Quantum Darboux theorem

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The problem of computing quantum mechanical propagators can be recast as a computation of a Wilson line operator for parallel transport by a flat connection acting on a vector bundle of wave functions. In this picture, the base manifold is an odd-dimensional symplectic geometry, or quite generically a contact manifold that can be viewed as a "phase-spacetime," while the fibers are Hilbert spaces. This approach enjoys a "quantum Darboux theorem" that parallels the Darboux theorem on contact manifolds which turns local classical dynamics into straight lines. We detail how the quantum Darboux theorem works for anharmonic quantum potentials. In particular, we develop a novel diagrammatic approach for computing the asymptotics of a gauge transformation that locally makes complicated quantum dynamics trivial.

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I. INTRODUCTION

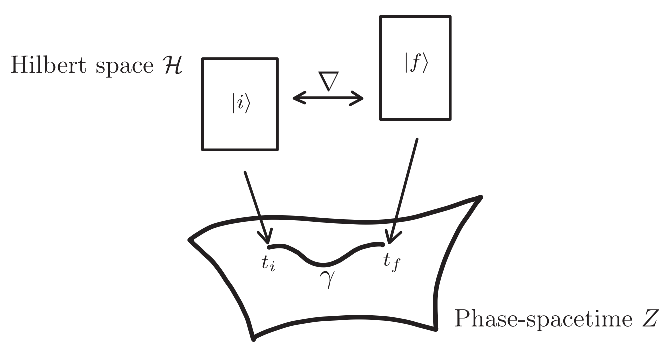
A fundamental problem in quantum mechanics is to compute correlators

$$\langle f|e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}|i\rangle,$$

where the states $|i\rangle$ and $|f\rangle$ are elements of some Hilbert space $\mathcal{H}$, the operator $\hat{H}$ is a quantum Hamiltonian, and t_i and t_f are classical times measured in some laboratory. It is useful to view the coordinates t_i and t_f as labels belonging to points in an odd-dimensional *phase-spacetime* manifold Z that corresponds to all possible classical laboratory measurements of generalized times, positions, and momenta. Then the unitary time evolution operator $\exp(-\frac{i}{\hbar}\hat{H}(t_f-t_i))$ can be replaced by a Wilson line,

$$P_\gamma \exp\left(-\int_\gamma \hat{A}\right).$$

Here $\hat{A}$ is the connection form for a connection $\nabla = d + \hat{A}$ acting on sections of a Hilbert bundle (see [1] and also [2]) $\mathcal{H}Z$, over the base manifold Z with Hilbert space fibers $\mathcal{H}$. Requiring that ∇ is flat (and if necessary, quotienting by nontrivial holonomies), the correlator $\langle f|P_\gamma \exp(-\int_\gamma \hat{A})|i\rangle$ only depends on the endpoints of γ and points $|i\rangle$ and $|f\rangle$ in the fibers of $\mathcal{H}Z$ above these two endpoints:



We attach the moniker *quantum dynamical system* to the data $(\mathcal{HZ},\nabla)$ of a Hilbert bundle equipped with a flat connection ∇. The goal of this article is to use the gauge covariance of Wilson line operators to map complicated quantum dynamics to simpler ones.

The article is structured as follows: We first review how to formulate a classical dynamical system in terms of an odd-dimensional analog of a symplectic geometry. We then explain, following [3], how to obtain a quantum dynamical

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system from the Becchi–Rouet–Stora–Tyutin (BRST) quantization of a classical dynamical system. Here the BRST charge corresponds to the flat connection ∇. We then treat the Hamiltonian-Jacobi theory in terms of contact geometry. (Note that a modern treatment of Hamilton-Jacobi actions and their formal quantization is given in [4].) Thereafter we describe the quantum analog of the Darboux theorem for quantum dynamical systems [5]. After that we primarily focus on the quantum mechanics of a particle on a line. The underlying classical dynamical system gives evolution on a three-dimensional phase-spacetime manifold Z, for which we give an explicit account of the (classical) Darboux theorem. The remainder of the article is devoted to developing a diagrammatic calculus for computing the asymptotics of the gauge transformations appearing in the quantum Darboux theorem of [5], and applying these to the computation of correlators.

II. DYNAMICAL SYSTEMS

Quite generally, dynamics is a rule governing the time evolution of a system, so a dynamical system is a one-parameter family of maps $\Phi_\tau\colon Z\to Z$ where points $\tau\in\mathbb{R}$ are viewed as times and Z is the state space of the system. Fixing a point $z_0\in Z$ and allowing τ to vary gives a parametrized path $\gamma\colon \mathbb{R}\to Z$ in Z with initial condition z_0. Thus, dynamics amounts to a set of parametrized paths (locally) foliating the space Z. Often, Z is taken to be a symplectic manifold or phase space, in which case it is even-dimensional and points in that space label generalized positions and momenta. However, to maintain general covariance also with respect to choices of clocks, we shall demand that Z is an odd-dimensional manifold which we term a phase-spacetime. We shall therefore view dynamics as a set of *unparametrized* paths (locally) foliating the odd-dimensional phase-spacetime Z^{2n+1}.

In general it is unusual to know explicitly the map Φ_τ determining a dynamical system; instead one has some kind of local rule generating dynamics. For example, on a phase-space or symplectic manifold one typically considers a Hamiltonian vector field X_H, specified by a Hamiltonian function H, whose integral flow determines dynamics in terms of *parametrized* paths. However, for Z a phase-spacetime, we only need to determine unparametrized paths. For that a local rule is generated by a maximally nondegenerate (so rank $2n$) two-form $\varphi\in\Omega^2 Z$, because an unparametrized path γ can be determined from the equation of motion

$$\varphi(\dot\gamma,\cdot)=0. \tag{2.1}$$

In the above $\dot\gamma$ is the tangent vector to γ with respect to *any* choice of parametrization.

Example 2.1. Massless relativistic particle: Let $Z=\mathbb{R}^7\ni(\vec k,x^0,\vec x)$ and

$$\varphi=d\vec k\,\hat{\wedge}\,(d\vec x+\hat k dx^0).$$

Then Eq. (2.1) is solved by

$$\dot\gamma\propto\frac{\partial}{\partial x^0}-\hat k\cdot\frac{\partial}{\partial\vec x},$$

which is the tangent vector to the trajectory of a massless particle in Minkowski space moving in the direction $\hat k$. ■

When the two-form φ is closed, we may write down an action principle for local dynamics, because locally $\varphi=d\alpha$ for some $\alpha\in\Omega^1 Z$. Then the action

$$S[\gamma]=\int_\gamma\alpha$$

is extremized under compactly supported variations of the path γ precisely when the equation of motion (2.1) holds. Changing α by an exact term $d\beta$ does not change the equation of motion. Because we wish to focus on systems with an action principle, from now on, we shall assume that φ is closed. When $\varphi\in\Omega^2 Z$ is closed and maximally nondegenerate, we call (Z,φ) a *dynamical phase-spacetime*. The closed, maximally nondegenerate two-form φ is termed an *odd symplectic form*. (Sometimes the additional data of a volume form is added to the definition of an odd symplectic manifold; see [6].) The data of α modulo gauge transformations $\alpha\mapsto\alpha+d\beta$, whose curvature $\varphi=d\alpha$ is maximally nondegenerate, also determines the dynamics, and we shall call this a *dynamical connection*.

Given a dynamical system (Z,φ), a function $Q\in C^\infty Z$ is said to be *conserved* when

$$\mathcal{L}_\rho Q=0,$$

for any vector field ρ obeying $\varphi(\rho,\cdot)=0$. Note that $\mathcal{L}_{f\rho}Q=f\mathcal{L}_\rho Q$ for any $f\in C^\infty Z$. A vector field u is said to generate a *symmetry* when

$$\mathcal{L}_u\varphi=0.$$

Conserved quantities and symmetries obey a Noether theorem: Given Q conserved, any solution u to

$$dQ=\varphi(u,\cdot) \tag{2.2}$$

is a symmetry because $\mathcal{L}_u\varphi=d\iota_u\varphi=d^2Q=0$. Vector fields $f\rho$ correspond to trivial (constant) conserved charges. The equation displayed above is always solvable for u because $\iota_\rho dQ=0$, and the solution for u is unique modulo a term $f\rho$. Conversely, given a symmetry u, then the one-form $\varphi(u,\cdot)$ is exact because $d\iota_u\varphi=\mathcal{L}_u\varphi=0$. Hence, locally, there always exists a smooth conserved Q solving the above display.

Experimentally, the initial conditions for a dynamical system cannot be determined with infinite precision. Instead, one associates an experimental uncertainty with an open ball in Z about some initial point $z_0 \in Z$. Therefore, a notion of volume is needed to ascertain the accuracy of such an initial measurement. Because φ is maximally nondegenerate, the form $\varphi^{\wedge n} \in \Omega^{2n} Z$ is nonvanishing. To make a top form, we need to exterior multiply this by some one-form. When $\varphi = d\alpha$—which is certainly true locally and for many physical systems the experimental apparatus can anyway only handle measurements in a finite range—a natural choice is the one-form α, in which case we define

$$\mathrm{Vol}_\alpha = \alpha \wedge \varphi^{\wedge n} \in \Omega^{2n+1} Z.$$

A priori, the "volume form" Vol_α need not be nondegenerate, and moreover it depends, up to an exact term, on the choice of α according to $\mathrm{Vol}_{\alpha+d\beta} = \mathrm{Vol}_\alpha + d(\beta\varphi^{\wedge n})$. For some systems, it may suffice only to have a nondegenerate volume form defined on suitable hypersurfaces of Z by $\varphi^{\wedge n}$, but generally we focus on systems where Vol_α is a volume form and view the choice of α as part of the data of the system required to give a good measurement theory. The case where φ is globally the d of a given α and Vol_α is nondegenerate is in some sense optimal. In this case α is called a *contact one-form*. The data (Z, α) is called a *strict contact structure*, and the dynamics on Z determined by the uniquely defined vector field $\rho \in \Gamma(TZ)$ such that

$$\varphi(\rho, \cdot) = 0, \qquad \alpha(\rho) = 1,$$

are called *Reeb dynamics*. The vector ρ is then called the *Reeb vector field*. The canonical parametrization of path γ in Z such that

$$\dot{\gamma} = \rho$$

is akin to that of geodesics in a Riemannian manifold by their proper length. A *contact structure* (Z, ξ) is the data of a hyperplane distribution ξ in TZ determined by the kernel of a contact one-form. A useful starting reference describing contact geometry is [7].

Example 2.2. Massive relativistic particle: Let $Z = \mathbb{R}^3 \ni (p, t, x)$ and

$$\alpha = p dx - \sqrt{p^2 + m^2} dt.$$

Then

$$\mathrm{Vol}_\alpha = \frac{m^2}{\sqrt{p^2 + m^2}} dp \wedge dt \wedge dx \neq 0,$$

so α is a contact one-form. It not difficult to verify that the Reeb trajectories correspond to those of a mass m, relativistic particle in two-dimensional Minkowski spacetime ■

III. QUANTIZATION

Our main focus is on the quantization of dynamical phase-spacetimes. We follow the treatment in [3]. The framework is quite close to that developed by Fedosov for deformation quantization of symplectic manifolds [8] (see also [9]). To quantize a dynamical phase-spacetime (Z, φ) we begin with an action on paths γ in Z,

$$S[\gamma] = \int_\gamma \alpha,$$

where α is any primitive of φ, so

$$\varphi = d\alpha.$$

For locally supported variations of γ, the potential failure of α to be unique or to exist globally is irrelevant. The above action can be reformulated as a Hamiltonian system on a coisotropic submanifold $\mathcal{C}$ of a larger symplectic manifold $\mathcal{Z}$, where

$$\mathcal{Z} = T^*Z \oplus \xi^*.$$

In the above, ξ^* is the bundle of hyperplanes in T^*Z defined by the kernel of the ray defined by the kernel of φ. So, for example, if $\varphi(r, \cdot) = 0$ for the ray r, then $\xi^* = \ker r$. In the case that α is a global contact form, this is the dual of the maximally nonintegrable distribution ξ defining a contact structure. Motivated by this correspondence, we call ξ^* a *codistribution*. The direct sum above is the Whitney vector bundle sum, so $\mathcal{Z}$ has base $Z \ni z^i$ and fiber $\mathbb{R}^{2n+1} \oplus \mathbb{R}^{2n} \ni (p_i, s_a)$. We call $\mathcal{Z}$ an *extended phase-space*; it has a symplectic current (or Liouville form) Λ obtained from the sum of the tautological one-form on T^*Z and the standard Liouville form λ_s on the $\mathbb{R}^{2n}$ fibers of ξ^*. In local coordinates (z^i, p_i, s_a) for $\mathcal{Z}$,

$$\Lambda = p_i dz^i + \frac{1}{2} s_a j^{ab} ds_b.$$

This makes $\mathcal{Z}$ into a symplectic manifold. Here $j^{ab} = -j^{ba}$ is an odd bilinear form defining the invariant tensor of $Sp(2n)$. Also, we employ the convention $X_a = j_{ab} X^b$. A coisotropic submanifold $\mathcal{C}$ of this is determined by the $2n + 1$ first class constraints

$$C_i = p_i - A_i(z, s),$$

where the one-form $A = \alpha + \kappa(z, s) + a(z, s)$ obeys the Cartan–Maurer equation

$$dA + \{A \overset{\wedge}{,} A\}_{PB} = 0. \tag{3.1}$$

Also, the leading fiberwise jet of the one-form $\kappa(z,s)$ must obey the maximal rank condition

$$\kappa(z,s) = e^a(z)s_a, \qquad \frac{1}{2} j_{ab} e^a \wedge e^b = \varphi,$$

and

$$a(z,s) = \mathcal{O}(s^2). \tag{3.2}$$

In the above, the $2n$ one-forms e^a are a basis, or adapted coframe, for the codistribution ξ^*, such that $e^a(\rho) = 0$. We shall often refer to these as *soldering forms*. The extended action for paths Γ in ξ, obtained by integrating out the momenta p_i by solving the constraints C_i, and given by

$$S[\Gamma] = \int_\Gamma (\lambda_s + A),$$

then gives a (gauge) equivalent description of the dynamics given by the original action $S[\gamma]$ above. Moreover, the constraints C_i are Abelian, so the classical Batalin–Fradkin–Vilkovisky (BFV)-BRST charge is simply $Q_{\mathrm{BRST}} = c^i(p_i - A_i(s,z))$ where c^i are ghosts. This charge [10] is "nilpotent" (strictly its BFV Poisson bracket with itself vanishes) by virtue of the Cartan-Maurer equation. In the above discussion we have effectively converted a system with a mixture of first and second class constraints to one with only first class constraints, which is an example of a general technique due to [11].

The extended action is easily quantized by viewing the ghosts c^i as one-forms on the base manifold Z (see for example [12]), so that $\frac{i}{\hbar} c^i p_i$ becomes the exterior derivative d acting on forms on Z and the fiber coordinates s_a become operators $\hat{s}_a \in \mathrm{End}\mathcal{H}$ acting on some choice of Hilbert space $\mathcal{H}$ and subject to

$$[\hat{s}_a, \hat{s}_b] = i\hbar j_{ba}.$$

In fact, since states are defined by complex rays, we only need to consider the projective Hilbert space $\mathbb{P}(\mathcal{H}) \ni [|\psi\rangle] = [e^{i\theta}|\psi\rangle]$ (for any real θ). We will abbreviate the notation $\mathbb{P}(\mathcal{H})$ by $\mathcal{H}$ in what follows.

The BRST Hilbert space $\mathcal{H}_{\mathrm{BRST}}$ is then differential forms on Z taking values in $\mathcal{H}$. At ghost number zero, these are sections of a Hilbert bundle $\mathcal{H}Z$ which is a vector bundle with fibers given by $\mathcal{H}$ and base manifold Z. In general BRST wave functions Ψ_{BRST} obey

$$\Psi_{\mathrm{BRST}} \in \Gamma(\mathcal{H}Z) \otimes \Omega Z = \mathcal{H}_{\mathrm{BRST}}.$$

The ghost number grading for the above space is given by form degree.

Note that the frame bundle of the dual $\xi \coloneqq (\xi^*)^*$ of the codistribution ξ^* canonically defines a principal $Sp(2n)$ bundle over Z, because φ endows ξ with a nondegenerate, skew symmetric bilinear form. This canonically and globally defines the associated vector bundle with fibers given by $\mathcal{H}$. In turn, the principal bundle of orthonormal frames with respect to the Hilbert space inner product has structure group $U(\mathcal{H})$. Let us denote by $\mathcal{H}Z$ the associated vector bundle with fibers $\mathcal{H}$ transforming under the fundamental representation of $U(\mathcal{H})$. This is the bundle of wave functions defined up to unitary equivalence where the base manifold Z plays the role of a generalized time coordinate.

The quantum BRST charge is a flat connection form on $\mathcal{H}Z$; this extends by linearity to higher forms in $\mathcal{H}_{\mathrm{BRST}}$. It is given by

$$\frac{i}{\hbar}\hat{Q}_{\mathrm{BRST}} = d + \hat{A} \eqqcolon \nabla,$$

where $\hat{A}$ is the quantization of the classical solution $A(z,s)$ to the CartanMaurer equation Eq. (3.1). It is a one-form taking values in Hermitean operators on $\mathcal{H}$, and decomposes as

$$\hat{A} = \frac{\alpha Id}{i\hbar} + \frac{\hat{\kappa}}{i\hbar} + \hat{a}. \tag{3.3}$$

We require that $\hat{A} \in \mathrm{End}(\Gamma(\mathcal{H}Z)) \otimes \Omega^1 Z$ gives a solution of the flatness condition

$$\nabla^2 = 0.$$

Given a connection form $d + \hat{A}$, the map

$$\hat{\kappa}\colon\ \Gamma(\mathcal{H}Z) \otimes \Gamma(TZ) \to \Gamma(\mathcal{H}Z)$$

is called the *quantum calibration map*. We require that it obeys the Heisenberg algebra, in the sense that for any $u, v \in \Gamma(TZ)$

$$\hat{\kappa}(u) \circ \hat{\kappa}(v) - \hat{\kappa}(v) \circ \hat{\kappa}(u) = i\hbar\varphi(u,v).$$

This can be solved locally using the coframe by writing $\hat{\kappa} = e^a \hat{s}_a$. Therefore this map calibrates quantum operators $\hat{s}$ to the underlying classical phase-spacetime manifold Z. Indeed, the above map always exists, because $\mathcal{H}$ comes equipped with a representation of the Heisenberg algebra; this is uniquely defined up to unitary equivalence by the Stone von Neumann theorem. The map $\hat{\kappa}$ is a symplectic analog of Clifford multiplication for spinor bundles; see [13].

For any quantum system with a classical limit, or that arises via quantization, there must be a flow with respect to some parameter $\hbar$ encoding how quantum quantities respond to changes in $\hbar$. Therefore, we introduce a grading operator

$$\mathrm{gr} = 2\hbar\frac{\partial}{\partial\hbar} + E,$$

where the operator $E\colon \Gamma(\mathcal{H}Z) \to \Gamma(\mathcal{H}Z)$ obeys

$$E \circ \hat{\kappa}(u) - \hat{\kappa}(u) \circ E = \hat{\kappa}(u), \qquad \forall\, u \in \Gamma(TZ).$$

This grading operator is also needed to state the quantum analog of the classical higher jet condition in Eq. (3.2). For example, in any choice of polarization $\hat{s}_a = (\hat{s}^A, \hat{s}_B)$ such that $[\hat{s}^A, \hat{s}_B] = i\hbar\delta^A_B$ acting on $\mathcal{H} = L^2(\mathbb{R}^n) \ni \psi(s^A)$ with $\hat{s}^A\psi = s^A\psi$, $\hat{s}_A\psi = \frac{\hbar}{i}\partial\psi/\partial s^A$, the map E is given by

$$E = \frac{i}{\hbar}\sum_{A=1}^{n} \hat{s}^A\hat{s}_A + 2\hbar\frac{\partial}{\partial\hbar}.$$

Let us say that an operator $\hat{O} \in \mathrm{End}(\Gamma(\mathcal{H}Z)$ has grade k when

$$\mathrm{gr} \circ \hat{O} + \hat{O} \circ \mathrm{gr} = k\hat{O}.$$

We require that the operator $\hat{a}$ in Eq. (3.3) has a grade greater than or equal to zero. Then, given the data of a dynamical connection α and a quantization map $\hat{\kappa}$, the solution

$$\nabla = \frac{\alpha Id}{i\hbar} + \frac{\hat{\kappa}}{i\hbar} + d + \hat{a}$$

to the flatness condition $\nabla^2 = 0$ will be called a *quantum connection*. When only a formal power series solution for ∇ is given, we call this a *formal quantum connection*. Note that the first and third terms of the above connection are the starting points for the geometric quantization of contact manifolds developed in [14]. Local existence of formal quantum connections given the data $(Z, \alpha, \hat{\kappa}, \mathrm{gr})$ is not difficult to establish [3] (alternately, see the Darboux construction of a flat quantum connection given in Sec. III A). Indeed, when the calibration map is given by coframes, the operator $\hat{a}$ can be expanded order by order in the grading

$$\hat{a} = \frac{1}{i\hbar}\sum_{\substack{j,\ell\geq 0\\ j+2\ell\geq 2}} \frac{\hbar^\ell}{j!}\omega^{a_1\cdots a_j}\hat{s}_{a_1}\cdots\hat{s}_{a_j}.$$

In the above, the one-forms $\omega^{a_1\cdots a_j}$ are totally symmetric in the labels $a_1, \ldots, a_j$ and are determined by solving a system of algebraic, zero-curvature, equations.

A. Quantum Darboux theorem

Locally, the contact Darboux theorem states that there exist coordinates $(\vec{\pi}, \vec{\chi}, \psi)$ such that any contact form α can be written as

$$\alpha = \vec{\pi} \cdot d\vec{\chi} - d\psi.$$

Here the Reeb vector is $\rho = -\frac{\partial}{\partial\psi}$ so that evolution is along straight lines of constant $\vec{\pi}$ and $\vec{\chi}$. In the case where only a dynamical phase-spacetime (Z, φ) is given, because φ is closed, we may always locally write $\varphi = d\alpha'$. Moreover, in the case that α' is not contact, because φ is nondegenerate, we may add to α' an exact term $d\beta$ such that $\alpha = \alpha' + d\beta$ is a contact form, at least locally. Therefore, the contact Darboux theorem applies to dynamical phase-spacetimes as well.

There is a quantum analog of the Darboux theorem for formal quantum connections [5]. Before discussing this we need to talk about gauge transformations for quantum connections. In the previous section we stipulated that the quantum connection ∇ was a flat connection form on the bundle $\mathcal{H}Z$. This is an associated vector bundle to a principal $U(\mathcal{H})$ bundle over Z. The connection form obeys a self-adjoint condition

$$\hat{A}_u = \hat{A}_u^\dagger \in \mathrm{End}(\Gamma(\mathcal{H}Z)),$$

for any $u \in \Gamma(TZ)$. Here the adjoint is defined fiberwise using the adjoint of $\mathcal{H}$.

The quantum Darboux theorem states that locally any pair of formal quantum connections, for a given choice of dynamical phase-spacetime (Z, φ), are formally gauge equivalent [5]. The result is established inductively in the grading gr by showing that there exists a formal $U(\mathcal{H})$ gauge transformation $\hat{U}$ such that

$$\hat{U}\nabla\hat{U}^{-1} = \nabla_{\mathrm{D}}. \tag{3.4}$$

Here ∇_{D} is a quantum connection whose quantum calibration map $\hat{\kappa}$ is closed so that

$$\nabla_{\mathrm{D}} \coloneqq \frac{\alpha}{i\hbar} + \frac{\hat{\kappa}}{i\hbar} + d$$

is obviously flat. To see that such a connection always exists locally, one can use a Darboux coordinate ball, for which $\varphi = d\alpha$ and where α is a contact with coordinates $(\vec{\pi}, \vec{\chi}, \psi)$ such that

$$\alpha = \vec{\pi} \cdot d\vec{\chi} - d\psi.$$

Then the quantum calibration map $\hat{\kappa} = e^a\hat{s}_a$ can be built from closed coframes

$$e^a = (d\vec{\pi}, d\vec{\chi}).$$

The quantum calibration map for a general quantum connection ∇ will not be given in terms of closed frames, but an $Sp(2n)$ gauge transformation in the frame bundle of ξ^* can be employed to achieve this. Locally, as discussed earlier, this lifts to an $Mp(2n)$ gauge transformation $\hat{U}_0$. The strategy to find $\hat{U}$ is first to find the metaplectic transformation $\hat{U}_0$. Then,

$$\nabla_0 \coloneqq \hat{U}_0^{-1} \nabla_{\mathrm{D}} \hat{U}_0 = \nabla + \hat{a}_0, \tag{3.5}$$

for some $\hat{a}_0$ of grade zero or greater. Thereafter one solves for a formal gauge transformation $\hat{U}_1$ of grade one higher, given as a formal series in the grading, such that $\hat{U}_1^{-1} \nabla_0 \hat{U}_1 = \nabla$. This means we must solve the equation

$$\nabla \hat{U}_1^{-1} = \hat{U}_1^{-1} \hat{a}_0, \tag{3.6}$$

where $\nabla \hat{U}_1^{-1} \coloneqq [\nabla, \hat{U}_1^{-1}]$ is the adjoint action of ∇. Note that acting with ∇ again on the above, just returns $\nabla_0^2 = 0$ as an integrability condition. The above display has a formal (and possibly only local) solution for $\hat{U}_1^{-1}$ [5]. The proof is by induction in the grading.

A main aim of this article is to study explicit, global (but possibly formal) solutions to the above equation for quantum mechanical systems describing dynamics on a line. Knowledge of the gauge transformation $\hat{U}_1$ is powerful, because it relates nontrivial interacting systems to their trivial Darboux counterparts. The first step is to study the classical Darboux theorem for these models.

IV. CONTACT HAMILTON-JACOBI THEORY

Let us consider a one-dimensional system with time-dependent Hamiltonian $H(p, q, t)$. The standard Hamilton-Jacobi theory for this system (see [4] for a modern treatment) can be recovered by studying diffeomorphisms on a three-dimensional dynamical phase-spacetime manifold Z with local coordinates (p, q, t) and odd symplectic form

$$\begin{aligned} \varphi &= dp \wedge dq - dH \wedge dt \\ &= \left(dp + \frac{\partial H}{\partial q} dt\right) \wedge \left(dq - \frac{\partial H}{\partial p} dt\right). \end{aligned}$$

This gives dynamics

$$\dot{\gamma} \propto \frac{\partial}{\partial t} - \frac{\partial H}{\partial q}\frac{\partial}{\partial p} + \frac{\partial H}{\partial p}\frac{\partial}{\partial q},$$

where $\propto$ denotes equality up to multiplication by some nonvanishing function on Z. Calling the worldline parameter τ, and choosing this function to be unity, the equations of motion are

$$\frac{\partial t}{\partial \tau} = 1, \qquad \frac{\partial p}{\partial \tau} = -\frac{\partial H}{\partial q}, \qquad \frac{\partial q}{\partial \tau} = \frac{\partial H}{\partial p}.$$

In the gauge $t(\tau) = \tau + c$ these are the standard Hamilton equations.

The odd symplectic form φ can be written as the exterior derivative of the one-form

$$\alpha = p dq - H(p, q, t) dt. \tag{4.1}$$

Away from the zero locus of $p \frac{\partial H}{\partial p} - H$, the above form is, in fact, contact. The contact Darboux theorem ensures that locally we can find a new local coordinate system (π, χ, ψ) such that

$$\alpha = \chi d\pi - d\psi. \tag{4.2}$$

Our aim in this section is to give an (as) explicit (as possible) formula for the diffeomorphism bringing α, at least on some open set U, to its Darboux form displayed above.

The Reeb vector for α as in Eq. (4.1) is given in these Darboux coordinates by $\rho = -\frac{\partial}{\partial \psi}$, while in the original coordinate system

$$\left(p\frac{\partial H}{\partial p} - H\right)\rho = \frac{\partial}{\partial t} - \frac{\partial H}{\partial q}\frac{\partial}{\partial p} + \frac{\partial H}{\partial p}\frac{\partial}{\partial q}. \tag{4.3}$$

To proceed we need to know one conserved quantity $K \in C^\infty U$,

$$\mathcal{L}_\rho K = \iota_\rho dK = 0. \tag{4.4}$$

This condition is always in principle *locally* solvable, but not in terms of explicit first integrals. Explicitly, it amounts to solving

$$\frac{\partial K}{\partial t} = \{H, K\}_{\mathrm{PB}},$$

where $\{\cdot,\cdot\}_{\mathrm{PB}}$ is the standard Poisson bracket $\{q, p\}_{\mathrm{PB}} = 1$, so $\{F, G\}_{\mathrm{PB}} = \frac{\partial F}{\partial q}\frac{\partial G}{\partial p} - \frac{\partial G}{\partial q}\frac{\partial F}{\partial p}$.

Of course, when the Hamiltonian function H is time independent, $H(p, q)$ is itself a solution. In what follows we assume that a solution for K is known (possibly approximately or even numerically). Then we make an ansatz for the sought after diffeomorphism:

$$\begin{aligned} \pi &= K(p, q, t), \\ \chi &= -t + \phi(p, q, t), \\ \psi &= \lambda(p, q, t). \end{aligned} \tag{4.5}$$

Since $\mathcal{L}_\rho \pi = 0 = \mathcal{L}_\rho \chi$ and $\mathcal{L}_\rho \psi = -1$, using Eq. (4.3) we must have

$$\frac{\partial K}{\partial t} = \{H, K\}_{\text{PB}}, \qquad \frac{\partial \phi}{\partial t} = \{H, \phi\}_{\text{PB}} + 1,$$
$$\frac{\partial \lambda}{\partial t} = \{H, \lambda, \}_{\text{PB}} + H - p\frac{\partial H}{\partial p}.$$

Comparing the right-hand sides of Eqs. (4.1) and (4.2) and using the Ansatz (4.5) give a triplet of partial differential equations (PDEs) which we wish to use to determine ϕ and λ:

$$\begin{aligned} K\frac{\partial \phi}{\partial p} - \frac{\partial \lambda}{\partial p} &= 0, \\ K\frac{\partial \phi}{\partial q} - \frac{\partial \lambda}{\partial q} &= p, \\ K\frac{\partial \phi}{\partial t} - \frac{\partial \lambda}{\partial t} &= K - H. \end{aligned} \tag{4.6}$$

Differentiating the second equation with respect to p and the first with respect to q and then taking the difference yields

$$\{\phi, K\}_{PB} = 1. \tag{4.7}$$

Assuming that the equation $\varepsilon = K(p, q, t)$ can be solved for $p = p(\varepsilon, q, t)$ we can solve the PDE given by the above display by first writing

$$\phi(p, q, t) =: \phi(K(p, q, t), q, t).$$

Using $\{K, K\}_{\text{PB}} = 0$, Eq. (4.7) now says that

$$\frac{\phi(\varepsilon, q, t)}{\partial q} \frac{\partial K(p, q, t)}{\partial p}\bigg|_{p=p(\varepsilon,q,t)} = 1.$$

Hence

$$\phi(\varepsilon, q, t) = \int^q \frac{dx}{\frac{\partial K(p,x,t)}{\partial p}}\bigg|_{p=p(\varepsilon,x,t)}.$$

Similarly, multiplying the second equation in (4.6) by $\partial K/\partial p$ and the first by $\partial K/\partial q$, the difference yields

$$K\{\phi, K\}_{\text{PB}} - \{\lambda, K\}_{\text{PB}} = p\frac{\partial K}{\partial p}.$$

This can be solved for $\lambda(p, q, t) =: \lambda(K(p, q, t), q, t)$ using the same method employed for ϕ:

$$\lambda(\varepsilon, q, t) = \int^q dx \frac{\varepsilon - p\frac{\partial K(p,x,t)}{\partial p}}{\frac{\partial K(p,x,t)}{\partial p}}\bigg|_{p=p(\varepsilon,x,t)}.$$

In summary, the diffeomorphism to the Darboux coordinate system is given by

$$\begin{aligned} \pi &= K(p, q, t), \\ \chi &= -t + \int^q \frac{dx}{\frac{\partial K(p,x,t)}{\partial p}}\bigg|_{p=p(K(p,q,t),x,t)}, \\ \psi &= \int^q dx \frac{K(p, q, t) - (p\frac{\partial K(p,x,t)}{\partial p})|_{p=p(K(p,q,t),x,t)}}{\frac{\partial K(p,x,t)}{\partial p}|_{p=p(K(p,q,t),x,t)}}. \end{aligned} \tag{4.8}$$

Example 4.1. For a time independent Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}q^2 + v(q)$$

we have

$$\begin{aligned} \pi &= \frac{1}{2}p^2 + \frac{1}{2}q^2 + v(q), \\ \chi &= -t + \int^q \frac{dx}{\sqrt{p^2 + q^2 - x^2 + 2(v(q) - v(x))}} \\ &\approx -t - \arctan\frac{p}{q} - \int^q dx \frac{v(q) - v(x)}{(p^2 + q^2 - x^2)^{3/2}}, \end{aligned} \tag{4.9}$$

$$\begin{aligned} \psi &= \int^q dx \frac{x^2 + 2v(x) - \frac{1}{2}p^2 - \frac{1}{2}q^2 - v(q)}{\sqrt{p^2 + q^2 - x^2 + 2(v(q) - v(x))}} \\ &\approx -\frac{1}{2}pq - \int^q dx \frac{\frac{1}{2}(p^2 + q^2)(v(q) - 3v(x)) + x^2 v(x)}{(p^2 + q^2 - x^2)^{3/2}}. \end{aligned} \tag{4.10}$$

The stated approximations are accurate in the limit when the deformation of the harmonic oscillator $v(q) \ll q^2$. In the harmonic oscillator limit when $v(q) = 0$, it is easily checked that indeed

$$\begin{aligned} \alpha = \pi d\chi - d\psi &= \frac{1}{2}(p^2 + q^2)d\left(-t - \arctan\frac{p}{q}\right) \\ &- d\left(-\frac{1}{2}pq\right) = pdq - \frac{1}{2}(p^2 + q^2)dt. \end{aligned}$$

■

Now that we can explicitly locally map a wide class of classical dynamical systems to one another using the Darboux theorem, we proceed to study the quantum analog that was discussed in Sec. III A. We shall focus on the quantum anharmonic oscillator.

V. THE QUANTUM ANHARMONIC OSCILLATOR

Let us consider the model with Hamiltonian

$$H = \frac{1}{2}p^2 + V(q), \tag{5.1}$$

and a single-well potential V that is smooth, is concave up, and obeys $V(0) = V'(0) = 0$. The classical phase-space curves for this model are concentric closed orbits. The phase-spacetime is $\mathbb{R}^3 \ni (p, q, t)$ and

$$\varphi = (dp + V'(q)dt) \wedge (dq - pdt).$$

In the Darboux coordinates (χ, π, ψ), the physical trajectories are straight lines. Clearly for this model, these can be *globally* mapped to the trajectories in (p, q, t) space. These are helixlike and foliate the phase-spacetime.

Standard quantization of the Hamiltonian (5.1) replaces the c-numbers p and q by quantum operators

$$p \mapsto \frac{\hbar}{i}\frac{\partial}{\partial S}, \qquad q \mapsto S,$$

acting on the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$ given by square integrable, complex-valued functions of S. A common choice of quantum Hamiltonian is then

$$\hat{H} \coloneqq -\frac{\hbar^2}{2}\frac{\partial^2}{\partial S^2} + V(S). \tag{5.2}$$

In principle, the space of *all* quantizations of the classical Hamiltonian in Eq. (5.1) ought to be encoded in the space of flat quantum connections on the phase-spacetime. This issue is of independent interest, but we avoid studying it for now and instead focus on the simple quantization in the above display.

Our aim is to compute the evolution operator $\exp(-\frac{i(t_f - t_i)}{\hbar}\hat{H})$ or its matrix elements

$$K(S_f, S_i; t_f, t_i) \coloneqq \langle S_f| \exp\left(-\frac{i(t_f - t_i)}{\hbar}\hat{H}\right)|S_i\rangle.$$

This the usual propagator problem in nonrelativistic quantum mechanics, which can be handled perturbatively by various quantum mechanical techniques. Here we want to demonstrate a rather different approach based on the quantum Darboux theorem.

First we need to rewrite the operator $\exp(-\frac{i}{\hbar}\hat{H}(t_f - t_i))$ as a path ordered line operator $P_\gamma \exp(-\int_\gamma \hat{A})$ for a quantum connection $\nabla = d + \hat{A}$ acting on a Hilbert bundle over phase-spacetime. For that, we need a solution for ∇ corresponding to the quantum Hamiltonian in Eq. (5.2). A solution is given by [3]

$$\nabla = d + \frac{dq}{i\hbar}\left(p + \frac{\hbar}{i}\frac{\partial}{\partial S}\right) - \frac{dp}{i\hbar}S - \frac{dt}{i\hbar}\left(\frac{1}{2}\left[p + \frac{\hbar}{i}\frac{\partial}{\partial S}\right]^2 + V(q + S)\right) \eqqcolon d + \hat{A}. \tag{5.3}$$

Observe that along the path

$$\gamma = \{(0, q, t_i(1 - \tau) + t_f\tau) : \tau \in [0, 1]\} \in Z,$$

the connection potential

$$\hat{A} = \frac{i}{\hbar}\hat{H}_q(t_f - t_i)d\tau,$$

where $\hat{H}_q \coloneqq -\frac{\hbar^2}{2}\frac{\partial^2}{\partial S^2} + V(S + q)$. It is tempting to take a path γ along which both p and q vanish. However, we avoid this choice because the Jacobian for a change of variables $(p, q) \mapsto (\pi, \phi)$ vanishes along such a path. Because $\partial/\partial S = \partial/\partial(S + q)$, there is no difficulty working along a path with constant $q \neq 0$, because this just shifts the variable S in wave functions.

The soldering forms for the above connection are given by

$$e^a = (dp + V'(q)dt, dq - pdt) \eqqcolon (f, e),$$

so that $\varphi = \frac{1}{2}j_{ab}e^a \wedge e^b = e \wedge f$ and $j_{12} = 1 = -j_{21} = j^{12} = -j^{21}$. These forms vanish along γ. Also note that $\hat{s}_a = (-S, \frac{\hbar}{i}\frac{\partial}{\partial S})$ and $[\hat{s}_1, \hat{s}_2] = -i\hbar$. It now follows that

$$P_\gamma \exp\left(-\int_\gamma \hat{A}\right) = \exp\left(-\frac{i(t_f - t_i)}{\hbar}\int_0^1 d\tau \hat{H}_q\right) = \exp\left(-\frac{i}{\hbar}\hat{H}_q(t_f - t_i)\right). \tag{5.4}$$

Our next goal is to find a gauge transformation mapping (at least formally) the connection ∇ to a far simpler one. Before doing that, it is useful to discuss quantum symmetries of this system.

A. Quantum Noether theorem

Since quantum dynamics is given by parallel transport with respect to a quantum connection $\nabla = d + \hat{A}$, quantum symmetries ought to be given by operators $\hat{\mathcal{O}}$ on the Hilbert bundle that obey

$$\nabla \circ \hat{\mathcal{O}} = \hat{\mathcal{O}}' \circ \nabla,$$

for any operator $\hat{\mathcal{O}}'$, since if $\Psi \in \Gamma(\mathcal{H}Z)$ solves $\nabla\Psi = 0$, then so too does $\hat{\mathcal{O}}\Psi$.

Such operators $\hat{\mathcal{O}}$ are easy to construct: Let $u \in \Gamma(TZ)$ be a vector field. Then, because ∇ is nilpotent, the operator $\{\iota_u, \nabla\}$ commutes with ∇. Acting on sections of the Hilbert bundle, this gives the operator

$$\mathcal{L}_u + \hat{A}_u.$$

Note that the Lie derivative is defined acting on sections of $\wedge^\bullet Z \otimes \mathcal{H}Z$ and is defined by the anticommutator $\{\iota_u, d\}$. Here we use that choosing the operator d in some gauge defines a connection. The particular choice of gauge is often determined by the explicit form of the system under study. Symmetries of the above type that hold for arbitrary vector fields u are tautological, in the sense that the first operator acts along the base Z, while the second acts on the Hilbert space fibers in a way that exactly compensates the former transformation. In BRST terms, these symmetries are BRST exact. However, specializing to vector fields u that solve

$$[\mathcal{L}_u, \nabla] = \frac{d\beta}{i\hbar} \tag{5.5}$$

for some $\beta \in C^\infty Z$, we can define a *conserved quantum charge*

$$\hat{Q}_u := i\hbar\{\iota_u, \nabla\} - i\hbar\mathcal{L}_u - \beta. \tag{5.6}$$

It is easy to verify that

$$[\nabla, \hat{Q}_u] = 0.$$

Note that the leading term of $\hat{Q}_u$ in the grading is $\alpha(u) - \beta$ which gives a classical conserved charge Q that solves Eq. (2.2) because

$$\mathcal{L}_\rho Q = \iota_\rho d(\iota_u\alpha) - \iota_\rho d\beta = \iota_\rho\mathcal{L}_u\alpha - \iota_\rho\iota_u\varphi - \iota_\rho d\beta = 0.$$

Here we used that Eq. (5.5) implies $\mathcal{L}_u\alpha = d\beta$ and $\varphi(\rho, \cdot) = 0$. Let us call vector fields u obeying Eq. (5.5) *quantum symmetries* of ∇.

The simple model in the next example will be important.

Example 5.1. Let $Z = \mathbb{R}^3 \ni (\pi, \chi, \psi)$ and

$$\varphi = d\pi \wedge d\chi.$$

This equals $d\alpha$ where $\alpha = \pi d\chi - d\psi$ is contact and the coordinates (π, χ, ψ) are Darboux. Then a quantum connection is

$$\nabla_{\rm D} = d + \frac{d\chi}{i\hbar}\left(\pi + \frac{\hbar}{i}\frac{\partial}{\partial S}\right) - \frac{d\pi}{i\hbar}S - \frac{d\psi}{i\hbar} =: d + \hat{A}_{\rm D}. \tag{5.7}$$

The vector fields

$$\frac{\partial}{\partial\pi}, \qquad \frac{\partial}{\partial\chi}, \qquad \frac{\partial}{\partial\psi},$$

are quantum symmetries with β equaling χ, 0, 0, respectively. Their conserved quantum charges are

$$\hat{Q}_{\frac{\partial}{\partial\pi}} = -\chi - S, \quad \hat{Q}_{\frac{\partial}{\partial\chi}} = \pi + \frac{\hbar}{i}\frac{\partial}{\partial S}, \quad \hat{Q}_{\frac{\partial}{\partial\psi}} = -1. \tag{5.8}$$

Acting on the Hilbert bundle, these charges obey the Heisenberg Lie algebra which is also the algebra of the three contact Hamiltonian vector fields $\frac{\partial}{\partial\pi} + \chi\frac{\partial}{\partial\psi}$, $\frac{\partial}{\partial\chi}$ and $\frac{\partial}{\partial\psi}$. ■

Returning to the anharmonic oscillator, we note that it has two nontrivial, independent, globally defined, conserved charges. One of these is the Hamiltonian $H = \frac{1}{2}p^2 + V(q)$, or simply π in Darboux coordinates. The other is $t - \phi(p, q)$, or equivalently $-\chi$. This says that the angle variable [see Eq. (4.8)]

$$\phi(p, q) = \int^q \frac{dx}{\sqrt{p^2 + 2V(q) - 2V(x)}} \tag{5.9}$$

obeys $\phi(p, q) = t + \text{const}$. Or in other words, the initial value of the angle variable is preserved along classical paths.

It is interesting to study the quantization of the conserved quantities H and $t - \phi$. The former is simple because

$$[\mathcal{L}_{\frac{\partial}{\partial t}}, \nabla] = 0$$

for the quantum connection form given in Eq. (5.3). Hence we can construct the quantum charge corresponding to the strict contactomorphism generated by $\frac{\partial}{\partial t}$. This gives

$$-\hat{Q}_{\frac{\partial}{\partial t}} = \frac{1}{2}\left[p + \frac{\hbar}{i}\frac{\partial}{\partial S}\right]^2 + V(q + S).$$

It is easy to verify that the above operator commutes with ∇. Moreover, at $p = 0 = q$, this recovers the standard quantum Hamiltonian $\hat{H}$.

The quantum charge corresponding to $t - \phi(p, q)$ is more involved. The quantization given by the quantum connection form ∇ in Eq. (5.3) does not obey condition (5.5) for the vector field $u = \frac{\partial}{\partial\pi} + \chi\frac{\partial}{\partial\psi}$. This does not mean that there is no corresponding charge, but rather that the formula (5.6) cannot be used. Instead, given a quantum gauge transformation $\hat{U}$ relating ∇ to $\nabla_{\rm D}$ as in Eq. (3.4), then the quantum charge $\hat{U}^{-1}\hat{Q}_{\frac{\partial}{\partial\pi}}\hat{U}$ commutes with ∇. Unfortunately we do not yet know the gauge transformation $\hat{U}$. The computation of this operator is the subject of the next section.

B. Quantum gauge transformation

We want to compute the quantum gauge transformation $\hat{U}$ given by a unitary endomorphism of the section space of the Hilbert bundle $\Gamma(\mathcal{H}Z)$ such that

$$\nabla = \hat{U}^{-1}\nabla_{\rm D}\hat{U},$$

where ∇ is the connection form corresponding to that the anharmonic oscillator in Eq. (5.3), while $\nabla_{\rm D}$ is the Darboux connection in Eq. (5.7). For this we will work iteratively order by order in the grading. The first step is to find a gauge transformation relating the calibration maps of the two connection forms.

1. Metaplectic transformation

To begin with, we need the relation between the soldering forms $(d\pi, d\chi)$ of the Darboux connection ∇_{D} to those—given by $(dp + H_q dt, dq - H_p)$—of ∇. (For brevity, from now on we often denote partial derivatives by subscripts.) This is given by

$$\begin{pmatrix} d\pi \\ d\chi \end{pmatrix} = \frac{\partial(\pi,\phi)}{\partial(p,q)}\begin{pmatrix} dp \\ dq \end{pmatrix} - dt\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \pi_p & \pi_q \\ \phi_p & \phi_q \end{pmatrix}\begin{pmatrix} dp + H_q dt \\ dq - H_p dt \end{pmatrix}.$$

The above display was computed using Eq. (4.5) specialized to the case $K = H(p,q)$ for which the functions ϕ and λ are t-independent. In the above

$$U_0 = \frac{\partial(\pi,\phi)}{\partial(p,q)} = \begin{pmatrix} \pi_p & \pi_q \\ \phi_p & \phi_q \end{pmatrix} \tag{5.10}$$

is the Jacobian of the change of variables $(p,q) \to (\pi,\phi)$. Notice also that the last equality was achieved using that the Poisson bracket of $\{\pi, H\}_{\mathrm{PB}} = 0$ and $\{\phi, H\}_{\mathrm{PB}} = 1$ [see Eq. (4.7)]. This implies that

$$\det U_0 = 1.$$

Hence the matrix U_0 is $Sp(2)$-valued with respect to the antisymmetric bilinear form

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} =: (j_{ab}).$$

We want to intertwine the $Sp(2)$ group element U_0 expressed in the fundamental representation in Eq. (5.10) to an operator $\hat{U}_0$ acting on sections of the Hilbert bundle. This operator must obey

$$\hat{U}_0^{-1}\left(\frac{d\chi}{i\hbar}\frac{\hbar}{i}\frac{\partial}{\partial S} - \frac{d\pi}{i\hbar}S\right)\hat{U}_0 = \frac{dq - H_p dt}{i\hbar}\frac{\hbar}{i}\frac{\partial}{\partial S} - \frac{dp + H_q dt}{i\hbar}S.$$

That is, the operator $\hat{U}_0$ transforms the Darboux solderings to those of ∇. The map from the matrix U_0 to the operator $\hat{U}_0$ is the intertwiner from the fundamental representation of $Sp(2)$ to its metaplectic representation on the projective Hilbert space $\mathbb{P}(\mathcal{H})$. Note that strictly only the double cover $Mp(2)$ of $Sp(2)$ has a metaplectic representation on the Hilbert space, but upon projectivizing, this gives a unitary $Sp(2)$ representation. Formally, the *projective* metaplectic action of any $Sp(2)$ matrix V is determined by the formulas

$$\widehat{\begin{pmatrix} 1 & 0 \\ t & 1 \end{pmatrix}} = \exp\left(\frac{it\hbar}{2}\frac{\partial^2}{\partial S^2}\right), \qquad \widehat{\begin{pmatrix} e^{-\ell} & 0 \\ 0 & e^{\ell} \end{pmatrix}} = \exp\left(-\ell S\frac{\partial}{\partial S}\right), \qquad \widehat{\begin{pmatrix} 1 & u \\ 0 & 1 \end{pmatrix}} = \exp\left(\frac{iu}{2\hbar}S^2\right).$$

The action of these operators on wave functions $\psi(S)$ can be computed using suitable Fourier transforms. In particular (up to irrelevant normalizations),

$$\widehat{\begin{pmatrix} 1 & 0 \\ t & 1 \end{pmatrix}}\psi(S) = \int dS' e^{\frac{i(S-S')^2}{2\hbar t}}\psi(S'), \qquad \widehat{\begin{pmatrix} e^{-\ell} & 0 \\ 0 & e^{\ell} \end{pmatrix}}\psi(S) = \psi(e^{-\ell}S), \qquad \widehat{\begin{pmatrix} 1 & u \\ 0 & 1 \end{pmatrix}}\psi(S) = e^{\frac{iu}{2\hbar}S^2}\psi(S). \tag{5.11}$$

Also, again up to an irrelevant normalization,

$$\widehat{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}}\psi(S) = \int dS' e^{-\frac{i}{\hbar}SS'}f(S'). \tag{5.12}$$

For future use, note that at the level of the Lie algebra $\mathfrak{sp}(2)$—recycling the hat notation for this—one has

$$\widehat{\begin{pmatrix} -a & b \\ c & a \end{pmatrix}} = \frac{i\hbar c}{2}\frac{\partial^2}{\partial S^2} - a\left(S\frac{\partial}{\partial S} + \frac{1}{2}\right) + \frac{ib}{2\hbar}S^2 = \frac{1}{2!i\hbar}M^{ab}\hat{s}_a\hat{s}_b. \tag{5.13}$$

In the above $(M^a{}_b) := \left(\begin{smallmatrix} -a & b \\ c & a \end{smallmatrix}\right)$ and $M^a{}_b =: j_{bc}M^{ac}$.

Also note that if $AD - BC = 1$, then

$$\widehat{\begin{pmatrix} A & B \\ C & D \end{pmatrix}} \circ \left(-\alpha S + \beta\frac{\hbar}{i}\frac{\partial}{\partial S}\right) \circ \widehat{\begin{pmatrix} D & -B \\ -C & A \end{pmatrix}} = -[A\alpha + B\beta]S + [C\alpha + D\beta]\frac{\hbar}{i}\frac{\partial}{\partial S}. \tag{5.14}$$

The above formula is the intertwiner between the fundamental representation of $Sp(2)$ and its projective metaplectic representation.

By now we have achieved that

$$\hat{U}_0^{-1}\nabla_{\mathrm{D}}\hat{U}_0 = \frac{pdq - Hdt}{i\hbar} + \frac{dq - H_p dt}{i\hbar}\frac{\hbar}{i}\frac{\partial}{\partial S} - \frac{dp + H_q dt}{i\hbar} S + \widehat{\begin{pmatrix} \phi_q & -\pi_q \\ -\phi_p & \pi_p \end{pmatrix}} \circ d \circ \widehat{\begin{pmatrix} \pi_p & \pi_q \\ \phi_p & \phi_q \end{pmatrix}}.$$

The difference between ∇_0 and ∇ in Eq. (3.5) is given by [see also Eq. (5.3)]

$$\hat{a}_0 = \widehat{\begin{pmatrix} \phi_q & -\pi_q \\ -\phi_p & \pi_p \end{pmatrix}} \left(d \widehat{\begin{pmatrix} \pi_p & \pi_q \\ \phi_p & \phi_q \end{pmatrix}} \right) + \frac{dt}{i\hbar}\left(-\frac{\hbar^2}{2}\frac{\partial^2}{\partial S^2} + v_2(q,S) \right).$$

In the above $v_2 \coloneqq V(q+S) - V(q) - V'(q)S$, and the above-displayed operator only has terms of grade zero and higher.

To complete the computation of $\hat{a}_0$, we must calculate $\hat{U}_0^{-1} d\hat{U}_0$. Because this one-form is Lie algebra-valued, we instead compute $U_0^{-1} dU_0$. Note that the matrix U_0 in Eq. (5.10) only depends on the variables p and q, or equivalently only on the pair (π, ϕ). Moreover, $\chi = -t + \phi$, so observe that—acting on functions that depend only on (p, q)—the exterior derivative can be written

$$d = d\pi \frac{\partial}{\partial \pi} + (d\chi + dt)\frac{\partial}{\partial \phi}.$$

Moreover,

$$\frac{\partial}{\partial \pi} = \phi_q \partial_p - \phi_p \partial_q = \{\phi, \cdot\}_{\mathrm{PB}}, \qquad \frac{\partial}{\partial \phi} = -V'\partial_p + p\partial_q = -\{\pi, \cdot\}_{\mathrm{PB}}.$$

Then, using $\{\phi, \pi\}_{\mathrm{PB}} = 1$, after some computation, it follows that

$$U_0^{-1}\frac{\partial}{\partial \pi}U_0 = \begin{pmatrix} -\phi_{pq} & -\phi_{qq} \\ \phi_{pp} & \phi_{pq} \end{pmatrix} = -J\mathrm{Hess}(\phi), \qquad U_0^{-1}\frac{\partial}{\partial \phi}U_0 = \begin{pmatrix} \pi_{pq} & \pi_{qq} \\ -\pi_{pp} & -\pi_{pq} \end{pmatrix} = J\mathrm{Hess}(\pi), \tag{5.15}$$

where the Hessian matrix $\mathrm{Hess}(f) \coloneqq \left(\begin{smallmatrix} f_{pp} & f_{pq} \\ f_{pq} & f_{qq} \end{smallmatrix}\right)$. Because the Hessian is symmetric, it follows that $J\,\mathrm{Hess}(f) \in \mathfrak{sp}(2)$.

Using Eq. (5.13), orchestrating the above computations gives

$$\hat{a}_0 = \widehat{\begin{pmatrix} 0 & V'' \\ -1 & 0 \end{pmatrix}} d\chi + \widehat{\begin{pmatrix} -\phi_{pq} & -\phi_{qq} \\ \phi_{pp} & \phi_{pq} \end{pmatrix}} d\pi + \frac{dt}{i\hbar} v_3(q,S),$$

where $v_3 \coloneqq V(q+S) - V(q) - V'(q)S - \frac{1}{2!}V''(q)S^2$ and the angle variable is given explicitly in Eq. (5.9). Happily—and necessarily on general grounds—the first two terms in the above display have grade zero and lie in the codistribution. Assuming real analyticity of $V(S)$, the last term has grades one and higher. Next we need to compute the higher order gauge transformation $\hat{U}_1$ subject to Eq. (3.6).

2. Higher order gauge transformations

To compute $\hat{U}_1$ we work in a formal power series in the grading. Examining (3.6), we see that it is simpler to compute $\hat{U}_1^{-1}$, which we expand as

$$\hat{U}_1^{-1} = 1 + \frac{W^{abc}\hat{s}_a\hat{s}_b\hat{s}_c}{3!i\hbar} + \cdots.$$

Here W^{abc} is some totally symmetric tensor to be determined. Then the lowest order contribution to Eq. (3.6) implies that

$$\left[\frac{e^a\hat{s}_a}{i\hbar}, \frac{W^{bcd}\hat{s}_b\hat{s}_c\hat{s}_d}{3!i\hbar}\right] = \frac{e^a j_{ab} W^{bcd}\hat{s}_c\hat{s}_d}{2!i\hbar} = \widehat{\begin{pmatrix} 0 & V'' \\ -1 & 0 \end{pmatrix}} d\pi + \widehat{\begin{pmatrix} -\phi_{pq} & -\phi_{qq} \\ \phi_{pp} & \phi_{pq} \end{pmatrix}} d\chi. \tag{5.16}$$

Using Eqs. (5.13) and (5.15) and calling $\Pi^a = (\pi, \phi)$ and $\partial_a = (\partial_p, \partial_q)$ we have that

$$W_{abc} = j_{fe}\partial_a \Pi^e \partial_b \partial_c \Pi^f.$$

Moreover, using that $\partial_{[a}\Pi^e \partial_{b]}\Pi^f$ is proportional to the Poisson bracket of Π^e and Π^f, and that $\{\phi, \pi\}_{\rm PB} = 1$, it follows that W_{abc} is totally symmetric.

We now examine higher order terms in $\hat{U}_1^{-1}$. Let us call the grade one object

$$\hat{W}_{(1)} \coloneqq \frac{W^{abc}\hat{s}_a \hat{s}_b \hat{s}_c}{3! i\hbar} \tag{5.17}$$

and search for the grade two correction

$$\hat{U}_1^{-1} = 1 + \hat{W}_{(1)} + \hat{W}_{(2)} + \cdots.$$

Also, let us decompose

$$\hat{a}_0 = a_{(0)} + a_{(1)} + \cdots,$$

where

$$\hat{a}_{(0)} = \widehat{\begin{pmatrix} 0 & V'' \\ -1 & 0 \end{pmatrix}} d\chi + \widehat{\begin{pmatrix} -\phi_{pq} & -\phi_{qq} \\ \phi_{pp} & \phi_{pq} \end{pmatrix}} d\pi \quad \text{and}$$

$$\hat{a}_{(1)} = \frac{dt}{3! i\hbar} V'''(q) S^3.$$

Along, similar lines, the grade zero part of ∇ in Eq. (5.3) is

$$\nabla_{(0)} \coloneqq d - \frac{dt}{i\hbar}\left(-\frac{\hbar^2}{2}\frac{\partial^2}{\partial S^2} + \frac{1}{2}V''(q)S^2\right).$$

Then, at grade one, Eq. (3.6) demands that

$$\left[\frac{e^a \hat{s}_a}{i\hbar}, \hat{W}_{(2)}\right] = -[\nabla_{(0)}, \hat{W}_{(1)}] + \hat{a}_{(1)} + \hat{W}_{(1)}\hat{a}_{(0)}. \tag{5.18}$$

To solve the above equation it is important to remember that $\hat{U}_1^{-1}$ must be a unitary operator. Thus we must require

$$(\hat{U}^{-1})^{-1} = 1 - \hat{W}_{(1)} - \hat{W}_{(2)} + \hat{W}_{(1)}^2 \cdots = 1 + \hat{W}_{(1)}^\dagger + \hat{W}_{(2)}^\dagger + \cdots = (\hat{U}^{-1})^\dagger, \tag{5.19}$$

so the Hermitian part of $\hat{W}_{(2)}$ is given by

$$\mathrm{He}(\hat{W}_{(2)}) = \frac{1}{2}\hat{W}_{(1)}^2.$$

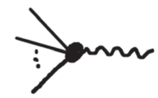
The anti-Hermitian part $\mathrm{aHe}(W_{(2)})$ is still undetermined. However Eq. (5.16) says that $[\frac{e^a \hat{s}_a}{i\hbar}, \hat{W}_{(1)}] = \hat{a}_{(0)}$ so Eq. (5.18) then gives

$$\left[\frac{e^a \hat{s}_a}{i\hbar}, \mathrm{aHe}(\hat{W}_{(2)})\right] = -\left[\nabla_{(0)} + \frac{1}{2}\hat{a}_{(0)}, \hat{W}_{(1)}\right] + \hat{a}_{(1)}. \tag{5.20}$$

To proceed we need to compute the right-hand side of the above expression. This is a tractable computation, but clearly as we move to even higher orders the complexity of such computations will grow dramatically. Hence, we digress to develop a diagrammatic representation of the operator-valued differential forms appearing in the above discussion.

3. Heaven and earth diagrams

Recall that $\Pi^a \coloneqq (\pi, \phi)$ and $\partial_a \coloneqq (\partial_p, \partial_q)$. Let us depict the tensor obtained from partial derivatives on Π^a by

$$\partial_{a_1}\partial_{a_2}\cdots\partial_{a_n}\Pi^b \coloneqq$$  .

Here the solid lines correspond to the indices $a_1, \ldots, a_n$, and these may be permuted at no cost because partial derivatives commute. The tensor j_{ab} and its inverse j^{ab} are denoted by directed line segments

$j_{ab} \coloneqq$  and $j^{ab} \coloneqq$  .

Concatenated lines indicated index contractions so, for example,

$\partial_{a_1}\partial_{a_2}\cdots\partial_{a_n}\Pi^b j_{bc} =$  ,

and

 $= j_{ab} j^{cb} = \delta_a^c\,.$ (5.21)

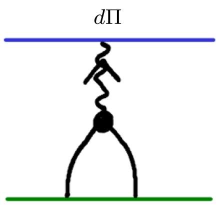
The identity above allows the depicted concatenation to be removed from a diagram. Also, note that reversing the direction of any arrow multiplies the tensor depicted by a minus sign.

More complicated diagrams obtained by such concatenations have the drawback that symmetry of external legs may be broken, and thus it may no longer be possible to uniquely associate a tensor with such a picture. Moreover, we are typically interested in Hilbert space operators taking values in differential forms built from tensors made from derivatives and products of Π^a's. Hence we adopt a "heaven and earth notation" in which a line attached to the earth (a horizontal green line) denotes contraction with the operator $\hat{s}^a$. Similarly, a line attached to heaven denotes contraction with a differential form, the choice of which will be labeled when this is not clear. For example,

$$\hat{s}^a \hat{s}^b \hat{s}^c\, \partial_a \partial_b \Pi^d j_{de} \partial_c \Pi^e =$$

and

$$\hat{s}^a \hat{s}^b \partial_a \partial_b \Pi^c j_{cd}\, d\Pi^d =$$



.

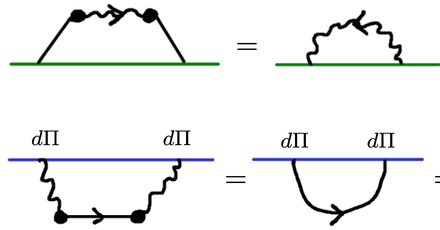
Now, the Poisson bracket $\{\phi, \pi\} = 1$ implies that $\partial_a \Pi^c j_{cd} \partial_b \Pi^d = j_{ba}$, so we have the diagrammatic identity

(5.22)

Similarly $\partial_a \Pi^c j^{ab} \partial_b \Pi^d = j^{cd}$ implies

(5.23)

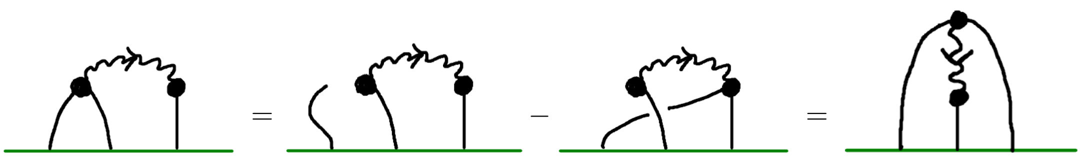
These relations imply two identities for heaven and earth diagrams



$= i\hbar,$ $= -2\varphi.$

The last equalities used that $[\hat{s}^a, \hat{s}^b] = i\hbar j^{ba}$ and $j_{ab} d\Pi^a \wedge d\Pi^b = 2\varphi$.

Since a solid line attached to a solid dot denotes a partial derivative of Π, there are further identities following from the product rule of, for example, the schematic type $(\partial\Pi)(\partial^2\Pi)(\partial^3\Pi) = \partial((\partial\Pi)^2(\partial^3\Pi)) - (\partial^2\Pi)(\partial\Pi)(\partial^3\Pi) - (\partial\Pi)^2(\partial^4\Pi)$. Hence, in a heaven and earth diagram, we can remove a leg from a solid dot and produce (minus) a sum of diagrams with that leg attached to all other solid dots plus a term where this derivative acts on the whole diagram. The latter is denoted by a solid line that ends midair between heaven and earth, and which denotes a partial derivative acting to the right. An example is the following identity:



.

The last equality used that $\hat{s}^a \partial_a i\hbar = 0$. The above is a diagrammatic demonstration that the tensor $W_{abc} = j_{fe} \partial_a \Pi^e \partial_b \partial_c \Pi^f$ is totally symmetric. To emphasize this we diagrammatically denote

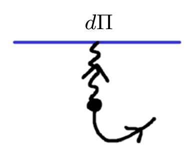
.

We need one further ingredient to attack Eq. (5.20): the exterior derivative. For that we note that acting on functions that are independent of t, we have

$$d = d\pi \partial_\pi + d\phi \partial_\phi = d\pi \{\phi, \cdot\}_{\rm PB} - d\phi \{\pi, \cdot\}_{\rm PB}$$
$$= d\Pi^a j_{ba} \partial_c \Pi^b j^{cd} \partial_d.$$

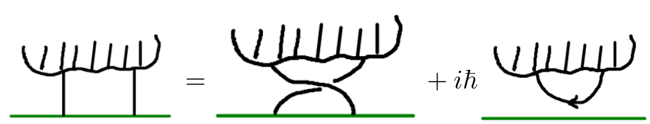
Thus we have the diagrammatic notation for the exterior derivative

$$d :=$$



.

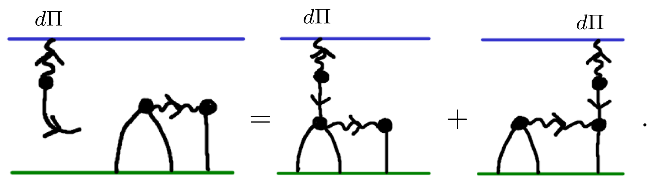
Before proceeding, we need one further diagrammatic identity expressing that $[\hat{s}^a, \hat{s}^b] = i\hbar j^{ba}$, namely



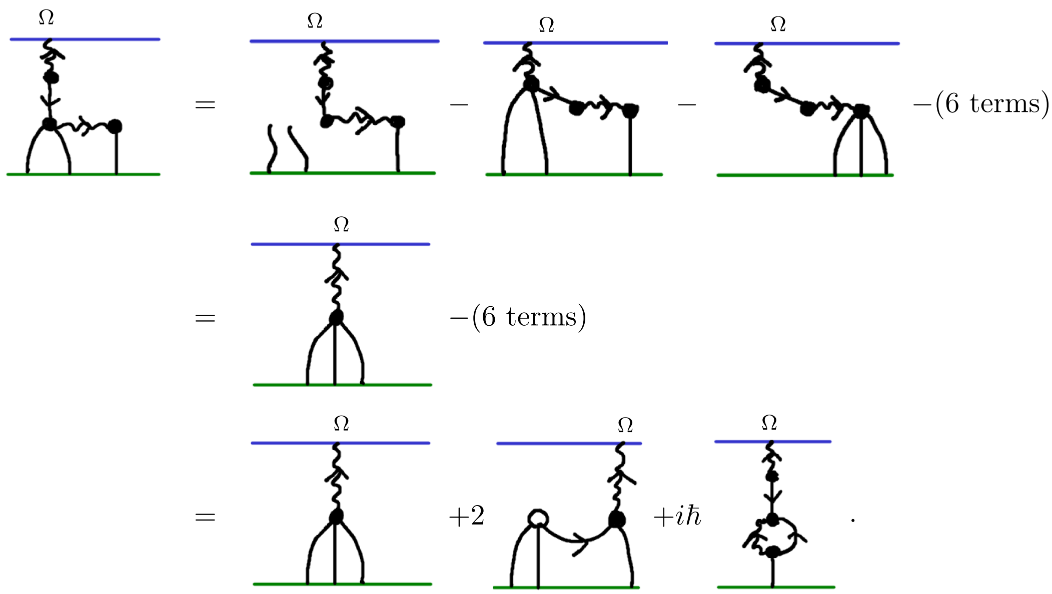
(5.24)

where the shaded blobs denote the (unspecified) remainder of the diagram.

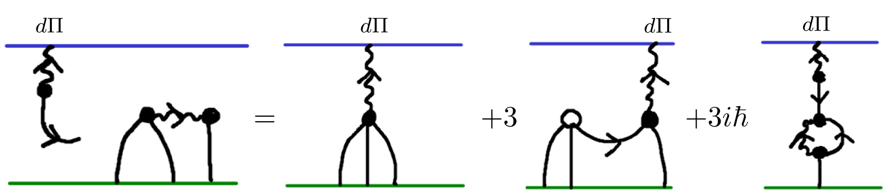
Now we are ready to diagrammatically compute the right-hand side of Eq. (5.20). We begin with $[d, \hat{W}_{(1)}]$:



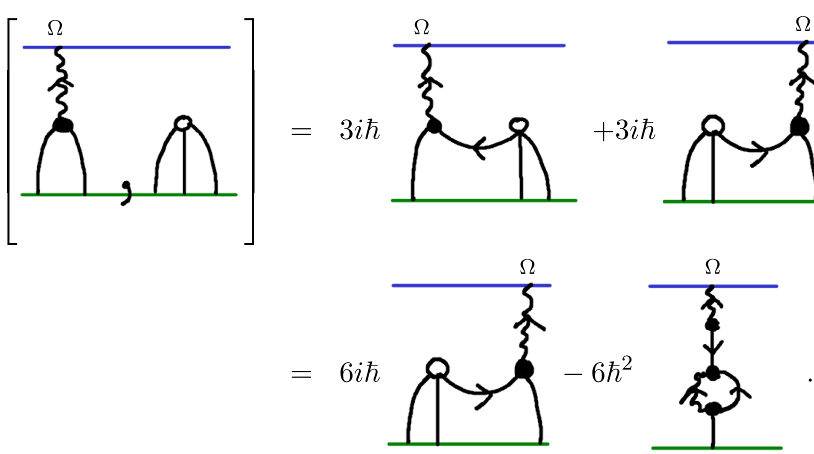
Now let Ω^a be any pair of differential forms. Then we have the following identities:



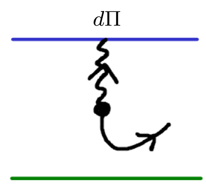
Hence

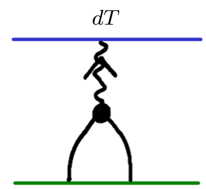


Here we used that  = and  = 0. For the remaining commutator terms in Eq. (5.20) we need the following computation:



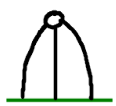
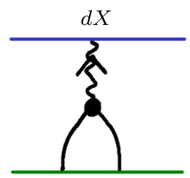
Now note that

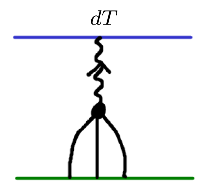
$$\nabla_{(0)} =$$


$$-\frac{1}{2i\hbar}$$


,

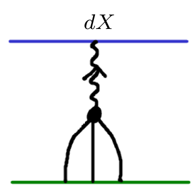
and

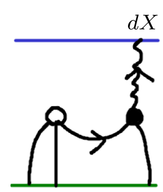
$$\hat{W}_{(1)} = -\frac{1}{3!i\hbar}$$

, $$\hat{a}_{(0)} = -\frac{1}{2i\hbar}$$


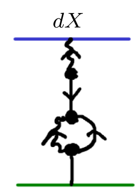
, $$\hat{a}_{(1)} = -\frac{1}{6i\hbar}$$


,

where $dT^a \coloneqq (0, dt) \eqqcolon d\Pi^a - dX^a$. Here $X^a = (\pi, \chi)$. Thus

$$-\left[\nabla_{(0)} + \frac{1}{2}\hat{a}_{(0)}, \hat{W}_{(1)}\right] + \hat{a}_{(1)} = \frac{1}{6i\hbar}$$


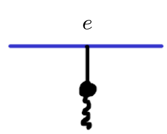
$$+\frac{1}{4i\hbar}$$


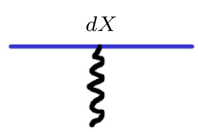
$$+\frac{1}{4}$$


.

A check of this result is that it is anti-Hermitian. This amounts to reversing the order of all the legs attached to the earth and then using the identity in Eq. (5.24) to restore these to the original pictures.

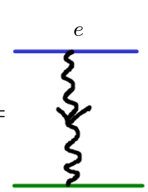
Now, using the Poisson bracket identity in Eq. (5.22) and the identity $dX^a = \partial_b \Pi^a e^b$, or in diagrams

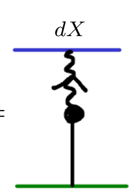


$$=$$


,

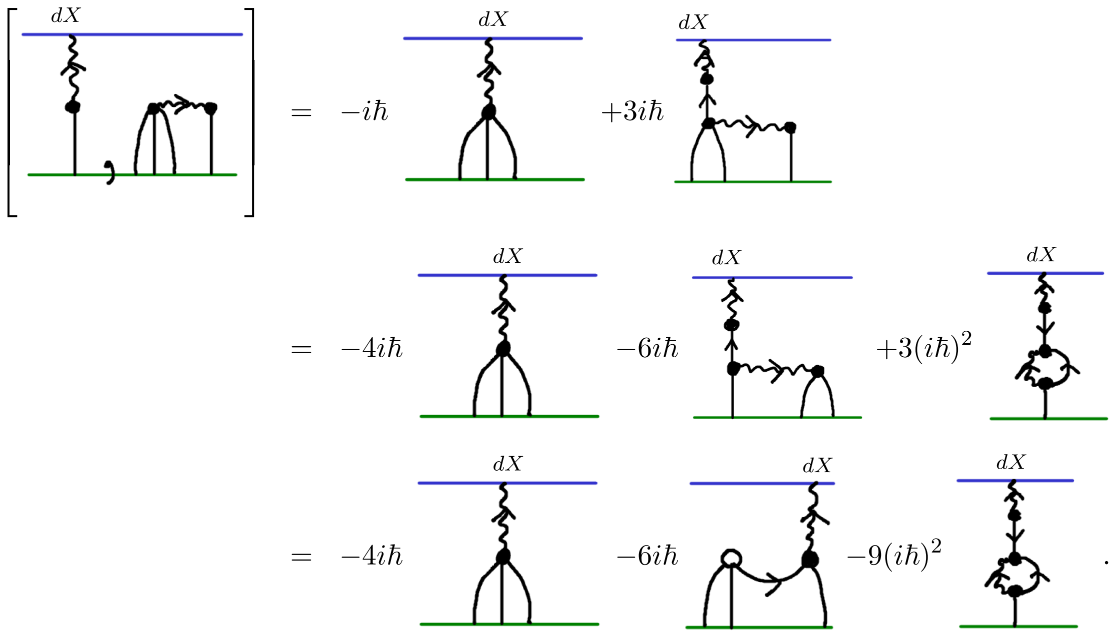
we have

$$e^a \hat{s}_a =$$


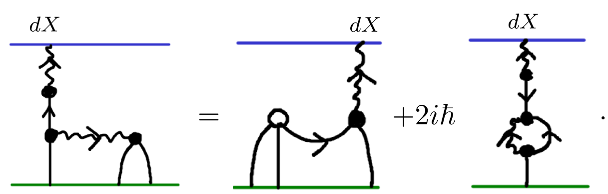
$$=$$


.

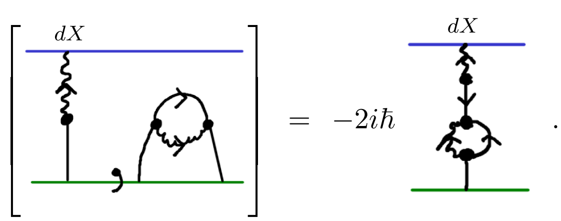
Hence we compute



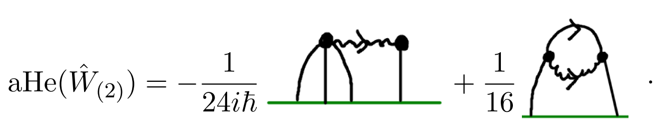
Here we used Eqs. (5.21) and (5.23) as well as the identity



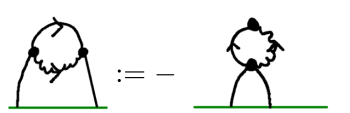
Similarly



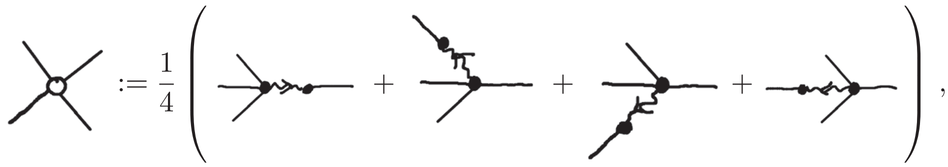
Thus we learn



Note that it is not difficult to see that the right-hand side above is anti-Hermitian using the identity



Let us define



where both sides of this diagrammatic picture define a totally symmetric rank four tensor. Then is not difficult to check that

$$\mathrm{aHe}(\hat{W}_{(2)}) = -\frac{1}{4!i\hbar}$$  . (5.25)

It is interesting to study even higher orders. For example, to compute $\hat{W}_{(3)}$, one can first consider the next order in Eq. (5.19) which determines

$$\mathrm{He}(\hat{W}_{(3)}) = \frac{1}{2}(-\hat{W}_{(1)}^3 + \hat{W}_{(1)}\hat{W}_{(2)} + \hat{W}_{(2)}\hat{W}_{(1)}).$$

The remaining difficulty now is to calculate the heaven and earth diagrams for $\mathrm{aHe}(\hat{W}_{(3)})$. Clearly this is possible but tedious. We have verified that in the model harmonic oscillator case where $V(q) = \frac{1}{2}q^2$, the obvious conjecture that symmetrizing the diagram

computes $\mathrm{aHe}(\hat{W}_{(3)})$, in fact, fails. The problem of computing an all order expression for $\hat{U}$ is related to the problem of finding deformation quantizations for Poisson and symplectic structures. These problems are solved by Kontsevich's formality theorem [15], which is neatly explained by the perturbative expansion of an all orders Poisson sigma model performed by Cattaneo and Felder [16]. It is possible that those ideas could be applied to the computation of a formal asymptotic series result for the gauge transformation $\hat{U}$.

C. Correlators

We are now ready to compute the evolution operator, which using Eq. (5.4) is given by

$$K(S_f, S_i; t_f - t_i) \coloneqq \langle S_f| \exp\left(-\frac{i(t_f - t_i)}{\hbar}\hat{H}_q\right)|S_i\rangle$$
$$= \langle S_f|P_\gamma \exp\left(-\int_\gamma \hat{A}\right)|S_i\rangle.$$

Here γ is any path between $z_i = (0, q, t_i)$ and $z_f = (0, q, t_f)$ [expressed in the (p, q, t) coordinate system]. For the moment, let us focus on the quantity on the right-hand side in the more general case that z_i and z_f are any two points in the manifold Z. In the previous section we computed the gauge transformation $\hat{U}$ such that

$$\hat{U}P_\gamma \exp\left(-\int_\gamma \hat{A}\right)\hat{U}^{-1} = P_\gamma \exp\left(-\int_\gamma \hat{A}_\mathrm{D}\right),$$

where $\hat{A}_\mathrm{D}$ is the quantum connection potential in Darboux form as in Eq. (5.7). The above operator is easy to compute (see, for example, [5]): Consider γ to be a path beginning at $z_i = (\pi_i, \chi_i, \psi_i)$ and ending at $z_f = (\pi_f, \chi_f, \psi_f)$. Because the connection ∇ is flat, we may take the path γ to be particularly simple, for example, one along which first only ψ changes by amount $\psi_f - \psi_i$, then π by $\pi_f - \pi_i$, and finally χ by $\chi_f - \chi_i$. This gives

$$P_\gamma \exp\left(-\int_\gamma \hat{A}_\mathrm{D}\right) = \exp\left(\frac{\psi_f - \psi_i + \pi_f(\chi_f - \chi_i)}{i\hbar}\right)$$
$$\times \exp\left((\chi_f - \chi_i)\frac{\partial}{\partial S}\right)$$
$$\circ \exp\left(\frac{\pi_f - \pi_i}{i\hbar}S\right).$$

Because γ is a path between $z_i = (0, q, t_i)$ and $z_f = (0, q, t_f)$, taking $H = \frac{1}{2}p^2 + V(q)$ with $V(0) = 0$, the above becomes [see Eq. (4.10)] simply a translation operator,

$$P_\gamma \exp\left(-\int_\gamma \hat{A}_\mathrm{D}\right) = \exp\left[(t_f - t_i)\left(\frac{V(q)}{i\hbar} - \frac{\partial}{\partial S}\right)\right]$$
$$\eqqcolon \exp\left(-\frac{i(t_f - t_i)}{\hbar}\hat{H}_\mathrm{D}\right). \quad (5.26)$$

We also need to compute $\hat{U}|S_i\rangle$. Viewed as a wave function, the state $|S_i\rangle$ is represented by $\delta(S - S_i)$. Now, remember that

$$\hat{U} = \hat{U}_0(1 + \hat{W}_{(1)} + \hat{W}_{(2)} + \cdots),$$

where $\hat{U}_0$ is the metaplectic representation of the matrix U_0 given in Eq. (5.10). Because p and q do not change along the path γ, at both the start and the endpoint we have

$$U_0 = \begin{pmatrix} 0 & V'(q) \\ -\frac{1}{V'(q)} & 0 \end{pmatrix}.$$

Then using Eq. (5.14), we have

$$\hat{U}_0^{-1} \circ P_\gamma \exp\left(-\int_\gamma \hat{A}_{\mathrm{D}}\right) \circ \hat{U}_0 = \exp\left[\frac{t_f - t_i}{i\hbar}(V(q) + V'(q)S)\right].$$

Next we imagine rewriting the remainder of the gauge transformation in normal order, i.e.,

$$1 + \hat{W}_{(1)} + \hat{W}_{(2)} + \cdots = :\mathcal{W}_N(S, P):,$$

where our normal ordering convention is

$$:S^k P^l: = S^k \left(\frac{\hbar}{i}\frac{\partial}{\partial S}\right)^l.$$

Then, if $|P_i\rangle$ and $|P_f\rangle$ are eigenstates of the momentum operator $\frac{\hbar}{i}\frac{\partial}{\partial S}$, we have

$$\begin{aligned}\langle P_f | P_\gamma \exp\left(-\int_\gamma \hat{A}\right) | P_i \rangle &= e^{\frac{V(q)\Delta t}{i\hbar}} \int dS e^{-\frac{iV'(q)\Delta t S}{\hbar}} \mathcal{W}_N^*(S, P_f)\mathcal{W}_N(S, P_i) \\ &=: e^{\frac{V(q)\Delta t}{i\hbar}} \mathcal{F}[\mathcal{W}_N^*(S, P_f)\mathcal{W}_N(S, P_i)](-V'(q)\Delta t),\end{aligned}$$

where $\Delta t := t_f - t_i$ and $\mathcal{F}$ denotes the Fourier transform $\mathcal{F}[f(x)](k) := \int dx e^{\frac{ikx}{\hbar}} f(x)$. To obtain the position space propagator two further Fourier transforms are needed, and this yields

$$K(S_i, S_f; \Delta t) = \mathcal{F}[\mathcal{W}_N^*(S, P')\mathcal{W}_N(S, P)] \times (-S_f, S_i, -V'(q)\Delta t), \qquad (5.27)$$

where the variables (P', P, S) are the respective Fourier dual variables to $(S_f, S_i, -V'(q)\Delta t)$. The above Fourier convolution result for quantum mechanical propagators is a very strong result, but it comes with a caveat which we now describe.

The equality in the above convolution result assumes that we can find an exact expression for the operator $\hat{U}_1$. However, in general, only an asymptotic series expression for $\hat{U}_1$ will exist. To see why this is, it is useful to study the harmonic oscillator example $V(q) = \frac{1}{2}q^2$. In that case the operator $\hat{U}_1$ must solve the condition

$$\hat{U}_1^{-1} \circ \exp\left[\frac{\Delta t}{i\hbar}\left(\frac{1}{2}q^2 + qS\right)\right] \circ \hat{U}_1 = \exp\left[\frac{\Delta t}{i\hbar}\left(-\frac{\hbar^2}{2}\frac{\partial^2}{\partial S^2} + \frac{1}{2}(q+S)^2\right)\right].$$

Because the spectrum of the harmonic oscillator Hamiltonian is discrete, while that of the operator qS is continuous, no unitary operator $\hat{U}_1$ solving the above operator equation can exist. However, there is an asymptotic series solution. Let us complete our study of the quantum Darboux theorem by demonstratng how these asymptotics work for the harmonic oscillator.

The first three asymptotic orders of the operator $\hat{U}$ were computed for general models using heaven and earth diagrams in Sec. V B 3. To explicate this series it is useful to introduce the new variables

$$\sigma := \frac{S}{\sqrt{\hbar}}, \qquad \varepsilon := \frac{\sqrt{\hbar}}{q},$$

in terms of which the display before last becomes

$$\hat{U}_1^{-1} \circ \exp\left[-i\Delta t\left(\frac{1}{2\varepsilon^2} + \frac{\sigma}{\varepsilon}\right)\right] \circ \hat{U}_1 = \exp\left[-i\Delta t\left(\frac{1}{2\varepsilon^2} + \frac{\sigma}{\varepsilon} - \frac{1}{2}\frac{\partial^2}{\partial\sigma^2} + \frac{1}{2}\sigma^2\right)\right]. \qquad (5.28)$$

For the harmonic oscillator, the pair $\Pi = (\pi, \phi) = (\frac{1}{2}p^2 + \frac{1}{2}q^2, -\arctan\frac{p}{q})$. Hence, at the starting point of a path γ with $p = 0$, the operator $\hat{W}_{(1)}$ given in Eq. (5.17) becomes

$$\hat{W}_{(1)} = \frac{\varepsilon}{3!}\left(\frac{\partial^3}{\partial\sigma^3} - 3\sigma^2\frac{\partial}{\partial\sigma} + 3\sigma\right),$$

while the anti-Hermitian part of $\hat{W}_{(2)}$ given in Eq. (5.25) is

$$\mathrm{aHe}(\hat{W}_{(2)}) = \frac{\varepsilon^2}{4!}\left(2\sigma\frac{\partial^3}{\partial\sigma^3} + 6\sigma^3\frac{\partial}{\partial\sigma} + 3\frac{\partial^2}{\partial\sigma^2} + 9\sigma^2\right).$$

Thus

$$\begin{aligned}\hat{U}_1 &= 1 + \hat{W}_{(1)} + \mathrm{aHe}(\hat{W}_{(2)}) + \frac{1}{2}\hat{W}_{(1)}^2 + \mathcal{O}(\varepsilon^3) \\ &= 1 + \frac{\varepsilon}{3!}\left(\frac{\partial^3}{\partial\sigma^3} - 3\sigma^2\frac{\partial}{\partial\sigma} + 3\sigma\right) \\ &\quad + \frac{\varepsilon^2}{4!}\left(\frac{1}{3}\frac{\partial^6}{\partial\sigma^6} - 2\sigma^2\frac{\partial^4}{\partial\sigma^4} + 3\sigma^4\frac{\partial^2}{\partial\sigma^2} - 6\sigma\frac{\partial^3}{\partial\sigma^3} \right. \\ &\quad \left. + 18\sigma^3\frac{\partial}{\partial\sigma} - 6\frac{\partial^2}{\partial\sigma^2} + 15\sigma^2\right) \\ &\quad + \mathcal{O}(\varepsilon^3). \end{aligned} \qquad (5.29)$$

It is not difficult to check that

$$\hat{U}_1^\dagger \hat{U}_1 = 1 + \mathcal{O}(\varepsilon^3),$$

and that

$$\hat{U}_1^\dagger \circ \sigma \circ \hat{U}_1 = \sigma + \frac{\varepsilon}{2}\left(-\frac{\partial^2}{\partial\sigma^2} + \sigma^2\right) + \mathcal{O}(\varepsilon^3). \qquad (5.30)$$

Note that as mentioned in the previous section, it can easily be checked that the antiHermitian part of $\hat{W}_{(3)}$ is not given solely by the five point diagram displayed there.

Now, for the sake of generality, imagine that we had solved for $\hat{U}_1$ asymptotically to order ε^k in the above display. Then, introducing the variable

$$\delta \coloneqq \frac{\Delta t}{\varepsilon},$$

we can develop an asymptotic series expansion in ε in the scaling limit where δ is held fixed for the evolution operator on the left-hand side of Eq. (5.28),

$$e^{-\frac{i\delta}{2\varepsilon}}\hat{U}_1^{-1} \circ \exp[-i\delta\sigma] \circ \hat{U}_1 = e^{-\frac{i\delta}{2\varepsilon}} \exp\left[-i\delta\left\{\sigma + \frac{\varepsilon}{2}\left(-\frac{\partial^2}{\partial\sigma^2} + \sigma^2\right)\right\}\right] + \mathcal{O}(\varepsilon^k).$$

Equation (5.30) ensures that the gauge transformation given in (5.29) solves the above displayed equality of asymptotic series for the case $k = 3$.

ACKNOWLEDGMENTS

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