ASYMPTOTICS OF THE QUANTUM INVARIANTS FOR SURGERIES ON THE FIGURE 8 KNOT

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Abstract. We investigate the Reshetikhin–Turaev invariants associated to $\mathfrak{sl}_2(\mathbb{C})$ for the 3–manifolds obtained by doing any rational surgery along the figure 8 knot. In particular, we express these invariants in terms of certain complex double contour integrals. These integral formulae allow us to propose a formula for the leading asymptotics of the invariants in the limit of large quantum level. We analyze this expression using the saddle point method. We prove that the stationary points for the relevant phase functions are in one to one correspondence with flat $\mathrm{SL}(2,\mathbb{C})$–connections on the 3–manifold and that the values of these phase functions at the relevant stationary points equals the classical Chern–Simons invariants of the corresponding flat $\mathrm{SU}(2)$–connections. Our findings are in agreement with the asymptotic expansion conjecture. Moreover, we calculate the leading asymptotics of the colored Jones polynomial of the figure 8 knot following Kashaev [Kash]. This leads to a slightly finer asymptotic description of the invariant than predicted by the volume conjecture [MM].

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1. Introduction

In this paper we investigate the large level asymptotics of the Reshetikhin–Turaev invariants of the 3–manifolds obtained by doing surgery on the figure 8 knot with an arbitrary rational surgery coefficient. Let X be a closed oriented 3-manifold and let $\tau_r(X)$ be the RT–invariant associated to $\mathfrak{sl}_2(\mathbb{C})$ at level r, some integer ≥ 2. The investigations of this paper are motivated by the following conjecture.

Conjecture 1.1 (Asymptotic expansion conjecture (AEC)). *There exist constants (depending on X) $d_j \in \mathbb{Q}$, $I_j \in \mathbb{Q}$ mod $8\mathbb{Z}$ and $v_j \in \mathbb{R}_+$ for $j = 0, 1, \dots, n$ and $a_j^l \in \mathbb{C}$ for $j = 0, 1, \dots, n$, $l = 1, 2, \dots$ such that the asymptotic expansion of $\tau_r(X)$ in the limit $r \to \infty$ is given by*

$$\tau_r(X) \sim \sum_{j=0}^{n} e^{2\pi i r q_j} r^{d_j} e^{i\frac{\pi}{4} I_j} v_j \left(1 + \sum_{l=1}^{\infty} a_j^l r^{-l}\right),$$

where $q_0 = 0, q_1, \dots q_n$ are the finitely many different values of the Chern–Simons functional on the space of flat $\mathrm{SU}(2)$*–connections on X.*

Here $\sim$ means **asymptotic expansion** in the Poincaré sense, which means the following: Let

$$d = \max\{d_0, \dots, d_n\}.$$

Then for any non-negative integer L, there is a $c_L \in \mathbb{R}$ such that

$$\left| \tau_r(X) - \sum_{j=0}^{n} e^{2\pi i r q_j} r^{d_j} e^{i\frac{\pi}{4} I_j} v_j \left(1 + \sum_{l=0}^{L} a_j^l r^{-l}\right) \right| \leq c_L r^{d-L-1}$$

for all levels r. Of course such a condition only puts limits on the large r behaviour of $\tau_r(X)$.

A little simple argument gives, that if $\tau_r(X)$ has an asymptotic expansion like this, then it is unique, that is the q_j's, the d_j's, I_j's, v_j's and the a_j^l's are all uniquely determined by the sequence $\tau_r(X)$, hence they are also topological invariants of X. There are topological formulae for the d_j's, I_j's and v_j's (see e.g. [A2] and the references given there). In this paper we will only pay attention to the formula for the d_j's.

For a flat SU(2)–connection A on X, consider the elliptic complex $d_A : \Omega^*(X; \mathfrak{su}(2)) \to \Omega^{*+1}(X; \mathfrak{su}(2))$, where $d_A f = df + [A, f]$ is the covariant derivative in the adjoint representation. Let h_A^i be the dimension of the ith cohomology group $H^i(X, d_A)$ of this complex.

Conjecture 1.2 (Topological interpretation of the d_j's). *Let $\mathcal{M}_j$ be the union of components of the moduli space of flat* $\mathrm{SU}(2)$*–connections on X which has Chern–Simons value q_j. Then*

$$d_j = \frac{1}{2} \max_{A \in \mathcal{M}_j} \left(h_A^1 - h_A^0\right),$$

where max *here means the maximum value $h_A^1 - h_A^0$ attains on a Zariski open subset of $\mathcal{M}_j$.*

We note that $H^1(X; d_A) = 0$ if A represents an isolated point in the moduli space, and $H^0(X, d_A) = 0$ if and only if A is irreducible.

In general, there should be expressions for each of the a_j^l in terms of sums over Feynman diagrams of certain contributions determined by the Feynman rules of the Chern–Simons theory. This has not yet been worked out in general, except in the case of an acyclic flat connection and the case of a smooth non-degenerate component of the moduli space of flat connections by Axelrod and Singer, cf. [AS1], [AS2], [Ax].

The AEC, Conjecture 1.1, however offers in a sense a converse point of view, where one seeks to derive the final output of perturbation theory after all cancellations have been made (i.e. collect all terms with the same Chern–Simons value). This seems actually rather reasonable in this case, since the exact invariant is known explicitly.

The AEC (and also Conjecture 1.2) was proved by Andersen in [A] in the case of mapping tori of finite order diffeomorphisms of orientable surfaces of genus at least two using the gauge-theoretic approach to the quantum invariants. Later on the AEC was proved by Hansen in [Ha2] for all Seifert manifolds with orientable base by supplementing the work of Rozansky [Ro] with the need analytic estimates. In [Ha3] the AEC is futher proved for the Seifert manifolds with nonorientable base of even genus.

Using the approach of Reshetikhin and Turaev to the quantum invariants, the AEC has not yet been proved for any hyperbolic 3–manifold. It is therefore particular interesting to consider surgeries on the figure 8 knot. Let $M_{p/q}$ be the manifold obtained by (rational) Dehn surgery on the figure 8 knot with surgery coefficient p/q. Then $M_{p/q}$ has a hyperbolic structure if and only if $|p| > 4$ or $|q| > 1$, see e.g. [Ra, Theorem 10.5.10] or [T]. We use here the convention of Rolfsen for surgery coefficients, cf. [Ro, Chap. 9]. In particular Dehn surgery on a knot K in S^3 with surgery coefficient $f \in \mathbb{Z}$ is equal to the boundary of the compact 4–manifold obtained by attaching a 2–handle to the 4–ball using the knot K with framing f, see [Ro, p. 261]. As usual $M_{p/q}$ is given the orientation induced by the standard right-handed orientation of S^3.

The advantage of working with surgeries on the figure 8 knot K, is that the normalized colored Jones polynomial $J'_K(\lambda)$ is known explicitly. In fact

$$J'_K(\lambda) = \sum_{m=0}^{\lambda-1} \xi^{-m\lambda} \prod_{l=1}^{m} (1-\xi^{\lambda-l})(1-\xi^{\lambda+l}),$$

where $\xi = \exp(2\pi i/r)$ (and the product is 1 for $m = 0$). The colors λ are here dimensions of irreducible representations of the quantum group associated to $\mathfrak{sl}_2(\mathbb{C})$ and the root of unity ξ, so $\lambda = 1, 2, \ldots, r$. By the above expression for $J'_K(\lambda)$ we have an explicit formula for the quantum invariant $\tau_r(M_{p/q})$ (see formula (6)). Although this formula is complete explicit, it is not clear from it what the leading order asymptotics of $\tau_r(M_{p/q})$ is. In order to study this asymptotics, we observe (generalizing from Kashaev's work) that the product in the expression for the colored Jones polynomial can be expressed in terms of a quotient of two evaluations of the Faddeev's quantum dilogarithm S_γ ($\gamma = \pi/r$):

$$J'_K(\lambda) = \sum_{m=0}^{\lambda-1} \frac{\xi^{-m\lambda}}{(1-\xi^{\lambda})} \frac{S_\gamma(-\pi + 2\gamma(\lambda - m) - \gamma)}{S_\gamma(-\pi + 2\gamma(\lambda + m) + \gamma)}. \tag{1}$$

This follows directly from the functional equation

$$(1 + e^{\sqrt{-1}\zeta}) S_\gamma(\zeta + \gamma) = S_\gamma(\zeta - \gamma)$$

which Faddeev's S_γ satisfies. Recall that for $\mathrm{Re}(\zeta) < \pi + \gamma$, we have the expression

$$S_\gamma(\zeta) = \exp\left(\frac{1}{4}\int_{C_R} \frac{e^{\zeta z}}{\sinh(\pi z)\sinh(\gamma z) z} \mathrm{d}z\right),$$

which together with the functional equation determines S_γ as a meromorphic function on $\mathbb{C}$. For the so-called top color, i.e. $\lambda = r$, we obtain the sligthly simpler expression

$$J'_K(r) = r \sum_{m=0}^{r-1} \frac{S_\gamma(\pi + (2m+1)\gamma)}{S_\gamma(-\pi + (2m+1)\gamma)}. \tag{2}$$

Then we simply use the residue formula to convert the sum (2) into a contour integral

$$J'_K(r) = \int_{C_r} \tan(\pi r x)\tilde{g}_r(x)\mathrm{d}x, \tag{3}$$

where C_r is contained in the strip $\{z \in \mathbb{C} \mid 0 < \mathrm{Re}(z) < 1\}$ and encloses $(m + \frac{1}{2})/r$ for $m = 0, \ldots, r-1$, and $\tilde{g}_r$ a holomorphic function in this strip expressed in terms of the above quotient of S_γ functions (see formula (19)).

Similarly we get for the quantum invariant with the use of (1) and the residue theorem, now a double contour integral, since the quantum invariant also involves a sum over colors:

$$\tau_r(M_{p/q}) = \int_{C_r \times C_r} \cot(\pi r x)\tan(\pi r y)\tilde{f}_{p,q,r}(x,y)\mathrm{d}x\mathrm{d}y, \tag{4}$$

where we furthermore require of C_r that it also encloses k/r for $k = 1, \ldots, r-1$ and $\tilde{f}_{p,q,r}$ is holomorphic on the double strip $\{z \in \mathbb{C} \mid 0 < \mathrm{Re}(z) < 1\}^2$ and given by some expression involving quotients of evaluations of S_γ–functions.

From this it is clear that we need to understand the small γ asymptotics of S_γ. We have that

$$S_\gamma(\zeta) = \exp\left(\frac{1}{2\sqrt{-1}\gamma}\mathrm{Li}_2(-e^{\sqrt{-1}\zeta}) + I_\gamma(\zeta)\right),$$

where Li_2 is Euler's dilogarithm function, and where we have certain analytic estimates on $I_\gamma(\zeta)$ (see Lemma 4.1).

Let us first explain how we use this to give a proof of the volume conjecture of Murakami and Murakami [MM] for the figure 8 knot, namely that

$$\lim_{r\to\infty} \frac{2\pi \mathrm{Log}(J'_K(r))}{r} = \mathrm{Vol}(4_1),$$

where the right-hand side is the hyperbolic volume of the figure 8 knot, i.e. the hyperbolic volume of the complement $S^3 \setminus K$. The basic idea in analyzing the above contour integral expression for $J'_K(r)$ is the following. In the upper half plane we approximate tan by i and by $-i$ in the lower half plane. Further we approximate S_γ by the above expression involving only the dilogarithm. In Appendix B we prove the needed estimates which allows us to do these approximations and we end up with the following formula for the leading order asymptotics

$$J'_K(r) \sim_{r\to\infty} r^2 \int_\epsilon^{1-\epsilon} e^{r\Phi(x)}\mathrm{d}x, \tag{5}$$

where

$$\Phi(x) = \frac{1}{2\pi\sqrt{-1}}\left(\mathrm{Li}_2(e^{-2\pi\sqrt{-1}x}) - \mathrm{Li}_2(e^{2\pi\sqrt{-1}x})\right).$$

Now we simply analyze the integral on the right-hand side of (5) by the saddle point method. This consists of finding the stationary points of Φ and also the so-called directions of steepest descend, see e.g. [B]. (In this paper we use critical point and stationary point interchangeable to mean a point in which the derivative is zero.) This analysis leads to two interesting results. Firstly, the search for stationary points leads to the hyperbolicity equation for the complement of the figure 8 knot in the 3–sphere. Recall that this complement can be decomposed into two so-called ideal hyperbolic tetrahedra each parametrized by a certain complex number. This decomposition then defines a hyperbolic structure on the complement exactly when the two parameters are equal and satisfy the hyperbolicity equation.

Secondly, we find that the value of the phase function in the relevant stationary point (there is only one such point in this case) is equal to the hyperbolic volume of the knot complement (divided by 2π), hence the leading asymptotics of $J'_K(r)$ is determined by this volume.

These phenomena were first observed by Kashaev [Kash] and have been conjectured by Thurston [Th] and Yokota [Y] to be generally true for hyperbolic knots (see Remark 4.3).

Ultimately our asymptotic analysis leads to the following

Theorem 1.3. *The leading order large r asymptotics of the colored Jones polynomial evaluated at the top color is given by*

$$J'_K(r) \sim_{r\to\infty} 3^{-1/4} r^{3/2} \exp\left(\frac{r}{2\pi}\mathrm{Vol}(4_1)\right).$$

As a corollary we obtain the volume conjecture for the figure 8 knot. We note that no of the proofs so far given in the literature for the volume conjecture for the figure 8 have been able to see the finer details of the asymptotic behaviour, namely the polynomial part $3^{-1/4} r^{3/2}$.

Let us now return to the study of the large r asymptotics of the quantum invariant $\tau_r(M_{p/q})$. We expect that an analysis of the expression (4) paralleling our analysis of $J'_K(r)$ should be applicable. I.e. tan and cot should be approximated by $\pm\sqrt{-1}$ depending on the sign of $\mathrm{Im}(y)$ and $\mathrm{Im}(x)$ and $\tilde{f}_{p,q,r}(x,y)$ by an appropriate expression involving the dilogarithm for some deformation of the part of $C_r \times C_r$. We have partial analytic results supporting this.

We propose the following analog of (5) for the quantum invariant. Let d be the inverse of $p \pmod q$. Let $(a,b) \in \{0,1\}^2$ and $n \in \mathbb{Z}$. Define

$$\Phi_n(x,y) = -\frac{dn^2}{q} - \frac{p}{4q}x^2 + \frac{n}{q}x - xy + \frac{1}{4\pi^2}\left(\mathrm{Li}_2(e^{2\pi i(x+y)}) - \mathrm{Li}_2(e^{2\pi i(x-y)})\right),$$

and

$$\Phi_n^{a,b}(x) = a(x-y) + b(x+y) + \Phi_n(x,y).$$

Conjecture 1.4. *There exist surfaces $\tilde{\Sigma}^n_{a,b} \subset \mathbb{C}^2$ for $(a,b) \in \{0,1\}^2$ and $n \in \mathbb{Z}/|q|\mathbb{Z}$ such that the leading order large r asymptotics of the quantum invariant is given by*

$$\bar{\tau}_r(M_{p/q}) \quad \sim_{r\to\infty} \quad \frac{i\mathrm{sign}(q)r}{4\sqrt{|q|}} e^{\frac{3\pi i}{4}\mathrm{sign}(pq)} \sum_{n\in\mathbb{Z}/|q|\mathbb{Z}} \sum_{(a,b)\in\{0,1\}^2} \int_{\tilde{\Sigma}^n_{a,b}} \tilde{g}_n(x) e^{2\pi i r \Phi_n^{a,b}(x,y)} \mathrm{d}x\mathrm{d}y, \quad (6)$$

where $\tilde{g}_n$ is some simple r-independent function of $x \in \mathbb{C}$. Moreover, the surfaces $\tilde{\Sigma}^n_{a,b} \subset \mathbb{C}^2$ can be chosen such that they pass through the critical points of $\Phi_n^{a,b}$ with vanishing $\mathrm{Im}(\Phi_n^{a,b})$. Furthermore, it can be arranged that $\mathrm{Im}(\Phi_n^{a,b}) \le 0$ along $\tilde{\Sigma}^n_{a,b}$ with equality only in the critical points.

Please see Conjecture 4.4 for the more detailed version of this conjecture, including the precise formula for $\tilde{g}_n$. (We have here for sign-reasons switched to the complex conjugate invariant $\bar{\tau}_r(M_{p/q}) = \overline{\tau_r(M_{p/q})} = \tau_r(M_{-p/q})$.)

We now proceed by making an asymptotics analysis of the right-hand side of (6) using the saddle point method like in our analysis of (5). Thus we need to analyze integrals of the form

$$I_n^{a,b} = \int_{\tilde{\Sigma}_{a,b}^n} \tilde{g}_n(x) e^{2\pi i r \Phi_n^{a,b}(x,y)} \mathrm{d}x\mathrm{d}y. \tag{7}$$

Again we have to determine the stationary points of $\Phi_n^{a,b}$ and the values of $\Phi_n^{a,b}$ in the relevant stationary points. The main idea behind the saddle point method is to deform $\tilde{\Sigma}_{a,b}^n$ so that it contains certain stationary points of $\Phi_n^{a,b}$ satisfying that the leading large r asymptotics of $I_n^{a,b}$ is determined solely by the contribution to $I_n^{a,b}$ coming from small neighborhoods of these stationary points.

If we let $v = e^{\pi i x}$ and $w = e^{2\pi i y}$, then by exponentiating the two equations for (x, y) being a stationary point of $\Phi_n^{a,b}(x, y)$ (see Theorem 1.5 below) we obtain the equations

$$\begin{aligned} v^{-p} &= \left(\frac{w - v^2}{1 - v^2 w} \right)^q, \\ v^2 w &= (1 - v^2 w)(w - v^2), \end{aligned} \tag{8}$$

which are independent of the integer parameters a, b, n. To link the asymptotics to the flat connections (as proposed by the AEC) we then have to relate the relevant stationary points of the phase functions $\Phi_n^{a,b}$ to the classical SU(2) Chern–Simons theory on the manifolds $M_{p/q}$. Fortunately, this Chern–Simons theory has been given a detailed description by Kirk and Klassen [KK] using the work of Riley [R1], [R2] on the $\mathrm{SL}(2, \mathbb{C})$ representation variety of the knot group of the figure 8 knot. According to Riley the nonabelian elements ρ of this variety can be parametrized by $\rho = \rho_{(s,u)}$, where $(s, u) \in \mathbb{C}^2$ satisfies a certain polynomial equation.

Using the results of Kirk and Klassen we show that $\rho_{(s,u)}$ defines a $\mathrm{SL}(2, \mathbb{C})$–representation of $\pi_1(M_{p/q})$ if and only if $(v, w) = (s, u + 1)$ is a solution to (8) and $v^2 \neq 1$. Moreover, this representation is conjugate to a SU(2)–representation if and only if $(s, u) \in S^1 \times \mathbb{R}$. Ultimately we arrive at

Theorem 1.5. *The map*

$$(x, y) \mapsto \rho_{(e^{\pi i x}, e^{2\pi i y} - 1)} = \rho_{(v, w-1)}$$

is a surjection from the set of critical points (x, y) of the functions $\Phi_n^{a,b}$ (with $x \notin \mathbb{Z}$) onto the nonabelian $\mathrm{SL}(2, \mathbb{C})$–representations of $\pi_1(M_{p/q})$. Moreover, $(x, y) \in \mathbb{C}^2$ is a critical point of $\Phi_n^{a,b}$ if and only if

$$\begin{aligned} 2a + \frac{n}{q} &= y + \left(\frac{p}{2q} + 1 \right) x + \frac{i}{\pi} \mathrm{Log}\left(1 - e^{2\pi i (x+y)} \right), \\ 2b + \frac{n}{q} &= y + \left(\frac{p}{2q} - 1 \right) x - \frac{i}{\pi} \mathrm{Log}\left(1 - e^{2\pi i (x-y)} \right). \end{aligned}$$

Futhermore, if (x, y) is a critical point of $\Phi_n^{a,b}$ such that $\rho_{(e^{\pi i x}, e^{2\pi i y} - 1)}$ is conjugate to a (nonabelian) SU(2)–representation $\bar{\rho}$ of $\pi_1(M_{p/q})$, then

$$\mathrm{CS}(\bar{\rho}) = \Phi_n^{a,b}(x, y) \mod \mathbb{Z},$$

where CS *is the* SU(2) *Chern–Simons functional.*

The results of Kirk and Klassen show that the moduli space of irreducible flat SU(2)–connections on $M_{p/q}$ is a discrete finite set, hence the covariant derivative complex $(\Omega^*(M_{p/q}, \mathfrak{su}(2)), d_A)$ is acyclic for all such connections A. If $p/q \neq 0$ the moduli space of reducible flat SU(2)–connections is also a discrete finite set, hence $h_A^1 = 0$ and $h_A^0 > 0$ for such connections A (using notation from Conjecture 1.2). According to Conjecture 1.2 the growth rate of $\tau_r(M_{p/q})$ in r should therefore be r^0 and the reducible connections should not contribute to the leading asymptotics of $\tau_r(M_{p/q})$ for $p/q \neq 0$.

Our results so far (see Corollary 4.5) are in agreement with these observations in relation to Conjecture 1.1 and 1.2 as far as the leading order asymptotics goes.

The invariant $\tau_r(M_0)$ and its full asymptotic expansion have been calculated by Jeffrey [J]. We show (see Appendix C) that Jeffrey's result is in agreement with the AEC. Again we see a growth rate of r^0, but in this case reducible flat SU(2)–connections contribute to the leading asymptotics. We note that the moduli space of reducible flat SU(2)–connections on M_0 is topologically a closed interval, so our findings are in accordance with Conjecture 1.2.

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2. The RT-invariant for surgeries on the figure-8 knot

This section is primarily intended to introduce notation. Moreover, we present some preliminary formulas for the colored Jones polynomial of the figure 8 knot and for the RT–invariants of the 3–manifolds $M_{p/q}$.

Let $t = \exp(2\pi\sqrt{-1}/(4r))$, r an integer ≥ 2, and let U_t be the modular Hopf algebra considered in [RT, Sect. 8], i.e. U_t is a finite-dimensional factor of the quantum group $U_\xi(\mathfrak{sl}_2(\mathbb{C}))$, $\xi = t^4$. (In [RT], and in most literature on the subject, ξ is denoted q, but we use in this paper q to mean something different.) For an integer k we let

$$[k] = \frac{t^{2k} - t^{-2k}}{t^2 - t^{-2}} = \frac{\sin(\pi k/r)}{\sin(\pi/r)},$$

sometimes called a quantum integer. For a knot K in S^3 we denote by K^0 the knot K considered as a framed knot with framing zero. The colored Jones polynomial associated to U_t of a framed oriented knot K with color $\lambda \in \{1, 2, \ldots, r\}$ is denoted $J_K(\lambda)$, and for an oriented knot K in S^3 we let $J'_K(\lambda) = J_{K^0}(\lambda)/[\lambda]$. Here the colors are the dimensions (as complex vector spaces) of irreducible U_t–modules.

Let N_f be the 3–manifold obtained by surgery on S^3 along K with surgery coefficient $f \in \mathbb{Z}$. By [KM1] or [RT] the RT–invariant (at level $r-2$) of N_f is

$$\tau_r(N_f) = \alpha \sum_{k=1}^{r-1} \xi^{(k^2-1)f/4} [k]^2 J'_K(k), \tag{9}$$

where K is given an arbitrary orientation. Here $\alpha = C^{\mathrm{sign}(f)} \mathcal{D}^{-2}$, where

$$\begin{aligned} \mathcal{D} &= \sqrt{\frac{r}{2}} \frac{1}{\sin(\pi/r)}, \\ C &= \exp\left(\frac{\sqrt{-1}\pi}{4} \frac{3(2-r)}{r} \right). \end{aligned}$$

We use here the normalization of [Tu]. This is $\mathcal{D}^{-1}$ times the normalization of [KM1] and $C^{-b_1(N_f)}\mathcal{D}^{-1}$ times the normalization of [RT], where $b_1(N_f)$ is the first betti number of N_f, see [Ha1, Appendix A]. (In the notation of [Tu], $C = \Delta \mathcal{D}^{-1}$.)

Let us next generalize to arbitrary rational surgery. Let p,q be a pair of coprime integers with $q \neq 0$, and let $N_{p/q}$ be the 3–manifold obtained by surgery along K with surgery coefficient p/q. Choose $c,d \in \mathbb{Z}$ such that $B = \begin{pmatrix} p & c \\ q & d \end{pmatrix} \in \mathrm{SL}(2,\mathbb{Z})$. Then (see e.g. [Ha1, Theorem 5.1 and the proofs of Corollary 8.3 and Theorem 8.4]),

$$\tau_r(N_{p/q}) = \left(e^{\frac{i\pi}{4}} \exp\left(-\frac{i\pi}{2r} \right) \right)^{\Phi(B)-3\mathrm{sign}(pq)} \sqrt{\frac{2}{r}} \sin\left(\frac{\pi}{r}\right) \sum_{\lambda=1}^{r-1} [\lambda] J'_K(\lambda) \tilde{B}_{\lambda,1},$$

where Φ is the Rademacher Phi function, see [RG], and $\tilde{\cdot}$ is the unitary representation of $P\mathrm{SL}(2,\mathbb{Z})$ given by

$$\begin{aligned} \tilde{B}_{j,k} &= \sqrt{-1}\frac{\mathrm{sign}(q)}{\sqrt{2r|q|}} e^{-\frac{\sqrt{-1}\pi}{4}\Phi(B)} \\ &\quad \times \sum_{\mu=\pm1} \sum_{n\in\mathbb{Z}/|q|\mathbb{Z}} \mu \exp\left(\frac{\sqrt{-1}\pi}{2rq} [pj^2 - 2\mu j(k+2rn\mu) + d(k+2rn\mu)^2] \right). \end{aligned}$$

By evaluating the sum over μ we get

$$\begin{aligned} \tau_r(N_{p/q}) &= a(r) \sum_{n\in\mathbb{Z}/|q|\mathbb{Z}} \exp\left(2\pi i r \frac{dn^2}{q} \right) \\ &\quad \times \sum_{k=1}^{r-1} \sin\left(\frac{\pi}{q}\left[2nd - \frac{k}{r} \right] \right) \exp\left(\frac{\pi i r}{2q} \left[p\left(\frac{k}{r}\right)^2 - 4n\frac{k}{r} \right] \right) [k] J'_K(k), \end{aligned} \tag{10}$$

where

$$a(r) = -\frac{2\mathrm{sign}(q)}{r\sqrt{|q|}} \sin\left(\frac{\pi}{r}\right) e^{-\frac{3\pi i}{4}\mathrm{sign}(pq)} \exp\left(\frac{\pi i}{2r} \left[3\mathrm{sign}(pq) - \frac{p}{q} + \mathrm{S}\left(\frac{p}{q}\right) \right] \right).$$

Here S is the Dedekind symbol, see e.g. [KM2]. We note that the quantum invariant τ_r is independent of the colored Jones polynomial $J'_K(k)$ for the top-color $k=r$.

In the remaining part of this paper K will denote the figure 8 knot unless explicitly stated otherwise. Recall that $M_{p/q}$ denotes the 3–manifold obtained by surgery on S^3 along K with surgery coefficient $p/q \in \mathbb{Q}$. By an R–matrix calculation (see e.g. [Ha4]) we find that

$$J'_K(\lambda) = \sum_{m=0}^{\lambda-1} \xi^{-m\lambda} \prod_{l=1}^{m} (1-\xi^{\lambda-l})(1-\xi^{\lambda+l}) \tag{11}$$

for $\lambda = 1,2,\ldots,r$, where $\prod_{l=1}^m (1-\xi^{k-l})(1-\xi^{k+l}) = 1$ for $m=0$. Le and Habiro have obtained a similar formula, cf. [Le].

Remark 2.1. Unitarity of $\mathcal{V}_t$ implies that

$$\tau_r(-M) = \overline{\tau_r(M)} \tag{12}$$

for any 3–manifold M, where $\bar{\cdot}$ means complex conjugation. This formula also follows directly from [KM1] and the remarks concerning normalization following (9).

Since the figure 8 knot is amphicheiral, $M_{-p/q}$ and $M_{p/q}$ are orientation reversing homeomorphic. By (12) we therefore have

$$\overline{\tau_r(M_{p/q})} = \tau_r(M_{-p/q}). \tag{13}$$

This formula also follows directly by (10) and the facts that $J'_K(\lambda)$ is real and $S(-p/q) = -S(p/q)$. That $J'_K(\lambda)$ is real follows by amphicheirality of K but can also be seen directly from (11) by

$$\begin{aligned} J'_K(\lambda) &= \sum_{m=0}^{\lambda-1}\prod_{l=1}^{m}\xi^{-\lambda/2}\xi^{l/2}(1-\xi^{\lambda-l})\xi^{-\lambda/2}\xi^{-l/2}(1-\xi^{\lambda+l}) \\ &= \sum_{m=0}^{\lambda-1}\prod_{l=1}^{m}(\xi^{(\lambda-l)/2}-\xi^{-(\lambda-l)/2})(\xi^{(\lambda+l)/2}-\xi^{-(\lambda+l)/2}) \\ &= \sum_{m=0}^{\lambda-1}(-4)^m\prod_{l=1}^{m}\sin(\pi(\lambda-l)/r)\sin(\pi(\lambda+l)/r). \end{aligned}$$

3. A complex double contour integral formula for $\tau_r(M_{p/q})$

In this section we derive a complex double contour integral formula for the RT–invariants $\tau_r(M_{p/q})$ by using methods similar to Kashaev [Kash]. By (10) and (11) we have

$$\begin{aligned} \tau_r(M_{p/q}) &= \frac{ia(r)}{2\sin(\pi/r)}\sum_{n\in\mathbb{Z}/|q|\mathbb{Z}}\exp\left(2\pi i r\frac{dn^2}{q}\right)\sum_{k=1}^{r-1}\sum_{m=0}^{r-1}\exp\left(\frac{\pi i r}{2q}\left[p\left(\frac{k}{r}\right)^2-4n\frac{k}{r}\right]\right) \\ &\quad\times\sin\left(\frac{\pi}{q}\left[2nd-\frac{k}{r}\right]\right)\frac{\xi^{-(m+1/2)k}}{(1-\xi^k)}\prod_{l=0}^{m}(1-\xi^{k-l})(1-\xi^{k+l}). \end{aligned} \tag{14}$$

When we consider the expression for the summand in this multi sum, we see that the expression as it stands only makes sense for non-negative integers m. In order to make sense of this expression for arbitrary complex values for m, let us consider the quantum dilogarithm of Faddeev

$$S_\gamma(\zeta) = \exp\left(\frac{1}{4}\int_{C_R}\frac{e^{\zeta z}}{\sinh(\pi z)\sinh(\gamma z)z}\mathrm{d}z\right) \tag{15}$$

defined on $\Delta_\gamma = \{\zeta\in\mathbb{C} \mid |\mathrm{Re}(\zeta)| < \pi+\gamma\ \}$, where $\gamma\in]0,1[$ and C_R is the contour $]-\infty,-R]+\Upsilon_R+[R,\infty[$, where $\Upsilon_R(t) = Re^{\sqrt{-1}(\pi-t)}$, $t\in[0,\pi]$ and $R\in]0,1[$.

The function $S_\gamma : \Delta_\gamma\to\mathbb{C}$ is holomorphic and it satisfies the well-known functional equation (see [F] or [Kash]).

Lemma 3.1. *For $\zeta\in\mathbb{C}$ with $|\mathrm{Re}(\zeta)|<\pi$ we have*

$$(1+e^{\sqrt{-1}\zeta})S_\gamma(\zeta+\gamma) = S_\gamma(\zeta-\gamma).$$

For the sake of completeness we have given a proof in Appendix A. We use Lemma 3.1 to extend S_γ to a meromorphic function on the complex plane $\mathbb{C}$.

From now on we fix $\gamma = \pi/r$. By Lemma 3.1 we get that

$$S_\gamma(\zeta) = S_\gamma(\zeta+2\pi)\prod_{j=0}^{r-1}\left(1+e^{\sqrt{-1}(\zeta+(2j+1)\pi/r)}\right).$$

If we write $\zeta = -\pi+2\pi x$ we get that

$$\prod_{j=0}^{r-1}\left(1+e^{\sqrt{-1}(\zeta+(2j+1)\pi/r)}\right) = \prod_{j=0}^{r-1}\left(1-w^je^{2\pi\sqrt{-1}(x+\frac{1}{2r})}\right),$$

where $w = e^{2\pi\sqrt{-1}/r}$. Using $1 - z^r = \prod_{j=0}^{r-1}(1 - w^j z)$ we get that

$$S_\gamma(-\pi + 2\pi x) = \left(1 + e^{2\pi\sqrt{-1}xr}\right) S_\gamma(-\pi + 2\pi(x+1)) \tag{16}$$

for $x \in \mathbb{C}$. Let

$$x_n = \frac{n}{r} + \frac{1}{2r}, \qquad n \in \mathbb{Z}.$$

Then $x \mapsto S_\gamma(-\pi + 2\pi x)$ is analytic on $\mathbb{C} \setminus \{x_n | n = r, r+1, \dots\}$. If m is a positive integer then $\{x_n | n = mr, mr+1, \dots, (m+1)r - 1\}$ are poles of order m, while the points $\{x_n | n = -mr, -mr+1, \dots, -mr+r-1\}$ are zeros of order m.

Let us use the function S_γ to give another expression for $\tau_r(M_{p/q})$. By Lemma 3.1 we have that

$$\prod_{l=0}^{m}(1 - \xi^{k \pm l}) = \prod_{l=0}^{m} \frac{S_\gamma(-\pi + 2\gamma(k \pm l) - \gamma)}{S_\gamma(-\pi + 2\gamma(k \pm l) + \gamma)}.$$

Therefore

$$\begin{aligned} \prod_{l=0}^{m}(1 - \xi^{k-l}) &= \frac{S_\gamma(-\pi + 2\gamma(k-m) - \gamma)}{S_\gamma(-\pi + 2\gamma k + \gamma)}, \\ \prod_{l=0}^{m}(1 - \xi^{k+l}) &= \frac{S_\gamma(-\pi + 2\gamma k - \gamma)}{S_\gamma(-\pi + 2\gamma(k+m) + \gamma)}. \end{aligned}$$

So

$$\prod_{l=0}^{m}(1 - \xi^{k-l})(1 - \xi^{k+l}) = (1 - \xi^k)\frac{S_\gamma(-\pi + 2\gamma(k-m) - \gamma)}{S_\gamma(-\pi + 2\gamma(k+m) + \gamma)},$$

and then by (14)

$$\tau_r(M_{p/q}) = \beta(r) \sum_{n \in \mathbb{Z}/|q|\mathbb{Z}} \sum_{k=1}^{r-1} \sum_{m=0}^{r-1} f_{n,r}\left(\frac{k}{r}, \frac{m + 1/2}{r}\right),$$

where

$$f_{n,r}(x,y) = \sin\left(\frac{\pi}{q}(x - 2nd)\right) e^{2\pi i r\left(\frac{dn^2}{q} + \frac{p}{4q}x^2 - \frac{n}{q}x - xy\right)} \frac{S_\gamma(-\pi + 2\pi(x-y))}{S_\gamma(-\pi + 2\pi(x+y))}$$

and

$$\beta(r) = -\frac{ia(r)}{2\sin(\pi/r)} = \frac{i\mathrm{sign}(q)}{r\sqrt{|q|}} e^{-\frac{3\pi i}{4}\mathrm{sign}(pq)} \exp\left(\frac{\pi i}{2r}\left[3\mathrm{sign}(pq) - \frac{p}{q} + \mathrm{S}\left(\frac{p}{q}\right)\right]\right). \tag{17}$$

Note that d is equal to the inverse of p (mod q) and that the functions $f_{n,r}$ are independent of the choice of this inverse. By the remarks following Lemma 3.1 the functions $f_{n,r}$ are holomorphic on $\Omega_r \times \Omega_r$, where

$$\Omega_s = \left\{ w \in \mathbb{C} \mid -\frac{1}{4s} < \mathrm{Re}(w) < 1 + \frac{1}{4s} \right\} \tag{18}$$

for $s \in]0, \infty]$. By the residue theorem we therefore end up with

Lemma 3.2. *The quantum invariants of $M_{p/q}$ are given by*

$$\tau_r(M_{p/q}) = \frac{\beta(r)r^2}{4} \sum_{n \in \mathbb{Z}/|q|\mathbb{Z}} \int_{C_r^1} \cot(\pi r x) \left(\int_{C_r^2} \tan(\pi r y) f_{n,r}(x,y)\mathrm{d}y\right)\mathrm{d}x,$$

where $\beta(r)$ is given by (17) *and*

$$f_{n,r}(x,y) = \sin\left(\frac{\pi}{q}(x-2nd)\right) e^{2\pi i r\left(\frac{dn^2}{q}+\frac{p}{4q}x^2-\frac{n}{q}x-xy\right)} \frac{S_\gamma(-\pi+2\pi(x-y))}{S_\gamma(-\pi+2\pi(x+y))},$$

and where C_r^1 is a closed curve in Ω_r such that the poles $\{k/r \mid k=1,2,\dots,r-1\}$ for $x\mapsto \cot(\pi r x)$ lies inside C_r^1 and all other poles for this function lies outside C_r^1, and C_r^2 is a closed curve in Ω_r such that the poles $\{(m+1/2)/r \mid m=0,1,\dots,r-1\}$ for $y\mapsto \tan(\pi r y)$ lies inside C_r^2 and all other poles for this function lies outside C_r^2. Both curves are oriented in the anti-clockwise direction.

Using the function S_γ we can also express $J_K'(r)$ as a contour integral. By Lemma 3.1 we get that

$$J_K'(r) = r\sum_{m=0}^{r-1} \frac{S_\gamma(\pi-(2m+1)\gamma)}{S_\gamma(-\pi+(2m+1)\gamma)}.$$

We have here used that

$$\frac{S_\gamma(-\pi+\gamma)}{S_\gamma(\pi-\gamma)} = \prod_{j=1}^{r-1}\frac{S_\gamma(\pi-(2j+1)\gamma)}{S_\gamma(-\pi+(2j+1)\gamma)} = \prod_{j=1}^{r-1}\left(1-e^{-2\pi\sqrt{-1}\frac{j}{r}}\right) = r.$$

If we put

$$g_r(x) = \frac{S_\gamma(\pi-2\pi x)}{S_\gamma(-\pi+2\pi x)}$$

for $x\in\Omega_{\frac{1}{2}r}$ we get

$$J_K'(r) = r\sum_{m=0}^{r-1} g_r\left(\frac{m+1/2}{r}\right),$$

and we can write this sum as the single contour integral

$$J_K'(r) = \frac{\sqrt{-1}r^2}{2}\int_{C_r^2} \tan(\pi r x) g_r(x)\mathrm{d}x, \tag{19}$$

where C_r^2 is given in Lemma 3.2.

4. The large r asymptotics of $J_K'(r)$ and $\tau_r(M_{p/q})$

In this section we investigate the large r asymptotics of $\tau_r(M_{p/q})$ or more precisely the leading term of this asymptotics, using the saddle point approximation method. We begin by calculating the large r asymptotics of $J_K'(r)$ using the expression (19). This calculation will demonstrate the use of the saddle point method and will serve as a warm up for the more difficult considerations of the asymptotics of $\tau_r(M_{p/q})$ in the final part of this section.

4.1. **Semiclassical asymptotics of the quantum dilogarithm.** It is well known that the semiclassical asymptotics, i.e. the small γ range of the quantum dilogarithm S_γ is given by Euler's dilogarithm

$$\mathrm{Li}_2(z) = -\int_0^z \frac{\mathrm{Log}(1-w)}{w}\mathrm{d}w \tag{20}$$

for $z\in\mathbb{C}\setminus]1,\infty[$. Here and elsewhere Log denotes the principal logarithm. For $|\mathrm{Re}(\zeta)|<\pi$ or $\zeta=\pm\pi$ one can check (see Appendix A) that

$$\frac{1}{2\sqrt{-1}\gamma}\mathrm{Li}_2(-e^{\sqrt{-1}\zeta}) = \frac{1}{4}\int_{C_R}\frac{e^{\zeta z}}{\sinh(\pi z)\gamma z^2}\mathrm{d}z,$$

hence we have that

$$S_\gamma(\zeta) = \exp\left(\frac{1}{2\sqrt{-1}\gamma}\mathrm{Li}_2(-e^{\sqrt{-1}\zeta}) + I_\gamma(\zeta)\right) \tag{21}$$

for such ζ, where

$$I_\gamma(\zeta) = \frac{1}{4}\int_{C_R} \frac{e^{\zeta z}}{z\sinh(\pi z)}\left(\frac{1}{\sinh(\gamma z)} - \frac{1}{\gamma z}\right)\mathrm{d}z.$$

Lemma 4.1. *If* $|\mathrm{Re}(\zeta)| < \pi$ *then*

$$|I_\gamma(\zeta)| \leq A\left(\frac{1}{\pi - \mathrm{Re}(\zeta)} + \frac{1}{\pi + \mathrm{Re}(\zeta)}\right)\gamma + B\left(1 + e^{-\mathrm{Im}(\zeta)R}\right)\gamma,$$

and for $|\mathrm{Re}(\zeta)| \leq \pi$ *we have*

$$|I_\gamma(\zeta)| \leq 2A + B\left(1 + e^{-\mathrm{Im}(\zeta)R}\right)\gamma,$$

where A *and* B *are positive constants only depending on* R.

A proof is given in Appendix A. On the unit circle the dilogarithm is given by Clausen's function Cl_2, i.e.

$$\mathrm{Im}\left(\mathrm{Li}_2(e^{i\theta})\right) = \mathrm{Cl}_2(\theta) = \sum_{n=1}^{\infty}\frac{\sin(n\theta)}{n^2} = -\int_0^\theta \mathrm{Log}\left|2\sin\left(\frac{t}{2}\right)\right|\mathrm{d}t \tag{22}$$

for $\theta \in \mathbb{R}$. One sees that Cl_2 is increasing on $[0,\pi/3] \cup [5\pi/3, 2\pi]$ and decreasing on $[\pi/3, 5\pi/3]$. In particular, Cl_2 attains its maximum value at $\pi/3$ and its minimum value at $5\pi/3$. Moreover

$$-\mathrm{Cl}_2\left(\frac{5\pi}{3}\right) = \mathrm{Cl}_2\left(\frac{\pi}{3}\right) = -2\int_0^{\pi/6}\mathrm{Log}|2\sin(\phi)|\mathrm{d}\phi = 2\mathbb{J}\left(\frac{\pi}{6}\right) = \frac{1}{2}\mathrm{Vol}(4_1), \tag{23}$$

where $\mathbb{J}$ is Lobachevsky's function and $\mathrm{Vol}(4_1)$ is the hyperbolic volume of the complement of the figure 8 knot, cf. [Ra, Sect. 10.4].

4.2. **The large r asymptotics of $J_K'(r)$.** We calculate the leading term of the large r asymptotics of $J_K'(r)$, using the saddle point approximation method like Kashaev [Kash]. Our calculation supplements the calculation of Kashaev with the needed analytic error estimates. Let

$$\begin{aligned} C_r^2 = C(\varepsilon) &= [\sqrt{-1}+\varepsilon, -\sqrt{-1}+\varepsilon] + [-\sqrt{-1}+\varepsilon, 1-\varepsilon-\sqrt{-1}] \\ &\quad + [1-\varepsilon-\sqrt{-1}, 1-\varepsilon+\sqrt{-1}] + [1-\varepsilon+\sqrt{-1}, \varepsilon+\sqrt{-1}], \end{aligned}$$

where $\varepsilon \in]0, \frac{1}{4r}[$. We let $C_+(\varepsilon)$ be the part of the contour $C(\varepsilon)$ above the real axes and $C_-(\varepsilon)$ the part below the real axes. By (19) we have

$$J_K'(r) = \frac{\sqrt{-1}r^2}{2}\left(J_+(r,\varepsilon) + J_-(r,\varepsilon)\right),$$

where

$$J_\pm(r,\varepsilon) = \int_{C_\pm(\varepsilon)} \tan(\pi r x) g_r(x)\mathrm{d}x.$$

The factor $\tan(\pi r x)$ can away from the real axis' be approximated by $\pm\sqrt{-1}$ depending on whether we are in the upper or lower half-plane:

$$|\tan(\pi r x) - \sqrt{-1}| \leq \begin{cases} 4e^{-2\pi r \mathrm{Im}(x)}, & \mathrm{Im}(x) \geq \frac{1}{\pi r}, \\ 2e^{-2\pi r\mathrm{Im}(x)}, & r\mathrm{Re}(x) \in \mathbb{Z}, \mathrm{Im}(x) \geq 0, \end{cases} \tag{24}$$

and

$$|\tan(\pi r x) + \sqrt{-1}| \leq \begin{cases} 4e^{2\pi r\sqrt{-1}\mathrm{Im}(x)}, & \mathrm{Im}(x) \leq -\frac{1}{\pi r}, \\ 2e^{2\pi r v}, & r\mathrm{Re}(x) \in \mathbb{Z}, \mathrm{Im}(x) \leq 0. \end{cases} \tag{25}$$

Therefore we write

$$J_\pm(r,\varepsilon) = \pm\sqrt{-1}\int_{C_\pm(\varepsilon)} g_r(x)\mathrm{d}x + \int_{C_\pm(\varepsilon)} (\tan(\pi r x) \mp \sqrt{-1})g_r(x)\mathrm{d}x.$$

The estimate on $\tan(\pi r x) \pm \sqrt{-1}$ can be used (see Appendix B) to prove that

$$\left| \sum_{\mu=\pm1} \int_{C_\mu(\varepsilon)} (\tan(\pi r x) - \mu\sqrt{-1})g_r(x)\mathrm{d}x \right| \leq K_1\frac{1}{r}, \tag{26}$$

where K_1 is a constant independent of r and ε. Let now

$$\Phi(x) = \frac{1}{2\pi\sqrt{-1}}\left(\mathrm{Li}_2(e^{-2\pi\sqrt{-1}x}) - \mathrm{Li}_2(e^{2\pi\sqrt{-1}x})\right). \tag{27}$$

Note that Φ is analytic on $D = \mathbb{C} \setminus \{\, x \in \mathbb{C} \,|\, \mathrm{Re}(x) \in \mathbb{Z} \,\}$ but not in the points $\mathbb{Z}$, so here we see the reason for using the small deformation parameter ε. We have

$$\begin{aligned} \int_{C_\pm(\varepsilon)} g_r(x)\mathrm{d}x &= \int_{C_\pm(\varepsilon)} e^{r\Phi(x)}\mathrm{d}x \\ &\quad + \int_{C_\pm(\varepsilon)} \left(\exp\left(I_\gamma(\pi - 2\pi x) - I_\gamma(-\pi + 2\pi x)\right) - 1\right) e^{r\Phi(x)}\mathrm{d}x, \end{aligned}$$

However, as we will see in Appendix B, the estimate in Lemma 4.1 implies that

$$\left| \int_{C_\mu(\varepsilon)} \left(\exp\left(I_\gamma(\pi - 2\pi x) - I_\gamma(-\pi + 2\pi x)\right) - 1\right) e^{r\Phi(x)}\mathrm{d}x \right| \leq \frac{K_2\mathrm{Log}(r)}{r} e^{\frac{r}{2\pi}\mathrm{Vol}(4_1)} \tag{28}$$

for $\mu = \pm1$, where K_2 is a constant independent of r and ε. We will see below that the estimates (26) and (28) imply that the leading order large r asymptotics of $J_K'(r)$ is given by

$$J_K'(r) \sim_{r\to\infty} \frac{r^2}{2}\left(\int_{C_-(\varepsilon)} e^{r\Phi(x)}\mathrm{d}x - \int_{C_+(\varepsilon)} e^{r\Phi(x)}\mathrm{d}x\right), \tag{29}$$

to which we can apply the saddle point method, see e.g. [B, Chap. 5]. First we determine the stationary points of the phase function Φ. On D we have

$$\Phi'(x) = \mathrm{Log}\left(1 - e^{2\pi\sqrt{-1}x}\right) + \mathrm{Log}\left(1 - e^{-2\pi\sqrt{-1}x}\right).$$

If we put $z = e^{2\pi\sqrt{-1}x}$, then $\Phi'(x) = 0$ implies that

$$z^2 - z + 1 = 0. \tag{30}$$

The equation (30) has the solutions $z_\pm = e^{\pm\sqrt{-1}\pi/3}$. We have $1 - z_\pm = 1/2 \mp i\sqrt{3}/2$ which both have norm 1 and are each others conjugate, so

$$\mathrm{Log}\,(1 - z_+) + \mathrm{Log}\,(1 - z_-) = 0.$$

We note that $z_\pm = e^{\pm 2\pi\sqrt{-1}\frac{1}{6}}$ correspond to the x–points $\pm1/6 + \mathbb{Z}$. These points are non-degenerate critical points. In fact,

$$\Phi''(x) = 2\pi\sqrt{-1}\frac{e^{2\pi\sqrt{-1}x} + 1}{e^{2\pi\sqrt{-1}x} - 1}$$

on D, so in particular $\Phi''(x_\pm) = \pm 2\pi\sqrt{3}$ for $x_\pm \in \pm 1/6 + \mathbb{Z}$. The imaginary part of $\Phi(x)$ is zero for $x \in \mathbb{R}$ and

$$\Phi(x) = \frac{1}{2\pi}\mathrm{Im}\left(\mathrm{Li}_2(e^{-2\pi\sqrt{-1}x}) - \mathrm{Li}_2(e^{2\pi\sqrt{-1}x})\right) = -\frac{1}{\pi}\mathrm{Cl}_2(2\pi x),$$

by (22). Let $x_\pm \in \pm 1/6 + \mathbb{Z}$. By (23) we have $\mathrm{Cl}_2(2\pi x_-) = -\mathrm{Cl}_2(2\pi x_+) = -\mathrm{Cl}_2(\pi/3) = -\mathrm{Vol}(4_1)/2$, i.e.

$$\Phi(x_\pm) = \mp\frac{1}{2\pi}\mathrm{Vol}(4_1).$$

By Cauchy's theorem we have

$$\int_{C_-(\varepsilon)} e^{r\Phi(x)}\mathrm{d}x - \int_{C_+(\varepsilon)} e^{r\Phi(x)}\mathrm{d}x = 2\int_{C_-(\varepsilon)} e^{r\Phi(x)}\mathrm{d}x = -2\int_{C_+(\varepsilon)} e^{r\Phi(x)}\mathrm{d}x.$$

Deform $C_-(\varepsilon)$ to $[\varepsilon, 1-\varepsilon]$ keeping the end points fixed. This does not change the integral $\int_{C_-(\varepsilon)} e^{r\Phi(x)}\mathrm{d}x$. Let $x_0 = 5/6$. By terminology borrowed from [B, Sect. 5.4] the axis of the saddle point x_0 is the real axis (i.e. the directions of steepest descent are along the real axis). From the analysis of [B, Sect. 5.7] it follows that we can find a $\delta > 0$ (independent of r and ε) such that $[x_0 - \delta, x_0 + \delta] \subseteq [1/(4r), 1 - 1/(4r)]$ and such that we have an asymptotic expansion

$$\int_{-\delta}^{\delta} e^{r\Phi(x_0+t)}\mathrm{d}t \sim \frac{1}{3^{1/4}\sqrt{r}} e^{\frac{r}{2\pi}\mathrm{Vol}(4_1)}\left(1 + \sum_{n=1}^{\infty} d_n r^{-n}\right)$$

in the limit $r \to \infty$, where d_n are certain complex numbers. Finally we note that

$$\left|\int_{\varepsilon}^{x_0-\delta} e^{r\Phi(t)}\mathrm{d}t + \int_{x_0+\delta}^{1-\varepsilon} e^{r\Phi(t)}\mathrm{d}t\right| \le e^{rc},$$

where $c = \max\{-\mathrm{Cl}_2(2\pi(x_0-\delta))/\pi, -Cl_2(2\pi(x_0+\delta))/\pi\} < \mathrm{Vol}(4_1)/2\pi$, see above (23). We have shown

Lemma 4.2. *The leading order large r asymptotics of $J'_K(r)$ is given by*

$$J'_K(r) \sim_{r\to\infty} 3^{-1/4} r^{3/2} \exp\left(\frac{r}{2\pi}\mathrm{Vol}(4_1)\right). \tag{31}$$

In fact

$$J'_K(r) = 3^{-1/4} r^{3/2} \exp\left(\frac{r}{2\pi}\mathrm{Vol}(4_1)\right) + \mathrm{O}\left(r\mathrm{Log}(r)\exp\left(\frac{r}{2\pi}\mathrm{Vol}(4_1)\right)\right)$$

in the limit $r \to \infty$. □

In particular

$$\lim_{r\to\infty} \frac{2\pi\mathrm{Log}(J'_K(r))}{r} = \mathrm{Vol}(4_1)$$

as predicted by the volume conjecture of Kashaev [Kash] and Murakami, Murakami [MM] and as proven by Ekholm and others, see [M1]. However, the arguments of Ekholm and others can't see the finer details of the asymptotic behaviour (31), namely the polynomial part $3^{-1/4}r^{3/2}$.

Remark 4.3. The complement $S^3 \setminus K$ of the figure 8 knot can be decomposed into two so-called ideal hyperbolic tetrahedra each parametrized by a certain complex number. This decomposition then defines a hyperbolic structure on this complement if and only if a certain set of conditions is satisfied. In fact, if the complex parameters for the two tetrahedra are respectively a and b, then these conditions are equivalent to $a = b$ and $b^2 - b + 1 = 0$, which is equation (30) after substituting b for z. We refer to [M2, Sect. 3] for more details. This phenomenon, that one finds the hyperbolicity equation for the figure 8 knot complement as the equation for the stationary points of the phase function, seems to be a general principal for hyperbolic knots as argued by Thurston and Yokota, cf. [Th], [Y]. However, there are major unsolved analytic difficulties in their approach. Basically they conjecture that one can carry out an asymptotic analysis similar to the one we carried out above for the figure 8 knot. To prove their conjecture one first has to show how to give an exact (multi-dimensional) contour integral formula for the Jones polynomial of a hyperbolic knot like our (19). A main part consists of choosing a correct (multi-dimensional) contour. Secondly, one has to carry out an asymptotic analysis similar to the one leading to (29). This analysis is relatively simple for the figure 8 knot due to the fact that we have a single (one-dimensional) contour in this case. In general one gets a contour of dimension > 1 and the asymptotic analysis is expected to be harder (as also illustrated by the asymptotic analysis of the double-contour integral expression for the invariant $\bar{\tau}_r(M_{p/q})$ in Lemma 3.2, see next section.)

4.3. **The large r asymptotics of $\tau_r(M_{p/q})$.** In Sect. 5 we will see that the signs of the phases in the asymptotics of $\bar{\tau}_r(M_{p/q}) = \overline{\tau_r(M_{p/q})}$ agrees with the Chern–Simons values, hence we work with this conjugate invariant. Because of (13) we can always obtain the asymptotic expansion of $\tau_r(M_{p/q})$ by complex conjugation or by replacing either p by $-p$ or q by $-q$. By Lemma 3.2 we have

$$\bar{\tau}_r(M_{p/q}) = \beta_1(r) \sum_{n\in\mathbb{Z}/|q|\mathbb{Z}} \int_{C_r^1\times C_r^2} \cot(\pi r x)\tan(\pi r y)\bar{f}_{n,r}(x,y)\mathrm{d}x\mathrm{d}y, \tag{32}$$

where

$$\beta_1(r) = \frac{i\mathrm{sign}(q) r}{4\sqrt{|q|}} e^{\frac{3\pi i}{4}\mathrm{sign}(pq)} \exp\left(-\frac{\pi i}{2r}\left[3\mathrm{sign}(pq) - \frac{p}{q} + \mathrm{S}\left(\frac{p}{q}\right)\right]\right), \tag{33}$$

and

$$\bar{f}_{n,r}(x,y) = \sin\left(\frac{\pi}{q}(x-2nd)\right) e^{2\pi i r\left(-\frac{dn^2}{q} - \frac{p}{4q}x^2 + \frac{n}{q}x - xy\right)} \frac{S_\gamma(-\pi + 2\pi(x-y))}{S_\gamma(-\pi+2\pi(x+y))},$$

where $\gamma = \pi/r$ as usual. Let for $k,l\in\mathbb{Z}$

$$\Omega_{k,l} = \{\ (x,y)\in\mathbb{C}^2 \mid \mathrm{Re}(x)+\mathrm{Re}(y)\in[k,k+1],\quad \mathrm{Re}(x)-\mathrm{Re}(y)\in[-l,-l+1]\ \}.$$

For $(x,y)\in\Omega_{k,l}$, we have by (16) and (21) that

$$\begin{aligned}\bar{f}_{n,r}(x,y) \;\; = \;\; & \sin\left(\frac{\pi}{q}(x-2nd)\right)\left(1+e^{2\pi i(x-y)r}\right)^l\left(1+e^{2\pi i(x+y)r}\right)^k e^{2\pi i r\Phi_n(x,y)} \\ & \times\exp\left(I_\gamma(-\pi+2\pi(x-y+l)) - I_\gamma(-\pi+2\pi(x+y-k))\right),\end{aligned}$$

where

$$\Phi_n(x,y) = -\frac{dn^2}{q} - \frac{p}{4q}x^2 + \frac{n}{q}x - xy + \frac{1}{4\pi^2}\left(\mathrm{Li}_2(e^{2\pi i(x+y)}) - \mathrm{Li}_2(e^{2\pi i(x-y)})\right).$$

We note that Φ_n is well-defined for $(x,y)\in\mathbb{C}^2$ satisfying the condition

$$(\mathrm{Re}(x)+\mathrm{Re}(y)\notin\mathbb{Z}\vee\mathrm{Im}(x)+\mathrm{Im}(y)\geq 0)\wedge(\mathrm{Re}(x)-\mathrm{Re}(y)\notin\mathbb{Z}\vee\mathrm{Im}(x)-\mathrm{Im}(y)\geq 0). \tag{34}$$

Observe that for $k,l\in\{0,1\}$, which corresponds to the four different $\Omega_{k,l}$ intersecting $C_r^1\times C_r^2$, we have that

$$\left(1+e^{2\pi i(x-y)r}\right)^l\left(1+e^{2\pi i(x+y)r}\right)^k = \sum_{(a,b)\in F_{k,l}} e^{2\pi i(a(x-y)+b(x+y))r},$$

where $F_{k,l} = \{(a,b) \in \{0,1\}^2 \mid a \leq k, \quad b \leq l\}$. Hence

$$\begin{aligned}\bar{f}_{n,r}(x,y) &= \sum_{(a,b)\in F_{k,l}} \sin\left(\frac{\pi}{q}(x-2nd)\right) e^{2\pi i r \Phi_n^{a,b}(x,y)} \\ &\quad \times \exp\left(I_\gamma(-\pi+2\pi(x-y+l)) - I_\gamma(-\pi+2\pi(x+y-k))\right),\end{aligned}$$

where

$$\Phi_n^{a,b}(x,y) = a(x-y) + b(x+y) + \Phi_n(x,y). \tag{35}$$

Let

$$\Omega_{k,l}^{\mu,\nu} = \{(x,y) \in \Omega_{k,l} \mid \mu \mathrm{Im}(x) \geq 0, \quad \nu \mathrm{Im}(x) \geq 0\}.$$

Conjecture 4.4. *There exists surfaces $\Sigma_{k,l,a,b}^{\mu,\nu,n} \subset \Omega_{k,l}^{\mu,\nu}$ for $(k,l) \in \{0,1\}^2$, $(a,b) \in F_{k,l}$, $(\mu,\nu) \in \{\pm 1\}^2$ and $n \in \mathbb{Z}/|q|\mathbb{Z}$ such that the leading order asymptotics of the quantum invariant is given by*

$$\begin{aligned}\bar{\tau}_r(M_{p/q}) &\sim_{r\to\infty} -\beta_1(r) \sum_{n\in\mathbb{Z}/|q|\mathbb{Z}} \sum_{(k,l)\in\{0,1\}^2} \sum_{(a,b)\in F_{k,l}} \\ &\quad \times \sum_{(\mu,\nu)\in\{\pm1\}^2} \mu\nu \int_{\Sigma_{k,l,a,b}^{\mu,\nu,n}} \sin\left(\frac{\pi}{q}(x-2nd)\right) e^{2\pi i r \Phi_n^{a,b}(x,y)} \mathrm{d}x\mathrm{d}y.\end{aligned} \tag{36}$$

Moreover, the surfaces $\Sigma_{k,l,a,b}^{\mu,\nu,n} \subset \Omega_{k,l}^{\mu,\nu}$ can be chosen such that they pass through the critical points of $\Phi_n^{a,b}$ with vanishing $\mathrm{Im}(\Phi_n^{a,b})$ which are contained in $\Omega_{k,l}^{\mu,\nu}$. Furthermore, it can be arranged that $\mathrm{Im}(\Phi_n^{a,b}) \leq 0$ along $\Sigma_{k,l,a,b}^{\mu,\nu,n}$ with equality only in the critical points.

The rational behind this conjecture is that we anticipate an analysis of the expression (32) paralleling our analysis of $J_K'(r)$ should be applicable. I.e. tan and cot should be approximated by $\pm\sqrt{-1}$ depending on the signs of $\mathrm{Im}(y)$ and $\mathrm{Im}(x)$ and $\bar{f}_{n,r}(x,y)$ by $\sin\left(\frac{\pi}{q}(x-2nd)\right) e^{2\pi i r \Phi_n^{a,b}(x,y)}$ for some deformation of the part of $C_r^1 \times C_r^2$ which is contained in $\Omega_{k,l}^{\mu,\nu}$. We have partial analytic results supporting this conjecture. Let us now compute the large r asymptotics of the right hand side of (36).

Let

$$I = \int_{\Sigma_{k,l,a,b}^{\mu,\nu,n}} \sin\left(\frac{\pi}{q}(x-2nd)\right) e^{2\pi i r \Phi_n^{a,b}(x,y)} \mathrm{d}x\mathrm{d}y, \tag{37}$$

where $k,l \in \{0,1\}$, $(a,b) \in F_{k,l}$, $\mu,\nu \in \{\pm 1\}$ and $n \in \mathbb{Z}$. By the properties of the surfaces $\Sigma_{k,l,a,b}^{\mu,\nu,n}$ postulated in Conjecture 4.4, the large r asymptotics of I can be calculated by the saddle point method. In order to apply this method, we need to compute the stationary points of $\Phi_n^{a,b}$. To this end, it is more convenient to work with the functions

$$\Psi_n^{a,b}(x,y) = ax + by + \Phi_n(x,y), \tag{38}$$

$a,b,n \in \mathbb{Z}$, so $\Phi_n^{a,b} = \Psi_n^{a+b,a-b}$.

Let $a,b,n \in \mathbb{Z}$ and put $\Psi = \Psi_n^{a,b}$. Let $z = e^{2\pi i x}$ and $w = e^{2\pi i y}$. Then

$$\begin{aligned}2\pi i \frac{\partial \Psi}{\partial x}(x,y) &= 2\pi i(a-y) - \frac{p}{2q} 2\pi i x + \frac{2\pi i n}{q} + \mathrm{Log}(1-zw) - \mathrm{Log}(1-zw^{-1}), \quad (39)\\ 2\pi i \frac{\partial \Psi}{\partial y}(x,y) &= 2\pi i(b-x) + \mathrm{Log}(1-zw) + \mathrm{Log}(1-zw^{-1}),\end{aligned}$$

where we have to assume (which we will also assume in what follows) that $zw, zw^{-1} \neq 1$.

We will need to specify a certain square root of z, namely let $v = e^{\pi i x}$. Then $\frac{\partial\Psi}{\partial x}(x,y) = 0$ implies that

$$v^{-p} = \left(\frac{w - v^2}{1 - v^2 w}\right)^q, \tag{40}$$

and $\frac{\partial\Psi}{\partial y}(x,y) = 0$ implies that

$$(1 - v^2 w)(w - v^2) = v^2 w. \tag{41}$$

Both equations (40) and (41) are independent of a, b, and n. We note that $(v,w) = (0,0)$ is the only solution to (41) with v or w equal to zero. Note, moreover, that (v,w) is a common solution to (40) and (41) if and only if $(\bar{v},\bar{w})$ is a common solution to these two equations. By writing (40) as

$$(-1)^q v^{p+2q} = \left(\frac{1 - v^2 w}{1 - v^{-2} w}\right)^q$$

and (41) as

$$(1 - v^2 w)(1 - v^{-2} w) = -w$$

we see that (v,w) is a nonzero solution to (40) and (41) if and only if (v^{-1},w) is such a solution.

Let us oppositely begin with a common solution $(v,w) \in \mathbb{C}^* \times \mathbb{C}^*$ to (40) and (41), where, as usual, $\mathbb{C}^* = \mathbb{C} \setminus \{0\}$. Write $v = e^{\pi i x}$ and $w = e^{2\pi i y}$ with $\mathrm{Re}(x) \in]-1,1]$ and $\mathrm{Re}(y) \in]-1/2,1/2]$, i.e. $x = \frac{1}{\pi i}\mathrm{Log}(v)$ and $y = \frac{1}{2\pi i}\mathrm{Log}(w)$. One now easily deduce from (41) that there exists a unique $b \in \mathbb{Z}$ such that

$$0 = 2\pi i(b - x) + \mathrm{Log}\left(1 - e^{2\pi i(x+y)}\right) + \mathrm{Log}\left(1 - e^{2\pi i(x-y)}\right), \tag{42}$$

and from (40) we deduce that there exists a unique $n \in \mathbb{Z}$ such that

$$0 = -2\pi i y - \frac{p}{q}\pi i x + \frac{2\pi i n}{q} + \mathrm{Log}\left(1 - e^{2\pi i(x+y)}\right) - \mathrm{Log}\left(1 - e^{2\pi i(x-y)}\right). \tag{43}$$

That is, there exists a unique pair of integers b, n such that (x,y) is a stationary point of $\Psi_n^{0,b}$.

Let us make a slight digression by giving some general remarks about the set of solutions to (41). Assume that $v, w \in \mathbb{C}^*$ and let $z = v^2$. Then (41) can be written in the following two ways

$$z^2 - \left(w + \frac{1}{w} + 1\right) z + 1 = 0, \tag{44}$$

$$w^2 - \left(z + \frac{1}{z} - 1\right) w + 1 = 0.$$

It is straightforward to see that if (z,w) is a solution to (44) with $w \in \mathbb{R}\setminus\{0\}$, then z is real and positive if $w > 0$, z is real and negative if $w \in]-\infty, -(3+\sqrt{5})/2] \cup [-(3-\sqrt{5})/2, 0[$, and $z \in S^1$ if

$$-(3+\sqrt{5})/2 \leq w \leq -(3-\sqrt{5})/2. \tag{45}$$

If (z,w) is a solution to (44) with $z \in \mathbb{R} \setminus \{0\}$, then w is real and negative if $z < 0$, w is real and positive if $z \in]0, (3-\sqrt{5})/2] \cup [(3+\sqrt{5})/2, \infty[$, and $w \in S^1$ if $z \in [(3-\sqrt{5})/2, (3+\sqrt{5})/2]$.

Later on we will be particularly interested in common solutions to (40) and (41) with $v \in S^1$ and $w \in \mathbb{R} \setminus \{0\}$. Assume that (v,w) is such a solution, and write $z = v^2 = e^{i\phi}$, $\phi \in]-\pi,\pi]$. By taking absolute values we get from (40) that $|1 - zw| = |w - z|$ and then from (41) that $|w| = |w-z|^2 = (w-z)(w-\bar{z}) = w^2 - 2\mathrm{Re}(z)w + 1$. If $w < 0$ this equation is equivalent to

$$w^2 + (1 - 2\mathrm{Re}(z))w + 1 = 0. \tag{46}$$

Since $z \in S^1$ we have $1 - 2\mathrm{Re}(z) \in [-1, 3]$ and since w is real we also have $|1 - 2\mathrm{Re}(z)| \geq 2$, so $1 - 2\mathrm{Re}(z) \in [2, 3]$ or equivalently $\phi \in]-\pi, -2\pi/3] \cup [2\pi/3, \pi]$. By (46) we find that

$$w = \cos(\phi) - \frac{1}{2} \pm \sqrt{\cos^2(\phi) - \cos(\phi) - \frac{3}{4}}.$$

If $w > 0$ we have already seen that $z \in]0, \infty[$. But then $z = 1$ so $w^2 - w + 1 = 0$ by (44) contradicting the fact that w is real.

Let us now turn to the second derivative of Ψ in a critical point (x_0, y_0), i.e. the Hessian $H = H(x_0, y_0)$ of Ψ in (x_0, y_0) (which is equal to the Hessian of Φ_n in (x_0, y_0)). Put $(v_0, w_0) = (e^{\pi i x_0}, e^{2\pi i y_0})$ and $z_0 = v_0^2$. By a small computation, using the fact that (v_0, w_0) is a solution to (41), we find that

$$\begin{aligned} H_{11} &= \frac{\partial^2 \Psi}{\partial x^2}(x_0, y_0) = \frac{1}{w_0} - w_0 - \frac{p}{2q}, \qquad (47)\\ H_{12} = H_{21} &= \frac{\partial^2 \Psi}{\partial x \partial y}(x_0, y_0) = z_0 - \frac{1}{z_0}, \\ H_{22} &= \frac{\partial^2 \Psi}{\partial y^2}(x_0, y_0) = \frac{1}{w_0} - w_0. \end{aligned}$$

Let us examine non-degeneracy of the critical point (x_0, y_0). We are particularly interested in critical points where $w_0 < 0$ and $z_0 \in S^1$. Writing $z_0 = e^{i\phi}$ so $z_0 - 1/z_0 = 2i\sin(\phi)$ we get

$$\det(H) = \left(\frac{1 - w_0^2}{w_0} - \frac{p}{2q}\right)\left(\frac{1 - w_0^2}{w_0}\right) + 4\sin^2(\phi). \tag{48}$$

We see immediately from this that if $w_0 \in]-1, 0[$ and $p/q \geq 0$ then $\det(H) > 0$. If $w_0 \in]-\infty, -1[$ and $p/q \leq 0$ then we also have $\det(H) > 0$. In connection to (46) we found that $\phi \in]-\pi, -2\pi/3] \cup [2\pi/3, \pi]$. If $w_0 = -1$ we see that $\det(H) > 0$ except if $\phi = \pi$, but $\phi = \pi$ is excluded by (46) since $w_0 = -1$. For any critical point we have

$$\det(H) = \left(w_0 + \frac{1}{w_0}\right)^2 - \left(z_0 + \frac{1}{z_0}\right)^2 + \frac{p}{2q}\left(w_0 - \frac{1}{w_0}\right).$$

By (44) we have $w_0 + \frac{1}{w_0} = z_0 + \frac{1}{z_0} - 1$ so

$$\det(H) = 1 - 2\left(z_0 + \frac{1}{z_0}\right) + \frac{p}{2q}\left(w_0 - \frac{1}{w_0}\right).$$

Now assume again that $w_0 < 0$ and $z_0 \in S^1$. Let $a = 1 - 2\mathrm{Re}(z_0) \in [2, 3]$ and get from (46) that $2w_0 = -a \pm \sqrt{a^2 - 4}$. In particular, we have $2/w_0 = -a \mp \sqrt{a^2 - 4}$ and therefore $w_0 - 1/w_0 = \pm\sqrt{a^2 - 4}$. But then

$$\det(H) = 2a - 1 \pm \frac{p}{2q}\sqrt{a^2 - 4}.$$

We see that $\det(H) = 0$ implies that

$$\left(4 - \frac{p^2}{4q^2}\right)a^2 - 4a + \left(1 + \frac{p^2}{q^2}\right) = 0.$$

If $4-p^2/(4q^2)=0$ or equivalently $|p/q|=4$ then $a=17/4>4$ which contradicts the fact that $a\leq 3$. Assume therefore that $|p/q|\neq 4$ and get that

$$a=\frac{4\pm\left|\frac{p}{q}\right|\sqrt{\frac{p^2}{q^2}-15}}{2\left(4-\frac{p^2}{4q^2}\right)}. \tag{49}$$

Since a is real we immediately conclude that $|p/q|\geq\sqrt{15}$. Assume that $|p/q|\in[\sqrt{15},4[$. Then (49) together with $a\in[2,3]$ leads to the condition

$$12-\frac{p^2}{q^2}\leq\pm\left|\frac{p}{q}\right|\sqrt{\left(\frac{p^2}{q^2}-15\right)}\leq 20-\frac{3p^2}{2q^2}.$$

Since $20-\frac{3p^2}{2q^2}$ is negative, we necessarily have a minus in front of $\left|\frac{p}{q}\right|\sqrt{\frac{p^2}{q^2}-15}$. Moreover, $-\left|\frac{p}{q}\right|\sqrt{\left(\frac{p^2}{q^2}-15\right)}\leq 20-\frac{3p^2}{2q^2}$ implies that

$$\frac{5}{4}\left(\frac{p}{q}\right)^4-45\left(\frac{p}{q}\right)^2+400\leq 0,$$

which forces $p^2/q^2\in[16,20]$ giving a contradiction.

Next assume that $|p/q|>4$. Then (49) together with $a\in[2,3]$ leads to the condition

$$12-\frac{p^2}{q^2}\geq\pm\left|\frac{p}{q}\right|\sqrt{\left(\frac{p^2}{q^2}-15\right)}\geq 20-\frac{3p^2}{2q^2}.$$

Since $12-\frac{p^2}{q^2}$ is negative, we necessarily have a minus in front of $\left|\frac{p}{q}\right|\sqrt{\left(\frac{p^2}{q^2}-15\right)}$. Moreover, $-\left|\frac{p}{q}\right|\sqrt{\left(\frac{p^2}{q^2}-15\right)}\geq 20-\frac{3p^2}{2q^2}$ implies that

$$\frac{5}{4}\left(\frac{p}{q}\right)^4-45\left(\frac{p}{q}\right)^2+400\geq 0,$$

which forces $p^2/q^2\leq 16$ or $p^2/q^2\geq 20$. Therefore $|p/q|\geq\sqrt{20}$. We have thus shown that if $|p/q|<\sqrt{20}$ then (x_0,y_0) is non-degenerate.

By the above we have

$$a=2\frac{\left|\frac{p}{q}\right|\sqrt{\left(\frac{p^2}{q^2}-15\right)}-4}{\frac{p^2}{q^2}-16} \tag{50}$$

for $|p/q|\geq\sqrt{20}$, if (x_0,y_0) is degenerate. Assuming that (x_0,y_0) is degenerate (so $|p/q|\geq\sqrt{20}$) we conclude that the only other solutions $(z,w)\in S^1\times]-\infty,0[$ to (46) satisfying that $1-2\mathrm{Re}(z)$ is equal to the right-hand side of (50) are $(z_0,1/w_0)$, $(\bar{z}_0,w_0)$ and $(\bar{z}_0,1/w_0)$. By the remarks following (48) we get that among these three points only the point $(\bar{z}_0,w_0)$ can actually satisfy, that the right-hand side of (48) is zero. We expect, that these arguments can be carried futher to show that all critical points are non-degenerate also in the case $|p/q|\geq\sqrt{20}$.

Let $\alpha,\beta\in S^1$ and let $\gamma_\alpha,\gamma_\beta: I_\delta\to\mathbb{C}$ be given by $\gamma_\alpha(s)=x_0+\alpha s$, $\gamma_\beta(s)=y_0+\beta s$, where $I_\delta=[-\delta,\delta]$ for a sufficiently small $\delta>0$. The main contributiton to the integral I in (37) in the large r limit can as stated below (37) be calculated using the saddle point method. This implies that the main contributions to I comes from integrating along the surface $\Sigma = \Sigma_{k,l,a,b}^{\mu,\nu,n}$ in small neighborhoods of the critical points on this surface. (One has also to consider boundary contributions. Except if there are saddle points on the boundary of Σ, these boundary contributions will, however, not contribute to the leading asymptotics. Saddle points on the boundary give contributions with the same growth rate in r as saddle points in the interior.) We are therefore lead to consider an integral of the form

$$\begin{aligned} K(x_0, y_0) &= \int_{\gamma_\alpha} \left(\int_{\gamma_\beta} \sin\left(\frac{\pi}{q}(x - 2nd)\right) e^{2\pi i r \Psi(x,y)} \mathrm{d}y \right) \mathrm{d}x \\ &= \alpha\beta \int_{-\delta}^{\delta} \left(\int_{-\delta}^{\delta} \sin\left(\frac{\pi}{q}(x_0 + \alpha s - 2nd)\right) e^{2\pi i r \Phi(x_0+\alpha s, y_0+\beta t)} \mathrm{d}t \right) \mathrm{d}s, \end{aligned}$$

where $\Psi = \Psi_n^{a,b}$ as above. (If (x_0, y_0) is a non-degenerate critical point on the boundary of Σ, then one or both or the integrals $\int_{-\delta}^{\delta}$ should be replaced by $\int_0^{\delta}$ (or $\int_{-\delta}^{0}$) and the contribution coming from that point in Corollary 4.5 should be multiplied by $\frac{1}{2}$ or $\frac{1}{4}$.) By a Taylor expansion we find that

$$\Psi(x_0 + \alpha s, y_0 + \beta t) = \Psi(x_0, y_0) + \frac{1}{2}\langle A \begin{pmatrix} s \\ t \end{pmatrix}, \begin{pmatrix} s \\ t \end{pmatrix} \rangle + h(s,t),$$

where

$$A = \mathrm{diag}(\alpha, \beta) H \mathrm{diag}(\alpha, \beta),$$

and

$$\langle \begin{pmatrix} x_1 \\ y_1 \end{pmatrix}, \begin{pmatrix} x_2 \\ y_2 \end{pmatrix} \rangle = x_1 x_2 + y_1 y_2$$

for $(x_1, y_1), (x_2, y_2) \in \mathbb{C}^2$, and where $h(s,t)$ is a remainder term being a sum of terms of the form $c_{n,m} s^n t^n$, $n, m \in \{0, 1, 2, \ldots, ...\}$, $n + m \geq 3$, $c_{n,m} \in \mathbb{C}$. We note that x_0 is a saddle point of the function $x \mapsto \Psi(x, y_0)$ and y_0 is a saddle point of the function $y \mapsto \Psi(x_0, y)$. We search for α and β such that there exists a $\delta > 0$ satisfying

$$\mathrm{Re}\left(2\pi i(\Psi(x_0 + \alpha s, y_0 + \beta t) - \Psi(x_0, y_0))\right) < 0 \tag{51}$$

for all $(s,t) \in I_\delta \times I_\delta \setminus \{(0,0)\}$. This amounts to finding α and β such that

$$\mathrm{Im}\left(\langle A \begin{pmatrix} s \\ t \end{pmatrix}, \begin{pmatrix} s \\ t \end{pmatrix} \rangle \right) > 0$$

for all $(s,t) \in \mathbb{R}^2 \setminus \{(0,0)\}$. Since

$$\mathrm{Im}\left(\langle A \begin{pmatrix} s \\ t \end{pmatrix}, \begin{pmatrix} s \\ t \end{pmatrix} \rangle \right) = \langle \mathrm{Im}(A) \begin{pmatrix} s \\ t \end{pmatrix}, \begin{pmatrix} s \\ t \end{pmatrix} \rangle$$

this corresponds to finding α and β such that $\mathrm{Im}(A)$ is positive definite. A main part of the process of finding surfaces $\Sigma_{k,l,a,b}^{\mu,\nu,n}$ as in Conjecture 4.4 consists of finding such α and β.

Since A is symmetric we have $\mathrm{Im}(A)_{ij} = \mathrm{Im}(A_{ij})$. Here $A_{11} = \alpha^2 H_{11}$, $A_{22} = \beta^2 H_{22}$, $A_{21} = A_{12} = \alpha\beta H_{12}$, where H is the Hessian in (47). Let us consider a general case. Therefore, let $M = \begin{pmatrix} a & c \\ c & b \end{pmatrix}$ be a real symmetric matrix. Then M has real eigenvalues, and M is positive definite if and only if both of these eigenvalues are positive, i.e. if and only if a and b are both positive and $ab > c^2$. Now assume that $M = \mathrm{Im}(A)$ and that

$z_0 \in S^1$ while $w_0 \in]-\infty, 0[$. Then H_{11} and H_{22} are real and $H_{12} = H_{21}$ is purely imaginary. If we write $\alpha = e^{i\phi}$, $\beta = e^{i\psi}$, $\phi, \psi \in]-\pi, \pi]$ we have

$$\begin{aligned} a &= \operatorname{Im}(\alpha^2 H_{11}) = \sin(2\phi) H_{11}, \\ b &= \operatorname{Im}(\beta^2 H_{22}) = \sin(2\psi) H_{22}, \\ c &= \operatorname{Im}(\alpha\beta H_{12}) = \cos(\phi + \psi) C, \end{aligned}$$

where $H_{12} = iC$, $C \in \mathbb{R}$. We see that the inequality $ab > c^2$ is equivalent to

$$\cos^2(\phi + \psi) < \sin(2\phi)\sin(2\psi)\frac{H_{11}H_{22}}{C^2}. \tag{52}$$

There are four cases to consider depending on the signs of H_{11} and H_{22}. If H_{11} and H_{22} are both negative then a and b are positive if and only if $\phi, \psi \in]-\pi/2, 0[\cup]\pi/2, \pi[$. In particularly M is positive definite if we put $\phi = \psi = -\pi/4$. If H_{11} and H_{22} are both positive, then a and b are positive if and only if $\phi, \psi \in]-\pi, -\pi/2[\cup]0, \pi/2[$. In particular we can let $\phi = \psi = \pi/4$ in which case (52) is obviously satisfied. Let us finally consider the case $H_{11} > 0$, $H_{22} < 0$ (the case $H_{11} < 0$, $H_{22} > 0$ is handled the same way). Then a and b are positive if and only if $\phi \in]-\pi, -\pi/2[\cup]0, \pi/2[$ and $\psi \in]-\pi/2, 0[\cup]\pi/2, \pi[$. If $-H_{11}H_{22}/C^2 > 1$ we can simply let $\psi = \phi + \pi/2$. The case $0 < -H_{11}H_{22}/C^2 \leq 1$ (or equivalently $\det(H) \geq 0$) is more difficult. We expect that either this case can be avoided or else one can find steepest descend directions also in that case.

If α and β are chosen so that $\operatorname{Im}(A)$ is positive definite, then the main contribution to the integral $K(x_0, y_0)$ in the limit of large r is given by

$$K_{\text{main}}(x_0, y_0) = \alpha\beta \sin\left(\frac{\pi}{q}(x_0 - 2nd)\right) e^{2\pi i r \Psi(x_0, y_0)} \int_{\mathbb{R}^2} e^{\pi i r \langle A \begin{pmatrix} s \\ t \end{pmatrix}, \begin{pmatrix} s \\ t \end{pmatrix} \rangle} \mathrm{d}s\mathrm{d}t,$$

and this integral can be evaluated using the results of [H, Sect. 3.4]. In fact,

$$\int_{\mathbb{R}^2} e^{\pi i r \langle A \begin{pmatrix} s \\ t \end{pmatrix}, \begin{pmatrix} s \\ t \end{pmatrix} \rangle} \mathrm{d}s\mathrm{d}t = \frac{1}{r}\left(\det(-iA)\right)^{-1/2},$$

where A is independent of r. Note here that the set S of complex symmetric 2×2–matrices B with $\operatorname{Re}(B)$ positive definite is an open convex set in the 3–dimensional complex vector space of symmetric 2×2–matrices. It follow that their is a unique analytic branch of $B \mapsto (\det(B))^{1/2}$ on S such that $(\det(B))^{1/2} > 0$ for B real. We have used that branch in the above result. In conclusion we can state the following corollary to Conjecture 4.4.

Corollary 4.5. *Assume that each of the surfaces $\Sigma = \Sigma^{\mu,\nu,n}_{k,l,a,b}$ follows the (2-dimensional) directions of steepest descend in the critical points of $\Psi = \Phi^{a,b}_n$ contained in Σ, i.e. (51) is satisfied in each of these critical points, and $\{(x_0 + \alpha s, y_0 + \beta t) \mid (s,t) \in I_\delta \times I_\delta\} \subseteq \Sigma$. Then the leading order asymptotics of the quantum invariant is given by*

$$\begin{aligned} \bar{\tau}_r(M_{p/q}) \quad \sim_{r\to\infty} \quad & -\frac{\beta_1(r)}{r} \sum_{n \in \mathbb{Z}/|q|\mathbb{Z}} \sum_{(k,l)\in\{0,1\}^2} \sum_{(a,b)\in F_{k,l}} \\ & \times \sum_{(\mu,\nu)\in\{\pm 1\}^2} \mu\nu \sum_{(x,y)\in C^{\mu,\nu,n}_{k,l,a,b}} \alpha(x,y)\beta(x,y)\left(\det(-iA(x,y))\right)^{-1/2} \\ & \times \sin\left(\frac{\pi}{q}(x - 2nd)\right) e^{2\pi i r \Phi^{a,b}_n(x,y)}, \end{aligned}$$

where $C^{\mu,\nu,n}_{k,l,a,b}$ is the set of non-degenerate critical points of $\Phi^{a,b}_n$ in $\Sigma^{\mu,\nu,n}_{k,l,a,b}$, and where $\alpha(x,y)$, $\beta(x,y)$ and $A(x,y)$ are as α, β and A above with $(x_0,y_0)=(x,y)$.

We note that the factor

$$\alpha(x,y)\beta(x,y)\left(\det(-iA(x,y))\right)^{-1/2}$$

is independent of r. Moreover, the leading term in the large r asymptotics of

$$\frac{\beta_1(r)}{r} = \frac{i\mathrm{sign}(q)}{4\sqrt{|q|}} e^{\frac{3\pi i}{4}\mathrm{sign}(pq)} \exp\left(-\frac{\pi i}{2r}\left[3\mathrm{sign}(pq) - \frac{p}{q} + \mathrm{S}\left(\frac{p}{q}\right)\right]\right)$$

is $\frac{i\mathrm{sign}(q)}{4\sqrt{|q|}} e^{\frac{3\pi i}{4}\mathrm{sign}(pq)}$. This implies, that the growth rate of the quantum invariants of $M_{p/q}$ is r^0. This is in agreement with our computer studies of the quantum invariants of $M_{p/q}$. The above corrollary gives a leading asymptotics as predicted by the AEC if we can prove that the union of the sets of critical points $C^{\mu,\nu,n}_{k,l,a,b}$ corresponds to the flat (irreducible) SU(2)–connections on $M_{p/q}$ and if we can prove that the values of the relevant phase functions $\Phi^{a,b}_n$ in these critical points are equal to the Chern–Simons invariants of these flat connections. This we will do in section 5.3.

In Sect. 5 we will show that the moduli space of irreducible flat SU(2)–connections on $M_{p/q}$ is a discrete finite set for all $p/q \in \mathbb{Q}$. Moreover, the set of reducible flat SU(2)–connections on $M_{p/q}$ is discrete, hence finite, if $p/q \in \mathbb{Q}\setminus\{0\}$ and is a closed interval for $p/q = 0$. According to the growth rate conjecture for the quantum invariants, i.e. Conjecture 1.2 (together with Conjecture 1.1), the growth rate of $\tau_r(M_{p/q})$ should therefore be r^0. Moreover, the reducible connections should only contribute to the leading asymptotics if $p/q = 0$. By the results in Appendix C, we see that the reducible connections in fact do give a contribution to the leading asymptotics in case $p/q = 0$.

5. Classical Chern–Simons theory on $M_{p/q}$

In this section we will describe the classical theory, that is the classical Chern–Simons theory on the manifolds $M_{p/q}$. The SU(2) Chern–Simons functional is a map with values in $\mathbb{R}/\mathbb{Z}$ defined on the set $\mathcal{A}$ of gauge equivalence classes of connections in a principal SU(2) bundle on $M_{p/q}$ (all such bundles being trivializable). Inside $\mathcal{A}$ sits the moduli space $\mathcal{M}_{p/q}$ of flat SU(2)–connections on $M_{p/q}$, that is the set of classical solutions to the SU(2) Chern–Simons field theory. Recall that

$$\mathcal{M}_{p/q} = \mathrm{Hom}(\pi_1(M_{p/q}), \mathrm{SU}(2))/\mathrm{SU}(2)$$

from which it is clear that $\mathcal{M}_{p/q}$ is a compact space. The Chern–Simons functional is constant on the connected components of $\mathcal{M}_{p/q}$, thus there are only finitely many different values on flat connections. Let $\mathcal{M}'_{p/q}$ be the subset of $\mathcal{M}_{p/q}$ consisting of nonabelian representations. Recall that these representations correspond to the irreducible connections, while the abelian representations correspond to the reducible connections.

The main results in this section are Theorem 5.8 and Theorem 5.9 which ties up the Chern–Simons theory to the large r asymptotics of $\bar{\tau}_r(M_{p/q})$ by showing that a certain subset of the critical points of the phase functions $\Phi^{a,b}_n$ are in bijection with $\mathcal{M}'_{p/q}$. Under this bijection, the Chern–Simons functional is taken to the phase functions $\Phi^{a,b}_n$.

We begin by giving a description of $\mathcal{M}_{p/q}$ following Riley [R1], [R2] and Kirk & Klassen [KK].

5.1. **The moduli space of flat $\mathrm{SU}(2)$–connections on $M_{p/q}$.** In the following $\pi = \pi_1\left(S^3 \setminus \mathrm{nbd}(K)\right)$ denotes the knot group of the figure 8 knot. We have a presentation

$$\pi = \langle\, x, y \,|\, wx = yw \,\rangle, \tag{53}$$

where $w = [x^{-1}, y]$, and where $\mu = x$ and $\lambda = yx^{-1}y^{-1}x^2y^{-1}x^{-1}y$ are the elements of π corresponding to the meridian and the preferred longitude of K. The $\mathrm{SL}(2,\mathbb{C})$ representation variety of π was analyzed by Riley [R1], [R2] relevant to our work. Consider a group G given by a presentation

$$G = \langle\, x, y \,|\, wx = yw \,\rangle,$$

where $w = x^{\varepsilon_1}y^{\varepsilon_2}x^{\varepsilon_3}\cdots y^{\varepsilon_{\alpha-1}}$, where α is odd and $\varepsilon_j = \varepsilon_{\alpha-j} = \pm 1$, $j = 1, 2, \ldots, \alpha - 1$. Such groups are denoted 2–bridge kmot groups by Riley since they generalize the 2–bridge knot groups. Following Riley we say that a representation $\psi : G \to \mathrm{SL}(2,\mathbb{C})$ is affine when the image of ψ fixes exactly one point in $\mathbb{CP}^1$ and not affine when this image has no fixed points. We note that if ψ is nonabelian then ψ is affine if and only if $\psi(x)$ and $\psi(y)$ have a common eigenvector, and ψ is not affine if these two matrices have no common eigenvector. Let H be some subgroup of $\mathrm{SL}(2,\mathbb{C})$. Then we will say that two representations $\psi_1, \psi_2 : G \to \mathrm{SL}(2,\mathbb{C})$ are H–equivalent if they are conjugate to each other by a matrix in H, i.e. if there exists a matrix $U \in H$ such that $\psi_2(\gamma) = U\psi_1(\gamma)U^{-1}$ for all $\gamma \in G$. In particular, we will say that ψ_1 and ψ_2 are equivalent if they are $\mathrm{SL}(2,\mathbb{C})$–equivalent. For $(t, u) \in \mathbb{C}^* \times \mathbb{C}$ we put

$$\begin{aligned}
C_0(t) &= \begin{pmatrix} t & 1 \\ 0 & 1 \end{pmatrix}, \quad D_0(t,u) = \begin{pmatrix} t & 0 \\ -tu & 1 \end{pmatrix}, \\
C_1(t) &= \begin{pmatrix} t & 1 \\ 0 & t^{-1} \end{pmatrix}, \quad D_1(t,u) = \begin{pmatrix} t & 0 \\ -u & t^{-1} \end{pmatrix}, \\
C_2(t) &= \begin{pmatrix} t & t^{-1} \\ 0 & t^{-1} \end{pmatrix}, \quad D_2(t,u) = \begin{pmatrix} t & 0 \\ -tu & t^{-1} \end{pmatrix}.
\end{aligned}$$

We note that $C_\nu(t)$ and $D_\nu(t,u)$ are elements of $\mathrm{SL}(2,\mathbb{C})$, $\nu = 1, 2$. If s is a square root of t and $V(s) = \mathrm{diag}(s, s^{-1})$ then

$$V(s)C_2(t)V(s)^{-1} = C_1(t), \quad V(s)D_2(t,u)V(s)^{-1} = D_1(t,u), \tag{54}$$

and

$$C_0(t) = sC_2(s), \quad D_0(t,u) = sD_2(s,u). \tag{55}$$

Let $W_\nu(t,u)$ denote the matrix obtained by replacing x and y by respectively $C_\nu(t)$ and $D_\nu(t,u)$ in the expression for w, and let

$$\phi(t,u) = W_{11} + (1-t)W_{12},$$

where $W = W(t,u) = W_0(t,u)$. We let $\rho_{(t,u)}$ be the assignment $x \mapsto C_2(t)$, $y \mapsto D_2(t,u)$. We have the following $\mathrm{SL}(2,\mathbb{C})$ version of [R1, Theorem 1].

Theorem 5.1. *Let $(s,u) \in \mathbb{C}^* \times \mathbb{C}$. None of the assignments $\rho_{(s,u)}$ extend to an abelian $\mathrm{SL}(2,\mathbb{C})$–representation of G. The assignment $\rho_{(s,u)}$ extends to a nonabelian representation $\rho_{(s,u)} : G \to \mathrm{SL}(2,\mathbb{C})$ if and only if*

$$\phi(s^2, u) = 0. \tag{56}$$

Conversely, if $\psi : G \to \mathrm{SL}(2,\mathbb{C})$ is a nonabelian representation, then there exists a pair $(s,u) \in \mathbb{C}^* \times \mathbb{C}$ satisfying (56) such that ψ and $\rho_{(s,u)}$ are equivalent. When ψ is affine this pair is unique, and when ψ is not affine the pair (s,u) can only be replaced by (s^{-1}, u).

Proof. The theorem follows by results of [R1], [R2]. The assignment $\rho_{(s,u)}$ extends to a $\mathrm{SL}(2,\mathbb{C})$–representation of G if and only if $W_2(s,u)C_2(s,u) = D_2(s,u)W_2(s,u)$. The matrices $C_2(s)$ and $D_2(s,u)$ commute if and only if $s = \pm 1$ and $u = 0$, and since $C_2(\pm 1) = \pm C_2(1)$ is different from $D_2(\pm 1, 0) = \pm D_2(1,0)$ we have that the assignment $\rho_{(\pm 1,0)}$ does not extend to a $\mathrm{SL}(2,\mathbb{C})$–representation of G. (We note that if $W = W(1,0)$ then $W_{21} = 0$ since the matices $C_0(1), D_0(1,0) = I$ and there inverses are upper triangular. But we also have that $\phi(1,0) = 0$ would imply that $W_{11} = 0$ contradicting the fact that W is invertible. Therefore $\phi(1,0) \neq 0$.)

Let $\sigma = \sum_{j=1}^{\alpha-1} \varepsilon_j$. Then $s^\sigma W_2(s,u) = W(s^2,u)$. By (the proof of) [R1, Theorem 1] we have $W(s^2,u)C_0(s^2) = D_0(s^2,u)W(s^2,u)$ if and only if $\phi(s^2,u) = 0$, so by (55) we find that $\rho_{(s,u)}$ extends to a (necessarily nonabelian) $\mathrm{SL}(2,\mathbb{C})$–representation of G if and only if $\phi(s^2,u) = 0$.

If $\psi : G \to \mathrm{SL}(2,\mathbb{C})$ is an arbitrary nonabelian representation it follows by [R2, Lemma 7] and (54) that there exists a pair $(s,u) \in \mathbb{C}^* \times \mathbb{C}$ (necessarily satisfying (56)) such that ψ and $\rho_{(s,u)}$ are equivalent. By the above any such pair is different from $(\pm 1, 0)$ and by [R2, Lemma 8] and (54) we then get the final statement of the theorem. □

If $(s,u) \in \mathbb{C}^* \times \mathbb{C}$ with $\phi(s^2,u) = 0$ then $\rho_{(s,u)}$ is affine if and only if $C_2(s)$ and $D_2(s,u)$ have a common eigenvector. But this happens exactly when $u = 0$ or $u = (s - s^{-1})^2$.

Let us now restrict to the case where G is the figure 8 knot group π. Then

$$\phi(t,u) = u^2 + \left(3 - (t + t^{-1})\right)(u+1) \tag{57}$$

so in particular $\phi(s^2,0) = 3 - s^2 - s^{-2} = 0$ if and only if $s^4 - 3s^2 + 1 = 0$ i.e. if and only if $s = \mu_1\sqrt{(3+\mu_2\sqrt{5})/2}$ for some $\mu_1, \mu_2 \in \{\pm 1\}$. If $u = (s - s^{-1})^2 = s^2 + s^{-2} - 2$ then $\phi(s^2,u) = u^2 + (3 - u - 2)(u+1) = u^2 + 1 - u^2 = 1$, so we conclude that $\rho_{(s,u)}$ is affine if and only if $u = 0$ and $s^4 - 3s^2 + 1 = 0$. Let

$$\mathcal{N} = \mathrm{Hom}(\pi, \mathrm{SL}(2,\mathbb{C}))/\mathrm{SL}(2,\mathbb{C}) \tag{58}$$

be the space of conjugacy classes of $\mathrm{SL}(2,\mathbb{C})$–representations of π and let $\mathcal{N}_{\mathrm{nab}}$ be the subset consisting of classes represented by nonabelian $\mathrm{SL}(2,\mathbb{C})$–representations. Moreover, let

$$\tilde{\mathcal{N}} = \{\, (s,u) \in \mathbb{C}^* \times \mathbb{C} \mid \phi(s^2,u) = 0 \,\}, \tag{59}$$

and let $\Phi : \tilde{\mathcal{N}} \to \mathcal{N}$ be the map which maps (s,u) to the class represented by $\rho_{(s,u)}$. We have shown

Corollary 5.2. *The image of Φ is $\mathcal{N}_{\mathrm{nab}}$. If we let*

$$\tilde{\mathcal{N}}_0 = \{\, (\mu_1\sqrt{(3+\mu_2\sqrt{5})/2}, 0) \mid \mu_1, \mu_2 \in \{\pm 1\} \,\}$$

then $\Phi|_{\tilde{\mathcal{N}}_0} : \tilde{\mathcal{N}}_0 \to \mathcal{N}$ is injective and $\Phi^{-1}(\Phi(s,u)) = \{(s,u), (s^{-1},u)\}$ for any $(s,u) \in \tilde{\mathcal{N}} \setminus \tilde{\mathcal{N}}_0$. □

Recall that $M_{p/q}$ denotes the closed oriented 3–manifold obtained by surgery on S^3 along the figure 8 knot with rational surgery coefficient p/q. The representation $\rho_{(s,u)}$, $(s,u) \in \tilde{\mathcal{N}}$, extends to a $\mathrm{SL}(2,\mathbb{C})$–representation of $\pi_1(M_{p/q})$ if and only if

$$\rho_{(s,u)}(\mu)^p \rho_{(s,u)}(\lambda)^q = 1.$$

To analyse this criterion it is an advantage to diagonalize $\rho_{(s,u)}(\lambda)$. Assume in the following that $(s,u) \in \tilde{\mathcal{N}}$. By a rather long but completely elementary and straightforward calculation we find that

$$\rho_{(s,u)}(\lambda) = \begin{pmatrix} \lambda_{11}(s,u) & \lambda_{12}(s,u) \\ 0 & \lambda_{11}(s^{-1},u) \end{pmatrix},$$

where

$$\lambda_{11}(s,u) = -1 + s^{-2} - 2s^2 + s^4 + u(s^{-2} - s^2)$$

and $\lambda_{12}(s,u) = 2u(1-u)$ if $s^2 = 1$ and

$$\lambda_{12}(s,u) = \frac{\lambda_{11}(s,u) - \lambda_{11}(s^{-1},u)}{s^2 - 1}$$

for $s^2 \neq 1$. We note that $\lambda_{11}(s^{-1},u) = \lambda_{11}(s,u)^{-1}$.

In general, if $A = \begin{pmatrix} \alpha & \beta \\ 0 & \alpha^{-1} \end{pmatrix} \in \mathrm{SL}(2,\mathbb{C})$, then A can be diagonalized if and only if A is not parabolic, i.e. if and only if $\mathrm{tr}(A) \neq \pm 2$ or equivalently if and only if $\alpha \neq \pm 1$ (except, of course, if $\beta = 0$). If $\alpha \neq \pm 1$ then $(1,0)$ is an eigenvector with eigenvalue α and $(-\beta/(\alpha - \alpha^{-1}), 1)$ is an eigenvector with eigenvalue α^{-1}. If $s^2 = 1$ then $\lambda_{11}(s,u) = -1$ and $\lambda_{12}(s,u) = \pm i2\sqrt{3}$. If $s^2 \neq 1$ then $\lambda_{11}(s,u) = \pm 1$ if and only if $\lambda_{12}(s,u) = 0$. Therefore $\rho_{(s,u)}(\lambda)$ is diagonalizable (or diagonal) if and only if $s^2 \neq 1$. In case $s^2 \neq 1$ and $\lambda_{12}(s,u) \neq 0$ we have

$$\frac{\lambda_{12}(s,u)}{\lambda_{11}(s,u) - \lambda_{11}(s,u)^{-1}} = \frac{1}{s^2 - 1} = \frac{s^{-1}}{s - s^{-1}}.$$

We conclude that if $s^2 \neq 1$, then $\mathbb{C}^2$ has a basis consisting of a set of common eigenvectors for the matrices $\rho_{(s,u)}(\mu)$ and $\rho_{(s,u)}(\lambda)$, namely $u_1 = (1,0)$ and $u_2 = (-1/(s^2-1), 1)$. If we let $\tilde{\rho}_{(s,u)} : \pi \to \mathrm{SL}(2,\mathbb{C})$ be the representation $\tilde{\rho}_{(s,u)}(\gamma) = U^{-1}\rho_{(s,u)}(\gamma)U$, where $U \in \mathrm{SL}(2,\mathbb{C})$ with jth column u_j, we therefore have

$$\tilde{\rho}_{(s,u)}(x) = \mathrm{diag}\left(s, s^{-1}\right), \qquad \tilde{\rho}_{(s,u)}(\lambda) = \mathrm{diag}\left(\lambda_{11}(s,u), \lambda_{11}(s,u)^{-1}\right). \tag{60}$$

In particular, $\rho_{(s,u)} : \pi \to \mathrm{SL}(2,\mathbb{C})$, $s^2 \neq 1$, extends to a representation of $\pi_1(M_{p/q})$ if and only if

$$s^{-p} = \lambda_{11}(s,u)^q. \tag{61}$$

Recall here that $\rho_{(s,u)}$ and $\rho_{(s^{-1},u)}$ are equivalent for $(s,u) \in \tilde{\mathcal{N}} \setminus \tilde{\mathcal{N}}_0$, cf. Corollary 5.2. But as noted above $\lambda_{11}(s^{-1},u) = \lambda_{11}(s,u)^{-1}$ in accordance with (61). For $(s,u) \in \tilde{\mathcal{N}}_0$ we have $\lambda_{11}(s,u) = 1$ and $|s| \neq 1$, so $\rho_{(s,u)}$ extends to a representation of $\pi_1(M_{p/q})$ if and only if $p = 0$.

A direct check shows that if $s^2 = 1$ then $\rho_{(s,u)}$ does not extend to a representation of $\pi_1(M_{p/q})$ for any rational number p/q. In fact, if $s = \pm 1$, then

$$\rho_{(s,u)}(\mu)^p = (\pm 1)^{|p|} \begin{pmatrix} 1 & p \\ 0 & 1 \end{pmatrix}$$

and

$$\rho_{(s,u)}(\lambda)^q = \left(- \begin{pmatrix} 1 & \varepsilon i2\sqrt{3} \\ 0 & 1 \end{pmatrix} \right)^q = (-1)^{|q|} \begin{pmatrix} 1 & \varepsilon i2q\sqrt{3} \\ 0 & 1 \end{pmatrix}$$

for a $\varepsilon \in \{-1,1\}$. On the other hand, since $\lambda_{11}(s,u) = -1$, we have that (61) is satisfied if $s = 1$ and q is even or $s = -1$ and both p and q are odd. For the following we note that if $s^2 = 1$ then $u^2 + u + 1 = \phi(1,u) = 0$ so u is not real.

We are mostly interested in the SU(2)–representations of π. Let in the following $\mathcal{M}_{\mathrm{nab}}$ be the set of conjugacy classes of nonabelian SU(2)–representations of π.

Proposition 5.3. *Let $(s,u) \in \tilde{\mathcal{N}}$. The representation $\rho_{(s,u)} : \pi \to \mathrm{SL}(2,\mathbb{C})$ is $\mathrm{SL}(2,\mathbb{C})$–equivalent to a representation $\pi \to \mathrm{SU}(2)$ if and only if $|s| = 1$ and u is real. If we write $s = e^{2\pi i\theta}$, $\theta \in]-1/2,1/2]$, then $u \in \{u_\pm\}$, where $u_\pm = u_\pm(\theta)$ are the two solutions to $\phi(e^{4\pi i\theta}, u) = 0$, i.e.*

$$u_\pm(\theta) = \cos(4\pi\theta) - \frac{3}{2} \pm \sqrt{\cos^2(4\pi\theta) - \cos(4\pi\theta) - \frac{3}{4}}.$$

Since u is real we have $\theta \in [-1/3,-1/6] \cup [1/6,1/3]$.
The representation $\rho_{(e^{2\pi i\theta},u_\pm)}$, $\theta \in [-1/3,-1/6] \cup [1/6,1/3]$, is $\mathrm{SL}(2,\mathbb{C})$–equivalent to a $\mathrm{SU}(2)$–representation $\bar{\rho}_{\theta,\pm}$ which satisfies

$$\bar{\rho}_{\theta,\pm}(\mu) = \mathrm{diag}\left(e^{2\pi i\theta}, e^{-2\pi i\theta}\right), \qquad \bar{\rho}_{\theta,\pm}(\lambda) = \mathrm{diag}(L_\pm, L_\pm^{-1}),$$

where μ and λ are the elements of π corresponding to the meridian and the preferred longitude of K, and

$$L_\pm = L_\pm(\theta) = \lambda_{11}\left(e^{2\pi i\theta}, u_\pm\right) = -1 + e^{-4\pi i\theta} - 2e^{4\pi i\theta} + e^{8\pi i\theta} + u_\pm\left(e^{-4\pi i\theta} - e^{4\pi i\theta}\right).$$

We note that $\bar{\rho}_{-\theta,\pm}$ and $\bar{\rho}_{\theta,\pm}$ are $\mathrm{SU}(2)$–equivalent. In particular, the space $\mathcal{M}_{\mathrm{nab}}$ can be parametrized by the two arcs $(e^{2\pi i\theta}, u_+(\theta))$, $\theta \in [1/6,1/3]$, and $(e^{2\pi i\theta}, u_-(\theta))$, $\theta \in [1/6,1/3]$. These two arcs only coincide at the endpoints, so topologically $\mathcal{M}_{\mathrm{nab}}$ is a circle.

This proposition follows from [R1, Proposition 4], see also [KK, Proposition 5.4]. For a more geometric argument determining the topological type of $\mathcal{M}_{\mathrm{nab}}$, see also [Kl].

For $\theta \in [-1/3,-1/6] \cup [1/6,1/3]$, the representation $\bar{\rho}_{\theta,\pm}$ extends to a representation of $\pi_1(M_{p/q})$ if and only if

$$\bar{\rho}_{\theta,\pm}(\mu)^p \bar{\rho}_{\theta,\pm}(\lambda)^q = 1,$$

i.e. if and only if

$$e^{-2\pi i p\theta} = L_\pm(\theta)^q. \tag{62}$$

¿From this (use e.g. (67)) we see that

Corollary 5.4. *Let $p/q \in \mathbb{Q}$ be arbitrary. The moduli space of irreducible flat $\mathrm{SU}(2)$–connections on $M_{p/q}$ is a finite set.* □

Let us end this section by finding the abelian SU(2)–representations of $\pi_1(M_{p/q})$ (up to equivalence). Therefore, let $\theta \in]-1/2,1/2]$ and let ρ_θ be the assignment

$$\rho_\theta(\mu) = \mathrm{diag}(e^{2\pi i\theta}, e^{-2\pi i\theta}). \tag{63}$$

By (53) this assignment extends to an abelian SU(2)–representation of π for any $\theta \in]-1/2,1/2]$ by letting $\rho_\theta(y) = \rho_\theta(x)$. Moreover, any abelian SU(2)–representation of π is SU(2)–equivalent to ρ_θ for some $\theta \in]-1/2,1/2]$. For any $\theta \in]-1/2,1/2]$ we have $\rho_\theta(\lambda) = 1$, and ρ_θ extends to a representation of $\pi_1(M_{p/q})$ if and only if $\rho_\theta(\mu)^p = 1$, i.e. if and only if $p\theta \in \mathbb{Z}$. If $A = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ then $A\rho_\theta(\mu)A^{-1} = \rho_{-\theta}(\mu)$ so we can assume that $\theta \in [0,1/2]$. Note, moreover, that two matrices $\mathrm{diag}(e^{i\phi}, e^{-i\phi})$ and $\mathrm{diag}(e^{i\psi}, e^{-i\psi})$, $\phi, \psi \in]-\pi,\pi]$, are conjugate in SU(2) if and only if $\phi = \psi$ or $\phi = -\psi$. We conclude

Proposition 5.5. *For $p \neq 0$ the set of conjugacy classes of abelian $\mathrm{SU}(2)$–representations of $\pi_1(M_{p/q})$ is given by*

$$\left\{ [\rho_{j/|p|}] \;\middle|\; j = 0, 1, \ldots, \left[\frac{|p|}{2}\right] \right\},$$

where $[x]$ is the integer part of x for $x > 0$. For $p = 0$ the set of conjugacy classes of abelian $\mathrm{SU}(2)$*–representations of $\pi_1(M_{p/q})$ is given by*

$$\left\{ [\rho_\theta] \;\middle|\; \theta \in [0, \frac{1}{2}] \right\},$$

so topologically this set is a closed interval. □

5.2. **Chern–Simons invariants.** We begin by recalling formulas from [KK] for the Chern–Simons invariants of the flat $\mathrm{SU}(2)$–connections on $M_{p/q}$. The basic tool will be Theorem 5.6 below due to P. A. Kirk and E. P. Klassen.

Let M be a closed oriented 3–manifold with a knot K in its interior and let X be the complement of a tubular neighborhood of K in M. Moreover, let μ be a meridian of K and λ a longitude, both in ∂X. Let G be $\mathrm{SU}(2)$ or $\mathrm{SL}(2,\mathbb{C})$. If $\rho : \pi_1(X) \to G$ is a representation, then ρ extends to a G–representation of $\pi_1(M)$ if and only if $\rho(\mu) = 1$. Now assume that $\rho_t : \pi_1(X) \to G$ is a piecewise smooth path of representations, $t \in I = [0, 1]$. Choose a piecewise smooth path $g : I \to G$ such that

$$\begin{aligned} g_t\rho_t(\mu)g_t^{-1} &= \mathrm{diag}\left(e^{2\pi i\alpha(t)}, e^{-2\pi i\alpha(t)}\right), \\ g_t\rho_t(\lambda)g_t^{-1} &= \mathrm{diag}\left(e^{2\pi i\beta(t)}, e^{-2\pi i\beta(t)}\right), \end{aligned} \tag{64}$$

for some piecewise smooth curves α, β. If $G = \mathrm{SU}(2)$ this is always possible by [KK, Lemma 3.1], and in that case α and β are real-valued. If $G = \mathrm{SL}(2,\mathbb{C})$ the above is possible if the path ρ avoids the parabolic representations (i.e. upper triangular with 1s or -1s on the diagonal), cf. [KK, Remark p. 354]. (See the text in connection to (60) for the case of the figure 8 knots.) In that case the curves α and β are complex-valued. We then have

Theorem 5.6 ([KK, Theorem 4.2])**.** *Assume that $\rho_0(\mu) = \rho_1(\mu) = 1$. Thinking of ρ_0 and ρ_1 as flat G–connections on M, we have*

$$\mathrm{CS}(\rho_1) - \mathrm{CS}(\rho_0) = -2\int_0^1 \beta(t)\alpha'(t)\mathrm{d}t \pmod{\mathbb{Z}},$$

where CS *is the Chern–Simons functional associated to G.* □

We note that in case $G = \mathrm{SL}(2,\mathbb{C})$ the Chern–Simons functional takes values in $\mathbb{C}/\mathbb{Z}$.

Next consider a knot K in S^3 and let X be the knot complement. Let p/q be a rational number and let $N_{p/q}$ be the closed oriented 3–manifold obtained by p/q surgery on S^3 along K. Let μ and λ be classes in $\pi_1(\partial X)$ represented by respectively a meridian and the preferred longitude of K. Choose integers $c, d \in \mathbb{Z}$ such that $pd - qc = 1$. Let V be a tubular neighborhood of K considered as a subspace of $N_{p/q}$. We note that $\mu' = p\mu + q\lambda$ and $\lambda' = c\mu + d\lambda$ are represented by respectively a meridian of V and a longitude of V. Assume that $\rho : I \to \mathrm{Hom}(\pi_1(X), G)$ is a piecewise smooth curve of representations from the trivial representation to a representation, which extends to a representation of $\pi_1(N_{p/q})$, i.e. $\rho(1)(\mu') = 1$. Assume, moreover, that ρ avoids the parabolic representations in case $G = \mathrm{SL}(2,\mathbb{C})$, and choose curves α, β as in (64) with $\alpha(0) = \beta(0) = 0$. By Theorem 5.6 we have

$$\begin{aligned} \mathrm{CS}(\tilde{\rho}(1)) &= -2\int_0^1 (c\alpha(t) + d\beta(t))(p\alpha'(t) + q\beta'(t))\mathrm{d}t \\ &= -2\int_0^1 \beta(t)\alpha'(t)\mathrm{d}t - cp\alpha^2(1) - dq\beta^2(1) - 2cq\alpha(1)\beta(1) \pmod{\mathbb{Z}}. \end{aligned} \tag{65}$$

(We have corrected a sign error in [KK, Formula (*) p. 361].) We note that this expression is independent of the choice of c, d. The condition $\rho(1)(\mu') = 1$ is equivalent to

$$p\alpha(1) + q\beta(1) \in \mathbb{Z}. \tag{66}$$

Now let K be the figure 8 knot and let $\bar{\rho}_{\theta,\varepsilon}$ be a SU(2)–representation of $\pi_1(M_{p/q})$, i.e. (62) is satisfied. Following [KK] we determine a formula for $\mathrm{CS}(\bar{\rho}_{\theta,\varepsilon})$. For later we will here pay special attention to the branches of the logarithm. By Proposition 5.3 we have

$$\begin{aligned} \mathrm{Re}\,(L_-(\theta)) &= \mathrm{Re}\,(L_+(\theta)) = 2\cos^2(4\pi\theta) - \cos(4\pi\theta) - 2, \\ \mathrm{Im}\,(L_\pm(\theta)) &= \mp 2\sin(4\pi\theta)\sqrt{\cos^2(4\pi\theta) - \cos(4\pi\theta) - \frac{3}{4}} \end{aligned} \tag{67}$$

for all $\theta \in [-1/3, -1/6] \cup [1/6, 1/3]$. From these identities we see that

$$L_\pm(1/3) = L_\pm(1/6) = -1, \quad L_\pm(1/4) = 1, \tag{68}$$

and that $\mathrm{Im}(L_+) < 0$ and $\mathrm{Im}(L_-) > 0$ on $]1/6, 1/4[$ with the opposite signs on $]1/4, 1/3[$. We conclude that $L_+(\theta)$ and $L_-(\theta)$ run through S^1 both beginning and ending in -1, L_+ in the anti-clockwise and L_- in the clockwise direction, as θ runs through $[1/6, 1/3]$. We can therefore use the principal logarithm Log to define continuous curves $\beta_\pm : [1/6, 1/3] \to \mathbb{R}$ by

$$\beta_\pm(\theta) = \frac{1}{2\pi i}\mathrm{Log}(L_\pm(\theta)) + f_\pm(\theta), \tag{69}$$

where

$$f_+(\theta) = \begin{cases} 0, & \theta = \frac{1}{6}, \\ 1, & \theta \in]\frac{1}{6}, \frac{1}{3}], \end{cases} \tag{70}$$

and

$$f_-(\theta) = \begin{cases} 0, & \theta \in [\frac{1}{6}, \frac{1}{3}[, \\ -1, & \theta = \frac{1}{3}. \end{cases} \tag{71}$$

We note that $\beta_\pm$ are smooth on $]\frac{1}{6}, \frac{1}{3}[$ but not in the end points $1/6$ and $1/3$. The terms $f_\pm$ have been chosen so that $\beta_\pm(1/6) = 1/2$. This is needed for the proof of

Proposition 5.7 ([KK, p. 362]). *Let $\theta \in [1/6, 1/3]$ and let $\bar{\rho}_{\theta,\pm}$ be as in* Proposition 5.3. *If $\bar{\rho}_{\theta,\varepsilon}$ extends to a representation of $\pi_1(M_{p/q})$ for a $\varepsilon \in \{\pm 1\}$ then*

$$\mathrm{CS}(\bar{\rho}_{\theta,\varepsilon}) = -\frac{1}{6} - cp\theta^2 - dq\beta_\varepsilon^2(\theta) - 2cq\theta\beta_\varepsilon(\theta) - 2\int_{1/6}^{\theta} \beta_\varepsilon(t)\mathrm{d}t \pmod{\mathbb{Z}},$$

where $\beta_\pm$ are the curves defined by (69). □

Kirk & Klassen prove the above result by explicitly constructing a piecewise smooth path $\rho : [0,1] \to \mathrm{Hom}(\pi, \mathrm{SL}(2,\mathbb{C}))$ from the trivial representation to $\bar{\rho}_{\frac{1}{6},+} = \bar{\rho}_{\frac{1}{6},-}$ with piecewise smooth curves $\alpha, \beta : [0,1] \to \mathbb{C}$ as in (64) satisfying $\alpha(1) = \frac{1}{6}$ and $\beta(1) = \frac{1}{2}$. Moreover, they use that $\int_0^1 \beta(t)\alpha'(t)\mathrm{d}t = \frac{1}{12}$ and the fact that $y \mapsto \bar{\rho}_{y,\varepsilon}$, $[1/6, \theta] \to \mathrm{Hom}(\pi, \mathrm{SU}(2))$ is a path from $\bar{\rho}_{\frac{1}{6},\varepsilon}$ to $\bar{\rho}_{\theta,\varepsilon}$ with associated functions $\alpha(y) = y$ and $\beta(y) = \beta_\varepsilon(y)$. By the choice of the functions $f_\pm$, these α– and β–functions are continuations of the ones used for the path ρ from the trivial representation to $\bar{\rho}_{\frac{1}{6},\pm}$.

Kirk & Klassen argue that $\int_0^1 \beta(t)\alpha'(t)\mathrm{d}t = \frac{1}{12}$ using a comparison between a computer calculation and the Chern–Simons invariants of flat SU(2)–connection on the Seifert manifold M_{-3}. By following Kirk & Klassen's arguments [KK, pp. 361–362] it is actually not hard to give an explicit calculation of this integral. Let us give some details. The path ρ from the trivial connection to $\bar{\rho}_{\frac{1}{6},\pm}$ consists of three parts, where β is identically zero along the first two parts. We can therefore concentrate on the third part. Let

$a = (3+\sqrt{5})/2$, and let $\alpha : [0,1] \to \mathbb{C}$ be a piecewise smooth curve from $\frac{1}{2\pi i}\mathrm{Log}(\sqrt{a})$ to $1/6$. Let $t(s) = e^{4\pi i\alpha(s)}$ and choose a piecewise smooth solution $u(s)$ to $\phi(t(s), u(s)) = 0$, where ϕ is given by (57). Then $s \mapsto \rho_{(e^{2\pi i\alpha(s)}, u(s))} =: \eta_s$ is the third piece of our curve ρ (reparametrized). Assuming $\alpha(s) \notin \frac{1}{2}\mathbb{Z}$ (so as to avoid the parabolic representations) we can diagonalize exactly as demonstrated after Corollary 5.2 and get

$$\tilde{\eta}_s(\mu) = \mathrm{diag}(T, T^{-1}), \qquad \tilde{\eta}_s(\lambda) = \mathrm{diag}\left(\lambda_{11}(T,u), \lambda_{11}(T,u)^{-1}\right),$$

where $T = T(s) = e^{2\pi i\alpha(s)}$, $u = u(s)$, λ_{11} is as below Corollary 5.2, and where $\tilde{\eta}_s(\gamma) = U^{-1}\eta_s(\gamma)U$ for $\gamma \in \pi$, where $U = U(s) = \begin{pmatrix} 1 & -1/(T^2-1) \\ 0 & 1 \end{pmatrix}$. This shows that $\alpha(s)$ indeed plays the role as the α–curve for our path η_s. The β–curve should be a piecewise smooth curve $\beta(s)$ starting at zero such that

$$e^{2\pi i\beta(s)} = \lambda_{11}(e^{2\pi i\alpha(s)}, u(s)) \tag{72}$$

for $s \in [0,1]$. We note that $\lambda_{11}(e^{2\pi i\alpha(1)}, u(1)) = -1$ so we must have $\beta(1) \in \frac{1}{2} + \mathbb{Z}$. Since $\bar{\rho}_{1/6,\pm}$ extends to a SU(2)–representation of $\pi_1(M_{-3})$ we get from (65) that

$$-2\int_0^1 \beta(s)\alpha'(s)\mathrm{d}s - \frac{1}{12} + \frac{1}{3}\beta(1) \pmod{\mathbb{Z}}$$

is a Chern–Simons value of a flat SU(2)–connection on M_{-3}, so $\int_0^1 \beta(s)\alpha'(s)\mathrm{d}s$ is real.

We now only have to choose a nice α–curve. Let δ be a small positive parameter less than $|\alpha(0)| < 1/6$, and let $\alpha = \alpha_1 + \alpha_2 + \alpha_3$, where α_1 is the line segment $[\alpha(0), -i\delta]$, α_2 is the part of the circle with centre zero and radius δ running from $-i\delta$ to δ, and $\alpha_3 = [\delta, 1/6]$. Here the parameter δ is introduced to avoid passing through zero (so as to avoid parabolic representations). With this choice it is not hard to show that there is a unique continuous solution $(u(s), \beta(s))$ to $\phi(t(s), u(s)) = 0$ and (72) with $\beta(0) = 0$ and $\beta(1) = \frac{1}{2}$ and to show that $\int_0^1 \beta(s)\alpha'(s)\mathrm{d}s = \frac{1}{12}$ for this solution. (Use that the integral is real and independent of δ and calculate its $\delta \to 0$ limit).

Proposition 5.7 gives a formula for the Chern–Simons invariants of the irreducible flat SU(2)–connections on $M_{p/q}$. Let us also determine the Chern–Simons invariants of the reducible flat SU(2)–connections on $M_{p/q}$. Therefore let $\rho_{j/|p|}$ be as in Proposition 5.5, $p \neq 0$, and let $\alpha(t) = jt/|p|$ and $\beta(t) = 0$, $t \in [0,1]$, and get by (65) that

$$\mathrm{CS}(\rho_{j/|p|}) = -cpj^2/p^2 = -cj^2/p \pmod{\mathbb{Z}}, \tag{73}$$

where c is the inverse of $-q \pmod{p}$.

In case $p = 0$ the moduli space of flat reducible SU(2)–connections on M_0 can be identified with a closed interval, cf. Proposition 5.5. Since the Chern–Simons functional is constant on each of the connected components of the moduli space of flat connections, we conclude that the Chern–Simons invariant of any of the reducible SU(2)–connections is equal to the Chern–Simons invariant of the trivial connection, i.e. it is equal to zero. This of course also follows from Kirk and Klassen's result. In fact, if ρ_θ denotes the abelian representation from Proposition 5.5, then we can put $\alpha(t) = \theta t$ and $\beta(t) = 0$, $t \in [0,1]$, and get by (65) that

$$\mathrm{CS}(\rho_\theta) = 0 \pmod{\mathbb{Z}}. \tag{74}$$

5.3. **A comparison between Chern–Simons invariants and critical values of the phase functions $\Phi_n^{a,b}$.** The purpose of this section is to combine the Chern–Simons theory described in the previous two sections with the asymptotic analysis in Sect. 4.3. First we will describe a correspondence between the critical points of the phase functions $\Phi_n^{a,b}$ in (35) and the nonabelian SL(2, $\mathbb{C}$)–representations of $\pi_1(M_{p/q})$. Thereafter we will show that the set of Chern–Simons invariants of flat irreducible SU(2)–connections on $M_{p/q}$ is a certain subset of the critical values of the functions $\Phi_n^{a,b}$. Like in Sect. 4.3 we will most of the time work with the shifted phase functions $\Psi_n^{a,b}$ in (38). We refer to Remark 5.10 for a comparison between the phase functions $\Phi_n^{a,b}$ and $\Psi_n^{a,b}$. Recall the set $\tilde{\mathcal{N}}$ given by (59).

Theorem 5.8. *The map $(x,y) \mapsto \rho_{(e^{\pi i x}, e^{2\pi i y}-1)}$ gives a surjection φ from the set of critical points (x,y) of the functions $\Psi_n^{a,b}$, $a,b,n \in \mathbb{Z}$, with $x \notin \mathbb{Z}$ onto the set of representations $\rho_{(s,u)} : \pi \to \mathrm{SL}(2,\mathbb{C})$, $(s,u) \in \tilde{\mathcal{N}}$, which extend to $\mathrm{SL}(2,\mathbb{C})$–representations of $\pi_1(M_{p/q})$.*

If (x,y) is a critical point, let us say of $\Psi_n^{a,b}$, then $(x+2k, y+l)$ is a critical point of $\Psi_{n+pk}^{a+l,b+2k}$ for any $k,l \in \mathbb{Z}$, so $\varphi^{-1}(\varphi(x,y)) = \{ (x+2k, y+l) \mid k,l \in \mathbb{Z} \}$ if $x \notin \mathbb{Z}$.

Proof. The last statement follows immediately from (39), so let us concentrate on the first part. Let $\psi : \mathbb{C}^2 \to \mathbb{C}$ be given by

$$\psi(z,w) = (1-zw)(w-z) - zw,$$

so $\psi(v^2, w) = 0$ if and only if (v,w) is a solution to (41). Then

$$\psi(z, u+1) = -z\phi(z,u)$$

for $(z,u) \in \mathbb{C}^* \times \mathbb{C}$, where ϕ is the function (57). It follows that (v,w) is a solution to (41) if and only if either $(v,w) = (0,0)$ or $(v, w-1) \in \tilde{\mathcal{N}}$.

Next assume that $(v,u) \in \tilde{\mathcal{N}}$ and put $(z,w) = (v^2, u+1)$. Since $\psi(z,w) = 0$ and $z \neq 0$ we have that $w \neq 0$ and $w - z \neq 0$. Therefore $1 - zw = wz/(w-z)$ and (v,w) is a solution to (40) if and only if

$$\begin{aligned} v^{-p} &= \left(\frac{(w-z)^2}{wz} \right)^q = \left(wz^{-1} - 2 + zw^{-1} \right)^q \\ &= \left(\lambda_{11}(v, w-1) - 1 - z^2 + zw^{-1} + wz + z \right)^q . \end{aligned}$$

But $\psi(z,w) = 0$ and $w \neq 0$ implies that $-1 - z^2 + zw^{-1} + wz + z = 0$. Thus (v,w) is a solution to (40) if and only if $(s,u) = (v,u)$ is a solution to (61).

The above shows together with the discussion around (61) that there is a one-one correspondence between common nonzero solutions (v,w) to (40),(41) with $v^2 \neq 1$ and representations $\rho_{(v,w-1)} : \pi \to \mathrm{SL}(2,\mathbb{C})$, $(v, w-1) \in \tilde{\mathcal{N}}$, which extend to $\mathrm{SL}(2,\mathbb{C})$–representations of $\pi_1(M_{p/q})$. By the remarks following (39) this proves the theorem. □

Let $(v,u) \in \tilde{\mathcal{N}}$ and recall that the representation $\rho_{(v,u)}$ is equivalent to a SU(2)–representation of $\pi_1(M_{p/q})$ if and only if $(v,u) \in S^1 \times \mathbb{R}$ and (v,u) is a solution to (61). The remaining part of this section is devoted to the proof of the following theorem, which is one of our main results.

Theorem 5.9. *Let $(x,y) \in \mathbb{C}^2$ such that $\rho_{(e^{\pi i x}, e^{2\pi i y}-1)}$ is equivalent to a nonabelian* SU(2)*–representation of $\pi_1(M_{p/q})$ and choose in accordance with* Theorem 5.8 *integers a,b,n such that (x,y) is a critical point of $\Psi_n^{a,b}$. If a',b',n' is another such set of integers, then $b' = b$ and $a' + n'/q = a + n/q$. In fact we have*

$$\begin{aligned} a + \frac{n}{q} &= y + \frac{p}{2q}x + \frac{i}{2\pi}\left(\mathrm{Log}\left(1 - e^{2\pi i(x+y)}\right) - \mathrm{Log}\left(1 - e^{2\pi i(x-y)}\right)\right), \\ b &= x + \frac{i}{2\pi}\left(\mathrm{Log}\left(1 - e^{2\pi i(x+y)}\right) + \mathrm{Log}\left(1 - e^{2\pi i(x-y)}\right)\right). \end{aligned}$$

Moreover, for any such set of integers a, b, n we have

$$\mathrm{CS}(\bar{\rho}_{\theta,\varepsilon}) = \Psi_n^{a,b}(x,y) \pmod{\mathbb{Z}},$$

where $\theta \in [-1/3,-1/6] \cup [1/6,1/3]$ and $\varepsilon \in \{\pm\}$ with $e^{2\pi i\theta} = e^{\pi i x}$ and $1 + u_\varepsilon(\theta) = e^{2\pi i y}$, and $\bar{\rho}_{\theta,\varepsilon}$ is a $\mathrm{SU}(2)$*–representation of $\pi_1(M_{p/q})$ equivalent to $\rho_{(e^{\pi i x}, e^{2\pi i y}-1)}$ and given by* Proposition 5.3.

Remark 5.10. In general we have $\Phi_n^{a,b} = \Psi_n^{a+b,a-b}$, so there is a ono to one correspondence between the phase functions $\Phi_n^{a,b}$ and the phase functions $\Psi_n^{a',b'}$ with $a'+b'$ and $a'-b'$ even. (We note that $a+b$ is even if and only if $a-b$ is even since $(a+b)+(a-b) = 2a$.) If (x,y) is a critical point of $\Psi_n^{a,b}$ with $a+b$ odd, then (x,y) is also a critical point of $\Psi_{n-q}^{a+1,b}$, by Theorem 5.9. In that way we see that any critical point of one of the functions $\Psi_n^{a,b}$ is also a critical point of one of the functions $\Phi_n^{a,b}$.

The phase functions $\Psi_n^{0,0}$, $\Psi_n^{1,-1}$, $\Psi_n^{1,1}$ and $\Psi_n^{2,0}$ are the ones entering Conjecture 4.4. By Theorem 5.9 the parameter b is fixed by a critical point of $\Psi_n^{a,b}$, while a and n can be varied as long as we keep fixed $a + n/q$. Because of this (see also Lemma 5.12) we only need to consider $\Psi_n^{0,0}$, $\Psi_n^{0,-1}$, and $\Psi_n^{0,1}$. We have the following corollary to Theorem 5.9 (the proof of this theorem and Proposition 5.3).

Corollary 5.11. *Let $(x,y) \in \mathbb{C}^2$ such that $\rho_{(e^{\pi i x}, e^{2\pi i y}-1)}$ is equivalent to a nonabelian* $\mathrm{SU}(2)$*–representation of $\pi_1(M_{p/q})$. Let $(x',y') \in \mathbb{C}^2$ such that $(e^{\pi i x'}, e^{2\pi i y'}) = (e^{\pi i x}, e^{2\pi i y})$ and* $\mathrm{Re}(x') \in]-1,1]$ *and* $\mathrm{Re}(y') \in]-1/2,1/2]$. *Moreover, let*

$$\begin{aligned} n &= q\left(y' + \frac{p}{2q}x' + \frac{i}{2\pi}\left(\mathrm{Log}\left(1-e^{2\pi i(x+y)}\right) - \mathrm{Log}\left(1-e^{2\pi i(x-y)}\right)\right)\right), \\ b &= x' + \frac{i}{2\pi}\left(\mathrm{Log}\left(1-e^{2\pi i(x+y)}\right) + \mathrm{Log}\left(1-e^{2\pi i(x-y)}\right)\right). \end{aligned}$$

Then $\theta := x'/2 \in [-1/3,-1/6] \cup [1/6,1/3]$ and

$$b = \begin{cases} -1, & \theta \in [-1/3,-1/4] \\ 0, & \theta \in]-1/4,-1/6] \cup [1/6,1/4] \\ 1, & \theta \in]1/4,1/3]. \end{cases}$$

Moreover, $n \in \mathbb{Z}$ and (x',y') is a critical point of $\Psi_n^{0,b}$ and

$$\mathrm{CS}(\bar{\rho}_{\theta,\varepsilon}) = \Psi_n^{0,b}(x',y') \pmod{\mathbb{Z}},$$

where $\varepsilon \in \{\pm\}$ with $1 + u_\varepsilon(\theta) = e^{2\pi i y}$, and $\bar{\rho}_{\theta,\varepsilon}$ is a $\mathrm{SU}(2)$*–representation of $\pi_1(M_{p/q})$ equivalent to $\rho_{(e^{\pi i x}, e^{2\pi i y}-1)}$ and given by* Proposition 5.3.

We note that the first part of Theorem 5.9 is an immediate consequence of (39). To prove the second part we start by observing that if if a, a', n, n', b are integers such that $a' + n'/q = a + n/q$ then $\Psi_n^{a,b}(x,y) - \Psi_{n'}^{a',b}(x,y)$ is an integer independent of $(x,y) \in \mathbb{C}^2$. The remaining part of the proof will consists of a series of lemmas. We start by

Lemma 5.12. *Let $a, b, n \in \mathbb{Z}$ and assume that (x,y) is a critical point of $\Psi_n^{a,b}$. Let $l, k \in \mathbb{Z}$ and put $a' = a + l$, $b' = b + k$, and $n' = n + pk$. Then $(x+2k, y+l)$ is a critical point of $\Psi_{n'}^{a',b'}$ and*

$$\Psi_{n'}^{a',b'}(x+2k, y+l) - \Psi_n^{a,b}(x,y) \equiv 0 \pmod{\mathbb{Z}}.$$

Proof. That $(x+2k, y+l)$ is a critical point of $\Psi_{n'}^{a',b'}$ is an immediate consequence of

(39) and was already observed in Theorem 5.8. Put $x' = x + 2k$ and $y' = y + l$. Since $e^{2\pi i x'} = e^{2\pi i x}$ and $e^{2\pi i y'} = e^{2\pi i y}$ we get

$$\begin{aligned}\Psi_{n'}^{a',b'}(x',y') - \Psi_n^{a,b}(x,y) &= a'x' + b'y' - x'y' + \frac{n'}{q}x' - \frac{p}{4q}x'^2 - \frac{d}{q}n'^2 \\ &\quad -ax - by + xy - \frac{n}{q}x + \frac{p}{4q}x^2 + \frac{d}{q}n^2 \\ &= 2(a+l)k + 2\frac{n}{q}(1-pd)k + \frac{p}{q}(1-pd)k^2.\end{aligned}$$

Here pd-cq =1 for an integer c so

$$\Psi_{n'}^{a',b'}(x',y') - \Psi_n^{a,b}(x,y) = 2(a+l-nc)k - pck^2.$$

□

By Proposition 5.3 and the above lemma we are thus left with the following to prove: Let $\theta \in [-1/3,-1/6] \cup [1/6,1/3]$ and assume that $\bar{\rho}_{\theta,\varepsilon}$ extends to a representation of $\pi_1(M_{p/q})$ for a $\varepsilon \in \{\pm\}$. Let $b = b(\theta)$ and $n = n(\theta)$ be the unique integers such that $(2\theta, y)$ is a stationary point of $\Psi_n^{0,b}$, where $y = \frac{1}{2\pi i}\mathrm{Log}(1 + u_\varepsilon(\theta))$ (so $\mathrm{Re}(y) = \frac{1}{2}$) (see around (42) and (43)). Then

$$\mathrm{CS}(\bar{\rho}_{\theta,\rho}) = \Psi_n^{0,b}(2\theta, y) \pmod{\mathbb{Z}}. \tag{75}$$

In the course of the proof of this identity we will prove that

$$\mathrm{CS}(\bar{\rho}_{\theta,\varepsilon}) = -\frac{1}{6} - \frac{p}{q}\theta^2 + \frac{m}{q}2\theta - \frac{d}{q}m^2 - 2\int_{1/6}^{\theta_0} \beta_\varepsilon(t)\mathrm{d}t \pmod{\mathbb{Z}}, \tag{76}$$

for $\theta \in [1/6, 1/3]$, where $m = p\theta_0 + q\beta_\varepsilon(\theta_0) \in \mathbb{Z}$ by (66). Unfortunately, the proof of (75) is rather technical, but we have tried to emphasize the main ideas of the proof here, and defer many technicalities to the appendices C and D.

The Chern–Simons invariants of SU(2)–connections are real, so we begin by investigating to what extend a general phase function $\Psi_n^{a,b}$, $a, b, n \in \mathbb{Z}$, is real in its critical points. Assume that (x, y) is such a critical point and write $z = e^{2\pi i x}$ and $w = e^{2\pi i y}$ as usual. From (39) we find that

$$a - \mathrm{Re}(y) = \frac{p}{2q}\mathrm{Re}(x) - \frac{n}{q} - \frac{1}{2\pi}\mathrm{Im}\left(\mathrm{Log}(1 - zw) - \mathrm{Log}(1 - zw^{-1})\right),$$

and

$$b - \mathrm{Re}(x) = -\frac{1}{2\pi}\mathrm{Im}\left(\mathrm{Log}(1 - zw) + \mathrm{Log}(1 - zw^{-1})\right).$$

Moreover, we have $\mathrm{Im}(x) = -\frac{1}{2\pi}\mathrm{Log}|z|$ and $\mathrm{Im}(y) = -\frac{1}{2\pi}\mathrm{Log}|w|$. By (38) we therefore get

$$\begin{aligned}\mathrm{Im}\left(\Psi_n^{a,b}(x,y)\right) &= (a - \mathrm{Re}(y))\mathrm{Im}(x) + (b - \mathrm{Re}(x))\mathrm{Im}(y) - \frac{p}{2q}\mathrm{Im}(x)\mathrm{Re}(x) + \frac{n}{q}\mathrm{Im}(x) \\ &\quad + \frac{1}{4\pi^2}\mathrm{Im}\left(\mathrm{Li}_2(zw) - \mathrm{Li}_2(zw^{-1})\right).\end{aligned}$$

This together with the above expressions for $a - \mathrm{Re}(y)$ and $b - \mathrm{Re}(x)$ leads to the formula

$$\begin{aligned}\mathrm{Im}\left(\Psi_n^{a,b}(x,y)\right) &= \frac{1}{4\pi^2}\Big(\mathrm{Im}(\mathrm{Log}(1 - zw) - \mathrm{Log}(1 - zw^{-1}))\mathrm{Log}|z| \\ &\quad + \mathrm{Im}(\mathrm{Log}(1 - zw) + \mathrm{Log}(1 - zw^{-1}))\mathrm{Log}|w| \\ &\quad + \mathrm{Im}\left(\mathrm{Li}_2(zw) - \mathrm{Li}_2(zw^{-1})\right)\Big).\end{aligned}$$

By introducing the Bloch–Wigner dilogarithm function

$$D(z) = \mathrm{Im}\left(\mathrm{Li}_2(z)\right) + \mathrm{Arg}(1-z)\mathrm{Log}|z|$$

we obtain

Lemma 5.13. *Let $a, b, n \in \mathbb{Z}$ and let (x, y) be a critical point of $\Psi_n^{a,b}$. Then*

$$\mathrm{Im}\left(\Psi_n^{a,b}(x,y)\right) = \frac{1}{4\pi^2}\left(D\left(e^{2\pi i(x+y)}\right) - D\left(e^{2\pi i(x-y)}\right)\right).$$

□

We note that D is analytic on $\mathbb{C} \setminus \{0,1\}$ and continuous on $\mathbb{C}$. Moreover, D satisfies the identities

$$D(z) + D(\bar{z}) = 0, \qquad D(z) + D(1/z) = 0 \tag{77}$$

for all $z \in \mathbb{C} \setminus \{0\}$. From this we have

Corollary 5.14. *Let $a, b, n \in \mathbb{Z}$ and let (x, y) be a critical point of $\Psi_n^{a,b}$ with $e^{2\pi i x} \in S^1$ and $e^{2\pi i y} \in \mathbb{R}$. Then*

$$\mathrm{Im}\left(\Psi_n^{a,b}(x,y)\right) = 0.$$

□

Remark 5.15. Let (v, w) be a non-zero solution to (40) and (41). Then $(\bar{v}, \bar{w})$ is also a solution to these two equations as already observed. Let $z = v^2$ and write $(z, w) = (e^{2\pi i x}, e^{2\pi i y})$. Then $(\bar{z}, \bar{w}) = (e^{-2\pi i \bar{x}}, e^{-2\pi i \bar{y}})$. If (x, y) is a critical point of $\Psi_n^{a,b}$, then $(-\bar{x}, -\bar{y})$ is a critical point of $\Psi_{-n}^{-a,-b}$. By Lemma 5.13 and (77) we have

$$\mathrm{Im}\left(\Psi_n^{a,b}(x,y)\right) = -\mathrm{Im}\left(\Psi_{-n}^{-a,-b}(-\bar{x},-\bar{y})\right)$$

for any $a, b, n \in \mathbb{Z}$. If these values are different from zero, then either $\exp(2\pi i r \Psi_{-n}^{-a,-b}(x,y))$ or $\exp(2\pi i r \Psi_n^{a,b}(-\bar{x},-\bar{y}))$ grows exponentially. By Conjecture 4.4 we claim that stationary points leading to such exponential growth do not contribute to the large r asymptotics of $\bar{\tau}_r(M_{p/q})$. In fact, we conjecture that the union of the sets of critical points $C_{k,l,a,b}^{\mu,\nu,n}$ in Corollary 4.5, via the correspondence Theorem 5.8, corresponds to the set of representations $\rho_{(s,u)}$ being equivalent to SU(2)–representations of $\pi_1(M_{p/q})$ (except for the case $p/q = 0$ where we have to include contributions from the reducible connections in the leading order large r asymptotics, see Appendix C).

We now embark upon proving (75). We start by reducing to the case $\theta \in [1/6, 1/3]$. By Proposition 5.3 we know that the representations $\bar{\rho}_{\theta,\varepsilon}$ and $\bar{\rho}_{-\theta,\varepsilon}$ are SU(2)–equivalent, so in particular they have the same Chern–Simons invariant.

Lemma 5.16. *Let the situation be as in* (75)*. Then*

$$\Psi_{n(\theta)}^{0,b(\theta)}(2\theta, y) - \Psi_{n(-\theta)}^{0,b(-\theta)}(-2\theta, y) \equiv 0 \pmod{\mathbb{Z}}.$$

To prove this and (75) we need the technical Lemma 5.17 keeping track of branches of the logarithm in certain expressions. Let $I = [-1/3, -1/6] \cup [1/6, 1/3]$ and put

$$\begin{aligned} Q_1^{\pm}(\theta) &= 1 - \left(1 + u_{\pm}(\theta)\right)^{-1} e^{4\pi i \theta}, \\ Q_2^{\pm}(\theta) &= 1 - \left(1 + u_{\pm}(\theta)\right) e^{4\pi i \theta}. \end{aligned} \tag{78}$$

for $\theta \in I$, where $u_{\pm}$ are defined in Proposition 5.3. We also put $Q_3^{\pm}(\theta) = 1 + u_{\pm}(\theta)$.

Lemma 5.17. *We have*

$$\mathrm{Log}\left(Q_1^{\pm}(\theta)\right) + \mathrm{Log}\left(Q_2^{\pm}(\theta)\right) = \mathrm{Log}\left(Q_1^{\pm}(\theta)Q_2^{\pm}(\theta)\right) \tag{79}$$

and

$$Q_1^{\pm}(\theta)Q_2^{\pm}(\theta) = e^{4\pi i\theta} \tag{80}$$

for all $\theta \in I$. Moreover

$$\mathrm{Log}\left(Q_1^{\pm}(\theta)\right) + \mathrm{Log}\left(Q_3^{\pm}(\theta)\right) - \mathrm{Log}\left(Q_2^{\pm}(\theta)\right) = \mathrm{Log}\left(\frac{Q_1^{\pm}(\theta)Q_3^{\pm}(\theta)}{Q_2^{\pm}(\theta)}\right) + e_{\pm}(\theta)2\pi i \tag{81}$$

for all $\theta \in I$, where

$$e_+(\theta) = \begin{cases} 1, & \theta \in]1/6, 1/4], \\ 0, & \theta \in]1/4, 1/3[, \end{cases}$$

and $e_-(\theta) = 1 - e_+(\theta)$ for $\theta \in]1/6, 1/3[$, $e_{\pm}(-1/4) = e_{\pm}(1/4)$, $e_{\pm}(\theta) = 1 - e_{\pm}(-\theta)$ for $\theta \in I \setminus \{\pm 1/6, \pm 1/4, \pm 1/3\}$, and $e_{\pm}(\theta) = 0$ for $\theta \in \{\pm 1/6, \pm 1/3\}$. Finally

$$\frac{Q_1^{\pm}(\theta)Q_3^{\pm}(\theta)}{Q_2^{\pm}(\theta)} = L_{\pm}(\theta) \tag{82}$$

for all $\theta \in I$, where $L_{\pm}$ are given by Proposition 5.3.

The proof of this lemma is given in Appendix D.

Proof of Lemma 5.16 By (42) and (43) we have

$$b(\theta) = 2\theta - \frac{1}{2\pi i}\left(\mathrm{Log}\left(Q_1^{\varepsilon}(\theta)\right) + \mathrm{Log}\left(Q_2^{\varepsilon}(\theta)\right)\right)$$

and

$$n(\theta) = p\theta + qy + q\frac{1}{2\pi i}\left(\mathrm{Log}\left(Q_1^{\varepsilon}(\theta)\right) - \mathrm{Log}\left(Q_2^{\varepsilon}(\theta)\right)\right).$$

By Lemma 5.17

$$b(\theta) = 2\theta - \frac{1}{2\pi i}\mathrm{Log}\left(e^{4\pi i\theta}\right). \tag{83}$$

Taking the real part of the expression for $n(\theta)$ we get

$$n(\theta) = p\theta + \frac{1}{2}q + \frac{q}{2\pi}\left(\mathrm{Arg}\left(Q_1^{\varepsilon}(\theta)\right) - \mathrm{Arg}\left(Q_2^{\varepsilon}(\theta)\right)\right). \tag{84}$$

By (83) we get that

$$b(-\theta) = -b(\theta), \quad \theta \in [-1/3, -1/6] \cup [1/6, 1/3] \setminus \{\pm 1/4\},$$

and

$$b(-1/4) = -1, \quad b(1/4) = 0.$$

By (84), (107), and (108) we get

$$n(-\theta) = q - n(\theta), \quad \theta \in [-1/3, -1/6] \cup [1/6, 1/3] \setminus \{\pm 1/4\},$$

and

$$n(-1/4) = n(1/4) - \frac{p}{2}.$$

Let $b = b(\theta)$ and $n = n(\theta)$. Since $\Psi_{n(\theta)}^{0,b(\theta)}(2\theta, y)$ is real by Corollary 5.14 and since $\mathrm{Re}\left(\mathrm{Li}_2(\bar{z})\right) = \mathrm{Re}\left(\mathrm{Li}_2(z)\right)$ for $z \in \mathbb{C}\backslash]1, \infty[$ we find that

$$\begin{aligned}\Psi_{n(\theta)}^{0,b(\theta)}(2\theta, y) - \Psi_{n(-\theta)}^{0,b(-\theta)}(-2\theta, y) &= (b - b(-\theta))\mathrm{Re}(y) - 4\theta\mathrm{Re}(y) \\ &\quad + \frac{(n + n(-\theta))}{q}2\theta - \frac{d(n^2 - n(-\theta)^2)}{q}.\end{aligned}$$

(If $\theta \in \{\pm 1/4\}$, use that $\mathrm{Li}_2(e^{2\pi i(2\theta+y)}) - \mathrm{Li}_2(e^{2\pi i(2\theta-y)})$ is the same for $\theta = 1/4$ and $\theta = -1/4$.) Assume first that $\theta \neq \pm 1/4$. Then, since $\mathrm{Re}(y) = 1/2$, we get

$$\Psi^{0,b(\theta)}_{n(\theta)}(2\theta, y) - \Psi^{0,b(-\theta)}_{n(-\theta)}(-2\theta, y) = b + dq - 2dn \in \mathbb{Z}.$$

Next assume that $\theta = 1/4$. Then

$$\begin{aligned}\Psi^{0,b(\theta)}_{n(\theta)}(2\theta, y) - \Psi^{0,b(-\theta)}_{n(-\theta)}(-2\theta, y) &= 1/2 - 1/2 + \frac{2n - p/2}{2q} - \frac{d}{q}\left(n^2 - (n-p/2)^2\right) \\ &= \frac{n}{q}(1-pd) - \frac{p}{4q}(1-pd).\end{aligned}$$

But $1 - pd = -qc$ for an integer c so

$$\Psi^{0,b(\theta)}_{n(\theta)}(2\theta, y) - \Psi^{0,b(-\theta)}_{n(-\theta)}(-2\theta, y) = \left(\frac{p}{4} - n\right)c.$$

By (66) $p/4 + q\beta_\varepsilon(1/4) \in \mathbb{Z}$. But $L_\pm(1/4) = 1$ so $\beta_\varepsilon(1/4) = f_\varepsilon(1/4) \in \mathbb{Z}$, so p is divisible by 4. □

By using that $y = \frac{1}{2\pi i}\mathrm{Log}\left(Q_3^\varepsilon(\theta)\right)$ together with Lemma 5.17 we obtain the alternative formula

$$n(\theta) = p\theta + qe_\varepsilon(\theta) + \frac{q}{2\pi i}\mathrm{Log}\left(L_\varepsilon(\theta)\right).$$

This and (69) immediately leads to

$$n(\theta) = p\theta + q\beta_\varepsilon(\theta) + q(e_\varepsilon(\theta) - f_\varepsilon(\theta)) \tag{85}$$

for $\theta \in [1/6, 1/3]$. In the proof of (75) we need certain symmetries for the functions $L_\pm$. First we note that

$$L_\pm\left(\frac{1}{2} - \theta\right) = L_\mp(\theta) \tag{86}$$

for $\theta \in [1/6, 1/3]$ by (67). Second, by the next lemma and Proposition 5.3, we have

$$L_-(\theta) = L_+(\theta)^{-1} \tag{87}$$

for $\theta \in [-1/3, -1/6] \cup [1/6, 1/3]$. (In particular, $\bar{\rho}_{\theta,\pm}$ extends to a representation of $\pi_1(M_{p/q})$ if and only if $\bar{\rho}_{\theta,\mp}$ extends to a representation of $\pi_1(M_{-p/q})$.)

Lemma 5.18. *Let $s \in \mathbb{C}^*$ and let $u_\pm$ be the two solutions to $\phi(s^2, u) = 0$. Then*

$$(1 + u_+)(1 + u_-) = 1,$$

and

$$\lambda_{11}(s, u_+)\lambda_{11}(s, u_-) = 1.$$

Proof. We have

$$1 + u_\pm = \frac{1}{2}(s^2 + s^{-2} - 1) \pm \frac{1}{2}\sqrt{s^4 + s^{-4} - 2(s^2 + s^{-2}) - 1}$$

so

$$(1 + u_+)(1 + u_-) = \frac{1}{4}(s^2 + s^{-2} - 1)^2 - \frac{1}{4}(s^4 + s^{-4} - 2(s^2 + s^{-2}) - 1) = 1.$$

Moreover,

$$\lambda_{11}(s, u_\pm) = \frac{1}{2}(s^4 + s^{-4}) - \frac{1}{2}(s^2 + s^{-2}) - 1 \pm \frac{1}{2}(s^{-2} - s^2)\sqrt{s^4 + s^{-4} - 2(s^2 + s^{-2}) - 1}$$

so

$$\begin{aligned}\lambda_{11}(s,u_+)\lambda_{11}(s,u_-) &= \left(\frac{1}{2}(s^4+s^{-4})-\frac{1}{2}(s^2+s^{-2})-1\right)^2\\ &\qquad -\frac{1}{4}(s^2-s^{-2})^2\left(s^4+s^{-4}-2(s^2+s^{-2})-1\right).\end{aligned}$$

By simple reductions one gets the result. □

We are now ready to finalize the proof of (75) and thereby the proof of Theorem 5.9.

Proof of (75) By Lemma 5.16 we can assume that $\theta \in [1/6,1/3]$. Write θ_0 for θ in the following. Let us first observe that formula (76) is an immediate consequence of Proposition 5.7. In fact, by letting c,d be integers as in Proposition 5.7 we get

$$-2cq\theta_0\beta_\varepsilon(\theta_0) = 2cp\theta_0^2 - 2cm\theta_0,$$
$$-dq\beta_\varepsilon^2(\theta_0) = -\frac{d}{q}\left(m^2-2pm\theta_0+p^2\theta_0^2\right),$$

and therefore

$$-cp\theta_0^2 - dq\beta_\varepsilon^2(\theta_0) - 2cq\theta_0\beta_\varepsilon(\theta_0) = \left(c-\frac{dp}{q}\right)p\theta_0^2 - 2\left(c-\frac{dp}{q}\right)m\theta_0 - \frac{d}{q}m^2.$$

But $c-dp/q=-1/q$, hence (76) follows. On the other hand we have

$$\Psi_n^{0,b}(2\theta_0,y) = (b-2\theta_0)y + \frac{n}{q}2\theta_0 - \frac{p}{q}\theta_0^2 - \frac{d}{q}n^2 + \frac{1}{4\pi^2}\left(\mathrm{Li}_2(z_0w_\varepsilon)-\mathrm{Li}_2(z_0w_\varepsilon^{-1})\right),$$

where $z_0=e^{4\pi i\theta_0}$ and $w_\varepsilon = 1+u_\varepsilon(\theta_0)$. By (83) and (85) we have $b-2\theta_0 = -\frac{1}{2\pi i}\mathrm{Log}(z_0)$ and $n = m+q\left(e_\varepsilon(\theta_0)-f_\varepsilon(\theta_0)\right)$ so

$$\begin{aligned}\Psi_n^{0,b}(2\theta_0,y) &= -\frac{p}{q}\theta_0^2 + \frac{m}{q}2\theta_0 - \frac{d}{q}m^2 + 2\left(e_\varepsilon(\theta_0)-f_\varepsilon(\theta_0)\right)\theta_0 - l_\varepsilon(\theta_0)\\ &\qquad +\frac{1}{4\pi^2}\left(\mathrm{Log}(z_0)\mathrm{Log}(w_\varepsilon)+\mathrm{Li}_2(z_0w_\varepsilon)-\mathrm{Li}_2(z_0w_\varepsilon^{-1})\right),\end{aligned}$$

where $l_\varepsilon(\theta_0) = 2dm\left(e_\varepsilon(\theta_0)-f_\varepsilon(\theta_0)\right)+dq\left(e_\varepsilon(\theta_0)-f_\varepsilon(\theta_0)\right)^2 \in \mathbb{Z}$. We therefore get that

$$\begin{aligned}\Psi_n^{0,b}(2\theta_0,y)-\mathrm{CS}(\bar\rho_{\theta_0,\varepsilon}) &= \frac{1}{6}+\frac{1}{4\pi^2}\left(\mathrm{Log}(z_0)\mathrm{Log}(w_\varepsilon)+\mathrm{Li}_2(z_0w_\varepsilon)-\mathrm{Li}_2(z_0w_\varepsilon^{-1})\right)\\ &\qquad +2\left(e_\varepsilon(\theta_0)-f_\varepsilon(\theta_0)\right)\theta_0 + 2\int_{1/6}^{\theta_0}\beta_\varepsilon(t)\mathrm{d}t \pmod{\mathbb{Z}}.\end{aligned}$$

For $\theta_0 \in [1/6,1/4]$ we note that $e_\varepsilon(\theta_0)=f_\varepsilon(\theta_0)$. We will consider the special cases $\theta_0 \in \{1/6,1/4,1/3\}$ first and then handle the other cases afterwards.

The cases $\theta_0 \in \{1/6,1/3\}$. In these cases we have $w_\varepsilon=-1$ so

$$\begin{aligned}&\Psi_n^{0,b}(2\theta_0,y)-\mathrm{CS}(\bar\rho_{\theta_0,\varepsilon})\\ &\quad = \frac{1}{6}+\frac{i}{4\pi}\mathrm{Log}(z_0)+2\left(e_\varepsilon(\theta_0)-f_\varepsilon(\theta_0)\right)\theta_0 + 2\int_{1/6}^{\theta_0}\beta_\varepsilon(t)\mathrm{d}t \pmod{\mathbb{Z}}.\end{aligned}$$

If $\theta_0=1/6$ we immmediately get that this is zero. If $\theta_0=1/3$ we get

$$\begin{aligned}\Psi_n^{0,b}(2\theta_0,y)-\mathrm{CS}(\bar\rho_{\theta_0,\varepsilon}) &= \frac{1}{6}+\frac{i}{4\pi}(4\pi i/3-2\pi i)+\frac{2}{3}\left(e_\varepsilon(\theta_0)-f_\varepsilon(\theta_0)\right)\\ &\qquad +2f_\varepsilon(1/4)(1/3-1/6)+\frac{1}{\pi i}\int_{1/6}^{1/3}\mathrm{Log}(L_\varepsilon(t))\mathrm{d}t \pmod{\mathbb{Z}}.\end{aligned}$$

But if $\theta \in [1/4, 1/3]$ then

$$\int_{1/4}^{\theta_0} \mathrm{Log}(L_\pm(\theta)\mathrm{d}\theta = -\int_{1/4}^{1/2-\theta_0} \mathrm{Log}(L_\mp(t))\mathrm{d}t = -\int_{1/2-\theta_0}^{1/4} \mathrm{Log}(L_\pm(t))\mathrm{d}t,$$

by (86) and (87) so

$$\int_{1/2-\theta_0}^{\theta_0} \mathrm{Log}(L_\pm(\theta)\mathrm{d}\theta = 0. \tag{88}$$

In particular,

$$\Psi_n^{0,b}(2\theta_0, y) - \mathrm{CS}(\bar{\rho}_{\theta_0,\varepsilon}) = \frac{1}{3} - \frac{2}{3}f_\varepsilon(1/3) + \frac{1}{3}f_\varepsilon(1/4) \pmod{\mathbb{Z}},$$

where we also use that $e_\pm(1/3) = 0$ by Lemma 5.17. By (70) and (71) this is zero.
The case $\theta_0 = 1/4$. In this case we have $z_0 = -1$ so

$$\begin{aligned}
&\Psi_n^{0,b}(2\theta_0, y) - \mathrm{CS}(\bar{\rho}_{\theta_0,\varepsilon}) \\
&\quad = \frac{1}{6} + \frac{1}{4\pi^2}\left(i\pi\mathrm{Log}(w_\varepsilon) + \mathrm{Li}_2(|w_\varepsilon|) - \mathrm{Li}_2(|w_\varepsilon|^{-1})\right) + 2\int_{1/6}^{1/4} \beta_\varepsilon(t)\mathrm{d}t \pmod{\mathbb{Z}}.
\end{aligned}$$

Since $(v_0, w_\varepsilon) = (e^{2\pi i\theta_0}, w_\varepsilon)$ is a solution to (41) we have $w_\varepsilon \in \{(-3-\sqrt{5})/2, (-3+\sqrt{5})/2\}$, and by (104) we then conclude that $w_\varepsilon = \frac{-3-\sqrt{5}}{2}$ if $\varepsilon = -$ and $w_\varepsilon = \frac{-3+\sqrt{5}}{2}$ if $\varepsilon = +$. By (102) we then get

$$\begin{aligned}
&\Psi_n^{0,b}(2\theta_0, y) - \mathrm{CS}(\bar{\rho}_{\theta_0,\varepsilon}) \\
&\quad = \frac{1}{6} + \frac{1}{4\pi^2}\left(-\pi^2 - \varepsilon\frac{\pi^2}{5}\right) + 2\int_{1/6}^{1/4} \beta_\varepsilon(t)\mathrm{d}t \\
&\quad = \frac{1}{6} + \frac{1}{4}\left(-1 - \varepsilon\frac{1}{5}\right) + \frac{1}{6}f_\varepsilon(1/4) + \frac{1}{\pi}\int_{1/6}^{1/4} \mathrm{Arg}(L_\varepsilon(t))\mathrm{d}t \pmod{\mathbb{Z}},
\end{aligned}$$

and this is zero by (70), (71), and (97).
The case $\theta \in]1/6, 1/3[\setminus\{1/4\}$. We have

$$\begin{aligned}
\Psi_n^{0,b}(2\theta_0, y) - \mathrm{CS}(\bar{\rho}_{\theta_0,\varepsilon}) &= \frac{1}{6} + \frac{1}{4\pi^2}\mathrm{Log}(z_0)\mathrm{Log}(w_\varepsilon) + 2\left(e_\varepsilon(\theta_0) - f_\varepsilon(\theta_0)\right)\theta_0 \\
&\qquad + 2\int_{1/6}^{\theta_0} \beta_\varepsilon(t)\mathrm{d}t + R(2\theta_0, y) \pmod{\mathbb{Z}},
\end{aligned}$$

where

$$R(x, y) = \frac{1}{4\pi^2}\left(\mathrm{Li}_2(e^{2\pi i(x+y)}) - \mathrm{Li}_2(e^{2\pi i(x-y)})\right).$$

Let us write u for u_ε in the following. By definition of the dilogarithm we have

$$4\pi^2 R(2\theta_0, y) = \int_0^{(1+u)^{-1}e^{4\pi i\theta_0}} \frac{\mathrm{Log}(1-t)}{t}\mathrm{d}t - \int_0^{(1+u)e^{4\pi i\theta_0}} \frac{\mathrm{Log}(1-t)}{t}\mathrm{d}t.$$

By (104) we have $1+u_-(\theta) \leq -1 \leq 1+u_+(\theta) < 0$ for all $\theta \in [1/6, 1/3]$ and $1+u_\pm(\theta) = -1$ if and only if $\theta \in \{1/6, 1/3\}$. Let $\theta_1 = 1/6$ if $\theta_0 \in [1/6, 1/4[$ and $\theta_1 = 1/3$ if $\theta_0 \in]1/4, 1/3[$.

We note that $z \mapsto \mathrm{Log}(1-z)/z$ is analytic on $\mathbb{C} \setminus [1,\infty[$ so by Cauchy's theorem

$$\begin{aligned} 4\pi^2 R(2\theta_0, y) &= \int_0^{-e^{4\pi i\theta_1}} \frac{\mathrm{Log}(1-t)}{t}\mathrm{d}t + \int_{-e^{4\pi i\theta_1}}^{(1+u)^{-1}e^{4\pi i\theta_0}} \frac{\mathrm{Log}(1-t)}{t}\mathrm{d}t \\ &\quad - \int_0^{-e^{4\pi i\theta_1}} \frac{\mathrm{Log}(1-t)}{t}\mathrm{d}t - \int_{-e^{4\pi i\theta_1}}^{(1+u)e^{4\pi i\theta_0}} \frac{\mathrm{Log}(1-t)}{t}\mathrm{d}t \\ &= \int_{-e^{4\pi i\theta_1}}^{(1+u)^{-1}e^{4\pi i\theta_0}} \frac{\mathrm{Log}(1-t)}{t}\mathrm{d}t - \int_{-e^{4\pi i\theta_1}}^{(1+u)e^{4\pi i\theta_0}} \frac{\mathrm{Log}(1-t)}{t}\mathrm{d}t. \end{aligned}$$

The curves $\gamma_\pm(\theta) = (1+u(\theta))^{\pm 1}e^{4\pi i\theta}$ are smooth on $]1/6, 1/3[$ so

$$4\pi^2 R(2\theta_0, y) = \lim_{\eta\to 0_+}\left(\int_{\theta_1+\mu\eta}^{\theta_0} \mathrm{Log}(1-\gamma_-(\theta))\frac{\gamma_-'(\theta)}{\gamma_-(\theta)}\mathrm{d}\theta - \int_{\theta_1+\mu\eta}^{\theta_0} \mathrm{Log}(1-\gamma_+(\theta))\frac{\gamma_+'(\theta)}{\gamma_+(\theta)}\mathrm{d}\theta\right),$$

where $\mu = 1$ if $\theta_1 = 1/6$ and $\mu = -1$ if $\theta_1 = 1/3$. (The parameter η is necessary because u is not differentiable in $1/6$ and $1/3$.) It follows that

$$4\pi^2 R(2\theta_0, y) = \lim_{\eta\to 0_+}\left(4\pi i R_1(\theta_0,\eta) - R_2(\theta_0,\eta)\right),$$

where

$$\begin{aligned} R_1(\theta_0,\eta) &= \int_{\theta_1+\mu\eta}^{\theta_0} \mathrm{Log}\left(Q_1^\varepsilon(\theta)\right) - \mathrm{Log}\left(Q_2^\varepsilon(\theta)\right)\mathrm{d}\theta, \\ R_2(\theta_0,\eta) &= \int_{\theta_1+\mu\eta}^{\theta_0} \left\{\mathrm{Log}\left(Q_1^\varepsilon(\theta)\right) + \mathrm{Log}\left(Q_2^\varepsilon(\theta)\right)\right\}\frac{u'(\theta)}{1+u(\theta)}\mathrm{d}\theta, \end{aligned}$$

where the functions $Q_i^\pm$ are defined above Lemma 5.17. By Lemma 5.17

$$\begin{aligned} R_2(\theta_0,\eta) &= \int_{\theta_1+\mu\eta}^{\theta_0} \mathrm{Log}\left(e^{4\pi i\theta}\right)\frac{u'}{1+u}\mathrm{d}\theta \\ &= 4\pi i\int_{\theta_1+\mu\eta}^{\theta_0} \theta\frac{u'(\theta)}{1+u(\theta)}\mathrm{d}\theta - 2\pi i b(\theta_0)\int_{\theta_1+\mu\eta}^{\theta_0}\frac{u'(\theta)}{1+u(\theta)}\mathrm{d}\theta. \end{aligned}$$

Since $u'(\theta)/(1+u(\theta)) = \frac{\mathrm{d}}{\mathrm{d}\theta}\log(1+u(\theta))$ for any branch log of the logarithm defined on an open section of $\mathbb{C}^*$ containing $]-\infty, 0[$ we have

$$\int_{\theta_1+\mu\eta}^{\theta_0} \theta\frac{u'(\theta)}{1+u(\theta)}\mathrm{d}\theta = \left[\theta\mathrm{Log}(1+u(\theta))\right]_{\theta_1+\mu\eta}^{\theta_0} - \int_{\theta_1+\mu\eta}^{\theta_0}\mathrm{Log}(1+u(\theta))\mathrm{d}\theta,$$

and

$$\int_{\theta_1+\mu\eta}^{\theta_0}\frac{u'(\theta)}{1+u(\theta)}\mathrm{d}\theta = \left[\mathrm{Log}(1+u(\theta))\right]_{\theta_1+\mu\eta}^{\theta_0}.$$

We therefore get

$$\begin{aligned} R(2\theta_0, y) &= \frac{1}{4\pi^2}\lim_{\eta\to 0_+}\left(4\pi i R_1(\theta_0,\eta) - R_2(\theta_0,\eta)\right) \\ &= \frac{b(\theta_0)}{2} - \theta_1 - \frac{1}{4\pi^2}\mathrm{Log}(z_0)\mathrm{Log}(w_\varepsilon) \\ &\quad + \frac{i}{\pi}\lim_{\eta\to 0_+}\left(R_1(\theta_0,\eta) + \int_{\theta_1+\mu\eta}^{\theta_0}\mathrm{Log}\left(Q_3^\varepsilon(\theta)\right)\mathrm{d}\theta\right), \end{aligned}$$

where we use that $1+u_\varepsilon(\theta)=Q_3^\varepsilon(\theta)=w_\varepsilon$ and (83). By Lemma 5.17 we get

$$R_1(\theta_0,\eta)+\int_{\theta_1+\mu\eta}^{\theta_0}\operatorname{Log}\left(Q_3^\varepsilon(\theta)\right)\mathrm{d}\theta=\int_{\theta_1+\mu\eta}^{\theta_0}\operatorname{Log}\left(L_\varepsilon(\theta)\right)+2\pi i e_\varepsilon(\theta)\mathrm{d}\theta,$$

so

$$\lim_{\eta\to 0_+}\left(R_1(\theta_0,\eta)+\int_{\theta_1+\mu\eta}^{\theta_0}\operatorname{Log}\left(Q_3^\varepsilon(\theta)\right)\mathrm{d}\theta\right)=e_\varepsilon(\theta_0)2\pi i(\theta_0-\theta_1)+\int_{\theta_1}^{\theta_0}\operatorname{Log}(L_\varepsilon(\theta))\mathrm{d}\theta.$$

But then

$$\begin{aligned}\Psi_n^{0,b}(2\theta_0,y)-\mathrm{CS}(\bar\rho_{\theta_0,\varepsilon}) &= \frac{1}{6}+2e_\varepsilon(\theta_0)\theta_1-2f_\varepsilon(\theta_0)\theta_0+\frac{b(\theta_0)}{2}-\theta_1\\ &\quad +2\int_{1/6}^{\theta_0}\beta_\varepsilon(t)\mathrm{d}t-\frac{1}{\pi i}\int_{\theta_1}^{\theta_0}\operatorname{Log}(L_\varepsilon(\theta))\mathrm{d}\theta \pmod{\mathbb{Z}}.\end{aligned}$$

Here

$$2\int_{1/6}^{\theta_0}\beta_\varepsilon(t)\mathrm{d}t=2f_\varepsilon(\theta_0)\left(\theta_0-\frac{1}{6}\right)+\frac{1}{\pi i}\int_{\theta_1}^{\theta_0}\operatorname{Log}(L_\varepsilon(\theta))\mathrm{d}\theta,$$

so

$$\begin{aligned}\Psi_n^{0,b}(2\theta_0,y)-\mathrm{CS}(\bar\rho_{\theta_0,\varepsilon}) &= \frac{1}{\pi i}\left(\int_{1/6}^{\theta_0}\operatorname{Log}(L_\varepsilon(\theta))\mathrm{d}\theta-\int_{\theta_1}^{\theta_0}\operatorname{Log}(L_\varepsilon(\theta))\mathrm{d}\theta\right)\\ &\quad +\frac{1}{6}+2e_\varepsilon(\theta_0)\theta_1-\frac{1}{3}f_\varepsilon(\theta_0)+\frac{b(\theta_0)}{2}-\theta_1 \pmod{\mathbb{Z}}.\end{aligned}$$

The subcase $\theta_0\in]1/6,1/4[$. Here we have $\theta_1=1/6$ and $b(\theta_0)=0$ so the result follows by the fact that $e_\varepsilon(\theta)=f_\varepsilon(\theta)$ for $\theta\in]1/6,1/4[$.
The subcase $\theta_0\in]1/4,1/3[$. In this case we have $b(\theta_0)=1$ and $\theta_1=1/3$ so

$$\begin{aligned}\Psi_n^{0,b}(2\theta_0,y)-\mathrm{CS}(\bar\rho_{\theta_0,\varepsilon}) &= \frac{1}{\pi i}\left(\int_{1/6}^{\theta_0}\operatorname{Log}(L_\varepsilon(\theta))\mathrm{d}\theta-\int_{1/3}^{\theta_0}\operatorname{Log}(L_\varepsilon(\theta))\mathrm{d}\theta\right)\\ &\quad +\frac{1}{3}+\frac{2}{3}e_\varepsilon(\theta_0)-\frac{1}{3}f_\varepsilon(\theta_0) \pmod{\mathbb{Z}}.\end{aligned}$$

By (88) we get

$$\int_{1/3}^{\theta_0}\operatorname{Log}(L_\pm(t))\mathrm{d}t=\int_{1/3}^{\frac{1}{2}-\theta_0}\operatorname{Log}(L_\pm(t))\mathrm{d}t=-\int_{1/6}^{\theta_0}\operatorname{Log}(L_\pm\left(\frac{1}{2}-t\right))\mathrm{d}t.$$

By (86) and (87) we then have

$$\int_{1/3}^{\theta_0}\operatorname{Log}(L_\pm(t))\mathrm{d}t=\int_{1/6}^{\theta_0}\operatorname{Log}(L_\pm(t))\mathrm{d}t,$$

so

$$\Psi_n^{0,b}(2\theta_0,y)-\mathrm{CS}(\bar\rho_{\theta_0,\varepsilon})=\frac{1}{3}+\frac{2}{3}e_\varepsilon(\theta_0)-\frac{1}{3}f_\varepsilon(\theta_0) \pmod{\mathbb{Z}},$$

and this is zero by Lemma 5.17, (70) and (71). □

Remark 5.19. If $u_\pm=u_\pm(v)$ are the two solutions to $\phi(v^2,u)=0$ for $v\in\mathbb{C}^*$ fixed, then $\lambda_{11}(v,u_-)=\lambda_{11}(v,u_+)^{-1}$ by Lemma 5.18. By the proof of Theorem 5.8 we therefore conclude that $(v,1+u_\pm)$ is a solution to (40) and (41) if and only if $(v,1+u_\mp)$ is a solution to (41) and

$$v^p=\left(\frac{w-v^2}{1-v^2w}\right)^q. \tag{89}$$

If we work with the invariants τ_r instead of the invariants $\bar{\tau}_r$, then by (13) we have to change p/q to $-p/q$ everywhere in the above. The equation (41) will be the same but (40) will change to (89). If $(v,u) \in \tilde{\mathcal{N}}$ then we find as in the proof of Theorem 5.8 that $(v,w) = (v,u+1)$ is a solution to (89) if and only if (v,u) is a solution to

$$v^p = \lambda_{11}(v,u)^q,$$

which is the "wrong" equation. This is one of the main reasons for working with $\bar{\tau}_r$ instead of τ_r. Another reason is that one would get the wrong signs in (75).

6. Appendices

We have in the following appendices collected material of a technical nature.

6.1. **Appendix A. Proofs of Lemma 3.1, Lemma 4.1 and (21).**

Proof of Lemma 3.1 Let $a > 0$. Let $\varepsilon = 1$ if $\mathrm{Im}(\zeta) \geq 0$ and let $\varepsilon = -1$ otherwise. Put $\delta_a^- = [-a, \sqrt{-1}\varepsilon a]$ and $\delta_a^+ = [\sqrt{-1}\varepsilon a, a]$. (Here, as usual, $[z_1, z_2]$ denotes the line segment in $\mathbb{C}$ beginning at z_1 and ending at z_2.) We have

$$\frac{S_\gamma(\zeta-\gamma)}{S_\gamma(\zeta+\gamma)} = \exp\left(-\frac{1}{2}\int_{C_R} \frac{e^{\zeta z}}{\sinh(\pi z)z}\mathrm{d}z\right).$$

By an elementary argument one finds that the integrals $\int_{\delta_a^\pm} \frac{e^{\zeta z}}{\sinh(\pi z)z}\mathrm{d}z$ converge to zero as $a \to \infty$. Therefore

$$\int_{C_R} \frac{e^{\zeta z}}{\sinh(\pi z)z}\mathrm{d}z = \varepsilon 2\pi\sqrt{-1}\left(b_\varepsilon + \sum_{n=1}^{\infty} \mathrm{Res}_{z=\varepsilon\sqrt{-1}n}\left\{\frac{e^{\zeta z}}{\sinh(\pi z)z}\right\}\right),$$

where $b_1 = 0$ and $b_{-1} = \mathrm{Res}_{z=0}\left\{\frac{e^{\zeta z}}{\sinh(\pi z)z}\right\} = \frac{\zeta}{\pi}$. For $n \in \mathbb{Z} \setminus \{0\}$ we have

$$\mathrm{Res}_{z=\sqrt{-1}n}\left\{\frac{e^{\zeta z}}{\sinh(\pi z)z}\right\} = \frac{(-1)^n e^{\sqrt{-1}\zeta n}}{\pi\sqrt{-1}n},$$

so

$$\int_{C_R} \frac{e^{\zeta z}}{\sinh(\pi z)z}\mathrm{d}z = -(1-\varepsilon)\sqrt{-1}\zeta - 2\mathrm{Log}\left(1 + e^{\varepsilon\sqrt{-1}\zeta}\right)$$

giving the result. □

To prove the identity (21) we use the power series expansion

$$\mathrm{Li}_2(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^2} \tag{90}$$

for the dilogarithm, valid for $|z| \leq 1$. In the course of the following proof we will establish the identity

$$\frac{\zeta^2}{2} - \frac{\pi^2}{6} - \mathrm{Li}_2(-e^{-\sqrt{-1}\zeta}) = \mathrm{Li}_2(-e^{\sqrt{-1}\zeta}) \tag{91}$$

valid for $\zeta = \pm\pi$ and all $\zeta \in \mathbb{C}$ with $|\mathrm{Re}(\zeta)| < \pi$.

Proof of (21) Note first that the integral $A_\gamma(\zeta) := \frac{1}{4}\int_{C_R} \frac{e^{\zeta z}}{\sinh(\pi z)\gamma z^2}\mathrm{d}z$ is convergent for all $\zeta \in \mathbb{C}$ with $|\mathrm{Re}(\zeta)| \leq \pi$ since

$$\int_{-\infty}^{-R} \frac{e^{\zeta t}}{\sinh(\pi t)t^2}\mathrm{d}t = -\int_R^{\infty} \frac{e^{-\zeta t}}{\sinh(\pi t)t^2}\mathrm{d}t$$

and

$$\left|\int_R^\infty \frac{e^{\zeta t}}{\sinh(\pi t)t^2}\mathrm{d}t\right| \leq \frac{2}{1-e^{-2\pi R}}\int_R^\infty e^{(\mathrm{Re}(\zeta)-\pi)t}\frac{1}{t^2}\mathrm{d}t.$$

Let $b = \mathrm{sign}(\mathrm{Im}(\zeta))$, where $\mathrm{sign}(0)$ can be put to both 1 and -1 in the following. Moreover, let h be a positive parameter and let $\delta_h^-(t) = (1+ib)ht+ibh$ for $t \in [-1,0]$ and let $\delta_h^+(t) = (1-ib)ht+ibh$ for $t \in [0,1]$. It is elementary to show that the integrals $\int_{\delta_h^\pm} \frac{e^{\zeta z}}{\sinh(\pi z)z^2}\mathrm{d}z$ converge to zero as h converges to infinity for $|\mathrm{Re}(\zeta)| \leq \pi$. By the residue theorem we conclude that

$$A_\gamma(\zeta) = \frac{1}{4\gamma}2\pi i\sum_{n=1}^\infty \mathrm{Res}_{z=in}\left\{\frac{e^{\zeta z}}{\sinh(\pi z)z^2}\right\}$$

for $\mathrm{Im}(\zeta) \geq 0$ and $|\mathrm{Re}(\zeta)| \leq \pi$ and

$$A_\gamma(\zeta) = -\frac{1}{4\gamma}2\pi i\sum_{n=0}^\infty \mathrm{Res}_{z=-in}\left\{\frac{e^{\zeta z}}{\sinh(\pi z)z^2}\right\}$$

for $\mathrm{Im}(\zeta) \leq 0$ and $|\mathrm{Re}(\zeta)| \leq \pi$. Using (90) this leads directly to

$$A_\gamma(\zeta) = \begin{cases} \frac{1}{2\sqrt{-1}\gamma}\mathrm{Li}_2(-e^{\sqrt{-1}\zeta}) & ,\mathrm{Im}(\zeta)\geq 0, \\ \frac{1}{2\sqrt{-1}\gamma}\left[\frac{\zeta^2}{2}-\frac{\pi^2}{6}-\mathrm{Li}_2(-e^{-\sqrt{-1}\zeta})\right] & ,\mathrm{Im}(\zeta)\leq 0. \end{cases}$$

for $|\mathrm{Re}(\zeta)| \leq \pi$. Left is to prove the identity (91). To this end, let

$$g(\zeta) = \frac{\zeta^2}{2} - \frac{\pi^2}{6} - \mathrm{Li}_2(-e^{-i\zeta}) - \mathrm{Li}_2(-e^{i\zeta})$$

for $\zeta \in \Omega := \{\zeta \in \mathbb{C} \mid |\mathrm{Re}(\zeta)| < \pi\}$. By (20) we have

$$g'(\zeta) = \zeta + i\left(\mathrm{Log}(1+e^{i\zeta}) - \mathrm{Log}(1+e^{-i\zeta})\right)$$

and therefore $e^{ig'(\zeta)} = 1$. Since Ω is connected, g is C^1 and $g'(0) = 0$ we get that g' is identically zero on Ω so g is constant on Ω. Now $g(0) = -\frac{\pi^2}{6} - 2\mathrm{Li}_2(-1)$ and

$$\mathrm{Li}_2(-1) = \sum_{n=1}^\infty \frac{(-1)^n}{n^2} = -\frac{\pi^2}{12}$$

so $g(0) = 0$. Finally we note that g is well-defined and continuous on $\Omega \cup \{\pm\pi\}$ so $g(\pm\pi) = 0$ by continuity. □

Note that the function g in the above proof is a well-defined analytic function on $W = \{\ \zeta \in \mathbb{C} \mid \mathrm{Re}(\zeta) \notin \pi + 2\pi\mathbb{Z}\ \}$ and that g is continuous on $W \cup \mathbb{R}$. As in the proof above we find that g is constant on each connected component of W. Moreover, we can on each of these connected components choose a branch of the dilogarithm such that g extends to a continuous (and hence a constant) function on the connected set $W \cup \mathbb{R}$.

Proof of Lemma 4.1 The function $1/\sinh(w)$ has a simple pole at $w = 0$ with principal part $1/w$, i.e.

$$\phi(w) = \frac{1}{\sinh(w)} - \frac{1}{w}$$

is holomorphic in a neighborhood of zero, in fact on the disk $D(0,\pi)$ with centre 0 and radius π. Let $a \geq R$, let $C_{R;a} = [-a,-R] \cup \Upsilon_R \cup [a,R]$, and write $I_\gamma(\zeta) = J_\gamma(\zeta) + K_\gamma(\zeta)$, where

$$\begin{aligned}
4J_\gamma(\zeta) &= \int_{C_{R;a}} \frac{e^{\zeta z}}{\sinh(\pi z) z}\phi(\gamma z)\mathrm{d}z, \\
4K_\gamma(\zeta) &= \int_{-\infty}^{-a} \frac{e^{\zeta z}}{\sinh(\pi z) z}\phi(\gamma z)\mathrm{d}z + \int_a^\infty \frac{e^{\zeta z}}{\sinh(\pi z) z}\phi(\gamma z)\mathrm{d}z.
\end{aligned}$$

To estimate $K_\gamma(\zeta)$ we simply use that

$$|\phi(\gamma t)| \leq \frac{1}{\sinh(\gamma t)} + \frac{1}{\gamma t} \leq \frac{2}{\gamma t}$$

for $t > 0$ leading to the bound

$$\begin{aligned}
|K_\gamma(\zeta)| &\leq \frac{1}{2\gamma}\int_a^\infty \frac{e^{\mathrm{Re}(\zeta)t} + e^{-\mathrm{Re}(\zeta)t}}{\sinh(\pi t)}\frac{1}{t^2}\mathrm{d}t \\
&\leq \frac{1}{\gamma(1-e^{-2\pi a})}\int_a^\infty \left(e^{-(\pi-\mathrm{Re}(\zeta))t} + e^{-(\pi+\mathrm{Re}(\zeta))t}\right)\frac{1}{t^2}\mathrm{d}t.
\end{aligned}$$

For $|\mathrm{Re}(\zeta)| \leq \pi$ we therefore get

$$|K_\gamma(\zeta)| \leq \frac{2}{\gamma(1-e^{-2\pi a})}\int_a^\infty \frac{1}{t^2}\mathrm{d}t = \frac{2}{a\gamma(1-e^{-2\pi a})}.$$

If $|\mathrm{Re}(\zeta)| < \pi$ we find that

$$\begin{aligned}
|K_\gamma(\zeta)| &\leq \frac{1}{\gamma a^2(1-e^{-2\pi a})}\int_a^\infty (e^{-(\pi-\mathrm{Re}(\zeta))t} + e^{-(\pi+\mathrm{Re}(\zeta))t})\mathrm{d}t \\
&= \frac{1}{\gamma a^2(1-e^{-2\pi a})}\left(\frac{1}{\pi-\mathrm{Re}(\zeta)}e^{-(\pi-\mathrm{Re}(\zeta))a} + \frac{1}{\pi+\mathrm{Re}(\zeta)}e^{-(\pi+\mathrm{Re}(\zeta))a}\right).
\end{aligned}$$

Next let us estimate $J_\gamma(\zeta)$. First we use the standard estimate

$$\left|\int_{\Upsilon_R} \frac{e^{\zeta z}}{\sinh(\pi z) z}\phi(\gamma z)\mathrm{d}z\right| \leq \pi R M(\zeta, R),$$

where $M(\zeta, R) = \max_{z\in\Upsilon_R}\left|\frac{e^{\zeta z}}{\sinh(\pi z)z}\phi(\gamma z)\right|$. We have

$$|\phi(w)| = \frac{\sinh(w) - w}{w\sinh(w)}.$$

Here $\sinh(w) - w = w^3 h(w)$ and $w\sinh(w) = w^2 k(w)$, where h and k are entire functions. Note that k is different from zero on $D(0, \pi)$. Since $\gamma \in]0, 1[$ we get

$$M(\zeta, R) = 2\gamma L(R) N(\zeta, R),$$

where $L(R) = \max_{|z|\leq R}|h(z)/k(z)|$ and $N(\zeta, R) = \max_{z\in\Upsilon_R}\left|\frac{e^{\zeta z}}{e^{\pi z} - e^{-\pi z}}\right|$. We note that

$$N(\zeta, R) \leq Q_\pm(R)\max_{z\in\Upsilon_R}\left|e^{(\zeta\pm\pi)z}\right|,$$

where $Q_\pm(R) = \max_{z\in\Upsilon_R}\frac{1}{|1-e^{\pm 2\pi z}|}$. Put $Q(R) = Q_-(R) + Q_+(R)$ and get

$$N(\zeta, R) \leq Q(R)\min_{\mu=\pm 1}\left(\max_{z\in\Upsilon_R}\left|e^{(\zeta+\mu\pi)z}\right|\right).$$

Since $\mathrm{Re}(z) \in [-R, R]$ and $\mathrm{Im}(z) \in [0, R]$ for $z \in \Upsilon_R$ we finally get

$$N(\zeta, R) \leq Q(R)e^{2\pi R}\left(1 + e^{-\mathrm{Im}(\zeta)R}\right).$$

We have thus obtained the estimate

$$\left|\frac{1}{4}\int_{\Upsilon_R}\frac{e^{\zeta z}}{\sinh(\pi z)z}\phi(\gamma z)\mathrm{d}z\right| \leq \gamma B\left(1+e^{-\mathrm{Im}(\zeta)R}\right),$$

where $B=\frac{\pi}{2}RL(R)Q(R)e^{2\pi R}$.

Finally we have to estimate $\int_R^a \frac{e^{\zeta t}-e^{-\zeta t}}{\sinh(\pi t)t}\phi(\gamma t)\mathrm{d}t$. First observe that

$$h(y)=\sum_{n=0}^{\infty}\frac{y^{2n}}{(2n+3)!}$$

and

$$k(y)=\sum_{n=0}^{\infty}\frac{y^{2n}}{(2n+1)!}$$

so $h(y)\leq k(y)/6$ for $y\in\mathbb{R}$. Therefore

$$\begin{aligned}\left|\int_R^a \frac{e^{\zeta t}-e^{-\zeta t}}{\sinh(\pi t)t}\phi(\gamma t)\mathrm{d}t\right| &\leq \frac{\gamma}{3}\int_R^a\frac{e^{\mathrm{Re}(\zeta)t}+e^{-\mathrm{Re}(\zeta)t}}{e^{\pi t}-e^{-\pi t}}\mathrm{d}t\\ &\leq \frac{\gamma}{3(1-e^{-2\pi R})}\int_R^a\left(e^{-(\pi-\mathrm{Re}(\zeta))t}+e^{-(\pi+\mathrm{Re}(\zeta))t}\right)\mathrm{d}t.\end{aligned}$$

For $|\mathrm{Re}(\zeta)|\leq\pi$ we get

$$\left|\int_R^a \frac{e^{\zeta t}-e^{-\zeta t}}{\sinh(\pi t)t}\phi(\gamma(t)\mathrm{d}t\right|\leq\frac{2a\gamma}{3(1-e^{-2\pi R})}.$$

If $|\mathrm{Re}(\zeta)<\pi$ we get

$$\begin{aligned}&\left|\int_R^a \frac{e^{\zeta t}-e^{-\zeta t}}{\sinh(\pi t)t}\phi(\gamma(t)\mathrm{d}t\right|\leq\frac{\gamma}{3(1-e^{-2\pi R})}\int_0^a\left(e^{-(\pi-\mathrm{Re}(\zeta))t}+e^{-(\pi+\mathrm{Re}(\zeta))t}\right)\mathrm{d}t\\ &=\frac{\gamma}{3(1-e^{-2\pi R})}\left(\frac{1}{\pi-\mathrm{Re}(\zeta)}\left(1-e^{-(\pi-\mathrm{Re}(\zeta))a}\right)+\frac{1}{\pi+\mathrm{Re}(\zeta)}\left(1-e^{-(\pi+\mathrm{Re}(\zeta))a}\right)\right).\end{aligned}$$

The lemma now follows by putting $a=1/\gamma>1>R$ and $A=\frac{13}{12(1-e^{-2\pi R})}$. ☐

6.2. **Appendix B. Proofs of the estimates (26) and (28).** Let

$$\begin{aligned}J'_\pm(r,\varepsilon) &= \int_{C_\pm(\varepsilon)}\exp\left(r\Phi(x)\right)\left(\exp\left(I_\gamma(\pi-2\pi x)-I_\gamma(-\pi+2\pi x)\right)-1\right)\mathrm{d}x,\\ J''_\pm(r,\varepsilon) &= \int_{C_\pm(\varepsilon)}(\tan(\pi r x)\mp\sqrt{-1})g_r(x)\mathrm{d}x,\end{aligned}$$

where Φ is given by (27). Note first that we are free to deform the contour $C_\pm(\varepsilon)$ as long as we stay inside the domain of analyticity of the integrands. For the integrals $J'_\pm(r,\varepsilon)$ we will deform $C_\pm(\varepsilon)$ to $\mp[\varepsilon,1-\varepsilon]$. Since the integrand of the integrals $J''_\pm(r,\varepsilon)$ is analytic on $\Omega_{\frac{1}{2}r}\setminus\{\,(m+1/2)/r\,|\,m=0,1,\ldots,r-1\,\}$, we can deform $C_\pm(\varepsilon)$ to $C_\pm(0)$ in these integrals without changing their sum, i.e.

$$J''_-(r,\varepsilon)+J''_+(r,\varepsilon)=J''_-(r)+J''_+(r),$$

where $J''_\pm(r)=J''_\pm(r,0)$. In the following calculations we will need the identity

$$\mathrm{Re}\left(\Phi(x)\right)=2\pi\mathrm{Re}(x)\mathrm{Im}(x)-\pi\mathrm{Im}(x)-\frac{1}{\pi}\mathrm{Im}\left(\mathrm{Li}_2\left(e^{-2\pi\mathrm{Im}(x)}e^{2\pi i\mathrm{Re}(x)}\right)\right), \tag{92}$$

valid for $x\in\Omega_\infty$. This identity is an immediate consequence of (91).

Proof of (26) Let us first estimate $J''_+(r)$. We partition $C_+(0)$ into the three pieces $C_+^1 = [\sqrt{-1}, 0]$, $C_+^2 = [1+\sqrt{-1}, \sqrt{-1}]$, and $C_+^3 = [1, 1+\sqrt{-1}]$. Put

$$I_+^i(r) = \int_{C_+^i} (\tan(\pi r x) - \sqrt{-1}) g_r(x) \mathrm{d}x.$$

By (24) we immediately get

$$|I_+^1(r)| \leq 2 \int_0^1 e^{-2\pi r t} |g_r(\sqrt{-1}t)| \mathrm{d}t.$$

To be able to use (21) we introduce the positive parameter ε again. In fact, we have by (21), Lemma 4.1 and Lebesgue's dominated convergence theorem that

$$|I_+^1(r)| \leq 2\exp(2A + 2B\pi/r) \lim_{\varepsilon \to 0_+} \int_0^1 e^{-2\pi r t} \left| e^{r\Phi(\varepsilon + \sqrt{-1}t)} \right| \mathrm{d}t.$$

By (92) we immediately get that

$$\left| e^{r\Phi(\varepsilon+\sqrt{-1}t)} \right| = \exp\left(r \left[2\pi\varepsilon t - \pi t - \frac{1}{\pi} \mathrm{Im}\left(\mathrm{Li}_2 \left(e^{2\pi\sqrt{-1}\varepsilon} e^{-2\pi t} \right) \right) \right] \right).$$

Now by continuity of $(t, \varepsilon) \mapsto \mathrm{Li}_2\left(e^{2\pi\sqrt{-1}\varepsilon} e^{-2\pi t}\right)$ on $[0,1] \times [0,1]$ we can remove the parameter ε again by using Lebusgue's dominated convergence theorem once more. This gives us

$$\lim_{\varepsilon \to 0_+} \int_0^1 e^{-2\pi r t} \left| e^{r\Phi(\varepsilon+\sqrt{-1}t)} \right| \mathrm{d}t = \int_0^1 e^{-3\pi r t} \mathrm{d}t$$

leading to the estimate

$$|I_+^1(r)| \leq \frac{2}{3\pi r} \exp(2A + 2B\pi/r) \left(1 - e^{-3\pi r}\right).$$

Next we estimate I_+^2. By (24) we get

$$|I_+^2(r)| \leq 4e^{-2\pi r} \int_0^1 |g_r(\sqrt{-1} + t)| \mathrm{d}t.$$

Similarly to the analysis of I_+^1 we introduce the parameter ε and get

$$|I_+^2(r)| \leq 4\exp(2A + 2B\pi/r) e^{-2\pi r} \lim_{\varepsilon \to 0_+} \int_\varepsilon^{1-\varepsilon} |e^{r\Phi(\sqrt{-1}+t)}| \mathrm{d}t.$$

Here

$$|e^{r\Phi(\sqrt{-1}+t)}| = e^{-\pi r(1-2t)} \exp\left(-\frac{r}{\pi} \mathrm{Im}\left(\mathrm{Li}_2(e^{-2\pi} e^{2\pi\sqrt{-1}t}) \right) \right)$$

by (92), so by Lebesgue's dominated convergence theorem we get

$$|I_+^2(r)| \leq 4\exp(2A + 2B\pi/r) e^{-3\pi r} \int_0^1 e^{2\pi r t} \exp\left(-\frac{r}{\pi} \mathrm{Im}\left(\mathrm{Li}_2(e^{-2\pi} e^{2\pi\sqrt{-1}t}) \right) \right) \mathrm{d}t.$$

By definition of the dilogarithm we have

$$\mathrm{Im}\left(\mathrm{Li}_2(e^{-2\pi} e^{2\pi\sqrt{-1}t}) \right) = -\int_0^1 \frac{\mathrm{Arg}\left(1 - s e^{-2\pi} e^{2\pi\sqrt{-1}t}\right)}{s} \mathrm{d}s,$$

which is non-negative for $t \in [0,1/2]$. For $t \in [1/2,1]$ we use that

$$\mathrm{Im}\left(\mathrm{Li}_2(e^{-2\pi}e^{2\pi\sqrt{-1}t})\right) = \mathrm{Im}\left(\mathrm{Li}_2(e^{2\pi\sqrt{-1}t})\right) + \int_{1-e^{-2\pi}}^{1} \frac{\mathrm{Arg}\left(1 - se^{2\pi\sqrt{-1}t}\right)}{s}\mathrm{d}s,$$

where the last integral is positive. The first term is bounded from below by $-\sum_{n=1}^{\infty}\frac{1}{n^2} = -\frac{\pi^2}{6}$ by (22). We therefore end up with

$$\begin{aligned} |I_+^2(r)| &\leq 4\exp(2A + 2B\pi/r)e^{-(3-1/6)\pi r}\int_0^1 e^{2\pi r t}\mathrm{d}t \\ &= \frac{2}{\pi r}\exp(2A+2B\pi/r)e^{-(3-1/6)\pi r}\left(e^{2\pi r} - 1\right). \end{aligned}$$

Finally, we estimate I_+^3. Similarly to the other cases we get

$$|I_+^3(r)| \leq 2\exp(2A+2B\pi/r)\lim_{\varepsilon\to 0_+}\int_0^1 e^{-2\pi r t}\left|e^{r\Phi(1-\varepsilon+\sqrt{-1}t)}\right|\mathrm{d}t.$$

By (92) we have

$$\left|e^{r\Phi(1-\varepsilon+\sqrt{-1}t)}\right| = \exp\left(r\left[\pi(1-2\varepsilon)t - \frac{1}{\pi}\mathrm{Im}\left(\mathrm{Li}_2(e^{-2\pi t}e^{-2\pi\sqrt{-1}\varepsilon})\right)\right]\right),$$

leading to

$$|I_+^3(r)| \leq 2\exp(2A+2B\pi/r)\int_0^1 e^{-\pi r t}\mathrm{d}t = \frac{2}{\pi r}\exp(2A+2B\pi/r)\left(1 - e^{-\pi r}\right).$$

By letting $C_-^1 = [-\sqrt{-1},0]$, $C_-^2 = [1-\sqrt{-1},-\sqrt{-1}]$, and $C_-^3 = [1, 1-\sqrt{-1}]$ and

$$I_-^i(r) = \int_{C_-^i}(\tan(\pi r x) + \sqrt{-1})g_r(x)\mathrm{d}x$$

we find an upper bound for $|I_-^i(r)|$ identical with the upper bound for $|I_+^i(r)|$, $i = 1,2,3$, with the exception that $\exp(2A+2B\pi/r)$ should be replaced by $\exp(2A+4B\pi/r)$ in these bounds. To conclude we have shown that there exists a constant K_1 independent of r and ε such that

$$|J_+''(r,\varepsilon) + J_-''(r,\varepsilon)| \leq \sum_{i=1}^{3}\left(|I_+^i| + |I_-^i|\right) \leq \frac{K_1}{r}$$

for all $r \in \mathbb{Z}_{\geq 2}$. □

Proof of (28) By the remarks prior to the proof of (26) we have

$$J_\pm'(r,\varepsilon) = \mp\int_\varepsilon^{1-\varepsilon}\exp\left(r\Phi(t)\right)h_\gamma(t)\mathrm{d}t,$$

where

$$h_\gamma(t) = \exp\left(I_\gamma(\pi - 2\pi t) - I_\gamma(-\pi + 2\pi t)\right) - 1.$$

The integrand is continuous on $[0,1]$. Therefore

$$\left|J_\pm'(r,\varepsilon)\right| \leq \int_0^1 \exp\left(r\mathrm{Re}\left(\Phi(t)\right)\right)|h_\gamma(t)|\,\mathrm{d}t$$

for all $\varepsilon \in]0,\frac{1}{4r}[$. By (22) and (23) and the remarks prior to (23) we have

$$\mathrm{Re}\left(\Phi(t)\right) = \frac{1}{2\pi}\mathrm{Im}\left(\mathrm{Li}_2(e^{-2\pi\sqrt{-1}t}) - \mathrm{Li}_2(e^{2\pi\sqrt{-1}t})\right) = -\frac{1}{\pi}\mathrm{Cl}_2(2\pi t) \leq \frac{1}{2\pi}\mathrm{Vol}(4_1).$$

Therefore

$$|J'_{\pm}(r,\varepsilon)| \leq \exp\left(\frac{r}{2\pi}\mathrm{Vol}(4_1)\right)\int_0^1 |h_\gamma(t)|\,\mathrm{d}t.$$

By definition we have

$$h_\gamma(t) = \sum_{n=1}^{\infty}\frac{1}{n!}\left(I_\gamma(\pi-2\pi t) - I_\gamma(-\pi+2\pi t)\right)^n.$$

From Lemma 4.1 we get

$$|I_\gamma(\pi-2\pi t) - I_\gamma(-\pi+2\pi t)| \leq (Cf(t)+D)\,\gamma$$

for $t \in]0,1[$, where C and D are positive constants independent of γ and t, and

$$f(t) = \frac{1}{t} + \frac{1}{1-t}.$$

Since $f :]0,1[\to \mathbb{R}$ is bigger than or equal to 4 we can choose C so big that

$$|I_\gamma(\pi-2\pi t) - I_\gamma(-\pi+2\pi t)| \leq Cf(t)\gamma$$

for $t \in]0,1[$. From Lemma 4.1 we also have

$$|h_\gamma(t)| \leq \exp\left(|I_\gamma(\pi-2\pi t) - I_\gamma(-\pi+2\pi t)|\right) \leq \exp(4A+4B\pi/r)$$

for $t \in [0,1]$, where A and B are as in Lemma 4.1, so $\frac{\pi}{r}\exp(4A+4B\pi/r)$ is an upper bound for both of the integrals $\int_0^\gamma |h_\gamma(t)|\mathrm{d}t$ and $\int_{1-\gamma}^1 |h_\gamma(t)|\mathrm{d}t$ (for $r \geq 4$). Left is to evaluate (for $r \geq 7$)

$$\int_\gamma^{1-\gamma} |h_\gamma(t)|\mathrm{d}t \leq \sum_{n=1}^{\infty}\frac{C^n\gamma^n}{n!}\int_\gamma^{1-\gamma} f(t)^n\mathrm{d}t.$$

By using that

$$f(t)^n = \sum_{k=0}^{n}\binom{n}{k}\frac{1}{t^k}\frac{1}{(1-t)^{n-k}}$$

we get

$$\begin{aligned}
\int_\gamma^{1-\gamma} f(t)^n\mathrm{d}t &= \sum_{k=0}^{n}\binom{n}{k}\int_\gamma^{1-\gamma}\frac{1}{t^k}\frac{1}{(1-t)^{n-k}}\mathrm{d}t \\
&\leq \sum_{k=0}^{n}\binom{n}{k}\left(2^{n-k}\int_\gamma^{1/2}\frac{1}{t^k}\mathrm{d}t + 2^k\int_{1/2}^{1-\gamma}\frac{1}{(1-t)^{n-k}}\mathrm{d}t\right) \\
&\leq 2^n\sum_{k=0}^{n}\binom{n}{k}\left(\int_\gamma^{1/2}\frac{1}{t^k}\mathrm{d}t + \int_\gamma^{1/2}\frac{1}{t^{n-k}}\mathrm{d}t\right) \\
&\leq 2^{n+1}\left(\sum_{k=0}^{n}\binom{n}{k}\right)\int_\gamma^{1/2}\frac{1}{t^n}\mathrm{d}t = 2^{2n+1}\int_\gamma^{1/2}\frac{1}{t^n}\mathrm{d}t.
\end{aligned}$$

Here

$$\int_\gamma^{1/2}\frac{1}{t}\mathrm{d}t = -\mathrm{Log}(2) - \mathrm{Log}(\gamma) \leq \mathrm{Log}(r)$$

and

$$\int_\gamma^{1/2}\frac{1}{t^n}\mathrm{d}t = \frac{1}{n-1}\left(\frac{1}{\gamma^{n-1}} - 2^{n-1}\right) \leq \frac{1}{n-1}\frac{1}{\gamma^{n-1}}$$

for $n \geq 2$. Therefore

$$\begin{aligned}\int_{\gamma}^{1-\gamma} |h_\gamma(t)|\mathrm{d}t &\leq 2\gamma\left(4C\mathrm{Log}(r) + \sum_{n=2}^{\infty}\frac{(4C)^n}{(n-1)n!}\right)\\ &\leq \frac{2\pi}{r}\left(4C\mathrm{Log}(r) + \exp(4C) - 4C - 1\right).\end{aligned}$$

We conclude that there exists a constant K_2 independent of r and ε such that

$$|J_+'(r,\varepsilon) + J_-'(r,\varepsilon)| \leq K_2\frac{\mathrm{Log}(r)}{r}\exp\left(\frac{r}{2\pi}\mathrm{Vol}(4_1)\right),$$

for all $r \in \mathbb{Z}_{\geq 2}$. □

6.3. **Appendix C. The case M_0.** The manifold M_0 is the mapping torus of a torus with monodromy matrix

$$\begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix},$$

see [KK, p. 366]. The invariant $\tau_r(M_0)$ has been calculated by Jeffrey [J, Theorem 4.1]. This theorem gives the large r asymptotics of the invariant as well. In fact, we have

$$\tau_r(M_0) = \frac{1}{2} - \frac{1}{2\sqrt{5}} - \frac{1}{\sqrt{5}}\left(\exp\left(2\pi\sqrt{-1}r\left(-\frac{1}{5}\right)\right) + \exp\left(2\pi\sqrt{-1}r\frac{1}{5}\right)\right) \tag{93}$$

which at the same time can be taken as the large r asymptotics of the invariant. Let us relate this result to our contour integral formula for the invariant $\tau_r(M_0) = \bar{\tau}_r(M_0)$. By Lemma 3.2

$$\tau_r(M_0) = \frac{r}{4i}\int_{C_r^1}\cot(\pi r x)\left(\int_{C_r^2}\tan(\pi r y) f_{0,r}(x,y)\mathrm{d}y\right)\mathrm{d}x,$$

where

$$f_{0,r}(x,y) = \sin(\pi x)e^{-2\pi i r x y}\frac{S_{\pi/r}(-\pi + 2\pi(x-y))}{S_{\pi/r}(-\pi + 2\pi(x+y))}.$$

Following the discussion in Sect. 4 the relevant (shifted) phase functions to consider are given by

$$\Psi_0^{a,b}(x,y) = ax + by - xy + \frac{1}{4\pi^2}\left(\mathrm{Li}_2(e^{2\pi i(x+y)}) - Li_2(e^{2\pi i(x-y)})\right),$$

where a, b are certain integers. If we put $\Psi = \Psi_0^{a,b}$, then by (39) (x,y) is a critical point of Ψ if and only if

$$\begin{aligned} 0 &= 2\pi i(a-y) + \mathrm{Log}(1-zw) - \mathrm{Log}(1-zw^{-1}), \\ 0 &= 2\pi i(b-x) + \mathrm{Log}(1-zw) + \mathrm{Log}(1-zw^{-1}), \end{aligned} \tag{94}$$

where $z = e^{2\pi i x}$ and $w = e^{2\pi i y}$ as usual, and this set of equations implies that

$$\begin{aligned} w - z &= 1 - zw, \\ (1-zw)(w-z) &= zw, \end{aligned} \tag{95}$$

compare with (40) and (41). We note that the first of these equations is equivalent to

$$w - 1 = z(1-w)$$

so $w = 1$ or $z = -1$. For $z = -1$ we get $w^2 + 3w + 1 = 0$ so $w = \frac{-3\pm\sqrt{5}}{2}$. For $w = 1$ we find that $z^2 - 3z + 1 = 0$ so $z = \frac{3\pm\sqrt{5}}{2}$. However, only the point $(z,w) = ((3-\sqrt{5})/2, 1)$

satisfies that $zw, zw^{-1} \notin [1, \infty[$. For this point we find that $y \in \mathbb{Z}$ and from (94) we get that $y = a$. But then

$$\Psi(x, y) = ax + by - xy + \frac{1}{4\pi^2}\left(\mathrm{Li}_2(z) - \mathrm{Li}_2(z)\right) = yx + ba - xy = ba \in \mathbb{Z}.$$

Let $\bar{\rho}_{\theta,\varepsilon}$ be the nonabelian SU(2)–representations of π from Proposition 5.3, where $\theta \in [-1/3, -1/6] \cup [1/6, 1/3]$ and $\varepsilon \in \{\pm\}$. Here $\bar{\rho}_{\theta,\varepsilon}$ and $\bar{\rho}_{-\theta,\varepsilon}$ are conjugate. By (62), $\bar{\rho}_{\theta,\varepsilon}$ extends to a representation of $\pi_1(M_0)$ if and only if

$$L_\varepsilon(\theta) = 1.$$

But this happens if and only if $\theta = \pm 1/4$ for both $\varepsilon = +$ and $\varepsilon = -$, i.e. the set of conjugacy classes of nonabelian SU(2)–representations of $\pi_1(M_0)$ is $\left\{[\bar{\rho}_{1/4,-}], [\bar{\rho}_{1/4,+}]\right\}$.

By (74) the flat reducible SU(2)–connections on M_0 all have a Chern–Simons invariant equal to zero, so we conclude that the image set of the SU(2) Chern–Simons functional on M_0 has at most three elements. By [KK, Theorem 5.6 and precedent text] we can therefore conclude that the set of Chern–Simons invariants of flat SU(2)–connections on M_0 is

$$\left\{0 \pmod{\mathbb{Z}}, -\frac{1}{5} \pmod{\mathbb{Z}}, \frac{1}{5} \pmod{\mathbb{Z}}\right\}. \tag{96}$$

In particular, the Chern–Simons invariants of $[\bar{\rho}_{1/4,\pm}]$ are $\left\{-\frac{1}{5} \pmod{\mathbb{Z}}, \frac{1}{5} \pmod{\mathbb{Z}}\right\}$. We note that (93) and (96) prove the AEC for the invariants $\tau_r(M_0)$.

By (68) and (69) we have $\beta_\pm(1/4) = f_\pm$, where $f_- = 0$ and $f_+ = 1$. By Proposition 5.7 and (69) we find

$$\mathrm{CS}(\bar{\rho}_{1/4,\pm}) = \pm\frac{1}{6} - \frac{1}{\pi}\int_{1/6}^{1/4} \mathrm{Arg}(L_\pm(t))\mathrm{d}t \pmod{\mathbb{Z}},$$

where we use that $L_\pm(t) \in S^1$. By (87) we have

$$\int_{1/6}^{1/4} \mathrm{Arg}(L_-(t))\mathrm{d}t = -\int_{1/6}^{1/4} \mathrm{Arg}(L_+(t))\mathrm{d}t$$

so we finally get

$$\mathrm{CS}(\bar{\rho}_{1/4,\pm}) = \pm\left(\frac{1}{6} - \frac{1}{\pi}\int_{1/6}^{1/4} \mathrm{Arg}(L_+(t))\mathrm{d}t\right) \pmod{\mathbb{Z}}.$$

Note that $\mathrm{Im}(L_+(t)) < 0$ on $]1/6, 1/4[$ so

$$-\frac{1}{12} = \frac{1}{\pi}(-\pi)(1/4 - 1/6) < \frac{1}{\pi}\int_{1/6}^{1/4} \mathrm{Arg}(L_+(t))\mathrm{d}t < 0.$$

Therefore

$$1/6 - \frac{1}{\pi}\int_{1/6}^{1/4} \mathrm{Arg}(L_+(t))\mathrm{d}t \in]\frac{1}{6}, \frac{1}{4}[.$$

Since this value $\pmod{\mathbb{Z}}$ belongs to the set $\{\pm 1/5 \pmod{\mathbb{Z}}\}$ we conclude that it is equal to $1/5$ so

$$\frac{1}{\pi}\int_{1/6}^{1/4} \mathrm{Arg}(L_-(t))\mathrm{d}t = -\frac{1}{\pi}\int_{1/6}^{1/4} \mathrm{Arg}(L_+(t))\mathrm{d}t = \frac{1}{30}. \tag{97}$$

Let us finally calculate the value of $\Psi = \Psi_0^{a,b}$ in the critical points corresponding to the solutions $(z, w) = ((3 + \sqrt{5})/2, 1)$ and $(z, w) = \left(-1, \frac{-3\pm\sqrt{5}}{2}\right)$ to (95). Since the set of solutions to (95) is in one-one correspondence with the set of nonabelian

$SL(2,\mathbb{C})$–representations of $\pi_1(M_0)$ by the proof of Theorem 5.8 and since the subset of solutions (z,w) with $z \in S^1$ and $w \in]-\infty,0[$ corresponds to the set of $SL(2,\mathbb{C})$–representations which are equivalent to $SU(2)$–representations we see that the points $(z,w) = \left(-1, \frac{-3\pm\sqrt{5}}{2}\right)$ correspond to nonabelian $SU(2)$–representations of $\pi_1(M_0)$ while the points $(z,w) = \left(\frac{3\pm\sqrt{5}}{2}, 1\right)$ correspond to nonabelian $SL(2,\mathbb{C})$–representations of $\pi_1(M_0)$ which are not equivalent to $SU(2)$–representations.

For $(z,w) = (e^{2\pi i x}, e^{2\pi i y}) = ((3+\sqrt{5})/2, 1)$ we find again that $y = a$ and then $\Psi(x,y) = ab$ (independent of the choice of branch of the dilogarithm along $]1,\infty[$).

Finally, let $(z,w) = (e^{2\pi i x}, e^{2\pi i y}) = \left(-1, \frac{-3\pm\sqrt{5}}{2}\right)$. The real values of the right-hand sides of (94) do not depend on a and b. Taking the imaginary values of these equations we get

$$\begin{aligned} 0 &= 2\pi\left(a - \mathrm{Re}(y)\right) + \mathrm{Im}\left(\mathrm{Log}(1+w) - \mathrm{Log}(1+w^{-1})\right), \\ 0 &= 2\pi(b-x) + \mathrm{Im}\left(\mathrm{Log}(1+w) + \mathrm{Log}(1+w^{-1})\right). \end{aligned}$$

The second of these equations is equivalent to

$$x - b = \frac{1}{2\pi}\left(\mathrm{Arg}(1+w) + \mathrm{Arg}(1+w^{-1})\right) = \frac{1}{2}$$

for both $w = \frac{-3\pm\sqrt{5}}{2}$, and the first is equivalent to

$$a - \mathrm{Re}(y) = \frac{1}{2\pi}\left(\mathrm{Arg}(1+w^{-1}) - \mathrm{Arg}(1+w)\right) = \begin{cases} \frac{1}{2}, & w = \frac{-3+\sqrt{5}}{2}, \\ -\frac{1}{2}, & w = \frac{-3-\sqrt{5}}{2}. \end{cases}$$

We have

$$\Psi(x,y) = ax + by - xy + \frac{1}{4\pi^2}\left(\mathrm{Li}_2(|w|) - \mathrm{Li}_2(1/|w|)\right),$$

and since this is real by Corollary 5.14, we get

$$\Psi(x,y) = ax + (b-x)\mathrm{Re}(y) + \frac{1}{4\pi^2}\mathrm{Re}\left(\mathrm{Li}_2(|w|) - \mathrm{Li}_2(1/|w|)\right).$$

Here

$$\begin{aligned} ax + (b-x)\mathrm{Re}(y) &= (b-x)\left(\mathrm{Re}(y) - a\right) + ab = ab + \frac{1}{2}\left(a - \mathrm{Re}(y)\right) \\ &= ab + \begin{cases} \frac{1}{4}, & w = \frac{-3+\sqrt{5}}{2}, \\ -\frac{1}{4}, & w = \frac{-3-\sqrt{5}}{2}. \end{cases} \end{aligned}$$

For $z \in \mathbb{C} \setminus [0,\infty[$ we have

$$\mathrm{Li}_2(z) + \mathrm{Li}_2(1/z) = -\frac{\pi^2}{6} - \frac{1}{2}\mathrm{Log}^2(-z).$$

This identity e.g. follows by differentiating the difference of the two sides in the identity, showing that this difference is constant on $\mathbb{C} \setminus [0,\infty[$, and then evaluating in $z = -1$ using that $\mathrm{Li}_2(-1) = -\pi^2/12$. Therefore

$$\mathrm{Li}_2(t) = -\frac{\pi^2}{6} - \frac{1}{2}\mathrm{Log}^2(-t) - \mathrm{Li}_2(t^{-1}) \tag{98}$$

for $t > 1$ for a branch of Li_2 continuously extended across $]1,\infty[$. Let $w_\pm = \frac{-3\pm\sqrt{5}}{2}$. We note that

$$w_+ w_- = 1. \tag{99}$$

Moreover, by [Lew, Formula (1.20) p. 7],

$$\mathrm{Li}_2\left(\frac{3-\sqrt{5}}{2}\right) = \frac{\pi^2}{15} - \mathrm{Log}^2\left(\frac{1+\sqrt{5}}{2}\right). \tag{100}$$

Note also that

$$\left(\frac{1+\sqrt{5}}{2}\right)^2 = \frac{3+\sqrt{5}}{2}. \tag{101}$$

Assume that $w = w_- = \frac{-3-\sqrt{5}}{2}$. Then, by (98),

$$\mathrm{Li}_2(|w|) = -\frac{\pi^2}{6} - \frac{1}{2}\mathrm{Log}^2(-|w|) - \mathrm{Li}_2(|w|^{-1}),$$

where $\mathrm{Log}(-|w|) = \mathrm{Log}(|w|) + i\pi$, so

$$\mathrm{Li}_2(|w|) = \frac{\pi^2}{2} - \frac{\pi^2}{6} - \frac{1}{2}\mathrm{Log}^2(|w|) - \mathrm{Li}_2(|w|^{-1}) - i\pi\mathrm{Log}(|w|).$$

But then

$$\mathrm{Li}_2(|w|) - \mathrm{Li}_2(|w|^{-1}) = \frac{\pi^2}{2} - \frac{\pi^2}{6} - \frac{1}{2}\mathrm{Log}^2(|w|) - 2\mathrm{Li}_2(|w|^{-1}) - i\pi\mathrm{Log}(|w|)$$

Here $|w|^{-1} = \frac{3-\sqrt{5}}{2}$ by (99) so by (100) and (101) we get

$$\mathrm{Li}_2(|w|) - \mathrm{Li}_2(|w|^{-1}) = \frac{\pi^2}{2} - \frac{\pi^2}{6} - \frac{2\pi^2}{15} - i\pi\mathrm{Log}(|w|) = \frac{\pi^2}{5} - i\pi\mathrm{Log}(|w|)$$

By (99) we conclude that

$$\mathrm{Li}_2(|w_\pm|) - \mathrm{Li}_2(|w_\pm|^{-1}) = \mp\frac{\pi^2}{5} - i\pi\mathrm{Log}(|w_\pm|). \tag{102}$$

For $w = w_\pm$ we therefore get

$$\Psi(x,y) = ab \pm \frac{1}{4} \mp \frac{1}{20} = ab \pm \frac{1}{5}.$$

We have thus shown that the set of values $\pmod{\mathbb{Z}}$ of $\Psi_0^{a,b}$ in its critical points is identical with the set (96) of Chern–Simons invariants of flat SU(2)–connections on M_0 for arbitrary $a, b \in \mathbb{Z}$. Note here that we use the identities (97) and (102) in the proof of Theorem 5.9 to handle the cases $\theta = \pm 1/4$, so we can not here refer to this theorem. The identity (102) was proved by using the explicit value of the dilogarithm in $(3-\sqrt{5})/2$, cf. (100). We note that only very few explicit values of the dilogaritm are known, see [Lew, Chap 1].

6.4. **Appendix D. Proof of Lemma 5.17.** Let us begin by showing the identitites (80) and (82). Let $\theta \in I$ and let $u = u_\pm(\theta)$, $Q_i = Q_i^\pm(\theta)$ and $t = e^{4\pi i\theta}$ and get

$$\begin{aligned} Q_1Q_2 &= \left(1-(1+u)^{-1}t\right)\left(1-(1+u)t\right) = 1 - t\left(1+u+(1+u)^{-1}\right) + t^2 \\ &= -t(1+u)^{-1}\left((1+u)^2 - (t+t^{-1})(u+1) + 1\right) = t, \end{aligned}$$

where the last equality follows by the fact that $\phi(t,u) = 0$, where ϕ is given by (57).

To show (82) we observe that

$$\begin{aligned} \frac{Q_1Q_3}{Q_2} &= \frac{Q_3Q_1^2}{Q_1Q_2} = t^{-1}Q_3Q_1^2 \\ &= t^{-1}(1+u)\left(1-t(1+u)^{-1}\right)^2 = t^{-1}(1+u) + t(1+u)^{-1} - 2 \end{aligned}$$

by (80). Now $\phi(t,u)=0$ implies that

$$t(1+u)^{-1}=t^2+1-t-t(u+1)$$

leading to the identity

$$\frac{Q_1Q_3}{Q_2}=-1+t^{-1}-2t+t^2+u(t^{-1}-t)=L_\pm(\theta).$$

To prove the identities (79) and (81) it is necessary to examine the arguments of the functions $Q_i^\pm(\theta)$, $i=1,2$. By Lemma 5.18 we note that

$$Q_1^\pm(\theta)=Q_2^\mp(\theta) \tag{103}$$

for $\theta\in I$.

Assume first that $\theta\in[1/6,1/3]$. An elementary calculation shows that

$$\begin{aligned} 1+u_+(\theta)&\in[-1,(\sqrt{5}-3)/2], \\ 1+u_-(\theta)&\in[-(3+\sqrt{5})/2,-1] \end{aligned} \tag{104}$$

for $\theta\in[1/6,1/3]$ and $1+u_\pm(\theta)=-1$ if and only if $\theta\in\{1/6,1/3\}$. In particular, $1+u_\pm(\theta)$ is negative. We therefore get

$$\mathrm{Im}\,(Q_1)=|1+u|^{-1}\sin(4\pi\theta)\begin{cases} >0, & \theta\in[1/6,1/4[, \\ =0, & \theta=1/4, \\ <0, & \theta\in]1/4,1/3]. \end{cases}$$

By (78), $\mathrm{Re}(Q_1)=1-(1+u)^{-1}\cos(4\pi\theta)$. Since $1+u$ is negative we see that $\mathrm{Re}(Q_1)$ have the same sign as $\cos(4\pi\theta)-(1+u)$, where $\mathrm{sign}(0)=0$ as usual. By (104) we conclude that

$$\mathrm{Re}\left(Q_1^-(\theta)\right)>0$$

for all $\theta\in[1/6,1/3]$. Let us next consider Q_1^+. First note that

$$\cos(4\pi\theta)-u_+(\theta)-1=\frac{1}{2}-\sqrt{\cos^2(4\pi\theta)-\cos(4\pi\theta)-\frac{3}{4}}.$$

We therefore get that $\mathrm{Re}\left(Q_1^+(\theta)\right)$ has the opposite sign as $\cos^2(4\pi\theta)-\cos(4\pi\theta)-1$. By the assumption on θ we have $\cos(4\pi\theta)\in[-1,-1/2]$, and we therefore get

$$\mathrm{Re}\left(Q_1^+(\theta)\right)\begin{cases} >0, & \theta\in[1/6,\theta_0[\cup]1/2-\theta_0,1/3], \\ =0, & \theta\in\{\theta_0,1/2-\theta_0\}, \\ <0, & \theta\in]\theta_0,1/2-\theta_0[, \end{cases}$$

where $\theta_0\in]1/6,1/4[$ is the unique element such that $\cos(4\pi\theta_0)=(1-\sqrt{5})/2\in]-1,-1/2[$ is the negative solution to $t^2-t-1=0$.

Let $\psi_i^\pm(\theta)\in]-\pi,\pi]$ be the principal argument of $Q_i^\pm(\theta)$. Then the above analysis shows, also using (103), that

$$\psi_2^-(\theta)=\psi_1^+(\theta)\begin{cases} \in]0,\frac{\pi}{2}[, & \theta\in[\frac{1}{6},\theta_0[, \\ =\frac{\pi}{2}, & \theta=\theta_0, \\ \in]\frac{\pi}{2},\pi[, & \theta\in]\theta_0,\frac{1}{4}[, \\ =\pi, & \theta=\frac{1}{4}, \\ \in]-\pi,-\frac{\pi}{2}[, & \theta\in]\frac{1}{4},\frac{1}{2}-\theta_0[, \\ =-\frac{\pi}{2}, & \theta=\frac{1}{2}-\theta_0, \\ \in]-\frac{\pi}{2},0[, & \theta\in]\frac{1}{2}-\theta_0,\frac{1}{3}], \end{cases} \tag{105}$$

and

$$\psi_2^+(\theta) = \psi_1^-(\theta) \begin{cases} \in]0, \frac{\pi}{2}[, & \theta \in [\frac{1}{6}, \frac{1}{4}[, \\ = 0, & \theta = \frac{1}{4}, \\ \in]-\frac{\pi}{2}, 0[, & \theta \in]\frac{1}{4}, \frac{1}{3}], \end{cases} \tag{106}$$

so

$$\psi_1^\pm(\theta) + \psi_2^\pm(\theta) \in \begin{cases}]0, \pi[, & \theta \in [\frac{1}{6}, \theta_0[, \\ ]\frac{\pi}{2}, \frac{3\pi}{2}[, & \theta \in]\theta_0, \frac{1}{4}[, \\ ]\frac{\pi}{2}, \pi], & \theta = \frac{1}{4}, \\ ]-\frac{3\pi}{2}, -\frac{\pi}{2}[, & \theta \in]\frac{1}{4}, \frac{1}{2} - \theta_0[, \\ ]-\pi, 0[, & \theta \in [\frac{1}{2} - \theta_0, \frac{1}{3}]. \end{cases}$$

By (80) we have

$$\psi_1^\pm(\theta) + \psi_2^\pm(\theta) \in 4\pi\theta + 2\pi\mathbb{Z},$$

so we conclude that

$$\psi_1^\pm(\theta) + \psi_2^\pm(\theta) = 4\pi\theta$$

for all $\theta \in [1/6, 1/3]$ proving (79) for these θ.

Next assume that $\theta \in [-1/3, -1/6]$. First observe that

$$Q_i^\pm(-\theta) = \overline{Q_i^\pm(\theta)}, \quad \theta \in I \setminus \{\pm 1/4\}, \tag{107}$$

and

$$Q_i^\pm(-1/4) = Q_i^\pm(1/4) \tag{108}$$

for $i = 1, 2$. By (108) we immediately get that (79) holds for $\theta = -1/4$. For $\theta \in [-1/3, -1/6] \setminus \{-1/4\}$, (79) follows by (107) and the fact that $\mathrm{Log}(\bar{p}) = \overline{\mathrm{Log}(p)}$ for $p \in \mathbb{C}\setminus]-\infty, 0]$.

Note that (81) is true if we choose $e_\pm(\theta) \in \mathbb{Z}$ such that

$$\psi_1^\pm(\theta) + \pi - \psi_2^\pm(\theta) - e_\pm(\theta) 2\pi \in]-\pi, \pi].$$

By (105) and (106) we have that $\psi_1^\pm(\theta) - \psi_2^\pm(\theta) \in]-\pi, \pi]$, and we conclude that we have to put $e_\pm(\theta) = 0$ if and only if $\psi_1^\pm(\theta) \le \psi_2^\pm(\theta)$ and $e_\pm(\theta) = 1$ elsewhere. By (105) and (106) we conclude that $e_-(1/4) = 0$ and $e_+(1/4) = 1$.

Assume that $\theta \in [1/6, 1/3] \setminus \{1/4\}$. Then $\psi_1^\pm(\theta)$ and $\psi_2^\pm(\theta)$ both belong to either $]-\pi, 0[$ or to $]0, \pi[$. We use this fact together with the fact that $\cot :]m\pi, (m+1)\pi[\to \mathbb{R}$ is strictly decreasing for any $m \in \mathbb{Z}$. In fact, $\cot(\psi_i) = \frac{\mathrm{Re}(Q_i)}{\mathrm{Im}(Q_i)}$ so

$$\begin{aligned} \cot(\psi_1) &= \cot(4\pi\theta) + \frac{|1+u|}{\sin(4\pi\theta)}, \\ \cot(\psi_2) &= \cot(4\pi\theta) + \frac{|1+u|^{-1}}{\sin(4\pi\theta)}. \end{aligned}$$

By this we find that

$$\operatorname{sign}\left(\psi_1^\pm(\theta) - \psi_2^\pm(\theta)\right) = \operatorname{sign}\left(\sin(4\pi\theta)\left(1 - (1 + u_\pm(\theta))^2\right)\right).$$

Since $(1 + u_+(\theta))^2 \le 1$ and $(1 + u_-(\theta))^2 \ge 1$ with equalities if and only if $\theta \in \{1/6, 1/3\}$, we get $\psi_1^\pm(\theta) = \psi_2^\pm(\theta)$ for $\theta \in \{1/6, 1/3\}$ and

$$\psi_1^\varepsilon(\theta) < \psi_2^\varepsilon(\theta)$$

for $\theta \in]1/6, 1/4[$ and $\varepsilon = -$ or for $\theta \in]1/4, 1/3[$ and $\varepsilon = +$. Moreover,

$$\psi_1^\varepsilon(\theta) > \psi_2^\varepsilon(\theta)$$

for $\theta \in]1/6, 1/4[$ and $\varepsilon = +$ or for $\theta \in]1/4, 1/3[$ and $\varepsilon = -$. We therefore get that (81) is true if we put $e_\pm(\theta) = 0$ for $\theta \in \{1/6, 1/3\}$ and

$$e_+(\theta) = \begin{cases} 1, & \theta \in]1/6, 1/4[, \\ 0, & \theta \in]1/4, 1/3[, \end{cases}$$

and let $e_-(\theta) = 1 - e_+(\theta)$ for $\theta \in]1/6, 1/3[\setminus\{1/4\}$.

Let us finally consider the case $\theta \in [-1/3, -1/6]$. First observe that

$$Q_3^\pm(-\theta) = Q_3^\pm(\theta) \tag{109}$$

for all $\theta \in I$. By this and (108) we conclude that $e_\pm(-1/4) = e_\pm(1/4)$. For $\theta \in [-1/3, -1/6] \setminus \{-1/4\}$ we get by (107) and (109) that

$$\begin{aligned} &\mathrm{Log}\left(Q_1^\pm(\theta)\right) + \mathrm{Log}\left(Q_3^\pm(\theta)\right) - \mathrm{Log}\left(Q_2^\pm(\theta)\right) \\ &= \mathrm{Log}\left(Q_3^\pm(\theta)\right) - \overline{\mathrm{Log}\left(Q_3^\pm(\theta)\right)} + \overline{\mathrm{Log}\left(Q_1^\pm(-\theta)\right) + \mathrm{Log}\left(Q_3^\pm(-\theta)\right) - \mathrm{Log}\left(Q_2^\pm(-\theta)\right)} \\ &= 2i\mathrm{Im}\left(\mathrm{Log}\left(Q_3^\pm(\theta)\right)\right) + \overline{\left(\mathrm{Log}\left(\frac{Q_1^\pm(-\theta)Q_3^\pm(-\theta)}{Q_2^\pm(-\theta)}\right) + e_\pm(-\theta)2\pi i\right)}. \end{aligned}$$

By using that Q_3 is negative and that $L_\pm(\theta) \in \mathbb{C}\setminus] - \infty, 0]$ for $\theta \in]1/6, 1/3[$ we get for $\theta \in] - 1/3, -1/6[\setminus\{-1/4\}$ that

$$\mathrm{Log}\left(Q_1^\pm(\theta)\right) + \mathrm{Log}\left(Q_3^\pm(\theta)\right) - \mathrm{Log}\left(Q_2^\pm(\theta)\right) = \mathrm{Log}\left(\frac{Q_1^\pm(\theta)Q_3^\pm(\theta)}{Q_2^\pm(\theta)}\right) + \left(1 - e_\pm(-\theta)\right)2\pi i,$$

so we conclude that $e_\pm(\theta) = 1 - e_\pm(-\theta)$ for these θ. Finally we get for $\theta \in \{-1/3, -1/6\}$ that $Q_1^\pm(\theta) = Q_2^\pm(\theta)$ so (81) is satisfied for $e_\pm(\theta) = 0$ for these θ.

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