Quantum Topology and Quantum Computing

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I. Introduction

This paper is a quick introduction to key relationships between the theories of knots,links, three-manifold invariants and the structure of quantum mechanics. In section 2 we review the basic ideas and principles of quantum mechanics. Section 3 shows how the idea of a quantum amplitude is applied to the construction of invariants of knots and links. Section 4 explains how the generalisation of the Feynman integral to quantum fields leads to invariants of knots, links and three-manifolds. Section 5 is a discussion of a general categorical approach to these issues. Section 6 is a brief discussion of the relationships of quantum topology to quantum computing. This paper is intended as an introduction that can serve as a springboard for working on the interface between quantum topology and quantum computing. Section 7 summarizes the paper.

This paper is a thumbnail sketch of recent developments in low dimensional topology and physics. We recommend that the interested reader consult the references given here for further information, and we apologise to the many authors whose significant work was not mentioned here due to limitations of space and reference.

II. A Quick Review of Quantum Mechanics

To recall principles of quantum mechanics it is useful to have a quick historical recapitulation. Quantum mechanics really got started when DeBroglie introduced the fantastic notion that matter (such as an electron) is accompanied by a wave that guides its motion and produces interference phenomena just like the waves on the surface of the ocean or the diffraction effects of light going through a small aperture.

DeBroglie's idea was successful in explaining the properties of

atomic spectra. In this domain, his wave hypothesis led to the correct orbits and spectra of atoms, formally solving a puzzle that had been only described in ad hoc terms by the preceding theory of Niels Bohr. In Bohr's theory of the atom, the electrons are restricted to move only in certain elliptical orbits. These restrictions are placed in the theory to get agreement with the known atomic spectra, and to avoid a paradox! The paradox arises if one thinks of the electron as a classical particle orbiting the nucleus of the atom. Such a particle is undergoing acceleration in order to move in its orbit. Accelerated charged particles emit radiation. Therefore the electron should radiate away its energy and spiral into the nucleus! Bohr commanded the electron to only occupy certain orbits and thereby avoided the spiral death of the atom - at the expense of logical consistency.

DeBroglie hypothesized a wave associated with the electron and he said that an integral multiple of the length of this wave must match the circumference of the electron orbit. Thus, not all orbits are possible, only those where the wave pattern can "bite its own tail". The mathematics works out, providing an alternative to Bohr's picture.

DeBroglie had waves, but he did not have an equation describing the spatial distribution and temporal evolution of these waves. Such an equation was discovered by Erwin Schrodinger. Schrodinger relied on inspired guesswork, based on DeBroglie's hypothesis and produced a wave equation, known ever since as the Schrodinger equation. Schrodinger's equation was enormously successful, predicting fine structure of the spectrum of hydrogen and many other aspects of physics. Suddenly a new physics, *quantum mechanics*, was born from this musical hypothesis of DeBroglie.

Along with the successes of quantum mechanics came a host of extraordinary problems of interpretation. What is the status of this wave function of Schrodinger and DeBroglie. Does it connote a new element of physical reality? Is matter "nothing but" the patterning of waves in a continuum? How can the electron be a wave and still have the capacity to instantiate a very specific event at one place and one time (such as causing a bit of phosphor to glow *there* on your television screen)? It came to pass that Max Born developed a

statistical interpretation of the wave-function wherein the wave determines a probability for the appearance of the localised particulate phenomenon that one wanted to call an “electron”. In this story the wavefunction ψ takes values in the complex numbers and the associated probability is $\psi^* \psi$, where ψ^* denotes the complex conjugate of ψ. Mathematically, this is a satisfactory recipe for dealing with the theory, but it leads to further questions about the exact character of the statistics. If quantum theory is inherently statistical, then it can give no complete information about the motion of the electron. In fact, there may be no such complete information available even in principle. Electrons manifest as particles when they are observed in a certain manner and as waves when they are observed in another, complementary manner. This is a capsule summary of the view taken by Bohr,Heisenberg and Born. Others, including DeBroglie, Einstein and Schrodinger, hoped for a more direct and deterministic theory of nature.

As we shall see, in the course of this essay, the statistical nature of quantum theory has a formal side that can be exploited to understand the topological properties of such mundane objects as knotted ropes in space and spaces constructed by identifying the sides of polyhedra. These topological applications of quantum mechanical ideas are exciting in their own right. They may shed light on the nature of quantum theory itself.

In this section we review a bit of the mathematics of quantum theory. Recall the equation for a wave:

$$f(x,t) = \sin((2\pi/\lambda)(x-ct)).$$

With x interpreted as the position and t and as the time, this function describes a sinusoidal wave travelling with velocity **c**. We define the wave number $k = 2\pi/\lambda$ and the frequency $w = (2\pi c/\lambda)$ where λ is the wavelength. Thus we can write

$$f(x,t) = \sin(kx - \omega t).$$

Note that the velocity, **c**, of the wave is given by the ratio of frequency to wave number, $c = \omega/k$.

DeBroglie hypothesized two fundamental relationships: between energy and frequency, and between momentum and wave number. These relationships are summarised in the equations

$$E = \hbar\omega,$$
$$p = \hbar k,$$

where **E** denotes the energy associated with a wave and **p** denotes the momentum associated with the wave**.** Here $\hbar = h/2\pi$ where **h** is Planck's constant (The relation $E = \hbar\omega$ originates with Max Planck in the context of black-body radiation.)

For DeBroglie the discrete energy levels of the orbits of electrons in an atom of hydrogen could be explained by restrictions on the vibrational modes of waves associated with the motion of the electron. His choices for the energy and the momentum in relation to a wave are not arbitrary. They are designed to be consistent with *the notion that the wave or wave packet moves along with the electron.* That is, the velocity of the wave-packet is designed to be the velocity of the "corresponding" material particle.

It is worth illustrating how DeBroglie's idea works. Consider two waves whose frequencies are very nearly the same. If we superimpose them (as a piano tuner superimposes his tuning fork with the vibration of the piano string), then there will be a new wave produced by the interference of the original waves. This new wave pattern will move at its own velocity, different (and generally smaller) than the velocity of the original waves. To be specific, let $\mathbf{f(x,t) = \sin(kx - \omega t)}$ and $\mathbf{g(x,t) = \sin(k'x - \omega' t).}$ Let $\mathbf{h(x,t) = \sin(kx - \omega t) + \sin(k'x - \omega' t) = f(x,t) + g(x,t).}$

A little trigonometry shows that

$$h(x,t) = \cos(((k-k')/2)x - ((\omega-\omega')/2)t)\sin(((k+k')/2)x - ((\omega+\omega')/2)t).$$

If we assume that k and k' are very close and that w and w' are very close, then $(k+k')/2$ is approximately k, and $(\omega+\omega')/2$ is approximately w. Thus h(x.t) can be represented by

$$\mathbf{H(x.t) = \cos((\delta k/2)x - (\delta\omega/2)t)\ f(x,t)}$$

where $\delta k=(k-k')/2$ and $\delta\omega=(\omega-\omega')/2$. This means that the

superposition, H(x,t), behaves as the waveform f(x,t) carrying a slower-moving "wave-packet"

$$G(x,t)=\cos((\delta k/2)x - (\delta\omega/2)t).$$

See Figure 1.

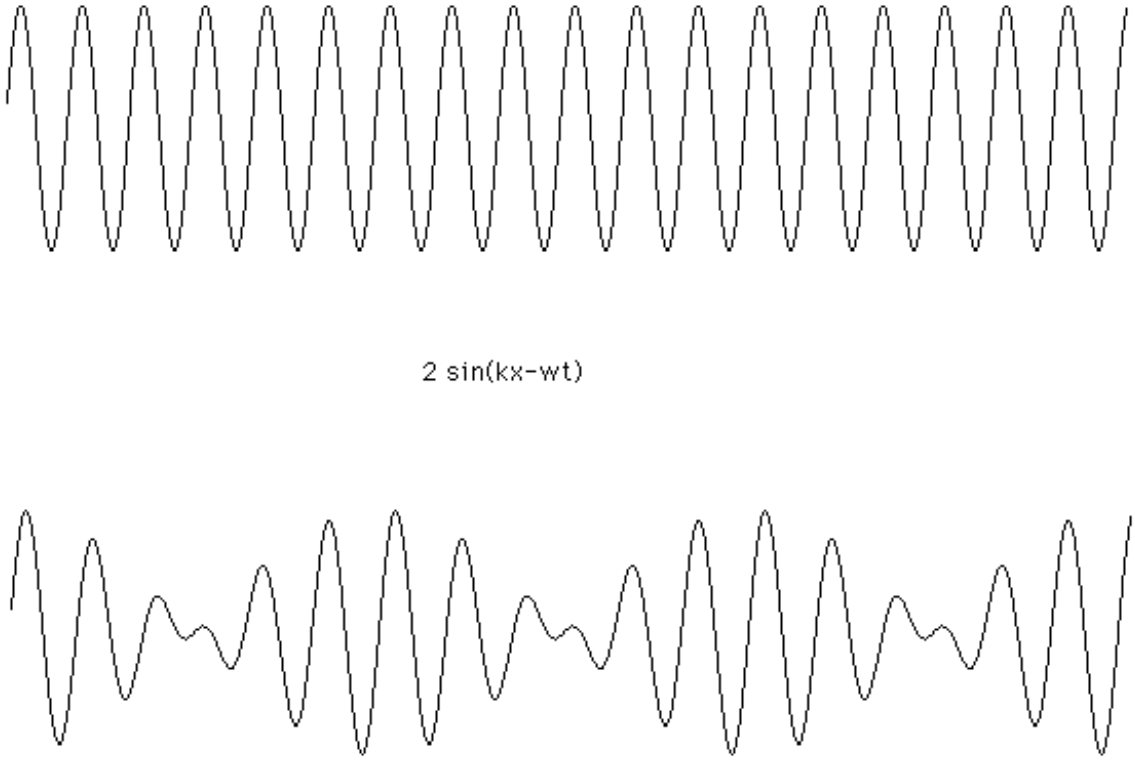


Figure 1

Since the wave packet (seen as the clumped oscillations in Figure1) has the equation $G(x,t)=\cos((\delta k/2)x - (\delta\omega/2)t)$, we see that that the velocity of this wave packet is $v_g = d\omega/dk$. Recall that wave velocity is the ratio of frequency to wave number. Now according to DeBroglie, $E = \hbar\omega$ and $p=\hbar k$, where E and p are the energy and momentum associated with this wave packet. Thus we get the formula

$v_g = dE/dp$. In other words, *the velocity of the wave-packet is the rate of change of its energy with respect to its momentum*. Now this is exactly in accord with the well-known classical laws for a material particle! For such a particle,

$E = mv^2/2$ and $p=mv$. Thus $E=p^2/2m$ and $dE/dp = p/m = v$.

It is this astonishing concordance between the simple wave model and the classical notions of energy and momentum that initiated the beginnings of quantum theory.

Schrodinger's Equation

Schrodinger answered the question:

Where is the wave equation for DeBroglie's waves?

Writing an elementary wave in complex form

$$\psi = \psi(x,t) = \exp(i(kx - \omega t))),$$

we see that we can extract DeBroglie's energy and momentum by differentiating:

$$i\hbar d\psi/dt = E\psi \quad \text{and} \quad -i\hbar d\psi/dx = p\psi.$$

This led Schrodinger to postulate *the identification of dynamical variables with operators* so that the first equation ,

$$i\hbar d\psi/dt = E\psi,$$

is promoted to the status of an equation of motion while the second equation becomes the definition of momentum as an operator:

$$p = -i\hbar d/dx .$$

Once **p** is identified as an operator, the numerical value of momentum is associated with an eigenvalue of this operator, just as in the example above. In our example $p\psi = \hbar k\psi$.

In this formulation, the position operator is just multiplication by **x** itself. Once we have fixed specific operators for position and momentum, the operators for other physical quantities can be expressed in terms of them. We obtain the energy operator by substitution of the momentum operator in the classical formula for

the energy:

$$E = (1/2)mv^2 + V$$
$$E = p^2/2m + V$$
$$E = -(\hbar^2/2m)\,d^2/dx^2 + V.$$

Here **V** is the potential energy, and its corresponding operator depends upon the details of the application.

With this operator identification for **E**, Schrodinger's equation

$$i\hbar d\psi/dt = -(\hbar^2/2m)\,d^2\psi/dx^2 + V\psi$$

is an equation in the first derivatives of time and in second derivatives of space. In this form of the theory one considers general solutions to the differential equation and this in turn leads to excellent results in a myriad of applications.

In quantum theory, observation is modelled by the concept of eigenvalues for corresponding operators. *The quantum model of an observation is a projection of the wave function into an eigenstate.* An energy spectrum $\{E_k\}$ corresponds to wave functions ψ satisfying the Schrodinger equation, such that there are constants E_k with $E\psi = E_k\psi$. An *observable* (such as energy) **E** is a Hermitian operator on a Hilbert space of wavefunctions. Since Hermitian operators have real eigenvalues, this provides the link with measurement for the quantum theory.

It is important to notice that there is no mechanism postulated in this theory for how a wave function is "sent" into an eigenstate by an observable. Just as mathematical logic need not demand causality behind an implication between propositions, the logic of quantum mechanics does not demand a specified cause behind an observation. The absence of an assumption of causality in logic does not obviate the possibility of causality in the world. Similarly, the absence of causality in quantum observation does not obviate causality in the physical world. Nevertheless, the debate over the interpretation of quantum theory has often led its participants into asserting that

causality has been demolished in physics.

Note that the operators for position and momentum satisfy the equation $xp - px = \hbar i$. This corresponds directly to the equation obtained by Heisenberg, on other grounds, that dynamical variables can no longer necessarily commute with one another. In this way, the points of view of DeBroglie, Schrodinger and Heisenberg came together, and quantum mechanics was born. In the course of this development, interpretations varied widely. Eventually, physicists came to regard the wave function not as a generalised wave packet, but as a carrier of information about possible observations. In this way of thinking $\psi^* \psi$ (ψ^* denotes the complex conjugate of ψ.) represents the probability of finding the "particle" (A particle is an observable with local spatial characteristics.) at a given point in spacetime.

Dirac Brackets

We now discuss Dirac's notation, **<b|a>**, [D58]. In this notation **<a|** and **|b>** are covectors and vectors respectively. **<b|a>** is the evaluation of **|a>** by **<b|**, hence it is a scalar, and in ordinary quantum mechanics it is a complex number. One can think of this as the amplitude for the state to begin in **"a"** and end in **"b"**. That is, there is a process that can mediate a transition from state **a** to state **b**. Except for the fact that amplitudes are complex valued, they obey the usual laws of probability. This means that if the process can be factored into a set of all possible intermediate states $c_1, c_2, ..., c_n$, then the amplitude for **a--->b** is the sum of the amplitudes for **a--->c_i--->b**. Meanwhile, the amplitude for **a--->c_i--->b** is the product of the amplitudes of the two subconfigurations **a--->c_i** and **c_i--->b**. Formally we have

$$\langle b|a\rangle = \Sigma_i \langle b|c_i\rangle\langle c_i|a\rangle$$

where the summation is over all the intermediate states **i=1, ..., n**.

In general, the amplitude for mutually disjoint processes is the *sum* of the amplitudes of the individual processes. The amplitude

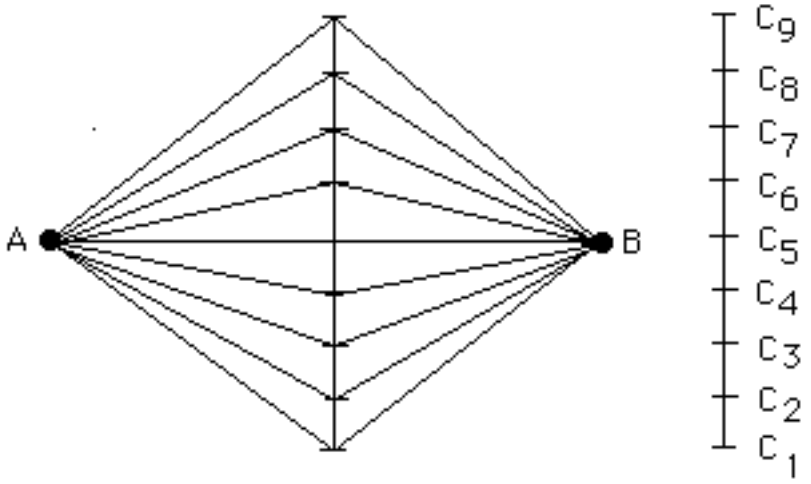
for a configuration of disjoint processes is the *product* of their individual amplitudes.

Dirac's division of the amplitudes into *bras* **<b|** and *kets* **|a>** is done mathematically by taking a vector space **V** (a Hilbert space, but it can be finite dimensional) for the kets: **|a>** belongs to **V**. The dual space **V *** is the home of the bras. Thus **<b|** belongs to **V *** so that **<b|** is a linear mapping
<b|:V -----> C where **C** denotes the complex numbers. We restore symmetry to the definition by realising that an element of a vector space **V** can be regarded as a mapping from the complex numbers to **V**. Given **|a>: C -----> V**, the corresponding element of **V** is the image of **1** (in **C**) under this mapping. In other words, **|a>(1)** is a member of **V.** Now we have **|a> :C -----> V** and **<b| : V -----> C**. The composition **<b| |a> = <b|a> : C -----> C** is regarded as an element of **C** by taking the specific value **<b|a>(1).** The complex numbers are regarded as the "vacuum", and the entire amplitude **<b|a>** is a "vacuum to vacuum" amplitude for a process that includes the creation of the state **a**, its transition to **b**, and the annihilation of **b** to the vacuum once more.

Dirac notation has a life of its own.
Let **P = |y><x|**.
Let **<x| |y> = <x|y>**.
Then **PP = |y><x| |y><x| = |y> <x|y> <x| = <x|y> P**.
Up to a scalar multiple, **P** is a projection operator. That is, if we let Q= P/<x|y>, then
QQ = PP/<x|y><x|y> = <x|y>P/<x|y><x|y> = P/<x|y> = Q.
Thus QQ=Q. In this language, the completeness of intermediate states becomes the statement that a certain sum of projections is equal to the identity:
Suppose that Σ_i $|c_i><c_i|$ = **1** (summing over i)
with $<c_i|c_i>=1$ for each i. Then

<b|a>
= <b| |a>
= <b| Σ_i $|c_i><c_i|$ |a>

$$= \Sigma_i \ \langle b| \ |c_i\rangle\langle c_i| \ |a\rangle$$



$$\langle b|a\rangle = \Sigma_i \ \langle b|c_i\rangle\langle c_i|a\rangle$$

Iterating this principle of expansion over a complete set of states leads to the most primitive form of the Feynman integral [Fey65]. Imagine that the initial and final states a and b are points on the vertical lines x=0 and x=n+1 respectively in the x-y plane, and that $(c(k)_{i(k)}, k)$ is a given point on the line x=k for 0<i(k)<m. Suppose that the sum of projectors for each intermediate state is complete. That is, we assume that following sum is equal to one, for each k from 1 to n-1:

$$|c(k)_1\rangle\langle c(k)_1| + \ldots + |c(k)_m\rangle\langle c(k)_m| = 1.$$

Applying the completeness iteratively, we obtain the following expression for the amplitude **<b|a>**:

$$\langle b|a\rangle =$$
$$\Sigma\Sigma\ldots\Sigma \langle b|c(1)_{i(1)}\rangle\langle c(1)_{i(1)}|c(2)_{i(2)}\rangle \ \ldots \ \langle c(n)_{i(n)}|a\rangle$$

where the sum is taken over all i(k) ranging between 1 and m, and k ranging between 1 and n. Each term in this sum can be

construed as a combinatorial path from a to b in the two dimensional space of the x-y plane. Thus the amplitude for going from a to b is seen as a summation of contributions from all the "paths" connecting a to b.

Feynman used this description to produce his famous path integral expression for amplitudes in quantum mechanics. His path integral takes the form

$$\int_{dP} \exp(iS)$$

where i is the square root of minus one, the integral is taken over all paths from point a to point b, and S is the *action* for a particle to travel from a to b along a given path. For the quantum mechanics associated with a classical (Newtonian) particle the action **S** is given by the integral along the given path from a to b of the difference **T - V** where **T** is the classical kinetic energy and **V** is the classical potential energy of the particle.

The beauty of Feynman's approach to quantum mechanics is that it shows the relationship between the classical and the quantum in a particularly transparent manner. Classical motion corresponds to those regions where all nearby paths contribute constructively to the summation. This classical path occurs when the variation of the action is null. To ask for those paths where the variation of the action is zero is a problem in the calculus of variations, and it leads directly to Newton's equations of motion. Thus with the appropriate choice of action, classical and quantum points of view are unified.

The drawback of this approach lies in the unavailability at the present time of an appropriate measure theory to support all cases of the Feynman integral.

On the other hand it is easy to see that a discretization of the Schrodinger equation leads to a sum over paths that is an exact solution to the discretization. To see this first write the time derivative as a difference quotient and get

$$\psi(x, t+\Delta t) = (1 - (i/\hbar)\Delta t\, E)\psi$$

where $E = -(\hbar^2/2m)\, d^2/dx^2 + V.$

Now approximate $d^2\psi/dx^2$ by

$$(\psi(x-\Delta x, t) - 2\psi(x,t) + \psi(x+\Delta x, t))/(\Delta x)^2.$$

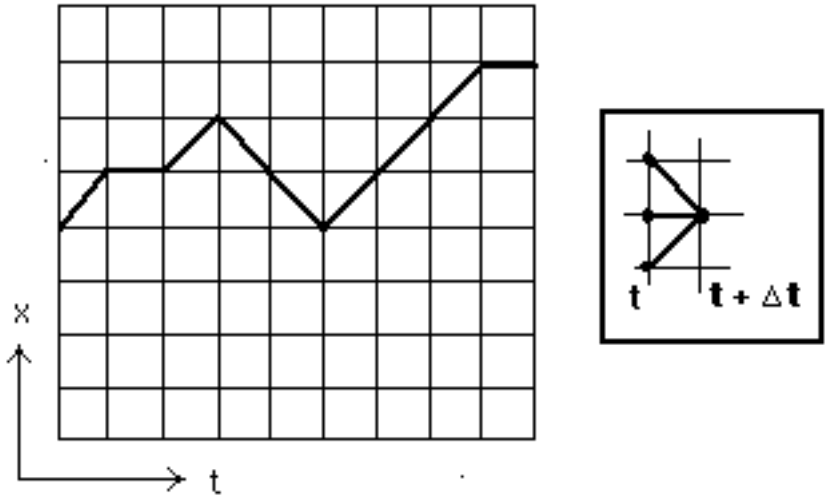
Putting this into the equation, we get a temporal recursion of the form

$$\psi(x, t + \Delta t) = A\psi(x-\Delta x, t) + B\psi(x,t) + A\psi(x+\Delta x, t)$$

where

$A = i\hbar\, \Delta t / (\Delta x)^2$ and $B = 1 - iV(x)/\hbar - 2i\hbar\, \Delta t / (\Delta x)^2$.

If we take $\psi(x,t)$ to be the sum over all lattice paths (in the spacetime lattice with steps Δx and Δt) where each path receives a product of weights A and B as defined above, then the recursion equation for the next time step of ψ is a tautology. In this sense it is easy to see that the discretized Schrodinger equation has a discrete path integral as its solution. Note that these lattice paths have exactly three possibilities entering $(x, t+\Delta t)$ from the past, namely $(x-\Delta x, t)$, (x,t) and $(x+\Delta x, t)$. Thus the “particle” travelling on the x-axis is executing a one-step random walk.



It is also worth noting that the equation

$$\psi(x, t+\Delta t) = (1 - (i/\hbar)\Delta t E)\psi$$

is the infinitesimal step of the formal equation

$$\psi(x,t) = e^{-i\hbar t E}\psi_0,$$

describing the wave function at later times as the result of a unitary evolution from an initial time. In devising algorithms for quantum computing the condition of unitary state evolution is the primary constraint that must be obeyed.

To summarize, Dirac notation shows at once how the probabilistic interpretation for amplitudes is tied with the vector space structure of the space of states of the quantum mechanical system. Our strategy for bringing forth relations between quantum theory and topology is to pivot on the Dirac bracket. The Dirac bracket intermediates between notation and linear algebra. In a very real sense, *the connection of quantum mechanics with topology is an amplification of Dirac notation.*

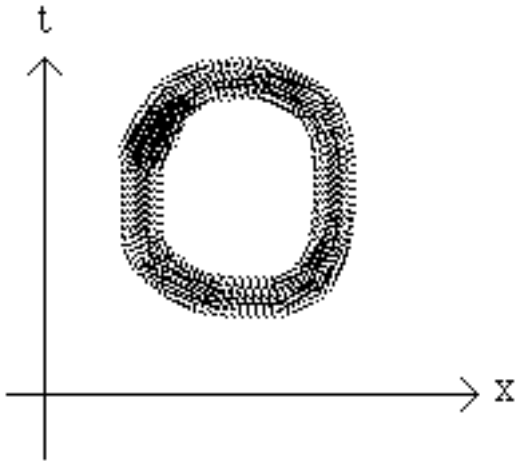
The next two sections discuss how topological invariants in low dimensional topology are related to amplitudes in quantum mechanics. In these cases the relationship with quantum mechanics

is primarily mathematical. Ideas and techniques are borrowed. It is not yet clear what the effect of this interaction will be on the physics itself.

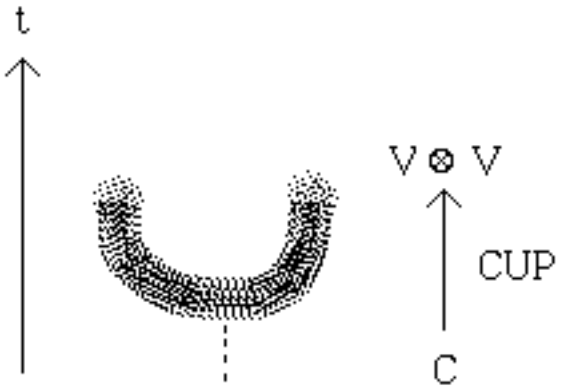
III. Knot Amplitudes

At the end of section1 we said: *the connection of quantum mechanics with topology is an amplification of Dirac notation.*

Consider first a circle in a spacetime plane with time represented vertically and space horizontally.



The circle represents a vacuum to vacuum process that includes the creation of two “particles”,



and their subsequent annihilation.

In accord with our previous description, we could divide the circle into these two parts (creation(a) and annihilation (b)) and consider the amplitude **<b|a>**. Since the diagram for the creation of the two particles ends in two separate points, it is natural to take a vector space of the form **V⊗V** as the target for the bra and as the domain of the ket.

We imagine at least one particle property being catalogued by each dimension of **V**. For example, a basis of **V** could enumerate the spins of the created particles. If $\{e_a\}$ is a basis for **V** then $\{e_a \otimes e_b\}$ forms a basis for **V⊗V**. The elements of this new basis constitute all possible combinations of the particle properties. Since such combinations are multiplicative, the tensor product is the appropriate construction.

In this language the creation ket is a map **cup**,

$$\mathbf{cup = |a> : C \text{ -----> } V \otimes V},$$

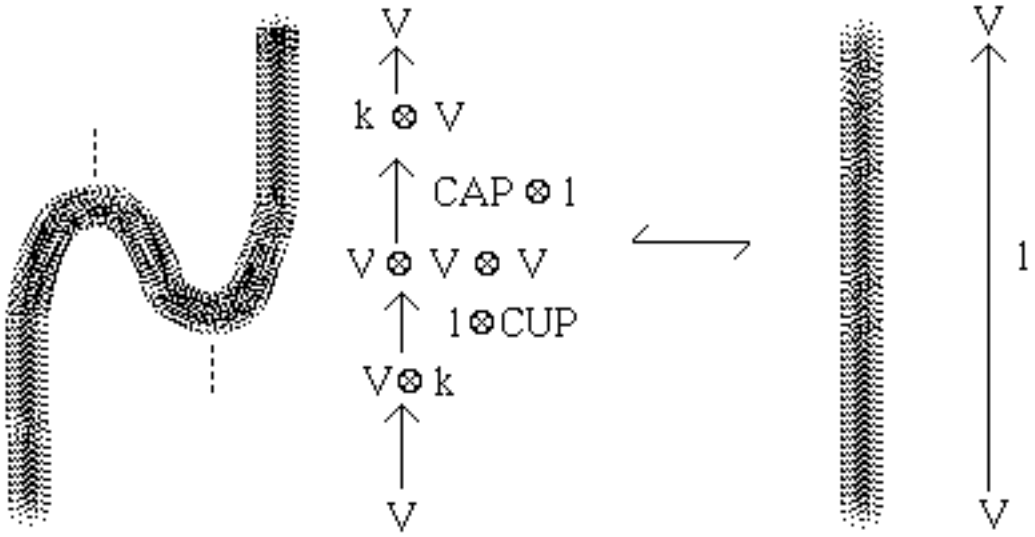
and the annihilation bra is a mapping **cap**,

$$\mathbf{cap = <b| : V \otimes V \text{ -----> } C.}$$

The first hint of topology comes when we realise that it is possible to draw a much more complicated simple closed curve in the plane that is nevertheless decomposed with respect to the vertical direction into many cups and caps. In fact, any non-selfintersecting differentiable curve can be rigidly rotated until it is in general position with respect to the vertical. It will then be seen to be decomposed into these minima and maxima. Our prescriptions for amplitudes suggest that we regard any such curve as an amplitude

via its description as a mapping from **C** to **C**.

Each simple closed curve gives rise to an amplitude, but any simple closed curve in the plane is isotopic to a circle, by the Jordan Curve Theorem. If these are *topological amplitudes*, then they should all be equal to the original amplitude for the circle. Thus the question: What condition on creation and annihilation will insure topological amplitudes? The answer derives from the fact that all isotopies of the simple closed curves are generated by the cancellation of adjacent maxima and minima as illustrated below.



In composing mappings it is necessary to use the identifications

$$(V \otimes V) \otimes V = V \otimes (V \otimes V) \quad \text{and}$$

$$V \otimes k = k \otimes V = V.$$

Thus in the illustration above, the composition on the left is given by

$$V = V \otimes k \xrightarrow{1 \otimes \text{cup}} V \otimes (V \otimes V) = (V \otimes V) \otimes V \xrightarrow{\text{cap} \otimes 1} k \otimes V = V.$$

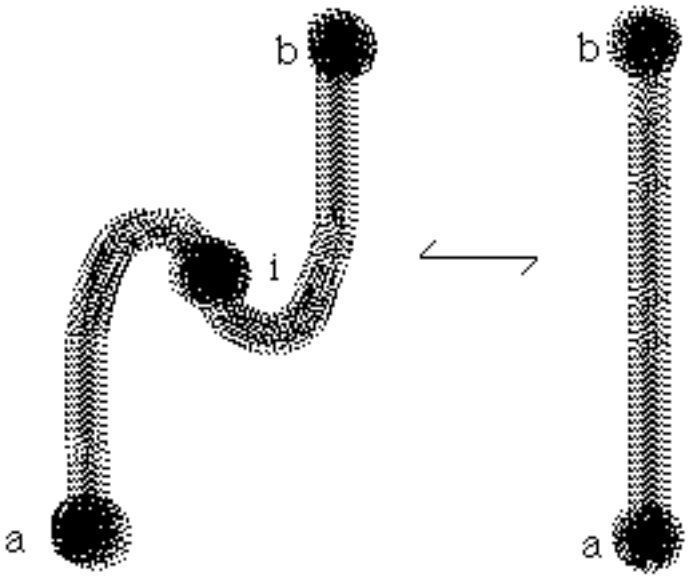
This composition must equal the identity map on V (denoted 1 here) for the amplitudes to have a proper image of the topological cancellation.

This condition is said very simply by taking a matrix representation for the corresponding operators.

Specifically, let $\{e_1, e_2, ..., e_n\}$ be a basis for V. Let $e_{ab} = e_a \otimes e_b$ denote the elements of the tensor basis for $V \otimes V$. Then there are matrices M_{ab} and M^{ab} such that

$cup(1) = \Sigma M_{ab} e_{ab}$ with the summation taken over all values of a and b from 1 to n. Similarly, cap is described by $cap(e_{ab}) = M^{ab}$. Thus the amplitude for the circle is $cap[cup(1)] = cap \Sigma M_{ab} e_{ab} = \Sigma M_{ab} M^{ab}$. In general, the value of the amplitude on a simple closed curve is obtained by translating it into an "abstract tensor expression" in the M_{ab} and M^{ab}, and then summing over these products for all cases of repeated indices.

Returning to the topological conditions we see that they are just that the matrices (M_{ab}) and (M^{ab}) are inverses in the sense that $\Sigma M_{a\,i} M^{i\,b} = I_a{}^b$ and $\Sigma M^{a\,i} M_{i\,b} = I^a{}_b$ are the identity matrices:



In the illustration above, we show the diagrammatic representative of the equation $\Sigma M_{a\,i} M^{i\,b} = I_a{}^b$.

In the simplest case cup and cap are represented by 2 x 2 matrices. The topological condition implies that these matrices are inverses of each other. Thus the problem of the existence of topological amplitudes is very easily solved for simple closed curves in the plane.

Now we go to knots and links. Any knot or link can be represented by a picture that is configured with respect to a vertical direction in the plane. The picture will decompose into minima (creations) maxima (annihilations) and crossings of the two types shown below. (Here I consider knots and links that are unoriented. They do not have an intrinsic preferred direction of travel.) See Figure 2. In Figure 2, next to each of the crossings we have indicated mappings of $\mathbf{V \otimes V}$ to itself , called $\mathbf{R}$ and $\mathbf{R^{-1}}$ respectively. These mappings represent the transitions corresponding to these elementary configurations.

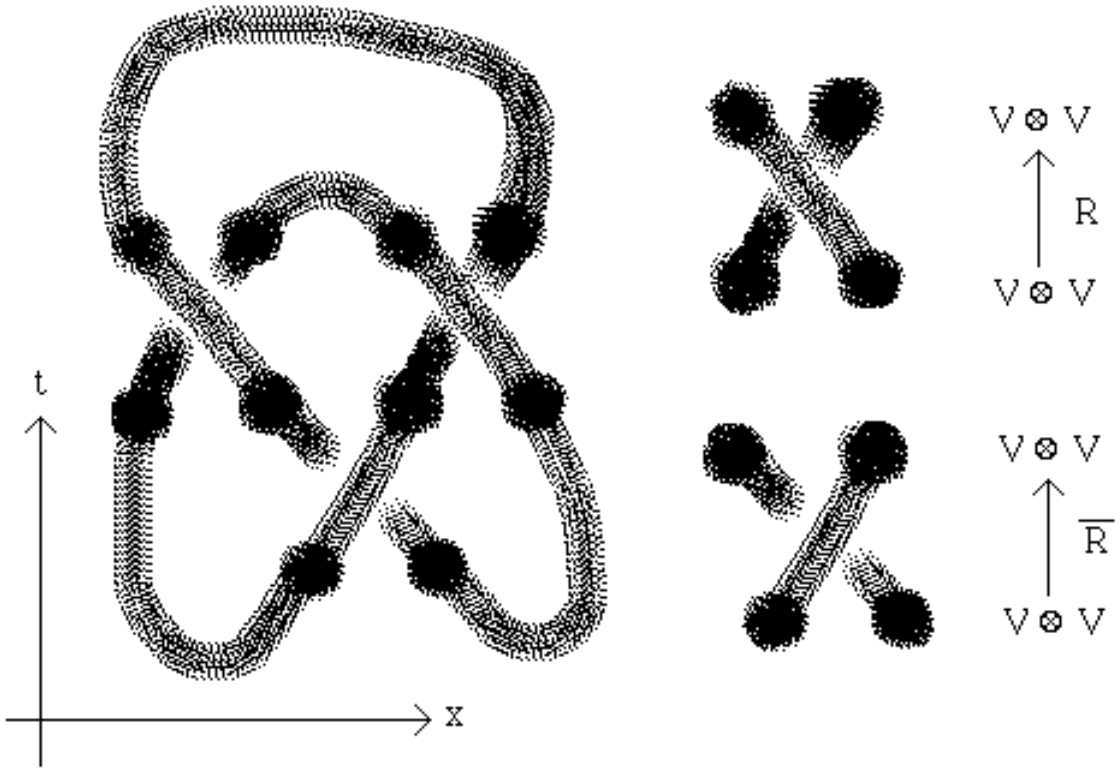
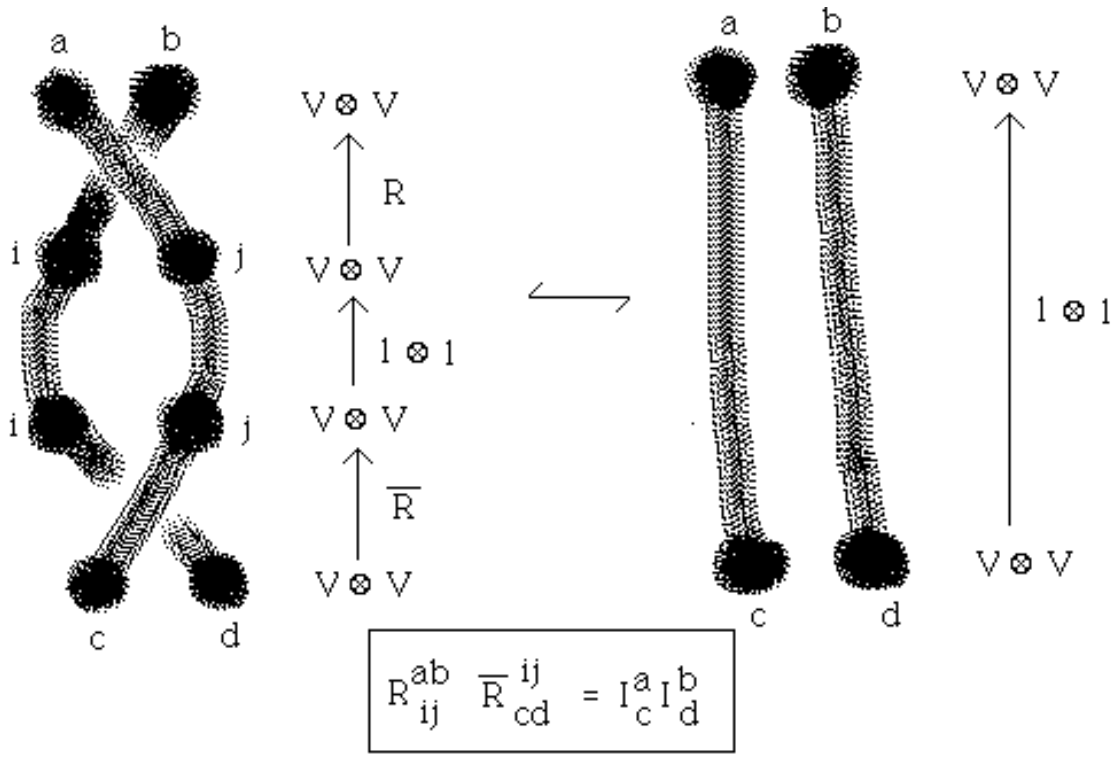


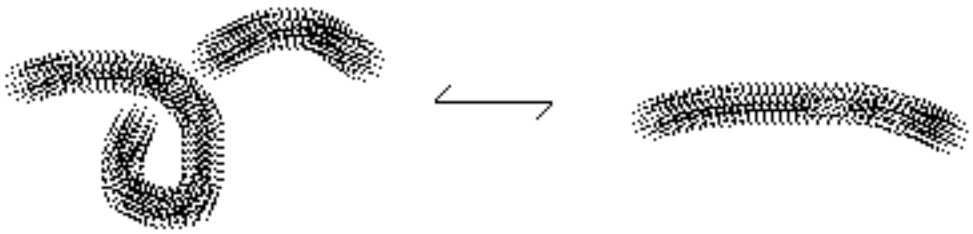
Figure 2

That $\mathbf{R}$ and $\mathbf{R^{-1}}$ really must be inverses follows from the isotopy

shown below (This is the second Reidemeister move.)



We now have the vocabulary of **cup,cap, R** and $\mathbf{R^{-1}}$. Any knot or link can be written as a composition of these fragments, and consequently a choice of such mappings determines an amplitude for knots and links. In order for such an amplitude to be topological we want it to be invariant under the list of local moves on the diagrams shown in Figure 3. These moves are an augmented list of the Reidemeister moves, adjusted to take care of the fact that the diagrams are arranged with respect to a given direction in the plane. The equivalence relation generated by these moves is called regular isotopy. It is one move short of the relation known as *ambient isotopy*. The missing move is the first Reidemeister move shown below.



In the first Reidemeister move, a curl in the diagram is created or destroyed. Ambient isotopy (generated by all the Reidemeister moves) corresponds to the full topology of knots and links embedded in three dimensional space. Two link diagrams are ambient isotopic via the Reidemeister moves if and only if there is a continuous family of embeddings in three dimensions leading from one link to the other. The moves give us a combinatorial reformulation of the spatial topology of knots and links.

By ignoring the first Reidemeister move, we allow the possibility that these diagrams can model framed links, that is links with a normal vector field or,equivalently, embeddings of curves that are thickened into bands. It turns out to be fruitful to study invariants of regular isotopy. In fact, one can usually normalise an invariant of regular isotopy to obtain an invariant of ambient isotopy. We shall see an example of this phenomenon with the bracket polynomial in a few paragraphs.

As the reader can see, we have already discussed the algebraic meaning of moves 0. and 2. The other moves translate into very interesting algebra. Move 3., when translated into algebra, is the famous Yang-Baxter equation. The Yang-Baxter equation occurred for the first time in problems related to exactly solved models in statistical mechanics (See [KA96].). All the moves taken together are directly related to the axioms for a quasi-triangular Hopf algebra (aka quantum group). We shall not go into this connection here.

There is an intimate connection between knot invariants and the structure of generalised amplitudes, as we have described them in terms of vector space mappings associated with link diagrams. This strategy for the construction of invariants is directly motivated by

the concept of an amplitude in quantum mechanics. It turns out that the invariants that can actually be produced by this means (that is by assigning finite dimensional matrices to the caps, cups and crossings) are incredibly rich. They encompass, at present, all of the known invariants of polynomial type (Alexander polynomial, Jones polynomial and their generalisations.).

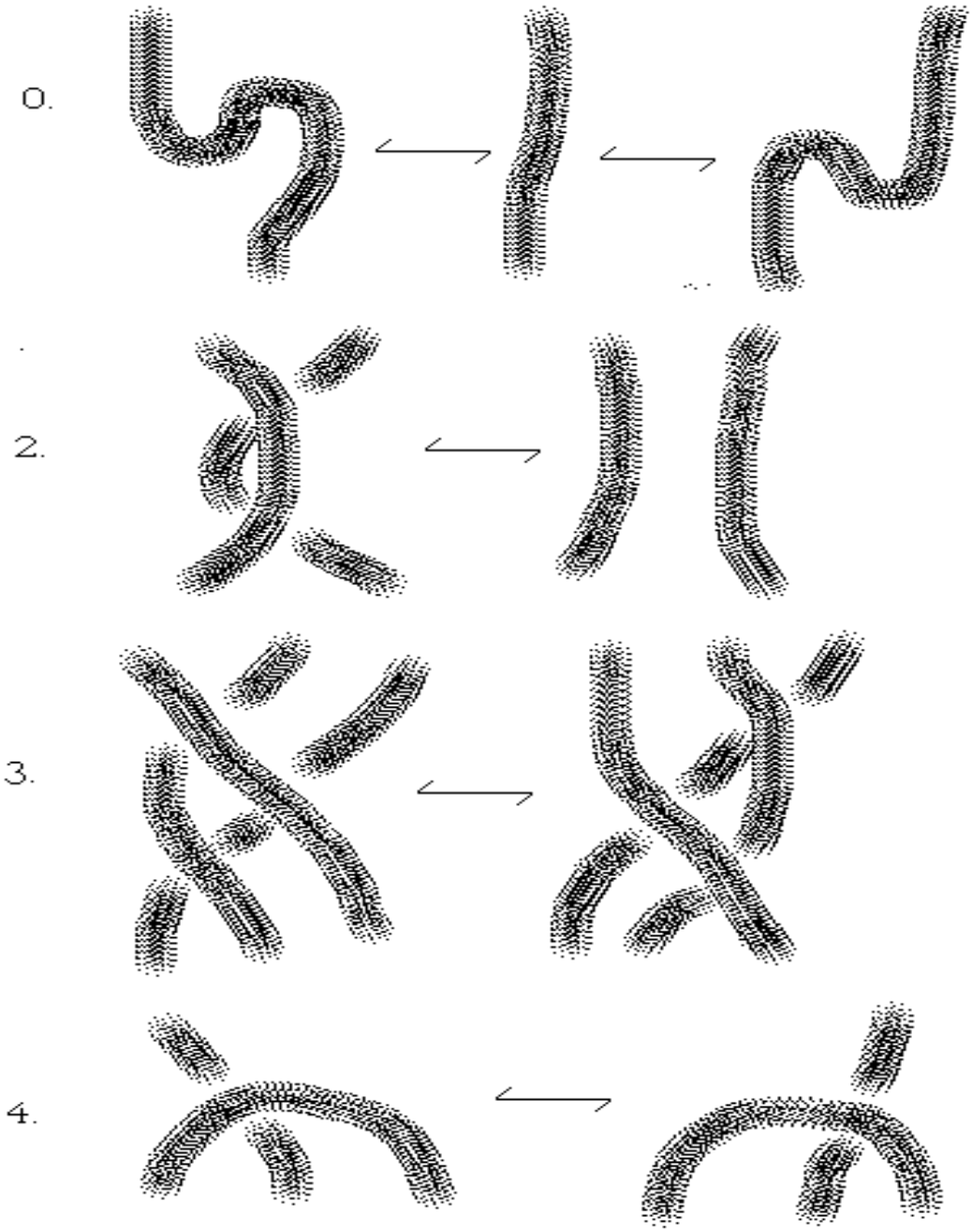


Figure 3

It is now possible to indicate the construction of the Jones polynomial via the bracket polynomial as an amplitude, by specifying its matrices.

The cups and the caps are defined by $(M_{ab}) = (M^{ab}) = M$ where M is the 2 x 2 matrix
(with ii=-1)

$$M = \begin{bmatrix} 0 & iA \\ -iA^{-1} & 0 \end{bmatrix}$$

Note that $MM = I$ where I is the identity matrix. Note also that the amplitude for the circle is

$$\Sigma M_{ab}M^{ab} = \Sigma M_{ab}M_{ab} = \Sigma (M_{ab})^2$$

$$= (iA)^2 + (-iA^{-1})^2 = -A^2 - A^{-2}.$$

The matrix R is then defined by the equation

$$R^{ab}{}_{cd} = AM^{ab}M_{cd} + AI^a{}_c I^b{}_d ,$$

or symbolically by

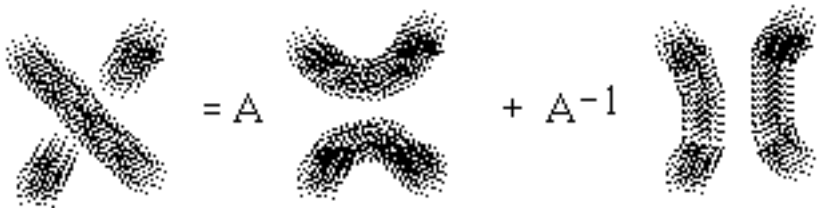
$$R = AM \otimes M + A^{-1} I \otimes I$$

For example, we have the specific evaluation

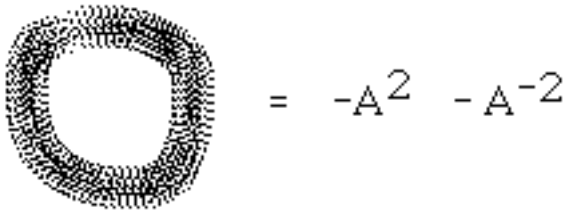
$$R^{12}_{12} = AM^{12}M_{12} + A^{-1} I^1_1 I^2_2$$

$$R^{12}_{12} = A(iA)(iA) + A^{-1}(1)(1)$$

Since, diagrammatically, we identify R with a (right handed) crossing, this equation can be written diagrammatically as



Taken together with the loop value of $-A^2 - A^{-2}$,



These equations can be regarded as a recursive algorithm for computing the amplitude.

This algorithm is the bracket state model for the (unnormalized) Jones polynomial [KA87]. This model can be studied on its own grounds. We end this section with some comments about this algorithm and its properties.

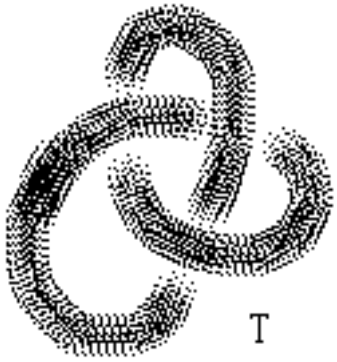
The Bracket Model

If we were to start with just the calculational formulas as indicated above but with arbitrary coefficients A and B for the two smoothings, and an arbitrary loop value d, then it is easy to see that the resulting method of calculating a three variable polynomial (in the commuting variables A,B and d) from a link diagram is well-defined, although not necessarily invariant under the Reidemeister moves. It is then an interesting exercise to see that asking for invariance under just the second Reidemeister move essentially forces $B=A^{-1}$ and $d=-A^2-A^{-2}$. Thus the parameters arising from the algebra that we

have sketched actually come directly from the topology. It is equally easy to see the the resulting Laurent polynomial is a well defined invariant of regular isotopy. Lets denote that invariant by **<K>**, the (unnormalised) bracket polynomial of K. In this version of the bracket we have $<O> = -A^{2} - A^{-2}$ where O denotes a circle in the plane. If we define $f_K(A) = (-A^3)^{-w(K)}<K>/<O>$ where w(K) denotes the sum of the signs of the crossings in an oriented link K (See [KA87] or [KA91].), then $f_K(A)$ is an invariant of ambient isotopy and the original Jones polynomial [JO86], $V_K(t)$ is given by the formula

$$V_K(t) = f_K(t^{-1/4}).$$

The bracket model for the Jones polynomial is quite useful both theoretically and in terms of practical computations. One of the neatest applications is to simply compute $f_K(A)$ for the trefoil knot T

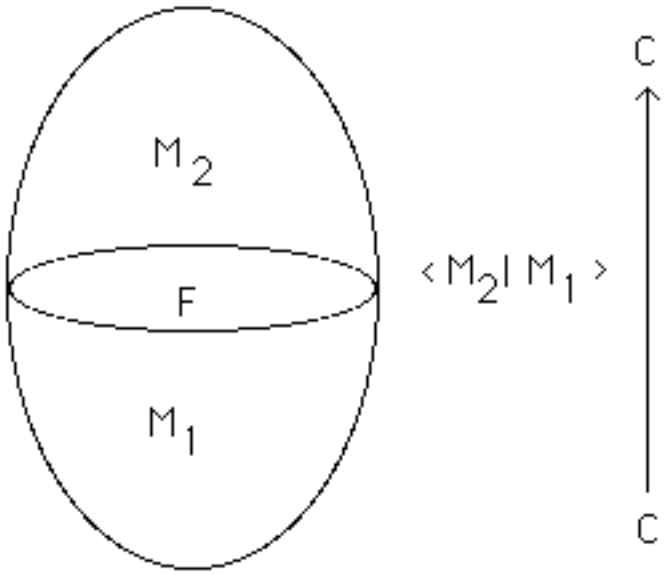


and determine that $f_K(A)$ is not equal to $f_K(A^{-1})$. This shows that the trefoil is not ambient isotopic to its mirror image, a fact that is quite tricky to prove by classical methods.

IV. Topological Quantum Field Theory - First Steps

In order to further justify this idea of the amplification of Dirac notation, consider the following scenario. Let **M** be a 3-dimensional manifold. Suppose that **F** is a closed orientable surface inside **M** dividing **M** into two pieces $\mathbf{M_1}$ and $\mathbf{M_2}$. These pieces are 3-manifolds with boundary. They meet along the surface **F**. Now consider an amplitude $\mathbf{<M_2|M_1> = Z(M)}$. The form of this amplitude generalises our previous considerations, with the surface **F** constituting the distinction between the “preparation” $\mathbf{M_1}$ and

the "detection" $\mathbf{M_2}$. This generalisation of the Dirac amplitude **<b|a>** amplifies the notational distinction consisting in the vertical line of the bracket to a topological distinction in a space **M**. The amplitude **Z(M)** will be said to be a *topological amplitude for **M*** if it is a topological invariant of the 3-manifold **M**. Note that a topological amplitude does not depend upon the choice of surface **F** that divides **M**.



From a physical point of view the independence of the topological amplitude on the particular surface that divides the 3-manifold is the most important property. An amplitude arises in the condition of one part of the distinction carved in the 3-manifold acting as "the observed" and the other part of the distinction acting as "the observer". If the amplitude is to reflect physical (read topological) information about the underlying manifold, then it should not depend upon this particular decomposition into observer and observed. The same remarks apply to 4-manifolds and interface with ideas in relativity. We mention 3-manifolds because it is possible to describe many examples of topological amplitudes in three dimensions. The matter of 4-dimensional amplitudes is a topic of current research. The notion that an amplitude be independent of the distinction producing it is prior to topology.

Topological invariance of the amplitude is a convenient and fundamental way to produce such independence.

This sudden jump to topological amplitudes has its counterpart in mathematical physics. In [WIT89] Edward Witten proposed a formulation of a class of 3-manifold invariants as generalised Feynman integrals taking the form **Z(M)** where

$$Z(M) = \int dA \exp[(ik/4p)S(M,A)].$$

Here **M** denotes a 3-manifold without boundary and A is a gauge field (also called a qauge potential or gauge connection) defined on **M.** The gauge field is a one-form on M with values in a representation of a Lie algebra. The group corresponding to this Lie algebra is said to be the *gauge group* for this particular field. In this integral the "action" **S(M,A)** is taken to be the integral over **M** of the trace of the Chern-Simons three-form

$$CS = AdA + (2/3)AAA.$$

(The product is the wedge product of differential forms.)

Instead of integrating over paths, the integral **Z(M)** integrates over all gauge fields modulo gauge equivalence. This generalisation from paths to fields is characteristic of quantum field theory. Quantum field theory was designed in order to accomplish the quantisation of electromagnetism. In quantum electrodynamics the classical entity is the electromagnetic field. The question posed in this domain is to find the value of an amplitude for starting with one field configuration and ending with another. The analogue of all paths from point a to point b is "all fields from field A to field B".

Witten's integral **Z(M)** is, in its form, a typical integral in quantum field theory. In its content **Z(M)** is highly unusual. The formalism of the integral, and its internal logic supports the existence of a large class of topological invariants of 3-manifolds and associated invariants of knots and links in these manifolds.

Invariants of three-manifolds were initiated by Witten as functional integrals in [WIT89] and at the same time defined in a combinatorial way by Reshetikhin and Turaev in [RT91]. The Reshetikhin-Turaev

definition proceeds in a way that is quite similar to the definition that we gave for the bracket model for the Jones polynomial in section 2. It is an amazing fact that Witten's definition seems to give the very same invariants. We are not in a position to go into the details of this correspondence here. However, one theme is worth mentioning: For k large, the Witten integral is approximated by those gauge connections A for which **S(M,A)** has zero variation with respect to change in A. These are the so-called *flat connections*. It is possible in many examples to calculate this contribution via both the functional integral and by the combinatorial definition of Reshetikhin and Turaev. In all cases, the two methods agree (See e.g. [GF91]). This is one of the pieces of evidence in a puzzle that everyone expects will eventually justify the formalism of the functional integral. Note how this case corresponds exactly to the relation of classical and quantum physics as it was discussed in Section 1.

In order to obtain invariants of knots and links from Witten's integral, one adds an extra bit of machinery to the brew. The new machinery is the *Wilson loop.* The Wilson loop is an exponentiated version of integrating the gauge field along a loop **K.** We take this loop **K** in three space to be an embedding (a knot) or a curve with transversal self-intersections. It is usually indicated by the symbolism

$$\mathbf{tr(Pexp(}S_K\mathbf{A))} \ .$$

Here the **P** denotes *path ordered integration* - that is we are integrating and exponentiating matrix valued functions, and one must keep track of the order of the operations. The symbol **t r** denotes the trace of the resulting matrix.

With the help of the Wilson loop function on knots and links, Witten [WIT89] writes down a functional integral for link invariants in a 3-manifold M:

$$\mathbf{Z(M,K)} = \int \mathbf{dAexp[(ik/4p)S(M,A)]} \quad \mathbf{tr(Pexp(}S_K\mathbf{A)).}$$

Here **S(M,A)** is the Chern-Simons Lagrangian, as in the previous

discussion.

If one takes the standard representation of the Lie algebra of SU(2) as 2x2 complex matrices then it is a fascinating exercise to see that the formalism of $\mathbf{Z(S^3,K)}$ (S^3 denotes the three-dimensional sphere.) yields up the original Jones polynomial with the basic properties as discussed in section 1. See Witten's paper or [WIT89] or [KA91],[KA95] for discussions of this part of the heuristics.

This approach to link invariants crosses boundaries between different methods. There are close relations between $\mathbf{Z(S^3,K)}$ and the invariants defined by Vassiliev (See [BAR95],[KA95].), to name one facet of this complex crystal.

This deep relationship between topological invariants in low dimensional topology and quantum field theory in the sense of Witten's functional integral is really still in its infancy. There will be many surprises in the future as we discover that what has so far been uncovered is only the tip of an iceberg.

V. Categorical Physics

We have seen that in quantum topology and topological quantum field theory, the Dirac notational viewpoint on quantum mechanics has become amplified into a framework that embraces amplitudes associated with topological spaces and with embeddings of one space within another (e.g. knots and links in three dimensional space). The brackets, kets and bras are generalized to become maps of vector spaces associated with these topological spaces in a category that allows tensor products (Thus we associated many tensor products of a single vector space V with itself in analyzing knots). The correct formal notion is that of a tensor category, but I will omit the precise definition in this informal discussion. On the other hand, the notion of category is worth examining in this context.

A *category* is a set with two types of elements called *objects* and *morphisms*. A morphism f is associated with two objects A and B and is written

f: A -----> B

where we say that f is a morphism from A to B. In a category if there is a morphism f:A -----> B and a morphism g:B----->C, then there is a morphism gf:A----->C called the *composition* of f and g. Composition of morphisms is associative and every object A has a morphism I(A):A----->A such that if f:A----->B is any other morphism then I(B)f = fI(A) = f. These properties comprise the definition of a category.

Given a category C and another category C' we say that
F:C---->C' is a *functor* from C to C' if F takes objects to objects, morphisms to morphisms, F applied to an identity morphism in C is an identity morphism in C' and F applied to a composition of morphisms in C is equal to the composition of the corresponding morphisms in C'. In other words, F(I(A)) = I(F(A)) for any object A in C, and F(ab) = F(a)F(b) for any composable morphisms a and b in C. A functor is a structural mapping from one category to another.

The morphisms in a category are not necessarily functions from some set to another set. Rather they are directed structural relations that are of significance in a particular domain. A case in point is our discussion of knots where we associated linear mappings to cups, caps, crossings and compositions of these forming all sorts of knots and tangles. The cups, caps and crossings can be regarded by themselves as the generating morphisms for a tensor category whose objects are just ordered collections of points (including the empty collection!) corresponding to the endpoints of arcs. Composition of morphisms corresponds to attaching endpoints together in the fashion that we described in that section. We call this category the (unoriented) *tangle category*. The association of linear mappings to elements in the tangle category that we so carefully described in our section on knots and links comprises a functor from the tangle category to the category of vector spaces and linear mappings.

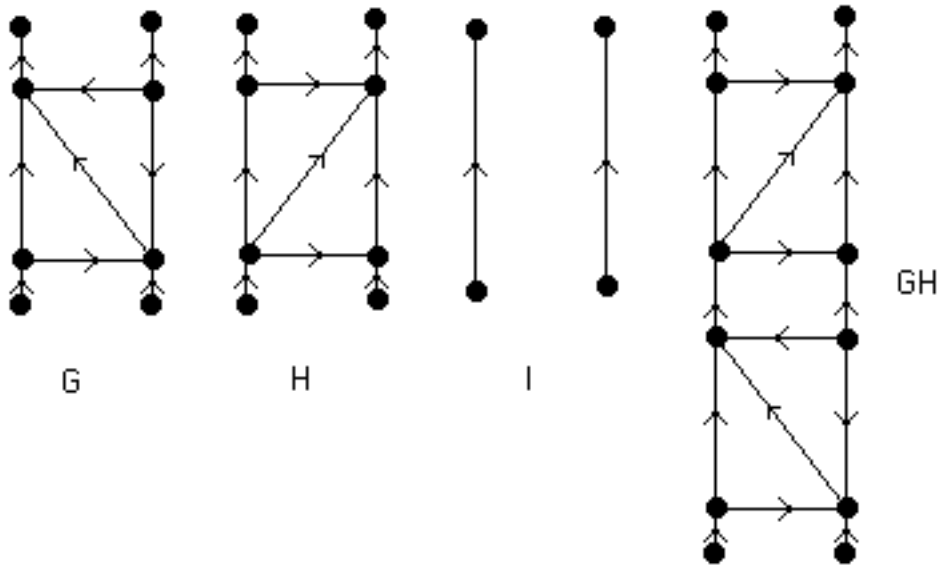
Quantum amplitudes are calculated in the vector space category.
The functor that we described from tangles to vector spaces tells us how to do "quantum mechanics" on the tangle category.
But this quantum mechanics is a generalization of the usual quantum mechanics. The underlying topological spaces (here the knots and

links) have quantum states, but they themselves are classical (at least in the sense that our abstraction of a knot from the physical rope embodies properties from classical physics). These same issues necessarily come up when trying to marry quantum mechanics and relativity theory since one wants to bring an underlying topological manifold (with changing topology and metric) into the discussion.

Furthermore, the issue of measurement is directly related to cutting the spaces apart or making distinctions in the underlying space. Thus in our example with three manifolds in the last section we divided the three manifold into parts M_1 and M_2 and then looked at the amplitude $<M_2|M_1>$. In this view either half of the manifold can be regarded as an observer of the other half.

This description of states of affairs is very similar to the time-honored discussion of the relationship of ordinary language and the classical description of measuring apparatus in relation to quantum mechanical calculations. Thus we could begin to formalize quantum mechanics as a special sort of functor whose domain category is a classical category analogous to knots, links and manifolds, and whose range category is an appropriate tensor category where amplitudes and observables can be computed. The classical category then gets structured in a non-classical way by this functor.

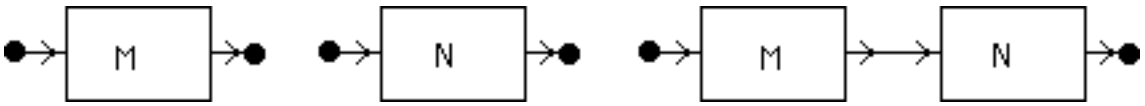
Here is another example of a structure of the sort that I just described. Consider the set of finite directed multi-graphs. Call a node in a graph G an *input node* if it has exactly one directed edge emanating from it and no edges entering it. Call a node an *output node* if it has exactly one edge entering it and no edges leaving it. Let **DG(n)** denote the set of digraphs of this kind that have n inputs and n outputs. Further assume that each such graph is equipped with an ordering of its inputs and an ordering of its outputs. Thus G in DG(n) will have inputs labelled 1,2,3,..., n and outputs labelled 1,2,3,...,n. Given G and H in DG(n) we define their *composition* GH by attaching the kth output of G to the kth input of H (by removing corresponding nodes and amalgamating the two directed edges at those nodes to a single edge). As shown below, the graph I consisting of n parallel edges is an identity for this composition.



The upshot is that G(n) is a category where the digraphs are the morphisms and the one object is the ordered set {1,2,...,n}. Juxtaposition of graphs gives a tensor structure and a mapping DG(n) x DG(m) -----> DG(n+m). With a little work, all the DG(n)'s can be put together in one category DG. When n=0, we have digraphs without inputs or outputs, analogous to knots and links. Clearly the categories DG(n) are analogous to n-strand tangles as we have discussed them in the section on knot amplitudes.

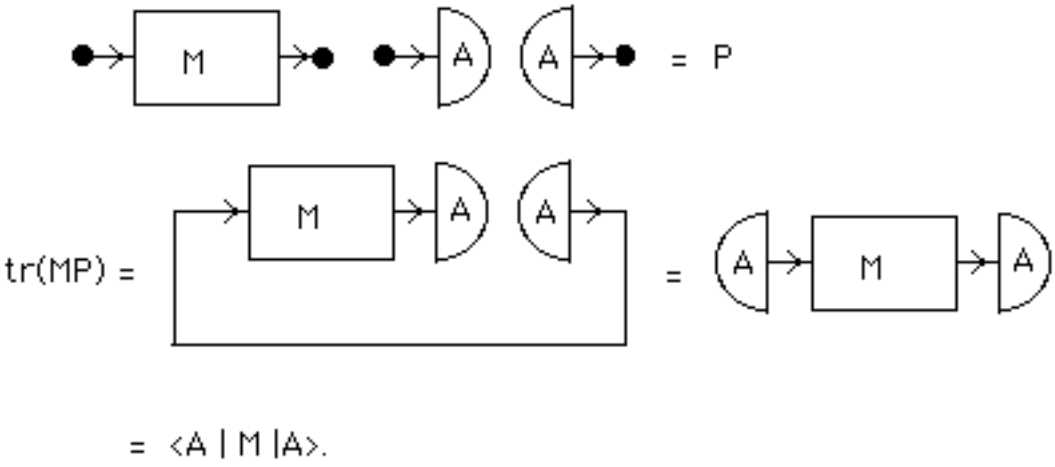
A functor on DG(n) that takes the category to vector spaces and linear maps can be constructed by associating a linear mapping or matrix to each different species of directed node in the graphs under consideration. Then compostion of graphs will correspond to matrix multiplication in much the same manner as our discussion for knots and links. To give a simple example, lets work in DG(1). Then each graph has one input and one output. Then we regard the input line of the graph as corresponding to the left index of a matrix and the output line as corresponding to the right index of a matrix. If G is the graph and F(G) the corresponding matrix then GH corresponds to F(G)F(H) if we regard the tying of the output line of G to the input line of H as connoting summation over all possibilities for the common index and take the sum of the products of the matrix entries for F(G) and F(H). This defines a functor from DG(1) to the category

of matrices where the morphisms are the matrices and composition is the matrix product.



In multiplying matrices M and N we have $(MN)_{i\ j} = S_k\ M_{i\ k} N_{k\ j}$.
In the graph category, the internal edge corresponds to the index susceptible to summation.

With this interpretation, many elementary formulas and patterns of quantum mechanics become simple matters of diagrammatics. For example, if we are computing tr(MP) (tr denotes trace) where P is a projection operator P=|A><A|, then it is easy to see in the graph category that tr(MP) = <A|M|A>.



This example also indicates how to conceptualize measurement in the graph category. An elementary measurement consists in inserting a projector P into a link in the graph. The effect of such an insertion is non-local since the amplitudes are computed via the functor to the matrix category and conseqently involve summations over all states of the graph (where a state consists in assignments of indices to all the internal lines of the graph and the amplitude is computed by summing over all the products of the resulting matrix elements).

The graph is a classical but abstract description of a set of relationships. The functor that computes amplitudes from the graph does a non-local computation involving the graph as a whole. If we imagine that the universe is a large network analogous to such a graph then it will be neccessary to understand how one part of the network becomes an observable for the rest and how this classical level of description intertwines with the quantum amplitude functor.

VI. Speculations on Quantum Computing

In this paper I have concentrated on giving a picture of the general framework of quantum topology and how it is related to a very general, in fact categorical, view of quantum mechanics.
Many algorithms in quantum topology are configured without regard to unitary evolution of the amplitude since the costraint has been topological invariance rather than conformation to physical reality. This gives rise to a host of problems (that we shall discuss elsewhere) of attempting to reformulate topological amplitudes as quantum computations. A particular case in point is the bracket model for the Jones polynomial. It would be of great interest to see a reformulation of this algorithm that would make it a quantum computation in the strict sense of quantum computing.

There are other ideas in the topology that deserve comparison with the quantum states. For example, topological entanglement in the sense of linking and braiding is intuitively related to the entanglement of quantum states. This is actually the case for the quantum topological states associated with the bracket polynomial, and undoubtedly would figure strongly in a quantum computing model of this algorithm. For this and many other reasons it is worthwhile to make the comparison between quantum computing and quantum computation.

VII. Summary

We have, in this short paper, given an almost unbroken line of argument from the beginnings of quantum mechanics to the construction of topological quantum field theories and link invariants associated with quantum amplitudes.

One of the most exciting prospects for these new invariants is the possibility of their application in quantum gravity. See [BAE94] for an account of these developments. Many other applications are possible, and the subject is just beginning. For a survey of past and present applications of knots and links we refer the reader to [KAU95] [KA98],[KAU98].

For a good survey of quantum computing we recommend [AH98] and for another view of topological issues see [FR98].

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