THE POLYLOG QUOTIENT AND THE GONCHAROV QUOTIENT IN COMPUTATIONAL CHABAUTY-KIM THEORY I

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Abstract

Polylogarithms are those multiple polylogarithms which factor through a certain quotient of the de Rham fundamental group of the thrice punctured line known as the polylogarithmic quotient. Building on work of Dan-Cohen–Wewers, Dan-Cohen, and Brown, we push the computational boundary of our explicit motivic version of Kim’s method in the case of the thrice punctured line over an open subscheme of Spec $\mathbb{Z}$. To do so, we develop a greatly refined version of the algorithm of Dan-Cohen tailored specifically to this case, and we focus attention on the polylogarithmic quotient. This allows us to restrict our calculus with motivic iterated integrals to the so-called depth-one part of the mixed Tate Galois group studied extensively by Goncharov. We also discover an interesting consequence of the symmetry-breaking nature of the polylog quotient that forces us to symmetrize our polylogarithmic version of Kim’s conjecture.

In this first part of a two-part series, we focus on a specific example, which allows us to verify an interesting new case of Kim’s conjecture.

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1. Introduction

1.1. Classical Chabauty’s Method. The Chabauty-Skolem method proves that certain equations have finitely many integral solutions, and, by innovations of Coleman, allows one to find all solutions. The idea is to embed the scheme $X$ defined by the equations (which, geometrically, should be a smooth irreducible curve of negative Euler characteristic) over an open integer scheme $Z = \mathcal{O}_K[1/S]$ (for $K$ a number field and $S$ a finite set of finite places of $K$) into a scheme $J$ with more structure, specifically that of a semiabelian variety (to do this, one takes a generalized Jacobian of $X$). One then choose a closed point $p$ of $Z$ and looks at the intersection of the $p$-adic closure of $J(Z)$ with $X(Z_p)$ (with $Z_p$ the completed local ring of $Z$ at $p$) inside the $p$-adic analytic space $J(Z_p)$ (where $p$ is a prime of good reduction for $X$ lying above $p$). The method of Coleman then sometimes allows one to find explicit $p$-adic analytic functions on $X(Z_p)$ that vanish on $X(Z)$ and have finitely many zeroes (i.e., Coleman functions).

1.2. Minhyong Kim’s Non-abelian Chabauty. This method often does not work, because $J(Z)$ can be too large. Philosophically, the reason why $J(Z)$ can be large while $X(Z)$ remains finite is because the geometric fundamental group of $J$ is abelian (as opposed to hyperbolic curves like $X$, whose fundamental groups are non-abelian, even center-free). The groundbreaking work of Minhyong Kim ([Kim05]) gets around this fact. First, it reinterprets the Chabauty-Skolem method by replacing $J(Z)$ (or its $p$-adic closure) by a corresponding $p$-adic Selmer group. By the work of Bloch-Kato ([BK90]), this can be expressed intrinsically in terms of the $p$-adic Tate module of $J$, which is the abelianization of the pro-$p$ étale fundamental group of $X_K$. Then, one replaces this abelianization by a mildly non-abelian version, namely, the $n$th quotient of the descending central series of the pro-$p$ étale fundamental group of $X_K$ for a natural number $n$.

\footnote{This is not to say that all varieties with abelian fundamental group have infinitely many integral points, but that in the context of the distinction between a curve and its Jacobian, this principle applies.}
Thus the $p$-adic Selmer group is replaced by the Selmer variety $\text{Sel}(X/Z)_n$ of [Kim09]. In particular, for a place $\mathfrak{p}$ of $K$ over $p$, Kim constructs a commutative diagram ([Kim05], [Kim09])

$$
\begin{array}{ccc}
X(Z) & \xrightarrow{\kappa} & X(Z_{\mathfrak{p}}) \\
\downarrow{\kappa_p} & & \downarrow{\kappa_p} \\
\text{Sel}(X/Z)_n & \xrightarrow{\text{loc}_n} & \text{Sel}(X/Z_{\mathfrak{p}})_n
\end{array}
$$

The goal, which was realized when $X = \mathbb{P}^1 \setminus \{0, 1, \infty\}$ in [Kim05], is to prove that the morphism of schemes $\text{loc}_n$ is non-dominant for sufficiently large $n$. This means that there is a nonzero ideal $\mathcal{I}_n^Z$ of functions on $\text{Sel}(X/Z_{\mathfrak{p}})_n$ that vanish on the image of $\text{loc}_n$. These functions pull back via $\kappa_p$ to Coleman functions on $X(Z_{\mathfrak{p}})$, which, by the commutativity of this diagram, vanish on $X(Z)$. We let $X(Z_{\mathfrak{p}})_n$ be the set of common zeroes of all pullbacks of elements of $\mathcal{I}_n^Z$, and we note that this sequence of sets is decreasing in $n$ and contains $X(Z)$. The map $\kappa_p$ can be expressed in terms of $p$-adic iterated integrals, which makes the method more concrete.

The original work of Kim ([Kim05]) dealt with the case of $X = \mathbb{P}^1 \setminus \{0, 1, \infty\}$. That work shows that $\mathcal{I}_n^Z$ is nonzero for sufficiently large $n$ and hence that $X(Z_{\mathfrak{p}})_n$ is finite for such $n$, thereby reproving a 1929 theorem of Siegel that $X(Z)$ is finite. This paper is part of the effort to develop algorithms for computing $X(Z_{\mathfrak{p}})_n$ and compute examples for specific $n$ and $Z$, in hopes of giving evidence for the conjecture of Kim ([BDCKW]) that $X(Z) = X(Z_{\mathfrak{p}})_n$ for sufficiently large $n$.

1.3. Motivic Chabauty-Kim Theory. In order to compute this set concretely (i.e., in terms that can be applied to computing elements of $\mathcal{I}_n^Z$), it is actually better to upgrade this Galois cohomology to a motivic version of the Selmer variety, as developed in [Had11] and [DCW16]. This motivic Selmer variety is just the group cohomology of the mixed Tate Galois group $\pi_1^{\text{MT}}(Z)$ of $Z$, as developed in [DG05], with coefficients in (a quotient depending on $n$ of) the unipotent fundamental group $\pi_1^{\text{un}}(X)$ of $X$. This group (as well as all of the quotients we take) has the structure of a mixed Tate motive, i.e., an action of $\pi_1^{\text{MT}}(Z)$.

We in fact work only with a certain quotient $\pi_1^{\text{PL}}(X)$ of $\pi_1^{\text{un}}(Z)$, known as the polylogarithmic quotient, as well as its finite-dimensional quotients $\pi_1^{\text{PL}}(X)_{n, m}$. In this case, we refer to the Chabauty-Kim ideal and loci by $\mathcal{I}_n^{\text{PL}}$ and $X(Z_{\mathfrak{p}})^{\text{PL}}$, respectively. The reason why this can be made explicit is that $\pi_1^{\text{MT}}(Z)$ can be described as an abstract (pro-algebraic) group over $\mathbb{Q}$, which ultimately results from Borel’s computation of the algebraic K-theory of integer rings. More specifically, $\pi_1^{\text{MT}}(Z) = \pi_1^{\text{un}}(Z) \rtimes \mathbb{G}_m$, where $\pi_1^{\text{un}}(Z)$ is isomorphic to a free pro-unipotent group on the graded vector space $(\bigoplus_{n=1}^{\infty} K_{2n-1}(Z)_{\mathbb{Q}})^\vee$. This is in contrast with classical Galois groups of number fields, which cannot be easily described as abstract profinite groups.

1.4. Motivic Periods. While we have an abstract description of the group $\pi_1^{\text{MT}}(Z)$ ultimately coming from algebraic K-theory and Voevodsky’s work on motives, we need to understand this group in more concrete terms. More specifically, we need to compute the image of the map $\text{loc}_n$ in the diagram, which is a $p$-adic regulator map. This leads to motivic polylogarithms of the form $\text{Li}_n^\text{un}(z)$ for $n \in \mathbb{Z}_{\geq 1}$ and $z \in \mathbb{Q}$, as well as motivic logarithms $\log^\text{un}(z)$ and motivic zeta values $\zeta^\text{un}(n)$ for $n \in \mathbb{Z}_{\geq 1}$ (Section 3.2). These are all elements of the coordinate ring $\mathcal{O}(\pi_1^{\text{un}}(Z))$ of $\pi_1^{\text{un}}(Z)$ whose $p$-adic realizations are the Coleman $p$-adic
polylogarithms \( \text{Li}_n^u(z) \). There is an explicit formula for the (reduced) coproduct of these elements in the Hopf algebra \( \mathcal{O}(\pi_1^{un}(Z)) \), due to Goncharov (Gon05a):

\[
\Delta' \text{Li}_n^u(z) := \Delta \text{Li}_n^u(z) - 1 \otimes \text{Li}_n^u(z) - \text{Li}_n^u(z) \otimes 1 = \sum_{i=1}^{n-1} \text{Li}_{n-i}^u(z) \otimes \frac{(\log^u(z))^i}{i!}.
\]

Our current paper, building on ideas in DCW16 and DC15, shows how this can be used to algorithmically compute bases of \( \mathcal{O}(\pi_1^{un}(Z)) \) in low degrees.

1.5. **This Project.** Before this work, the only cases that had been computed were those for which \( Z = \mathbb{Z}, \mathbb{Z}[1/2] \), both in weights \( n = 2, 4 \) (in DCW16). In addition, an algorithm had been proposed, and this algorithm was shown to compute the set of points assuming various conjectures (DC15).

In this work, we make the algorithm more efficient and explicit and use it to find an element of \( I_{\mathbb{Z}}^{PL,4} \) for \( Z = \mathbb{Z}[1/3] \). More specifically, we have:

**Theorem 1.1 (Theorem 4.6).** The element

\[
\zeta^u(3) \log^u(3) \text{Li}_4^u - \left( -\frac{12}{w_2(9)} \text{Li}_3^u(3) + (2w_2(9))^{-1} \text{Li}_3^u(9) \right) \log^u \text{Li}_3^u
\]

\[
- \frac{(\log^u)^3 \text{Li}_3^u}{24} \left( \zeta^u(3) \log^u(3) - 4 \left( -\frac{12}{w_2(9)} \text{Li}_3^u(3) + (2w_2(9))^{-1} \text{Li}_3^u(9) \right) \right)
\]

of \( \mathcal{O}(\Pi_{PL,4} \times \pi_1^{un}(Z)) \) (defined in Section 2.4) is in \( I_{PL,4}^Z \) for \( Z = \text{Spec} \mathbb{Z}[1/3] \), where \( w_2(9) \) is a number \( p \)-adically close to \(-\frac{26}{3}\) for \( p = 5, 7 \).

By computing values of this function at elements of \( X(Z_p)_{PL,2} \) already found in BDCKW, we get:

**Theorem 1.2 (Theorem 4.7).** For \( Z = \text{Spec} \mathbb{Z}[1/3] \), we have \( X(Z_p)_{PL,4} \subseteq \{-1\} \) for \( p = 5, 7 \).

We note that \( X(\text{Spec} \mathbb{Z}[1/3]) = \emptyset \).

Part of the reason for computing information about these Chabauty-Kim loci is that they help verify cases of the following conjecture of Kim:

**Conjecture 1.3 (Conjecture 3.1 of BDCKW).** \( X(Z) = X(Z_p)_n \) for sufficiently large \( n \).

In order to do computations, it is easier to work only with polylogarithms, i.e., only with the polylogarithmic quotient. Luckily, not only is \( I_{n}^{PL} \) nonzero for sufficiently large \( n \), but \( I_{PL,n}^{Z} \) is as well, and hence \( X(Z_p)_{PL,n} \) is finite for such \( n \). To make the method truly computable, one would like an analogue of Conjecture 1.3 for the polylogarithmic quotient, which leads one to ask the question:

**Question 1.4 (Question 2.24).** Does \( X(Z) = X(Z_p)_{PL,n} \) for sufficiently large \( n \)?

A positive answer would be a strengthening of Conjecture 1.3. However, we prove:

**Theorem 1.5 (Theorem 5.2).** For any prime \( \ell \) and positive integer \( n \), we have

\[-1 \in X(Z_p)_{PL,n},\]

where \( Z = \text{Spec} \mathbb{Z}[1/\ell] \).

In particular, for \( \ell \) odd, Question 1.4 has a negative answer.
In particular, it does not make sense to make a version of Kim’s conjecture with $X(Z_p)^{S_3}_{PL,n}$ in place of $X(Z_p)_n$. However, there is an action of $S_3$ on the scheme $X$, and we may use it to propose a strengthening of Kim’s conjecture. We write

$$X(Z_p)^{S_3}_{PL,n} := \bigcap_{\sigma \in S_3} \sigma(X(Z_p)_{PL,n}).$$

Our strengthened Kim’s conjecture is the following:

**Conjecture 1.6 (Conjecture 2.25).** $X(Z) = X(Z_p)^{S_3}_{PL,n}$ for sufficiently large $n$.

As explained in Section 2.7, Conjecture 1.6 implies Conjecture 1.3.

We then use our computation from Theorem 1.2 to verify Conjecture 1.6 for $Z = \mathbb{Z}[1/3]$ and $p = 5, 7$:

**Theorem 1.7 (Theorem 5.4).** For $Z = \text{Spec} \mathbb{Z}[1/3]$ and $p = 5, 7$, Conjecture 1.6 (and hence Conjecture 2.23) holds (with $n = 4$).

1.6. **Notation.** For a scheme $Y$, we let $\mathcal{O}(Y)$ denote its coordinate ring. If $R$ is a ring, we let $Y \otimes R$ or $Y_R$ denote the product (or ‘base-change’) $Y \times \text{Spec} R$. If $Y$ and $\text{Spec} R$ are over an implicit base scheme $S$ (often $\text{Spec} \mathbb{Q}$), we take the product over $S$. Similarly, if $M$ is a linear object (such as a module, an algebra, a Lie algebra, or a Hopf algebra), then $M_R$ denotes $M \otimes R$ (again, with the tensor product taken over an implicit base ring).

If $f : Y \to Z$ is a morphism of schemes, we denote by $f^\#: \mathcal{O}(Z) \to \mathcal{O}(Y)$ the corresponding homomorphism of rings. Similarly, if $\alpha \in Y(R)$, we have a homomorphism $\alpha^\#: \mathcal{O}(Y) \to R$.

2. **Technical Preliminaries**

This paper builds on the work of [DCW16], [DC15], and [Bro17]. We recall some of the important objects in the theory.

2.1. **Generalities on Graded Pro-Unipotent Groups.**

2.1.1. **Conventions for Graded Vector Spaces.** Our definition of graded vector space is the following:

**Definition 2.1.** A graded vector space is a collection of vector spaces $V_i$ indexed by $i \in \mathbb{Z}$.

**Definition 2.2.** A graded vector space is positive (respectively negative, strictly positive, strictly negative) if $V_i = 0$ for $i < 0$ (respectively, for $i > 0$, for $i \leq 0$, for $i \geq 0$).

In general, we will only consider graded vector spaces satisfying one of these four conditions.

Furthermore, unless otherwise stated, we will only consider graded vector spaces $\{V_i\}$ such that each $V_i$ is finite-dimensional, which ensures that the double dual is the identity. One must then be careful when taking tensor constructions, as follows. Specifically, we only consider the tensor product between two graded vector spaces if they are either both positive or both negative, and we consider the tensor algebra only of a strictly positive or strictly negative graded vector space.

We now make a technical remark. For a collection

$$V = \{V_i\}_{i \in \mathbb{Z}}$$

...
of (finite-dimensional) vector spaces indexed by the integers, we may either take the direct sum
\[ V^{\oplus} := \bigoplus_i V_i \]
or the direct product
\[ V^{\prod} := \prod_i V_i \]
as our notion of a graded vector space. In general, we use the former for coordinate rings and Lie coalgebras and the latter for universal enveloping algebras and Lie algebras. As all of our pro-unipotent groups will be negatively graded, we use the \( \oplus \) notion for positively graded vector spaces and the \( \prod \) notion for negatively graded vector spaces.

When considering the \( \prod \) notion, we take completed tensor product instead of tensor product (and similarly for tensor algebras and universal enveloping algebras), and a coproduct is a complete coproduct, i.e., a homomorphism \( V \to V \hat{\otimes} V \). In addition, a set of homogeneous elements is considered a basis if it generates \( V \) in each degree, and a similar remark applies to bases of algebras and Lie algebras. When taking the dual of a negatively graded vector space, we take the graded dual and then view the resulting (positively) graded vector space via the \( \oplus \) notion. In particular, the double dual is always the original vector space. Nonetheless, we have the following relation between graded and ordinary (non-graded) duals:
\[ (V^{\oplus})^\vee = (V^\vee)^{\prod}. \]

2.1.2. Graded Pro-unipotent Groups. Let \( U \) be a pro-unipotent group over \( \mathbb{Q} \).

Then \( U \) is a group scheme over \( \mathbb{Q} \), so its coordinate ring \( \mathcal{O}(U) \) is a Hopf algebra over \( \mathbb{Q} \). We recall that if \( \mathcal{O}(U) \) is a Hopf algebra over \( \mathbb{Q} \), then it is equipped with a product \( \mathcal{O}(U) \otimes \mathcal{O}(U) \to \mathcal{O}(U) \), a coproduct \( \Delta: \mathcal{O}(U) \to \mathcal{O}(U) \otimes \mathcal{O}(U) \), and a counit \( \epsilon: \mathcal{O}(U) \to \mathbb{Q} \).

The kernel \( I(U) \) of \( \epsilon \) is known as the augmentation ideal. We also write \( \Delta'(x) := \Delta(x) - x \otimes 1 - 1 \otimes x \) for the reduced coproduct. Finally, we say that an element is primitive if it is in the kernel of \( \Delta' \).

We say that a Hopf algebra \( A \) is a graded Hopf algebra if the multiplication \( A \otimes A \to A \), the coproduct \( A \to A \otimes A \), unit \( \mathbb{Q} \to A \), and counit \( A \to \mathbb{Q} \), are morphisms of graded vector spaces, where \( A \otimes A \) has the standard grading on a tensor product, and \( \mathbb{Q} \) is in degree zero.

**Definition 2.3.** By a grading on \( U \), we mean a positive grading on \( \mathcal{O}(U) \) as a \( \mathbb{Q} \)-vector space such that the degree zero part of \( \mathcal{O}(U) \) is one-dimensional over \( \mathbb{Q} \).

**Definition 2.4.** If \( A \) is a Hopf algebra graded in the sense of Definition 2.3 we let \( \Delta_n \) and \( \Delta'_n \) denote the restrictions of \( \Delta \) and \( \Delta' \), respectively, to \( A_n \), the \( n \)th graded piece.

Furthermore, \( \Delta_n \) and \( \Delta'_n \) map \( A_n \) into the \( n \)th graded piece of \( A \otimes A \), which is
\[ \bigoplus_{i+j=n} A_i \otimes A_j. \]

**Definition 2.5.** For \( i + j = n \) and \( i, j \geq 0 \), we let \( \Delta_{ij} \) and \( \Delta'_{ij} \) denote the projections of \( \Delta_n \) and \( \Delta'_n \), respectively, to \( A_i \otimes A_j \). One may check via the axioms defining a Hopf algebra that \( \Delta'_{ij} = 0 \) when either of \( i \) or \( j \) is zero.

The reduced coproduct \( \Delta' \) induces a (graded) Lie coalgebra structure on \( I(U)/I(U)^2 \), and the dual Lie algebra \( (I(U)/I(U)^2)^\vee \) is the Lie algebra \( \mathfrak{n} \) of \( U \). It is a strictly negatively
graded pro-nilpotent Lie algebra. We let $\mathcal{U}U = \mathcal{U}\mathfrak{n}$ denote the dual Hopf algebra of $\mathcal{O}(U)$, which is the (completed) universal enveloping algebra of $\mathfrak{n}$. The composition

$$\ker(\Delta') \hookrightarrow \mathcal{U}U = \mathcal{O}(U)^\vee \twoheadrightarrow I(U)^\vee$$

induces an isomorphism between the set of primitive elements of $\mathcal{U}U$ and the Lie algebra $\mathfrak{n} = (I(U)/I(U)^2)^\vee \subseteq I(U)^\vee$.

Furthermore, for a $\mathbb{Q}$-algebra $R$, we may identify $U(R)$ with the group of grouplike elements in $(\mathcal{U}U)_R$, i.e., $x$ such that $\Delta x = x \otimes x$.

Evaluation of an an element of $\mathcal{O}(U)$ on an element of $U(R)$ is given by evaluation on the corresponding grouplike element of $(\mathcal{U}U)_R$.

The functor sending $U$ to $\mathfrak{n}$ is known to be an equivalence of categories between graded pro-unipotent groups and strictly negatively graded pro-nilpotent Lie algebras. For each positive integer $n$, the set of elements $n < -n$ is a Lie ideal, and we denote by $n \geq -n$ the quotient $n/n < -n$.

We denote the corresponding quotient pro-unipotent group by $U_{\geq -n}$, and it is a unipotent algebraic group. In fact, $U$ is the inverse limit

$$\lim_{\leftarrow n} U_{\geq -n}.$$  

**Example 2.6.** If $\mathfrak{n}$ is a one-dimensional Lie algebra generated by an element $x$, then $\mathfrak{n}$ is nilpotent. We have $\mathcal{U}\mathfrak{n} = \mathbb{Q}[\![x]\!]$, and $\mathcal{O}(U) = \mathbb{Q}[f_x]$, with both $x$ and $f_x$ primitive. Then $U$ is the group $G_a$, and the set of grouplike elements of $\mathcal{U}\mathfrak{n}$ is the set of elements of the form $\exp(rx)$ for $r \in \mathbb{Q}$. In particular, this demonstrates the usefulness of taking completed universal enveloping algebras.

2.1.3. **Free Pro-unipotent Groups.**

**Definition 2.7.** If $V$ is a strictly negative graded vector space, we may form the free pro-nilpotent Lie algebra on $V$ as follows. We take the graded tensor algebra $TV$ on $V$ and put the unique coproduct on it such that all elements of $V$ are primitive. The subspace of primitive elements of $TV$ forms a graded pro-nilpotent Lie algebra, denoted $\mathfrak{n}(V)$, with corresponding pro-unipotent group $U(V)$. Then $\mathfrak{n}(V)$, $U(V)$ are known as the **free pro-nilpotent Lie algebra** and **free pro-unipotent group**, respectively, on the graded vector space $V$.

The construction $V \mapsto \mathfrak{n}(V)$ is left adjoint to the forgetful functor from graded pro-nilpotent Lie algebras to graded vector spaces.

Finally, if $I$ is an index set with a degree function $d : I \to \mathbb{Z}_{<0}$ with finite fibers, then the **free pro-unipotent group on the set $I$** is just the free pro-unipotent group on the free graded vector space on the set $I$. In particular, the free pro-unipotent group on a graded vector space is isomorphic to the free pro-unipotent group on a (graded) basis of that vector space. The Lie algebra is the pro-nilpotent completion\footnote{In fact, if one takes a free Lie algebra in the graded sense and views it via the $\prod$ notion, then it is already pro-nilpotent.} of the free Lie algebra on the set $I$ and as such is generated by the elements of $I$.

The graded dual Hopf algebra of $TV = \mathcal{U}\mathfrak{n}(V)$ is the coordinate ring $\mathcal{O}(U(V))$. Let $\{x_i\}$ be a graded basis of $V$, so that words $w$ in the $\{x_i\}$ form a basis of $\mathcal{U}\mathfrak{n}(V)$, and let $\{f_w\}_w$ denote...
the basis of $\mathcal{O}(U(V))$ dual to $\{w\}$. Then $\mathcal{O}(U(V))$ is isomorphic to the free shuffle algebra on the graded vector space $V^\vee$. Its coproduct is known as the deconcatenation coproduct and is given by
\[
\Delta f_w := \sum_{w_1 w_2 = w} f_{w_1} \otimes f_{w_2},
\]
and the (commutative) product $\Pi$ on $\mathcal{O}(U(V))$, known as the shuffle product, is given by:
\[
f_{w_1} \Pi f_{w_2} := \sum_{\sigma \in \Pi(\ell(w_1), \ell(w_2))} \sigma(f_{w_1} w_2),
\]
where $\ell$ denotes the length of a word, $\Pi(\ell(w_1), \ell(w_2)) \subseteq S_{\ell(w_1) + \ell(w_2)}$ denotes the group of shuffle permutations of type $(\ell(w_1), \ell(w_2))$, and $w_1 w_2$ denotes concatenation of words.

**Remark 2.8.** It follows from the definition of the deconcatenation coproduct that a word consisting of a single letter is a primitive element of the free shuffle algebra.

2.1.4. **Conventions for Products.** Let $\alpha$ and $\beta$ be two paths in a space $X$. Then in the literature, the symbol $\alpha \beta$ can have two different meanings. It can either denote:

(i) The path given by going along $\alpha$ and then $\beta$  
(ii) The path given by going along $\beta$ and then $\alpha$

The first is known as the ‘lexical’ order and the second as the ‘functional’ order. In this paper, we will use the lexical order, in contrast to the convention of [DCW16] (but consistent with [Bro17]). However, we would like to take a moment to explain how these two conventions help clarify differing conventions in the literature for iterated integrals, multiple zeta values, polylogarithms, and more. We will refer to these differing conventions as the lexical and functional conventions, respectively.

In fact, either convention necessitates a particular convention for iterated integrals. In general, one wants a “coproduct” formula to hold for iterated integrals (c.f. Section 2.1 of [Bro12b], 5.1(ii) of [Hai94], or Proposition 5 of [Hai05]), by which we mean

\[
\int_{\alpha \beta} \omega_1 \cdots \omega_n = \sum_{i=0}^n \int_\alpha \omega_1 \cdots \omega_i \int_\beta \omega_{i+1} \cdots \omega_n
\]

In order for the coproduct to take this nice form $\Pi$, our convention for path composition determines our convention for iterated integrals. More specifically, those that use the lexical order for path composition use the formula

\[
I(\gamma(0); \omega_1, \cdots, \omega_n; \gamma(1)) := \int_\gamma \omega_1 \cdots \omega_n = \int_{0 \leq t_1 \leq \cdots \leq t_n \leq 1} f_1(t_1) \cdots f_n(t_n) dt_1 \cdots dt_n,
\]

where $\gamma^*(\omega_i) = f_i(t)dt$, and those that use the function order for path composition use the formula

\[
I(\gamma(0); \omega_1, \cdots, \omega_n; \gamma(1)) := \int_\gamma \omega_1 \cdots \omega_n = \int_{0 \leq t_n \leq \cdots \leq t_1 \leq 1} f_1(t_1) \cdots f_n(t_n) dt_1 \cdots dt_n.
\]

Given that these conventions are opposite, the corresponding conventions for the iterated integral expression for polylogarithms must be opposite. More precisely, the iterated integral
defining a multiple polylogarithm must always begin with \( \frac{dz}{1-z} \) in the lexical convention, while it must always end with \( \frac{dz}{1-z} \) in the functional convention. More precisely, let us define

\[
\textstyle{\text{Li}}_{s_1, \ldots, s_r}(z) := \sum_{0 < k_1 < \cdots < k_r} \frac{z^{k_r}}{k_1^{s_1} \cdots k_r^{s_r}}.
\]

Set \( e^0 = \frac{dz}{z} \) and \( e^1 = \frac{dz}{1-z} \). Then using the lexical convention for iterated integration, we have:

\[
\textstyle{\text{Li}}_{s_1, \ldots, s_r}(z) = I(0; e^1, e^0, \ldots, e^0, e^1, e^0, \ldots, e^0, e^1, e^0, \ldots, e^0; z).
\]

In fact, the definition itself of \( \textstyle{\text{Li}}_{s_1, \ldots, s_r}(z) \) depends on the convention. More specifically, if we were to use the functional convention for iterated integrals in tandem with (2), we would get:

\[
\textstyle{\text{Li}}_{s_1, \ldots, s_r}(z) = I(0; e^0, \ldots, e^0, e^1, e^0, \ldots, e^0, e^1, e^0, \ldots, e^0, e^1; z).
\]

This is precisely the formula that appears in \([\text{BL11} \text{ (1.4)}]\). However, most authors prefer the \( s_i \)'s to appear in the iterated integral in the same order as they do in the argument of the function. Therefore, almost all papers that use the functional convention for iterated integration will write:

\[
\textstyle{\text{Li}}_{s_1, \ldots, s_r}(z) := \sum_{k_1 > \cdots > k_r > 0} \frac{z^{k_r}}{k_1^{s_1} \cdots k_r^{s_r}}.
\]

As a result, one then writes:

\[
\textstyle{\text{Li}}_{s_1, \ldots, s_r}(z) = I(0; e^0, \ldots, e^0, e^1, e^0, \ldots, e^0, e^1, e^0, \ldots, e^0, e^1; z).
\]

Thus, the convention one uses for path composition determines the convention one uses for \( \textstyle{\text{Li}}_{s_1, \ldots, s_r}(z) \) (except in \([\text{BL11}]\)). Similarly, the two conventions for multiple zeta values follow this paradigm. Specifically, those who use the lexical convention write

\[
\zeta(s_1, \cdots, s_r) = \sum_{k_1 > \cdots > k_r > 0} \frac{1}{k_1^{s_1} \cdots k_r^{s_r}},
\]

and those who use the functional convention write

\[
\zeta(s_1, \cdots, s_r) = \sum_{k_1 > \cdots > k_r > 0} \frac{1}{k_1^{s_1} \cdots k_r^{s_r}}.
\]

Note, however, that \( \textstyle{\text{Li}}_n \) always denotes the same function (both as a multi-valued complex analytic function, a Coleman function, and an abstract function on the de Rham fundamental group), no matter which convention one uses. In fact, this brings us back to the two conventions for path composition. The fact that some write \( \textstyle{\text{Li}}^\text{u}_n \) (c.f. Section 3.1) as \( e^1 \frac{e^0 \cdots e^0}{n-1} \) and others write it as \( \frac{e^0 \cdots e^0}{n-1} e^1 \), yet both denote the exact same regular function on the unipotent de Rham fundamental group of \( \mathbb{P}^1 \setminus \{0, 1, \infty\} \), is due to the differing conventions for path composition.
As we use the lexical convention, one will find the coproduct formula
\[ \Delta' \text{Li}_u^n = \sum_{i=1}^{n-1} \text{Li}_{n-i}^i \otimes \frac{(\log u)^{\text{III}_i}}{i!} \]
in this paper (3.1). With the other convention, one must write
\[ \Delta' \text{Li}_u^n = \sum_{i=1}^{n-1} \frac{(\log u)^{\text{III}_i}}{i!} \otimes \text{Li}_{n-i}^i. \]

More subtly, these conventions affect the convention one uses for the motivic coproduct. More specifically, if we use the lexical convention, we want to also be able to write
\[ \Delta' \text{Li}_u^n(z) = \sum_{i=1}^{n-1} \text{Li}_{n-i}^i(z) \otimes \frac{(\log u(z))^\text{III}_i}{i!} \]
rather than its opposite. This formula is correct as long as we use the lexical order for composition in \( \pi_{1,\text{un}}(X) \) and another for composition in \( \pi_{1,\text{un}}(Z) \), but that would cause formulas (3) and (4) not to appear identical.

One important implication of the difference in formulas for the motivic coproduct is:

**Remark 2.9.** Our \( f_{\sigma\tau} \) is actually the \( \phi_{1,3} \) of 7.6.1 of [DCW16], even though the notation would suggest it is \( \phi_{3,1} \).

In terms of authors and sources, one may find the lexical convention and/or the other conventions that go along with it in [Bro14] (Section 1.2), [Hai94] (Section 5), [Hai05] (Definition 2), [Bro17] (9.1), [Hai87] (Definition 1.1), [Bro12b] (Definition 2.1), [Gon05a], [Che77] (1.1.1), [Fur04] (0.1), [Gon05b] (3.4.3), [Gon] (Formula (4) and Definition 1.2), [Gon95] (Section 12), [Zag93], [Zag94], [Ter02], and [Rab96]. One may also find conventions for multiple zeta values consistent with this convention in other articles by Francis Brown, e.g., [Bro12a], [Bro], and [Bro13].

The sources [DCW16] (1.16), [DG05] (5.16.1), [Car02] (Formula (79), [Del10] (Formula 0.1 and 5.1A), [Del13], [Hof97], [Rac02], [Sou10], [DC15] (2.2.4), and [Bro04] use the functional conventions.

### 2.2. The Various Fundamental Groups.

#### 2.2.1. The Mixed Tate Fundamental Group of Z.

**Definition 2.10.** An open integer scheme is an open subscheme of \( \text{Spec} \, \mathcal{O}_K \), where \( K \) is a number field and \( \mathcal{O}_K \) its ring of integers.

Let \( Z \subseteq \text{Spec} \, \mathcal{O}_K \) be an open integer scheme, \( \text{MT}(Z, \mathbb{Q}) \) its Tannakian category of mixed Tate motives with \( \mathbb{Q} \)-coefficients, which exists by [DG05]. This is a category with realization functors
\[ \text{real}^g : \text{MT}(Z, \mathbb{Q}) \rightarrow \text{MHS}_\mathbb{Q} \]

\[ \text{real}^g : \text{MT}(Z, \mathbb{Q}) \rightarrow \text{MHS}_\mathbb{Q} \]

\[ \text{real}^g : \text{MT}(Z, \mathbb{Q}) \rightarrow \text{MHS}_\mathbb{Q} \]

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\[ \text{real}^g : \text{MT}(Z, \mathbb{Q}) \rightarrow \text{MHS}_\mathbb{Q} \]

\[ \text{real}^g : \text{MT}(Z, \mathbb{Q}) \rightarrow \text{MHS}_\mathbb{Q} \]
to mixed Hodge structures with \(\mathbb{Q}\)-coefficients for each embedding \(\sigma: K \hookrightarrow \mathbb{C}\) and
\[
\text{real}^\ell: \text{MT}(Z, \mathbb{Q}) \to \text{Rep}_\mathbb{Q}(G_K)
\]
to \(\ell\)-adic representations of \(G_K\) for each prime \(\ell\). The image of each realization functor consists of mixed Tate objects, i.e., objects with a composition series consisting of tensor powers of the image of the Tate object \(\mathbb{Q}(1) := h_2(P^1; \mathbb{Q})\).

**Definition 2.11.** A continuous \(\mathbb{Q}_\ell\)-representation of \(G_K\) for a number field \(K\) is said to have good reduction at a non-archimedean place \(v\) of \(K\) if either \(v \nmid \ell\), and the representation is unramified at \(v\), or if \(v \mid \ell\), and the representation is crystalline at \(v\).

The \(\ell\)-adic realizations of an object of \(\text{MT}(Z, \mathbb{Q})\) form a compatible system of \(\mathbb{Q}_\ell\)-Galois representations with good reduction at closed points of \(Z\) (in particular, crystalline at primes dividing \(\ell\)). If \((X, D)\) is a pair of a scheme and codimension 1 subscheme, both smooth and proper over \(Z\) and rationally connected, then the relative cohomology \(h^*(X, D; \mathbb{Q})\) is an object of this category such that
\[
\text{real}^*(h^*(X, D; \mathbb{Q})) = H_\text{Betti}(X^\text{an}(\mathbb{C}), D^\text{an}(\mathbb{C}); \mathbb{Q}),
\]
real\(^\ell(h^*(X, D; \mathbb{Q})) = H_\sigma^*(X_{\overline{K}}, D_{\overline{K}}; \mathbb{Q}_\ell),
\]
with their associated mixed Hodge structure and continuous \(G_K\)-action, respectively.

The only simple objects of \(\text{MT}(Z, \mathbb{Q})\) are the objects \(\mathbb{Q}(n) := \mathbb{Q}(1)^{\otimes n}\) for \(n \in \mathbb{Z}\), each object has a finite composition series, and the extensions are determined by the fact that
\[
\text{Ext}^1(\mathbb{Q}(0), \mathbb{Q}(n)) = K_{2n-1}(Z)_\mathbb{Q}
\]
\[
\text{Ext}^i = 0 \quad \forall i \geq 2.
\]

The groups \(K_{2n-1}(Z)_\mathbb{Q}\) are known by the work of Borel ([Bor74]). For \(n = 1\), we have \(K_1(Z) = \mathcal{O}(Z)^*\), and for \(n \geq 2\), \(K_{2n-1}(Z)_\mathbb{Q} = K_{2n-1}(\mathbb{Q})_\mathbb{Q}\) has dimension \(r_2\) for \(n\) even and \(r_1 + r_2\) for \(n\) odd, where \(r_1\) and \(r_2\) are the numbers of real and complex places of \(K\), respectively.

**Definition 2.12.** Let \(M\) be an object of \(\text{MT}(Z, \mathbb{Q})\). Then \(M\) has an increasing filtration \(W_iM\) known as the weight filtration. The quotient \(W_iM/W_{i-1}M\) is trivial when \(i\) is odd and is isomorphic to a direct sum of copies of \(\mathbb{Q}(-i)/2\) when \(i\) is even.

We let
\[
\text{Can}(M) := \bigoplus_{i \in \mathbb{Z}} \text{Hom}_{\text{MT}(Z, \mathbb{Q})}(\mathbb{Q}(-i), W_2M/W_{2i-1}M),
\]
and we call this the canonical fiber functor.

Then the category \(\text{MT}(Z, \mathbb{Q})\) is a neutral \(\mathbb{Q}\)-linear Tannakian category with fiber functor \(\text{Can}\), and we let \(\pi_1^\text{MT}(Z)\) denote its Tannakian fundamental group, which is therefore a pro-algebraic group over \(\mathbb{Q}\).

The subcategory of simple objects of \(\text{MT}(Z, \mathbb{Q})\) consists of direct sums of tensor powers of \(\mathbb{Q}(1)\) and is therefore equivalent as a Tannakian category to the category of representations of \(G_m\). This inclusion induces a quotient map \(\pi_1^\text{MT}(Z) \twoheadrightarrow G_m\), and we let \(\pi_1^\text{un}(Z)\) denote the kernel of this quotient. The functor sending an object \(M\) of \(\text{MT}(Z, \mathbb{Q})\) to the direct sum \(\bigoplus_{i \in \mathbb{Z}} W_iM/W_{i-1}M\) gives a splitting of this inclusion of categories, which implies that the quotient map \(\pi_1^\text{MT}(Z) \twoheadrightarrow G_m\) splits.

This implies that \(\text{MT}(Z, \mathbb{Q})\) has fundamental group
\[
\pi_1^\text{MT}(Z) = \pi_1^\text{un}(Z) \rtimes G_m.
\]
where \( \pi^\text{un}_1(Z) \) the maximal pro-unipotent subgroup of \( \pi^\text{MT}_1(Z) \). The action of \( \mathbb{G}_m \) on \( \pi^\text{un}_1(Z) \) by conjugation gives an action of \( \mathbb{G}_m \), or equivalently, a grading, on the Hopf algebra of \( \pi^\text{un}_1(Z) \). This associated graded Hopf algebra is denoted

\[
\bigoplus_{i=0}^{\infty} A(Z)_i = A(Z) := \mathcal{O}(\pi^\text{un}_1(Z)),
\]

where \( A(Z)_i \) denotes the \( n \)th graded piece. We refer to the degree on \( A(Z) \) as the \textit{half-weight}, as it is half the ordinary motivic weight.

In fact, the description of the \( \text{Ext} \) groups gives us the following information. It gives a canonical embedding of graded vector spaces

\[
\bigoplus_{n=1}^{\infty} K_{2n-1}(Z)_\mathbb{Q} \hookrightarrow A(Z),
\]

with \( K_{2n-1}(Z)_\mathbb{Q} \) in degree \( n \), and whose image is the set of primitive elements of \( A(Z) \). Equivalently, this gives a canonical isomorphism

\[
\pi^\text{un}_1(Z)^\text{ab} \cong \left( \bigoplus_{n=1}^{\infty} K_{2n-1}(Z)_\mathbb{Q} \right)^\vee.
\]

In fact, this canonical isomorphism extends to an isomorphism between \( \pi^\text{un}_1(Z) \) and the free pro-unipotent group (Definition 2.7) on the graded vector space \( \left( \bigoplus_{n=1}^{\infty} K_{2n-1}(Z)_\mathbb{Q} \right)^\vee \), with \( (K_{2n-1}(Z))\vee \) in degree \( -n \), but this extension is not canonical. This last fact tells us that there is a non-canonical isomorphism between \( A(Z) \) and the free shuffle algebra on the graded vector space \( \bigoplus_{n=1}^{\infty} K_{2n-1}(Z)_\mathbb{Q} \), with \( K_{2n-1}(Z) \) in degree \( n \). This non-canonicity is the key to a later consideration; see Remark 4.2.

Furthermore, in Proposition 4.3 we will show that \( \text{Ext}^1(\mathbb{Q}(0), \mathbb{Q}(n)) \) is isomorphic to the space of degree \( n \) primitive elements of \( A(Z) \).

For \( Z' \subseteq Z \) an open subscheme, we have an inclusion \( \text{MT}(Z, \mathbb{Q}) \subseteq \text{MT}(Z', \mathbb{Q}) \), which gives rise to a quotient map \( \pi^\text{MT}_1(Z') \twoheadrightarrow \pi^\text{MT}_1(Z) \) that is an isomorphism on \( \mathbb{G}_m \) and hence to an inclusion

\[
A(Z) \subseteq A(Z')
\]

of graded Hopf algebras. There is also a graded Hopf algebra \( A(\text{Spec} \mathcal{O}_K) \), which is the union of \( A(Z) \) for \( Z \subseteq \text{Spec} \mathcal{O}_K \), and we may view all such \( A(Z) \) as lying inside \( A(\text{Spec} \mathcal{O}_K) \). If \( p \) is a point of \( \text{Spec} \mathcal{O}_K \setminus Z \) and \( \alpha \in A(Z) \), we say \( \alpha \) is \textit{unramified at} \( p \) if

\[
\alpha \in A(Z \cup \{p\}) \subseteq A(Z).
\]

2.2.2. The de Rham Unipotent Fundamental Group of \( X \). For the rest of this paper, we let \( X = \mathbb{P}^1 \setminus \{0, 1, \infty\} \) over \( \mathbb{Z} \).

**Definition 2.13.** We let

\[
\pi^\text{un}_1(X)
\]

denote the unipotent de Rham fundamental group of \( X_\mathbb{Q} \). It is the fundamental group of the Tannakian category of algebraic vector bundles with connection on \( X_\mathbb{Q} \).

This pro-unipotent group over \( \mathbb{Q} \) is a free pro-unipotent group the graded vector space consisting of \( H^1_\text{dR}(X_\mathbb{Q}) \) in degree \(-1\) (and zero in other degrees). Dually, its coordinate ring is generated by words in holomorphic differential forms on \( X \), which are integrands of iterated integrals.
By the construction in Section 3 of [DG05], $\pi_1^{un}(X)$ is in $\mathbf{MT}(Z, \mathbb{Q})$ (in the sense that its coordinate ring and Lie algebra are each an Ind-object and pro-object, respectively, of $\mathbf{MT}(Z, \mathbb{Q})$). It therefore carries an action of $\pi_1^{MT}(Z)$, whose restriction to $\mathbb{G}_m$ induces the grading. While the group $\pi_1^{MT}(Z)$ is not, and we always use the tangential basepoint $\overline{0}$. Remark 2.14. By an argument analogous to the proof of Corollary 2.9 of [BDCKW], one may check that all of these constructions (in particular, the Chabauty-Kim locus, c.f., Section 2.5) are the same if we replace $\overline{0}$ by any other $Z$-integral basepoint of $X$.

Remark 2.15. We will often consider $\pi_1^{MT}(Z)$-equivariant quotients $\pi_1^{un}(X) \twoheadrightarrow \Pi$, especially when $\Pi$ is finite-dimensional as a scheme over $\mathbb{Q}$ (hence an algebraic group). Unless otherwise stated, it is always understood that $\Pi$ is such a quotient.

A standard example is $\Pi_n := \pi_1^{un}(X)_{\geq -n}$. However, in most of our calculations, we will be concerned with quotients that factor through $\pi_1^{PL}(X)$, a specific quotient to be introduced in Section 2.6.

We write $\mathfrak{n}(Z)$, $\mathfrak{n}(X)$, and $\mathfrak{n}^{PL}(X)$ for the corresponding Lie algebras.

2.3. Cohomology and Cocycles. We let $H^1(\pi_1^{MT}(Z), \pi_1^{un}(X))$ denote the (pointed) set of $\pi_1^{MT}(Z)$-equivariant torsor schemes under $\pi_1^{un}(X)$.

For $b \in X(Z)$, there is the torsor of paths $\overline{b}P_{\overline{1}_0}$ constructed in Section 3 of [DG05] (as [DG05] uses the functional convention for path composition; this is in fact the torsor of paths from $\overline{1}_0$ to $b$). It is a $\pi_1^{MT}(Z)$-equivariant torsor under $\overline{1}_0P_{\overline{1}_0} = \pi_1^{un}(X)$.

We therefore have the Kummer map

$$X(Z) \xrightarrow{\kappa} H^1(\pi_1^{MT}(Z), \pi_1^{un}(X)),$$

and by composition with the map induced by $\pi_1^{un}(X) \twoheadrightarrow \Pi$,

$$X(Z) \xrightarrow{\kappa} H^1(\pi_1^{MT}(Z), \Pi).$$

Definition 2.16. For any $\mathbb{Q}$-algebra $R$, we define

$$Z_{\Pi}^{1,\mathbb{G}_m}(R) := Z^1(\pi_1^{un}(Z)_R, \Pi_R)^{\mathbb{G}_m},$$

which is the set of morphisms of schemes from $\pi_1^{un}(Z)_R$ to $\Pi_R$ over $R$, equivariant with respect to the $\mathbb{G}_m$-action, and satisfying the cocycle condition on the $R'$-points for any $R$-algebra $R'$.

Proposition 6.4 of [Bro17] ensures that this is representable by a scheme (also see Corollary 3.10). We thus write

$$Z_{\Pi}^{1,\mathbb{G}_m}(Z) := Z^1(\pi_1^{un}(Z), \Pi)^{\mathbb{G}_m}$$

for the scheme of $\mathbb{G}_m$-equivariant cocycles. If $\Pi$ is finite-dimensional, then this is in fact a finite-dimensional variety over $\mathbb{Q}$.

By Proposition 5.2.1 of [DCW16], we have

$$H^1(\pi_1^{MT}(Z), \Pi) = Z_{\Pi}^{1,\mathbb{G}_m}(\mathbb{Q}).$$

We have a universal cocycle evaluation map

$$C_\Pi : Z_{\Pi}^{1,\mathbb{G}_m} \times \pi_1^{un}(Z) \rightarrow \Pi \times \pi_1^{un}(Z).$$
It is defined on the functor of points as follows. For a \( \mathbb{Q} \)-algebra \( R \) and an element \( (c, \gamma) \in (\mathbb{Z}_{\Pi}^{1, G_m})(R) \times \pi^{un}_1(Z)(R) = (\mathbb{Z}_{\Pi}^{1, G_m} \times \pi^{un}_1(Z))(R) \), we have \( c(\gamma) \in \Pi_R(R) = \Pi(R) \). We define \( C_{\Pi}(c, \gamma) \) to be the pair \( (c(\gamma), \gamma) \).

In fact, the morphism \( C_{\Pi} \) lies over the identity morphism on \( \pi^{un}_1(Z) \), so letting \( K \) denote the function field of \( \pi^{un}_1(Z) \), we also have the base change from \( \pi^{un}_1(Z) \) to \( \text{Spec} K \).

\[
\Phi_{\Pi}: (\mathbb{Z}_{\Pi}^{1, G_m})_K \to \Pi_K.
\]

**Remark 2.17.** If \( \Pi \) is finite dimensional, it will turn out that this is a morphism of affine spaces over the field \( K \), and our “geometric step” (see 4.2) consists in computing its scheme-theoretic image.

**Definition 2.18.** We let \( I^Z_{\Pi} \) denote the ideal of functions in the coordinate ring of \( \Pi_K \) vanishing on the image of \( C_{\Pi} \). This is known as the Chabauty-Kim ideal (associated to \( \Pi \)). For \( \Pi = \Pi_n \), we denote it by \( I^Z_n \).

### 2.4. \( p \)-adic Realization and Kim’s Cutter

Let \( p \) be a closed point of \( Z \). For simplicity, we suppose that \( Z_p \cong \text{Spec} \mathbb{Z}_p \).

If \( \omega \in \mathcal{O}(\pi^{un}_1(X)) \), and \( a, b \) are \( \mathbb{Z}_p \)-basepoints of \( X \) (rational or tangential), then we can extract an element of \( \mathbb{Q}_p \) known as the Coleman iterated integral \( \int_a^b \omega \). The Coleman iterated integral is originally due to Coleman ([Col82]) and was reformulated by Besser ([Bes02]) into the form that is used in [DCW16]. Fixing \( a = \overline{0} \) and letting \( b \) vary over \( X(Z_p) \), one may define local Kummer map

\[
\overline{X}(Z_p) \xrightarrow{\kappa_p} \pi^{un}_1(X)(\mathbb{Q}_p)
\]

by sending a regular function \( \omega \) on \( \pi^{un}_1(X) \) to the Coleman function \( \kappa_p(\omega): X(Z_p) \to \mathbb{Q}_p \) defined by \( b \mapsto \int_a^b \omega \).

Its composition with \( \pi^{un}_1(X)(\mathbb{Q}_p) \to \Pi(\mathbb{Q}_p) \) is also denoted by \( \kappa_p \). This map is Coleman-analytic, meaning that regular functions on \( \pi^{un}_1(X) \) pull back to Coleman functions on \( X(Z_p) \). These are locally analytic functions, and a nonzero such function has finitely many zeroes.

**Remark 2.19.** The local Kummer map in this form was originally referred to in [Kim05] as the \( p \)-adic unipotent Albanese map. It is the same as the map \( \alpha \) of 1.3 of [DCW16]. The latter is defined by sending \( b \) to the torsor of paths from \( a \) to \( b \) (with its structure as a filtered \( \phi \)-module)

#### 2.4.1. \( p \)-adic Period Map

In addition, there is a morphism \( \text{Spec} \mathbb{Q}_p \to \pi^{un}_1(Z) \), or equivalently, a \( \mathbb{Q} \)-algebra homomorphism

\[
\text{per}_p: A(Z) \to \mathbb{Q}_p,
\]

known as the \( p \)-adic period map. While elements of \( A(Z) \) are represented by formal (motivic) iterated integrals, this homomorphism takes the value of the iterated integral in the sense of Coleman integration.

The following may be regarded as a \( p \)-adic analogue of a small piece of the Kontsevich-Zagier period conjecture ([KZ01]). It has been in folklore for some time and appears in the literature for \( K/\mathbb{Q} \) abelian as Conjecture 4 of [Yam10].

**Conjecture 2.20** (\( p \)-adic Period Conjecture). For any open integer scheme \( Z \), the period map \( \text{per}_p: A(Z) \to \mathbb{Q}_p \) is injective.
2.4.2. Kim’s Cutter. Viewing $C_\Pi$ as a morphism of schemes over $\pi_1^{un}(Z)$ and base-changing along the $p$-adic period map $\text{Spec} \mathbb{Q}_p \to \pi_1^{un}(Z)$, we get a morphism $(\mathbb{Z}_\Pi^{1,Grm})_{\mathbb{Q}_p} \to \Pi_{\mathbb{Q}_p}$. The induced map on $\mathbb{Q}_p$-points is denoted by $\text{loc}_\Pi$. Denoting the composition $X(Z) \to H^1(\pi_1^{MT}(Z), \Pi) = \mathbb{Z}_\Pi^{1,Grm}(\mathbb{Q}) \subseteq \mathbb{Z}_\Pi^{1,Grm}(\mathbb{Q}_p)$ by $\kappa$ as well, this fits into a diagram:

\[
\begin{array}{ccc}
X(Z) & \xrightarrow{\kappa} & X(Z_p) \\
\downarrow & & \downarrow \\
\mathbb{Z}_\Pi^{1,Grm}(\mathbb{Q}_p) & \xrightarrow{\text{loc}_\Pi} & \Pi(\mathbb{Q}_p)
\end{array}
\]

which we call Kim’s Cutter.

This diagram is commutative (c.f. [DCW16], 4.9). In Section 3.4, we will describe $\kappa$ and $\kappa_p$ explicitly in terms of coordinates.

2.6. Chabauty-Kim Locus. Let $f \in \mathcal{O}(\Pi \times \pi_1^{un}(Z))$. Now $\text{per}_p$ induces a morphism $\Pi_{\mathbb{Q}_p} \to \Pi \times \pi_1^{un}(Z)$, and $f$ pulls back via this morphism to an element of the coordinate ring of $\Pi_{\mathbb{Q}_p}$, hence a function $\Pi(\mathbb{Q}_p) \xrightarrow{f} \mathbb{Q}_p$. The composite $f \circ \kappa_p$ with $X(Z_p) \xrightarrow{\kappa_p} \Pi(\mathbb{Q}_p)$ is a Coleman function on $X(Z_p)$ and is denoted $f \mid_{X(Z_p)}$.

We then define

$X(Z_p)_\Pi = X(Z_p)_{\Pi} := \{z \in X(Z_p) : f \mid_{X(Z_p)}(z) = 0 \, \forall \, f \in \mathcal{O}(\Pi \times \pi_1^{un}(Z)) \cap \mathbb{Z}_\Pi^Z \}$.

While this set depends on $Z$, we write $X(Z_p)_\Pi$ when there is no confusion.

Any $f \in \mathcal{O}(\Pi \times \pi_1^{un}(Z)) \cap \mathbb{Z}_\Pi^Z$ vanishes on the image of $C_\Pi : \mathbb{Z}_\Pi^{1,Grm} \times \pi_1^{un}(Z) \to \Pi \times \pi_1^{un}(Z)$, hence also on the image of $\text{loc}_\Pi$. By the commutativity of Kim’s Cutter, $f \mid_{X(Z_p)}$ vanishes on $X(Z)$, hence

$X(Z) \subseteq X(Z_p)_\Pi$.

We note that if $\Pi'$ dominates $\Pi$ (i.e., we have $\pi_1^{un}(X) \to \Pi' \xrightarrow{p} \Pi$), then $\text{per}_p^#(\mathbb{Z}_\Pi^Z) \subseteq \mathbb{Z}_\Pi^Z$, hence $X(Z_p)_{\Pi'} \subseteq X(Z_p)_\Pi$.

For $\Pi = \Pi_n$, we denote $X(Z_p)_\Pi$ by $X(Z_p)_n$. The importance of Kim’s method lies in the fact that $X(Z_p)_n$ is known to be finite for sufficiently large $n$ when $K$ is totally real by [Kim05] and [Kim12].

Remark 2.21. The locus defined in [DCW16] differs slightly from our own in that it uses a version of $\mathbb{Z}_\Pi^Z$ defined as the ideal of functions vanishing on the image of the base change of $C_\Pi$ along $\text{per}_p$, which could in principle be larger than our own. However, as explained in 4.2.6 of [DC13], Conjecture 2.20 implies that these two are the same, which is why we see no harm in doing it this way. Furthermore, our version of Kim’s conjecture is a priori stronger than the original version, so our theorems apply to his conjecture either way.

2.6. The Polylogarithmic Quotient. We let $N$ denote the kernel of the homomorphism $\pi_1^{un}(X) \to \pi_1^{un}(\mathbb{G}_m)$ induced by the inclusion $X \hookrightarrow \mathbb{G}_m$, where $\pi_1^{un}(\mathbb{G}_m)$ refers to the unipotent de Rham fundamental group of $\mathbb{G}_m$. Then, following [Del89], we define the polylogarithmic quotient

$\pi_1^{PL}(X) := \pi_1^{un}(X)/[N, N]$.

The group $\pi_1^{MT}(Z)$ acts on $\pi_1^{un}(\mathbb{G}_m)$ as well as $\pi_1^{un}(X)$, and because $\pi_1^{un}(X) \to \pi_1^{un}(\mathbb{G}_m)$ is induced by a map of schemes over $\mathbb{Z}$, it is $\pi_1^{MT}(Z)$-equivariant. Therefore, $N$ and hence $[N, N]$ are $\pi_1^{MT}(Z)$-stable, so $\pi_1^{PL}(X)$ has a structure of a motive, i.e., an action of $\pi_1^{MT}(Z)$. 
As a motive, it has the structure

$$\pi_1^{PL}(X) = \mathbb{Q}(1) \times \prod_{i=1}^{\infty} \mathbb{Q}(i),$$

so in particular the action of $\pi_1^{MT}(Z)$ factors through $G_m$.

**Remark 2.22.** In Section 3.1, we will describe $\pi_1^{PL}(X)$ more explicitly in coordinates.

In the specific case $\Pi = \Pi_{PL,n} := \pi_1^{PL}(X)_{\geq n}$ for a positive integer $n$, we write $Z^{1,G_m}_{\Pi_{PL,n}}$, $C_{PL,n}$, loc$_{PL,n}$, $I^Z_{PL,n}$, and $X(Z_p)_{PL,n}$ to denote $Z^{1,G_m}_{\Pi}$, $C_{\Pi}$, loc$_{\Pi}$, $I^Z_{\Pi}$, and $X(Z_p)_{\Pi}$, respectively.

Since $\pi_1^{un}(Z)$ acts trivially on $\pi_1^{PL}(X)$, a $G_m$-equivariant cocycle

$$c: \pi_1^{un}(Z) \to \pi_1^{PL}(X)$$

is just a $G_m$-equivariant homomorphism.

If $\Pi$ is a quotient of $\Pi_{PL,n}$, then any $G_m$-equivariant homomorphism $\pi_1^{un}(Z) \to \Pi$ must be zero on $\pi_1^{un}(Z)_{<n}$ by the $G_m$-equivariance, so $Z^{1,G_m}_{\Pi}$ is the same as

$$Z^{1}(\pi_1^{un}(Z)_{\geq n}, \Pi)^{G_m}_{\Pi}. $$

It follows that we can in fact view $C_{PL,n}$ as a morphism

$$Z^{1,G_m}_{\Pi_{PL,n}} \times \pi_1^{un}(Z)_{\geq n} \to \Pi_{PL,n} \times \pi_1^{un}(Z)_{\geq n}$$

lying over the identity on $\pi_1^{un}(Z)_{\geq n}$. Letting $\mathcal{K}_n$ denote the function field of $\pi_1^{un}(Z)_{\geq n}$, it induces a map

$$C^{\mathcal{K}_n}_{PL,n} \cdot (Z^{1,G_m}_{\Pi_{PL,n}})_{\mathcal{K}_n} \to (\Pi_{PL,n})_{\mathcal{K}_n}$$

of finite-dimensional affine spaces over the field $\mathcal{K}_n$, and we view $I^Z_{PL,n}$ as an ideal in $\mathcal{O}((\Pi_{PL,n})_{\mathcal{K}_n})$.

### 2.7. Kim’s Conjecture.

We recall Conjecture 1.3 from the introduction:

**Conjecture 2.23.** $X(Z) = X(Z_p)_n$ for sufficiently large $n$.

In fact, dimension counts show that $I^Z_{PL,n}$ is nonzero and hence $X(Z_p)_{PL,n}$ is finite for sufficiently large $n$. One might wonder the following:

**Question 2.24.** Does $X(Z) = X(Z_p)_{PL,n}$ for sufficiently large $n$?

This is a strengthening of Conjecture 2.23. However, as we will show in Section 3, this question has a negative answer as stated (at least for $Z = \text{Spec} \mathbb{Z}[1/\ell]$ and odd primes $\ell$) and needs to be modified by an $S_3$-symmetrization.

More specifically, there is an action of $S_3$ on the scheme $X$. This induces an action of $S_3$ on $\pi_1^{un}(X)$. For a quotient $\Pi$ and $\sigma \in S_3$, we may define $\sigma(\Pi)$ by

$$\ker(\pi_1^{MT}(Z) \to \sigma(\Pi)) = \sigma(\ker(\pi_1^{MT}(Z) \to \Pi)).$$

It follows by independence of basepoint (Remark 2.14) and functoriality of all the constructions that $\sigma(X(Z_p)_{\Pi}) = X(Z_p)_{\sigma(\Pi)}$. We then write

$$X(Z_p)_{S_3}^{\Pi_{PL,n}} := \bigcap_{\sigma \in S_3} \sigma(X(Z_p)_{PL,n}) = \bigcap_{\sigma \in S_3} X(Z_p)_{\sigma(\Pi_{PL,n})}.$$ 

Our symmetrized conjecture is that

**Conjecture 2.25.** $X(Z) = X(Z_p)_{S_3}^{\Pi_{PL,n}}$ for sufficiently large $n$. 

We note that $\Pi_n$ dominates $\sigma(\Pi_{PL,n})$ for all $\sigma \in S_3$; hence $X(Z_p)_n \subseteq \sigma(X(Z_p)_{PL,n})$, and so

$$X(Z_p)_n \subseteq X(Z_p)_{PL,n}^{S_3},$$

so Conjecture 2.25 implies Conjecture 2.23. In Theorem 5.4 we use our computations to verify Conjecture 2.25 for $Z = \text{Spec} \mathbb{Z}[1/3]$ and $p = 5, 7$.

3. COORDINATES

3.1. Coordinates on the Fundamental Group. Let $\{e_0, e_1\}$ be a basis of $H^1_{dR}(X_{\mathbb{Q}})$ dual to the basis $\{dz, \frac{dz}{z}\}$ of $H^1_{dR}(X_{\mathbb{Q}})$. The algebra $\mathcal{U} \pi^\text{un}_1(X)$ is the free (completed) non-commutative algebra on the generators $e_0$ and $e_1$, with coproduct given by declaring that $e_0$ and $e_1$ are primitive and grading given by putting both in degree $-1$. We refer to the words $e_0, e_1, e_1e_0, e_1e_0e_0, \ldots$ as the polylogarithmic words. We let the elements

$$\log^u, Li_1^u, Li_2^u, \ldots \in \mathcal{O}(\pi^\text{un}_1(X))$$

be the duals of these words with respect to the standard basis of $\mathcal{U} \pi^\text{un}_1(X)$. More generally, for a word $w$ in $e_0, e_1$, we let $Li_w^u$ denote the dual basis element of $\mathcal{O}(\pi^\text{un}_1(X))$.

Proposition 3.1. We have

$$\Delta' \log^u = 0$$

$$\Delta' Li_n^u = \sum_{i=1}^{n-1} Li_{n-i}^u \otimes \frac{(log^u)^{\Pi_i}}{i!}.$$

Proof. The first equation follows from Remark 2.8. By the discussion following Definition 2.7 we have the formula

$$\Delta' Li_n^u = \Delta' Li_{e_1e_0\ldots e_0}^u = Li_{e_1} \otimes Li_{e_0\ldots e_0}^u + Li_{e_1e_0} \otimes Li_{e_0\ldots e_0}^u + \cdots + Li_{e_1e_0\ldots e_0} \otimes Li_{e_0}^u.$$

By the definition of the shuffle product, we have the formula

$$(log^u)^{\Pi_i} = (Li_{e_i}^u)^{\Pi_i} = i! Li_{(e_i)}^u.$$

The previous two formulas together with the definition of $Li_n^u$ then imply the proposition. \qed

Letting $\mathcal{P}^{PL}$ be the subalgebra generated by $\log^u, Li_1^u, Li_2^u, \ldots$, the formula above implies that $\mathcal{P}^{PL}$ is a Hopf subalgebra. It therefore corresponds to a quotient group of $\pi^\text{un}_1(X)$. It follows from Proposition 7.1.3 of [DCW16] that this quotient group is the group $\pi^\text{PL}_1(X)$.

Furthermore, we have

$$\mathcal{O}((\Pi_{PL,n}) = \mathbb{Q}[\log^u, Li_1^u, \ldots, Li_n^u]$$

as a Hopf subalgebra of $\mathcal{P}^{PL} = \mathcal{O}(\pi^\text{PL}_1(X))$.

Given a cocycle $c \in Z^1_{PL,\mathbb{Q}}$, we write $c^\sharp : \mathcal{P}^{PL} \to A(Z)$ for the associated homomorphism of $\mathbb{Q}$-algebras, and we write

$$\log^u(c) := c^\sharp \log^u,$$

$$Li_n^u(c) := c^\sharp Li_n^u.$$
Corollary 3.2. For $c \in Z_{PL}^{1,G_m}(\mathbb{Q})$, we have

$$\Delta' \log^u(c) = 0$$

$$\Delta' \text{Li}_n^u(c) = \sum_{i=1}^{n-1} \text{Li}_{n-i}^u(c) \otimes \frac{(\log^u(c))^{i!}}{i!}.$$ 

Proof. The cocycle condition reduces to the homomorphism conditions (as we are restricting ourselves to the polylogarithmic quotient), which means, dually, that $c^2$ respects the coproduct. The corollary then follows immediately from Proposition 3.1. \hfill \Box

3.2. Generating $A(Z)$. We take a moment to discuss coordinates for the Galois group $\pi_1^{un}(Z)$. On an abstract level, this is a free unipotent group, and its structure is governed by the theory of 2.1. However, we need to be able to write elements of $A(Z)$ in a way that allows us to compute their $p$-adic periods. This essentially means writing them as explicit combinations of special values of polylogarithms and zeta functions.

We introduce the notation

$$\log^u(z) := \log^u(\kappa(z)) \in A(Z)_1$$

$$\text{Li}_n^u(z) := \text{Li}_n^u(\kappa(z)) \in A(Z)_n$$

for $z \in X(Z)$. It is the same as the motivic period $\text{Li}_n^u(z)$ mentioned in (9.1) of [Bro17] and 2.2.4 of [DC15], which justifies the notation $\text{Li}_n^u(c)$ in the previous section.

Because $\log^u$ is pulled back from $G_m$, we in fact have $\log^u(z) \in A(Z)$ whenever $z \in G_m(Z)$.

We also note:

Fact 3.3. For $z, w \in X(Z)$, we have

$$\log^u(zw) = \log^u(z) + \log^u(w)$$

and

$$\text{Li}_1^u(z) = -\log^u(1-z).$$

Letting $c_1$ denote the cocycle corresponding to the class of the path torsor $\pi_1 P_{1_0}$ in $H^1(\pi_1^{MT}(Z), \pi_1^{un}(X))$, we write

$$\zeta^u(n) := \text{Li}_n^u(c_1) \in A(Z)_n.$$ 

It is not clear a priori that the special values $\text{Li}_n^u(z)$ for $z \in X(Z)$ span the space $A(Z)$ (whether we leave $Z$ fixed or take a union over various $Z$, such as all $Z$ with a fixed function field $K$ or all $Z$ whose function field is cyclotomic). However, there is the following conjecture of Goncharov:

Conjecture 3.4 ([Gon], Conjecture 7.4). The ring $A(\mathbb{Q})$ is spanned by elements of the form $\text{Li}_w^u(z)$ for $z$ a rational point or rational tangential basepoint of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ and $w$ a word in $\epsilon_0, \epsilon_1$.

Similar to [DC15], we state a version of this conjecture with control on ramification.

Definition 3.5. We say that an integral scheme $Z$ with function field $\mathbb{Q}$ is saturated if there exists $N \in \mathbb{Z}_{\geq 0} \cup \{\infty\}$ such that $Z \cong \text{Spec} \mathbb{Z}[1/S]$ for $S = \{p \text{ prime}; p \leq N\}$.

Conjecture 3.6. If $Z$ is saturated, then the ring $A(Z)$ is spanned by elements of the form $\text{Li}_w^u(z)$ for $z$ a $Z$-integral point or tangential basepoint of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$. 
This is a strengthening of Conjecture 2.2.6 of [DC15] and is in fact the motivation behind that conjecture. It is known in the cases \( N = 1 \) ([Bro12a]) and \( N = 2 \) ([Del10]), and the case \( N = \infty \) is Conjecture 3.4.

In Section 4.3, we will demonstrate this in practice by writing elements of \( A(\mathbb{Z}[1/3]) \) in terms of values of polylogarithms at elements of \( \mathbb{P}^1 \setminus \{0, 1, \infty\}(\mathbb{Z}[1/6]) \).

Remark 3.7. In doing so, we will find that all of these may be written in terms of single (rather than multiple) polylogarithms. This is in line with a conjecture of Goncharov about the depth filtration, as we now describe. We let

\[
\pi^G_1(Z) := \pi(Z) / [\pi(Z)_{< -1}, [\pi(Z)_{< -1}, \pi(Z)_{< -1}]],
\]

\( \pi^G_1(Z) \) the corresponding quotient group, and \( A^G(Z) \) its coordinate ring. It follows by the definition of \( \pi^\text{PL}_1(X) \) that

\[
Z^1\text{PL}_{n,n} = Z^1(\pi^G_1(Z) \geq n, \Pi_{\text{PL}, n})^{\text{PL}}.
\]

In particular, each \( \text{Li}^n_\text{Li}(z) \) is in \( A^G(Z) \), and Goncharov’s conjecture (Conjecture 7.6 of [Gon]) says that \( A^G(Z) \) is spanned by elements of the form \( \text{Li}^n_\text{Li}(z) \), at least when \( Z = \text{Spec} \mathbb{Q} \). We might expect this to hold whenever \( Z \) is saturated. Whenever \( K \) is totally real, \( \mathfrak{n}^G(Z) \) agrees with \( \mathfrak{n}(Z) \) in degrees \( \geq -4 \); hence \( A^G(Z)_{\leq 4} = A(Z)_{\leq 4} \) should be spanned by elements of the form \( \text{Li}^n_\text{Li}(z) \).

3.3. Coordinates on the Space of Cocycles. Fix an arbitrary family \( \Sigma = \{\sigma_{n,i}\} \) of homogeneous free generators for \( \mathfrak{n}(Z) \) with \( \sigma_{n,i} \) in half-weight \(-n\), and for each word \( w \) of half-weight \(-n\) in the above generators, let \( f_w \) denote the associated element of \( A_n = A(Z)_n \).

The following proposition was communicated to the authors in an unpublished letter by Francis Brown. It provides equivalent information to the geometric algorithm in [DC15], but it allows one to avoid computing the logarithm in a unipotent group, making the algorithm much more practical.

Definition 3.8. For an arbitrary cocycle \( c \in Z^r_{\text{PL}}(R) \) for a \( \mathbb{Q} \)-algebra \( R \), a polylogarithmic word \( \lambda \) of half-weight \(-n\), and a word \( w \) in the elements of \( \Sigma \) of half-weight \(-n\), let

\[
\phi^\lambda_w(c) \in \mathbb{Q}
\]

denote the associated matrix entry of \( c^\lambda \), so that in the notation above, we have

\[
\text{Li}^n_\lambda(c) = \sum_w \phi^\lambda_w(c) f_w.
\]

Proposition 3.9. Let \( c \in Z^r_{\text{PL}}(R) \) for a \( \mathbb{Q} \)-algebra \( R \). For \( 0 \leq r < n \), \( \tau_1, \ldots, \tau_r \in \Sigma_{-1} \), and \( \sigma \in \Sigma_{r - n} \), we have

\[
\phi^\lambda_{e_1 \cdots e_0}(-\sigma_{1, \tau_1} \cdots \sigma_{r, \tau_r} c) = \phi^\lambda_{e_0}(-\sigma c) \cdots \phi^\lambda_{e_0}(-\sigma c) \phi^\lambda_{e_1 \cdots e_0}(-\sigma_{1, \tau_1} \cdots \sigma_{r, \tau_r} c),
\]

and all other matrix entries \( \phi^\lambda_w(c) \) vanish.

Proof. This amounts to a straightforward verification, but we nevertheless give the details. We begin with a formal calculation, in which \( \Sigma_{-1} \) may be an arbitrary finite set, and \( \{a^\tau\}_{\tau \in \Sigma_{-1}} \) a family of commuting coefficients. In this abstract setting, we claim that

\[
\left( \sum_{\tau \in \Sigma_{-1}} a^\tau f_\tau \right)^{\Pi_{\text{ln}}} = n! \sum_{\tau_1, \ldots, \tau_n \in \Sigma_{-1}} a^{\tau_1} \cdots a^{\tau_n} f_{\tau_1 \cdots \tau_n}.
\]
Indeed, the left side of the equation
\[
= \sum_{\tau_1, \ldots, \tau_n} (a^{\tau_1} f_{\tau_1}) \cdots (a^{\tau_n} f_{\tau_n}) \\
= \sum_{\tau_1, \ldots, \tau_n} a^{\tau_1} \cdots a^{\tau_n} \left( \sum_{\text{permutations } p \text{ of } \tau_1, \ldots, \tau_n} f_{\tau_{p_1} \cdots \tau_{p_n}} \right) \\
= \sum_p \sum_{\tau_1, \ldots, \tau_n} a^{\tau_1} \cdots a^{\tau_n} f_{\tau_{p_1} \cdots \tau_{p_n}}, \text{ independent of } p
\]
which equals the right side of the equation.

Returning to our concrete situation, we apply the reduced coproduct \(\Delta'\) to both sides of
\[
\sum_{|w| = -(n+1)} \phi_{n+1}^w(c) f_w = \text{Li}_{n+1}^u(c),
\]
and compute:

\[
(5) \quad \sum_{w', w''} \phi_{n+1}^{w'w''}(c) f_{w'} \otimes f_{w''} = \sum_{i=1}^n \text{Li}_{n+1-i}^u(c) \otimes \frac{\text{Li}_i^u}{i!} \\
= \sum_{i=1}^n \left( \text{Li}_{n+1-i}^u(c) \otimes \frac{\sum_{\tau \in \Sigma_{-1}} \phi_{\tau_0}^\tau(c) f_{\tau} \text{Li}_i^u}{i!} \right) \\
= \sum_{i=1}^n \sum_{\tau_1, \ldots, \tau_i \in \Sigma_{-1}} \sum_{|w| = n+1-i} \phi_{\tau_1}^{\tau_0}(c) \cdots \phi_{\tau_i}^{\tau_0}(c) \phi_{n+1-i}^w(c) f_w \otimes f_{\tau_1 \cdots \tau_i}
\]

Taking the coefficient of \(f_v \otimes f_{\tau}\), with \(\tau \in \Sigma_{-1}\), and \(v\) an arbitrary word of length \(n \geq 1\), we obtain
\[
\phi_{n+1}^{v\tau}(c) = \phi_{\tau_0}^{\tau}(c) \cdot \phi_{n}^{v}(c),
\]
while taking the coefficient of \(f_v \otimes f_{\sigma}\), with \(\sigma \in \Sigma_{-i < -1}\), and \(v\) an arbitrary word of length \(n + 1 - i \geq 1\), we obtain
\[
\phi_{n+1}^{v\sigma}(c) = 0. \quad \square
\]

We have a morphism
\[
\mathcal{C}_{\text{PL}} : Z_{\text{PL}}^{1,G_m} \times \pi_1^{\text{un}}(Z) \to \pi_1^{\text{PL}}(X)
\]
given by
\[
(c, \gamma) \mapsto c(\gamma).
\]
We refer to \(\mathcal{C}_{\text{PL}}\) as the universal polylogarithmic cocycle, and it is just the first component of the universal cocycle evaluation morphism \(\mathcal{C}_{\Pi}\) for \(\Pi = \pi_1^{\text{PL}}(X)\). We define a morphism
\[
\Psi : Z_{\text{PL}}^{1,G_m} \to \text{Spec } \mathbb{Q} \left[ \{ \Phi_\lambda \}_{\text{wt}(<\lambda)} \right],
\]
where $\rho$ ranges over $\Sigma$ and $\lambda$ ranges over the set of polylogarithmic words, by

$$c \mapsto (\phi^\rho_\lambda(c))_{\rho,\lambda}.$$  

We define a homomorphism of rings

$$\theta^\#: \mathbb{Q}[\log u, \text{Li}_1^u, \text{Li}_2^u, \ldots] \to A(Z)[\{\Phi^\rho_\lambda\}]$$

by

$$\log u \mapsto \sum_{\tau \in \Sigma} f_\tau \Phi^\tau_{e_0}$$

and

$$\text{Li}_n^u \mapsto \sum_{\tau_1, \ldots, \tau_r \in \Sigma_{-1-1}} f_{\sigma \tau_1 \ldots \tau_r} \Phi^\tau_{e_0} \Phi^\sigma_{e_1} \cdots e_0.$$

**Corollary 3.10.** The morphism $\Psi$ is an isomorphism. In particular, $Z_{1, \mathbb{G}_m}^{\text{PL}}$ is canonically an affine space endowed with coordinates. Moreover, the triangle

$$Z_{1, \mathbb{G}_m}^{\text{PL}} \times \pi_{1}^\text{un}(Z) \xrightarrow{\Psi \times \text{id}} \text{Spec} \mathbb{Q}[\{\Phi^\rho_\lambda\}] \times \pi_{1}^\text{un}(Z)$$

commutes.

**Proof.** The injectivity of $\Psi$, as well as the commutativity of the diagram, follow directly from Proposition 3.9. The surjectivity of $\Psi$ amounts to the statement that given any family $a^\rho_\lambda$ of elements of a $\mathbb{Q}$-algebra $R$, the $R$-algebra homomorphism

$$c^\#: R[\log u, \text{Li}_1^u, \text{Li}_2^u, \ldots] \to R \otimes A(Z)$$

given by

$$\log u \mapsto \sum_{\tau \in \Sigma_{-1}} a^\tau_{e_0} f_\tau$$

and

$$\text{Li}_n^u \mapsto \sum_{\tau_1, \ldots, \tau_r \in \Sigma_{-1-1}} a^{\tau_1}_{e_0} \cdots a^{\tau_r}_{e_0} a^{\sigma}_{e_1} \cdots e_0 f_{\sigma \tau_1 \ldots \tau_r}$$

is compatible with the coproduct. For $\log u$, this is because both sides are primitive. For $\text{Li}_n^u$, this follows by the computation of (5)–(7) and the fact that the terms for which $r = 0$ are primitive.

$\square$
3.3.1. **Variant in Bounded Weight.** Let \( n \) be a positive integer. Then there is a natural isomorphism \( Z_{PL,n}^{1,Gm} \overset{\Psi}{\longrightarrow} (\text{Spec } \mathbb{Q}[\{\Phi_\rho^\rho\}_{\rho,|\lambda|\leq n}]) \) such that the square

\[
\begin{array}{ccc}
Z_{PL,n}^{1,Gm} & \overset{\Psi}{\longrightarrow} & \text{Spec } \mathbb{Q}[\{\Phi_\rho^\rho\}_{\rho,|\lambda|\leq n}] \\
\downarrow & & \downarrow \\
Z_{PL,n}^{1,Gm} & \overset{\sim}{\longrightarrow} & \text{Spec } \mathbb{Q}[\{\Phi_\rho^\rho\}_{\rho,|\lambda|\leq n}]
\end{array}
\]

commutes, where the vertical arrows are the natural projections.

3.4. **Kummer and Period Maps in Coordinates.** Given \( z \in X(Z) \), we recall that, by definition,

\[
\log^u(z) = \log^u(\kappa(z)), \\
\text{Li}_n^u(z) = \text{Li}_n^u(\kappa(z)).
\]

We describe \( \kappa_p \) in these coordinates. More precisely, for \( z \in X(Z_p) \), the value \( \kappa_p \) is the element of \( \Pi_{PL,n}(Q_p) \) sending \( \log^u \) to \( \log^p(z) \) and \( \text{Li}_n^u \) to \( \text{Li}_n^p(z) \).

Finally, we describe \( \text{per}_p \) in these coordinates. More precisely, we have

\[
\text{per}_p(\log^u(z)) = \log^p(z), \\
\text{per}_p(\text{Li}_n^u(z)) = \text{Li}_n^p(z),
\]

which in particular expresses the commutativity of Kim’s cutter.

4. **Computations for \( Z = \text{Spec } \mathbb{Z}[1/S] \)**

4.1. **Abstract Coordinates for \( Z = \text{Spec } \mathbb{Z}[1/S] \).** We let \( \ell \) denote a prime number. We want to fix free generators \((\tau_\ell)_{\ell \in S}\) and \((\sigma_{2n+1})_{n \geq 1}\) for \( n(Z) \), with \( \tau_\ell \) in degree \(-1\) and \( \sigma_{2n+1} \) in degree \(-2n-1\). We first recall some notation from Section 3.2 of [DC15].

Letting \( A_n = A(Z)_n \) denote the degree \( n \) part of \( A(Z) \), and \( A_{>0} = \bigoplus_{n=1}^{\infty} A_n \), we let \( E_n = E_n(Z) \) denote the kernel of \( \Delta' \mid_{A_n} \) and \( D_n = D_n(Z) \) the subspace of decomposable elements of degree \( n \), i.e., the degree \( n \) elements in the image of

\[
A_{>0} \otimes A_{>0} \xrightarrow{\text{mult}} A.
\]

We let \( P_n = P_n(Z) \) denote a vector subspace of \( A_n \) complementary to \( E_n \) and \( D_n \). The symbols \( E_n, D_n, \) and \( P_n \) refer to bases of \( E_n, D_n, \) and \( P_n \), respectively.

**Proposition 4.1.** One may choose free generators \((\tau_\ell)_{\ell \in S}\) and \((\sigma_{2n+1})_{n \geq 1}\) for \( n(Z) \), with \( \tau_\ell \) in degree \(-1\) and \( \sigma_{2n+1} \) in degree \(-2n-1\), such that \( f_{\tau_\ell} = \log^u(\ell) \) and \( f_{\sigma_{2n+1}} = \zeta^u(2n+1) \).

Furthermore a choice of \( P_{2n+1} \) uniquely determines \( \sigma_{2n+1} \).

**Proof.** A computation using Corollary 3.2 shows that \( \log^u(\ell) \) and \( \zeta^u(2n+1) \) are primitive elements of the Hopf algebra \( A(Z) \) (or, in the terminology of [DC15], they lie in the space \( E_n \) of extensions). In fact, by our knowledge of the rational algebraic K-theory of \( Z \), we know that \( E_n \) is one-dimensional when \( n \) is odd and zero-dimensional otherwise. Therefore, the elements \( \log^u(\ell) \) and \( \zeta^u(2n+1) \) must span the spaces \( E_n \), and we take them as our \( E_n \).

By Proposition 3.2.3 of [DC15], for a choice of \( E_n, D_n, \) and \( P_n \), we get a set of generators for the Lie algebra, which are dual to the elements of \( E_n \). In fact, the part of the condition of being dual that depends on \( D_n \) and \( P_n \) is that the element of the Lie algebra pairs to
zero with all of $D_n \cup P_n$, so it in fact depends only on $P_n$ and $D_n$. The latter is uniquely determined, so a choice of $P_n$ determines such a choice of generators.

\begin{proof}
We have the reduced cobar complex
\[
\Delta' : A >_0 \otimes A >_0 \otimes A >_0 \otimes A >_0 \otimes A >_0 \otimes A >_0 \otimes A >_0 \otimes A >_0 \otimes A >_0 \rightarrow \cdots,
\]
which is a complex of graded vector spaces. The proof of Lemma 3.8 of [Gon] shows that the $k$th cohomology of this complex is the graded vector space $\bigoplus_n \text{Ext}^k_{\text{GrComod}(A)}(Q(0), Q(n))$ (graded by $n$). The result then follows because the category of graded comodules over $A$ is the same as the category of representations of $\pi^1_{\text{MT}}(Z)$, or equivalently, the category $\text{MT}(Z, Q)$, and we know that $\text{Ext}^2_{\text{MT}(Z, Q)}(Q(0), Q(n)) = K_{2n-1}(Z)_Q$.

from our knowledge of the Ext-groups in the category $\text{MT}(Z, Q)$.
\end{proof}

We recall Definitions 2.4 and 2.5. In those definitions, we let $\Delta_n'$ denote the restriction of $\Delta'$ to $A_n$. For $i + j = n$, we let $\Delta_{i,j}'$ denote the component of $\Delta_n'$ landing in $A_i \otimes A_j$.

The following corollary will be useful for computations in half-weight 4:

\begin{corollary}
If $K$ is totally real, then $\ker(\Delta_1') = \ker(\Delta_3') = E_3$.
\end{corollary}

\begin{proof}
Let $\alpha \in A_3$. Since $\Delta_1'$ is zero (by Remark 2.8), we have
\[
(\Delta_2' \otimes \text{id} - \text{id} \otimes \Delta_2')(\Delta_3'(\alpha)) = (\Delta_2' \otimes \text{id})(\Delta_3'(\alpha)) - (\text{id} \otimes \Delta_2')(\Delta_3'(\alpha)) = 0.
\]
As $K$ is totally real, it has no complex places, so we have $K_3(Z)_Q = 0$. Then by Proposition 4.3, we have that $E_2 = 0$. Therefore, $\Delta_2'$ is injective, hence $\Delta_2' \otimes \text{id}$ is injective on $A_2 \otimes A_1$. By the displayed equation and the previous sentence, it follows that if $\Delta_{1,2}'(\alpha) = 0$, then $\Delta_{2,1}'(\alpha) = 0$ as well. Therefore, $\ker(\Delta_{1,2}') = \ker(\Delta_3') = E_3$.
\end{proof}

Remark 4.2. The choice of $\log^u(\ell)$ and $\zeta^u(2n + 1)$ corresponds to choosing generators for the rational algebraic $K$-groups of $Z$. The arbitrariness in choosing $P_n$ then corresponds precisely to the non-canonicity discussed toward the end of Section 2.2.1.

Give such a set of generators, we get an abstract basis for $A(Z)$. For each word $w$ of half-weight $-n$ in the above generators, we have an element $w \in \mathcal{U}_n(Z)$, and these form a basis of $\mathcal{U}_n(Z)$. We let $(f_w)_w$ denote the dual basis for $A(Z)$. With the choices above, we have
\[
f_{\tau} = \log^u(\ell),
f_{\sigma_{2n+1}} = \zeta^u(2n + 1).
\]
In order to find bases of $P_n$ and verify relations between different $\text{Li}^u_n(z)$’s, we need to apply the reduced coproduct to reduce the computation in degree $n$ to the computation in degrees $m < n$. For this, we need the exact sequence

\begin{proposition}
The sequence
\[
0 \rightarrow E_n \rightarrow A_n \overset{\Delta'}{\rightarrow} \bigoplus_{i+j=n, i,j \geq 1} A_i \otimes A_j \overset{\Delta' \otimes \text{id} - \text{id} \otimes \Delta'}{\rightarrow} \bigoplus_{i+j+k=n, i,j,k \geq 1} A_i \otimes A_j \otimes A_k
\]
is exact, and $E_n = \text{Ext}^1_{\text{MT}(Z, Q)}(Q(0), Q(n)) = K_{2n-1}(Z)_Q$.
\end{proposition}

\begin{proof}
We have the reduced cobar complex
\[
A >_0 \overset{\Delta'}{\rightarrow} A >_0 \otimes A >_0 \overset{\Delta' \otimes \text{id} - \text{id} \otimes \Delta'}{\rightarrow} A >_0 \otimes A >_0 \otimes A >_0 \otimes A >_0 \rightarrow \cdots,
\]
which is a complex of graded vector spaces. The proof of Lemma 3.8 of [Gon] shows that the $k$th cohomology of this complex is the graded vector space $\bigoplus_n \text{Ext}^k_{\text{GrComod}(A)}(Q(0), Q(n))$ (graded by $n$). The result then follows because the category of graded comodules over $A$ is the same as the category of representations of $\pi^1_{\text{MT}}(Z)$, or equivalently, the category $\text{MT}(Z, Q)$, and we know that $\text{Ext}^2_{\text{MT}(Z, Q)}(Q(0), Q(n)) = K_{2n-1}(Z)_Q$.

We recall Definitions 2.4 and 2.5. In those definitions, we let $\Delta_n'$ denote the restriction of $\Delta'$ to $A_n$. For $i + j = n$, we let $\Delta_{i,j}'$ denote the component of $\Delta_n'$ landing in $A_i \otimes A_j$.

The following corollary will be useful for computations in half-weight 4:

\begin{corollary}
If $K$ is totally real, then $\ker(\Delta_{1,2}') = \ker(\Delta_3') = E_3$.
\end{corollary}

\begin{proof}
Let $\alpha \in A_3$. Since $\Delta_1'$ is zero (by Remark 2.8), we have
\[
(\Delta_2' \otimes \text{id} - \text{id} \otimes \Delta_2')(\Delta_3'(\alpha)) = (\Delta_2' \otimes \text{id})(\Delta_3'(\alpha)) - (\text{id} \otimes \Delta_2')(\Delta_3'(\alpha)) = 0.
\]
As $K$ is totally real, it has no complex places, so we have $K_3(Z)_Q = 0$. Then by Proposition 4.3, we have that $E_2 = 0$. Therefore, $\Delta_2'$ is injective, hence $\Delta_2' \otimes \text{id}$ is injective on $A_2 \otimes A_1$. By the displayed equation and the previous sentence, it follows that if $\Delta_{1,2}'(\alpha) = 0$, then $\Delta_{2,1}'(\alpha) = 0$ as well. Therefore, $\ker(\Delta_{1,2}') = \ker(\Delta_3') = E_3$.
\end{proof}
4.1.1. Coordinates on the Space of Cocycles for $Z = \text{Spec } Z[1/\ell]$. Relative to the chosen coordinates, we name coordinates for $Z_{\text{PL}, n}^{1, G_n}$ when $S = \{\ell\}$. Specifically, we set

\[
\begin{align*}
w_0 & := \phi_{\ell e_0}^\tau \\
w_1 & := \phi_{e_1 e_0}^\tau \\
w_k & := \phi_{2e_1 e_0 \cdots e_0}^{\sigma_2 k+1} 2 \leq k \leq n
\end{align*}
\]

in the notation of Proposition 3.9. In fact, for $k \geq 2$, this makes sense even when $|S| > 1$, and we use it in Section 4.3.3.

If $z \in X(Z)$, we write $w_k(z)$ for $w_k(\kappa(z))$. In this notation, $w_0(z) = \text{ord}_\ell z$, and $w_1(z) = -\text{ord}_\ell (1 - z)$, both by Fact 3.3.


4.2.1. Coordinates for the Galois Group. Let $Z = Z[1/\ell]$. Then $n(Z)_{\geq -4}$ is three-dimensional as a vector space, generated by $\tau = \tau_\ell$, $\sigma = \sigma_3$, and $[\sigma, \tau]$. As $P_3 = 0$ when $|S| = 1$, the elements $\tau, \sigma$ are already well-defined. We choose $f_\tau, f_\sigma$, and $f_{\sigma\tau}$ as a set of affine coordinates on $\pi_{1, \text{un}}^{\text{un}}(Z)_{\geq -4}$.

4.2.2. Coordinates for the Selmer Variety. In this case, the only nonzero coordinates are $w_0$, $w_1$, and $w_2$.

4.2.3. The Universal Cocycle Evaluation Morphism. We now write the morphism $C_{\text{PL}, 4}$ in these coordinates. We have $C_{\text{PL}, 4}(f_i) = f_i$ for $i = \tau, \sigma, \sigma\tau$.

Using Equation (8), we find that $C_{\text{PL}, 4}(\log^u) = w_0 f_\tau$, $C_{\text{PL}, 4}(\text{Li}_1^u) = w_1 f_\tau$, and $C_{\text{PL}, 4}(\text{Li}_2^u) = w_0 w_1 f_\tau^2/2$. 

At this point, we already see that the function on $\Pi_{\text{PL}, 4} \times \pi_{1, \text{un}}^{\text{un}}(Z)_{\geq -4}$ given by

\[
\text{Li}_2^u - \frac{1}{2} \log^u \text{Li}_1^u
\]

vanishes on the image of $C_{\text{PL}, 4}$, i.e., is in $\mathcal{T}_{\text{PL}, 4}^Z$.

Again, by Equation (8), we have

\[
\begin{align*}
C_{\text{PL}, 4}(\text{Li}_3^u) & = w_1 w_0^2 f_\tau^3/6 + w_2 f_\sigma, \\
C_{\text{PL}, 4}(\text{Li}_4^u) & = w_1 w_0^3 f_\tau^4/24 + w_0 w_2 f_{\sigma\tau}.
\end{align*}
\]
To construct a second element of $I_{PL,4}$, we first eliminate $w_2$ by considering
\[ C_{PL,4}^*(f_\sigma f_\tau \text{Li}_4^u - f_\sigma \log^u \text{Li}_3^u) = w_1 w_0^3 f_\sigma f_\tau^5/24 - f_\sigma w_1 w_0^3 f_\tau^4/6 \]
\[ = \frac{w_1 w_0^3 f_\tau^4}{24} (f_\sigma f_\tau - 4 f_\sigma \tau) \]
\[ = \frac{C_{PL,4}^*(\log^u)^3 \text{Li}_1^u}{24} (f_\sigma f_\tau - 4 f_\sigma \tau) \]

It follows that
\[ C_{PL,4}^* \left( f_\sigma f_\tau \text{Li}_4^u - f_\sigma \log^u \text{Li}_3^u - \frac{(\log^u)^3 \text{Li}_1^u}{24} (f_\sigma f_\tau - 4 f_\sigma \tau) \right) = 0 \]

In other words,

**Proposition 4.5.** The two functions

\[ \text{Li}_2^u - \frac{1}{2} \log^u \text{Li}_1^u \]
\[ f_\sigma f_\tau \text{Li}_4^u - f_\sigma \log^u \text{Li}_3^u - \frac{(\log^u)^3 \text{Li}_1^u}{24} (f_\sigma f_\tau - 4 f_\sigma \tau) \]

on $\Pi_{PL,4} \times \pi_{1,u}(Z)_{\geq 4}$ are in $I_{PL,4}^*$ for $Z = \text{Spec}\mathbb{Z}[1/\ell]$.

4.3. **Coordinates on the Galois Group for** $Z = \mathbb{Z}[1/\ell]$. In order to evaluate the functions of Proposition 4.5 we need to choose a prime $p \neq \ell$ and interpret $f_\tau$, $f_\sigma$, and $f_\sigma \tau$ in such a way that we can take (approximate) their $p$-adic periods. Essentially, this means writing them as special values of polylogarithms. As mentioned in Proposition 4.1 we have chosen the first two to correspond to $\log^u(\ell)$ and $\zeta^u(3)$, respectively. It remains to understand $f_\sigma \tau$.

This will depend on $\ell$. We start with the case $\ell = 2$, in an effort to re-derive Theorem 1.16 of [DCW10].

4.3.1. **The Case** $Z = \mathbb{Z}[1/2]$. We let $A = A(Z)$ as usual. We compute using Corollary 3.2 and Fact 3.3 that

\[ \Delta_{1,2}^*(\text{Li}_5^u(1/2)) = \text{Li}_5^u(1/2) \otimes (\log^u(1/2))^2/2 = -\log^u(1/2) \otimes (\log^u(2))^2/2 = f_\tau \otimes f_\tau^2/2. \]

Using the fact that $\Delta$ is a ring homomorphism, we note that $\Delta_{1,2}(\log^u(2)^3) = 3 \log^u(2) \otimes \log^u(2)^2$. Therefore, Corollary 4.4 implies that

\[ \text{Li}_5^u(1/2) - \frac{(\log^u(2))^3}{6} \]

is in $E_3$. As $E_3 = K_5[Z]_{\mathbb{Q}}$ is one-dimensional, this is a rational multiple of $\zeta^u(3)$.

The identity in the appendix to [DCW16] says that

\[ (9) \quad \text{Li}_5^u(1/2) = \frac{(\log^u(2))^3}{6} + \frac{7}{8} \zeta^u(3). \]

By Definition 3.8 we have

\[ C_{PL,4}^*(\text{Li}_4^u) = w_1 w_0^3 f_\tau^4/24 + w_0 w_2 f_\sigma \tau. \]

It is easy to check using the formulas at the end of Section 4.1.1 that $w_0(\kappa(1/2)) = -1$ and $w_1(\kappa(1/2)) = 1$, and (9) together with Definition 3.8 implies that $w_2(\kappa(1/2)) = 7/8$.  

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We therefore get
\[ \text{Li}_3^u(1/2) = -(\log^u(2))^4/24 - \frac{7}{8} f_{\sigma \tau}. \]

It follows that
\[ f_{\sigma \tau} = -\frac{8}{7} \left( \frac{\log^u(2)^4}{24} + \text{Li}_3^u(1/2) \right). \]

4.3.2. Choosing \( P_3(\text{Spec } \mathbb{Z}[1/6]) \). To deal with the case \( Z = \text{Spec } \mathbb{Z}[1/3] \), we have to consider \( Z' = \text{Spec } \mathbb{Z}[1/6] \), as \( Z \) is not saturated. In this case, the Lie algebra \( \mathfrak{n}(Z') \) is generated by \( \tau_2, \tau = \tau_3, \) and \( \sigma = \sigma_3. \)

In this case, \( P_1(Z') \) is zero. As \( P_3(Z') \) is nonzero, there is some choice in the definition of \( \sigma \) as an element of \( \mathfrak{n}(Z') \). We therefore seek to choose a set \( P_3(Z') \).

While \( A(Z')_1 \) has basis \( \{\log^u(2), \log^u(3)\} \), we must first find a basis of \( A(Z')_2. \) As \( E_2(Z') = 0 \), the map \( \Delta_2 \) is injective. We may take \( D_2(Z') = \{\log^u(2)^2, \log^u(2) \log^u(3), \log^u(3)^2\}. \) Then
\[ \Delta'(\text{Li}_2^u(-2)) = \text{Li}_1^u(-2) \otimes \log^u(-2) = -\log^u(3) \otimes \log^u(2), \]
which is independent from
\[ \{\Delta' \log^u(2)^2, \Delta' \log^u(2) \log^u(3), \Delta' \log^u(3)^2\} \]
in \( A_1(Z') \otimes A_1(Z') \) (as seen by checking via the basis of \( A_1(Z') \otimes A_1(Z') \) induced by the basis \( \{\log^u(2), \log^u(3)\} \) of \( A_1(Z') \)). In fact, \( \text{Li}_2^u(-2) = -f_{\tau \tau_2} \), as they have the same reduced coproduct.

This gives us a basis \( \{\log^u(2)^2, \log^u(2) \log^u(3), \log^u(3)^2, \text{Li}_2^u(-2)\} \) of \( A_2(Z') \), so by taking all degree 3 products of basis elements of \( A_1(Z') \) and \( A_2(Z') \), we may take
\[ D_3(Z') = \{\log^u(2)^3, \log^u(3)^3, \log^u(2)^2 \log^u(3), \log^u(2) \log^u(3)^2, \log^u(2) \text{Li}_2^u(-2), \log^u(3) \text{Li}_2^u(-2)\}. \]

We would like to show that
\[ B := \{\log^u(2)^3, \log^u(3)^3, \log^u(2)^2 \log^u(3), \log^u(2) \log^u(3)^2, \log^u(2) \text{Li}_2^u(-2), \log^u(3) \text{Li}_2^u(-2), \text{Li}_3^u(-2), \text{Li}_3^u(3)\} \]
is a basis of \( A_3(Z')/E_3(Z') \), which would imply that \( \{\text{Li}_3^u(-2), \text{Li}_3^u(3)\} \) can be taken as \( P_3(Z') \). To do this, we apply \( \Delta'_{1,2} \) to each element of \( B \) and expand in the basis
\[ \{\log^u(2) \otimes \log^u(2)^2, \log^u(2) \otimes \log^u(2) \log^u(3), \log^u(2) \otimes \log^u(3)^2, \log^u(2) \otimes \text{Li}_2^u(-2), \]
\[ \log^u(3) \otimes \log^u(2)^2, \log^u(3) \otimes \log^u(2) \log^u(3), \log^u(3) \otimes \log^u(3)^2, \log^u(3) \otimes \text{Li}_2^u(-2)\} \]
of \( A_1(Z') \otimes A_2(Z') \). Using Corollary 3.2, this produces the matrix

| \( \log^u(2) \otimes \log^u(2)^2 \) | 3 | 0 | 0 | 0 | 0 | 0 | 0 |
| \( \log^u(2) \otimes \log^u(2) \log^u(3) \) | 0 | 0 | 2 | 0 | 0 | 0 | 0 |
| \( \log^u(2) \otimes \log^u(3)^2 \) | 0 | 0 | 1 | 0 | 0 | 0 | \(-1/2\) |
| \( \log^u(2) \otimes \text{Li}_2^u(-2) \) | 0 | 0 | 0 | 1 | 0 | 0 | 0 |
| \( \log^u(3) \otimes \log^u(2)^2 \) | 0 | 0 | 1 | 0 | \(-1\) | 0 | \(-1/2\) |
| \( \log^u(3) \otimes \log^u(2) \log^u(3) \) | 0 | 0 | 2 | 0 | \(-1\) | 0 | 0 |
| \( \log^u(3) \otimes \log^u(3)^2 \) | 0 | 3 | 0 | 0 | 0 | 0 | 0 |
| \( \log^u(3) \otimes \text{Li}_2^u(-2) \) | 0 | 0 | 0 | 0 | 1 | 0 | 0 |

where the columns correspond to the element of \( B \). This matrix has determinant 9, which by Corollary 4.4 and the fact that \( A_3(Z')/E_3(Z') \) is eight-dimensional (by our knowledge of the shuffle algebra \( A(Z') \)) implies that \( B \) is in fact a basis of \( A_3(Z')/E_3(Z') \). We choose
$P_3(Z')$ to be the space generated $Li_3^u(-2)$ and $Li_3^u(3)$, and $\sigma$ such that it pairs to 0 with this choice of $P_3(Z')$.

4.3.3. The Case $Z = \mathbb{Z}[1/3]$. Armed with our choice of $\sigma \in \mathfrak{n}(Z')$, we seek to write $f_\sigma \in A(Z)$ as an explicit combination of motivic polylogarithms. With our choice of $\sigma$, we have $w_2(-2) = w_2(3) = 0$ because $Li_3^u(-2)$ and $Li_3^u(3)$ are elements of $\mathcal{P}_3$.

From the matrix above, we see that

$$\Delta_{1,2}' Li_3^u(3) = -\log^u(2) \otimes \log^u(3)^2/2.$$  

We also compute

$$\Delta_{1,2}' Li_3^u(9) = Li_1^u(9) \otimes \log^u(9)^2/2 = -6 \log^u(2) \otimes \log^u(3)^2,$$

so $Li_3^u(9) = 12 Li_3^u(3)$ is in $E_3(Z')$, hence a rational multiple of $\zeta^u(3)$ (because $E_3(Z') = K_5(Z') \mathbb{Q}$ is one-dimensional). In fact, since $w_2(3) = 0$, this rational number is the $f_\sigma$-coordinate of $Li_3^u(9)$ in the basis $(f_w)_w$ of $A(Z')$, hence it equals $w_2(9)$ because $f_\sigma = \zeta^u(3)$.

Numerical computation using the code [DCC] in the 5-adic and 7-adic realizations suggests that

$$w_2(9) = \frac{Li_3^u(9) - 12 Li_3^u(3)}{\zeta^u(3)} = -\frac{26}{3}.$$  

We may now compute using Definition 3.8 that

$$Li_3^u(3) = w_2(3) \phi_e^\tau(3) f_\sigma + \phi_e(3) \phi_e^\tau(3)^3 f_{\tau\tau\tau\tau} = -f_{\tau\tau\tau\tau}$$

and

$$Li_3^u(9) = w_2(9) \phi_e(9) f_\sigma + \phi_e(3) \phi_e^\tau(9)^3 f_{\tau\tau\tau\tau} = 2w_2(9) f_\sigma - 24 f_{\tau\tau\tau\tau}.$$  

This implies that

$$-\frac{12}{w_2(9)} Li_3^u(3) + (2w_2(9))^{-1} Li_3^u(9) = f_\sigma.$$  

We note that this corresponds precisely to $f_\sigma$ in the image of $\mathcal{O}(\pi_1^{un}(Z)) \hookrightarrow \mathcal{O}(\pi_1^{un}(Z'))$.

Plugging this into the second equation of Proposition 4.5, we find

**Theorem 4.6.** The element

$$\zeta^u(3) \log^u(3) Li_3^u - \left( -\frac{12}{w_2(9)} Li_3^u(3) + (2w_2(9))^{-1} Li_3^u(9) \right) \log^u Li_3^u$$

$$-\frac{(\log^u)^3 Li_3^u}{24} \left( \zeta^u(3) \log^u(3) - 4 \left( -\frac{12}{w_2(9)} Li_3^u(3) + (2w_2(9))^{-1} Li_3^u(9) \right) \right)$$

of $\mathcal{O}(\Pi_{PL,4} \times \pi_1^{un}(Z))$ is in $\mathcal{T}_{PL,4}^Z$ for $Z = \text{Spec } \mathbb{Z}[1/3]$, where $w_2(9)$ is a number $p$-adically close to $-\frac{26}{3}$ for $p = 5, 7$.

For $p \neq 2, 3$, the corresponding Coleman function is

$$\zeta^p(3) \log^p(3) Li_3^p + \left( -\frac{12}{w_2(9)} Li_3^p(3) + (2w_2(9))^{-1} Li_3^p(9) \right) \log^p(z) Li_3^p(z)$$

$$-\frac{(\log^p(z))^3 Li_3^p(z)}{24} \left( \zeta^p(3) \log^p(3) - 4 \left( -\frac{12}{w_2(9)} Li_3^p(3) + (2w_2(9))^{-1} Li_3^p(9) \right) \right).$$
4.4. The Chabauty-Kim Locus for $Z[1/3]$ in Half-Weight 4. As noted in Section 8.2 of BDCKW, the function $\text{Li}_p^2(z) - \frac{1}{2} \log^p(z) \log^p(1 - z)$ has the zero set $\{2, \frac{1}{2}, -1\}$ for $p = 5, 7$. By numerical evaluation of (10) at $\text{BDCKW}$, the function

$$
\text{The Chabauty-Kim Locus for 4.4.}
$$

Theorem 4.7. For $Z = \text{Spec } Z[1/3]$, we have $X(Z_p)_{\text{PL},4} \subset \{ -1 \}$ for $p = 5, 7$.

5. Answer to Question 2.24 and $S_3$-Symmetrization

5.1. Answer to Question 2.24. We fix a set of generators as in Section 4.1.

We first need the following lemma:

Lemma 5.1. We have $\text{Li}_k^p(-1) = 0$ for $k \geq 2$ even.

Proof. This follows from the identity $2^{-k} \text{Li}_k^p(z^2) = \text{Li}_k^p(z) + \text{Li}_k^p(-z)$, which is Proposition 6.1 of [Col82] for $m = 1$. Indeed, setting $z = 1$ in the identity shows $\text{Li}_k^p(-1) = (2^{-k} - 1) \text{Li}_k^p(1)$, and since $\text{Li}_k^p(1) = \zeta^p(k)$, which is 0 for $k$ even, we have $\text{Li}_k^p(-1) = 0$.

Theorem 5.2. For any prime $\ell$ and positive integer $n$, we have

$$
-1 \in X(Z_p)_{\text{PL},n},
$$

where $Z = \text{Spec } Z[1/\ell]$.

In particular, for $\ell$ odd, Question 2.24 has a negative answer.

Proof. We use the coordinates of Section 4.1. We also write $\tau = \tau_\ell$. We have $f_\tau = \log^n(\ell)$.

To prove the theorem, we produce an element $c_{-1}$ of $Z_{\text{PL},n}^*(K)$ whose image $\alpha_{-1}$ under $C_{\text{PL},n}$ lies in $\Pi_{\text{PL},n}(A(Z)) \subset \Pi_{\text{PL},n}(K)$ and satisfies $\text{per}_p(\alpha_{-1}) = \kappa_p(-1) \in \Pi_{\text{PL},n}(Q_p)$. Since any element of $O(\Pi_{\text{PL},n} \times (\mathbb{Z}_p^{un}(Z)) \cap Z_{\text{PL},n}$ vanishes on the image of $C_{\text{PL},n}^K$, it vanishes on $\alpha_{-1}$ and therefore on $\kappa_p(-1)$, which proves the theorem.

We define $c_{-1}$ by setting

$$
w_0(c_{-1}) := 0,
$$

$$
w_1(c_{-1}) := \frac{\text{Li}_1^u(-1)}{\log^u(\ell)},
$$

$$
w_k(c_{-1}) := \frac{\text{Li}_{2k-1}^u(-1)}{\zeta^u(2k - 1)} \quad k = 2, \ldots, n.
$$

Setting $\alpha_{-1} := C_{\text{PL},n}(c_{-1})$, we now compute $\log^u(\alpha_{-1})$ and $\text{Li}_k^u(\alpha_{-1})$ for $1 \leq k \leq n$.

We have $C_{\text{PL},n}^K(\log^u) = w_0 f_\tau$, so

$$
\log^u(\alpha_{-1}) = w_0(c_{-1}) f_\tau = 0.
$$

We have $C_{\text{PL},n}^K(\text{Li}_1^u) = w_1 f_\tau$, so

$$
\text{Li}_1^u(\alpha_{-1}) = w_1(c_{-1}) f_\tau = \frac{\text{Li}_1^u(-1)}{\log^u(\ell)} \log^u(\ell) = \text{Li}_1^u(-1).
$$
For $k \geq 2$ even, we have
\[
\mathcal{C}_{PL,n}^\#(\text{Li}_k^u) = w_1 w_0^{k-1} f_k / k! + \sum_{i=2}^{[\frac{k}{2}]} w_i w_0^{k-2i+1} f_{\sigma_{2i-1}} \tau^{k-2i+1},
\]
\[
= w_0 \left( w_1 w_0^{k-1} f_k / k! + \sum_{i=2}^{[\frac{k}{2}]} w_i w_0^{k-2i} f_{\sigma_{2i-1}} \tau^{k-2i+1} \right),
\]
and since $w_0(c_{-1}) = 0$, we have $\text{Li}_k^u(\alpha_{-1}) = 0$.

For $k \geq 3$ odd, we have
\[
\mathcal{C}_{PL,n}^\#(\text{Li}_k^u) = w_1 w_0^{k-1} f_k / k! + \sum_{i=2}^{[\frac{k}{2}]} w_i w_0^{k-2i+1} f_{\sigma_{2i-1}} \tau^{k-2i+1},
\]
\[
= w_0 \left( w_1 w_0^{k-1} f_k / k! + \sum_{i=2}^{[\frac{k}{2}]-1} w_i w_0^{k-2i} f_{\sigma_{2i-1}} \tau^{k-2i+1} \right) + w_{k+1} f_{\sigma_k},
\]
so by $w_0(c_{-1}) = 0$, we have
\[
\text{Li}_k^u(\alpha_{-1}) = w_{k+1} (-1)^{f_{\sigma_k}}
\]
\[
= \text{Li}_k^u(-1) \zeta^u(k)
\]
\[
= \text{Li}_k^u(-1).
\]

We have thus shown that $\log^u(\alpha_{-1}) = 0$, $\text{Li}_k^u(\alpha_{-1}) = 0$ for $k$ even, and $\text{Li}_k^u(\alpha_{-1}) = \text{Li}_k^u(-1)$ for $k$ odd. This shows that $\alpha_{-1} \in \Pi_{PL,n}(A(Z))$.

The key fact is that $\text{Li}_k^p(-1) = 0$ for $k \geq 2$ even. This follows from the identity $2^{-k}\text{Li}_k^p(z^2) = \text{Li}_k^p(z) + \text{Li}_k^p(-z)$, which is Proposition 6.1 of [Col82] for $m = 1$. Indeed, setting $z = 1$ in the identity shows $\text{Li}_k^p(-1) = (2^{-k} - 1)\text{Li}_k^p(1)$, and since $\text{Li}_k^p(1) = \zeta^p(k)$, which is $0$ for $k$ even, we have $\text{Li}_k^p(-1) = 0$.

By Lemma 5.1, $\text{Li}_k^p(-1) = 0$ for $k \geq 2$ even. Since we also have $\log^p(-1) = 0$, we get that $\text{Li}_k^p(-1) = \log^p(-1)$ for $k \geq 2$. This implies that $\text{per}_k(\alpha_{-1}) = \kappa_\langle-1\rangle$, as desired. 

5.2. $S_3$-Symmetrization. We recall our strengthening of Conjecture 2.23. The $S_3$-action on $X$ induces an $\pi_1^{\text{MT}}(Z)$-equivariant action on $\pi_1^{\text{un}}(X)$, and for a quotient $\Pi$ and $\sigma \in S_3$, we may refer to $\sigma(\Pi)$. We then write
\[
X(Z_p)^{S_3}_{PL,n} := \bigcap_{\sigma \in S_3} \sigma(X(Z_p)_{PL,n}) = \bigcap_{\sigma \in S_3} X(Z_p)_{\sigma(\Pi)}.
\]

Our symmetrized conjecture is that

**Conjecture 5.3.** $X(Z) = X(Z_p)^{S_3}_{PL,n}$ for sufficiently large $n$.

5.2.1. Verification for $Z = \text{Spec} \mathbb{Z}[1/3]$. We can use our computations in Section 4 to show verify a case of this conjecture:

**Theorem 5.4.** For $Z = \text{Spec} \mathbb{Z}[1/3]$ and $p = 5, 7$, Conjecture 5.3 (and hence Conjecture 2.23) holds (with $n = 4$).
Proof. By Theorem 4.7, \( X(Z_p)^{PL,4} \subseteq \{-1\} \). But \(-1\) is not fixed by the action of \( S_3 \), so

\[
X(Z_p)^{S_3}_{PL,4} := \bigcap_{\sigma \in S_3} \sigma(X(Z_p)^{PL,4}) = \emptyset
\]

for \( p = 5, 7 \). In particular, Conjecture 5.3 and hence Conjecture 2.23 holds in these cases. 

\[\square\]

References


