Topology, Decoherence, and Semiclassical Gravity*

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Abstract

We address the issue of recovering the time-dependent Schrödinger equation from quantum gravity in a natural way. To reach this aim it is necessary to understand the nonoccurrence of certain superpositions in quantum gravity. We explore various possible explanations and their relation. These are the delocalisation of interference terms through interaction with irrelevant degrees of freedom (decoherence), gravitational anomalies, and the possibility of $\theta$ states. The discussion is carried out in both the geometrodynamical and connection representation of canonical quantum gravity.

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Complex numbers play a fundamental role in quantum theory. This was not easily accepted in the early days of quantum mechanics, and only in the last of his seminal papers on quantization as an eigenvalue problem \cite{1} did Schrödinger introduce the $i$ in his equation. Again, Ehrenfest \cite{2} expressed his uneasiness about complex wave functions. In his response, Pauli \cite{3} argued that they are unavoidable if one is interested in conserved positive probabilities which are bilinear in the wave function and which do not contain its time derivatives.

A second, powerful, argument is due to Stueckelberg \cite{4} who showed that if one starts with a real Hilbert space the uncertainty relations cannot hold unless a new operator, $\hat{J}$, with $\hat{J}^2 = -1$, is introduced. The use of Hilbert spaces as a convenient mathematical framework for quantum theory has been motivated by Wootters \cite{5} who argued that an appropriately defined notion of "statistical distance", as suggested by the probabilistic character of quantum theory, coincides with the angle between rays in an appropriate Hilbert space.

Thus, as far as ordinary quantum theory is concerned, Ehrenfest’s question was answered in a satisfactory way. The problem, however, shows up again within the framework of quantum gravity since there is no term containing $i\partial/\partial t$ at a fundamental level \cite{6}. Although a consistent theory of quantum gravity does not yet exist, there has been some progress in the context of applying canonical quantization rules to general relativity. Basically, two different approaches can be distinguished within this scheme. The first uses the three-metric on a three-dimensional space and its extrinsic curvature as the basic variables (the geometrodynamical formulation), the second uses a complex $SO(3)$ connection and the densitized triad defined on the same three-space (the connection or, alternatively, loop space formulation). The central equations in both frameworks are the quantum version of the classical constraint equations which are implemented, in the sense of Dirac, as conditions on physically allowed wave functionals. The most important equation is the Hamiltonian constraint equation,

$$H \Psi = 0,$$  \hspace{1cm} (1)

where $H$ is the total Hamiltonian including both gravitational and non-gravitational fields. In the geometrodynamical formulation, where $\Psi$ depends on the three-metric, (1) is referred to as the Wheeler-DeWitt equation \cite{7}. In the connection formulation it depends on the complex connection referred to above. A major development in recent years had been the discovery of exact
formal solutions to (1) (without matter) [8], [9]. If one takes for definiteness a massive scalar field for the matter part, the Hamiltonian reads explicitly, in the geometrodynamical formulation,

$$H_g = -\frac{1}{2M} G_{abcd} \frac{\delta^2}{\delta h_{ab} \delta h_{cd}} - 2M \sqrt{h}(R - 2\Lambda)$$

$$- \frac{1}{2\sqrt{h}} \frac{\delta^2}{\delta \phi^2} + \frac{\sqrt{h}}{2}(h^{ab} \partial_a \phi \partial_b \phi + m^2 \phi^2),$$

(2)

where $M = (32\pi G)^{-1}$, and $G$, $R$, $\Lambda$ are respectively the gravitational constant, the three-dimensional Ricci scalar, and the cosmological constant. The coefficients $G_{abcd}$ depend on the metric and play themselves the role of a metric on $\text{Riem}(\Sigma)$, the space of all three-metrics. Its distinguished property is its hyperbolicity at each space point which gives rise to an intrinsic ("many-fingered") timelike variable. We do not consider any factor ordering terms and regularization prescriptions since we are not interested in finding exact solutions to (1) but in making contact with established physics from a conceptual point of view. Since we will remain in the realm of the semi-classical approximation, such prescriptions can be consistently neglected.

In the connection representation, the Hamiltonian is given by the expression

$$H_c = \frac{G}{4\pi} \epsilon^{ijk} F_{ab}^k \frac{\delta^2}{\delta A^i_a \delta A^j_b} + \frac{\delta^2}{\delta \phi^2} + 2G^2 \partial_a \phi \partial_b \phi \frac{\delta^2}{\delta A^i_a \delta A^j_b}$$

$$+ \frac{\sqrt{2}}{3}(G^3 m^2 \phi^2 + G^2 \Lambda) \eta_{abc} \epsilon^{ijk} \frac{\delta^3}{\delta A^i_a \delta A^j_b \delta A^k_c},$$

(3)

where $F_{ab}^k = \partial_a A^k_b - \partial_b A^k_a - \epsilon^{klm} A^l_a A^m_b$ is the field strength tensor associated with the complex connection $A$, and $\eta_{abc}$ is the metric-independent totally skew-symmetric density of weight $-1$. $F_{ab}^k$ plays the role of a metric in the space of all connections. In contrast to (2), it is complex and not hyperbolic. Moreover, it is not even ultralocal. The important difference between (2) and (3) is that $H_c$ does not contain the Ricci scalar, that it contains only terms with functional derivatives (even third order derivatives) and that it is intrinsically complex since $A$ is complex. Note that a factor of $G$ is associated with each functional derivative with respect to $A^i_a$ which comes with a term containing $\phi$.

As mentioned above, the important feature about both formulations is the absence of any external time parameter in (1). A necessary condition
for the whole formalism is of course that it be possible to recover, at least approximately, the familiar, and well-tested, Schrödinger equation with its $i\partial/\partial t$ term, independent of whether a sensible concept of time can be introduced at the fundamental level of Eq. (1) itself or not. A straightforward possibility to get the desired term would be to include a matter field with linear momentum into the fundamental Hamiltonian. This has been discussed through the introduction of a dust field \[15\]. Since, however, this approach may create its own problems \[16\], we will not take into account such dust fields and work directly with the Hamiltonian (2) or (3).

The Schrödinger equation can then be recovered, at least in a formal way, through a Born-Oppenheimer kind of expansion with respect to the Planck mass \[17\]. This approximation scheme should make it transparent how complex numbers enter into ordinary quantum theory. Let us briefly review how it works.

One starts by writing the total state in the form $\Psi = e^{iS}$ (with a complex function $S$) and expanding $S$ in powers of the Planck mass (we use $M \equiv (32\pi G)^{-1}$ in the geometrodynamical and $M \equiv G^{-1}$ in the connection formulation), $S = MS_0 + S_1 + M^{-1}S_2 + \ldots$. This ansatz is inserted into Eq. (1) and leads to a series of equations at consecutive orders in $M$.

We discuss first the geometrodynamical approach. The highest order ($M^2$) leads to the condition that $S_0$ must not depend on the matter fields. If there were, say, $N$ scalar fields $\phi_i$ in the matter Hamiltonian, this equation would read

$$\sum_{i,j} \left( \frac{\delta S_0}{\delta \phi_i} \right) \left( \frac{\delta S_0}{\delta \phi_j} \right) g_{ij}(\phi) = 0,$$

where $g_{ij}$ denotes a positive definite quadratic form. It is crucial for the success of the present approximation scheme that one can conclude from (1) that $S_0$ does not depend on the fields $\phi_i$. Since non-gravitational fields possess positive kinetic energy, this conclusion can be drawn if one requires that $S_0$ is either real or pure imaginary. It is an interesting observation that, due to the indefinite nature of the gravitational kinetic energy, one cannot derive in this scheme the opposite limit of classical matter fields coupled to quantum gravity. This is in contrast to, say, electromagnetism coupled to matter where each part can be treated semiclassically in an appropriate limit \[13\].

The next order ($M^1$) yields the Hamilton-Jacobi equation for gravity
\[ \frac{1}{2} G_{abcd} \frac{\delta S_0}{\delta h_{ab}} \frac{\delta S_0}{\delta h_{cd}} - 2 \sqrt{\hbar (R - 2\Lambda)} = 0. \] (5)

Eq. (5) is equivalent to Einstein’s field equations \[13\] and thus corresponds to the description of a (semi)classical gravitational background.

The most important step happens in the next order \((M^0)\) where the time-dependent Schrödinger equation can be recovered \textit{provided} that \(S_0\) is chosen to be real (strictly speaking, with a negligible imaginary part). This corresponds to the \textit{choice of a complex wave function} at this order. It happens at this point that complex numbers come into play, and it is exactly this step that has been criticized as being ad hoc \[1\]. The procedure continues by introducing a wave functional \(\chi \equiv D e^{i S_1}\) (and demanding a certain condition on the real prefactor \(D\)), which obeys \[20\]

\[ i G_{abcd} \frac{\delta S_0}{\delta h_{ab}} \frac{\delta \chi}{\delta h_{cd}} \equiv i \frac{\delta \chi}{\delta \tau} = H \chi, \] (6)

where \(H\) is the matter part of the Hamiltonian density \[3\]. Eq. (6) is the functional Schrödinger equation or Tomonaga-Schwinger equation for matter fields propagating in the classical background given by (3); \(\tau(x; h_{ab})\) is a ”many-fingered” time parameter. The emergence of a time parameter in the semiclassical limit reflects the fact that time is not an absolute entity but is inextricably entangled with the actual world: It is defined, in this approach, by ”evolving” three-geometries. It is interesting to observe that this concept corresponds exactly to the way time is most accurately ”measured” in practice – to \textit{ephemeris time} \[22\]. Briefly speaking, ephemeris time is determined by inverting solutions of the equations of motion to give time as a function of the (observed) position of a celestial body. All astronomical data that have been collected in the last centuries are implemented in the definition of ephemeris time which can only be determined, for a certain event, in retrospect. It is impressive to recognize that, as can be seen from the timing of the binary pulsar PSR 1913+16 \[23\], already the motion of the whole Galaxy has to be taken into account. Eventually all available data of the cosmological evolution will have to be implemented in the determination of ephemeris (”WKB”) time.

We will not pursue the present approximation scheme further which in the next order leads to small correction terms to the Schrödinger equation induced by quantum gravity \[24\] showing that unitary time evolution is only an approximate concept. We also note that there exist proposals to
generalize the above notion of semiclassical time to a full definition of time in quantum gravity [25]. Time is there defined exactly by the total phase of the wave functional, but, again, this demands the presence of a complex state as a solution to Eq. (1).

The choice of an imaginary solution for $S_0$ in (3) would lead to a diffusion type of equation instead of the Schrödinger equation (6). In quantum gravity this choice is sometimes interpreted as describing a euclidean spacetime [26]. The problem discussed here is, however, not so much related to the possible existence of euclidean worlds than to the fact that superpositions of WKB states would not allow the recovery of the Schrödinger equation as presented above. The superposition $\frac{1}{\sqrt{2}} e^{iS_0} + \frac{1}{\sqrt{2}} e^{-iS_0}$ (which is a real solution to the Wheeler-DeWitt equation (1) at order $M$), for example, does not lead to Eq. (6). The above derivation has therefore been criticized by several authors [6, 16, 21] since it heavily relies on the choice of a very special, complex, state in this order of approximation.

We now repeat briefly the above derivation of the Schrödinger equation in the connection representation. Since the connection is complex, a complex structure enters the scene already at the fundamental level of the configuration space. It is important to note that the wave functional is a holomorphic functional of the connection (analogously to the Bargmann representation for the harmonic oscillator). There is, however, still the problem that only a special WKB-state allows one to derive the Schrödinger equation for matter fields. Expanding, again, $S[A^i, \phi]$ in powers of the gravitational constant and inserting the state into (1) with the Hamiltonian given by (3), one finds that $S_0$ does not depend on matter fields and that it obeys the Hamilton-Jacobi equation

$$\frac{\epsilon^{ijk}}{4\pi} F^k_{ab} \frac{\delta S_0}{\delta A^a_i} \frac{\delta S_0}{\delta A^b_j} + \frac{i\sqrt{2}}{3} \Lambda \eta_{abc} \epsilon_{ijk} \frac{\delta S_0}{\delta A^a_i} \frac{\delta S_0}{\delta A^b_j} \frac{\delta S_0}{\delta A^c_k} = 0.$$ (7)

Note that since the momentum conjugate to $A^i_a$, $E^a_i$, is replaced by $\frac{\delta}{\delta A^i_a}$ (without an $i$) in the Schrödinger representation, the momentum is given by $E^a_i \equiv i\delta S_0/\delta A^i_a$. The triad $E^a_i$ is not necessarily real, but it can be chosen to be real by making use of one of the remaining constraint equations. Note that $S_0 = constant$ is always a solution of this equation.

The next order ($G^0$) yields the functional Schrödinger equation for the wave functional $\chi \equiv De^{iS_1}$,

$$i \frac{\epsilon^{ijk}}{4\pi} F^k_{ab} \frac{\delta S_0}{\delta A^a_i} \frac{\delta \chi}{\delta A^b_j} = i \frac{\delta \chi}{\delta \tau} = \tilde{H}_m \chi,$$ (8)
where the Hamiltonian density $\tilde{H}_m$ is now given by the expression

$$\tilde{H}_m = -\frac{1}{2} \frac{\delta^2 \chi}{\delta \phi^2} + \frac{\delta S_0}{\delta A^k_a} \frac{\delta S_0}{\delta A^k_b} \partial_a \phi \partial_b \phi + \frac{i}{3\sqrt{2}} \mu^2 \phi^2 \eta_{abc} \epsilon_{ijk} \frac{\delta S_0}{\delta A^k_a} \frac{\delta S_0}{\delta A^k_b} \frac{\delta S_0}{\delta A^k_c}$$

\[ + \sqrt{2} \Lambda \eta_{abc} \epsilon_{ijk} \frac{\delta S_0}{\delta A^k_a} \left( \frac{\delta S_0}{\delta A^k_b} \frac{\delta \chi}{\delta A^k_c} \right) \frac{\delta S_0}{\delta A^k_c} \frac{\delta S_0}{\delta D^k} \chi + \frac{\delta^2 S_0}{\delta A^k_a} \frac{\delta \chi}{\delta A^k_b} \chi \right). \quad (9)\]

At this stage, some comments are in order.

Firstly, the Hamiltonian density $\tilde{H}_m$ is equal to $H_c$ (3) as evaluated on the classical gravitational background determined by the Hamilton-Jacobi equation except for the last three $\Lambda$-dependent terms in (9) which arise due to the presence of the third functional derivatives in (3). This does not happen in the geometrodynamical formulation. The last two terms can be absorbed in an $A$-dependent phase but the first term may contain the matter field and may thus lead to a modification of the Hamiltonian (3). The interpretation of this term is not yet understood.

The second point has to do with the complex nature of the connection. Eq. (8) can be written as a functional Schrödinger equation if, in an appropriate region of configuration space, a time functional $\tau(x; A)$ can be introduced such that

$$\delta (x - y) = \epsilon_{ijk} F_{ab}^k(y) \frac{\delta S_0}{\delta A^k_a(y)} \frac{\delta \tau(x; A)}{\delta A^k_b(y)}. \quad (10)$$

This time functional, however, is in general complex. Since the wave functional is assumed to be a holomorphic functional in any order of approximation, its derivative with respect to $\tau$ is fully determined by its derivative with respect to the real part of $\tau$ which may thus serve to play the role of physical time. The semiclassical expansion in this approach has, of course, also to include an expansion of the reality conditions [12] which, in highest order, leads to a restriction of the original configuration space onto a subspace.

Thirdly, the above derivation of the Schrödinger equation has to be contrasted with the corresponding derivation in [12]. A Schrödinger equation has there been found by expanding the classical Hamiltonian constraint to second order around a chosen classical background and then applying this truncated constraint as a condition on the wave functional. Using arguments similar to above, the holomorphicity of the wave functional enabled one to identify a certain functional of the imaginary part of the trace part of $A$.
with physical time. The gravitational part alone then satisfies a Schrödinger equation with respect to this time variable. This is the main difference to our approach which only attempts to derive such an equation for quantum matter fields in a semiclassical gravitational background. The derivation in \cite{12} is analogous to a similar derivation in the geometrodynamical approach \cite{27} where time has been constructed from the extrinsic curvature. The similarity is not surprising since the imaginary part of the connection is given by the extrinsic curvature.

How, then, can one justify the use of a single state $D^{-1} e^{i S_0}$ in the derivation of the Schrödinger equation? One attempt at a possible solution makes use of the notion of decoherence \cite{28, 29}. The key ingredient is the fact that only a tiny fraction of the configuration space is accessible to observation. The unobservable degrees of freedom can thus be considered as being irrelevant and have to be traced out. Since there exist in general quantum correlations between all degrees of freedom, this leads to a nonunitary master equation for the relevant system describing the suppression of interference terms. In the geometrodynamic approach, the simplest superposition is (to order $M^0$)

$$\Psi \approx \frac{1}{D} e^{iS_0} \chi + \frac{1}{D} e^{-iS_0} \chi^*,$$

(11)

where both $\chi$ and $\chi^*$ may be consistently assumed to satisfy the time-dependent Schrödinger equation ($\chi^*$ with the sign-reversed time-parameter).

While $S_0$ depends only on the three-metric (say, the scale factor of the Universe in a simple minisuperspace model), $\chi$ depends on the three-metric as well as on all nongravitational fields. The idea is that most of these degrees of freedom contained in $\chi$ are inaccessible. The relevant object on which one has to focus is thus the reduced density matrix for the gravitational part,

$$\rho[h_{ab}, h'_{ab}] = \text{Tr}_{\phi} \Psi^* [h'_{ab}, \phi] \Psi [h_{ab}, \phi],$$

(12)

where $\phi$ symbolically denotes the fields which are traced out. Decoherence then occurs if in the total density matrix

$$\Psi^* \Psi = \frac{1}{D^2} (2|\chi|^2 + e^{2iS_0} \chi^2 + e^{-2iS_0} \chi^* 2^2)$$

the last two terms become small after integration over the $\phi$-variables. The reduced density matrix then describes an approximate ensemble of the two states in (11). In a typical model one takes for $\phi$ the inhomogeneous modes.
of a scalar field and restricts attention only to the radius of the Universe as the relevant degree of freedom. For the superposition (11) one can then find a suppression of interferences. It has been found, for example, that the suppression factor is proportional to \( \exp\left(-\frac{\pi m H_0^2 a^3}{128}\right) \), where \( m, H_0, a \) are respectively the mass of the scalar field, the Hubble parameter, and the scale factor \([29]\). Except for small scales and near the turning point of the corresponding classical Universe one can consistently treat the two components in (11) as being dynamically independent. One has to emphasize, of course, that the degree of decoherence depends on the total state and on the choice of relevant and irrelevant variables. As the discussed examples indicate, decoherence should become effective if a huge number of degrees of freedom as well as large masses (in our case it is the large Planck mass) are involved.

In the general case one has, instead of (11), many WKB components,

\[
\Psi \approx \sum_r e^{i S_r} \chi_r,
\]

where each component has its own WKB time. Decoherence then should explain why the second sum in the total density matrix,

\[
\Psi^\ast \Psi \approx \sum_r |\chi_r|^2 + \sum_{r \neq s} e^{i (S_r - S_s)} \chi_s \chi_r^\ast,
\]

becomes negligible after integrating out the irrelevant degrees of freedom.

Independent of this approach through decoherence it has been suggested to introduce complex numbers on the level of (11) itself so that it will be natural to start with a complex WKB state from the very beginning. This can be achieved, for example, if the functional derivative in (2) is replaced according to the prescription \([6]\)

\[
\frac{\delta}{\delta h_{ab}} \rightarrow \frac{\delta}{\delta h_{ab}} - i A^{ab}[h_{cd}],
\]

where \( A^{ab} \) are the components of some “super-gauge potential” defined on the configuration space (an analogous proposal can be made with respect to (3)–see below). How could one justify the introduction of such a super gauge potential? We provide three different answers which are, however, not independent of each other and which may also be connected to the notion of decoherence discussed above.

The first possibility is connected with the occurrence of anomalies. It is well known that, for example, Weyl fermions in an external electromagnetic background may acquire an anomaly leading to the violation of gauge
invariance (see, e.g., [30]). This, in turn, is intimately connected with the emergence of a "functional" Berry phase $\gamma$,

$$\gamma = \oint D A^a A_a(x; A),$$

(14)

where $A$ denotes the usual vector potential, and

$$A_a(x; A) = i \langle \Psi | \frac{\delta}{\delta A_a(x)} | \Psi \rangle$$

(15)

is a super-gauge potential defined on the configuration space of all vector potentials. It stands in close analogy to the potential $A^{ab}$ in (13). The state $\Psi$ in (15) is a fermionic state which also depends on the external electromagnetic field. One can restore gauge invariance (but loses Lorentz invariance) if one replaces the electromagnetic field momentum according to

$$\delta \rightarrow \delta - i A_a(x; A).$$

(16)

This introduces complex numbers into the electromagnetic field Hamiltonian.

The standard model of gauge theories, however, does not possess such anomalies, at least perturbatively. Are there gravitational anomalies of this kind? It has been shown that the determinant of the Weyl operator for handed fermions in a gravitational background is not invariant under frame rotations if the dimension $d$ of spacetime is $d = 4n + 2 = 2, 6, 10, \ldots$ [32]. Such Lorentz anomalies thus do not exist in four spacetime dimensions. An external gravitational field influences chiral anomalies in four dimensions but not in the standard model. Thus, as far as canonical quantum gravity in three space dimensions is concerned, anomalies do not seem to be a realistic option to justify the substitution (13) (they may become relevant in the framework of Kaluza-Klein theories).

Before we embark on a more promising explanation we note that the presence of torsion [33] could become important in this context. The action for a Dirac field in an external gravitational field, for example, is complex if torsion is nonvanishing. This in turn would also lead to a complex Hamiltonian and could thus also produce a nontrivial Berry phase in analogy to the case discussed above.

Perhaps the most promising attempt to justify a substitution like (13) arises from the possibility to have $\theta$ states in quantum gravity [34]. Since the
situation in the geometrodynamical formulation is somewhat different from
the connection formulation, we treat both cases separately. \( \theta \) states can
arise from the possibility to have large symmetry transformations, i.e., sym-
metry transformations which are not connected with the identity. In general
relativity, the relevant symmetry is the invariance under the group of diffeo-
morphisms. The momentum constraints secure only the invariance of the
wave functional under infinitesimal diffeomorphisms \[35\] that are asymptot-
ically trivial \[36\]. One thus has to deal with \( \theta \) states if the diffeomorphism
group is not connected, i.e., if \( \pi_0(\text{Diff}\Sigma) \equiv \text{Diff}\Sigma/\text{Diff}_{id}\Sigma \) is non-vanishing.
One would thus expect, in analogy to ordinary quantum theory, that the
wave functional
transforms according to a one-dimensional, irreducible, representation of
\( \pi_0(\text{Diff}\Sigma) \), and the \( \theta \) sectors are then labelled by the elements of the group
\( \text{Hom}(\pi_0(\text{Diff}\Sigma), U(1)) \), i.e., the group of homomorphisms of \( \pi_0 \) into \( U(1) \).
It has to be emphasized that the restriction to such representations is an
assumption which one might have to generalize after a better understanding
of quantum gravity will have been achieved. We note, however, that higher
dimensional representations appear even in standard quantum mechanics in
the presence of discrete groups \[38\].

The emergence of a \( \theta \) parameter is well known from Yang-Mills theo-
ries (see, e.g., \[39\]). For the gauge group \( G : S^3 \to SU(N) \), e.g., one has
\( \pi_0(G) = \pi_3(SU(N)) = Z \). Thus, \( \theta \) states are simply labelled by the elements
of
\( \text{Hom}(Z, U(1)) \). In the connection approach to quantum gravity, the situa-
tion will be analogous, as discussed below. Instead of taking the gauge group
as the starting point, one can take an alternative viewpoint and focus on
the topological properties of the physical configuration space, \( \mathcal{Q} \), of the the-
ory. In the Yang-Mills case this is the space of vector potentials modulo \( \mathcal{G} \),
while in gravity this is the space of Riemannian metrics, \( \text{Riem}\Sigma \), on \( \Sigma \) mod-
ulo diffeomorphisms. Quantum theory on nontrivial configuration spaces
has been extensively discussed in the literature (see, e.g., \[40\]). It was
found that \( \theta \) structures may emerge if the first fundamental group, \( \pi_1(\mathcal{Q}) \),
is nonvanishing. The quantum mechanical propa-
gator, \( K(q_2, q_1) \), of a system can then be expressed as a sum of prop-
agators \( K[p] \) where in each \( K[p] \) the paths lie in the same homotopy class. Thus,
\[
K(q_2, q_1) = \sum_{[p]} \chi([p])K[p](q_2, q_1),
\] (17)
where $\chi \in \text{Hom}(\pi_1(Q), U(1))$. In the functional Schrödinger equation wave functionals can be viewed as cross sections of a complex bundle over $Q$ which gives rise to a connection over $Q$ precisely in the way as it was envisaged in \cite{13}. One considers flat connections only since there is no hint of a ”super connection” with non-vanishing curvature in the framework of the Wheeler-DeWitt equation.

Both viewpoints can be unified if the symmetry group acts freely on $\text{Riem}\Sigma$, since then $\pi_1(Q)$ is homeomorphic to $\pi_0(\mathcal{G})$ and the $\theta$ parameter can be directly connected with the nontrivial structure of the configuration space itself. In gravity, however, $\text{Diff}(\Sigma)$ does not act freely because of the existence of isometries. These can be removed if one goes to the ”extended superspace” \cite{11, 12}. (We emphasize that the compact and open cases can be discussed on the same footing within this framework since the corresponding configuration spaces are diffeomorphic.) $\theta$ states are then classified by the elements of $\text{Hom}(\pi_1(\text{Riem}\Sigma/\text{Diff}_\Sigma) \equiv \pi_0(\text{Diff}_\Sigma, U(1))$, where $\text{Diff}_\Sigma$ is the subgroup of $\text{Diff}\Sigma$ consisting of diffeomorphisms which leave the tangent space at some fixed base point invariant. It acts freely on $\text{Riem}\Sigma$ \cite{14}. Even if the action of the group is not free, one can discuss $\theta$ sectors which correspond to representations of the group acting on configuration space \cite{13}. One can even find such sectors if the first fundamental group is vanishing \cite{14}.

It is sometimes suggested that the configuration space has to be reduced further from three degrees of freedom per space point to two degrees of freedom by extracting some intrinsic time variable \cite{34}. This would amount to solve the Hamiltonian constraint before quantization through the choice of an appropriate time function. The corresponding framework would be different from the one considered here since there would be no equation like \cite{1}. As far as the topological properties of the new configuration space are concerned, one would, however, not expect drastic modifications since $\text{Riem}\Sigma$ is in that case only factored by the multiplicative group of conformal factors which is a topologically trivial operation \cite{15}.

The most interesting question of course is: Which three-manifolds $\Sigma$ can lead to a nontrivial $\theta$ structure? Since $\pi_0(\text{Diff}_{S^3}) = \text{id}$ for orienting preserving diffeomorphisms, there is no such structure in the simplest case of a three-sphere, $\Sigma = S^3$, except for the case that reflections are included. Nontrivial structures emerge, e. g., in the case $\Sigma = S^1 \times S^2$ (”wormhole”) and $\Sigma = S^1 \times S^1 \times S^1$ (the three-torus) \cite{34}.

The next question is: Might the presence of a $\theta$ structure be the reason why one can focus consistently on complex solutions to \cite{1} and, moreover, to only one WKB component $D^{-1} e^{i\xi}$ in the semiclassical approximation?
The first part of this question can be answered easily. If \( \pi_0 \neq 0 \), and if the group is represented by a one-dimensional, irreducible representation, the superposition \((\Pi)\) does not belong to the class of allowed quantum states since one component would transform, under the assumption that it is an eigenstate of a large symmetry transformation, with the complex conjugate of the other (always assuming, of course, that the \( \theta \) parameter is nonvanishing). The state \((\Pi)\) would thus not be an eigenstate of a large symmetry transformation. This would correspond to an *exact* superselection rule – much stronger than the approximate notion of decoherence discussed above from which it could in principle be distinguished. We note that \( \theta \) is a parameter which can in principle be measured (in QCD, for example, it can be determined by measuring the electric dipole moment of the neutron).

The second part of this question is more difficult to answer. A single semiclassical state is in general not, even within the limits of the semiclassical approximation, an eigenstate of a large symmetry transformation. If the \( \theta \) structure indeed gave rise to an exact superselection rule, one would have to select amongst all possible WKB solutions those which are eigenstates of a large symmetry transformation. This could turn out to be a viable principle in finding physically relevant solutions since most eigenstates are superpositions of several WKB components \[43\]. Because of the complexity of the problem, concrete examples have to be discussed within the context of very simple minisuperspace models. Consider, e. g., a model which is defined in *three* spacetime dimensions, with spatial sections \( \Sigma = S^1 \times S^1 \) \[43, 46\], by the metric

\[
\begin{align*}
  ds^2 &= -N^2(t)dt^2 + a^2(t)dx^2 + b^2(t)dy^2,
\end{align*}
\]

where \( x \) and \( y \) are identified periodically with period \( 2\pi \). The Wheeler-DeWitt equation reads, for this model,

\[
H\psi \equiv \left( \frac{\partial^2}{\partial a \partial b} + \frac{\pi^2 \Lambda ab}{4G^2} \right) \psi = 0,
\]

where \( G \) and \( \Lambda \) denote again the gravitational constant and the cosmological constant, respectively. The minisuperspace analogue of \( \pi_0(\text{Diff}\Sigma) \) is here played by the permutation group of the two scale factors, which has only two one-dimensional, irreducible, representations. Note that the coupling to matter only produces additional terms containing the combination \( ab \) so
that this symmetry will not be spoiled. Semiclassical solutions are of the form
\[ \psi = Ce^{iS}, \]  
where \( S \) is a solution to the Hamilton-Jacobi equation
\[ -\frac{\partial S}{\partial a} \frac{\partial S}{\partial b} + \frac{\pi^2 \Lambda ab}{4G^2} = 0. \]
In [43, 46] interest was focused on the class of solutions that correspond to the "no-boundary proposal." These states are not eigenstates of the permutation operator so one has to superpose two semiclassical states of the form \( \psi = Ce^{iS} \) to arrive at states which are either symmetric or antisymmetric under the action of the permutation group. Such superpositions, however, do not allow one to recover the Schrödinger equation for matter fields. This is possible if one chooses one of the two solutions
\[ \psi_{\pm}(a, b) = \left( \frac{1}{a} + \frac{\beta}{b} \right) \exp \left( \pm \frac{i\pi}{2G} \sqrt{\Lambda} ab \right) \]  
with either \( \beta = 1 \) (symmetric state) or \( \beta = -1 \) (antisymmetric state). It is important that the WKB prefactor can be chosen in such a way that the wave function acquires the desired transformation properties. Note that \( \psi_{\pm} \) is an exact solution of \( \psi = Ce^{iS} \). It is an artifact of this simple model, which allows only real representation to occur, that the superposition of the two states \( \psi_{+} \) and \( \psi_{-} \), which does not allow the derivation of the Schrödinger equation, is again an eigenstate of the permutation operator. In the generic case of complex representations this is no longer possible. In the nontrivial examples in [43] only the trivial representations are possible if single WKB states are required to be eigenstates.

The situation is somewhat different from the point of view of the connection representation. Since the wave functional is defined on a space of connections, one has, in addition to the diffeomorphism group, a \( SO(3) \) gauge group [47], and hence one may have \( \theta \) states in analogy to the Yang-Mills case [48] independent of whether the action of the diffeomorphism group is represented trivially or not. As discussed above, these states arise since \( \pi_0(\mathcal{G}) = Z \). Thus, as long as \( \theta \neq 0 \), the wave functional transforms under a large gauge transformation with winding number \( n \) as
\[ \Psi[A] \rightarrow e^{in\theta} \Psi[A]. \]
Superpositions like (11) are thus "forbidden" if one assumes, in analogy to the Yang-Mill case, that physical states are eigenstates of the operator which generates large gauge transformations. This would correspond to the decomposition of the full theory into inequivalent superselection sectors. To say that superpositions are "forbidden" is equivalent to saying that they are indistinguishable from an ensemble of states living in different sectors if only gauge-invariant observables are available [50]. Whether gauge-noninvariant observables, which can bridge between these sectors, are present at a more fundamental level, is an open question. The situation is analogous to QED where one might speculate whether the charge superselection rule has its prime origin in the invariance of the theory under rigid gauge transformations or in decoherence [29, 49]. A further example is provided by the spontaneous symmetry breaking in the early Universe [49] where the various "true vacua" are separated by a superselection rule.

Instead of demanding that the wave functional transforms like in (23), one can alternatively demand that it be invariant but that instead the field momentum changes according to

\[ \frac{\delta}{\delta A^i_a} \to \frac{\delta}{\delta A^i_a} - i\theta G^2 \frac{1}{8\pi^2} \tilde{B}^a_i, \]  

(24)

where \( \tilde{B}^a_i \equiv \eta^{abc} F^i_{cb} \) is the "magnetic field" corresponding to \( A^i_a \). The gravitational constant enters explicitly in (24). Note that this is just the desired substitution (13).

To conclude, we have presented some possible avenues which may lead to a deeper understanding of the derivation of the Schrödinger equation from quantum gravity. A non vanishing \( \theta \) parameter could lead to a strong selection principle amongst possible WKB solutions. Moreover, it might be that at a fundamental level decoherence and \( \theta \) sectors are actually related, i. e., that the \( \theta \)-superselection rule is caused by decoherence in a dynamical way. A detailed discussion would, however, need to invoke a specific "environment" which is able to decohere different \( \theta \) eigenstates. Furthermore, since the structures of the respective configuration spaces in the geometrodynamical and the connection dynamical formulations are different, semiclassical considerations could perhaps provide a way to distinguish between both approaches to quantum gravity. We hope to address these issues in a future publication.

It should be emphasized that the whole paper rests on the assumption
that general relativity is the starting point for quantization. Higher derivatives, for example, would change the situation and lead to a Schrödinger equation even at the fundamental level of full quantum gravity \[51\].

It is interesting to see that the possible connection of symmetries with the \(i\) in the Schrödinger equation is similar to the one envisaged in \[52\], although it emerges here at a much more fundamental level.

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**References**


[9] They were found in the *loop-space representation* which is related to the connection representation by an integral transform, see Ref. 10.

[11] We use a rescaled connection $A^i_o \equiv G \bar{A}^i_o$, where $\bar{A}^i_o$ denotes the connection as it is introduced in Ref. 12. This rescaling is convenient for performing the semiclassical expansion and is analogous to a corresponding rescaling in QED where $G$ is replaced by the electric charge, see Ref. 13. Such a rescaling has also been exploited in the study of the strong gravity limit, see Ref. 14.


[18] An expansion with respect to $G$ does not allow to consider "macroscopic" sources in (4). They can be included in the description if the expansion if performed with respect to some other parameter ("large mass") of the theory.


[20] We do not consider factor ordering terms which may arise from the coupling of gravity to the kinetic matter terms, see Ref. 21.


If one allows for rotations at spatial infinity, there is also a possibility to get half-integer spin states in case that a $2\pi$ rotation acts nontrivially, see Ref. 37 (the manifold $\Sigma = R^3 \# T^3$, e. g., allows such states). In this paper we restrict ourselves to the compact case.


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One might again be concerned about the complex nature of the connection in this context. Since the wave functional is, however, holomorphic with respect to the connection, it is determined by its restriction to its real part, see Ref. 48.


