Knots and Quantum Gravity:
Progress and Prospects

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Abstract

Recent work on the loop representation of quantum gravity has revealed previously unsuspected connections between knot theory and quantum gravity, or more generally, 3-dimensional topology and 4-dimensional generally covariant physics. We review how some of these relationships arise from a 'ladder of field theories' including quantum gravity and BF theory in 4 dimensions, Chern-Simons theory in 3 dimensions, and the G/G gauged WZW model in 2 dimensions. We also describe the relation between link (or multiloop) invariants and generalized measures on the space of connections. In addition, we pose some research problems and describe some new results, including a proof (due to Sawin) that the Chern-Simons path integral is not given by a generalized measure.

1 Introduction

The relation between knots and quantum gravity was discovered in the course of a fascinating series of developments in mathematics and physics. In 1984, Jones [34] announced the discovery of a new link invariant, which soon led to a bewildering profusion of generalizations. It was clear early on that these new invariants were intimately related to conformal field theory in 2 dimensions. Atiyah [9], however, conjectured that there should be an intrinsically 3-dimensional definition of these invariants using gauge theory. Witten [53] gave a heuristic proof of Atiyah's conjecture by deriving the Jones polynomial and its generalizations from Chern-Simons theory. The basic idea is simply that the vacuum expectation values of Wilson loops in Chern-Simons theory are link invariants because of the diffeomorphism-invariance of the theory. To calculate these expectation values, however, Witten needed to use the relation between Chern-Simons theory and a conformal field theory known as the Wess-Zumino-Witten (or WZW) model.

In parallel to this work, a new approach to quantum gravity was being developed, initiated by Ashtekar's [1] discovery of the 'new variables' for general relativity. In this approach, the classical configuration space is a space of connections, and states of the quantum theory are (roughly speaking) measures on the space of connections which satisfy certain constraints: the Gauss law, the diffeomorphism constraint, and the Hamiltonian constraint. In an effort to find such states, Rovelli and Smolin [46] used a 'loop representation' in which one works, not with the measures per se, but with the expectation values of Wilson loops with respect to these measures. In these terms, the diffeomorphism constraint amounts to requiring that the Wilson loop expectation values are link invariants. In itself this was not surprising; the surprise was that knot theory could be applied to obtain explicit solutions of the Hamiltonian constraint, as well!

Indeed, in Rovelli and Smolin's original paper they gave a heuristic construction assigning to each isotopy class of unoriented links a solution of all the constraints of quantum gravity in the loop representation. Later, Kodama [37] showed how to obtain another sort of solution using Chern-Simons theory. From Witten's work it is clear that in the loop representation this solution is just the Jones polynomial — or more precisely, the closely related Kauffman bracket invariant [35].

At first these developments may appear to be an elaborate series of coincidences. Some of the mystery is removed when we note that the 'Chern-Simons state' of quantum gravity is the only state of a simpler diffeomorphism-invariant theory in 4 dimensions known as BF theory [22, 33]. However, a truly systematic explanation would require understanding the following 'ladder' of field theories as a unified structure: general relativity and BF theory in dimension 4, Chern-Simons theory in dimension 3, and the WZW model in dimension 2. The concept of a ladder of field theories has appeared in other contexts and appears to be an important one [9, 51]. In Section 1, after an introduction to the 'new variables', we review this ladder of field theories and its relation to the new knot invariants.

In addition to understanding the Chern-Simons state as a bridge between knot theory and quantum gravity, there is the much larger task of making the loop representation of quantum gravity into a mathematically rigorous theory and justifying, if possible, Rovelli and Smolin's construction of solutions of the constraint equations from link classes. One key aspect of this task is to understand the precise sense in which diffeomorphism-invariant measures on the space of connections correspond to isotopy invariants of links (or more generally, 'multiloops'). In Section 2 we review recent work by Ashtekar, Isham, Lewandowski and the author [6, 7, 13, 14, 15, 38] on this problem.

In what follows we will not concentrate on the loop representation *per se*, as it is already the subject of a number of excellent review articles [2, 3, 25, 39, 48] and books [4].

2 The New Variables and the Dimensional Ladder

Traditionally, general relativity has been viewed as a theory in which a metric is the basic field. In these terms, the Einstein-Hilbert action with cosmological constant term is given by

$$S_{EH}(g) = \int_M (R + 2\Lambda) \,\mathrm{vol}, \tag{1}$$

where R is the Ricci scalar curvature and vol is the volume form associated to the metric g on the oriented 4-manifold M. The equation we get by varying g is, of course,

$$R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu} - \Lambda g_{\mu\nu} = 0.$$

Recent advances in quantizing the theory, however, have taken advantage of the techniques of gauge theory by emphasizing the role of *connections*. This approach is also what allows one to relate general relativity to the 'ladder' of simpler field theories shown below.

$$\begin{array}{lccc}
\text{4d:} & \textbf{General relativity} & \rightarrow & BF\ \textbf{theory} \\
 & & & \downarrow \\
\text{3d:} & & & \textbf{Chern-Simons theory} \\
 & & & \downarrow \\
\text{2d:} & \textbf{WZW model} & \rightarrow & G/G\ \textbf{gauged WZW model}
\end{array}$$

Figure 1. The dimensional ladder

Historically, the first step towards viewing general relativity as a gauge theory was the Palatini formalism. (For a discussion of various Lagrangians for general relativity, see the review article by Peldan [41].) In this approach, we fix an oriented bundle $\mathcal{T}$ over M (usually called the 'internal space') that is isomorphic to TM and equipped with a Lorentzian metric η, and we assume that the spacetime metric g is obtained from η via an isomorphism $e\colon TM \rightarrow \mathcal{T}$. We may also think of e as a $\mathcal{T}$-valued 1-form, the 'soldering form', and in the Palatini formalism the basic fields are this soldering form and a connection A on $\mathcal{T}$ preserving the metric η, usually called a 'Lorentz connection'. Interestingly, however, most of what we say below makes sense even when $e\colon TM \rightarrow \mathcal{T}$ is *not* an isomorphism. Thus the Palatini formalism provides a generalization of general relativity to situations where the metric $g(v, w) = \eta(e(v), e(w))$ is degenerate.

To clarify the relationship to gauge theory, it is useful to work with the algebra of differential forms on M taking values in the exterior algebra bundle $\Lambda\mathcal{T}$. In particular, the orientation and internal metric on $\mathcal{T}$ gives rise to an 'internal volume form', i.e.

a section of $\Lambda^4\mathcal{T}$, and this in turn gives a map from $\Lambda^4\mathcal{T}$-valued forms to ordinary differential forms, which we denote by 'tr'. The Palatini action is then given by

$$S_{Pal}(A,e) = \int_M \mathrm{tr}(e\wedge e\wedge F + \frac{\Lambda}{12} e\wedge e\wedge e\wedge e) \qquad (2)$$

where we use η to regard the curvature F of A as a $\Lambda^2\mathcal{T}$-valued 2-form on M. When A corresponds to the Levi-Civita connection of g via the isomorphism $e\colon TM\to\mathcal{T}$, the Palatini action equals the Einstein-Hilbert action. More importantly, we can obtain Einstein's equations by computing the variation of the Palatini action. Using d_A to denote the exterior covariant derivative of $\Lambda\mathcal{T}$-valued forms, we have:

$$\begin{aligned} \delta S_{Pal} &= \int \mathrm{tr}(2\delta e\wedge e\wedge F + e\wedge e\wedge\delta F + \frac{\Lambda}{3}\delta e\wedge e\wedge e\wedge e) \\ &= \int \mathrm{tr}(2\delta e\wedge(e\wedge F + \frac{\Lambda}{6} e\wedge e\wedge e) + e\wedge e\wedge d_A\delta A) \\ &= 2\int \mathrm{tr}(((e\wedge F + \frac{\Lambda}{6} e\wedge e\wedge e)\wedge\delta e - e\wedge d_A e\wedge\delta A) \end{aligned}$$

where we have ignored boundary terms. The classical equations of motion are thus

$$e\wedge F + \frac{\Lambda}{6} e\wedge e\wedge e = 0, \quad e\wedge d_A e = 0.$$

If e is nondegenerate, the latter equation implies that $d_A e = 0$, i.e., the soldering form is flat, which means that the connection on TM corresponding to A via the isomorphism e is torsion-free, hence equal to the Levi-Civita connection of g. Then the first equation is equivalent to Einstein's equation (with cosmological constant).

The self-dual formulation of general relativity is based on a slight variant of the Palatini action, the Plebanski action, that is especially suited to canonical quantum gravity. The self-dual formulation applies very naturally to complex general relativity, and some extra work is needed to restrict to real-valued metrics. (In what follows we will gloss over these very important 'reality conditions', on which progress is just beginning [3, 8].) The idea is to work with a *complex-valued* soldering form, that is, 1-form on M with values in the complexified bundle $\mathbf{C}\mathcal{T}$, and a *self-dual* connection A_+. To understand this concept of self-duality, note that the internal metric η extends naturally to $\mathbf{C}\mathcal{T}$, making the orthonormal frame bundle of $\mathbf{C}\mathcal{T}$ into a principal bundle P with structure group $\mathrm{SO}(4,\mathbf{C})$. Now assume we have a spin structure for $\mathbf{C}\mathcal{T}$, that is, a double cover $\tilde{P}$ of P with structure group $\widetilde{SO}(4,\mathbf{C}) = \mathrm{SL}(2,\mathbf{C})\times\mathrm{SL}(2,\mathbf{C})$. Then $\tilde{P}$ is the sum $P_+\oplus P_-$ of 'right-handed' and 'left-handed' principal bundles with structure group $\mathrm{SL}(2,\mathbf{C})$. This splitting is what lets us define chiral spinors on M. It is also closely related to duality, since by using the isomorphism between $\Lambda^2\mathbf{C}\mathcal{T}$ and $\mathrm{ad}P$ it lets us write a section ω of $\Lambda^2\mathbf{C}\mathcal{T}$ as a sum of two parts, which are precisely the self-dual and anti-self-dual parts with respect to the 'internal' Hodge star operator $*$ coming from the internal metric and orientation on $\mathbf{C}\mathcal{T}$:

$$\omega = \omega_+ + \omega_-, \qquad *\omega_\pm = \pm i\omega_\pm.$$

We call connections on P_+ 'self-dual' because, fixing one, we can identify all the rest with $\Lambda^2 \mathbf{C}\mathcal{T}$-valued 1-forms that are internally self-dual. Note that a connection A on P is equivalent to a pair of connections $A_\pm$ on $P_\pm$, which we call its self-dual and anti-self-dual parts. The curvature F of A is then a $\Lambda^2 \mathbf{C}\mathcal{T}$-valued 2-form which is the sum of the curvatures $F_\pm$ of $A_\pm$. Moreover, we have

$$*F_\pm = \pm i F_\pm .$$

The Plebanski action is then:

$$S_{Ple}(A_+, e) = \int_M \mathrm{tr}(e \wedge e \wedge F_+ + \frac{\Lambda}{12} e \wedge e \wedge e \wedge e). \tag{3}$$

Just as before, the classical equations of motion are

$$e \wedge F_+ + \frac{\Lambda}{6} e \wedge e \wedge e = 0, \quad e \wedge d_{A_+} e = 0.$$

To relate these equations to the Palatini formalism, we interpret A_+ as the self-dual part of A, so that F_+ is the self-dual part of F. When e is nondegenerate, the second equation then implies that A_+ is the self-dual part of the connection on P corresponding via e to the Levi-Civita connection on M. The algebraic Bianchi identity then implies that $e \wedge F_+ = e \wedge F$, so the first equation is equivalent to the corresponding equation in the Palatini formalism, i.e., Einstein's equation.

Now let us turn to BF theory, which is a diffeomorphism-invariant gauge theory that makes sense in any dimension. Suppose that the spacetime manifold M is oriented and n-dimensional, and that P is a G-bundle over M, where G is a connected Lie group and Lie algebra of G is equipped with an invariant bilinear form which we write as 'tr'. Then the basic fields in BF theory are a connection A on P and an $(n-2)$-form B with values in $\mathrm{ad}P$, and the action for the theory is

$$\int_M \mathrm{tr}(B \wedge F).$$

After attention was drawn to it by the work of Blau and Thompson [22] and Horowitz [33], this theory has been extensively studied in dimensions 2, 3, and 4. In dimension 2, it is closely related to Yang-Mills theory [54]. In dimension 3, it has gravity in the Palatini formalism as a special case [5, 52]. In dimension 4, it is also known as 'topological gravity' when we take $G = \mathrm{SL}(2, \mathbf{C})$ and take P to be the bundle P_+ used in the self-dual formulation of general relativity [29, 30]. Mathematically, BF theory is closely related to moduli spaces of flat connections, and thereby to the Ray-Singer torsion, the Alexander-Conway polynomial invariant of links, and the Casson invariant of homology 3-spheres [21, 22, 28, 47].

In what follows we will focus on dimension 4, and consider a variant of the BF action that includes a $B \wedge B$ term:

$$S_{BF}(A, B) = \int_M \mathrm{tr}(B \wedge F + \frac{\Lambda}{12} B \wedge B). \tag{4}$$

Ignoring boundary terms, the variation of the action is then

$$\delta S_{BF} = \int \mathrm{tr}((F + \frac{\Lambda}{6}B) \wedge \delta B - d_A B \wedge \delta A),$$

where $d_A B$ denotes the exterior covariant derivative of B. Setting $\delta S_{BF} = 0$ we obtain the classical equations of motion:

$$F + \frac{\Lambda}{6}B = 0, \quad d_A B = 0.$$

Note that the case $\Lambda \neq 0$ is very different from the case $\Lambda = 0$. When $\Lambda \neq 0$, the second equation follows from the first one and the Bianchi identity, so A is *arbitrary* and it determines B. When $\Lambda = 0$, A must be *flat* and B is any section with $d_A B = 0$.

Note that BF theory is very similar to general relativity in its self-dual formulation, with B playing the role of $e \wedge e$. To compare these theories more precisely, we will write simply P for the 'right-handed' $\mathrm{SL}(2, \mathbf{C})$ principal bundle P_+ discussed above, and drop the subscript '+' on the A and F fields. Now, there is a mapping from the space of fields (A, e) for general relativity to the space of fields (A, B) for BF theory (with $G = \mathrm{SL}(2, \mathbf{C})$) given by

$$(A, e) \mapsto (A, B) = (A, e \wedge e).$$

If $(A, e \wedge e)$ is a solution of the BF equations of motion, then (A, e) is a solution of Einstein's equations. Of course, we obtain only a limited class of solutions of Einstein's equations this way: for $\Lambda = 0$ we obtain precisely the flat solutions, while for $\Lambda \neq e$ we obtain those with $F = -\frac{\Lambda}{6} e \wedge e$.

Amazingly, BF theory appears to yield solutions of the constraint equations of *quantum* gravity by a similar mechanism. Moreover, these solutions are closely related to well-known link invariants. No formalism for quantum gravity has been worked out to the point where we can feel full confidence in these results, but the work of various authors using the connection [37] and loop [27] representations, as well as the BRST formalism [30], all seems to point in the same direction. In what follows we will describe these results in terms of Dirac's approach to canonical quantization of constrained systems.

Suppose, then, that $M = \mathbf{R} \times S$, and identify S with the slice $\{t = 0\}$. Working in temporal gauge, both classical BF theory and classical general relativity in the Ashtekar formalism can be described in terms of a 'kinematical' phase space $T^*\mathcal{A}$ together with certain constraints. Here the configuration space $\mathcal{A}$ consists of connections on the bundle $P|_S$. A tangent vector $\delta A \in T_A\mathcal{A}$ can be identified with an $\mathrm{ad}P$-valued 1-form on S, so a cotangent vector can be identified with an $\mathrm{ad}P$-valued 2-form B, using the pairing

$$\langle B, \delta A \rangle = \int_S \mathrm{tr}(B \wedge \delta A).$$

In BF theory, one obtains a point in the kinematical phase space from a solution of the equations of motion by restricting A and B to S, while in general relativity one does the same with A and the self-dual part of $e \wedge e$, regarded as an $\mathrm{ad}P$-valued 2-form. In general relativity, however, it is conventional to use the isomorphism

$$\Lambda^2 T^*M \cong TM \otimes \Lambda^3 T^*M$$

to think of $(e \wedge e)_+$ as an $\mathrm{ad}P$-valued 'vector density', usually written $\tilde{E}$. This is precisely where the advantage of the self-dual formalism over the Palatini one appears: one can attempt a similar trick in the Palatini formalism, but in that case, extra constraints negate the advantage of working with this formalism. In the self-dual formalism, no conditions on $\tilde{E}$ need hold for it to come from a complex soldering form e.

Since the kinematical phase space for BF theory is the same as that for general relativity, the difference between the theories lies in the constraints. To describe these, it is handy to introduce indices $i, j, k, \ldots$ labeling a basis of sections of TS, and indices $a, b, c, \ldots$ labeling an orthonormal basis of sections of $\mathrm{ad}P|_S$. (Note that TS and $P|_S$ are trivial so we can find global bases of sections.) In BF theory the canonically conjugate variables can then be written as A_i^a and a vector density $\tilde{B}_a^i = \frac{1}{2}\epsilon^{ijk} B_{jka}$, and the constraints are the Gauss law

$$\mathcal{G}^a = \partial_i \tilde{B}^{ia} + [A_i, \tilde{B}^i]^a = 0$$

and

$$\mathcal{C}_{ij}^a = F_{ij}^a + \frac{\Lambda}{6}\epsilon_{ijk}\tilde{B}^{ka} = 0.$$

In general relativity, on the other hand, working with the lapse and shift as Lagrange multipliers, the canonically conjugate variables are A_i^a and $\tilde{E}_a^i$, and the constraints are the Gauss law

$$\mathcal{G}^a = \partial_i \tilde{E}^{ia} + [A_i, \tilde{E}^i]^a,$$

together with the Hamiltonian and diffeomorphism constraints:

$$\mathcal{H} = \epsilon_{abc}\tilde{E}^{ia}\tilde{E}^{jb}F_{ij}^c + \frac{\Lambda}{6}\epsilon_{abc}\epsilon_{ijk}\tilde{E}^{ia}\tilde{E}^{jb}\tilde{E}^{jc}, \qquad \mathcal{H}_j = \tilde{E}_a^i F_{ij}^a.$$

We now turn to the canonical quantization of general relativity and BF theory. (We emphasize that the remarks above could be made rigorous in a rather straightforward way, while the rest of this section is heuristic in character.) In either theory, we begin with a 'kinematical state space' consisting of functions on $\mathcal{A}$, the space of connections on $P|_S$. In BF theory, we then quantize the canonically conjugate fields A_i^a and $\tilde{B}_a^i$, making them into operators on the kinematical state space by

$$(\hat{A}_i^a(x)\psi)(A) = A_i^a(x)\psi(A), \quad (\hat{\tilde{B}}{}_a^i(x)\psi)(A) = \frac{\delta\psi}{\delta A_i^a(x)}(A).$$

For a function on $\mathcal{A}$ to represent a physical state, it must be annihilated by the quantized constraints:

$$\hat{\mathcal{G}}^a \psi = 0, \quad \hat{\mathcal{C}}^a_{ij} \psi = 0.$$

Classically the Gauss law generates gauge transformations, so the best interpretation of the first equation is simply that ψ is invariant under small gauge transformations. The second equation is a first-order partial differential equation on $\mathcal{A}$:

$$\frac{\Lambda}{6} \epsilon_{ijk} \frac{\delta}{\delta A_{ka}} \psi = -F^a_{ij} \psi.$$

For $\Lambda \neq 0$ this has a single solution, the so-called 'Chern-Simons state':

$$\psi_{CS}(A) = e^{-\frac{6}{\Lambda} \int_S \mathrm{tr}(A \wedge dA + \frac{2}{3} A \wedge A \wedge A)},$$

which is automatically invariant under small gauge transformations. For $\Lambda = 0$, any gauge-invariant ψ supported on the space of *flat* connections is a solution. We call such solutions 'flat states'. For $\Lambda = 0$ we can also use the 'constrain before quantizing' strategy and describe the flat states as functions on the moduli space of flat connections on $P|_S$, which has the advantage over $\mathcal{A}$ of being finite-dimensional. (For more on the flat states, see the work of Blencowe [24].)

One can attempt to quantize gravity in a similar fashion, defining operators on $\mathbf{H}_{kin}$ by

$$(\hat{A}^a_i(x)\psi)(A) = A^a_i(x)\psi(A), \quad (\hat{\tilde{E}}^i_a(x)\psi)(A) = \frac{\delta \psi}{\delta A^a_i(x)}(A),$$

and seeking solutions of the constraint equations:

$$\hat{\mathcal{G}}^a \psi = \hat{\mathcal{H}}_j \psi = \hat{H} \psi = 0.$$

The remarkable thing is that the solutions we found for BF theory are also annihilated by these constraints, at least if we take the operator ordering for $\hat{\mathcal{H}}$ given by

$$\hat{\mathcal{H}} = \epsilon^{abc} \frac{\delta}{\delta A^a_i} \frac{\delta}{\delta A^b_j} F_{ijc} + \frac{\Lambda}{6} \epsilon^{abc} \epsilon_{ijk} \frac{\delta}{\delta A^a_i} \frac{\delta}{\delta A^b_j} \frac{\delta}{\delta A^c_k}.$$

The reason is simple. In classical general relativity the constraint $\mathcal{G}^a$ generates gauge transformations, while $\mathcal{H}_j$ generates diffeomorphisms, so we should interpret the quantized constraint equations $\hat{G}^a \psi = \hat{\mathcal{H}}_j \psi = 0$ as saying that ψ is invariant under small gauge transformations and diffeomorphisms. A mathematically more proper way to state this is to say that ψ is invariant under small automorphisms of the bundle $P|_S$. (It is unclear whether one should also demand invariance under 'large' bundle automorphisms; we will not do so here.) The solutions we found for BF theory are indeed invariant under small bundle automorphisms! The Hamiltonian constraint, on the other hand, can be expressed in terms of the constraints of BF theory by

$$\hat{\mathcal{H}} = \epsilon^{abc} \frac{\partial}{\partial A_{ia}} \frac{\partial}{\partial A_{jb}} \hat{\mathcal{C}}_{ijc},$$

if we identify $\tilde{E}^{ia}$ in general relativity with $\tilde{B}^{ia}$ in BF theory. Thus $\hat{\mathcal{C}}^a_{ij}\psi = 0$ implies $\hat{\mathcal{H}}\psi = 0$.

In short, the relationship between BF theory and general relativity gives us some *explicit* solutions of the constraint equations of quantum gravity: the Chern-Simons state when $\Lambda \neq 0$, and the flat states when $\Lambda = 0$. What is the physical significance of these solutions? As noted by Kodama [37], if $S = S^3$, the Chern-Simons state appears to represent a 'quantized deSitter universe' (or anti-deSitter, depending on the sign of Λ). Smolin and Soo have recently done some fascinating work on the 'problem of time' using this idea [49]. Similarly, if $S = \mathbf{R}^3$ it appears that the single flat state represents a 'quantized Minkowski space'! However, there has been some debate over whether the Chern-Simons state is normalizable, and the same could be asked of the flat states. We will have more to say about this question in the next section, but it can only really be settled when we understand the problem of the inner product in quantum gravity. It is worth noting here that some approaches to the inner product problem rely heavily on ideas from knot theory and 3-dimensional topology. For example, Rovelli has drawn inspiration from the Turaev-Viro theory, a topological quantum field theory in 3 dimensions, to give a formula for the physical inner product [45], which unfortunately is purely formal at present. An alternative strategy, which is mathematically rigorous but physically more radical, is to split S into two manifolds with boundary, and to use the Chern-Simons state on S to define inner products of 'relative states' on each of the two halves [15, 31].

Now let us return to the Chern-Simons state of BF theory with arbitrary gauge group G. An interesting relation to knot theory shows up when we try to compute the 'loop transform' of this state. Given loops γ_i in S, the loop transform of ψ_{CS} is formally given by

$$\hat{\psi}_{CS}(\gamma_1, \ldots, \gamma_n) = \int_{\mathcal{A}} \prod_{i=1}^{n} \mathrm{tr}(Te^{\int_{\gamma_i} A})\, \psi_{CS}(A)\, \mathcal{D}A,$$

where $\mathcal{D}A$ is purely formal 'Lebesgue measure' on $\mathcal{A}$. Since ψ_{CS} is invariant under small bundle automorphisms, if we assume $\mathcal{D}A$ shares this invariance property we can conclude that $\hat{\psi}_{CS}$ is a 'multiloop invariant', that is, it should not change when we apply a given small diffeomorphism to all of the loops γ_i. In particular, if we restrict to *links* (embedded collections of loops), $\hat{\psi}_{CS}$ should give a link invariant.

This reasoning is merely heuristic, due to the mysterious nature of '$\mathcal{D}A$', but in fact Witten [53] was able to compute the link invariant corresponding to $\hat{\psi}_{CS}$ for $G = \mathrm{SU}(n)$, and similar computations are now possible for many other groups. For $\mathrm{SU}(2)$ the result is simply the Kauffman bracket, which is a link invariant defined by the skein relations shown below, and normalized so that its value on the empty link is 1.

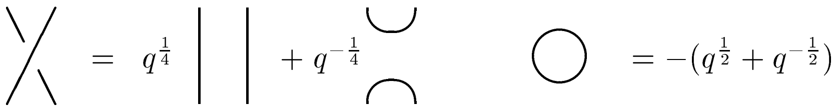

Figure 2. Skein relations for the Kauffman bracket

Here

$$q = e^{2\pi i/(k+2)}, \qquad k = \frac{24\pi i}{\Lambda}.$$

Only for integer k is ψ_{CS} invariant under large gauge transformations. It is important to note that the Kauffman bracket is an invariant of *framed* links, reflecting the fact that one must regularize the Wilson loops to properly calculate their expectation value

For the groups $\mathrm{SU}(n)$ one obtains a link invariant generalizing the Kauffman bracket known as the HOMFLY polynomial, while for $\mathrm{SO}(n)$ one obtains yet another invariant, the Kauffman polynomial [35, 43]. All of these link invariants are also defined by skein relations. Since ψ_{CS} may be defined as the unique function on $\mathcal{A}$ annihilated by the constraint $\hat{\mathcal{C}}^a_{ij}$, while $\hat{\psi}_{CS}$ is determined (at least on links) by the skein relations, it appears that the skein relations are simply a rewriting of the constraint $\hat{\mathcal{C}}^a_{ij}$ in the language of Wilson loops. The author has speculated on the implications of this idea for physics elsewhere [16], but it also suggests the following essentially mathematical problem:

Problem 1. *Derive the skein relations for the Kauffman and HOMFLY polynomials as directly as possible from the corresponding* $\mathrm{SU}(n)$ *and* $\mathrm{SO}(n)$ *BF theories in 4 dimensions. (Hint: study the existing work on deriving the skein relations via loop deformations [26], and consider the possibility of a relation to the theory of surfaces immersed in 4-manifolds [29].)*

It is often tacitly assumed that the Chern-Simons state for $\mathrm{SL}(2,\mathbf{C})$, which is the one relevant to quantum gravity, has the Kauffman bracket as its loop transform just as the $\mathrm{SU}(2)$ Chern-Simons state does. Perturbative calculations on S^3 appear to support this [18], but nonperturbatively, especially on 3-manifolds with nontrivial fundamental group, the situation is far from clear:

Problem 2. *Describe Chern-Simons theory with noncompact gauge group (in particular,* $\mathrm{SL}(2,\mathbf{C})$*) as a topological quantum field theory satisfying axioms similar to those listed by Atiyah [10], and compute the vacuum expectation values of Wilson loops in this theory. (Hint: see the work of Bar-Natan and Witten [19, 55].)*

Let us now turn to how one computes the link invariant corresponding to $\hat{\psi}_{CS}$. For reasons of space we will be very sketchy here. First, writing

$$\psi_{CS}(A) = e^{-\frac{6}{\Lambda} S_{CS}(A)},$$

the quantity

$$S_{CS}(A) = \int_S \mathrm{tr}(A \wedge dA + \frac{2}{3} A \wedge A \wedge A) \tag{5}$$

can be interpreted as the action for a 3-dimensional field theory, Chern-Simons theory. Note that the 3-manifold S, which played the role of 'space' in BF theory, now plays the role of 'spacetime', and that the loop transform of ψ_{CS} can now be thought of as a path integral. To compute this path integral, one chops up S (and the link in S) into simple pieces, deals with these pieces, and then glues them together using the axioms of a topological quantum field theory. In particular, it is useful to begin by considering Chern-Simons theory on a spacetime $S = \mathbf{R} \times \Sigma$, with Σ a Riemann surface. This lets us descend the dimensional ladder yet another rung, since in this situation the states of Chern-Simons theory correspond exactly to the conformal blocks of the WZW model [53], and we can derive the Kauffman bracket skein relations from the transformation properties of n-point functions under elements of the mapping class group. However, more recently it has become clear that the more fundamental relation is that between Chern-Simons theory and a 2-dimensional *topological* quantum field theory, the G/G gauged WZW model [23]. From this point of view, the WZW model itself serves mainly as a computational tool.

What is the real meaning of the dimensional ladder? Most importantly, one climbs down it by considering 'boundary values'. For example, on 4-manifolds without boundary, when Λ is nonzero S_{BF} is unchanged by infinitesimal transformations of the form

$$A \mapsto A + \delta A, \qquad B \mapsto B - \frac{6}{\Lambda} d_A \delta A,$$

since such transformations change the Lagrangian by an exact form:

$$\delta \mathrm{tr}(B \wedge F + \frac{\Lambda}{12} B \wedge B) \;\; = \;\; -\frac{6}{\Lambda} d\, \mathrm{tr}(\delta A \wedge F)$$

This symmetry is the reason why any connection A gives a solution of the classical equations of motion. On a 4-manifold with boundary, the exact form gives a boundary term. Up to a constant factor, this is precisely the variation of the Chern-Simons action:

$$\delta S_{CS}(A) = 2 \int_S \mathrm{tr}(\delta A \wedge F).$$

(It is the relation between the BF Lagrangian and the 2nd Chern form $\mathrm{tr}(F \wedge F)$ that makes this computation work [51].) In a similar but subtler manner, $S_{CS}(A)$ is invariant under small gauge transformations when the 3-manifold S has no boundary, but by considering how it changes when S has boundary we may derive the action of the G/G gauged WZW model [23].

Problem 3. *Give, if possible, a construction of BF theory in 4 dimensions as a topological quantum field theory. (In the $\Lambda = 0$ case, the Atiyah axioms [10] will need to be generalized to treat situations where the Hilbert space of states is infinite-dimensional.)*

We conclude this section with a few words about the $\Lambda \to 0$ limit of the Chern-Simons state and Vassiliev invariants. If we regard ψ_{CS} as a function of Λ, the $\Lambda \to 0$ limit appears to be very singular. And indeed, we have seen that the character of BF theory becomes very different when Λ vanishes. However, when we consider *imaginary* Λ, corresponding to integer k, the formula for $\hat{\psi}_{CS}$ becomes an oscillatory integral which can be approximated as $\Lambda \to 0$ using the method of stationary phase [53]. The points of stationary phase are, by the above formula for δS_{CS}, precisely the *flat* connections. Thus we expect that as $\Lambda \to 0$, the Chern-Simons state approaches a particular flat state. Indeed, the HOMFLY and Kauffman polynomials can all be expanded as power series in Λ, with coefficients being link invariants of a special sort known as invariants of finite type, or Vassiliev invariants [17]. If we accept the assumption that the Chern-Simons state for $\mathrm{SL}(2, \mathbf{C})$ corresponds to the Kauffman bracket, at least on S^3, we obtain a fascinating relation between quantum gravity and Vassiliev invariants. For more on this, we urge the reader to the references [11, 27, 32, 36, 42].

3 Multiloop Invariants and Generalized Measures

In the previous section, much of the discussion of *quantum* gravity in 4 dimensions was heuristic in character. In particular, we imagined starting with a kinematical state space $\mathbf{H}_{kin}$ consisting of functions on the space of connections $\mathcal{A}$, and defining the physical state space $\mathbf{H}_{phys}$ to consist of those $\psi \in \mathbf{H}_{kin}$ satisfying the Gauss law, diffeomorphism constraint, and Hamiltonian constraint. To make this rigorous, we should try to give a precise definition $\mathbf{H}_{kin}$, and then make sense of the constraints.

As already noted, the Gauss law and diffeomorphism constraints have such a simple geometrical meaning that we can make sense of them quite nicely without defining operators corresponding to these constraints, or even choosing a specific definition of $\mathbf{H}_{kin}$. Namely, we can take these constraints to say that ψ is invariant under small automorphisms of the bundle $P|_S$. It is far more difficult to treat the Hamiltonian constraint properly. In what follows we will discuss a particular way of definining $\mathbf{H}_{kin}$, first suggested by Rovelli and Smolin under the name of the 'loop representation' [46], and subsequently made rigorous by Ashtekar, Isham, Lewandowski and the author [6, 7, 13, 14, 15, 38]. According to the original heuristic work of Rovelli and Smolin [46], a large space of solutions of the Hamiltonian constraint can be described explicitly using the loop representation! However, finding a rigorous formulation of the Hamiltonian constraint in the loop representation of quantum gravity remains one of the outstanding challenges of the subject.

At the heuristic level, the key ingredient of the loop representation is the loop transform

$$\hat{\psi}(\gamma_1, \ldots, \gamma_n) = \int_{\mathcal{A}} \prod_{i=1}^{n} \mathrm{tr}(Te^{\int_{\gamma_i} A})\, \psi(A)\, \mathcal{D}A$$

taking functions on the space of connections to functions of multiloops. Unfortunately, the 'Lebesgue measure' $\mathcal{D}A$ is a purely formal object! There is, however, a way to avoid this problem. The idea is to treat states in $\mathbf{H}_{kin}$ not as *functions* on the space of connections, but as 'generalized measures' on the space of connections. This amounts to treating the combination $\psi(A)\mathcal{D}A$ as a single object, to be made sense of in its own right. As we shall see, there is a way to do this which gives us access to a large class of $\psi \in \mathbf{H}_{kin}$ that are invariant under small bundle automorphisms. Since much of what follows is applicable to any smooth manifold M and principal G-bundle P over M, where G is a compact connected Lie group, we will work at this level of generality, and let $\mathcal{A}$ denote the space of smooth connections on P.

Working with measures on an infinite-dimensional space like $\mathcal{A}$ is a notoriously tricky business, but if we take the attitude that the job of a measure is to let us integrate functions, we can simply specify an algebra of functions on $\mathcal{A}$ that we would like to integrate, and define generalized measures on $\mathcal{A}$ to be continuous linear functionals on this algebra. In the case at hand we want this algebra to contain the Wilson loop functions $\mathrm{tr}(Te^{\int_\gamma A})$. So, suppose that γ is a piecewise smooth path in M, and let $\mathcal{A}_\gamma$ denote the space of smooth maps $F\colon P_{\gamma(a)} \to P_{\gamma(b)}$ that are compatible with the right action of G on P:

$$F(xg) = F(x)g.$$

Note that for any connection $A \in \mathcal{A}$, the parallel transport map

$$Te^{\int_\gamma A} : P_{\gamma(a)} \to P_{\gamma(b)}$$

lies in $\mathcal{A}_\gamma$. Of course, if we fix a trivialization of P at the endpoints of γ, we can identify $\mathcal{A}_\gamma$ with the group G. Now let $\mathrm{Fun}_0(\mathcal{A})$ be the algebra of functions on $\mathcal{A}$ generated by those of the form

$$f(Te^{\int_\gamma A})$$

where f is a continuous function on $\mathcal{A}_\gamma$. Let $\mathrm{Fun}(\mathcal{A})$ denote the completion of $\mathrm{Fun}_0(\mathcal{A})$ in the sup norm:

$$\|\psi\|_\infty = \sup_{A \in \mathcal{A}} |\psi(A)|.$$

It is easy to check that the Wilson loops lie in this algebra, taking the trace in any finite-dimensional representation of G. Thus we define the space of 'generalized measures' on $\mathcal{A}$ to be the dual $\mathrm{Fun}(\mathcal{A})^*$. Given a function $\psi \in \mathrm{Fun}(\mathcal{A})$, we can write $\mu(\psi)$ as an integral

$$\int_{\mathcal{A}} \psi(A)\, d\mu(A)$$

if we wish to emphasize that μ serves the same purpose as a measure on $\mathcal{A}$.

We can now make the relation between knot theory and diffeomorphism-invariant gauge theory precise, as follows. For simplicity we consider only the case $G = \mathrm{SU}(n)$. Suppose μ is a generalized measure on $\mathcal{A}$ that is invariant under all small bundle automorphisms. Then the quantity

$$\hat{\mu}(\gamma_1, \ldots, \gamma_n) = \int_{\mathcal{A}} \prod_{i=1}^{n} \mathrm{tr}(Te^{\int_{\gamma_i} A}\, d\mu(A),$$

where we take traces in the fundamental representation, is a multiloop invariant. Conversely, knowing the multiloop invariant $\hat{\mu}$ determines μ uniquely! A basic problem is:

Problem 4. *Characterize the multiloop invariants that arise from generalized measures on the space $\mathcal{A}$ of smooth connections on a given bundle P.*

It is worth emphasizing that while $\hat{\mu}$ restricts to a link invariant, the link invariant is not enough to determine $\hat{\mu}$. The point is that generalized measures on $\mathcal{A}$ can give multiloop invariants that detect singularities: self-intersections, corners, cusps and the like [13]. This may be a good thing for quantum gravity, since the Hamiltonian constraint is also sensitive to self-intersections [46]. Also, within knot theory itself, more and more attention is being paid to multiloops with self-intersections [17, 20].

It is typical that the measures appearing in quantum field theory (either as path-integrals or as states in the canonical formalism) are not supported on the space of smooth fields[40], but on a larger space of 'distributional fields'. And indeed, generalized measures on $\mathcal{A}$ can alternatively be described as honest measures on a space $\overline{\mathcal{A}}$ of 'generalized connections' containing $\mathcal{A}$ as a dense subset. These 'generalized connections' are objects that allow parallel transport along paths in M, but without some of the smoothness conditions characteristic of connections in $\mathcal{A}$. In particular, like a connection, a generalized connection A associates to each piecewise smooth path $\gamma\colon [a,b] \to M$ an element of $\mathcal{A}_\gamma$, which we write formally as $Te^{\int_\gamma A}$. Generalized connections are only required to satisfy the following property: given any finite set of piecewise smooth paths γ_i, $1 \le i \le n$, and any continuous function $F\colon \prod A_{\gamma_i} \to \mathbf{C}$, if

$$F(Te^{\int_{\gamma_1} A}, \ldots, Te^{\int_{\gamma_n} A}) = 0$$

for all smooth connections $A \in \mathcal{A}$, then the same equation holds for any generalized connection. (It follows that parallel transport using generalized connections composes when one composes paths, is independent of the parametrization of the path, and so on.) We equip $\overline{\mathcal{A}}$ with the weakest topology such that all the maps

$$A \mapsto Te^{\int_\gamma A}$$

are continuous from $\overline{\mathcal{A}}$ to $\mathcal{A}_\gamma$ (identifying the latter space with G). In this topology $\overline{\mathcal{A}}$ is a compact Hausdorff space, and $\mathcal{A}$ is dense in $\overline{\mathcal{A}}$. Finally, generalized measures on $\mathcal{A}$ are in one-to-one correspondence with measures on $\overline{\mathcal{A}}$. (Here and in what follows by 'measure' we implicitly mean 'finite regular Borel measure.')

Now, it is common in quantum field theory to avoid certain infinities in integrals over $\mathcal{A}$ by integrating instead over $\mathcal{A}/\mathcal{G}$, where $\mathcal{G}$ is the gauge group of P. It is worth digressing for a moment to explain why this is unnecessary here. While much work on the loop representation uses generalized measures on $\mathcal{A}/\mathcal{G}$, these are in one-to-one correspondence with gauge-invariant generalized measures on $\mathcal{A}$, as follows. First, define the 'holonomy C*-algebra' $\mathrm{Fun}(\mathcal{A}/\mathcal{G})$ to be the algebra of functions on $\mathcal{A}/\mathcal{G}$ that pull back under the quotient map $p\colon \mathcal{A} \to \mathcal{A}/\mathcal{G}$ to elements of $\mathrm{Fun}(\mathcal{A})$. The functions $p^*\psi \in \mathrm{Fun}(\mathcal{A})$ one obtains this way are precisely the gauge-invariant elements of $\mathrm{Fun}(\mathcal{A})$. Next, define a generalized measure on $\mathcal{A}/\mathcal{G}$ to be an element of the dual $\mathrm{Fun}(\mathcal{A}/\mathcal{G})^*$. Then given a gauge-invariant generalized measure $\tilde{\mu}$ on $\mathcal{A}$, there is a generalized measure μ on $\mathcal{A}/\mathcal{G}$ given by

$$\mu(\psi) = \tilde{\mu}(p^*\psi)$$

for all $\psi \in \mathrm{Fun}(\mathcal{A}/\mathcal{G})$. Conversely, given a generalized measure μ on $\mathcal{A}/\mathcal{G}$, we can obtain the corresponding gauge-invariant generalized measure $\tilde{\mu}$ on $\mathcal{A}$ as follows. There is a rigorous way to average over the gauge group action, giving a continuous linear map $q\colon \mathrm{Fun}(\mathcal{A}) \to \mathrm{Fun}(\mathcal{A}/\mathcal{G})$ with the property that qp^* is the identity on $\mathrm{Fun}(\mathcal{A}/\mathcal{G})$. Given μ, we then define $\tilde{\mu}$ by

$$\tilde{\mu}(\psi) = \mu(q\psi)$$

for all $\psi \in \mathrm{Fun}(\mathcal{A})$. (These results follow from a slight extension of published work [15].)

Almost everything one does with measures can be done with generalized measures. This should not be surprising, since generalized measures on $\mathcal{A}$ *are* measures on $\overline{\mathcal{A}}$. However, it is rarely necessary to refer to the big space $\overline{\mathcal{A}}$. For example, a generalized measure μ is said to be 'strictly positive' if $\psi \geq 0$ and $\psi \neq 0$ implies $\mu(\psi) > 0$. Given a strictly positive generalized measure $\tilde{\mu}$ on $\mathcal{A}$, we can form a Hilbert space $L^2(\mathcal{A}, \mu)$ by completing $\mathrm{Fun}(\mathcal{A})$ in the norm

$$\|\psi\|_2 = \mu(\overline{\psi}\psi)^{1/2}.$$

If in addition $\tilde{\mu}$ is invariant under some group, then this group will have a unitary representation on $L^2(\mathcal{A}, \tilde{\mu})$. In particular, if $\tilde{\mu}$ is gauge-invariant, the corresponding generalized measure μ on $\mathcal{A}/\mathcal{G}$ will also be strictly positive, allowing us to form $L^2(\mathcal{A}/\mathcal{G}, \mu)$ in a similar fashion, and $L^2(\mathcal{A}/\mathcal{G}, \mu)$ will be isomorphic as a Hilbert space to the subspace of gauge-invariant elements of $L^2(\mathcal{A}, \tilde{\mu})$.

How does one *construct* generalized measures on $\mathcal{A}$, however? Without a way to do this, the theory would be of little interest. There are various ways; unfortunately, most of them currently require one to work with piecewise analytic paths rather than piecewise smooth paths as we have done so far. (The reason is that piecewise smooth paths can have horribly complicated self-intersections.) Everything we have said so far about the loop representation is still true if we assume that M is real-analytic and all paths are piecewise analytic; the bundle P and the connections in $\mathcal{A}$ can still be merely smooth. Henceforth we will assume this is the case, and define $\mathrm{Diff}(M)$ to consist of *analytic* diffeomorphisms of M, and $\mathrm{Aut}(P)$ to consist of bundle automorphisms that act on the base space M by analytic diffeomorphisms.

Problem 5. *Determine which of the results below can be generalized to the smooth category.*

The most basic recipe for constructing generalized measures is a nonlinear version of the theory of 'cylinder measures' widely used to study linear quantum fields. Interestingly, this recipe is based on ideas from lattice gauge theory. In lattice gauge theory one approximates the space of connections on $\mathbf{R}^n$ by the space of connections on a lattice in $\mathbf{R}^n$, where a connection on the lattice assigns a group element to each edge of the lattice. In the present diffeomorphism-invariant context we must consider all graphs embedded in the manifold M. An 'embedded graph' ϕ in M is a collection analytic paths $\phi_i\colon [0,1] \to M$, $1 \le i \le n$, called 'edges', such that:

1. for all i, ϕ_i is an embedding when restricted to $(0,1)$,
2. for all $i \neq j$, $\phi_i[0,1]$ and $\phi_j[0,1]$ intersect, if at all, only at their endpoints.

Given an embedded graph ϕ, we define the space $\mathcal{A}_\phi$ of connections on ϕ as follows:

$$\mathcal{A}_\phi = \prod_{i=1}^n \mathcal{A}_{\phi_i}.$$

If we trivialize P at the endpoints of the edges of ϕ, we can identify $\mathcal{A}_\phi$ with a product of copies of G.

Now, given embedded graphs ϕ and ψ, let us write $\phi \hookrightarrow \psi$ if every edge of ϕ is, up to reparametrization, a product of edges of ψ and their inverses. If $\phi \hookrightarrow \psi$, there is a natural map from $\mathcal{A}_\psi$ onto $\mathcal{A}_\phi$. We say that a family of measures $\{\mu_\phi\}$ on the spaces $\mathcal{A}_\phi$ is 'consistent' if whenever $\phi \hookrightarrow \psi$, the measure μ_ψ pushes forward to the measure μ_ϕ under this natural map. Every generalized measure on $\mathcal{A}$ uniquely determines a consistent family of measures $\{\mu_\phi\}$. Conversely — and this is how one can construct generalized measures — every consistent family of measures $\{\mu_\phi\}$ that is uniformly bounded in the usual norm determines a unique generalized measure on $\mathcal{A}$.

For example, if one uses products of copies of the normalized Haar measure on G to define measures on the spaces $\mathcal{A}_\phi$, one can easily check the consistency and boundedness conditions and obtain a generalized measure $\tilde{\mu}$ on $\mathcal{A}$ called the 'uniform' generalized measure [15]. This is a kind of partial substitute for the nonexistent

Lebesgue measure $\mathcal{D}A$. In particular, $\tilde{\mu}$ is strictly positive and invariant under all automorphisms of the bundle P. It therefore gives rise to a generalized measure on $\mathcal{A}/\mathcal{G}$, the 'Ashtekar-Lewandowski' generalized measure [7].

Moreover, given a function $\psi \in \mathrm{Fun}(\mathcal{A})$ that is invariant under small bundle automorphisms, the product $\psi\tilde{\mu}$ will be a generalized measure invariant under small automorphisms, or in other words, a solution to the Gauss law and diffeomorphism constraints. We do not expect to find many solutions this way, though; there are simply not enough functions ψ with this property. However, a more sophisticated version of this approach *does* give many solutions, indeed, one for each isotopy class of links [3]! It would be very interesting to know whether, as in the heuristic work of Rovelli and Smolin, these are also solutions of the Hamiltonian constraint.

One can use the same basic recipe to construct other generalized measures on $\mathcal{A}$ that are invariant under small bundle automorphisms. Examples include those whose loop transforms are multiloop invariants detecting singularities [13].

Let us conclude by returning to the exact solutions we discussed in the previous section: the Chern-Simons state and flat states. Are these given by generalized measures on the space of connections? In the case of the flat states the answer is yes: it is easy to see that every measure on the moduli space of flat connections on P gives a generalized measure on $\mathcal{A}$ that is invariant under small bundle automorphisms [13].

For the Chern-Simons state the question is not quite well-posed as it stands! The problem is that the Kauffman bracket of a link depends on a framing, while the multiloop invariants coming from generalized measures do not. One strategy to deal with framing issues is to work with an algebra generated by regularized Wilson loop observables, such as the 'tube algebra' [14]. This leads to an alternate definition of generalized measure, and such generalized measures determine framed link invariants. However, the following argument due to Sawin [50] shows that the Kauffman bracket cannot come from such a generalized measure, at least not for q a root of unity near 1.

Suppose there were such a generalized measure corresponding to the Kauffman bracket for some root of unity q very close to 1. If there were, for some constant $C > 0$ the Kauffman bracket would satisfy $|\langle K\rangle| < C$ for all framed knots K. However, let T be the trefoil knot (with any framing). Since $\langle T\rangle = (-A^5 - A^{-3} + A^{-7})\langle\circ\rangle$ where $A = q^{1/4}$ is the principal branch of the fourth root and $\circ$ denotes the unknot, for q sufficiently close to 1 we have $|\langle T\rangle| > |\langle\circ\rangle|$. On the other hand, for any two knots we have $\langle K\#K'\rangle = \langle K\rangle\langle K'\rangle/\langle\circ\rangle$, so by induction, the Kauffman bracket of a connected sum of n trefoil knots approaches infinity (in absolute value) as $n \to \infty$, contradicting the supposed bound.

Alternatively, we can work with the Jones polynomial, an invariant of oriented links arising from Chern-Simons theory with gauge group $\mathrm{SU}(2) \times \mathrm{U}(1)$. This does not depend on a framing, so *a priori* it could arise from a generalized measure of the sort defined in this section. However, since the Jones polynomial of a knot K is simply the Kauffman bracket times $(-A^{-3})^{w(K)}$, where $w(K)$ is the writhe, the above argument also shows that the Jones polynomial cannot come from a generalized measure. There is thus some mathematically well-defined sense in which the Chern-Simons state is not 'normalizable.' This does not yet rule it out as a physical state, however, since it is possible that physical states of quantum gravity can be more singular than generalized measures.

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