Conserved currents for Mobius Domain Wall Fermions

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We derive the exactly conserved vector, and almost conserved axial currents for rational approximations to the overlap operator with a general Mobius kernel. The approach maintains manifest Hermiticity, and allows matrix elements of the currents to be constructed at no extra cost after solution of the usual 5d system of equations, similar to the original approach of Furman and Shamir for domain wall Fermions.
RBC and UKQCD have recently adopted the Möbius generalisation of the domain wall action [1, 2, 3]. Our conventions are as follows. The usual Wilson matrix is 

\[ D_W(M) = M + 4 - \frac{1}{2}D_{\text{hop}}, \]

where 

\[ D_{\text{hop}} = (1 - \gamma_\mu U_\mu(x))\delta_{\epsilon + \mu, y} + (1 + \gamma_\mu U_\mu^\dagger(y))\delta_{\epsilon - \mu, y}. \]

We introduce the five dimensional action 

\[ S^5 = \bar{\psi} D_{GDW}^5 \psi \]

where

\[ D_{GDW}^5 = \begin{pmatrix} D - P_+ & 0 & \ldots & 0 & mP_+ \\ -P_+ & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & \ddots & -P_+ \\ mP_- & 0 & \ldots & 0 & -P_+ & D \end{pmatrix}, \]

and we define 

\[ D_+ = (b D_W + 1) ; \quad D_- = (1 - c D_W) ; \quad \tilde{D} = (D_-)^{-1} D_+. \]

This generalized set of actions reduces to the standard Shamir action in the limit \( b = 1, c = 0 \), and it can also be taken to give the polar approximation to the Neuberger overlap action as another limiting case [4, 5]. In all of our simulations we take the coefficients \( b \) and \( c \) as constant across the fifth dimension, as in the Shamir domain wall fermion formulation we identify “physical”, four-dimensional quark fields \( q \) and \( \bar{q} \) whose Green’s functions define our domain wall fermion approximation to continuum QCD. We choose to construct these as simple chiral projections of the five-dimensional fields \( \psi \) and \( \bar{\psi} \) which appear in the action.

\[ q_R = P_\gamma \psi_L, \quad q_L = P_- \bar{\psi}_1, \quad \bar{q}_R = \bar{\psi}_L P_+, \quad \bar{q}_L = \bar{\psi}_1 P_. \]

The choice of physical quark fields given in Eq. (2) has the added benefit that the corresponding four-dimensional propagators satisfy a simple \( \gamma^5 \) hermiticity relation and a hermitian, partially conserved axial current can be easily defined. If we introduce the so-called transfer matrix as

\[ T^{-1} = -(Q_-)^{-1} Q_+ = -[H_M - 1]^{-1} [H_M + 1], \]

and define the Möbius kernel as

\[ H^M = \gamma_5 \frac{(b + c) D_W}{2 + (b - c) D_W}. \]

One can show that \( D_{GDW}^5 \) takes the following form [1, 2, 3],

\[ D_{GDW}^5 = \begin{pmatrix} P_- - mP_+ & -T^{-1} & 0 & \ldots & 0 \\ 0 & 1 & -T^{-1} & 0 & \vdots \\ \vdots & 0 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \ldots & 0 & 1 & -T^{-1} \\ -T^{-1} (P_+ - mP_-) & 0 & \ldots & 0 & 1 \end{pmatrix}, \]

for which we can perform a UDL decomposition around the top left block:

\[ \begin{pmatrix} D & C \\ B & A \end{pmatrix} = \begin{pmatrix} 1 & CA^{-1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} S_{\chi} & 0 \\ 0 & A \end{pmatrix} \begin{pmatrix} 1 & 0 \\ A^{-1} B & 1 \end{pmatrix}. \]
Denoting the left and right factors as \( U \) and \( L(m) \) respectively, we write this factorisation as \( D^5_\chi = UDS(m)L(m). \) The determinants of the \( U \) and \( L(m) \) are unity, and the determinant of the product is 

\[
\det D^5_\chi = \det A \det S_\chi = \det S_\chi,
\]

where

\[
S_\chi(m) = -(1 + T^{-L}\gamma_s \left[ \frac{1 + m}{2} \gamma_s + \frac{1 - m}{2} T^{-L} - 1 \right]).
\]

We can see that after the removal of the determinant of the Pauli Villars fields we are left with the determinant of an effective overlap operator, which is the following rational function of the kernel:

\[
\det D^5_{\psi}D(m) = \det D_{\text{ov}} = \det \left( \frac{1 + m}{2} + \frac{1 - m}{2} \gamma_s (1 + H_M)^{L} - (1 - H_M)^{L} \right). \tag{8}
\]

We identify \( D_{\text{ov}} \) as an approximation to the overlap operator with approximate sign function

\[
\epsilon(H_M) = \frac{(1 + H_M)^{L} - (1 - H_M)^{L}}{(1 + H_M)^{L} + (1 - H_M)^{L}}. \tag{9}
\]

The approximate overlap operator can be written as \( D_{\text{ov}} = S_\chi(m = 1)^{-1}S_\chi(m) \). If we solve the following 5d system of equations and substitute the UDL decomposition,

\[
D^5_\chi(m = 1)^{-1}D^5_{\text{ov}}(m)\phi = (q, 0, \ldots, 0)^T, \tag{10}
\]

the approximate overlap operator can be expressed in terms of the \( \psi \) basis fields,

\[
D_{\text{ov}} = S_\chi(m = 1)^{-1}S_\chi(m) = \left[ \mathcal{P}^{-1}D_{\text{GDW}}^5(m = 1)^{-1}D_{\text{GDW}}^5(m)\mathcal{P} \right]_{11}. \tag{11}
\]

The cancellation the Pauli-Villars term can be expressed in terms of unmodified generalised domain wall matrix \( D_{\text{GDW}}^5 \). The contact term can be subtracted from the overlap propagator. We define

\[
D_{\text{ov}}^{-1} = \frac{1}{1 - m} \left[ D_{\text{ov}}^{-1} - 1 \right] = \frac{1}{1 - m} \left\{ \mathcal{P}^{-1}D_{\text{GDW}}^5(m = 1)^{-1} \left[ D_{\text{GDW}}^5(m = 1) - D_{\text{GDW}}^5(m) \right] \mathcal{P} \right\}_{11}. \tag{12}
\]

Now, the difference \( \left[ D_{\text{GDW}}^5(m = 1) - D_{\text{GDW}}^5(m) \right]_{ij} = (1 - m) [P_+ \delta_{i,1} \delta_{j,1} + P_- \delta_{i,1} \delta_{j,L_{s}}] \). This relation is simpler to interpret in our convention than with the convention from [3]: the mass term is applied to our five dimensional surface fields without field rotation. With this,

\[
\tilde{D}_{\text{ov}}^{-1} = \left\{ \mathcal{P}^{-1}D_{\text{GDW}}^5(m = 1)^{-1}R_{5}\mathcal{P} \right\}_{11}. \tag{13}
\]

This is just the normal valence propagator of the physical DWF fields \( q = (\mathcal{P}^{-1}\psi)_1 \) and \( \tilde{q} = (\psi R_{5}\mathcal{P})_1 \). We see that the usual domain wall valence propagator has always contained both the contact term subtraction and the appropriate multiplicative renormalisation of the overlap fermion propagator. As a result, the issues of lattice artefacts in NPR raised in reference [6] have never been present in domain wall valence analyses. This was guaranteed to be the case because Shamir’s 5d construction is designed to exactly suppress chiral symmetry breaking in the limit of infinite \( L_{s} \), including any contact term. For later use, we may also consider the propagator into the bulk from a surface field \( q \) for Mobius fermions

\[
\langle Q_1 \bar{q} \rangle = \left[ \mathcal{P}^{-1}D_{\text{GDW}}^5(m)^{-1}R_{5}\mathcal{P} \right]_{11} = \frac{1}{1 - m} \left\{ L^{-1}(m) \left( \frac{S_\chi^{-1}(m)S_\chi(1)}{0} \right) L(1) - I \right\}_{11}. \tag{14}
\]
Now,

\[
L(m) = \begin{pmatrix}
-T^{-1}(m_0-1)(P_+ - mP_-) & 0 \\
\vdots & \ddots \\
-T^{-1}(P_+ - mP_-) & 0 \\
\end{pmatrix} ;
L(m)^{-1} = \begin{pmatrix}
-T^{-1}(m_0-1)(P_+ - mP_-) & 0 \\
\vdots & \ddots \\
T^{-1}(P_+ - mP_-) & 0 \\
\end{pmatrix}
\]

Finally, applying \( \mathcal{P} \), we have the five dimensional propagator from a physical field,

\[
G_y = \mathcal{P} \langle Q, \bar{Q} \rangle = [P_+ + P_- T^{-1}] \begin{pmatrix}
T^{-1}(m_0-1) \\
T^{-1}(m_0-2) \\
\vdots \\
T^{-1} \\
1 \\
\end{pmatrix} [1 + T^{-1}L_s]^{-1} D_{yv}^{-1}.
\]

The connection between domain wall systems and the overlap, well established in the literature and reproduced in this section, is needed in the following derivation of conserved currents.

1. **Conserved vector and axial currents**

The standard derivation of lattice Ward identities proceeds as follows. A change variables of the fermion fields \( \psi \) and \( \bar{\psi} \) at a single site \( y \) is performed: \( \psi'_y = \psi_y - i\alpha \psi_y ; \bar{\psi}'_y = \bar{\psi}_y + i\psi_y \alpha \) under the path integral, the Jacobian is unity, and the partition function is left invariant

\[
Z' = \int d\bar{\psi}d\psi e^{-S[\bar{\psi}, \psi]} \left\{ 1 - i\alpha \left[ \frac{\delta S}{\delta \psi_y} \psi_y - \bar{\psi}_y \frac{\delta S}{\delta \bar{\psi}_y} \right] \right\} = Z.
\]

Hence,

\[
\frac{\delta S}{\delta \bar{\psi}_y} \psi_y - \bar{\psi}_y \frac{\delta S}{\delta \psi_y} = 0.
\]

The Wilson action gives eight terms from varying \( \bar{\psi}_y \) and eight terms from varying \( \psi_y \):

\[
\bar{\psi}_y \delta_y (D_W) \psi = \Delta^\mu \psi^W_\mu (y) = \Delta^\mu \left[ \psi_y \frac{1 - \gamma_\mu}{2} U_\mu (y) \psi_{y + \mu} - \bar{\psi}_{y + \mu} U^\dagger_\mu (y) \psi_y \right] = 0,
\]

where \( \Delta^\mu \) is the backwards discretized derivative. An equivalent alternate approach may be taken, however, and this is a better way to approach non-local actions such as the chiral fermions. Gauge symmetry leaves the action invariant at \( O(\alpha) \) under the simultaneous active substitution,

\[
U_\mu (y) \to (1 + i\alpha) U_\mu (y) ; \quad U_{\mu} (y \rightarrow \mu) \to U_{\mu} (y - \mu) (1 - i\alpha); \quad \psi_y \to (1 + i\alpha) \psi_y ; \quad \bar{\psi}_y \to \bar{\psi}_y (1 - i\alpha).
\]

A change variables on the fermion fields at site \( y \) may be performed simultaneously to absorb the phase on the fermions, \( \psi'_y = (1 + i\alpha) \psi_y ; \bar{\psi}'_y = \bar{\psi}_y (1 - i\alpha) \). Under the path integral, the Jacobian is unity, and the phase associated with the fermion is absorbed. We can now view the change in action as being associated with the unabsorbed phases on the eight gauge links connected to site \( y \).

\[
Z' = Z = \int d\bar{\psi}' d\psi' e^{-S[\bar{\psi}', \psi']} \left\{ 1 + i\alpha \sum_\mu \left[ \frac{\delta S}{\delta U_\mu (y)} U_\mu (y) U_\mu (y) - \frac{\delta S}{\delta U_\mu (y - \mu)} U_\mu (y - \mu) U_\mu (y) \right] \right\}.
\]
For a gauge invariant Lagrangian we can always use a picture where the same change in action, and same current conservation law may be arrived at by differentiating with respect to the eight links connected to a site
\[
\left\langle \sum_{\mu} \left[ \frac{\delta S}{\delta U_{\mu}(y)} U_{\mu}(y)_{ij}^{y} - \frac{\delta S}{\delta U_{\mu}(y - \mu)} U_{\mu}(y - \mu)_{ij}^{y} \right] \right\rangle = 0. \tag{1.6}
\]

This arises because the phase freedom of fermions and of gauge fields are necessarily coupled and inseparable in a gauge theory. For the nearest neighbour Wilson action this generates the same eight terms entering \( \Delta \mu J_\mu = 0 \). In the case of non-local actions, the Dirac matrix, whatever it is, can be viewed as a sum of gauge covariant paths. When we generating a current conservation law from \( U(1) \) rotation of the fermion field at site \( y \), we sum over all fields \( \bar{\psi}(x) \) and \( \psi(x) \) connecting through the Dirac matrix \( D(x,y) \) to the fixed site \( \psi(y) \) and \( \bar{\psi}(y) \). The following sum is always constrained to be zero for all \( y \), and is identical to that found by Kikukawa and Yamada \[7\]:
\[
\sum_x \bar{\psi}_x D(x,y) \psi_y - \bar{\psi}_y D(y,x) \psi_x = 0. \tag{1.7}
\]
The partitioning of this sum of terms, into a paired discrete divergence operator and current is not obvious, and it is cumbersome to generate Kikukawa and Yamada’s non-local kernel. We may derive the same sum of terms by differentiating with respect to the 8 links connected to site \( y \).
\[
\left\langle \sum_{\mu} \left[ \frac{\delta S}{\delta U_{\mu}(y)} U_{\mu}(y)_{ij}^{y} - \frac{\delta S}{\delta U_{\mu}(y - \mu)} U_{\mu}(y - \mu)_{ij}^{y} \right] \right\rangle = 0 \tag{1.8}
\]
The structure of eqn. 1.8 always lends itself interpretation as a backwards finite difference. For a non-local action the differentiation eqn. 1.8 appears to generate a lot more terms than the fermion field differentiation eqn. 1.7. The reason is clear: these extra terms are constrained by gauge symmetry to sum to zero, but only after cancellation between the different terms in eqn. 1.8. Specifically, we consider an action constructed as the product of Wilson matrices:
\[
S = \sum_{xycw} \bar{\psi}_x D_W(x,y) D_W(y,z) D_W(z,w) \psi(w). \tag{1.9}
\]
The link variation approach gives three terms, each of which are conserved under a nearest neighbour difference divergence: varying with respect to the 8 links we obtain via the product rule
\[
\delta_y (\bar{\psi} D_W D_W \psi) \psi = \psi \left[ (\delta_y D_W) D_W + D_W (\delta_y D_W) + D_W D_W (\delta_y D_W) \right] \psi \tag{1.10}
\]
Each of these contributions contain a backwards difference operator and it is trivial to split this into a divergence and corresponding conserved current using eqn. (1.3). The above comment is generally applicable to any function of the Wilson matrix. We take this approach to establish the exactly conserved vector current of an approximate overlap operator, where the approximation is represented by a rational function. We will also establish that matrix elements of this current are identical to those of the Furman and Shamir approach \[8\] in the case of domain wall fermions. The Furman and Shamir approach will then be used to also establish an axial Ward identity for our generalised Möbius domain wall fermions, under which an explicitly known defect arises. This
is important in both renormalising lattice operators and also in determining the most appropriate measure of residual chiral symmetry breaking in our simulations. We construct the conserved vector current by determining the variation in the overlap Dirac operator $\delta_{\mu}D_{ov}$

$$\delta_{\mu}D_{ov} = \frac{1 - m}{2} \gamma_{S} \left\{ \delta_{\mu} \left[ \frac{1}{1 + T - L_s} \right] \delta_{\mu} \right\} = \frac{1 - m}{1 + T - L_s} \gamma_{S} \left\{ \delta_{\mu} \left[ \frac{1}{1 + T - L_s} \right] \delta_{\mu} \right\} .$$

We can similarly find the variation in $T^{-1}$ induced by a variation in $D_{W}$, where the variation in $D_{W}$ is just the backwards divergence of the standard Wilson conserved current operator. Denoting,

$$T^{-1} = -(\hat{Q})^{-1} \hat{Q},$$

$$\hat{Q}_{-} = D_{\mu} P_{-} - D_{-} P_{-} = D_{-} \gamma_{S} Q_{-},$$

$$\hat{Q}_{+} = D_{\mu} P_{+} - D_{+} P_{+} = D_{+} \gamma_{S} Q_{+},$$

we see that

$$\delta_{\mu}(T^{-1}) = -\hat{Q}_{-}^{-1} \delta_{\mu}(D_{W}) \left\{ (b P_{-} + c P_{+}) T^{-1} + b P_{+} + c P_{-} \right\} .$$

Since

$$\hat{Q}_{-} P_{-} = (1 + b D_{W}) P_{-} ; \hat{Q}_{+} P_{-} = (c D_{W} - 1) P_{-}$$

$$\hat{Q}_{-} P_{+} = (c D_{W} - 1) P_{+} ; \hat{Q}_{+} P_{+} = (1 + b D_{W}) P_{+},$$

we may reexpress the identity

$$\hat{Q}_{-}^{-1} (P_{+} + P_{-}) = \frac{\hat{Q}_{-}^{-1}}{b + c} \left[ \hat{Q}_{+} (c P_{+} - b P_{-}) + \hat{Q}_{-} (c P_{-} - b P_{+}) \right] ,$$

and this lets us find a symmetrical form:

$$(b + c)\delta_{\mu}(T^{-1}) = [b P_{+} - T^{-1} P_{-} + c [T^{-1} P_{+} - P_{-}]] \delta_{\mu}(D_{W}) \left[ b [P_{+} + P_{-} T^{-1}] + c [P_{-} T^{-1} + P_{-}] \right] .$$

We may now look at the variation of the term $T^{-L_s}$

$$\delta_{\mu}(T^{-L_s}) = \sum_{s=1}^{L_s} T^{-(s-1)} \left[ b P_{+} - T^{-1} P_{-} \right] \delta_{\mu}(D_{W}) \left[ b P_{+} + P_{-} T^{-1} + c [P_{-} T^{-1} + P_{-}] \right] .$$

Pulling these results together, we find

$$\delta_{\mu}D_{ov} = \frac{1 - m}{b + c} \gamma_{S} \frac{1}{1 + T - L_s} \left( \sum_{s=0}^{L_s} T^{-(s-1)} \delta_{\mu}(T^{-1}) T^{-(L_s-s)} \right) \frac{1}{1 + T - L_s} .$$

The terms may be expanded until insertions of the the backwards divergence of the Wilson current are reached, eqn. 1.3. Gauge symmetry then implies the conservation of the obvious current and the vector Ward identities can be constructed. For example, we may take as source $\eta^{J_{\mu}a\alpha'}(z) = \delta_{\mu,\alpha} \alpha' \delta^{4}(z - x)$ and a two point function of the conserved current may be constructed as

$$\Delta_{\mu} \langle \tilde{\eta} \gamma_{S} \gamma_{\mu}(x) \gamma_{\mu}(y) \rangle = \text{Tr} \gamma_{S} \gamma_{\mu} \eta^{J_{\mu}a\alpha'}(1 + T - L_s)^{-1} \left( \sum_{s=0}^{L_s} T^{-s} \delta_{\mu}(T^{-1}) T^{-(L_s-s)} \right) [1 + T^{-L_s}]^{-1} D_{ov}^{-1} \eta .$$

(1.16)
Note that when $c = 0$ the insertion of eqn. 1.14 contains only terms such as $[P_+ T^{-1} + P_-]$, which are also present in the surface to bulk propagator eqn. 16. As one would expect, when we take $b$ and $c$ to represent domain wall fermions, the two point function of our exactly conserved vector current - derived from the four dimensional effective action - exactly matches the matrix element of the vector current constructed by Furman and Shamir [8], eqn. (2.21), from a five dimensional interpretation of the action. Since the Furman and Shamir current was easily constructed from the five dimensional propagator eqn. (16) one might hope to do the same in the generalised approach to domain wall fermions. To play a similar trick for the $c$ term we would need to generate the terms $P_+ [1 + T^{-L_1}]^{-1} D_{ov}^{-1}$, and $P_+ T^{-1}_1 [1 + T^{-L_1}]^{-1} D_{ov}^{-1}$. These are not manifestly present in eqn. 1.16. However, the presence of the contact term on the $s = 0$ slice can be removed after a propagator calculation. We define this slice as $S(x) = \langle Q_0 \bar{q} \rangle = \frac{1}{1-m} \langle D_{ov}^{-1}(m) - 1 \rangle$. In a practical calculation the source vector $\eta$ may be used to eliminate the contact term by forming

$$(1-m)S(x)\eta + \eta = D_{ov}^{-1}(m)\eta = [1 + T^{-L_1}] [1 + T^{-L_2}]^{-1} D_{ov}^{-1} \eta. \quad (1.17)$$

By applying $P_+$ and $P_-$ we find we have the following set of vectors

$$( P_+ P_- T^{-L_1} P_+ [1 + T^{-L_2}] P_- [1 + T^{-L_1}] )^T [1 + T^{-L_2}]^{-1} D_{ov}^{-1}, \quad (1.18)$$

and we may eliminate to form a $L_d + 1$ vectors from a 4d source $\eta$

$$T(s) = \left( 1, T^{-1}, \ldots, T^{-L_1} \right)^T [1 + T^{-1}_{L_1} \cdots T^{-1}_{L_2}]^{-1} D_{ov}^{-1}(m) \eta. \quad (1.19)$$

This may be used to construct

$$[b[P_+ P_- T^{-1}] + c[P_+ T^{-1} + P_-)] T^s, \quad (1.20)$$

for $s \in \{0 \ldots L_d - 1\}$, and by contracting these vectors through the Wilson conserved current the the matrix element eqn. 1.16 can be formed a very similar manner to the standard DWF conserved vector current. When $c = 0$ the matrix element reduces to being identical to that for the Furman and Shamir vector current. A flavour non-singlet axial current, almost conserved under a backwards difference operator, can now also be constructed following Furman and Shamir. We associate a fermion field rotation

$$\psi(x,s) \rightarrow \left\{\begin{array}{cc} e^{i\alpha \Gamma(s)\psi(x,s)} & ; x = x_0 \\ \psi(x,s) & ; x \neq x_0 \end{array}\right\} \Gamma(s) \rightarrow \left\{\begin{array}{cc} -1 & ; 0 \leq s < L_3/2 \\ 1 & ; L_3/2 \leq s \end{array}\right\}. \quad (1.21)$$

We acquire a related (almost) conserved axial current, whose pseudoscalar matrix element is

$$\Delta_{\mu}^{-} \langle \bar{\psi} \gamma_{5} \psi(x) | \sigma_{\mu}(y) \rangle = \text{Tr}[\eta^T D_{ov}^{-1} \bar{\gamma}_{5}] [1 + T^{-L_1}]^{-1}\left\{ \sum_{s=0}^{L_2-1} T^{-s} \delta_{y,0} \right\} [1 + T^{-L_2}]^{-1} D_{ov}^{-1} \eta \quad (1.22)$$

This generalisation of the Furman and Shamir approach induces the same $J_{s\theta}$ midpoint density defect that arose for DWF, and the axial Ward identity is

$$\Delta_{\mu}^{-} \langle \bar{\psi} \gamma_{5} \psi(x) | \sigma_{\mu}(y) \rangle = \langle \bar{\psi} \gamma_{5} \psi(x) | 2mP(y) + 2J_{s\theta}(y) \rangle. \quad (1.23)$$


This allows us to retain the usual definition of the residual mass in the case of Möbius domain wall fermions. We emphasize that the definition,

\[
m_{\text{res}} = \frac{\langle \pi (\vec{p} = 0) | J_{5q} \rangle}{\langle \pi (\vec{p} = 0) | P \rangle} \bigg|_{m=-m_{\text{res}}},
\]

via the zero-momentum pion matrix element of \( J_{5q} \) is important, because the PCAC relation,

\[
\langle \pi (\vec{p} = 0) | 2mP + 2J_{5q} \rangle = 0,
\]

guarantees that the low momentum lattice pions are massless. This is the appropriate measure of chiral symmetry breaking for the analysis of the chiral expansion.

Figure 1: As a numerical proof of the correctness we display the difference of the left and right hand sides of the axial Ward identity evaluated on a 16\(^3\) configuration with a point source. The defect is of order the convergence error.

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