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THREE-DIMENSIONAL EXTENSIONS OF THE ALDAY–GAIOTTO–TACHIKAWA RELATION

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An extension of the two-dimensional (2d) Alday–Gaiotto–Tachikawa (AGT) relation to three dimensions starts from relating the theory on the domain wall between some two S-dual supersymmetric Yang–Mills (SYM) models to the 3d Chern–Simons (CS) theory. The simplest case of such a relation would presumably connect traces of the modular kernels in 2d conformal theory with knot invariants. Indeed, the two quantities are very similar, especially if represented as integrals of quantum dilogarithms. But there are also various differences, especially in the "conservation laws" for the integration variables holding for the monodromy traces but not for the knot invariants. We also consider another possibility: interpreting knot invariants as solutions of the Baxter equations for the relativistic Toda system. This implies another AGT-like relation: between the 3d CS theory and the Nekrasov–Shatashvili limit of the 5d SYM theory.

Keywords: Alday–Gaiotto–Tachikawa relation, Chern–Simons theory, knot invariant

1. Introduction

A long-expected relation was suggested in [1] (also see [2]–[12]), which can be considered one possible 3+3 counterpart of the celebrated 2+4 Alday–Gaiotto–Tachikawa (AGT) relation [13] between conformal blocks and Nekrasov functions. This new relation is assumed to identify the modular transformation kernels $M(a,a')$ of conformal blocks and the matrix elements in the three-dimensional (3d) Chern–Simons (CS) theory. In its simplest version, the relation is between the trace of the modular kernel as a function of the external dimensions and the Hikami integrals [14] representing the CS partition functions on $S^3 \setminus K$ (a 3d sphere with a knot K removed) considered as functions of monodromies around K. Our task here is to discuss possible explicit formulations of such a relation, omitting all the general context and reasoning considered in detail in [1]. We indicate some problems with the exact identification of the modular trace and knot invariants. We also emphasize the importance of another relation between knot invariants and the 5d Seiberg–Witten (SW) theory, which implies another form of the AGT relation involving the 3d CS theory.

2. Modular kernel

The conformal block $B_\Gamma(a|m|q)$ for a given graph Γ depends on three kinds of variables: a and m are parameters (α-parameters) on the respective internal lines and external legs (the corresponding conformal dimensions are quadratic in these parameters), and q parameterizes the graph itself. The modular transformation does not change the graph Γ (while changing $q \to q'$ and permuting the members of the set α of

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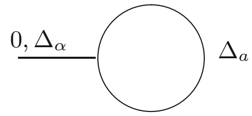

Fig. 1. Toric conformal block diagram: $\Delta_a = (\epsilon^2/4 + a^2)/\epsilon_1\epsilon_2$, $\Delta_\alpha = (\epsilon^2/4 + \alpha^2)/\epsilon_1\epsilon_2$.

external-leg parameters) and is realized as an integral transformation in the a variables:

$$B_\Gamma(a|\alpha|q) = \int d\mu(a')\, M(a,a')B_\Gamma(a'|\alpha'|q').$$

The function $M(a,a')$ depends on Γ and α but not on q and is called the modular kernel associated with the particular modular transformation $q \to q'$. In spirit, it is a Fourier kernel: $M(a,a') \sim e^{4\pi i a a'/\epsilon_1\epsilon_2 + \cdots}$, where the corrections are less singular at small ϵ_1 and ϵ_2.

The simplest example is provided by the modular transformation of the toric one-point function (see Fig. 1), which on the Yang–Mills theory side describes the theory with adjoint matter with the mass $m = -i\alpha + \epsilon/2 = -2i\widetilde{\alpha}$:

$$\mathcal{B}(a|\alpha| -1/\tau) = \int d\mu(a')\, \mathcal{M}(a,a'|\alpha)\mathcal{B}(a'|\alpha|\tau). \tag{1}$$

Here (see [15]),

$$\mathcal{B}(a|\alpha|\tau) = q^{-(\nu+1)/24}\eta^\nu(q)e^{2\pi i\tau a^2/\epsilon_1\epsilon_2} \times$$
$$\times\left(1 + 2q\frac{(\epsilon_1 - m)(\epsilon_2 - m)}{\epsilon_1\epsilon_2}\frac{(\epsilon^2 - 4a^2 + m(m-\epsilon))}{\epsilon^2 - 4a^2} + O(q^2)\right), \tag{2}$$

where

$$\nu = 1 - \frac{2m(\epsilon - m)}{\epsilon_1\epsilon_2}, \qquad \epsilon = \epsilon_1 + \epsilon_2, \qquad q = e^{2\pi i\tau}, \qquad \eta(q) = q^{1/24}\prod_{k=1}^{\infty}(1 - q^k).$$

According to [16], the modular kernel in (1) is given by

$$\mathcal{M}(a,a'|\alpha) = \frac{2^{3/2}}{s(\alpha)}\int \frac{s(a + r + \widetilde{\alpha})s(a - r + \widetilde{\alpha})}{s(a + r - \widetilde{\alpha})s(a - r - \widetilde{\alpha})}e^{4\pi i r a'/\epsilon_1\epsilon_2}\, dr, \tag{3}$$

where the measure is $d\mu(a') = 4\sinh(2\pi\epsilon_1 a')\sinh(2\pi\epsilon_2 a')\, da'$. The function $s(z)$ is the "quantum dilogarithm" [17], [18] (also see Appendix A below), i.e., the ratio of two digamma functions,

$$s(z|\epsilon_1,\epsilon_2) \sim \prod_{m,n\geq 0}\frac{(m + 1/2)\epsilon_1 + (n + 1/2)\epsilon_2 - iz}{(m + 1/2)\epsilon_1 + (n + 1/2)\epsilon_2 + iz}. \tag{4}$$

In (3) and everywhere below except Sec. A.1 in Appendix A (which is for reference purposes), we omit the parameters ϵ_1 and ϵ_2 from the dilogarithm arguments: $s(z) \equiv s(z|\epsilon_1,\epsilon_2)$.

We note that $\mathcal{M}(a,a'|\alpha)$ depends on the external momentum $\widetilde{\alpha}$, the internal dimension $\Delta(\alpha)$, and the central charge $c = 1 + 6\epsilon^2/\epsilon_1\epsilon_2$, but not on the modular parameter τ.

When $\alpha \to 0$, the conformal block becomes purely classical,

$$\mathcal{B}(a|\alpha|\tau) \to \frac{1}{\eta(q)}e^{2i\pi\tau a^2/\epsilon_1\epsilon_2}$$

(the last factor in the parentheses in the right-hand side of (2)) becomes $q^{1/12}\eta^{-2}(q)$ at $m = 0$), and the modular transformation becomes the ordinary Fourier transformation,

$$\mathcal{M}(a, a'|0)\mu'(a) \overset{\widetilde{\alpha}=i\epsilon/2}{=} \sqrt{2}\,\cos\biggl(4\pi i\frac{aa'}{\epsilon_1\epsilon_2}\biggr). \tag{5}$$

Hence, indeed

$$\frac{e^{-2\pi i\tau^{-1}a^2/\epsilon_1\epsilon_2}}{\eta(-\tau^{-1})} = \int da'\, e^{4\pi i a a'/\epsilon_1\epsilon_2}\frac{e^{2\pi i\tau(a')^2/\epsilon_1\epsilon_2}}{\eta(\tau)}\frac{1}{\sqrt{\epsilon_1\epsilon_2}}.$$

We note that the monodromy kernel satisfies the unitarity relation

$$\int d\mu(a)\, M(a,b)M^*(a,b') = \frac{d\mu(b')}{db'}\delta(b-b'),$$

and it is therefore natural to define the trace as

$$\mathrm{tr} \sim \int da'\frac{d\mu(a)}{d\mu(a')}\delta(a-a').$$

The trace of monodromy kernel (3) thus defined contains two integrals, which split:

$$\int da\,\mathcal{M}(a,a|\alpha) = \frac{2^{3/2}}{s(\alpha)}\iint dr\,da\frac{s(a+r+\widetilde{\alpha})s(a-r+\widetilde{\alpha})}{s(a+r-\widetilde{\alpha})s(a-r-\widetilde{\alpha})}e^{4\pi i r a} = \frac{2^{3/2}}{s(\alpha)}T_+(\widetilde{\alpha})T_-(\widetilde{\alpha}),$$

where

$$T_\pm(\widetilde{\alpha}) = \int\frac{s(z+\widetilde{\alpha})}{s(z-\widetilde{\alpha})}e^{\pm i\pi z^2}\,dz. \tag{6}$$

In fact, the quantities like (6) are well known from the CS theory, and this opens a way towards 3d extensions of the AGT conjecture.

3. Examples from knot theory

Polynomial knot invariants can be defined as averages of the Wilson loop along the knot in the topological CS theory [19]:

$$\langle K\rangle_R = \Bigl\langle \mathrm{tr}_R\,\mathrm{Pexp}\oint_K A\Bigr\rangle_{\mathrm{CS}}. \tag{7}$$

This invariant depends on the knot K, the Lie algebra G, its representation R, the coupling constant of the theory $\hbar = \log q = 2\pi i/k$ (sometimes k is shifted to $k + C_A$, as in the WZNW model [20]), and also the monodromy u, which describes the deviation from the periodicity of the field A while circling around the knot. We can assume that u is an eigenvalue of the matrix of the monodromy of the passage around the knot K. On the other hand, we can consider that u takes values in the Cartan subalgebra of the gauge group $SU(2)$ and thus describes the representation R on the knot K.

The averages $\langle K\rangle_R$ are reasonable generalizations of the ordinary characters and, like all exact correlators, have hidden integrability properties [21], [22]. We note an explicit example of this hidden structure: the averages $\langle K\rangle_R$ satisfy K-dependent difference equations in R [23], which allows regarding them as belonging to the family of generalized q-hypergeometric series. The $q \to 1$ limit of these equations defines the spectral curve $\Sigma(K)$, and the saddle point of the corresponding integral representation defines the associated SW differential. After that, the full $\hbar$-dependence can be reconstructed using the topological recursion [24] from this SW data [9].

Invariants (7) have the remarkable property that at $u = 0$, they are finite polynomials in $q = e^{2\pi i/k}$. In the literature, these polynomials normalized by the quantum dimension have different conventional names corresponding to the choice of the group and representation. Here, for convenience, we present Table 1 explaining the correspondence.

Table 1

Group/ Representation	Fundamental representation	General representation with weight λ
$N = 0$	Convey–Alexander polynomial	—
$SU(2)$	Jones polynomial	Colored Jones polynomial
$SU(N)$	HOMFLY polynomial	Colored HOMFLY polynomial
$SO(N)$	Kauffmann polynomial	Colored Kauffman polynomial
$\{SU(N)\}_t$	Superpolynomial	Colored superpolynomial

The last line in Table 1 describes an extension from (quantum) groups to MacDonald characters, which leads to a one-parameter deformation (t-deformation) of (7), to superpolynomials [25], [26] involving the Khovanov homology [27]. The further extension of the MacDonald functions to the Askey–Wilson–Kerov level remains uninvestigated.

Six kinds of representations are currently known for the Wilson averages in CS theory. We briefly describe them in the following subsections and present some explicit examples in Appendix B.

3.1. Representation in terms of the quantum *R*-matrix. The material in this subsection is presented in more detail in [28].

The representation in terms of the quantum R-matrix appears when calculations in the CS theory are done in the temporal gauge $A_0 = 0$ [29]. The propagator is then ultralocal, and only the crossings (c) and extremal points (e) in the projection of K on the xy plane contribute. The answer can therefore be written schematically as

$$\langle K\rangle_R = \operatorname{tr}_R \overrightarrow{\prod_{\mathrm{e,c}}} \mathcal{U}_{\mathrm{e}} \mathcal{R}_{\mathrm{c}},$$

where the ordered product is taken along the line K, $\mathcal{R}$ is the quantum R-matrix in the representation R, and $\mathcal{U} = q^\rho$ is the "enhancement" of the $\mathcal{R}$-matrix in the same representation. For the braid representation of the knot, this formula reduces to the well-known formula for quantum group invariants of the knot:

$$\langle K\rangle_R = q^{-w(b_K)\Omega_2(R)}\, \operatorname{qtr}_R(b_K), \qquad \Omega_2(R) = \frac{\operatorname{tr}_R(T^aT^a)}{\dim R}, \qquad \operatorname{qtr}_R b_K = \operatorname{tr}_R b^K q^{\rho^{\otimes n}}. \tag{8}$$

Here, $b_K \in B_n$ is the element of the braid group representing the knot K, i.e., its closure gives K, $\Omega_2(R)$ is the value of the quadratic Casimir function in the representation R, and qtr_R is the quantum trace over the representation R, $\operatorname{qtr}_R b_K = \operatorname{tr}_R b^K q^{\rho^{\otimes n}}$. The function $w(b_k)$ is the so-called writhe number of the braid b_K and is equal to the total sum of orientations of the crossings:

$$b_K = \prod_{\{k\}} g_k^{n_k} \quad \Longrightarrow \quad w(b_K) = \sum_{\{k\}} n_k.$$

Calculating (8) for a particular knot reduces to multiplying and taking the trace of relatively large matrices. The braid representations of the first few knots and the writhe numbers of the corresponding closures are presented in Table 2.

Table 2

Knot	Braid representation	Writhe number
3_1	$b = g_1^3 \in B_2$	$w(\hat{b}) = 3$
4_1	$b = g_2^2 g_1^{-1} g_2 g_1^{-1} \in B_3$	$w(\hat{b}) = 1$
5_1	$b = g_1^5 \in B_2$	$w(\hat{b}) = 5$
5_2	$b = g_2^3 g_1 g_2^{-1} g_1 \in B_3$	$w(\hat{b}) = 4$
6_1	$b = g_1 g_2^{-1} g_3 g_1 g_2^{-1} g_3^{-2} \in B_4$	$w(\hat{b}) = -1$

3.2. Representation in terms of the classical *R*-matrix and quantum associator. In this subsection, we rely on the results in [30].

A similar representation for $\langle K\rangle_R$ in terms of classical instead of quantum R-matrices appears in the calculation of (7) in the holomorphic gauge $A_{\bar{z}} = 0$. But instead of the trivial insertions of q^ρ factors, we now need to insert sophisticated Drinfeld associators [31]. In the holomorphic gauge, the theory reduces to the Kontsevich integral of the knot [32]. In this case, the representation of the braid group B_n in $R^{\otimes n}$ can be constructed in terms of the Drinfeld associators as follows. For the element $g_k \in B_n$, we have $g_k \to \Psi_k R_k \Psi_k^{-1}$, where

$$R_k = \underbrace{1\otimes\cdots\otimes 1}_{k-1} \otimes R \otimes \underbrace{1\otimes\cdots\otimes 1}_{n-k}, \qquad R = q^{T^a\otimes T^a}, \qquad \Psi_k = \Phi_k \otimes 1^{\otimes(n-k)},$$

where Φ_k is the kth Drinfeld associator. If $b_K \in B_n$ is the braid representing some knot K, then we obtain

$$\langle K\rangle_R = \mathrm{qtr}_R(1)^n q^{-w(b_K)\Omega_2(R)}\, \mathrm{qtr}_R(b_K) \tag{9}$$

for quantum invariant (7). The classical R-matrices $R = q^{T^a\otimes T^a}$ again appear just at the intersection points of the K projection on a plane. But instead of the simple enhancement factors q^ρ, between them, we must now insert the quantum associators [31] acting on k lines simultaneously. The Drinfeld associators are solutions of the Knizhnik–Zamolodchikov equations [33] in the WZNW conformal theory [20]. In particular, the kth associator describes the monodromy of the $(k+2)$-point function in the WZNW model, and the Kontsevich integral is just the trace of the monodromy associated with the braid b_K. A more detailed description of this representation can be found in [34].

3.3. Representation in terms of Vassiliev invariants and Kontsevich integrals. In the perturbative expansion of the CS theory, the dependences of the Wilson average $\langle K\rangle_R$ on the knot K and on the group structure G, R are nicely separated:

$$\langle K\rangle_R = \dim_q(R) \prod_{m=0}^{\infty} \prod_{n=1}^{d_m} \exp\{\hbar^m \alpha_{m,n}(K) r_{m,n}(R)\}, \tag{10}$$

where $\dim_q(R)$ is the quantum dimension of the representation:

$$\dim_q(R) = \frac{q^{N/2} - q^{-N/2}}{q^{1/2} - q^{-1/2}}.$$

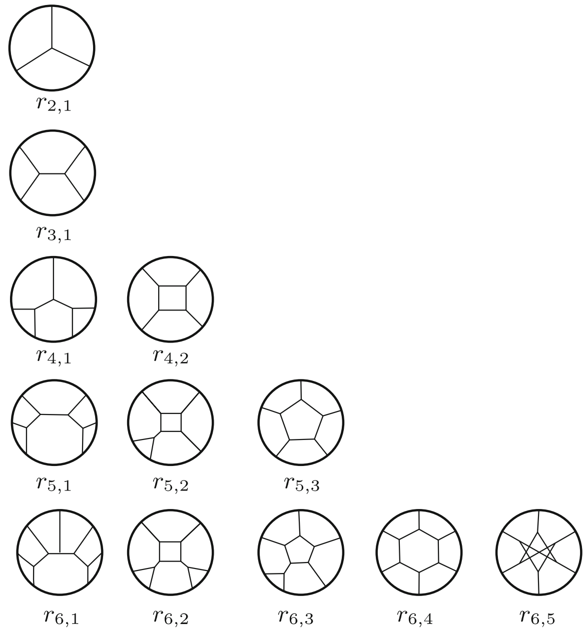

Fig. 2. A basis of independent Casimir functions up to degree 6.

The quantities $\alpha_{m,n}(K)$ are the primary Vassiliev invariants [35], which are rational (!) numbers, naturally represented either as modifications of the Gauss linking integrals in the Lorentz gauge $\partial_\mu A_\mu = 0$ [36] or as the Kontsevich integrals in the holomorphic gauge $A_{\bar{z}} = 0$ or in terms of the writhe numbers [37] in the temporal gauge $A_0 = 0$.

The group factors $r_{m,n}(R)$ are the eigenvalues of the operators in the cut-and-join algebra [38] on the $GL(\infty)$ characters χ_R and form a basis of the *multiplicative independent* Casimir eigenvalues of order m. In each order m, we have d_m independent Casimirs; the first few values of d_m are

$$d_1 = 0, \qquad d_2 = 1, \qquad d_3 = 1, \qquad d_4 = 2, \qquad d_5 = 3, \qquad d_6 = 5.$$

The Casimir functions $r_{m,n}$ are polynomials of the rank and weight of the representations. Table 3 lists the first four Casimirs for $SU(n)$ and $SO(n)$ in the fundamental representation and for $SU(2)$ in the spin-J representation.

Table 3

Group	$r_{2,1}$	$r_{3,1}$	$r_{4,1}$	$r_{4,2}$
$SU(n)$	$-\frac{(n^2-1)}{4}$	$-\frac{n(n^2-1)}{8}$	$-\frac{n^2(n^2-1)}{6}$	$-\frac{(n^2+2)(n^2-1)}{16}$
$SO(n)$	$-\frac{(n-2)(n-1)}{16}$	$-\frac{(n-2)^2(n-1)}{64}$	$-\frac{(n-2)^3(n-1)}{256}$	$\frac{(n-1)(n-2)(n^2-5n+10)}{256}$
$SU(2)$	$-J(J+1)$	$-J(J+1)$	$-J(J+1)$	$2J^2(J+1)^2$

Our choice of the basis of $r_{m,n}$ is shown in Fig. 2 in the form of chord diagrams: the circle denotes the trace over the representation R, and the trivalent vertices depict the structure constants f^{abc} of the algebra. This notation is clear from the two examples

$$r_{2,1} = \frac{1}{\dim_R} f^{abc}\,\mathrm{tr}_R(T^a T^b T^c), \qquad r_{3,1} = \frac{1}{\dim_R} f^{abe} f^{ecd}\,\mathrm{tr}_R(T^a T^b T^d T^c).$$

In the case of $G = SL(2)$, the relevant representations R are labeled by the value of the spin J, and $r_{kj}(J)$ are kth-degree polynomials in J. The series in exponential (10) can be reexpanded in the new variables $\hbar$ and $N = 2J + 1 = u/\hbar$:

$$F(K, \hbar, u) = \log\langle K\rangle_R - \log N = \sum_{k=0}^{\infty} \hbar^k \sum_{j=1}^{d_k} \alpha_{kj}(K) r_{kj}(N/\hbar) = \sum_k \hbar^k F_k(K, u). \tag{11}$$

These $F_k(K, u)$ are infinite combinations of Vassiliev invariants of all orders. Such a reexpansion obscures the K and R separation, which is obvious in (10), and all the information about the gauge group ($r_{m,n}$) and the knot ($\alpha_{m,n}$) is intermixed. Instead, this expansion is the knot theory counterpart of the genus $1/N$-expansion in matrix models, and $u = \hbar N$ plays the role of the 't Hooft coupling.

We note that for some knots (called *hyperbolic*), $F(K)$ behaves as $V(K, u)\hbar^{-1}$ at small $\hbar$ [39], although all terms in the series have positive powers of $\hbar$. This is typical for genus expansion series: contributions of each particular genus are all convergent series, but the sum over genera diverges. This sum can be analyzed using the Padé summation methods (see [40], [41] for a recent description in the matrix model context). The value of the coefficient $V(K, u)$ at $u = 1$ coincides with the volume of $S^3 \setminus K$ in the uniquely defined hyperbolic metric [42]. The situation is far more interesting for nonhyperbolic knots (*toric* or satellite; see the plots in Appendix C).

3.4. Representation in terms of the quantum dilogarithm. In [23], polynomial invariants (7) for the gauge group $SU(2)$ with the spin J were systematically interpreted as generalized q-hypergeometric functions. Such representations were previously widely used in particular examples. This means that these Wilson averages can be represented in the form of finite sums:

$$\langle K\rangle_J = \dim_q(R) \sum_{k_1,\dots,k_n} \frac{(q, N)_{k_1} \cdots (q, N)_{k_{i_1}}}{(q, N)_{k_{i_2}} \cdots (q, N)_{k_n}} q^{p_2(k_1,\dots,k_n)}. \tag{12}$$

Here, $N = 2J + 1$, $(q, N)_k$ is the q-Pochhammer symbol,

$$(q, N)_k = \prod_{i=1}^{k} \bigl(q^{(N-i)/2} - q^{-(N-i)/2}\bigr),$$

and $p_2(k_1, \dots, k_n)$ is a certain quadratic function. The numbers of k_i in sum (12), the quadratic polynomial p_2, and the arrangement of the Pochhammer symbols are determined by the knot K, and the summation limits are determined by J. The existence of such a representation for knots directly follows from the AJ conjecture for the colored Jones polynomials [43], which states that $\langle K\rangle_j$ is a solution of a certain hypergeometric difference equation (also see Sec. 3.6 below). At the same time, the Pochhammer symbols can be expressed in terms of the ratio of quantum dilogarithms:

$$(q, N)_k = (-i)^k \frac{s(i\epsilon_2(N - 1 - k) + i(\epsilon_1 + \epsilon_2)/2)}{s(i\epsilon_2(N - 1) + i(\epsilon_1 + \epsilon_2)/2)},$$

and expression (12) can be rewritten schematically as

$$\langle K\rangle_J = \dim_q(R) \sum_{k_1,\dots,k_n} \frac{s_{k_1} \cdots s_{k_{i_1}}}{s_{k_{i_2}} \cdots s_{k_n}} q^{p_2(k_1,\dots,k_n)}.$$

This expression provides a discrete version of the Hikami invariants.

3.5. The Hikami formalism in the Chern–Simons theory. The idea of the Hikami formalism is to calculate the CS partition functions using a triangulation of the 3d manifold M, i.e., decomposing it into elementary symplices, tetrahedra. Each tetrahedron has four faces, we can choose two and call them white. The other two are then black, and we glue black faces only to white faces. With each site, we associate a number p with the white faces and p^* with the black faces. When two sites are identified, the two numbers are identified, $p_i = p_j^*$. Finally, with each tetrahedron, we associate a function $G(p_1^*, p_2^*|p_1, p_2)$ and integrates over all p-variables on identified faces. With each triangulation of S^3, we thus associate a multiple integral over all p-variables, one per each two-face of triangulation:

$$H(K|u) = \int \prod_{\text{simplices}} dp_{i_1}\, dp_{i_2}\, dp_{i_1}\, dp_{i_2}\, G(p_{i_1}^*, p_{i_2}^*|p_{i_1}, p_{i_2}) \prod_{\text{2-faces}} \delta_{p_{k_m}^* - p_{k_n}} \prod_{\text{1-cycles}} \delta\biggl(\sum_j p_j - u\biggr).$$

At the same time, geometrically, we can associate a knot K with the system of glued tetrahedra. Moreover, the u-variables, which are associated with the one-cycles, can be interpreted as the $U(1)$-monodromies around the knot K. Most importantly, the functions G were proved in [14] to be

$$G(p_{i_1}^*, p_{i_2}^*|p_{i_1}, p_{i_2}) = \delta(p_1 + p_2 - p_1^*) s(p_2^* - p_2 - i\pi + \hbar) e^{p_1(p_2^* - p_2)/2\hbar + \hbar^2/6},$$

and the Hikami integral $H(K|u)$ for the given K has exactly the same form as the Wilson average $\langle K\rangle_R$ in Sec. 3.4 in the $(\hbar, u)$ variables, only the sum is replaced with an integral (see examples in Appendix B below). Passing from sums to integrals is associated with switching from compact to noncompact groups.

3.6. Spectral curves and topological recursion. At least for $G = SL(2)$, the average $\langle K\rangle_R$ is annihilated by a K-dependent difference operator, i.e., satisfies a recursive relation in the spin J. This statement is sometime called the AJ conjecture [43] (see [44], [45] for the first few examples except $SL(2)$). In the variables $u = N\hbar$, where $N = D_{2J+1} = 2J + 1$, we obtain

$$\mathcal{A}(e^{\hbar\partial_u}, e^u)\langle K\rangle_R = 0. \tag{13}$$

In the $\hbar$=0 limit, this operator becomes a (polynomial) function, and the difference equation becomes an algebraic equation,

$$\mathcal{A}(w, \lambda) = 0, \tag{14}$$

defining the spectral curve $\Sigma(K)$. We can further define the SW differential $dS = \log w\, d\log\lambda$. In the typical examples of the knots 4_1 and $m009$, Eq. (14) is quadratic in w (we note that an additional $U(1)$-factor $w - 1$ splits away, decreasing the degree of the equations by one):

$$\Sigma(K)\colon\ \mathcal{A}(w, \lambda) = w + \frac{1}{w} - 2f\left(\lambda + \frac{1}{\lambda}\right) = 0, \qquad w_\pm(\lambda) = f \pm \sqrt{f^2 - 1}, \tag{15}$$

and

$$dS = \bigl(\log w_+(\lambda) - \log w_-(\lambda)\bigr)\, d\log\lambda = \log\frac{f + \sqrt{f^2 - 1}}{f - \sqrt{f^2 - 1}}\, d\log\lambda. \tag{16}$$

Free energy (11), $F = \log\langle K\rangle_R$, is in fact an exact SW prepotential, reconstructed in all orders of the genus expansion in $\hbar$ from this data $\bigl(\Sigma(K), dS\bigr)$ using the topological recursion in [24] (see [9] for detailed examples of this reconstruction). One may wonder what the corresponding SW theory is. The formulas in [46] describing the 5d version of the classical SW theory in terms of the relativistic Toda integrable system can be easily recognized in (15) and (16). Equation (13) should then be a Baxter equation, which is now known to describe the Nekrasov–Shatashvili (NS) deformation of the classical SW theory [47], [48] (or, equivalently, the NS limit of the full SW theory). This observation implies a new kind of AGT duality, which we discuss in Sec. 5 below. When $\mathcal{A}(w, \lambda) = 0$ does not reduce to a quadratic equation in w, the analysis is more complicated.

4. A 3d AGT relation

The suggestion in [1] is to identify the modular kernels $M(a, a')$ associated with modular transformations $S(q) \longrightarrow S(q')$ of a punctured Riemann surface and amplitudes in the CS theory on the 3d space that is the cylinder of the homotopy of $S(q)$ to $S(q')$. In particular, the trace of $M(a, a')$ should coincide with the invariant of the knot K formed by the trajectory of punctures under the homotopy in the 3d manifold, and external momenta should coincide with monodromies around the knot. Of course, K depends on the choice of the modular transformation. Indeed, there is an understandable analogy between quantities (18) and (19) defined below. Both are multiple integrals of products of quantum dilogarithms $s(\,\cdot\,)$, and there is a natural identification of the parameters [1]:

$$2\pi i\hbar = \log q = \frac{2\pi i}{k + C_{\mathrm{G}}} = 2\pi i b^2 = \frac{2\pi i \epsilon_2}{\epsilon_1}. \tag{17}$$

But (18) and (19) differ in the number of s-functions, the number of arguments, and the integration contours. Perhaps, the most striking difference is that the integration variables obey "conservation laws" in the expressions for knot invariants, but this does not happen with the trace of the monodromy matrix. To see this, we can use the property $s(z) = 1/s(-z)$ to bring the integral to the canonical form with all the s functions in the numerator:

$$\prod_i \int_{C_i} dp_i \prod_m s(A_{m,i} p_i + B_m) e^{C_{ij} p_i p_j + D_i p_i + E}.$$

Then $\sum_m A_{m,i} = 0$ in (6), but this relation is not satisfied for knot invariants, at least for some i, i.e., for some integration variables. The simplest example of such a discrepancy is between the expression for the trace of the toric transformation,

$$T_\pm(\alpha) = \int dz\, \frac{s(z + \widetilde{\alpha})}{s(z - \widetilde{\alpha})} e^{\pm i\pi z^2}, \tag{18}$$

and the expression for the Wilson–Hikami average associated with the knot 4_1,

$$\langle 4 \rangle_1 \sim \int s(z + u) s(z - u) e^{6\pi i u z/\epsilon_1\epsilon_2}\, dz. \tag{19}$$

We hence see that together with similar appearances, the two constructions have serious differences, which do not allow formulating an explicit 3d relation.

5. A route to an alternative AGT relation

The seeming failure of the 3+3 AGT relation can attract additional attention to possible alternative variants of this relation: we can expect many different AGT-like relations to exist. The simplest possibility is to extend the known 2+4 case to the case of 3+5 dimensions, i.e., to identify quantities in the 3d CS theory and the quantities in a 5d Yang–Mills-type theory. This should be a much simpler exercise. The equations in Sec. 3.6 describe knot invariants, but it is easy to recognize (15) as the spectral curve for the relativistic Toda system and (16) as the corresponding SW differential [46]. These equations thus yield a relation between the 3d CS theory and the 5d version of the SW theory formulated as a direct q-deformation of the ordinary 4*d* SW theory. In the light of this relation, difference equation (13) is identified with the Baxter equation for the same system. At the same time, the Baxter equations arise [47] in the NS limit [49] of the Losev–Moore–Nekrasov–Shatashvili (LMNS) prepotential [50], and we thus obtain a new AGT-like relation, supplementing the usual AGT relation [51]:

$$\text{3d CS theory} \overset{\text{new AGT}}{\longleftrightarrow} \text{NS limit of 5d LMNS prepotential} \overset{\text{ordinary AGT}}{\longleftrightarrow}$$

$$\overset{\text{ordinary AGT}}{\longleftrightarrow} q\text{-Virasoro conformal blocks.}$$

More precisely, in accordance with [47], the solution of the Baxter equation, i.e., $\langle K\rangle_R$, must be associated with the SW differential, its monodromies around the A- and B-cycles on the spectral curve yielding the 5d Nekrasov functions in the NS limit via the SW equations.

There are a few interesting points to be mentioned already at this stage. The dilogarithm formulas in Secs. 3.4 and 3.5 for the knot invariants provide integral representations for solutions of Eqs. (13). They are similar to the solutions in [52] for the open quantum relativistic Toda chain system. Such solutions are unavailable for the closed chain, but solution (15) is just of this type! The point is that, first, solution (13) defines a Baxter equation at some special point of the moduli space, for some special values of "energies." Hence, the fact that solutions are unavailable in such a form at a generic point does not preclude their existence at some special point. Second, while classical solution (15) relates to the relativistic Toda type, its quantization is ambiguous, and (13) is not the standard version of the Baxter equation considered in the literature. It is important that when dealing with difference (and not differential) equations, we obtain infinitely many solutions. To cope with this ambiguity, we consider two difference equations where there might be only one differential equation. And this pair of equations is usually related by the symmetry $\epsilon_1 \leftrightarrow \epsilon_2$, which is explicitly broken in our construction of knot invariants. In particular, it is explicitly broken in basic AGT relation (17).

An unresolved interesting question remains. What should replace the knot invariants if this new AGT duality is lifted to the entire LMNS deformation of the 5d LMNS theory and not only in the NS limit?

6. Conclusion

After the discovery of the AGT relation [13], using which we can describe the 2d conformal theory in the general context of the SW and integrability theories [53], a search was immediately initiated for its extension, which would do the same with the 3d CS theory. The goal of this paper is to switch the discussion of the 3d AGT relations from the qualitative to a quantitative level. This became possible because of the progress in the theory of knot invariants, which was briefly reviewed in Sec. 3 above (in fact, some consequences of the CS theory have not yet been obtained, but this is mostly due to the insufficient attention of researchers studying quantum field theory). Given a set of directly explicit formulas, we can easily test various hypotheses. In this direction, we encountered several problems arising when studying the hypothesis [1] that relates knot invariants to modular kernels based on the AGT relation. Instead of this, using the AGT relation, we demonstrated that these invariants are connected with the 5d SYM theory. This is a more direct and less intriguing possibility nevertheless also deserving attention.

Appendix A: Dilogarithm properties

A serious problem when discussing 3d AGT relations is the lack of a common notation: for the same quantities, specialists from various fields use different notations that are distinguished by different rescalings. The purpose of this appendix is to list some relations between various definitions of quantum dilogarithms used in the literature. We also demonstrate the trick needed for taking the massless limit $\alpha \to 0$ of the modular kernel $M(a, a')$, i.e., for deriving Eq. (5).

A.1. Various dilogarithms. The "quantum dilogarithm" [18] is defined as the ratio of two digamma functions [17]:

$$s(z|\epsilon_1, \epsilon_2) = \prod_{m,n\geq 0} \frac{(m+1/2)\epsilon_1 + (n+1/2)\epsilon_2 - iz}{(m+1/2)\epsilon_1 + (n+1/2)\epsilon_2 + iz} = \frac{\Gamma_2(\epsilon/2 + iz|\epsilon_1, \epsilon_2)}{\Gamma_2(\epsilon/2 - iz|\epsilon_1, \epsilon_2)}.$$

It has several periodicity properties:

$$s\left(z-\frac{i\epsilon_2}{2}\,\middle|\,\epsilon_1,\epsilon_2\right)=2\,\mathrm{ch}\left(\frac{\pi z}{\epsilon_1}\right)s\left(z+\frac{i\epsilon_2}{2}\,\middle|\,\epsilon_1,\epsilon_2\right),$$
$$s\left(z-\frac{i\epsilon_1}{2}\,\middle|\,\epsilon_1,\epsilon_2\right)=2\,\mathrm{ch}\left(\frac{\pi z}{\epsilon_2}\right)s\left(z+\frac{i\epsilon_1}{2}\,\middle|\,\epsilon_1,\epsilon_2\right),\tag{A.1}$$
$$s\left(z-\frac{i\epsilon}{2}\,\middle|\,\epsilon_1,\epsilon_2\right)=4\sinh\left(\frac{\pi z}{\epsilon_1}\right)\sinh\left(\frac{\pi z}{\epsilon_2}\right)s\left(z+\frac{i\epsilon}{2}\,\middle|\,\epsilon_1,\epsilon_2\right).$$

The definition of the quantum dilogarithm allows finding its integral representation

$$i\log s(z|\epsilon_1,\epsilon_2)=\int_0^\infty\frac{dw}{w}\left(\frac{\sin(2zw)}{2\sinh(\epsilon_1 w)\sinh(\epsilon_2 w)}-\frac{z}{\epsilon_1\epsilon_2 w}\right),$$

which can be used to obtain the asymptotic formula

$$i\log s(z|\epsilon_1,\epsilon_2)=\frac{\pi z^2}{2\epsilon_1\epsilon_2}-\frac{\pi}{24}\frac{2\epsilon_1\epsilon_2-\epsilon^2}{\epsilon_1\epsilon_2}+i\sum_{n=0}^{\infty}\frac{B_n(1/2)}{n!}\left(2\pi i\frac{\epsilon_2}{\epsilon_1}\right)^{n-1}\mathrm{Li}_{2-n}(-e^{2\pi z/\epsilon_1}).\tag{A.2}$$

The resummation expansion

$$i\log s(z_0+z|\epsilon_1,\epsilon_2)=\frac{\pi(z_0+z)^2}{2\epsilon_1\epsilon_2}-\frac{\pi}{24}\frac{2\epsilon_1\epsilon_2-\epsilon^2}{\epsilon_1\epsilon_2}+$$
$$+\sum_{k=-1}^{\infty}\sum_{j=0}^{\infty}\frac{i^{k+1}B_{k+1}(1/2)}{(k+1)!\,j!}(2\pi)^{k+j}\frac{\epsilon_2^k}{\epsilon_1^{k+j}}\mathrm{Li}_{1-j-k}(-e^{2\pi z_0/\epsilon_1})z^j$$

is also useful. The quantum dilogarithm is symmetric with respect to ϵ_1 and ϵ_2, but we have explicitly chosen ϵ_2 to be small here, this expansion playing a crucial role in the NS limit.

The definition of the quantum dilogarithm presented above is convenient for applications in the context of the AGT conjecture, where the parameters $\epsilon_{1,2}$ are explicitly specified, but another variant that differs by rescaling is encountered in the literature,

$$S_b(z)=\exp\left\{\frac{1}{i}\int_0^\infty\frac{dw}{w}\left(\frac{\sin(2zw)}{2\sinh(bw)\sinh(b^{-1}w)}-\frac{z}{w}\right)\right\},\tag{A.3}$$

and hence

$$s(z|\epsilon_1,\epsilon_2)=S_{\sqrt{\epsilon_1/\epsilon_2}}\left(\frac{z}{\sqrt{\epsilon_1\epsilon_2}}\right).$$

A.2. Modular kernel. In this section, we present a standard trick for computing modular kernel (3) in the simple limit of zero external dimension $\widetilde{\alpha}\to i\epsilon/2$. Considering the modular kernel in this limit naively, we derive

$$M(a,a')=2^{3/2}\int dr\,\frac{e^{4\pi i a' r}}{16\sinh\bigl(\pi(a+r)/\epsilon_1\bigr)\sinh\bigl(\pi(a+r)/\epsilon_2\bigr)\sinh\bigl(\pi(a-r)/\epsilon_1\bigr)\sinh\bigl(\pi(a-r)/\epsilon_2\bigr)}$$

from Eq. (A.1). The denominator in the integrand has double poles, which are glued together in the limit $\widetilde{\alpha}\to i\epsilon/2$, and the chosen integration contour is pinched between them. Hence, we must take the limit more carefully:

$$\mathcal{M}(a,a'|0)=\oint_{r=-a}dr\frac{s(a+r+i\epsilon/2+i\lambda)}{s(a+r-i\epsilon/2-i\lambda)}\frac{e^{4\pi i a' r}}{4\sinh\bigl(\pi(a-r)/\epsilon_1\bigr)\sinh\bigl(\pi(a-r)/\epsilon_2\bigr)}+$$
$$+\oint_{r=a}dr\frac{s(a-r+i\epsilon/2+i\lambda)}{s(a-r-i\epsilon/2-i\lambda)}\frac{e^{4\pi i a' r}}{4\sinh\bigl(\pi(a+r)/\epsilon_1\bigr)\sinh\bigl(\pi(a+r)/\epsilon_2\bigr)}.$$

Further, we have

$$\frac{s(a+r+i\epsilon/2+i\lambda)}{s(a+r-i\epsilon/2-i\lambda} = \prod_{m,n\geq 0} \frac{(m+1/2)\epsilon_1+(n+1/2)\epsilon_2 - i(a+r+i\epsilon/2+i\lambda)}{(m+1/2)\epsilon_1+(n+1/2)\epsilon_2 + i(a+r+i\epsilon/2+i\lambda)} \times$$

$$\times \frac{(m+1/2)\epsilon_1+(n+1/2)\epsilon_2 + i(a+r-i\epsilon/2-i\lambda)}{(m+1/2)\epsilon_1+(n+1/2)\epsilon_2 - i(a+r-i\epsilon/2-i\lambda)} =$$

$$= \prod_{m,n\geq 0} \frac{(m+1)\epsilon_1+(n+1)\epsilon_2 - i(a+r+i\lambda)}{m\epsilon_1+n\epsilon_2+i(a+r+i\lambda)} \times$$

$$\times \frac{(m+1)\epsilon_1+(n+1)\epsilon_2 + i(a+r-i\lambda)}{m\epsilon_1+n\epsilon_2-i(a+r-i\lambda)} \underset{m,n=0}{\sim}$$

$$\underset{m,n=0}{\sim} \frac{1}{(a+r)^2-\lambda^2} \underset{\lambda\to 0}{\sim} \delta(a+r).$$

As a result, we obtain

$$\mathcal{M}(a,a'|0) \to \frac{\sqrt{2}\,\cos(4\pi i a a'/\epsilon_1\epsilon_2)}{\mu'(a)}.$$

A.3. Chern–Simons average. A different definition of the dilogarithm is commonly used to calculate the standard quantities in the CS theory. For instance, the average for the knot 4_1 is usually written as a function of the coupling constant h and the knot monodromy parameter u as (we note that $\hbar$ in our formulas differs from h in [14] by a factor of 2)

$$\langle 4_1\rangle = H(u,\hbar) = \frac{1}{\sqrt{\pi\hbar}} \int dp \frac{\Phi_\hbar(p+i\pi+\hbar/2)}{\Phi_\hbar(-2u-p-i\pi-\hbar/2)} e^{-4u(u+p)/\hbar - u},$$

where

$$\Phi_\hbar(z) = \Phi\left(\frac{z}{\pi i\hbar}\,\middle|\,\frac{\hbar}{2\pi i}\right), \qquad \Phi(z|\tau) = \exp\left(\frac{1}{4}\int \frac{dw}{w}\frac{e^{2xz}}{\sinh w \sinh \tau w}\right).$$

In the previously discussed context of conformal field theory, we can encounter a similar function but with rescaled parameters,

$$e_b(z) = \exp\left(\frac{1}{4}\int \frac{dw}{w}\frac{e^{-2izw}}{\sinh(bw)\sinh(b^{-1}w)}\right) = \Phi(-ibz|b^2),$$

and hence

$$\langle 4_1\rangle = \frac{1}{\sqrt{2\pi(\pi i b^2)}} \int dp \frac{e_b((p+i\pi+\pi i b^2)/2\pi b)}{e_b((-2u-p-i\pi-\pi i b^2)/2\pi b)} e^{-2\pi i b^2 u(u+p)/2\pi b^2 - u}.$$

Introducing the new variables $z = p/2\pi b$, $u' = u/2\pi b$, and $Q = b + b^{-1}$, we obtain

$$\langle 4_1\rangle = \frac{2\pi b}{\sqrt{2\pi(\pi i b^2)}} \int dz \frac{e_b(z+iQ/2)}{e_b(-2u'-z-iQ/2)} e^{8\pi i u'(u'+z) - 2\pi b u'}.$$

We note that the functions e_b and S_b given by (A3), although similar, differ slightly, in particular, they differ by a factor: $e_b(z) = e^{\pi i z^2/2} e^{-i\pi(2-Q^2)/24} S_b(z)$. Therefore,

$$\langle 4_1\rangle = \sqrt{-2i}\int dz\,\frac{S_b(z+iQ/2)}{S_b(-2u'-z-iQ/2)} e^{6\pi i u'(z+u') - \pi u'(b-b^{-1})} \underset{z\to z-u'-iQ/2}{=}$$

$$\underset{z\to z-u'-iQ/2}{=} \sqrt{-2i}\int dz\, S_b(z-u')S_b(z+u') e^{6\pi i u' z + 2\pi u'/b + 4\pi u' b}.$$

Finally, the same expression in terms of the $s(z)$ dilogarithms is

$$H\left(\frac{2\pi u}{\sqrt{\epsilon_1\epsilon_2}}, \pi i\frac{\epsilon_2}{\epsilon_1}\right) = \sqrt{\frac{-2i}{\epsilon_1\epsilon_2}} \int dz\, s(z-u)s(z+u)\exp\left\{\frac{6\pi i u z}{\epsilon_1\epsilon_2} + \frac{2\pi u}{\epsilon_2} + \frac{4\pi u}{\epsilon_1}\right\}.$$

A.4. Pochhammer symbols as dilogarithm ratios. We consider the Pochhammer symbols

$$(q,N)_k = \prod_{j=1}^{k}(q^{(N-j)/2} - q^{-(N-j)/2}) = 2^k \prod_{j=1}^{k} \sinh\bigl(\pi i\hbar(N-j)\bigr),$$

$$(q,N)_k^* = \prod_{j=1}^{k}(q^{(N+j)/2} - q^{-(N+j)/2}) = 2^k \prod_{j=1}^{k} \sinh\bigl(\pi i\hbar(N+j)\bigr).$$

Using periodicity conditions (A1), we can rewrite the hyperbolic sine products as

$$\sinh\left(\frac{\pi i\epsilon_2 z}{\epsilon_1}\right) = -\frac{i}{2}\frac{s(i\epsilon_2 z + i(\epsilon_1-\epsilon_2)/2)}{s(i\epsilon_2 z + i(\epsilon_1+\epsilon_2)/2)},$$

i.e., the Pochhammer symbols are

$$(q,N)_k = (-i)^k \prod_{j=1}^{k}\frac{s(i\epsilon_2(N-1-j)+i\epsilon/2)}{s(i\epsilon_2(N-j)+i\epsilon/2)} = (-i)^k\frac{s(i\epsilon_2(N-1-k)+i\epsilon/2)}{s(i\epsilon_2(N-1)+i\epsilon/2)} \tag{A.4}$$

and, similarly,

$$(q,N)_k^* = (-i)^k\frac{s(i\epsilon_2(N)+i\epsilon/2)}{s(i\epsilon_2(N+k)+i\epsilon/2)}.$$

We note that the average $\langle 4_1\rangle$ can be expressed in terms of the symbol $\bigl(q,N/\sqrt{\hbar}\bigr)_{k/\sqrt{\hbar}}$, which has the symmetry under the change $\hbar\to\hbar^{-1}$:

$$\langle 4_1\rangle = \frac{i}{\cosh(i\epsilon_2(N-1/2)+i\epsilon/2)}\sum_{k\in\mathbb{Z}+1/2}(-1)^k\frac{s(i\epsilon_2(N-1/2-k)+i\epsilon/2)}{s(i\epsilon_2(N-1/2+k)+i\epsilon/2)}.$$

In the limit $\epsilon_2\to 0$, $N\to\infty$, $i\epsilon_2(N-1/2)+i\epsilon/2=\tilde{u}$, the sum can be replaced with the integral to give

$$\langle 4_1\rangle = -\frac{1}{\epsilon_2\cosh\tilde{u}}\int dz\, e^{\pi z/\epsilon_2} s(z-\tilde{u})s(z+\tilde{u}),$$

which is quite similar to the Hikami formula, although the correct exponential factor is not restored in the integrand.

Appendix B: Examples of knot invariants

In this section, we describe a few simplest examples of knots and also calculate some invariants in Sec. 3: for each knot K, we find the corresponding annihilating operator $\mathcal{A}$, the spectral curve, the braid-group element, the combination of the classical R-matrix and Drinfeld associator, the expansion of $F=\log\langle K\rangle_R$ in the primitive Vassiliev invariants, and the Hikami integral $H(K|u)$ in terms of the relevant combination of s-functions.

B.1. Unknot.

B.1.1. Quantum *R*-matrix representation. The simplest braid representation of the unknot U_0 is the braid of a single strand, i.e., the closure of the only element in the group B_1: $b_{U_0}=1\in B_1$. Hence, the value of the polynomial invariant is given by the character

$$\langle U_0\rangle = \operatorname{qtr}_R(1) = \operatorname{tr}_R(q^\rho) = \chi_R(z_i)\big|_{z_i=q^{N-2i+1}},$$

where χ_R is the character of the representation R (i.e., the corresponding Schur polynomial).

B.1.2. Representation in terms of the Drinfeld associator. Formula (9) for the unknot gives the average in the form of the trace of the first Drinfeld associator Φ_3 (the so-called hump). The relation to the invariant in the preceding subsection is not entirely trivial: $\langle\text{hump}\rangle$ is given as the inverse of $\langle U_0\rangle$. The associator is a tensor with six indices, and the corresponding trace is defined as the contraction

$$\langle\text{hump}\rangle = \sum_{i,k,m=1}^{\dim_R} (\Phi_3)^{i,i,k}_{k,m,m}. \tag{B.1}$$

In the case of the fundamental representation of $SU(N)$, this sum is computed explicitly, and the result is represented as a particular value of the hypergeometric function (see [34]):

$$\langle\text{hump}\rangle = \frac{N}{F\big([(N-1)\hbar,(N+1)\hbar],[1+N\hbar],1\big)} = \frac{N(q^{1/2}-q^{-1/2})}{q^{N/2}-q^{-N/2}} = \frac{N}{[N]_q}.$$

B.1.3. Representation in terms of the Vassiliev invariant. The first few Vassiliev invariants of the unknot are

$$\alpha_{2,1} = -\frac{2}{3}, \qquad \alpha_{3,1} = 0, \qquad \alpha_{4,1} = \frac{2}{45}, \qquad \alpha_{4,2} = -\frac{2}{45}, \qquad \alpha_{5,1} = \alpha_{5,2} = \alpha_{5,3} = 0.$$

For example, using Table 3 and these invariants for the group $SU(2)$ with spin J, we obtain[1]

$$\langle U_0\rangle_J = N\exp\left\{h^2\frac{2}{3}J(J+1) - h^4\frac{2}{45}(J+1)(2J^2+2J+1)J+\ldots\right\} =$$
$$= \frac{q^{N/2}-q^{-N/2}}{q^{1/2}-q^{-1/2}} = [N]_q, \quad N = 2J+1.$$

B.1.4. $\mathcal{A}$-polynomial. The colored Jones polynomial in the case with no knot,

$$K_N(U_0|q) = \langle U_0\rangle_J = \frac{q^{J+1/2}-q^{-(J+1/2)}}{q^{1/2}-q^{-1/2}} = \frac{q^{N/2}-q^{-N/2}}{q^{1/2}-q^{-1/2}},$$

is given by character (B.1), and it therefore satisfies the quantum Laplace equation on the Cartan lattice:

$$K_{N+1} - [2]_q K_N + K_{N-1} = 0.$$

As a result, the $\mathcal{A}$-polynomial for the unknot can be defined as $\mathcal{A}(l,m) = (l-1)^2/2$, and the quantum $\mathcal{A}$-polynomial is the q-Laplace operator

$$\hat{\mathcal{A}} = \Delta_q = \hat{l} - [2]_q + \hat{l}^{-1}, \qquad \Delta_q K_N = 0,$$

where the operators $\hat{l}$ and $\widehat{m}$ act on the Jones polynomial as $\hat{l}K_N = K_{N+1}$ and $\widehat{m}K_N = q^N K_N$.

B.1.5. Polynomial invariants. The colored HOMFLY polynomial is given by [54]

$$\langle U_0\rangle_Y = \dim_q(Y) = \prod_{i,j\in Y}\frac{q^{(N+j-i)/2}-q^{-(N+j-i)/2}}{q^{h(i,j)/2}-q^{-h(i,j)/2}}.$$

Here, Y is the Young diagram corresponding to the representation of $SU(N)$, and $h(i,j)$ is the hook length of a box in Y.

The superpolynomial is

$$P_0(a,q,t) = \frac{a^{1/2}-a^{-1/2}}{q^{1/2}-q^{-1/2}}.$$

The colored superpolynomial can be found in [26] (see formulas (67) and (68) there).

[1] Here and hereafter, we use the expansion in the parameter $h := 2\pi i\hbar$, and hence $q = e^h$.

B.2. Knot 3_1.

B.2.1. Representation in terms of the quantum $\boldsymbol{R}$-matrix and Drinfeld associator. The polynomial invariant for the knot 3_1 can be constructed using formulas (8) and (9). In this case, 3_1 is the closure of the element $b_{3_1} = g_1^3 \in B_2$. In this representation, the knot has three positively oriented crossings ($w(b) = 3$) and two strands ($n = 2$ in (9)).

B.2.2. Representation in terms of the Vassiliev invariant. The first few Vassiliev invariants of the knot 3_1 are

$$\alpha_{2,1} = 4, \qquad \alpha_{3,1} = -8, \qquad \alpha_{4,1} = \frac{62}{3}, \qquad \alpha_{4,2} = \frac{10}{3},$$
$$\alpha_{5,1} = -\frac{176}{3}, \qquad \alpha_{5,2} = -\frac{31}{3}, \qquad \alpha_{5,3} = -8.$$

For example, using Table 3 for $SU(2)$ gives

$$\langle 3_1 \rangle = [2J+1]_q \exp\biggl\{-4J(1+J)h^2 + 8J(1+J)h^3 + \\ + \frac{2}{3}J(1+J)(-31+10J+10J^2)h^4 + \dots\biggr\}, \qquad h = 2\pi i\hbar.$$

B.2.3. Representation in terms of the quantum dilogarithm. The colored Jones polynomial for the knot 3_1 with $N = 2J+1$ can be represented in the hypergeometric form:

$$K_N(3_1|q) = [N]_q \sum_{i=0}^{N-1} (-1)^i q^{i(i+3)/2} (q,N)_i (q,N)_i^* \equiv [N]_q J_N(3_1|q). \tag{B.2}$$

Using (A.4), we obtain

$$J_N \sim \sum_{k=0}^{N-1} q^{k(k+3)/2} \frac{s(i\epsilon_2(N-1-k) + i(\epsilon_1+\epsilon_2)/2)}{s(i\epsilon_2(N-1) + i(\epsilon_1+\epsilon_2)/2)} \frac{s(i\epsilon_2 N + i(\epsilon_1+\epsilon_2)/2)}{s(i\epsilon_2(N+k) + i(\epsilon_1+\epsilon_2)/2)}.$$

In the limit as $N \to \infty$ with $|q| > 1$, this expression becomes

$$J_N \sim q^{3N^2/2 - 3N/4}. \tag{B.3}$$

B.2.4. $\boldsymbol{\mathcal{A}}$-polynomial. The $\mathcal{A}$-polynomial and the spectral curve for the knot 3_1 have the forms

$$\mathcal{A}_{3_1}(l,m) = m^3 + l, \qquad \Sigma_{3_1} = \{(m,l) \in \mathbb{C}^2 \colon m^3 + l = 0\}.$$

We note that this spectral curve corresponds to the sphere and to the open relativistic Toda system. To compute the quantum $\mathcal{A}$-polynomial, we note that the Jones polynomial for the trefoil,

$$J_{N+1} + q^{3N+2} \frac{1-q^N}{1-q^{N+1}} J_N = q^N \frac{q^{2N+1}-1}{q^{N+1}-1}, \tag{B.4}$$

satisfies difference equation (B.2), which can be rewritten as

$$\frac{1}{\widehat{B}(\widehat{m})} \hat{A}(\hat{l}, m) J_N(q) = 1, \tag{B.5}$$

where $\hat{A} = q\widehat{m}^3(\widehat{m}-1) + (q\widehat{m}-1)\hat{l}$ and $\widehat{B} = (q\widehat{m}^2-1)\widehat{m}$. Equivalently, (B.5) can be rewritten as

$$\sqrt{\frac{q}{\widehat{m}^3}}\,\frac{1-\widehat{m}}{1-q\widehat{m}^2}(\hat{l} + q^{3/2}\widehat{m}^3)K_N(q) = 1. \tag{B.6}$$

In the leading order in the large-N limit, this equation reduces to

$$(\hat{l} + q^{3/2}\widehat{m}^3)K_N(q) = 0, \tag{B.7}$$

i.e., the quantum $\mathcal{A}$-polynomial is[2]

$$\hat{\mathcal{A}}_{3_1}(\hat{l}, \widehat{m}|q) = \hat{l} + q^{3/2}\widehat{m}^3.$$

We note that polynomial (B.3) solves (B.7). For finite N, Eq. (B.6) can be rewritten as [55]

$$\hat{\mathcal{A}}_{\mathrm{G}} J_N(q) \equiv (\hat{l}-1)\frac{1}{\widehat{B}(\widehat{m})}\hat{A}(\hat{l},\widehat{m})J_N(q) = 0,$$

where

$$\hat{\mathcal{A}}_{\mathrm{G}} = -\frac{1}{q\widehat{m}}\frac{1-q^2\widehat{m}}{1-q^2\widehat{m}^2}\hat{l}^{\,2} - \left[\frac{1}{\widehat{m}}\frac{1-q\widehat{m}}{1-q\widehat{m}^2} - q^2\widehat{m}^2\frac{1-q\widehat{m}}{1-q^3\widehat{m}}\right]\hat{l} - q^2\widehat{m}^2\frac{1-\widehat{m}}{1-q^2\widehat{m}}.$$

B.2.5. Polynomial invariants. The colored polynomial is known only for $SU(3)$ (see Theorem 1 in [45]).

The superpolynomial (noncolored) has the form

$$P_{3_1}(a,q,t) = P_0(a,q,t)(aq^{-1} + aqt^2 + a^2t^3).$$

Substituting $t=-1$, we obtain the HOMFLY polynomial from this superpolynomial. If we set $a = q^N$ in it, then it corresponds to the $SU(N)$ CS theory. The case $a = q^2$ gives the Jones polynomial, and $a = q^0 = 1$ gives the Alexander polynomial.

B.3. Knot 4_1.

B.3.1. Representation in terms of the quantum R-matrix and Drinfeld associator. The polynomial invariant for the knot 4_1 can be constructed using formulas (8) and (9). In this case, knot 4_1 can be represented as the closure of the element $b_{4_1} = g_2^2 g_1^{-1} g_2 g_1^{-1} \in B_3$. In this representation, the knot has three positively oriented crossings, two negatively oriented crossings ($w(b)=1$), and two strands ($n=3$ in (9)).

B.3.2. Representation in terms of the Vassiliev invariant. The first few Vassiliev invariants of knot 4_1 are

$$\alpha_{2,1} = -4, \qquad \alpha_{3,1} = 0, \qquad \alpha_{4,1} = \frac{33}{3}, \qquad \alpha_{4,2} = \frac{14}{3}, \qquad \alpha_{5,1} = \alpha_{5,2} = \alpha_{5,3} = 0.$$

For instance, using Table 3 for $SU(2)$ gives

$$\begin{aligned}\langle 4_1\rangle = [N]_q \exp\biggl\{ J(J+1)h^2\biggl[4 + \frac{2}{3}(14J^2 + 14J - 17)h^2 +{}\\ + \frac{1}{90}(2416J^4 + 4832J^3 - 9212J^2 - 11628J + 8013)h^4 +{}\\ + \frac{1}{1260}(109552J^6 + 328656J^5 - 973888J^4 - 2495536J^3 +{}\\ + 1783146J^2 + 3085690J - 1645097)h^6 + \dots\biggr]\biggr\}.\end{aligned}$$

[2]A different choice of the variables is often made in the literature: $q \to q^2$ and $\widehat{m} \to \widehat{m}^2$.

In the limit as $N \to \infty$ ($N = 2J+1$) with finite $u = hN$, only the terms of the zeroth degree in N survive, and the series becomes

$$\begin{aligned}\lim_{N\to\infty} \log\langle 4_1\rangle &= 1 + u^2 + \frac{7}{12}u^4 + \frac{151}{360}u^6 + \cdots = \\ &= \sum_{n=0}^{\infty} \frac{2u^{2n}}{(2n)!} \sum_{k=0}^{\infty} \frac{k^{2n-1}}{\left((1+\sqrt{5}\,)/2\right)^2} = -\log\biggl(\Bigl(1 - \frac{m}{\gamma}\Bigr)\Bigl(1 - \frac{1}{\gamma m}\Bigr)\biggr),\end{aligned}$$

where $\gamma = \bigl(3+\sqrt{5}\,\bigr)/2$ and $m = e^u$. We note that a $1/\hbar$ term would correspond to the genus 1/2 in the 't Hooft expansion.

B.3.3. Representation in terms of the quantum dilogarithm. The colored Jones polynomial for the knot 4_1 with $N = 2J+1$ can be represented in the hypergeometric form:

$$K_N(4_1|q) = [N]_q \sum_{i=0}^{N-1} (q,N)_i (q,N)_i^* \equiv [N]_q J_N(4_1|q).$$

Formula (A.4) then gives

$$K_N \sim \sum_{k=0}^{N-1} (-1)^k \frac{s(i\epsilon_2(N-1-k) + i(\epsilon_1+\epsilon_2)/2)}{s(i\epsilon_2(N-1) + i(\epsilon_1+\epsilon_2)/2)} \frac{s(i\epsilon_2 N + i(\epsilon_1+\epsilon_2)/2)}{s(i\epsilon_2(N+k) + i(\epsilon_1+\epsilon_2)/2)}. \tag{B.8}$$

B.3.4. Hikami representation. To obtain the Hikami integral representation from (B.8), we must take the double limit $\epsilon_2 \to 0$ and $N \to \infty$ such that $i\epsilon_2(N-1/2) + i\epsilon/2 = \tilde{u}$. In this limit, the sum in (B.8) should be replaced with the integral, and we finally obtain

$$K_N = -\frac{1}{\epsilon_2 \cosh\tilde{u}} \int dz\, e^{\pi z/\epsilon_2} s(z-\tilde{u}) s(z+\tilde{u}). \tag{B.9}$$

In Hikami's terms, the presence of two dilogarithm functions in this integral shows that the hyperbolic space $S^3 \setminus 4_1$ can be obtained by gluing two tetrahedra. This representation for $S^3 \setminus 4_1$ is well studied in the literature (see, e.g., [56]).

B.3.5. $\mathcal{A}$-polynomial. The $\mathcal{A}$-polynomial and the spectral curve for the knot 4_1 have the forms

$$\begin{aligned}\mathcal{A}_{4_1}(l,m) &= m^2 + l(-1 + m + 2m^2 + m^3 - m^4) + l^2 m^2, \\ A\Sigma_{4_1} &= \{(m,l) \in \mathbb{C}^2 \colon \mathcal{A}_{4_1}(l,m) = 0\}.\end{aligned}$$

To find the quantum $\mathcal{A}$-polynomial, we note that the Jones polynomial for the knot 4_1 vanishes under the action of the difference operator

$$\begin{aligned}\hat{A} = q^2\widehat{m}^2(1-\widehat{m})(1-q^3\widehat{m}^2) - (q\widehat{m}+1)(1 - q\widehat{m} - q\widehat{m}^2 - \\ - q^3\widehat{m}^2 - q^3\widehat{m}^3 + q^4\widehat{m}^4)(1-q\widehat{m})^2\hat{l} + q^2\widehat{m}^2(1-q\widehat{m}^2)(1-q^2\widehat{m})\hat{l}^{\,2}.\end{aligned}$$

Moreover, in this case,

$$\widehat{B} = q\widehat{m}(1-q^3\widehat{m}^2)(1-q\widehat{m}^2)(1+q\widehat{m})$$

(see formula (B.5)). In the large-N limit, the difference equation reduces to

$$[q^{3/2}\widehat{m}^2(1-q^3\widehat{m}^2)-(1-q^2\widehat{m}^2)(1-q\widehat{m}-q\widehat{m}^2-q^3\widehat{m}^2-q^3\widehat{m}^3+q^4\widehat{m}^4)\hat{l}+ \\ +q^{5/2}\widehat{m}^2(1-q\widehat{m}^2)\hat{l}^{\,2}\big]K_N(q)=0.$$

Hence, the quantum $\mathcal{A}$-polynomial is

$$\hat{\mathcal{A}}_{4_1}(\hat{l},\widehat{m}|q)=q^{3/2}\widehat{m}^2(1-q^3\widehat{m}^2)-(1-q^2\widehat{m}^2)(1-q\widehat{m}-q\widehat{m}^2- \\ -q^3\widehat{m}^2-q^3\widehat{m}^3+q^4\widehat{m}^4)\hat{l}+q^{5/2}\widehat{m}^2(1-q\widehat{m}^2).$$

For finite N, the Jones polynomial satisfies the equation

$$\hat{\mathcal{A}}_{\mathrm{G}}J_N(q)\equiv(\hat{l}-1)\frac{1}{\widehat{B}(\widehat{m})}\hat{A}(\hat{l},\widehat{m})J_N(q)=0,$$

where

$$\begin{aligned}\hat{\mathcal{A}}_{\mathrm{G}}=&-\frac{q^2\widehat{m}(1-q^3\widehat{m})}{(1+q^2\widehat{m})(1-q^5\widehat{m}^2)}\,\hat{l}^{\,3}+\\ &+\frac{1}{q}\frac{(1-q^2\widehat{m})(1+q\widehat{m}-2q^2\widehat{m}-q^3\widehat{m}^2+q^4\widehat{m}^2-q^5\widehat{m}^2-2q^6\widehat{m}^3+q^7\widehat{m}^3+q^8\widehat{m}^4)}{\widehat{m}(1+q\widehat{m})(1-q^5\widehat{m}^2)}\,\hat{l}^{\,2}-\\ &-\frac{1}{q}\frac{(1-q\widehat{m})(1-2q\widehat{m}+q^2\widehat{m}-q\widehat{m}^2+q^2\widehat{m}^2-q^3\widehat{m}^2+q^2\widehat{m}^3-2q^3\widehat{m}^3+q^4\widehat{m}^4)}{\widehat{m}(1+q^2\widehat{m})(1-q\widehat{m}^2)}\,\hat{l}+\\ &+\frac{q\widehat{m}(1-\widehat{m})}{(1+q\widehat{m})(1-q\widehat{m}^2)}.\end{aligned}$$

B.3.6. Polynomial invariants. The superpolynomial is given by

$$P_{4_1}(a,q,t)=P_0(a,q,t)(a^{-1}t^{-2}+q^{-1}t^{-1}+1+qt+at^2). \tag{B.10}$$

B.4. Knot 5_2.

B.4.1. Representation in terms of the quantum *R*-matrix and Drinfeld associator. The polynomial invariant for the knot 5_2 can be constructed using formulas (8) and (9). In this case, the knot can be represented as the closure of the element $b_{5_2}=g_2^3g_1g_2^{-1}g_1\in B_3$. In this representation, the knot has five positively oriented crossings, one negatively oriented crossing ($w(b)=4$), and two strands ($n=3$ in (9)).

B.4.2. Representation in terms of the Vassiliev invariant. The first few Vassiliev invariants of the knot 5_2 are

$$\alpha_{2,1}=8,\qquad \alpha_{3,1}=-24,\qquad \alpha_{4,1}=\frac{268}{3},\qquad \alpha_{4,2}=\frac{43}{3},$$
$$\alpha_{5,1}=-368,\qquad \alpha_{5,2}=-64,\qquad \alpha_{5,3}=-56.$$

For instance, using Table 3 for $SU(2)$ gives

$$\langle 5_2\rangle=[N]_q\exp\bigg\{-8J(1+J)h^2+24J(1+J)h^3+ \\ +\frac{4}{3}J(1+J)(-67+22J+22J^2)\hbar^4+\ldots\bigg\},\qquad h=2\pi i\hbar.$$

B.4.3. Representation in terms of the quantum dilogarithm. The colored Jones polynomial for the knot 5_2 with $N=2J+1$ can be represented in the hypergeometric form:

$$K_N(5_2|q)=[N]_q\sum_{0\le k\le l\le N-1}\frac{(q,N)_l(q,N)_l}{(q,N)^*_k}q^{-k(l+1)}\equiv[N]_qJ_N(5_2|q).$$

Hence, formula (A.4) gives

$$J_N\sim\sum_{0\le k\le l\le N-1}(-i)^{k+2l}q^{-k(l+1)}\frac{s^2(i\epsilon_2(N-1-l)+i(\epsilon_1+\epsilon_2)/2)}{s^2(i\epsilon_2(N-1)+i(\epsilon_1+\epsilon_2)/2)}\times$$
$$\times\frac{s(i\epsilon_2(N+k)+i(\epsilon_1+\epsilon_2)/2)}{s(i\epsilon_2N+i(\epsilon_1+\epsilon_2)/2)},$$
$$J_N=\frac{i}{s^3(u)}\int dz_1\int dz_2\,s^2(u-z)s(u+z)\times$$
$$\times\exp\biggl\{-\frac{2\pi z_1z_2}{\epsilon_1\epsilon_2}+\frac{\pi i(z_1-z_2)}{\epsilon_1}+\frac{2\pi i(2z_1+z_2)}{\epsilon_2}\biggr\}.$$

Again, the presence of three dilogarithms in this integral implies that the space $S^3\setminus 5_2$ can be realized by gluing three tetrahedrons in the Hikami model.

B.4.4. $\mathcal{A}$-polynomial. In the 5_2 case, we have

$$\mathcal{A}(l,m)=1+l(-1+2m+2m^2-m^4+m^5)+l^2(m^2-m^3+2m^5+2m^6-m^7)+l^3m^7.$$

The quantum $\mathcal{A}$-polynomial can be calculated as in the preceding cases, and we obtain the result

$$\hat{\mathcal{A}}(l,m)=q^{1/2}(1-q^4\widehat{m}^2)(1-q^5\widehat{m}^2)-(1-q^2\widehat{m}^2)(1-q^5\widehat{m}^2)\bigl(1-2q\widehat{m}-q(q+q^3)\widehat{m}^2+$$
$$+q^2(1-q)(1-q^2)\widehat{m}^3+q^5\widehat{m}^4-q^6\widehat{m}^5\bigr)\hat{l}+q^{5/2}(1-q\widehat{m}^2)(1-q^4\widehat{m}^2)\widehat{m}^2\times$$
$$\times\bigl(1-q^2\widehat{m}-q^2(1-q)(1-q^2)\widehat{m}^2+q^4(1+q^3)\widehat{m}^3+2q^7\widehat{m}^4-q^9\widehat{m}^5\bigr)\hat{l}^2+$$
$$+q^{14}(1-q\widehat{m}^2)(1-q^2\widehat{m}^2)\widehat{m}^7\hat{l}^3.$$

We note that this is the simplest example where $\hat{\mathcal{A}}(l,m)$ is not quadratic but cubic in l. In this case, the spectral curve is not hyperelliptic.

B.4.5. Polynomial invariants. The superpolynomial has the form

$$P_{5_2}(a,q,t)=P_0(a,q,t)(aq^{-1}+at+aqt^2+a^2q^{-1}t^2+a^2t^3a^2qt^4+a^3t^5).$$

Appendix C: Examples of the volume conjecture

The volume conjecture states that in the large-N limit, the logarithm of the colored Jones polynomial of a hyperbolic knot K is proportional to the volume of the complement of the knot in the three-dimensional sphere S^3:

$$\log|J_N(K)|\sim\frac{N}{2\pi}\mathrm{Vol}(S^3\setminus K)$$

for $q=e^{2\pi i/N}$ and $J_N(K)=\langle K\rangle/\dim_q(R)$.

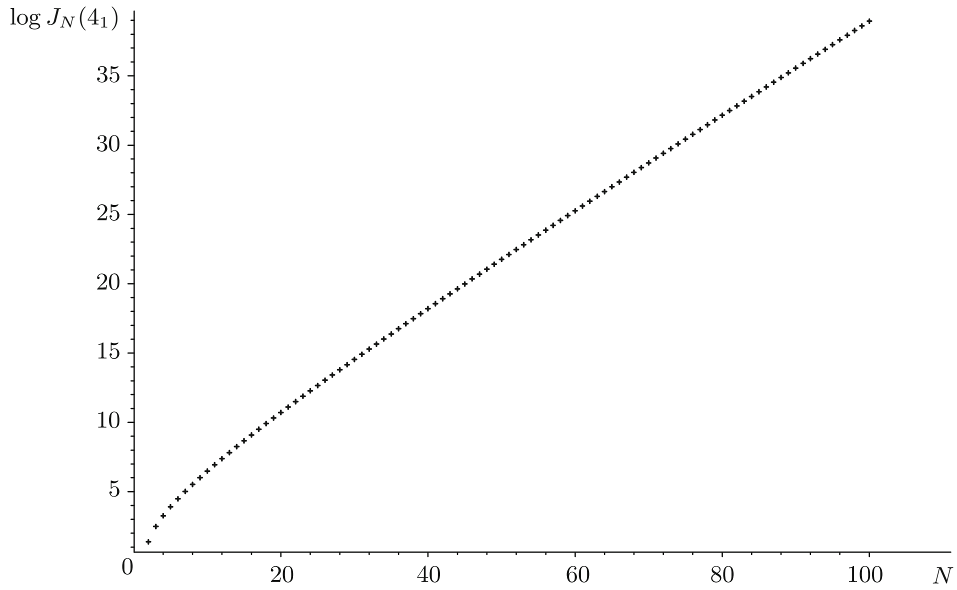

Fig. 3. The plot of $\log J_N(4_1)$ for $N = 3, \ldots, 100$: the plot becomes linear for large N.

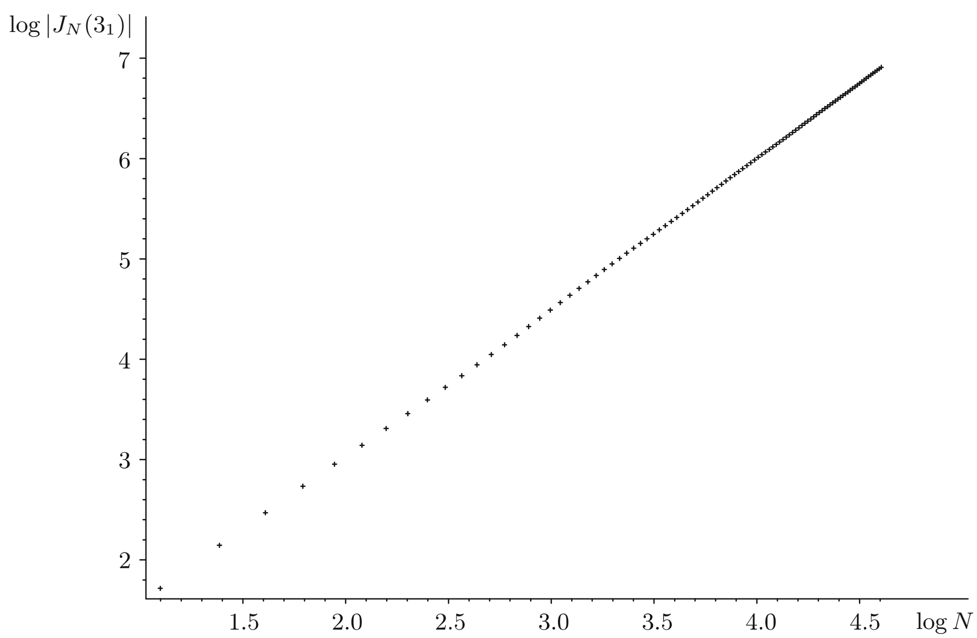

Fig. 4. The plot of $\log |J_N(3_1)|$ for $N = 3, \ldots, 100$ as a function of $\log N$: the plot behaves linearly with the slope $3/2$ for large N.

In the case of the hyperbolic knot 4_1, formula (B.9) for $q = e^{2\pi i/N}$ gives

$$J_N(4_1) = \sum_{k=1}^{N-1} \prod_{j=1}^{k} 4 \sin^2 \frac{\pi j}{N}.$$

We note that all terms in this formula are positive. The graph of this function for $N = 3, \ldots, 100$ is shown in Fig. 3. Using representation (B.8) and expansion (A.2) of the quantum dilogarithm function for large N, we can approximate this sum by the integral

$$J_N(4_1) \sim \int dz \exp\left\{\frac{N}{2\pi i}\big(\mathrm{Li}_2(-e^{-iz}) - \mathrm{Li}_2(-e^{iz})\big)\right\}.$$

Using the saddle point approximation, we obtain

$$\frac{d}{dz}\big(\mathrm{Li}_2(-e^{-iz}) - \mathrm{Li}_2(-e^{iz})\big) = 0,$$

consequently $\log\big((1+e^{-iz})(1+e^{iz})\big) = 0$, and hence $e^{iz} = e^{2\pi i/3}$. As a result, we obtain

$$\mathrm{Vol}(4_1) = -i\big(\mathrm{Li}_2(-e^{-2\pi i/3}) - \mathrm{Li}_2(-e^{2\pi i/3})\big) \approx 2.02688 \tag{C.1}$$

for the volume. This value can be measured directly as the slope in the plot in Fig. 3.

For the toric knot 3_1, the quantity $J_N(3_1)$ can take complex values, and the saddle point approximation is therefore subtler. In Fig. 4, we present the graph of $\log\big|J_N(3_1)\big|$ as a function of $\log N$ for $N = 3, \ldots, 100$. The asymptotic behavior of $|J_N(3_1)|$ can be seen as expected [57] and is consistent with the volume conjecture for the torus knot, $|J_N(3_1)| \sim N^{3/2}$. The phase of $J_N(3_1)$ behaves in a much more complicated way (see [58]).

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