

Anomaly of topological phase transition in one-dimensional fermionic systems at nonzero temperature

Xiao-Dong Cui¹

¹*Naval Aeronautical and Astronautics University, 264000 Yantai, China*

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Abstract

It was realized as an important progress in the field of topological matters that the nontrivial topological phase will be violated when temperature hits or exceeds a nonzero threshold. However, the concept of anomaly of topological phase transition is firstly introduced in the paper, referring to the nontrivial topological phase at nonzero temperature transitioned from a trivial one at zero temperature. A no-go theorem is here proved that the anomaly cannot happen to one-dimensional fermionic flat-band systems. Besides, the existence of the anomaly is obtained and analyzed by reexamining the mapping of the parameters of the system Hamiltonian in momentum space which plays a pivotal role in the anomaly rather than energy band.

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I. INTRODUCTION

Topological invariance is consistently at the core of topology in mathematics, which is usually characterized by topological invariants to classify topological objects. Often a newly-found topological invariant implies an even finer partition of topological equivalence classes; namely, two topological objects corresponding to different topological invariants must be topologically nonequivalent. Nowadays such an abstract mathematical concept has been widely applied in physics, especially in the field of topological matters [1–4], due to the celebrated TKNN's formula analogous to Gauss-Bonnet formula in differential topology, where the quantized Hall transversal conductivity σ_{xy} in units of e^2/h is 2π times an integer equaling to the integral of Berry curvature over two-dimensional Brillouin zone or equivalently two-dimensional torus [5, 7].

In the last decade, topological Uhlmann index or number was introduced as a new topological invariant via Uhlmann phase to characterize topological phases in nonzero-temperature quantum systems described by mixed quantum states [19–27]. It allows that classification of topological matters can no longer be confined to the case of pure quantum states describing zero-temperature quantum systems. Besides, available studies have evidently indicated that there exists a nonzero critical temperature T_c for topological phase transition [24–27], *i.e.*, the nontrivial topological index can be sustained below T_c but will be violated at and above T_c , in accordance with physical intuition. However, it is unaware whether a nontrivial

topological phase at nonzero temperature may be transitioned from a trivial one at zero temperature. The issue is here addressed and answered by reexamining the planar mapping of parameters of one-dimensional fermionic system Hamiltonians in momentum space. It will be seen that the geometric configuration of the mapping is an important factor making the phenomenon happen.

Topological Uhlmann index is based on the concept of Uhlmann phase which is briefly and practically reviewed here by the language of fiber bundles. Uhlmann's pioneer work generalizes the notion of Berry phase from pure quantum states to mixed quantum states [19–21]. Mixed quantum states ρ whose collection is denoted by ϱ are intrinsically operators, not as well as pure quantum states $|\psi\rangle$ constituting a Hilbert space endowed with the common inner product $(\psi_1, \psi_2) = \langle\psi_1|\psi_2\rangle$. To constitute a Hilbert space endowed with a proper inner product, mixed quantum states need a purification or homomorphism procedure: a mixed quantum state ρ is decomposed as $\rho = \omega\omega^\dagger$ by Hilbert-Schmidt decomposition theorem, where ω is a Hilbert-Schmidt operator and commonly called amplifier; next, given the non-uniqueness of Hilbert-Schmidt decomposition, the amplifier ω can be expressed via spectral decomposition $\rho = \sum_{j=1}^n p_j |\varphi_j\rangle\langle\varphi_j|$ as $\omega = \sqrt{\rho}u = \sum_{j=1}^n \sqrt{p_j} |\varphi_j\rangle\langle\varphi_j|u$ where $u \in U(n)$; and then, there exists an bijective mapping between the operator ω and the state $|\omega\rangle$, *i.e.*, $\omega \longleftrightarrow |\omega\rangle = \sum_{j=1}^n \sqrt{p_j} |\varphi_j\rangle \otimes \langle\varphi_j|u$; at last, all those states $|\omega\rangle$ constitute a Hilbert space $\mathcal{H}_\omega := \mathcal{H} \otimes \mathcal{H}^*$ endowed with Hilbert-Schmidt product $(\omega_1, \omega_2) = \text{Tr}(|\omega_1\rangle\langle\omega_2|)$ as inner product. So far, the quadruple $(\mathcal{H}_\omega, \varrho, \pi, U(n))$ has formed a fiber bundle where $\mathcal{H}_\omega/U(n) = \varrho$ or equivalently $\pi(\mathcal{H}_\omega) = \varrho$.

Following the prevailing practice in developing Berry phase [6–28], which begins from Berry's parallel transport condition by minimizing the distance between two pure quantum states $|\psi_1\rangle$ and $|\psi_2\rangle$, *i.e.*, $\min_{a_1, a_2 \in U(1)} \|\psi_1 a_1 - \psi_2 a_2\|$, to obtain the Berry's U(1) holonomy $a_2 a_1^\dagger = \langle\psi_2|\psi_1\rangle/|\langle\psi_2|\psi_1\rangle|$ and furthermore the Berry's connection 1-form $A_B = daa^\dagger = -i\text{Im}\langle\psi|d\psi\rangle$, Uhlmann's parallel transport condition by minimizing the distance between two amplifiers ω_1 and ω_2 , *i.e.*, $\min_{u_1, u_2 \in U(n)} \|\omega_1 u_1 - \omega_2 u_2\|$, can derive the Uhlmann's U(n) holonomy $u_2 u_1^\dagger = \sqrt{\rho_2}^{-1} \sqrt{\rho_1}^{-1} \sqrt{\sqrt{\rho_1} \rho_2 \sqrt{\rho_1}}$ and moreover the Uhlmann's connection 1-form $A_U = duu^\dagger = \sum_{i,j} |\psi_i\rangle \frac{\langle\psi_i|[d\sqrt{\rho}, \sqrt{\rho}]\psi_j\rangle}{p_i + p_j} \langle\psi_j|$ [22, 26]. Exactly as Berry's U(1) phase factor stemming from the accumulation of the Berry's connection 1-form along a closed trajectory, *i.e.*, $e^{i\Phi_B} = e^{\int A_B}$, Uhlmann's U(n) phase factor originates from the accumulation of the Uhlmann's connection 1-form along a closed trajectory, *i.e.*, $u = \mathcal{P}e^{\int A_U}$, where \mathcal{P} represents

the path ordering operator. Thus far, Uhlmann phase can be properly defined as

$$\Phi_U := \arg \text{Tr}(\rho \mathcal{P} e^{\oint A_U})$$

which possesses a $U(n)$ -gauge invariance as well as Berry phase $\Phi_B = -i \oint A_B$ possesses a $U(1)$ -gauge invariance [6–8].

II. TOPOLOGICAL UHLMANN INDEX DESCRIBED BY TWO-BAND HAMILTONIAN'S PARAMETERS

Two-band hamiltonians for one-dimensional fermionic systems are considered in this paper, which can be abstractly described as a quadratic form $H = \sum_k \Psi_k^\dagger H_k \Psi_k$ in units of Boltzmann constant and

$$\begin{aligned} H(k) &= h(k) + \mathbf{p}(k) \cdot \boldsymbol{\sigma} \\ &= h(k) + p_x(k)\sigma_x + p_y(k)\sigma_y + p_z(k)\sigma_z \end{aligned}$$

where $h(k)$ denotes the band offset and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices. The band eigenvalues of H_k can be written as

$$E_{\pm}(k) = h(k) \pm \Delta(k)$$

where $\Delta(k) = |\mathbf{p}(k)| = \sqrt{p_x^2(k) + p_y^2(k) + p_z^2(k)}$ denotes the half of the gap of $H(k)$, and the corresponding eigenvectors can be represented by

$$|\psi_{\pm}(k)\rangle = \frac{1}{\sqrt{2\Delta(k)[\Delta(k) \mp p_z(k)]}} \begin{pmatrix} p_x(k) - ip_y(k) \\ \pm\Delta(k) - p_z(k) \end{pmatrix}$$

When the system is at thermal equilibrium with particle number conserved and Fermi level in the gap, its one-particle Gibbs states can be expressed via $\text{Tr}(\mathbf{p}(k) \cdot \boldsymbol{\sigma}) = 0$ as

$$\rho(k) = \frac{e^{-\frac{H(k)}{T}}}{\text{Tr}(e^{-\frac{H(k)}{T}})} = \frac{1}{2} \left[1 - \frac{\tanh \frac{\Delta(k)}{T}}{\Delta(k)} \mathbf{p}(k) \cdot \boldsymbol{\sigma} \right].$$

Since p_x, p_y, p_z are on equal terms in the Hamiltonian $H(k)$ and the Gibbs state $\rho(k)$ is independent of the band offset $h(k)$, $p_z(k) \equiv 0$ and $h(k) \equiv 0$ can be set throughout this paper without loss of generality, which also means $H(k)$ has a chiral symmetry.

By applying the following equation

$$\mathbf{p}(k) \cdot \boldsymbol{\sigma} |\psi_{\pm}(k)\rangle = \pm \Delta(k) |\psi_{\pm}(k)\rangle,$$

the Uhlmann's connection 1-form A_U for $\rho(k)$ proves to be

$$\begin{aligned} A_U &= \sum_{i,j=+,-} |\psi_i(k)\rangle \frac{\langle \psi_i(k) | [d\sqrt{\rho}, \sqrt{\rho}] | \psi_j(k) \rangle}{p_i + p_j} \langle \psi_j(k) | \\ &= \left[1 - \operatorname{sech} \frac{\Delta(k)}{T} \right] \left(\langle \psi_-(k) | d\psi_+(k) \rangle |\psi_-(k)\rangle \langle \psi_+(k)| + \langle \psi_+(k) | d\psi_-(k) \rangle |\psi_+(k)\rangle \langle \psi_-(k)| \right). \end{aligned}$$

The planar mapping $\mathbf{p} : \mathbb{R} \rightarrow \mathbb{R}^2$ winds around a contour ∂S on the $O - p_x p_y$ plane as k changes as cycle of 2π , provided here that S denotes a simply connected and open area surrounded by the contour ∂S . The eigenvalues and eigenvectors are now expressed by p_x and p_y as

$$E_{\pm} = \pm \Delta(p_x, p_y), \quad |\psi_{\pm}\rangle = \frac{1}{\sqrt{2[p_x^2 + p_y^2]}} \begin{pmatrix} p_x - ip_y \\ \pm \sqrt{p_x^2 + p_y^2} \end{pmatrix},$$

and in the basis of which the Uhlmann's connection 1-form A_U comes to be

$$A_U = i \frac{1 - \operatorname{sech} \frac{\sqrt{p_x^2 + p_y^2}}{T}}{2(p_x^2 + p_y^2)} [p_y dp_x - p_x dp_y] \sigma_x.$$

Due to algebraic identity $\sigma_x^2 = 1$, the Uhlmann's $U(n)$ phase factor turns out to be

$$\begin{aligned} u &= \mathcal{P} e^{\oint A_U} \\ &= \frac{1}{2} \left[e^{i \oint_{\partial S} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)} - i \oint_{\partial S} \operatorname{sech} \frac{\sqrt{p_x^2 + p_y^2}}{T} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)}} + e^{-i \oint_{\partial S} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)} + i \oint_{\partial S} \operatorname{sech} \frac{\sqrt{p_x^2 + p_y^2}}{T} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)}} \right] \\ &\quad + \frac{\sigma_x}{2} \left[e^{i \oint_{\partial S} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)} - i \oint_{\partial S} \operatorname{sech} \frac{\sqrt{p_x^2 + p_y^2}}{T} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)}} + e^{-i \oint_{\partial S} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)} + i \oint_{\partial S} \operatorname{sech} \frac{\sqrt{p_x^2 + p_y^2}}{T} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)}} \right]. \end{aligned}$$

Furthermore, the corresponding Uhlmann phase can be derived as

$$\begin{aligned} \Phi_U &= \arg \operatorname{Tr}(\rho \mathcal{P} e^{\oint A_U}) \\ &= \arg \left[\cos \oint_{\partial S} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)} \cos \oint_{\partial S} \operatorname{sech} \frac{\sqrt{p_x^2 + p_y^2}}{T} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)} \right], \end{aligned}$$

whose possible value is merely 0 or π so that the topological Uhlmann index can be defined by

$$n_U := \Phi_U / \pi = \begin{cases} 0, & \Phi_U = 0 \\ 1, & \Phi_U = \pi \end{cases},$$

where the indices 0 and 1 correspond to the trivial and nontrivial topological phase, respectively.

III. ANOMALY OF TOPOLOGICAL PHASE TRANSITION AT NONZERO TEMPERATURE

Considering the identity

$$\oint_{\partial S} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)} = \begin{cases} 0, & (p_x, p_y) = (0, 0) \notin S \cup \partial S \\ \pi, & (p_x, p_y) = (0, 0) \in S \end{cases}$$

where the point $(0, 0)$ on the $O - p_x p_y$ plane is the unique singular point of the integral, the topological Uhlmann index for one-dimensional fermionic systems with two-band hamiltonians at zero temperature is followed by

$$\begin{aligned} n_U^0 &= \lim_{T \rightarrow 0} \arg \left[\cos \oint_{\partial S} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)} \cos \oint_{\partial S} \operatorname{sech} \frac{\sqrt{p_x^2 + p_y^2}}{T} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)} \right] \\ &= \frac{1}{\pi} \arg \left[\cos \oint_{\partial S} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)} \right] \\ &= \begin{cases} 0, & (p_x, p_y) = (0, 0) \notin S \cup \partial S \\ 1, & (p_x, p_y) = (0, 0) \in S \end{cases} \end{aligned}$$

where the interchangeability between limitation and integration holds. Namely, the system at zero temperature is at the trivial and nontrivial topological phase when the singular point $(0, 0)$ is outside and inside the contour ∂S , respectively. It had already been indicated that there exists a nonzero critical temperature T_c for the nontrivial topological phase which can be sustained below T_c but will be transitioned to the trivial one at and above T_c [24]. Such kind of topological phase transition is called normal.

However, it is to be naturally asked if the trivial topological phase may be transitioned to the nontrivial one as temperature rises from zero. Such kind of topological transition is in the paper called anomaly. To be more precisely, the definition of anomaly is given below:

Definition. *Provided the point $(0, 0)$ on the $O - p_x p_y$ plane is not a singularity, i.e., $(0, 0) \notin S \cup \partial S$, if the topological Uhlmann index which now reduces to*

$$n_U = \frac{1}{\pi} \arg \left[\cos \oint_{\partial S} \operatorname{sech} \frac{\sqrt{p_x^2 + p_y^2}}{T} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)} \right].$$

jumps from 0 to 1 as temperature T rises from zero, then such kind of topological phase transition is called anomaly.

The issue whether and how the anomaly may happen will be subsequently answered.

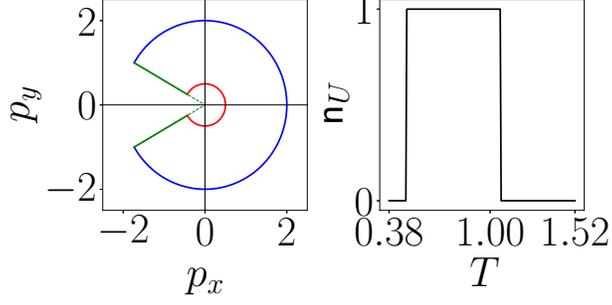


FIG. 1. The planar mapping \mathbf{p} “Pac-Man” in momentum space (left) and the corresponding anomaly of topological Uhlmann index driven by temperature (right). The contour is composed of a red curve, a blue curve and two green line, where the red curve denotes the constant lower bound function $\Delta_l(\theta) \equiv 0.5$ and the blue curve denotes the constant upper bound function $\Delta_u(\theta) \equiv 2$ of modulus r , respectively. The pair of green dashed lines starting from original point are tangent rays of the contour to confine the azimuth θ in $[-5\pi/6, 5\pi/6]$. The range of temperature T is set between 38% of the minimum gap and 38% of the maximum gap as considered. All parameters are dimensionless.

Theorem. *The anomaly cannot happen to one-dimensional fermionic flat-band systems.*

The theorem is equivalently to say there does not exist a transition temperature of the anomaly.

Proof. Considering $\varphi(T) := \oint_{\partial S} \text{sech} \frac{\sqrt{p_x^2 + p_y^2}}{T} \frac{p_y dp_x - p_x dp_y}{2(p_x^2 + p_y^2)}$ as a function of temperature T , topological Uhlmann index n_U may change with temperature T , especially that $n_U = 1$ is equivalent to that $\cos \varphi(T) < 0$. For the further calculation of $\varphi(T)$, it is convenient to transform the $O - p_x p_y$ plane to the polar coordinate plane. Here, every point (θ, r) of $S \cup \partial S$ in polar coordinate representation satisfies

$$\theta_{\min} := \left(\arctan \frac{p_y}{p_x} \right)_{\min} \leq \theta \leq \left(\arctan \frac{p_y}{p_x} \right)_{\max} =: \theta_{\max}$$

and

$$\Delta_l(\theta) \leq r \leq \Delta_u(\theta)$$

where $\Delta_l(\theta)$ and $\Delta_u(\theta)$ as the two segments of the contour ∂S divided by two tangent rays $\theta = \theta_{\min}$ and $\theta = \theta_{\max}$ are the lower and the upper bound functions, respectively.

Via Green’s formula in calculus, $\varphi(T)$ is calculated to be

$$\varphi(T) = \frac{1}{2} \int_{\theta_{\min}}^{\theta_{\max}} \left[\text{sech} \frac{\Delta_l(\theta)}{T} - \text{sech} \frac{\Delta_u(\theta)}{T} \right] d\theta.$$

By virtue of the inequality

$$\operatorname{sech} \frac{\Delta_l(\theta)}{T} - \operatorname{sech} \frac{\Delta_u(\theta)}{T} < \operatorname{sech} \frac{\Delta_{\min}}{T} - \operatorname{sech} \frac{\Delta_{\max}}{T} < 1$$

where Δ_{\min} and Δ_{\max} represent the half of the minimum and maximum gap, respectively, a necessary estimate must be

$$\pi < \frac{\pi}{\operatorname{sech} \frac{\Delta_{\min}}{T} - \operatorname{sech} \frac{\Delta_{\max}}{T}} < \theta_{\max} - \theta_{\min} < 2\pi$$

or equivalently

$$\operatorname{sech} \frac{\Delta_{\min}}{T} - \operatorname{sech} \frac{\Delta_{\max}}{T} > \frac{1}{2}$$

in order that $\cos \varphi(T) < 0$ possibly holds. Furthermore, due to the inequality $0 < \operatorname{sech} \frac{\Delta_{\max}}{T} < \operatorname{sech} \frac{\Delta_{\min}}{T} < 1$, a reasonable estimate of transition temperature of the anomaly T_c^a is followed by the inequality

$$\operatorname{sech} \frac{\Delta_{\max}}{T} < \frac{1}{2} < \operatorname{sech} \frac{\Delta_{\min}}{T}$$

which must hold and defines the admissible range of T_c^a , *i.e.*,

$$\frac{\Delta_{\min}}{\ln(2 + \sqrt{3})} < T_c^a < \frac{\Delta_{\max}}{\ln(2 + \sqrt{3})}$$

namely, T_c^a is situated approximately between 38% of the minimum gap and 38% of the maximum gap. It immediately implies there cannot exist any T_c^a for one-dimensional fermionic flat-band systems. And the proof is completed. \square

Besides, the theorem also implies the existence of the anomaly can merely happen to one-dimensional fermionic non-flat-band systems.

To demonstrate the existence of the anomaly, the planar mapping $\mathbf{p}(k)$ should be selected as simple as possible in order to simplify the calculation of $\varphi(T)$. Apparently it is the case that the upper and lower bound functions $\Delta_{u,l}(\theta)$ are both selected as constant functions, *i.e.*, $\Delta_u(\theta) \equiv \Delta_{\max}$ and $\Delta_l(\theta) \equiv \Delta_{\min}$. Accordingly, the contour of the planar mapping $\mathbf{p}(k)$ looks like ‘‘Pac-Man’’, a famous video-game character as illustrated in Fig.1(left). As expected, the topological Uhlmann index n_U indeed happens to jump from 0 to 1 and to be sustained within a certain temperature range; T_c^a appears in the range between 38% of the minimum gap and 38% of the maximum gap, *i.e.*, $T_c^a \in (0.38, 1.52)$, as illustrated in Fig.1(right). Such a simple example indicates that the concavity of planar mapping $\mathbf{p}(k)$ about the point $(0, 0)$ on the $O - p_x p_y$ plane plays a pivotal role in inducing the anomaly.

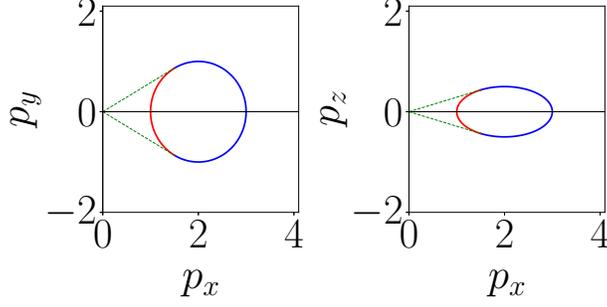


FIG. 2. The planar mapping \mathbf{p} of Polyacetylene (left) with $J_1 = -2$, $J_2 = 1$ and Creutz Ladder (right) with $m = 2$, $\Theta = \pi/6$ in momentum space. Every contour is composed of a red curve and a blue one which denote the lower bound function $\Delta_l(\theta)$ and the upper bound function $\Delta_u(\theta)$ of modulus r , respectively. Every pair of green dashed lines starting from original point are tangent rays of the contour to describe the range of azimuth θ . All parameters are dimensionless.

IV. DISCUSSION AND CONCLUSION

The following examples provide the reason why the anomaly of topological phase transition in one-dimensional fermionic systems was not found. Polyacetylene or a SSH model introduced for topological insulating phase in momentum space is written by

$$H_{\text{SSH}} = (-J_1 - J_2 \cos k)\sigma_x + J_2 \sin k\sigma_y.$$

The corresponding planar mapping is a circle on the $O - p_x p_y$ plane represented by the equation

$$\frac{(p_x + J_1)^2}{J_2^2} + \frac{p_y^2}{J_2^2} = 1,$$

whose convexity about the point $(0, 0)$ leads to $\theta_{\max} - \theta_{\min} < \pi$ as illustrated in Fig.1(left), and it is therefore impossible to cause the anomaly no matter how the temperature T changes. Similarly, the same situation happens to Creutz Ladder (as illustrated in Fig.2(right))

$$H_{\text{CL}} = (m + \cos k)\sigma_x + \sin \Theta \sin k\sigma_z$$

whose planar mapping is an ellipse on the $O - p_x p_z$ plane represented by the equation

$$\frac{(p_x - m)^2}{1} + \frac{p_z^2}{\sin^2 \Theta} = 1,$$

and so does Majorana Chain

$$H_{\text{MC}} = -\sin k\sigma_y + (-m + c \cos k)\sigma_z,$$

whose planar mappings is also an ellipse on the $O - p_y p_z$ plane.

Finally, it is here stressed that the admissible range of transition temperature of the anomaly T_c^a as a reasonable but rough estimate based on two simple energy band indices, the minimum and maximum gap, is a necessary rather than sufficient condition for the anomaly of topological phase transition, which may be useful only after examining the geometric configuration of the mapping of parameters of the system Hamiltonian.

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