the transformation in Eq. (122) is invertible by applying our method. Although the method we developed above does not apply to metric transformations in general because a metric is a tensor and has more than two components (except in a one-dimensional spacetime), we can use it when applied to particular ansatze that contain scalar functions only. Indeed, let us restrict ourselves to the case of the homogeneous cosmology,

$$g_{\mu\nu}dx^\mu dx^\nu = -\mathfrak{n}(t)dt^2 + \mathfrak{a}(t)d\mathbf{x}^2, \qquad \chi = \chi(t), \tag{123}$$

where $\mathfrak{a}(t)$ is the square of the scale factor and $\mathfrak{n}(t)$ is the square of the lapse function. Note that we keep $\mathfrak{n}(t)$ in the ansatz of Eq. (123), since it changes under the transformation in Eq. (122). For Eq. (123) we obtain, under the disformal transformation in Eq. (122),

$$\tilde{\mathfrak{n}} = C\mathfrak{n} - D\dot{\chi}^2, \qquad \tilde{\mathfrak{a}} = C\mathfrak{a}, \tag{124}$$

where a dot denotes a t derivative, and

$$C = C(\chi, X) = C\left(\chi(t), -\frac{\dot{\chi}^2(t)}{\mathfrak{n}(t)}\right), \qquad D = D\left(\chi(t), -\frac{\dot{\chi}^2(t)}{\mathfrak{n}(t)}\right). \tag{125}$$

Note that the above transformation can be considered as the change of variables $\{\mathfrak{n}, \mathfrak{a} \to \tilde{\mathfrak{n}}, \tilde{\mathfrak{a}}\}$ (with the time-dependent external function $\chi(t)$), which does not involve derivatives. Therefore, by virtue of the standard theorem on invertibility, the transformation in Eq. (124) is invertible if $\det B_{ia} \neq 0$, where B_{ia} is given by

$$B_{ia} = \begin{pmatrix} C - XC_X - X^2 D_X & 0 \\ -\frac{\mathfrak{a}}{\mathfrak{n}} XC_X & C \end{pmatrix}, \tag{126}$$

so that we obtain $C\big(C - \frac{dC}{dX}X - \frac{dD}{dX}X^2\big) \neq 0$, which reproduces the result we cited above.

On the other hand, one can consider a more general disformal transformation by including two derivatives of the scalar as follows:

$$\tilde{g}_{\mu\nu} = C(\chi, X)g_{\mu\nu} + D(\chi, X)\nabla_\mu\chi\nabla_\nu\chi + E(\chi, X)\nabla_\mu\nabla_\nu\chi. \tag{127}$$

For the above transformation one cannot directly express $g_{\mu\nu}$ in terms of $\tilde{g}_{\mu\nu}$, since the last term of the right-hand side of Eq. (127) also contains the metric $g_{\mu\nu}$. Therefore, it has been conjectured that the inverse transformation of Eq. (127) does not exist [9]. However, to the best of our knowledge, this has not yet been proven. Indeed, although the simple inverse of Eq. (127) does not exist, this does not necessarily mean that there is no more complicated inverse transformation. Using our method, however, we are able to demonstrate that the transformation in Eq. (127) with non-zero E is indeed not invertible.

To do this, let us assume that the transformation in Eq. (127) is invertible, and we will see that this assumption leads to a contradiction. The Friedmann–Robertson–Walker (FRW) homogeneous ansatz in Eq. (G3) expresses a subspace of functional space described with $g_{\mu\nu}$ and χ. Invertibility limited to this subspace gives the necessary condition of invertibility for the full functional space. Here, we will show the violation of this necessary condition, which leads to a contradiction. From Eqs. (127) and (123) we have

$$\tilde{\mathfrak{n}} = C\mathfrak{n} - D\dot{\chi}^2 - E\left(\ddot{\chi} - \frac{\dot{\chi}\dot{\mathfrak{n}}}{2\mathfrak{n}}\right), \qquad \tilde{\mathfrak{a}} = C\mathfrak{a} - E\frac{\dot{\chi}\dot{\mathfrak{a}}}{2\mathfrak{n}}, \tag{128}$$

which is a generalization of Eq. (124) for the case of non-zero E.

As in the case considered above, we treat Eq. (128) as a transformation relating a set of two variables $\big(\mathfrak{n}(t), \mathfrak{a}(t)\big)$ with $\big(\tilde{\mathfrak{n}}(t), \tilde{\mathfrak{a}}(t)\big)$ with the time-dependent external function $\chi(t)$. Contrary to standard disformal transformation, in this case the transformation involves first derivatives of the variables $\mathfrak{n}(t)$ and $\mathfrak{a}(t)$, and therefore we should apply our method to check whether the conditions for this transformation to be invertible are satisfied. We have

$$A_{ia} = \frac{E\dot{\chi}}{2\mathfrak{n}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{129}$$

According to our discussion above, the leading-order condition for the transformation given by Eq. (127) to be invertible is the vanishing of the determinant of Eq. (129). As we can see, this condition is clearly violated for non-zero E, and therefore we arrive at the conclusion that the transformation in Eq. (127) is not invertible unless $E = 0$.

Once we generalize the structure of the higher-derivative term as [10,11]

$$\tilde{g}_{\mu\nu} = \mathcal{F}_0 g_{\mu\nu} + \mathcal{F}_1\chi_\mu\chi_\nu + \mathcal{F}_2\chi_{\mu\nu} + \mathcal{F}_3\chi_{(\mu}X_{\nu)} + \mathcal{F}_4 X_\mu X_\nu + \mathcal{F}_5\chi^\alpha_\mu\chi_{\nu\alpha}, \tag{130}$$

where $\mathcal{F}_i = \mathcal{F}_i(\phi, X, \mathcal{B}, \mathcal{Y}, \mathcal{Z}, \mathcal{W})$ and

$$\mathcal{B} = \nabla_\mu\nabla^\mu\chi, \qquad \mathcal{Y} = \nabla_\mu\chi\nabla^\mu X, \qquad \mathcal{Z} = \nabla_\mu X\nabla^\mu X, \qquad \mathcal{W} = \nabla^\mu\nabla^\nu\chi\nabla_\mu\nabla_\nu\chi, \tag{131}$$

the structure of A_{ia} is changed and the no-go result obtained above for the transformation in Eq. (127) could be avoided. We examine such a possibility in Appendix G.

6. Discussions

In this work we have focused on field transformations that involve up to the first-order derivative of fields, $\phi_i = \bar{\phi}_i(\psi_a, \partial_\alpha\psi_a, x^\mu)$, between two fields ψ_a and another two fields ϕ_i, and shown conditions for this transformation to be invertible. A field transformation of this type changes the number of derivatives acting on the fields, and hence in general it changes the number of degrees of freedom. When the transformation function satisfies certain conditions, however, the appearance of additional degrees of freedom is hindered and the transformation can then be invertible.

We emphasize that the degeneracy conditions and the procedure to derive the complete set of invertibility conditions given in Sect. 2.1 apply to field transformations that involve arbitrary numbers of fields and arbitrary-order derivatives, though we have presented expressions only for transformations with first derivatives just for simplicity. We then, for simplicity, limited our scope to the simplest case where the transformation maps two fields ϕ_i ($i = 1, 2$) to other two fields ψ_a ($a = 1, 2$), and then derived the conditions for this transformation to be invertible. This is because, as we have shown, there is no invertible transformation with derivatives for the one-field case and hence the two-field case is the simplest. To derive the necessary conditions for invertibility, we employed the method of characteristics for partial differential equations in Sect. 2. If a transformation is invertible, the number of characteristic surfaces, which corresponds to the number of physical degrees of freedom, must be invariant. The derivatives contained in the transformation generate extra characteristic surfaces in general, and then the necessary conditions are obtained by demanding that the extra characteristic surfaces are removed so that the total number of characteristic surfaces is invariant. After deriving the necessary conditions, in Sect. 3 we confirmed that they are actually sufficient. It turned out that the invertibility conditions are composed of two degeneracy conditions, Eqs. (50) and (68), and the two non-degeneracy conditions given in Eq. (73).

As an application of the thus derived invertibility conditions, in Sect. 4 we showed some examples of invertible transformations satisfying the invertibility conditions. The invertibility conditions can be regarded as equations for a function of the field transformation, and if we could construct their general solution we could obtain the most general invertible transformation. Instead of finding the general solution, we proposed some ansatze for the transformation for which part of the invertibility conditions are automatically satisfied, and as a result we obtained three kinds of invertible transformations as non-trivial examples. Although they may not be the most general, they span a broad class of invertible transformations and would provide a basis for the construction and classification of various invertible transformations.

As another application, in Sect. 5 we considered a higher-derivative extension of the disformal transformation in gravity and examined its invertibility. Using our invertibility conditions, just by simple calculations we showed explicitly that a disformal-type transformation associated with the second derivative of the scalar field cannot be invertible, which is the first rigorous proof as far as we are aware.

Several directions of future research are indicated. In this work we considered the simplest case that the transformation involves only two scalar fields up to their first derivatives. Provided that our method can be generalized to transformations involving both a scalar field and a metric, we will be able to apply our results to studies on scalar–tensor theories and various modified gravity theories. For example, invertible disformal transformations were utilized to generate and classify the so-called degenerate higher-order scalar–tensor theories from a simpler theory, the Horndeski theory. This scheme may be generalized to incorporate higher-order derivatives if we could generalize the disformal transformation by introducing higher derivatives. Such an application to modified gravity theory will be an ultimate goal of this study. As a first step toward such a goal, it would be useful to consider a generalization to involve more than two scalar fields and more than first-order derivatives. Such generalizations within transformations of scalar fields, and also further generalizations including more fields such as metric, will be discussed in future work.

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Appendix A. Non-invertibility of field-number-changing transformations

Let us consider a transformation $\phi_i = \phi_i(\psi_1, \partial\psi_1)$ $(i = 1, 2)$ for which the number of fields decreases but the number of derivatives increases. Naively, this transformation should preserve the degrees of freedom because the product of the number of fields and the order of derivatives is invariant under the transformation. To examine this expectation, let us evaluate the invertibility conditions. For simplicity we work in the one-dimensional case where the fields depend on only one variable, i.e. we work in a point-particle system. The first degeneracy condition, Eq. (50), is given by

$$A_{ia} = \frac{\partial\phi_i}{\partial\dot{\psi}_a} = \begin{pmatrix} \frac{\partial\phi_1}{\partial\dot{\psi}_1} & 0 \\ \frac{\partial\phi_2}{\partial\dot{\psi}_1} & 0 \end{pmatrix} = aV_iU_a, \qquad V_i = \frac{1}{a}\frac{\partial\phi_i}{\partial\dot{\psi}_1}, \qquad U_a = (1, 0), \tag{A1}$$

where a is chosen to normalize V_i as $V_iV_i = 1$. Then, using $n_i = \epsilon_{ij}V_j$ and $m_a = \epsilon_{ab}U_b = (0, -1)$, the second degeneracy condition, Eq. (68), and the non-degeneracy conditions, Eq. (73), are given by

$$B_{ia} = \frac{\partial\phi_i}{\partial\psi_a} = \begin{pmatrix} \frac{\partial\phi_1}{\partial\psi_1} & 0 \\ \frac{\partial\phi_2}{\partial\psi_1} & 0 \end{pmatrix} = \tilde{V}_iU_a, \qquad \tilde{V}_i = \frac{\partial\phi_i}{\partial\psi_1}, \tag{A2}$$

$$n_iB_{ia}m_a = 0, \qquad n_iB_{ia}U_a = n_i\tilde{V}_i, \qquad \left(V_iB_{ia} - a\dot{U}_a\right)m_a = 0. \tag{A3}$$

While $n_iB_{ia}U_a = n_i\tilde{V}_i$ may not hold, $\left(V_iB_{ia} - a\dot{U}_a\right)m_a$ vanishes identically and hence the non-degeneracy condition among the invertibility conditions is violated. Then, we can judge that the transformation $\phi_i = \phi_i(\psi_1, \partial\psi_1)$ $(i = 1, 2)$ is not invertible. This result can be understood as follows. If the transformation were invertible, then an inverse transformation $\psi_1 = f_1(\phi_1, \phi_2)$, $\dot{\psi}_1 = f_2(\phi_1, \phi_2)$ would exist. This implies that there exists a constraint $\dot{f}_1 = f_2$ between ϕ_1 and ϕ_2. This is in contradiction with the fact that ϕ_1 and ϕ_2 are independent variables, implying that the transformation cannot be invertible.

Appendix B. Derivation of Eq. (6)

In this section we sketch the derivation of the formula in Eq. (6), based on which the necessary conditions for invertibility are derived. Acting ∂_{μ_n} on $\phi_i = \bar{\phi}_i(\psi_a, \partial_\alpha\psi_a, x^\mu)$ gives

$$\partial_{\mu_n}\phi_i(\psi_a, \partial_\alpha\psi_a, x^\mu) = \frac{\partial\bar{\phi}_i}{\partial\psi_a}\partial_{\mu_n}\psi_a + \frac{\partial\bar{\phi}_i}{\partial\left(\partial_\alpha\psi_a\right)}\partial_{\mu_n}\partial_\alpha\psi_a + \frac{\partial\bar{\phi}}{\partial x^{\mu_n}}, \tag{B1}$$

where the third term is the partial derivative with respect to the explicit x^μ dependence of $\bar{\phi}_i$. Then, the highest-derivative term of ψ_a contained in $\partial_{\mu_1\ldots\mu_n}\phi_i$ is generated when all the derivatives other than ∂_{μ_n} act on $\partial_{\mu_n}\partial_\alpha\psi_a$ in Eq. (B1), i.e.

$$\partial_{\mu_1\cdots\mu_n}\phi_i \ni \frac{\partial\bar{\phi}_i}{\partial\left(\partial_\alpha\psi_a\right)}\partial_{\mu_1\cdots\mu_n\alpha}\psi_a = A^\alpha_{ia}\partial_{\mu_1\cdots\mu_n\alpha}\psi_a. \tag{B2}$$

This term is the origin of the leading $\partial^{n+1}\psi_a$ term of Eq. (6). The subleading $\partial^n\psi_a$ term is composed of the following two contributions. The first one is generated when $\partial_{\mu_1\cdots\mu_{n-1}}$ acts on $\partial_{\mu_n}\psi_a$ in Eq. (B1):

$$\partial_{\mu_1\cdots\mu_n}\phi_i \ni \frac{\partial\bar{\phi}_i}{\partial\psi_a}\partial_{\mu_1\cdots\mu_n}\psi_a = B_{ia}\partial_{\mu_1\cdots\mu_n}\psi_a. \tag{B3}$$

The second one is generated when $n-1$ derivatives among $\partial_{\mu_1\cdots\mu_n}$ are consumed to generate $A^{\mu_n}_{ia}\partial^n\psi_a$ and the other one derivative acts directly on ϕ_i, i.e.

$$\partial_{\mu_1\cdots\mu_n}\phi_i \ni \sum_{k=1}^{n}\frac{\partial^2\bar{\phi}_i}{\partial x^{\mu_k}\partial\left(\partial_\alpha\psi_a\right)}\partial_{\mu_1\cdots\mu_{k-1}\mu_{k+1}\cdots\mu_n\alpha}\psi_a = \sum_{k=1}^{n}\partial_{\mu_k}A^\alpha_{ia}\partial_{\mu_1\cdots\mu_{k-1}\mu_{k+1}\cdots\mu_n\alpha}\psi_a. \tag{B4}$$

Contracting with a totally symmetric coefficient $K_{bi}^{(\mu_1\cdots\mu_n)}$, the expression appearing in Eq. (6) is obtained as

$$\begin{aligned} &K_{bi}^{(\mu_1\cdots\mu_n)}\partial_{\mu_1\cdots\mu_n}\phi_i \\ &\quad\ni K_{bi}^{(\mu_1\cdots\mu_n)}\sum_{k=1}^{n}\partial_{\mu_k}A^\alpha_{ia}\partial_{\mu_1\cdots\mu_{k-1}\mu_{k+1}\cdots\mu_n\alpha}\psi_a = n\,K_{bi}^{(\alpha\mu_1\cdots\mu_{n-1})}\partial_\alpha A^{\mu_n}_{ia}\partial_{\mu_1\cdots\mu_n}\psi_a. \end{aligned} \tag{B5}$$

The $\partial^{n-k}\psi_a$ term of Eq. (6) is obtained in a similar manner. The ∂^kB_{ia} term is obtained by using $n-k$ derivatives to generate $\partial^{n-k}\psi_a$, and by acting the other derivatives on ϕ_i directly. The $\partial^{k+1}A^\mu_{ia}$ term is obtained by using $n-k-1$ derivatives to generate $\partial^{n-k}\psi_a$, and by acting the other derivatives on ϕ_i directly. The coefficients of each term, $\binom{n}{k}$ and $\binom{n}{k+1}$, correspond to the number of combinations of the derivatives among ∂^n that are used to generate $\partial^k\psi_a$.

Appendix C. Derivation of Eq. (40)

We give the derivation of Eq. (40) based on Eq. (6) and using the degeneracy conditions in the two-field case, Eqs. (32) and (37). We also use results given in Sect. 2.2.

We start the derivation from

$$\begin{aligned}
&\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\bar{A}_{bi}^{\mu_{n+1}}\bar{A}^{2,\mu_{n+2}\mu_{n+3}}\partial_{\mu_1\cdots\mu_{n+3}}\phi_i\\
&\quad-\Big[\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\mathcal{A}_{2,bc}^{\mu_{n+1}}\tilde{A}_{ci}^{\mu_{n+2}}\\
&\quad-\left(n\,\overset{\approx}{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\bar{A}^{2,\mu_n\mu_{n+1}}+2\,\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{2,\mu_{n+1}\alpha}\right)\partial_\alpha\bar{A}_{bi}^{\mu_{n+2}}\Big]\partial_{\mu_1\cdots\mu_{n+2}}\phi_i,
\end{aligned}\tag{C1}$$

which is given by the $\partial^{n+2}\psi$ and lower-order terms once rewritten in terms of ψ using Eq. (6), as explained in Sect. 2.2.

Using Eq. (6), the first term of Eq. (C1) is expressed in terms of ψ as

$$\begin{aligned}
&\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\bar{A}_{bi}^{\mu_{n+1}}\bar{A}^{2,\mu_{n+2}\mu_{n+3}}\partial_{\mu_1\cdots\mu_{n+3}}\phi_i\\
&=\left[\partial^{n+3}\psi\text{ term}\right]\\
&\quad+\Bigg\{\Bigg[\frac{n(n-1)}{2}\,\overset{\approx}{K}^{(\alpha_1\alpha_2\mu_1\cdots\mu_{n-2})}\bar{A}_{bi}^{\mu_{n-1}}\bar{A}^{2,\mu_n\mu_{n+1}}+n\,\overset{\approx}{K}^{(\alpha_1\mu_1\cdots\mu_{n-1})}\bar{A}_{bi}^{\alpha_2}\bar{A}^{2,\mu_n\mu_{n+1}}\\
&\quad+2n\,\overset{\approx}{K}^{(\alpha_1\mu_1\cdots\mu_{n-1})}\bar{A}_{bi}^{\mu_n}\bar{A}^{2,\mu_{n+1}\alpha_2}+\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\left(2\bar{A}_{bi}^{\alpha_1}\bar{A}^{2,\mu_{n+1}\alpha_2}+\bar{A}_{bi}^{\mu_{n+1}}\bar{A}^{2,\alpha_1\alpha_2}\right)\Bigg]\partial_{\alpha_1\alpha_2}A_{ia}^{\mu_{n+2}}\\
&\quad+\Bigg[n\,\overset{\approx}{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\bar{A}_{bi}^{\mu_n}\bar{A}^{2,\mu_{n+1}\mu_{n+2}}\\
&\quad+\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\left(\bar{A}_{bi}^{\alpha}\bar{A}^{2,\mu_{n+1}\mu_{n+2}}+2\bar{A}_{bi}^{\mu_{n+1}}\bar{A}^{2,\mu_{n+2}\alpha}\right)\Bigg]\partial_\alpha B_{ia}\Bigg\}\partial_{\mu_1\ldots\mu_{n+2}}\psi_a\\
&\quad+\mathcal{O}\left(\partial^{n+1}\psi_a\right),
\end{aligned}\tag{C2}$$

where the terms appearing on the right-hand side are classified according to the positions of the indices α, α_1, α_2. Likewise, the second term of Eq. (C1) is expressed as

$$\begin{aligned}
&\left[\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\mathcal{A}_{2,bc}^{\mu_{n+1}}\tilde{A}_{ci}^{\mu_{n+2}}-\left(n\,\overset{\approx}{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\bar{A}^{2,\mu_n\mu_{n+1}}+2\,\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{2,\mu_{n+1}\alpha}\right)\partial_\alpha\bar{A}_{bi}^{\mu_{n+2}}\right]\partial_{\mu_1\cdots\mu_{n+2}}\phi_i\\
&=\left[\partial^{n+3}\psi\text{ term}\right]\\
&\quad+\Bigg\{\Bigg[\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\mathcal{A}_{2,bc}^{\mu_{n+1}}\tilde{A}_{ci}^{\mu_{n+2}}-\left(n\,\overset{\approx}{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\bar{A}^{2,\mu_n\mu_{n+1}}+2\,\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{2,\mu_{n+1}\alpha}\right)\partial_\alpha\bar{A}_{bi}^{\mu_{n+2}}\Bigg]B_{ia}\\
&\quad+\Big\{n\,\overset{\approx}{K}^{(\alpha_2\mu_1\cdots\mu_{n-1})}\mathcal{A}_{2,bc}^{\mu_n}\tilde{A}_{ci}^{\mu_{n+1}}+2\,\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\mathcal{A}_{2,bc}^{(\alpha_2}\tilde{A}_{ci}^{\mu_{n+1})}\\
&\quad-n\Big[(n-1)\,\overset{\approx}{K}^{(\alpha_1\alpha_2\mu_1\cdots\mu_{n-2})}\bar{A}^{2,\mu_{n-1}\mu_n}\partial_{\alpha_1}\bar{A}_{bi}^{\mu_{n+1}}\\
&\quad+\overset{\approx}{K}^{(\alpha_1\mu_1\cdots\mu_{n-1})}\left(2\bar{A}^{2,\alpha_2\mu_n}\partial_{\alpha_1}\bar{A}_{bi}^{\mu_{n+1}}+\bar{A}^{2,\mu_n\mu_{n+1}}\partial_{\alpha_1}\bar{A}_{bi}^{\alpha_2}\right)\Big]\\
&\quad-2\left(n\,\overset{\approx}{K}^{(\alpha_2\mu_1\cdots\mu_{n-1})}\bar{A}^{2,\mu_n\alpha_1}\partial_{\alpha_1}\bar{A}_{bi}^{\mu_{n+1}}+2\,\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{2,\alpha_1(\alpha_2}\partial_{\alpha_1}\bar{A}_{bi}^{\mu_{n+1})}\right)\Big\}\partial_{\alpha_2}A_{ia}^{\mu_{n+2}}\Bigg\}\partial_{\mu_1\ldots\mu_{n+2}}\psi_a\\
&\quad+\mathcal{O}\left(\partial^{n+1}\psi_a\right),
\end{aligned}\tag{C3}$$

where the $\partial^{n+3}\psi$ term on the right-hand side is the same as that in Eq. (C2). Then, in Eq. (C1) the $\partial^{n+3}\psi$ terms cancel out, and the remaining terms are given by the difference between Eqs. (C2) and (C3). Reorganizing the terms according to their tensor structures, it can be expressed as

$$\begin{aligned}
&\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{\mu_{n+1}}_{bi}\bar{A}^{2,\mu_{n+2}\mu_{n+3}}\partial_{\mu_1\cdots\mu_{n+3}}\phi_i-\Bigg[\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\mathcal{A}^{\mu_{n+1}}_{2,bc}\tilde{A}^{\mu_{n+2}}_{ci}-\Bigg(n\,\overset{\approx}{K}^{(\alpha\mu_1\cdots\mu_{n-1})}\bar{A}^{2,\mu_n\mu_{n+1}}\\
&\quad+2\,\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\bar{A}^{2,\mu_{n+1}\alpha}\Bigg)\partial_\alpha\bar{A}^{\mu_{n+2}}_{bi}\Bigg]\partial_{\mu_1\cdots\mu_{n+2}}\phi_i\\
&=\Bigg\{\frac{n(n-1)}{2}\,\overset{\approx}{K}^{(\alpha_1\alpha_2\mu_1\cdots\mu_{n-2})}\bar{A}^{2,\mu_{n-1}\mu_n}\left[\bar{A}^{\mu_{n+1}}_{bi}\partial_{\alpha_1\alpha_2}A^{\mu_{n+2}}_{ia}+2\left(\partial_{\alpha_1}\bar{A}^{\mu_{n+1}}_{bi}\right)\partial_{\alpha_2}A^{\mu_{n+2}}_{ia}\right]\\
&\quad+n\,\overset{\approx}{K}^{(\alpha_1\mu_1\cdots\mu_{n-1})}\Big\{-\mathcal{A}^{\mu_n}_{2,bc}\tilde{A}^{\mu_{n+1}}_{ci}\partial_{\alpha_1}A^{\mu_{n+2}}_{ia}\\
&\quad+2\bar{A}^{2,\mu_n\alpha_2}\left[\bar{A}^{\mu_{n+1}}_{bi}\partial_{\alpha_1\alpha_2}A^{\mu_{n+2}}_{ia}+\left(\partial_{\alpha_1}\bar{A}^{\mu_{n+1}}_{bi}\right)\partial_{\alpha_2}A^{\mu_{n+2}}_{ia}+\left(\partial_{\alpha_2}\bar{A}^{\mu_{n+1}}_{bi}\right)\partial_{\alpha_1}A^{\mu_{n+2}}_{ia}\right]\\
&\quad+\bar{A}^{2,\mu_n\mu_{n+1}}\left[\bar{A}^{\mu_{n+2}}_{bi}\partial_{\alpha_1}B_{ia}+\left(\partial_{\alpha_1}\bar{A}^{\mu_{n+2}}_{bi}\right)B_{ia}+\bar{A}^{\alpha_2}_{bi}\partial_{\alpha_1\alpha_2}A^{\mu_{n+2}}_{ia}+\left(\partial_{\alpha_1}\bar{A}^{\alpha_2}_{bi}\right)\partial_{\alpha_2}A^{\mu_{n+2}}_{ia}\right]\Big\}\\
&\quad+\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\Big[\bar{A}^{\alpha_1}_{bi}\bar{A}^{2,\mu_{n+1}\mu_{n+2}}\partial_{\alpha_1}B_{ia}-2\mathcal{A}^{(\alpha_2}_{2,bc}\tilde{A}^{\mu_{n+1})}_{ci}\partial_{\alpha_2}A^{\mu_{n+2}}_{ia}-\mathcal{A}^{\mu_{n+1}}_{2,bc}\tilde{A}^{\mu_{n+2}}_{ci}B_{ia}\\
&\quad+2\bar{A}^{2,\mu_{n+1}\alpha_1}\left(\partial_{\alpha_1}\bar{A}^{\mu_{n+2}}_{bi}B_{ia}+\bar{A}^{\mu_{n+2}}_{bi}\partial_{\alpha_1}B_{ia}+\bar{A}^{\alpha_2}_{bi}\partial_{\alpha_1\alpha_2}A^{\mu_{n+2}}_{ia}+\partial_{\alpha_1}\bar{A}^{\alpha_2}_{bi}\partial_{\alpha_2}A^{\mu_{n+2}}_{ia}\right)\\
&\quad+\bar{A}^{2,\alpha_1\alpha_2}\left(\bar{A}^{\mu_{n+1}}_{bi}\partial_{\alpha_1\alpha_2}A^{\mu_{n+2}}_{ia}+2\partial_{\alpha_1}\bar{A}^{\mu_{n+1}}_{bi}\partial_{\alpha_2}A^{\mu_{n+2}}_{ia}\right)\Big]\Bigg\}\partial_{\mu_1\cdots\mu_{n+2}}\psi_a\\
&\quad+\mathcal{O}\left(\partial^{n+1}\psi_a\right)\\
&=\Bigg\{-\frac{n(n-1)}{2}\,\overset{\approx}{K}^{(\alpha_1\alpha_2\mu_1\cdots\mu_{n-2})}\bar{A}^{2,\mu_{n-1}\mu_n}\left(\partial_{\alpha_1\alpha_2}\bar{A}^{\mu_{n+1}}_{bi}\right)A^{\mu_{n+2}}_{ia}\\
&\quad+n\,\overset{\approx}{K}^{(\alpha_1\mu_1\cdots\mu_{n-1})}\Big[-\mathcal{A}^{\mu_n}_{2,bc}\tilde{A}^{\mu_{n+1}}_{ci}\partial_{\alpha_1}A^{\mu_{n+2}}_{ia}-2\bar{A}^{2,\mu_n\alpha_2}\left(\partial_{\alpha_1\alpha_2}\bar{A}^{\mu_{n+1}}_{bi}\right)A^{\mu_{n+2}}_{ia}+\bar{A}^{2,\mu_n\mu_{n+1}}\partial_{\alpha_1}\mathcal{A}^{\mu_{n+2}}_{ba}\Big]\\
&\quad+\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}\Big[\bar{A}^{2,\mu_{n+1}\mu_{n+2}}\bar{A}^{\alpha}_{bi}\partial_\alpha B_{ia}-2\mathcal{A}^{(\alpha}_{2,bc}\tilde{A}^{\mu_{n+1})}_{ci}\partial_\alpha A^{\mu_{n+2}}_{ia}-\mathcal{A}^{\mu_{n+1}}_{2,bc}\tilde{A}^{\mu_{n+2}}_{ci}B_{ia}\\
&\quad+2\bar{A}^{2,\mu_{n+1}\alpha}\partial_\alpha\mathcal{A}^{\mu_{n+2}}_{2,ba}-\bar{A}^{2,\alpha_1\alpha_2}\left(\partial_{\alpha_1\alpha_2}\bar{A}^{\mu_{n+1}}_{bi}\right)A^{\mu_{n+2}}_{ia}\Big]\Bigg\}\partial_{\mu_1\cdots\mu_{n+2}}\psi_a\\
&\quad+\mathcal{O}\left(\partial^{n+1}\psi_a\right).
\end{aligned}\tag{C4}$$

At the final equality we used Eq. (28) and the identity that follows from the second derivative of Eq. (12) in the two-field case, which is given by

$$\partial_\mu\partial_\nu\left(\bar{A}^{(\alpha}_{bi}A^{\beta)}_{ia}\right)=\left(\partial_\mu\partial_\nu\bar{A}^{(\alpha}_{bi}\right)A^{\beta)}_{ia}+\left(\partial_\mu\bar{A}^{(\alpha}_{bi}\right)\partial_\nu A^{\beta)}_{ia}+\left(\partial_\nu\bar{A}^{(\alpha}_{bi}\right)\partial_\mu A^{\beta)}_{ia}+\bar{A}^{(\alpha}_{bi}\left(\partial_\mu\partial_\nu A^{\beta)}_{ia}\right)=0.\tag{C5}$$

As argued in Sect. 2.2, to find the last condition for invertibility we should focus on the coefficient of the highest-derivative term in the $\psi^\perp$ space, and this coefficient is obtained by replacing $\partial_{\mu_1\cdots\mu_{n+2}}\psi_a$ by $\bar{A}^{\mu_3}_{aj}$ and symmetrizing over μ_1, μ_2, μ_3 in Eq. (C4). Below, we evaluate each term in Eq. (C4) after this replacement. First, the $\overset{\approx}{K}^{(\alpha_1\alpha_2\mu_1\cdots\mu_{n-2})}$ term vanishes because it contains $A^{(\mu_{n+2}}_{ia}\bar{A}^{\mu_3)}_{aj}=0$, which is enforced by Eq. (28). Next, the $\overset{\approx}{K}^{(\alpha_1\mu_1\cdots\mu_{n-1})}$ term also vanishes as follows:

$$\Big[-\mathcal{A}^{(\mu_n}_{2,bc}\tilde{A}^{\mu_{n+1}}_{ci}\partial_{\alpha_1}A^{\mu_{n+2}}_{ia} - 2\bar{A}^{2,\alpha_2(\mu_n}\left(\partial_{\alpha_1\alpha_2}\bar{A}^{\mu_{n+1}}_{bi}\right)A^{\mu_{n+2}}_{ia} + \bar{A}^{2,(\mu_n\mu_{n+1}}\partial_{\alpha_1}\mathcal{A}^{\mu_{n+2}}_{ba}\Big]\bar{A}^{\mu_3)}_{aj}$$
$$= \left(-\mathcal{A}^{(\mu_n}_{2,bc}\tilde{A}^{\mu_{n+1}}_{ci}\partial_{\alpha_1}A^{\mu_{n+2}}_{ia} + \bar{A}^{2,(\mu_n\mu_{n+1}}\partial_{\alpha_1}\mathcal{A}^{\mu_{n+2}}_{ba}\right)\bar{A}^{\mu_3)}_{aj}$$
$$= \left(\mathcal{A}^{(\mu_n}_{2,bc}\tilde{A}^{\mu_{n+1}}_{ci}A^{\mu_{n+2}}_{ia} - \bar{A}^{2,(\mu_n\mu_{n+1}}\mathcal{A}^{\mu_{n+2}}_{ba}\right)\partial_{\alpha_1}\bar{A}^{\mu_3)}_{aj}$$
$$= \left[\mathcal{A}^{(\mu_n}_{2,bc}\tilde{A}^{\mu_{n+1}}_{ci}A^{\mu_{n+2}}_{ia} - \mathcal{A}^{(\mu_n}_{bc}\left(\bar{A}^{\mu_{n+1}}_{ci}\bar{A}^{\mu_{n+2}}_{ai} + \tilde{A}^{\mu_{n+1}}_{ci}A^{\mu_{n+2}}_{ia}\right)\right]\partial_{\alpha_1}\bar{A}^{\mu_3)}_{aj} = 0. \quad \text{(C6)}$$

The first equality follows from Eq. (28). The second equality follows from Eq. (14) and the first derivative of Eq. (37), i.e.

$$\partial_{\alpha_1}\mathcal{A}^{(\mu_{n+2}}_{ba}\bar{A}^{\mu_3)}_{aj} = -\mathcal{A}^{(\mu_{n+2}}_{ba}\partial_{\alpha_1}\bar{A}^{\mu_3)}_{aj}. \quad \text{(C7)}$$

At the third equality we replaced $\bar{A}^{2,\mu_n\mu_{n+1}}$ using Eq. (30). Then, this equation can be shown to vanish using Eq. (37). Lastly, in the $\overset{\approx}{K}^{(\mu_1\cdots\mu_n)}$ term of Eq. (C4), the last part with $A^{\mu_{n+2}}_{ia}$ vanishes thanks to Eq. (12). The remaining term gives Eq. (41), once ∂B is rewritten into $\mathcal{B}$ using Eq. (28).

Appendix D. Absence of invertible field transformation with derivatives for the one-field case

We show here that there is no invertible field transformation of one field involving up to the first derivative by using the conditions obtained for the two-field case. We consider the transformation

$$\phi_1 = \bar{\phi}_1(\psi_1, \partial_\alpha\psi_1, x^\mu), \qquad \phi_2 = \psi_2, \quad \text{(D1)}$$

which essentially represents a one-field transformation with derivatives. Then, the first degeneracy condition, Eq. (50), is satisfied as follows:

$$A^\mu_{ia} = \frac{\partial\phi_i}{\partial\left(\partial_\mu\psi_a\right)} = \begin{pmatrix} \frac{\partial\phi_1}{\partial(\partial_\mu\psi_1)} & 0 \\ 0 & 0 \end{pmatrix} = \frac{\partial\phi_1}{\partial\left(\partial_\mu\psi_1\right)}U_aV_i, \quad \text{(D2)}$$

where $\frac{\partial\phi_1}{\partial(\partial_\mu\psi_1)}$ is assumed to be non-zero and

$$U_a = (1, 0) = V_i, \qquad m_a = (0, -1) = n_i. \quad \text{(D3)}$$

On the other hand, the second degeneracy condition, Eq. (68), is never satisfied, because

$$B_{ia} = \frac{\partial\phi_i}{\partial\psi_a} = \begin{pmatrix} \frac{\partial\phi_1}{\partial\psi_1} & 0 \\ 0 & 1 \end{pmatrix}, \qquad n_iB_{ia}m_a = 1 \neq 0. \quad \text{(D4)}$$

Note that one can also easily check that the third conditions, Eq. (73), are also violated because $n_iB_{ia}U_a = 0$ and $(V_jB_{jb} - a^\beta\partial_\beta U_b)m_b = 0$ in this case. Thus, there is no invertible field transformation of one field involving first derivatives. A similar argument also applies to a case with more derivatives, $\phi_1 = \bar{\phi}_1(\psi_1, \partial_\alpha\psi_1, \partial_\alpha\partial_\beta\psi_1, \ldots; x^\mu)$, and we can show that it can never be invertible.

Appendix E. Inverse function theorem applied directly to the functional space, and implicit function theorem to finite-dimensional subspaces

In our proof in Sects. 2 and 3, we do not apply the inverse function theorem to the mapping from $\psi(x)$ to $\phi(x)$, but instead use the implicit function theorem for the mapping from $(\psi, \partial\psi, \ldots)$ to $(\phi, \partial\phi, \ldots)$. This is because the former indeed does not work in cases with derivatives. In this appendix we explain why it is not applicable in Sect. E.1, and show the idea of our proof in Sect. E.2.

E.1 Inapplicability of the inverse function theorem to the functional space

The inverse function theorem can be applied to the mapping from a Banach space X to another Banach space Y. Functional spaces that are discussed in physics are mainly Hilbert spaces, and thus one might naively think that the inverse function theorem is directly applicable to a field redefinition with derivatives from $\psi(x)$ to $\phi(x)$ by analyzing all spacetime points simultaneously. However, if derivatives of fields are involved in the field redefinition, the inverse function theorem cannot be applied to the functional space. This means that linearized analysis in the functional space does not give correct statements. Let us see that the inverse function theorem in functional spaces does not work in cases with derivatives.

We have the condition for degeneracy of the coefficients of the highest-order derivative,

$$\det(A^{\mu}_{ia}\xi_\mu) = 0. \tag{E1}$$

In the (wrong) linear analysis, this is obtained as an equation which has to be satisfied for a fixed value of ψ_a. However, we know from the analysis of the necessary condition discussed in Sect. 2 that Eq. (E1) should be interpreted as an identity, i.e. the equality has to be satisfied for any ψ_a. Since the sufficient condition, which can be obtained from the inverse function theorem, should be stronger than the necessary condition, Eq. (E1) should be obtained as an identity (or replaced by a stronger condition).

We shall see in detail why the inverse function theorem is not directly applicable to the field redefinition with derivatives. For this purpose, let us carefully inspect the statement of the inverse function theorem for a mapping between Banach spaces [12]:

Let X and Y be Banach spaces. Let U be an open neighborhood of a point $x_0 \in X$ and F be a continuously differentiable mapping from U to Y, F: $U \to Y$. Suppose that there exists the Fréchet derivative dF_0 at $x_0 \in U$ which gives a bounded linear isomorphism that maps U onto an open neighborhood of $F(x_0) \in Y$. Then, there exists an open neighborhood U' of $x_0 \in X$ and V of $F(x_0) \in Y$, and a continuously differentiable map G from V to U', G: $V \to U'$, satisfying $F(G(y)) = y$.

The important point is that, in the application of the theorem, a mapping is required to be continuously differentiable. To see the argument clearly, we consider an example given by

$$\phi_1 = \psi_1\dot{\psi}_2 + \psi_1, \qquad \phi_2 = \dot{\psi}_1 + \psi_2. \tag{E2}$$

We denote this mapping as Φ: $\psi_a(x) \to \phi_i(x)$. Let us apply the linear analysis to Φ (although it gives an incorrect result). We linearize Eq. (E2) as

$$\delta\phi_1 = \delta\psi_1\dot{\psi}_2 + \psi_1\delta\dot{\psi}_2 + \delta\psi_1, \qquad \delta\phi_2 = \delta\dot{\psi}_1 + \delta\psi_2. \tag{E3}$$

If we consider $\psi_1(x) = \psi_2(x) = 0$ for any x, a point in the phase space, the above equations become

$$\delta\phi_1 = \delta\psi_1, \qquad \delta\phi_2 = \delta\dot{\psi}_1 + \delta\psi_2, \tag{E4}$$

and they can be solved uniquely for $\delta\psi_1$ and $\delta\psi_2$ as

$$\delta\psi_1 = \delta\phi_1, \qquad \delta\psi_2 = \delta\phi_2 - \delta\dot{\phi}_1. \tag{E5}$$

Since the linearized equation is uniquely solved, one might think the inverse function theorem is applicable, but this is not true. This is because, if the inverse function theorem is applicable, the mapping Φ must also be invertible for $\psi_1(x) = \epsilon(\neq 0)$ and $\psi_2(x) = 0$, which is in the neighborhood of $\psi_1(x) = \psi_2(x) = 0$ for sufficiently small ϵ. However, this is not the case because the linearized equations for $\psi_1(x) = \epsilon$, $\psi_2(x) = 0$ become

$$\delta\phi_1 = \epsilon\delta\dot{\psi}_2 + \delta\psi_1, \qquad \delta\phi_2 = \delta\dot{\psi}_1 + \delta\psi_2. \tag{E6}$$

These equations cannot be solved uniquely for $\delta\psi_1$ and $\delta\psi_2$, and hence the transformation Φ is not invertible.

What was wrong in this example? Actually, the derivative of the mapping $\Phi\big(\psi_a(x)\big)$ (that is, the field redefinition in Eq. (E2)) cannot be obtained in the linearized analysis. The Fréchet derivative of Φ is defined as follows.

If there exists a bounded linear operator A satisfying

$$\lim_{||\delta\psi_a(x)||_M \to 0} \frac{||\Phi\big(\psi_a(x) + \delta\psi_a(x)\big) - \Phi\big(\psi_a(x)\big) - A\,\delta\psi_a(x)||_M}{||\delta\psi_a(x)||_M} = 0, \tag{E7}$$

the Fréchet derivative is defined as

$$D\Phi\big(\psi_a(x)\big) = A. \tag{E8}$$

Otherwise, the Fréchet derivative does not exist. Here, M is an open region in spacetime that we consider, and $||\cdot||_M$ is a norm for the phase space covered by $\phi_i(x)$ or $\psi_a(x)$.

For the existence of the Fréchet derivative that is necessary to establish the invertibility, the linear part of

$$\Phi\big(\psi_a(x) + \delta\psi_a(x)\big) - \Phi\big(\psi_a(x)\big) = \big(\delta\psi_1\dot{\psi}_2 + \psi_1\delta\dot{\psi}_2 + \delta\psi_1\delta\dot{\psi}_2 + \delta\psi_1, \delta\dot{\psi}_1 + \delta\psi_2\big) \tag{E9}$$

must be close to $A\delta\psi_a(x)$, where A is a *bounded* linear operator. One may expect that the linear part of Eq. (E9) can be approximated by $A\delta\psi_a(x)$. However, Eq. (E9) includes derivatives of $\delta\psi$, which may not be bounded. Hence, the inverse function theorem is not applicable.

The inverse functional theorem roughly means that, if it is applicable, the linear analysis works well. However, in the application to an infinite-dimensional space, such as a functional space, the existence of the Fréchet derivative is required. Without confirmation of this, the result of invertibility by linear analysis cannot be trusted, and, in the case of the field redefinition with derivative, it generically does not work.

E.2 Our idea: Application of the implicit function theorem to finite-dimensional subspaces

To avoid complication due to the derivatives involved in the mapping, we take a different approach by working in the function space spanned by $\phi_i(x_0)$, $\partial_\mu\phi_i(x_0)$, $\partial_\mu\partial_\nu\phi_i(x_0)$, … as follows. The field redefinition in Eq. (5) from ψ_a to ϕ_i is obviously unique; Eq. (5) shows that ψ_a is uniquely obtained from a fixed ϕ_i. Hence, if the mapping from ϕ_i to ψ_a is also unique, the field redefinition becomes invertible.

Let us give ϕ_i in an open region of spacetime; then, its derivatives $\partial_\mu\phi_i$, $\partial_\mu\partial_\nu\phi_i$, … are uniquely obtained. Thus, if we can show that ψ_a is uniquely fixed for given ϕ_i along with its derivatives $\partial_\mu\phi_i$, $\partial_\mu\partial_\nu\phi_i$, …, we can say the inverse mapping is unique. To show this, we use the implicit function theorem.

The problem appearing in the direct application of the inverse function theorem in Sect. E.1 stems from the dimension of the space being infinite. Even if we use the implicit function theorem, we have a similar problem. However, if we use the equations shown in Sect. 3, we can consider the implicit function theorem at each point of spacetime separately, i.e. for $\psi_a(x_0)$ with fixed $\phi_i(x_0)$ and its derivatives ($\partial_\mu\phi_i(x_0)$, $\partial_\mu\partial_\nu\phi_i(x_0)$, …) at each spacetime point x_0. Note that now we (are trying to) apply the implicit function theorem to ($\phi_i(x_0)$; $\phi_i(x_0)\partial_\mu\phi_i(x_0)$, $\partial_\mu\partial_\nu\phi_i(x_0)$, ...) with fixed x_0, and thus the dimension of the space is finite. (Here, we consider the case where the number of derivatives of ϕ is finite.)

Since the dimension of the space is finite, we are not concerned with infinite dimensions and the implicit function theorem can be easily applied. Note that the neighborhood in the implicit function theorem here means for the values of $\phi_i(x_0)$, $\partial_\mu\phi_i(x_0)$, $\partial_\mu\partial_\nu\phi_i(x_0)$, ..., not the space-time point. Hence, the neighborhood or "locality" in our argument means a local region of functional space, where the deviations of $\phi_i(x)$, $\partial_\mu\phi_i(x)$, $\partial_\mu\partial_\nu\phi_i(x)$, ... from a reference value should be small. This should be acceptable in physics, which usually has the ultraviolet cutoff scale.

Note that the "neighborhood" in the implicit (or inverse) function theorem is not necessarily small. Let us take a simple example, $f(x) = x^2$. The inverse function theorem is applicable except at $x = 0$. At $x = 3$, one might take an open neighborhood $2 < x < 4$. Then, we take the inverse function theorem again near $x = 2$ and the "neighborhood" can be extended to $0 < x$. This extension of the "neighborhood" is general and it is done just before the condition is violated.

Appendix F. Setting $U_a = (0, 1)$ in $\phi_i = \phi_i(\psi_a, U_a(\psi_a)\partial_\mu\psi_a)$

In this appendix we consider a transformation in which a derivative of ψ_a appears only in a combination $U_a(\psi_a)\partial_\mu\psi_a$, i.e.

$$\phi_i = \phi_i\left(\psi_a, U_a(\psi_a)\partial_\mu\psi_a\right), \tag{F1}$$

and show that $U_a(\psi_a)$ can be set to a constant vector $U_a = (0, 1)$ without loss of generality by a field transformation $\psi_a = \psi_a(\tilde{\Psi}_a)$. This technique is used in Sect. 4 to simplify examples of invertible transformations.

F.1 Field transformation to set $U_a = (0, 1)$

As a first step to setting $U_a(\psi_a)$ to a constant vector, we rewrite this transformation as

$$\phi_i = \phi_i\big(\psi_a, \tilde{U}_a(\psi_a)\partial_\mu\psi_a\big), \tag{F2}$$

where

$$\tilde{U}_a \equiv c(\psi_a)U_a(\psi_a) \tag{F3}$$

is a local rescaling of U_a such that $\tilde{U}_a$ is an irrotational vector in the ψ_a space, i.e.

$$\frac{\partial\tilde{U}_1}{\partial\psi_2} - \frac{\partial\tilde{U}_2}{\partial\psi_1} = 0. \tag{F4}$$

This $\tilde{U}_a$ can be obtained by choosing the rescaling factor $c(\psi_a)$ appropriately. We show the construction method of $c(\psi_a)$ and $\tilde{U}_a(\psi_a)$ in the next section.

When Eq. (F4) is satisfied, due to the Poincaré lemma there exists a scalar function $\Psi_1(\psi_k)$ satisfying

$$\tilde{U}_a = \frac{\partial\Psi_2}{\partial\psi_a}. \tag{F5}$$

Let us also introduce another scalar function $\Psi_1(\psi_a)$ that is functionally independent of $\Psi_1(\psi_a)$ (i.e. $\det(\partial\Psi_a/\partial\psi_b) \neq 0$). Then, there exists a one-to-one mapping between ψ_a and Ψ_a, and the transformation in Eq. (F2) may be expressed in terms of Ψ_a as

$$\phi_i = \phi_i\big(\Psi_a, \partial_\mu\Psi_2\big). \tag{F6}$$

This is equivalent to setting $U_a = (0, 1)$ in the transformation in Eq. (F1). Hence, we may impose $U_i = (0, 1)$ without loss of generality in the transformation in Eq. (F1), as long as there exists a rescaling $c(\psi_i)$ satisfying the condition in Eq. (F4).

F.2 Finding irrotational $\tilde{U}_i$

In the argument above, it is crucial that a rescaling such as Eq. (F3) exists to make $\tilde{U}_a$ an irrotational vector satisfying Eq. (F4). We show how to find such a rescaling in this section.

Using Eq. (F3), the condition in Eq. (F4) can be rewritten as

$$U_1 \frac{\partial c}{\partial \psi_2} - U_2 \frac{\partial c}{\partial \psi_1} + c\left(\frac{\partial U_1}{\partial \psi_2} - \frac{\partial U_2}{\partial \psi_1}\right) = 0. \tag{F7}$$

This equation is a first-order partial differential equation for $\log c(\psi_1, \psi_2)$, and it can be solved a least locally once an appropriate boundary condition for c is given. For example, when $U_1 \neq 0$ we may solve Eq. (F7) as an evolution equation in the "time" direction ψ_2 for an initial condition given by $c = 1$ on a $\psi_2 =$ constant line in the ψ_a space, regarding ψ_1 as the "spatial" coordinate.

Appendix G. Disformal transformation with higher derivatives for the FRW ansatz

In Sect. 5 we examined a generalization of the disformal transformation to introduce the second derivative of the scalar field $\nabla\nabla\chi$, and found it non-invertible unless such a second-derivative term is absent. In this appendix we consider a further generalization of this transformation, and find that there may be an invertible disformal transformation with higher derivatives if the metric is limited to the FRW type. Note that the investigation of the FRW type gives a necessary condition. While the violation of invertibility in the FRW subspace shows the same in the full space of the metric, establishing it in the subspace does not result in that in the full space.

G.1 Generalized disformal transformation with second derivatives

Let us consider the following generalization of the disformal transformation [10,11]:

$$\tilde{g}_{\mu\nu} = \mathcal{F}_0 g_{\mu\nu} + \mathcal{F}_1 \chi_\mu \chi_\nu + \mathcal{F}_2 \chi_{\mu\nu} + \mathcal{F}_3 \chi_{(\mu} X_{\nu)} + \mathcal{F}_4 X_\mu X_\nu + \mathcal{F}_5 \chi^\alpha_\mu \chi_{\nu\alpha}, \tag{G1}$$

where $\mathcal{F}_i$ depends on X, $\mathcal{B}$, $\mathcal{Y}$, $\mathcal{Z}$, and $\mathcal{W}$, which are scalar quantities involving up to the square of the second derivative of the scalar field $\nabla\nabla\chi$, i.e.

$$X = \chi^\mu \chi_\mu, \qquad \mathcal{B} = \Box\chi, \qquad \mathcal{Y} = \chi^\mu X_\mu, \qquad \mathcal{Z} = X_\mu X^\mu, \qquad \mathcal{W} = \chi^{\mu\nu}\chi_{\mu\nu}. \tag{G2}$$

The subscripts denote covariant derivatives (e.g. $\chi_\mu = \nabla_\mu \chi$, $\chi_{\mu\nu} = \nabla_\mu \nabla_\nu \chi$).

Let us take the FRW homogeneous ansatz for the metric $g_{\mu\nu}$,

$$g_{\mu\nu} dx^\mu dx^\nu = -\mathfrak{n}(t) dt^2 + \mathfrak{a}(t) d\mathbf{x}^2, \qquad \chi = \chi(t). \tag{G3}$$

For this ansatz we have

$$X=-\frac{\dot\chi^2}{\mathfrak{n}},\tag{G4}$$

$$\mathcal{B}=\frac{1}{2\mathfrak{n}}\left(\dot\chi\frac{\dot{\mathfrak{n}}}{\mathfrak{n}}-3\dot\chi\frac{\dot{\mathfrak{a}}}{\mathfrak{a}}-2\ddot\chi\right)=\frac{\mathcal{Y}}{2X}-\frac{3\dot\chi}{2\mathfrak{n}}\frac{\dot{\mathfrak{a}}}{\mathfrak{a}},$$

$$\mathcal{Y}=-\frac{\dot\chi^2}{\mathfrak{n}^2}\left(\dot\chi\frac{\dot{\mathfrak{n}}}{\mathfrak{n}}-2\ddot\chi\right),$$

$$\mathcal{Z}=\frac{\dot\chi^2}{\mathfrak{n}^3}\left(-\dot\chi^2\frac{\dot{\mathfrak{n}}^2}{\mathfrak{n}^2}+4\dot\chi\ddot\chi\frac{\dot{\mathfrak{n}}}{\mathfrak{n}}-4\ddot\chi^2\right)=-\frac{\dot\chi^2}{\mathfrak{n}^3}\left(\dot\chi\frac{\dot{\mathfrak{n}}}{\mathfrak{n}}-2\ddot\chi\right)^2=\frac{\mathcal{Y}^2}{X},$$

$$\mathcal{W}=\frac{1}{\mathfrak{n}^2}\left(\frac{\dot\chi^2}{4}\frac{\dot{\mathfrak{n}}^2}{\mathfrak{n}^2}+\frac{3\dot\chi^2}{4}\frac{\dot{\mathfrak{a}}^2}{\mathfrak{a}^2}-\dot\chi\ddot\chi\frac{\dot{\mathfrak{n}}}{\mathfrak{n}}+\ddot\chi^2\right)=\left(\frac{\mathcal{Y}}{2X}\right)^2+\frac{1}{3}\left(\frac{\mathcal{Y}}{2X}-\mathcal{B}\right)^2.$$

Hence, for the FRW ansatz, $\mathcal{Z}$ and $\mathcal{W}$ are expressed by X, $\mathcal{B}$, and $\mathcal{Y}$ and are not independent. Also evaluating the terms appearing in Eq. (G1), we find that the metric after the transformation $\tilde g$ is expressed by the FRW ansatz

$$\tilde g_{\mu\nu}=\tilde{\mathfrak{n}}(t)dt^2+\tilde{\mathfrak{a}}(t)dx^2,\tag{G5}$$

and $\tilde{\mathfrak{n}}$ and $\tilde{\mathfrak{a}}$ are given by

$$\tilde{\mathfrak{n}}=\mathfrak{n}\left(\mathcal{F}_0+\mathcal{F}_1X+\mathcal{F}_2\frac{\mathcal{Y}}{2X}+\mathcal{F}_3\mathcal{Y}+\mathcal{F}_4\frac{\mathcal{Y}^2}{X}+\mathcal{F}_5\left(\frac{\mathcal{Y}}{2X}\right)^2\right):=\mathfrak{n}F_{\mathfrak{n}}(X,\mathcal{B},\mathcal{Y}),\tag{G6}$$

$$\tilde{\mathfrak{a}}=\mathfrak{a}\left(\mathcal{F}_0-\mathcal{F}_2\frac{1}{3}\left(\frac{\mathcal{Y}}{2X}-\mathcal{B}\right)+\mathcal{F}_5\frac{1}{9}\left(\frac{\mathcal{Y}}{2X}-\mathcal{B}\right)^2\right):=\mathfrak{a}F_{\mathfrak{a}}(X,\mathcal{B},\mathcal{Y}).$$

This result implies that the generalized disformal transformation in Eq. (G1) is completely governed by the functions $F_{\mathfrak{n}}(X,\mathcal{B},\mathcal{Y})$ and $F_{\mathfrak{a}}(X,\mathcal{B},\mathcal{Y})$ for the FRW ansatz.

G.2 The general disformal transformation reduced on the FRW spacetime

The transformation in Eq. (G6) involves only $\mathfrak{n}$, $\mathfrak{a}$, and their first derivatives, and hence its invertibility can be analyzed within the framework explained in Sect. 2. Based on this, we derive the invertibility conditions for the transformation in Eq. (G6) below.

Since the transformation in Eq. (G6) involves $\dot{\mathfrak{n}}$ and $\dot{\mathfrak{a}}$, A_{ia} must be degenerate for invertibility:

$$A_{ia}=\begin{pmatrix}\partial\tilde{\mathfrak{n}}/\partial\dot{\mathfrak{n}} & \partial\tilde{\mathfrak{n}}/\partial\dot{\mathfrak{a}}\\ \partial\tilde{\mathfrak{a}}/\partial\dot{\mathfrak{n}} & \partial\tilde{\mathfrak{a}}/\partial\dot{\mathfrak{a}}\end{pmatrix}=\frac{1}{2}\sqrt{\frac{-X}{\mathfrak{n}}}\begin{pmatrix}F_{\mathfrak{n},\mathcal{B}}+2XF_{\mathfrak{n},\mathcal{Y}} & -\frac{3\mathfrak{n}}{\mathfrak{a}}F_{\mathfrak{n},\mathcal{B}}\\ \frac{\mathfrak{a}}{\mathfrak{n}}\left(F_{\mathfrak{a},\mathcal{B}}+2XF_{\mathfrak{a},\mathcal{Y}}\right) & -3F_{\mathfrak{a},\mathcal{B}}\end{pmatrix},\tag{G7}$$

$$\det A=\frac{3X^2}{2\mathfrak{n}}\left(F_{\mathfrak{a},\mathcal{B}}F_{\mathfrak{n},\mathcal{Y}}-F_{\mathfrak{n},\mathcal{B}}F_{\mathfrak{a},\mathcal{Y}}\right)=0.\tag{G8}$$

Below we assume that the rank of the matrix A_{ia} is 1. When the rank of A_{ia} is zero, all the components of A_{ia} vanish and then the transformation in Eq. (G6) does not involve $\dot{\mathfrak{n}}$ and $\dot{\mathfrak{a}}$. In this case, the invertibility condition is simply given by $\det B_{ia}\neq 0$.

When the degeneracy condition in Eq. (G8) is satisfied, there exist zero eigenvectors n_i, m_a and their dual vectors V_i, U_a satisfying

$$n_iA_{ia}=0=A_{ia}m_a,\qquad n_in_i=1=m_am_a,\qquad n_i=\epsilon_{ij}V_j,\qquad m_a=\epsilon_{ab}U_b.\tag{G9}$$

They are given explicitly as

$$\begin{aligned}n_i&=N^{-1}\left(F_{\mathfrak{a},\mathcal{B}},-\tfrac{\mathfrak{n}}{\mathfrak{a}}F_{\mathfrak{n},\mathcal{B}}\right), & m_a&=M^{-1}\left(\tfrac{3\mathfrak{n}}{\mathfrak{a}}F_{\mathfrak{n},\mathcal{B}},2XF_{\mathfrak{n},\mathcal{Y}}+F_{\mathfrak{n},\mathcal{B}}\right),\\ V_i&=N^{-1}\left(-\tfrac{\mathfrak{n}}{\mathfrak{a}}F_{\mathfrak{n},\mathcal{B}},-F_{\mathfrak{a},\mathcal{B}}\right), & U_a&=M^{-1}\left(2XF_{\mathfrak{n},\mathcal{Y}}+F_{\mathfrak{n},\mathcal{B}},-\tfrac{3\mathfrak{n}}{\mathfrak{a}}F_{\mathfrak{n},\mathcal{B}}\right),\end{aligned}\tag{G10}$$

where M and N are normalization coefficients given by

$$M = \sqrt{(F_{\mathfrak{n},\mathcal{B}} + 2XF_{\mathfrak{n},\mathcal{Y}})^2 + (3\mathfrak{n}F_{\mathfrak{n},\mathcal{B}}/\mathfrak{a})^2}, \qquad N = \sqrt{F_{\mathfrak{a},\mathcal{B}}^2 + (\mathfrak{n}F_{\mathfrak{n},\mathcal{B}}/\mathfrak{a})^2}. \tag{G11}$$

We assume $M, N \neq 0$ below, and discuss the case where either M or N vanishes separately.

Using these expressions, the second degeneracy condition in Eq. (68) in the invertibility conditions is evaluated as

$$\begin{aligned} 0 &= n_i B_{ia} m_a \\ &= \frac{1}{MN}\frac{\mathfrak{n}F_{\mathfrak{n},\mathcal{B}}}{\mathfrak{a}}\left[3F_{\mathfrak{n}}F_{\mathfrak{a},\mathcal{B}} - F_{\mathfrak{a}}\left(F_{\mathfrak{n},\mathcal{B}} + 2XF_{\mathfrak{n},\mathcal{Y}}\right) + 3X\left(F_{\mathfrak{a},X}F_{\mathfrak{n},\mathcal{B}} - F_{\mathfrak{a},\mathcal{B}}F_{\mathfrak{n},X}\right)\right], \end{aligned} \tag{G12}$$

where we eliminated $F_{\mathfrak{a},\mathcal{Y}}$ using the first degeneracy condition in Eq. (G8).

The non-degeneracy conditions in Eq. (73) in the invertibility conditions are given as follows:

$$0 \neq n_i B_{ia} U_a = \frac{MF_{\mathfrak{a}}}{3N}, \tag{G13}$$

where we used the first and second degeneracy conditions in Eqs. (G8) and (G12) to simplify the expression. The other non-degeneracy condition can be derived after some calculations as

$$\begin{aligned} 0 &\neq \left(V_i B_{ia} - a\dot{U}_a\right) m_a \\ &= \frac{3N}{M}\left[-(-X)^{3/2}F_{\mathfrak{n},\mathcal{B}}\left(\frac{F_{\mathfrak{n},\mathcal{Y}}}{F_{\mathfrak{n},\mathcal{B}}}\right)' - F_{\mathfrak{n}} + XF_{\mathfrak{n},X} + \mathcal{B}F_{\mathfrak{n},\mathcal{B}} + \mathcal{Y}F_{\mathfrak{n},\mathcal{Y}}\right], \end{aligned} \tag{G14}$$

where a prime ($'$) denotes a derivative with respect to the proper time, i.e. $f' \equiv \mathfrak{n}^{-1/2}\dot{f}$. To simplify this equation we used the degeneracy conditions in Eqs. (G8) and (G12) and their t derivatives; that is, we assumed the degeneracy conditions in Eqs. (G8) and (G12) are satisfied identically at any t.

To summarize, the transformation in Eq. (G6) becomes invertible when the conditions in Eqs. (G8), (G12), (G13), and (G14) are satisfied. These conditions should be regarded as necessary conditions for the invertibility of the generalized disformal transformation in Eq. (G1) for a general metric, because the above results are derived only for the FRW ansatz in Eq. (G3), in which the degrees of freedom of the metric are reduced to two functions $\mathfrak{n}(t)$, $\mathfrak{a}(t)$ depending only on t. The invertibility conditions for a general metric should encompass the conditions in Eqs. (G8), (G12), (G13), and (G14), while they may contain more stringent conditions in general. An obvious next step is to derive the invertibility conditions for a more general metric, and also it would be interesting to construct examples of invertible transformations based on the invertibility conditions obtained above. We reserve those issues for future work.

Let us briefly mention the case that either M or N given by Eq. (G11) vanishes. In this case, it turns out that the degeneracy conditions imply that $F_{\mathfrak{n},\mathcal{B}} = F_{\mathfrak{n},\mathcal{Y}} = F_{\mathfrak{a},\mathcal{B}} = 0$, i.e. $F_{\mathfrak{n}} = F_{\mathfrak{n}}(X)$ and $F_{\mathfrak{a}} = F_{\mathfrak{a}}(X, \mathcal{Y})$. For these functions, it follows that

$$A_{ia} = -\left(\frac{-X}{\mathfrak{n}}\right)^{3/2}\begin{pmatrix} 0 & 0 \\ \mathfrak{a}F_{\mathfrak{a},\mathcal{Y}} & 0 \end{pmatrix}, \tag{G15}$$

and $V_i = (0, 1)$, $U_a = (1, 0)$. It can be shown that the first and second degeneracy conditions are automatically satisfied, and the non-degeneracy conditions are given by

$$F_{\mathfrak{n}} - XF_{\mathfrak{n},X} \neq 0, \qquad F_{\mathfrak{a}} \neq 0. \tag{G16}$$

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