Semiclassical Analysis of Constrained Quantum Systems

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Abstract. Exact procedures that follow Dirac’s constraint quantization of gauge theories are usually technically involved and often difficult to implement in practice. We overview an “effective” scheme for obtaining the leading order semiclassical corrections to the dynamics of constrained quantum systems developed elsewhere. Motivated by the geometrical view of quantum mechanics, our method mimics the classical Dirac-Bergmann algorithm and avoids direct reference to a particular representation of the physical Hilbert space. We illustrate the procedure through the example of a relativistic particle in Minkowski spacetime.

Keywords: Dirac’s constraint quantization, semiclassical states, effective equations

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INTRODUCTION

Full phase-space of fundamental gauge theories does not represent the physical degrees of freedom: constraint functions restrict the part of the phase-space that is physically accessible and the transformations they generate identify points that are physically equivalent. Direct quantization of the physical degrees of freedom requires global knowledge of the solutions to the constraint functions and the corresponding gauge orbits which, in general is unavailable. In its absence one can follow a method due to Dirac [1], which postpones enforcement of the constraints until after quantization. Constraints are to be promoted to quantum operators and solved by demanding that they annihilate physical states. Often the most challenging part of this procedure is determining the physical inner product on the space of solutions. Explicit constructions of the physical Hilbert space are only available in few specific cases.

Here we overview an “effective” scheme for solving constraints at the quantum level developed in [2] and [3]. Focusing on kinematically semiclassical states we obtain quantitative description of the leading order quantum corrections without a rigorous definition of the physical inner product. In its current form, the method applies to theories with finite number of classical degrees of freedom, such as symmetry-reduced minisuperspace models. In each section of the report we illustrate the corresponding part of our construction using the example of a free relativistic particle.
KINEMATICAL REPRESENTATION

According to Dirac’s prescription, one is first to quantize the free system to obtain what is commonly referred to as a **kinematical representation**. We assume that in this process some closed Poisson algebra with a finite number of generators, that completely describes the classical phase-space, is quantized canonically. Explicitly, there are \( N \) real phase-space functions \( a_i, i = 1, \ldots, N \) that are closed with respect to the Poisson bracket \( \{ a_i, a_j \} = \sum_k \alpha_{ij}^k a_k \), where \( \alpha_{ij}^k \) are structure constants. Quantization identifies these with self-adjoint operators \( a_i \), whose commutation relations represent the quantized version of the classical Poisson bracket \( [a_i, a_j] = i\hbar \sum_k \alpha_{ij}^k a_k \). For our purposes we assume that the kinematical operators generate an associative unital algebra \( \mathcal{A} \) containing all finite polynomials in \( a_i \). The issue of domains of definition of unbounded operators may be kinematically addressed by using a non-Cauchy-complete pre-Hilbert inner product space representation. This algebra has a countable linear basis \( a_n a_n^1 \ldots a_n^N \)—due to the commutation relations, other orderings of these polynomials are related through addition of lower order polynomial terms.

We further assume that there is a single constraint \( C \), which is a given element of \( \mathcal{A} \). The case of several commuting constraints may be treated in an analogous manner. In order to sidestep the issue of the physical inner product we will avoid direct reference to a Hilbert space, instead a state in our construction is a complex-valued linear functional on \( \mathcal{A} \). This is a more general notion than a Hilbert-space state, in particular it includes density states and states that are non-positive with respect to the kinematical \( \star \)-relations. A state can be specified completely by specifying the values it assigns to a linear basis on \( \mathcal{A} \). We restrict to states that assign 1 to the identity element—a rather weak version of normalization.

**Free Relativistic Particle.** The classical phase-space of a relativistic point particle of rest-mass \( m \) in Minkowski spacetime with one space and one time dimension is coordinatized by two canonical pairs \( t, p_t \) and \( q, p \) with the non-zero Poisson brackets \( \{ t, p_t \} = 1 = \{ q, p \} \). The dynamics is governed by a single constraint

\[
C = p_t^2 - p^2 - m^2.
\]

The standard quantum kinematical representation of this system is given by the action of differential operators on smooth wavefunctions in two variables \( x_0 \) and \( x_1 \):

\[
t = x_0 \quad , \quad p_t = \frac{\hbar}{i} \frac{\partial}{\partial x_0} \quad , \quad q = x_1 \quad , \quad p = \frac{\hbar}{i} \frac{\partial}{\partial x_1}.
\]

The associative algebra these generate has a linear basis \( t^k p_t^l q^m p^n \)—terms with a different ordering may be expressed using the well-known commutation relations

\[
[t, p_t] = i\hbar \mathbb{1} \quad , \quad [q, p] = i\hbar \mathbb{1}.
\]

Henceforth we will no longer refer to a concrete representation of \( \mathcal{A} \) in terms of operators on a vector space—unless stated otherwise, we will treat a state as an assignment of a complex number to each basis polynomial. There is no product-ordering ambiguity in the case of the above constraint and quantization identifies it with the element \( C = p_t^2 - p^2 - m^2 \mathbb{1} \) of \( \mathcal{A} \).
QUANTUM VARIABLES

In the previous section we have defined a state as a complex linear functional on $\mathcal{A}$, which is then an element of its vector-space dual, henceforth referred to as $\mathcal{A}^*$. We will denote the value assigned by the state $\psi \in \mathcal{A}^*$ to the element $A \in \mathcal{A}$ by $\langle A \rangle_{\psi}$. Dropping the reference to a particular state we write $\langle A \rangle$ to denote the corresponding complex-valued function on the space of all states. In particular, the set of functions induced by the linear basis $\langle a_1^n a_2^m \ldots a_N^N \rangle$ completely coordinatizes the space $\mathcal{A}^*$.

Functions on the space of states inherit a Poisson bracket from the commutation relations on $\mathcal{A}$:

$$\{ \langle A \rangle, \langle B \rangle \} = \frac{1}{i\hbar} \langle [A, B] \rangle.$$

The bracket satisfies the Jacobi identity and can be extended to non-linear functions by using Leibnitz’s rule. A flow induced on observables by a Hamiltonian operator may be expressed entirely using this bracket. In ordinary quantum mechanics the evolution of the expectation value of an observable is governed by the equation

$$\frac{d}{dt} \langle O \rangle = \frac{1}{i\hbar} \langle [O, H] \rangle + \frac{\partial \langle O \rangle}{\partial t}.$$

By our earlier definition, the first term on the right-hand side is simply the quantum Poisson bracket $\{ \langle O \rangle, \langle H \rangle \}$. The evolution of any function on $\mathcal{A}^*$ induced by the Hamiltonian can be expressed using a generalization of this equation

$$\frac{d}{dt} f = \{ f, \langle H \rangle \} + \frac{\partial f}{\partial t}.$$

This construction is related to the various geometrical formulations of quantum mechanics [4] [5] and can be used to replace the single partial-differential Schrödinger equation by an infinite number of coupled ordinary differential equations, which can be of advantage in certain regimes [6].

To investigate semiclassical properties, we use coordinates on $\mathcal{A}^*$, that are adapted to the semiclassical expansion, namely the $N$ expectation values $\langle a_i \rangle$ and the infinite number of moments $\langle (a_1 - \langle a_1 \rangle)^{n_1} \ldots (a_N - \langle a_N \rangle)^{n_N} \rangle_{\text{Weyl}}$, where the subscript “Weyl” indicates the total symmetrization of terms in the product. Semiclassical states are close to maximum localization in the phase-space variables (bounded from below by the various uncertainty relations). We assume that for such a state the moments fall off as $\hbar^{\frac{1}{2} \sum_{i=1}^{N} n_i}$, this assumption can be concretely realized using Gaussian wavefunctions.

**Free Relativistic Particle.** The system’s quantum state is completely determined by the values of $\langle t^k p^l q^m p^n \rangle$, or alternatively the expectation values of the four basic observables $\langle t \rangle, \langle p_t \rangle, \langle q \rangle, \langle p \rangle$, and their moments. The lowest order moments correspond to $k + l + m + n = 2$ (see below) and are easy to identify as the standard deviations and covariances in the observables. For example, $\langle (q - \langle q \rangle)^2 \rangle$ is precisely the spread of the wavefunction in the $x_1$ coordinate. Using a sharply peaked Gaussian wavefunction in $x_0$ and $x_1$ it is straightforward to verify the semiclassical fall-off of the moments

$$\langle (t - \langle t \rangle)^k (p_t - \langle p_t \rangle)^l (q - \langle q \rangle)^m (p - \langle p \rangle)^n \rangle_{\text{Weyl}} \propto \hbar^{\frac{1}{2} (k+l+m+n)}.$$
CONSTRAINT FUNCTIONS

Once the free system has been quantized, Dirac’s prescription for enforcing a constraint is to restrict to the subspace of vector states that are annihilated by the constraint operator. In other words, physical wavefunctions are solutions to the equation

\[ \mathbf{C} | \psi \rangle = 0. \]

In many interesting cases, this equation can be solved, but the solutions have an infinite norm with respect to the kinematical inner product. Exact techniques, such as group averaging [7], provide a method for \textit{formally} defining the physical inner product on the space of solutions, with exact calculations typically being fairly involved.

We observe that, in general, solutions of the quantum constraint have no kinematical dual and therefore, there is no \textit{a priori} method for taking expectation values. In fact, there is typically an infinite number of ways to define a state, in the sense of a linear functional on \( \mathcal{A} \), using such a wave-function. For example a momentum eigenstate \( \exp(i \omega x) \), is not square-integrable with respect to \( x \), however we can define expectation values using a suitably well-behaved distribution \( f(x) \) as

\[ \langle A \rangle_f := \int \! \! dx f(x) A \exp(i \omega x). \]

The weak normalization condition would only require that \( \int \! \! dx f(x) \exp(i \omega x) = 1 \), for the given value of \( \omega \), which can be satisfied by a large variety of distributions. The fact that the state was constructed using an eigenfunction of momentum manifests itself by momentum acting multiplicatively on such a state when the corresponding element appears to the right but not on the left, i.e. \( \langle A p \rangle_f = \hbar \omega \langle A \rangle_f \neq \langle p A \rangle_f \). By analogy, we demand that states be annihilated when the constraint appears on the right, that is

\[ \langle A C \rangle = 0, \quad \forall A \in \mathcal{A}. \]

Choosing the constraint to annihilate states when appearing on the left is entirely equivalent. Enforcing this condition leads to an infinite countable set of constraint functions on the space of states, which can be imposed systematically by setting \( \langle a^n_1 \ldots a^n_N C \rangle = 0 \) for all values of \( n_1, \ldots, n_N \). The complete set of these conditions is closed with respect to the Poisson bracket on \( \mathcal{A} \), the system is thus analogous to a classical system with first-class constraints.

The states, such as \( \langle \rangle_f \) above, are not always positive with respect to the kinematical \( \star \)-relations, in the algebraic sense that \( \langle A A^\star \rangle \geq 0 \) will in general not hold for all \( A \). Consequently the states can assign complex values to expectation values and moments of \( \star \)-invariant elements. It is our observation that kinematically non-positive states are needed in order to impose the quantum constraint in the above sense. We note, that the states can still be positive with respect to a subalgebra of \( \mathcal{A} \), for instance the elements that commute with the constraint.

\textit{Free Relativistic Particle}. In terms of wavefunctions in \( x_0 \) and \( x_1 \), \( \mathbf{C} | \psi \rangle = 0 \) takes the form of the usual Klein-Gordon equation. Here we impose the quantum constraint systematically by demanding \( \langle t^k p_l q^m p^n C \rangle = 0 \) for all values of \( k, l, m, n \). We adapt
these conditions to semiclassical expansion by expressing them in terms of expectation values and moments. Below are examples of two of the quantum constraints expressed in this way, where short-hand notation was used for the expectation values $a := \langle a \rangle$ and the moments of second order: $(\Delta a)^2 := \langle (a - \langle a \rangle)^2 \rangle$ and $\Delta(ab) := \langle (a - \langle a \rangle)(b - \langle b \rangle) \rangle_{\text{Weyl}}$

\[ C = \langle C \rangle = p_t^2 - p^2 - m^2 + (\Delta p_t)^2 - (\Delta p)^2 = 0 \]
\[ C_t = \langle (t - \langle t \rangle)C \rangle = 2p_t\Delta(tp_t) + ihp_t - 2p\Delta(tp) + (3\text{rd order moments}) = 0 \]

For convenience, we have replaced the constraint function $\langle tC \rangle$ with $\langle (t - \langle t \rangle)C \rangle$, which is equivalent when other constraint functions are taken into account as the two are related by adding $t\langle C \rangle$. Other constraint functions may be expanded similarly.

**GAUGE FREEDOM**

As one may recall from analysis of classical constrained systems, first-class constraints, through Poisson bracket, generate transformations that preserve the constraint surface and are regarded as gauge. In our case, infinitesimal gauge transformations are generated by the action of the constraint element when it appears on the left, since our constraint condition only demands that the states are annihilated by the constraint element appearing to the right. Constraint functions introduced in the previous section are only meant to be analogous to imposing $C|\psi\rangle = 0$. In particular, we have introduced no analogue of the physical inner product. Consequently, it does not come as a surprise that we are still left with a number of gauge choices. One may be puzzled here as the exact Hilbert space constructions, such as group averaging, typically provide a unique physical inner product on the space of solutions—where then does this ambiguity in taking the expectation values come from?

To address this question, we point out that such a physical inner product is defined only on the space of solutions and does not in general extend to other wavefunctions in a natural way. As a result, the expectation values of operators that do not preserve the space of solutions, are not well-defined. The gauge transformation generated by a constraint function $\langle AC \rangle$ on the expectation value of some observable $\langle O \rangle$ is given by

\[ \delta \langle O \rangle = \{ \langle O \rangle, \langle AC \rangle \} = \frac{1}{ih} \langle A[O,C] \rangle + \frac{1}{ih} \langle [O,A]C \rangle \]

It is easy to see that the function generated by an operator that commutes with the constraint on the solution space, and therefore preserves it, has a vanishing Poisson bracket with all of the constraint functions. Therefore, in our formalism, there is also no ambiguity in taking expectation values of observables that preserve solutions to the constraint. These are the true physical degrees of freedom of the system.

To extract invariant quantities one can fix all of the gauge freedom or solve the differential equations for all the gauge flows. For the quantities that do not commute with the constraint, one may attempt to ask how they vary along the gauge orbits relative to each other [8] [9]. This is a physically meaningful question especially when one is dealing with a so-called Hamiltonian constraint, which itself should govern the dynamics. Classically, a Hamiltonian constraint produces a single gauge flow on the
constraint surface. Multiplying the constraint function by any other function that does not vanish on the constraint surface results in the same gauge-orbit structure with a different parametrization. One can take two functions on the constraint surface and parameterize the gauge flow of one relative to the other
\[ \frac{df}{dg} = \left( \frac{dg}{d\tau} \right)^{-1} \frac{d}{d\tau} f = \{ f, C \} \]

where \( \tau \) is the parameter along the orbits generated by \( C \). This is well-defined so long as the bracket \( \{ g, C \} \) does not vanish. In our quantum analysis, a single Hamiltonian constraint gives rise to an infinite number of first-class quantum constraint functions, which generate an infinite number of gauge flows. One could guess that the flow induced by the expectation value of the original constraint operator itself is somehow “preferred”. However, classically, the constraint function is only fixed up to multiplication by a non-vanishing function, so that even with quantization ambiguities set aside, there is no preferred constraint operator. From the kinematical perspective, any operator with the same zero-eigenspace as \( C \) will yield the same set of solutions, but would in general produce a different flow. For example if \( A \) is invertible, kinematically self-adjoint and commutes with \( C \), the operator product \( C' = AC \) is just as good as a constraint operator but produces a different unitary flow. For our purposes we assume that all combinations of transformations induced by the quantum constraint functions are equally viable directions of evolution. Thus in order to use one of the functions on the constraint surface as an evolution parameter we first need a way to reduce the infinite number of gauge directions to a single one.

Below we summarize a method that achieves such a gauge reduction order-by-order within semiclassical analysis. Let \( X \) be an observable chosen to serve as a “clock”. We would like \( \langle X \rangle \) to measure time and the element itself to act on states simply as a multiplication by \( \langle X \rangle \). In principle, we once again have the option to demand that \( X \) acts as a multiplicative operator when appearing on the left or on the right. We require that \( \langle XA \rangle = \langle X \rangle \langle A \rangle \) for all \( A \) as the gauge condition, since it is the only choice consistent with our constraint functions, namely \( \langle XAC \rangle = 0 = \langle X \rangle \langle AC \rangle \). The preferred flow is the one that preserves this gauge. We do not possess a proof or a strong argument that suggests that these conditions always result in a reduction to one and only one preferred gauge transformation. In the examples studied so far, however, we have found that order-by-order in semiclassical analysis, the method does yield the correct number of gauge fixing conditions leaving \( \langle X \rangle \) free to vary along the single remaining flow.

**Free Relativistic Particle.** For the particle, is natural to choose the element corresponding to its time coordinate \( t \)—as the evolution variable. In terms of the moments the gauge conditions are \( (\Delta t)^2 = 0, \Delta (tp_t) = -\frac{i\hbar}{2}, \Delta (tq) = 0, \Delta (tq) = 0 \) as well as similar conditions for higher order moments.

### SEMICLASSICAL ANALYSIS

In order to extract the leading order quantum corrections to the classical equations of motion we restrict our analysis to the states that are kinematically semiclassical in the
sage defined earlier. Namely, we assume that M-th order moments have magnitudes of the order $\hbar^M$ and truncate constraint functions at some chosen power of $\hbar$. For a constraint that is polynomial in the basic observables, the truncation yields a finite system of polynomial equations in expectation values and moments. The set of equations may have more than one solution, each of which needs to be tested for consistency with the original semiclassical assumption. The complete infinite set of constraint functions is first-class, the finite truncated set of constraint functions is generally only first-class to the relevant order in $\hbar$. Adding gauge-fixing conditions breaks the first-class nature of the system, where the residual gauge freedom is given by the linear combinations of constraint functions that have a vanishing bracket with the gauge conditions.

The final problem, which can be complicated in general, is ensuring positivity of the gauge-fixed state with respect to the gauge invariant algebra elements. In principle it is equivalent to enforcing reality of the expectation values and quantum uncertainty relations on moments, however gauge-fixing conditions in general force us to modify Poisson brackets between variables making them more difficult to interpret.

*Free Relativistic Particle.* Here we consider a semiclassical truncation at order $\hbar$—we discard all terms of order $\hbar^3$ and higher, dropping moments above second order as well as products of second order moments. The truncated versions of the constraint functions used as an example earlier are

$$
C = p_t^2 - p^2 - m^2 + (\Delta p_t)^2 - (\Delta p)^2 = 0 \\
C_t = 2p_t\Delta(tp_t) + i\hbar p_t - 2p\Delta(tp)
$$

Truncating constraint functions of the relativistic particle one is left with only five non-trivial constraints and fourteen variables describing the state up to the second order in moments. The truncated system of equations has two solutions compatible with the semiclassical assumption

$$
p_t = \pm E \\
\Delta(tp_t) = \pm \frac{p}{E} \Delta(tp) - \frac{i\hbar}{2} \\
(\Delta p_t)^2 = p^2 + m^2 + (\Delta p)^2 - E^2 \\
\Delta(p_tq) = \pm \frac{p}{E} \left(\Delta(qp) + \frac{i\hbar}{2}\right) \\
\Delta(p tp) = \pm \frac{p}{E} (\Delta p)^2,
$$

where $E = \sqrt{p^2 + m^2} \left(1 + \frac{m^2(\Delta p)^2}{2(p^2 + m^2)^2}\right)$.

The two constraint surfaces are clearly the extensions of the two classical solutions $p_t = \pm \sqrt{p^2 + m^2}$. We use the above solutions to completely eliminate the variables generated by $p_t$.

The five non-trivial constraints produce only four independent gauge flows, which ultimately is a consequence of the degeneracy of the Poisson structure on $\mathcal{M}$. In the previous section we have identified four gauge conditions associated with choosing $t$ as
time, it may appear that after gauge-fixing we will have no flow left to label as evolution along parameter $\langle t \rangle$. However a linear combination of these gauge conditions is already encoded in the constraint $C_t$, since it is equivalent to the gauge condition $\langle tC \rangle = \langle t \rangle \langle C \rangle$ which is automatically satisfied on the constraint surface. Following through with the gauge-fixing we find that a single gauge generator $C_{\text{Ham}}$ remains, its parametrization is fixed by demanding that $\{t, C_{\text{Ham}}\} = 1$. We find that $C_{\text{Ham}} = p_t \pm E$, where the sign depends on the solution chosen. To order $\hbar$ the expression for $E$ agrees with the semiclassical expectation value of the Klein-Gordon Hamiltonian $H = (p^2 + m^2 \mathbb{1})^{\frac{1}{2}}$.

Finally, we enforce positivity by demanding

$$q, p, (\Delta q)^2, \Delta(qp), (\Delta p)^2 \in \mathbb{R}$$

$$(\Delta p)^2, (\Delta q)^2 \geq 0$$

$$(\Delta p)^2 (\Delta q)^2 - (\Delta(qp))^2 \geq \frac{1}{4}\hbar^2.$$ 

In this particular example, the gauge conditions do not affect the Poisson algebra of the variables generated by $q$ and $p$ and the difficulty mentioned earlier is avoided. Given an initial state we can now evolve its leading order moments for as long as the semiclassical approximation remains valid. For details of this example see [3].

**CONCLUDING REMARKS**

We have developed a technique for deriving leading order semiclassical corrections for the evolution of quantum systems with constraints. Within our treatment, a quantum mechanical system is described by a point on an infinite-dimensional phase-space of expectation values and moments. Quantum constraint produces an infinite number of first-class constraint functions. Semiclassical approximation allows us to truncate the system to a finite dimensional one at which point the local structure of quantum constraint surface and gauge orbits can be analyzed using essentially classical techniques. We have identified a set of gauge conditions related to the choice of a time variable. Since the procedure makes use of semiclassical states on kinematical observables, imposing positivity in general remains complicated. The scheme is of immediate use in quantizing minisuperspaces such as the various quantum cosmological models, this venue to be pursued elsewhere.

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