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Heisenberg evolution WKB and symplectic area phases

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Abstract

The Schrödinger and Heisenberg evolution operators are represented in phase space $T^*\mathbb{R}^n$ by their Weyl symbols. Their semiclassical approximations are constructed in the short and long time regimes. For both evolution problems, the WKB representation is purely geometrical: the amplitudes are functions of a Poisson bracket and the phase is the symplectic area of a region in $T^*\mathbb{R}^n$ bounded by trajectories and chords. A unified approach to the Schrödinger and Heisenberg semiclassical evolutions is developed by introducing an extended phase space $\chi_2 \equiv T^*(T^*\mathbb{R}^n)$. In this setting, Maslov's pseudodifferential operator version of WKB analysis applies and represents these two problems via a common higher dimensional Schrödinger evolution, but with different extended Hamiltonians. The evolution of a Lagrangian manifold in χ_2 , defined by initial data, controls the phase, amplitude and caustic behaviour. The symplectic area phases arise as a solution of a boundary condition problem in χ_2 . Various applications and examples are considered. Physically important observables generally have symbols that are free from rapidly oscillating phases. The semiclassical Heisenberg evolution in this context has been traditionally realized as an \hbar power series expansion whose leading term is classical transport. The extended Heisenberg Hamiltonian has a reflection symmetry that ensures this behaviour. If the WKB initial phase is zero, it remains so for all time, and semiclassical dynamics reduces to classical flow plus finite order \hbar corrections.

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1. Introduction

The version of quantum mechanics most suitable for semiclassical dynamics is Moyal's [1] representation. This classical-like statement of quantum mechanics is achieved by the Wigner–Weyl [2, 3] correspondence, which uniquely associates Hilbert space operators with Weyl

symbols (functions) on phase space. This correspondence transforms the non-commutative product of operators into a non-commutative $*$ product of symbols. Expectation values are realized as integrals over phase space.

For systems whose coordinate manifold is Cartesian, the Wigner–Weyl isomorphism is compactly described [4–6] in terms of the quantizer. Let $T(x) = \exp[i(p \cdot \hat{q} - q \cdot \hat{p})/\hbar]$ be the Heisenberg translation operator. Here $x = (q, p)$ are the position, momentum coordinates of the linear phase space $\chi_1 \equiv T^*\mathbb{R}_q^n$, and $\hat{x} = (\hat{q}, \hat{p})$ are the corresponding quantum counterparts. The parity operator on Hilbert space is $P\psi(q) = \psi(-q)$, $\psi \in L^2(\mathbb{R}_q^n)$. The product of these two unitary operators defines the quantizer, $\Delta(x) \equiv 2^n T(2x)P$. In terms of $\Delta(x)$, the one-to-one Weyl symbol–operator pairing is

$$\hat{A} = h^{-n} \int_{\chi_1} dx A(x) \Delta(x) \quad A(x) = [\hat{A}]_w(x) = \text{Tr} \hat{A} \Delta(x)$$

where $h = (2\pi\hbar)$. The first statement above is Weyl quantization; the second is de-quantization. Whenever the operator is a density matrix $\hat{\rho}$, the quantity $h^{-n} \rho(x)$ is the Wigner distribution.

The star product is defined by the requirement that $[\hat{A}\hat{B}]_w = A * B$. For small \hbar , the $*$ multiplication is approximately the commutative product of symbols,

$$A * B(x) = A(x)B(x) + i\hbar/2\{A, B\}(x) + O(\hbar^2).$$

The Poisson bracket term measures, to leading \hbar order, the non-commutative character of the star product.

The two basic statements of quantum dynamics are the Schrödinger and Heisenberg pictures. On the space, $L^2(\mathbb{R}_q^n)$, each self-adjoint Hamiltonian \hat{H} generates a unitary Schrödinger evolution, $\hat{U}(t) = \exp[-it\hat{H}/\hbar]$. An initial density matrix $\hat{\rho}_0$ has Heisenberg evolution, $\hat{\rho}(t) = \hat{U}(t)\hat{\rho}_0\hat{U}(t)^\dagger$. Let $H, U(t)$ and $\rho(t)$ be the Weyl symbols of $\hat{H}, \hat{U}(t)$ and $\hat{\rho}(t)$, respectively. In this setting, the equations of motion are

$$i\hbar \partial U(t, x) / \partial t = H(x) * U(t, x) \quad (1.1)$$

$$\partial \rho(t, x) / \partial t = \{H, \rho(t)\}_M(x) \quad (1.2)$$

with initial conditions $U(0, x) = 1$ and $\rho(0, x) = \rho_0(x)$. In (1.2), the bracket operation is defined by

$$\{A, B\}_M \equiv \frac{1}{i\hbar} [\hat{A}, \hat{B}]_w = \frac{1}{i\hbar} (A * B - B * A).$$

This is the Moyal bracket. Like the quantum commutator, it is bilinear, skew and obeys the Jacobi identity.

It is evident that the Weyl–Heisenberg symbol evolution problem (1.2) is formally as close as it can be to classical dynamics. Since $\{A, B\}_M = \{A, B\} + O(\hbar^2)$, Bohr’s correspondence principle is realized in a transparent form. The time-dependent expectation value of an observable \hat{A} is conveniently given by the phase space integral,

$$\langle \hat{A} \rangle_t \equiv \text{Tr} \hat{A} \hat{\rho}(t) = h^{-n} \int_{\chi_1} dx A(x) \rho(t, x). \quad (1.3)$$

The main goal of this paper is to obtain both short and long time WKB approximate solutions for the Weyl symbol evolution problems (1.1) and (1.2). In theorems 1 and 2, we prove that the phases entering these semiclassical representations are invariant geometrical quantities—namely the symplectic areas defined by certain closed loops in phase space. Furthermore, the amplitude functions are given by determinants of a Poisson bracket.

We introduce a unified approach to solve both problems (1.1) and (1.2). Standard Weyl symbol calculus identities show that $H*$ and $\{H, \cdot\}_M$ are pseudodifferential operators; in other words they are functions of ∇_x and multiplication by x . If one introduces an extended phase space $\chi_2 \equiv T^*(T^*\mathbb{R}_q^n)$, then Maslov's [7] WKB analysis applies. In particular, the semiclassical approximations for the evolutions $U(t, x)$ and $\rho(t, x)$ are characterized by a Lagrangian manifold, and the time evolution of this manifold is determined by an extended Hamiltonian in χ_2 . In order to distinguish these two phase spaces we label χ_1 the primary phase space (PPS), and χ_2 the secondary phase space (SPS). Projecting the χ_2 analysis back onto the primary phase space provides explicit WKB representations of $U(t, x)$ and $\rho(t, x)$.

In spite of the importance of problem (1.2), it has received insufficient study. The version of the Heisenberg problem that has been investigated in detail [8–11] occurs for the case where the observable \hat{A} is semiclassically admissible, namely its Weyl symbol is \hbar dependent and allows a finite order small \hbar asymptotic expansion, cf (3.7). In [12] a connected graph method was constructed to obtain the coefficients of the \hbar asymptotic expansion of $[\hat{U}(t)^\dagger \hat{A} \hat{U}(t)]_w(x)$. Based on this latter formalism, numerical calculations have shown [13] that the \hbar^2 -order semiclassical expansion accurately describes noble gas atom–atom scattering. However, semiclassically admissible symbols are not suitable for representing [14] density matrices. The requirement that one has a pure state, $\rho_0 * \rho_0 = \rho_0$, means that $\rho_0(x)$ is an $\hbar \rightarrow 0$ rapidly oscillating function, cf (2.12).

The results in the literature which form the point of departure for this investigation are found in three seminal works: by Karasev and Nazaikinskii [15], Berry [16] and Marinov [17]. In the first of these, an analytical approach to a generalized semiclassical expansion based on a SPS with its associated left–right representation of $*$ -product and Hamilton–Jacobi equation was developed. In the second pair of works, the geometrical (symplectic phase) interpretation of the Wigner eigenfunction and of the dynamical WKB approximation was achieved. Specifically, in the small time sector, where the time evolving χ_2 Lagrangian manifold remains single sheeted, Marinov found the WKB amplitude and phase for $U(t, x)$.

This paper is organized as follows. Section 2 presents the extended Schrödinger equation in the SPS setting and shows how problems (1.1) and (1.2) are particular examples of this extended evolution. Also, the geometric, commutative and coordinate relationships between the PPS and SPS are reviewed. The trajectories entering the WKB expansion are determined by the solutions of a boundary condition problem. In section 3, a detailed analysis of the BC problem and the manner in which it constructs phase space loops is carried out. The semiclassical expansions for $\rho(t, x)$ and $U(t, x)$ are consolidated in theorems 1 and 2. Finally, in section 4 the group generated phase addition rules are obtained; the mutual compatibility of the Schrödinger and Heisenberg semiclassical evolution is established; the exact solutions for quadratic Hamiltonian systems are compared and the $\hbar \rightarrow 0$ asymptotics of $[\hat{U}(t)^\dagger \hat{A} \hat{U}(t)]_w(x)$ for semiclassically admissible operators \hat{A} is realized as a special case of theorem 1. There are two appendices containing specialized aspects of Jacobi fields and a Poincaré–Cartan identity.

2. Secondary phase space dynamics

The first part of this section shows how to interpret the $H*$ structure in the equations of motion as the action of a pseudodifferential operator (Ψ DO). The normal ordered symbols of these operators are then functions on the secondary phase space. For the Schrödinger and Heisenberg problem, we demonstrate how the classical flow in χ_2 is composed in terms of the standard Hamiltonian mechanics on χ_1 . The necessity of representing the initial value

form of the density matrix as a rapidly oscillating \hbar function is confirmed by constructing the semiclassical Weyl symbol for a pure state.

Introduce the SPS canonical operators X, Y acting on functions $f(x)$: $Xf(x) = xf(x)$ and $Yf(x) = -i\hbar\nabla_x f(x)$. Let $\mathcal{H}(\overset{2}{X}, \overset{1}{Y})$ be a normal ordered, symmetric Ψ DO defined by symbol $\mathcal{H}(x, y)$. On the coordinate domain \mathbb{R}_x^{2n} , the extended Schrödinger evolution problem is

$$i\hbar\partial\Psi(t, x)/\partial t = \mathcal{H}(\overset{2}{X}, \overset{1}{Y})\Psi(t, x). \quad (2.1)$$

The two problems (1.1) and (1.2) are particular cases of (2.1). The appropriate realization of \mathcal{H} in each case is determined by employing the left–right $*$ product representation [18], namely

$$f_1 * f_2(x) = f_1\left(\overset{2}{X} - \frac{1}{2}J\overset{1}{Y}\right)f_2(x) \quad f_1 * f_2(x) = f_2\left(\overset{2}{X} + \frac{1}{2}J\overset{1}{Y}\right)f_1(x).$$

Setting $\mathcal{H}(x, y) = \mathcal{H}_1 \equiv H(x - \frac{1}{2}Jy)$ selects the Schrödinger problem (1.1) whereas the choice $\mathcal{H}_2 \equiv H(x - \frac{1}{2}Jy) - H(x + \frac{1}{2}Jy)$ gives the Heisenberg problem (1.2). The solution $\Psi(t, x)$ is either $U(t, x)$ or $\rho(t, x)$ depending on the choice of \mathcal{H} .

Throughout the paper, symbols with SPS arguments (x, y) correspond to normal ordered operators while symbols with PPS argument x denote Weyl ordering. Consistency of the extended Schrödinger problem requires that the normal ordered symbol $H(x \pm \frac{1}{2}Jy)$ defines a symmetric operator on $L^2(\mathbb{R}_x^{2n})$. That this is so is a consequence of the argument structure $(x \pm \frac{1}{2}Jy)$ which implies that the normal ordered and Weyl ordered symbols are the same function. Since the Weyl ordered symbol is real, one has that the Ψ DO Hamiltonians in (2.1) are formally self-adjoint.

Consider the coordinate systems of χ_1 and χ_2 and their interconnections. Let y be the momentum variable in SPS so that a general point $m \in \chi_2$ has Cartesian coordinates $z(m) = (x, y)$. The symplectic structure of χ_1 and χ_2 is determined by their respective canonical 2-forms

$$\begin{aligned} \omega^{(1)} &\equiv dp \wedge dq = \frac{1}{2}J_{\alpha\beta} dx_\beta \wedge dx_\alpha & J &= \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix} \\ \omega^{(2)} &\equiv dy \wedge dx = \frac{1}{2}\tilde{J}_{jk} dz_k \wedge dz_j \end{aligned}$$

where I_n is the $n \times n$ identity matrix, and \tilde{J} is the symplectic matrix having the block form of J with I_{2n} substituted for I_n . Given the 2-forms, $\omega^{(1)}$ and $\omega^{(2)}$, the corresponding Poisson brackets are

$$\{f, g\}_1(x) = \nabla f(x) \cdot J \nabla g(x) \quad \{F, G\}_2(z) = \nabla F(z) \cdot \tilde{J} \nabla G(z).$$

The coordinate functions, $x = (q, p)$ and $z = (x, y)$, are canonical in χ_1 and χ_2 , namely $\{x_\alpha, x_\beta\}_1 = J_{\alpha\beta}$ and $\{z_j, z_k\}_2 = \tilde{J}_{jk}$. In order that (2.1) be a standard Schrödinger equation the coordinates $x = (q, p)$ must commute. This is the case since $\{x_\alpha, x_\beta\}_2 = 0$. Although (2.1) has the appearance of an equation of motion for a ‘wavefunction’ $\Psi(t, x)$, it needs to be recalled that $\Psi(t, x)$ is a Weyl symbol and always represents an operator on $L^2(\mathbb{R}_x^{2n})$.

As one sees from functional the forms of \mathcal{H} , a second natural coordinate system for χ_2 is defined by the (l, r) variables

$$\begin{aligned} l &= x - \frac{1}{2}Jy & r &= x + \frac{1}{2}Jy & l, r &\in \mathbb{R}^{2n} \\ x &= \frac{1}{2}(l + r) & y &= J(l - r). \end{aligned} \quad (2.2)$$

The link between the coordinate systems (x, y) and (l, r) and their commutative structures is the following.

Lemma 1.

(i) The SPS commutative properties of the projections $l, r : \mathbb{R}_z^{4n} \rightarrow \mathbb{R}_x^{2n}$ are

$$\{l_\alpha, l_\beta\}_2 = J_{\alpha\beta} \quad \{r_\alpha, r_\beta\}_2 = -J_{\alpha\beta} \quad \{l_\alpha, r_\beta\}_2 = 0.$$

(ii) The l variables are Poisson; the r variables are anti-Poisson, namely

$$\{f \circ l, g \circ l\}_2 = \{f, g\}_1 \circ l \quad \{f \circ r, g \circ r\}_2 = -\{f, g\}_1 \circ r.$$

(iii) The χ_2 Poisson bracket and symplectic form have the $l \times r$ decomposition

$$\begin{aligned} \{F, G\}_2 &= (\nabla_l F)_\alpha J_{\alpha\beta} (\nabla_l G)_\beta - (\nabla_r F)_\alpha J_{\alpha\beta} (\nabla_r G)_\beta \\ \tilde{J}_{jk} dz_k \wedge dz_j &= J_{\alpha\beta} dl_\beta \wedge dl_\alpha - J_{\alpha\beta} dr_\beta \wedge dr_\alpha. \end{aligned}$$

The space structure for the left–right variables is $\chi_1 \otimes \chi'_1 \ni (l, r)$. Here χ'_1 denotes the phase space defined by the 2-form $-\frac{1}{2}J_{\alpha\beta} dr_\beta \wedge dr_\alpha$. Often the space $\chi_1 \otimes \chi'_1$ is called [19] the double phase space. We use the name secondary phase space for cotangent bundle $\chi_2 = T^*(T^*R_q^n)$ in order to distinguish it from $\chi_1 \otimes \chi'_1$. The left–right map (2.2) is diffeomorphic.

The basic ingredients in any semiclassical approximation are the classical action phase and the amplitude functions determined by classical transport. Because the extended Hamiltonians are the simple composite functions $H \circ l$ and $H \circ l - H \circ r$, it is possible to describe the χ_2 phase space motion as appropriately weighted sums of χ_1 trajectories. Let $g(\tau|x_0) = (q(\tau|x_0); p(\tau|x_0))$ denote the solution of the PPS Hamiltonian system

$$\dot{g}(\tau|x_0) = J\nabla H(g(\tau|x_0)) \quad g(0|x_0) = x_0. \tag{2.3}$$

The SPS motion is labelled $G(\tau|z_0) = (x(\tau|z_0); y(\tau|z_0))$, where

$$\dot{G}(\tau|z_0) = \tilde{J}\nabla\mathcal{H}(G(\tau|z_0)) \quad G(0|z_0) = z_0. \tag{2.4}$$

The initial data z_0 for system (2.4) also has the left–right form $l_0 = l(z_0), r_0 = r(z_0)$.

Lemma 2. The solution of the SPS Hamiltonian system, in terms of χ_1 flows, takes the form

(i) for the Schrödinger problem with $\mathcal{H}_1 = H \circ l$

$$x(\tau|z_0) = \frac{1}{2}(g(\tau|l_0) + r_0) \quad y(\tau|z_0) = J(g(\tau|l_0) - r_0), \tag{2.5}$$

(ii) for the Heisenberg problem with $\mathcal{H}_2 = H \circ l - H \circ r$

$$x(\tau|z_0) = \frac{1}{2}(g(\tau|l_0) + g(\tau|r_0)) \quad y(\tau|z_0) = J(g(\tau|l_0) - g(\tau|r_0)). \tag{2.6}$$

Proof. Consider part (i). Using the Poisson equations of motion, it is convenient to state the SPS flow in the l, r variables. Lemma 1(iii) implies

$$\dot{l}_\alpha(\tau) = \{l_\alpha, H \circ l\}_2 = J_{\alpha\beta} \nabla_\beta H(l(\tau)) \quad \dot{r}_\alpha(\tau) = \{r_\alpha, H \circ l\}_2 = 0. \tag{2.7}$$

So $l(\tau|l_0) = g(\tau|l_0)$ and the r -motion is a constant, $r(\tau|r_0) = r_0$. Using (2.2) recovers (2.5). A similar argument verifies part (ii). \square

The identities (2.7) show that the left–right motions are decoupled. This decoupling occurs because $\{l_\alpha(\tau), r_\beta(\tau)\}_2 = 0$. Further note that the system $\mathcal{H}_1 = H \circ l$ has $2n$ constants of motion; $r_\alpha(\tau) = \text{const}$ for $\alpha = 1, \dots, 2n$. Nevertheless, \mathcal{H}_1 is not completely integrable since the functions $r_\alpha(\tau)$ are not in involution, i.e. $\{r_\alpha(\tau), r_\beta(\tau)\}_2 = -J_{\alpha\beta} \neq 0$.

Lagrangian manifolds in SPS create canonical transformations in PPS. Let us clarify how this is realized in terms of the left–right projections. Suppose Λ is a χ_2 manifold which is

locally defined by the smooth phase $S : U \subseteq \mathbb{R}_x^{2n} \rightarrow \mathbb{R}$, i.e. $y = \nabla S(x)$, $x \in U$. This identity relates l to r by

$$r - l = J \nabla S \left(\frac{1}{2}(l + r) \right). \quad (2.8)$$

If $\det \left(I \pm \frac{1}{2} J S'' \right) \neq 0$, $x \in U$ then the implicit function theorem defines $l = l(r)$ and $r = r(l)$. These transformations are canonical. This follows from

$$\frac{dl}{dr} = \frac{\left(I - \frac{1}{2} J S'' \right)}{\left(I + \frac{1}{2} J S'' \right)}.$$

The right-hand side in the equation above is the Cayley transform of the symmetric S'' and so defines a symplectic matrix. A systematic study of generating functions of this type is found in [20]

An important aspect of WKB analysis is the \hbar singularity structure of the Cauchy initial data. As noted in the introduction, a pure state density matrix must be a rapidly oscillating function. Let us clarify this situation with an example. Suppose $\psi_0(q) = n(q) \exp[i s(q)/\hbar]$ is a unit normalized $L^2(\mathbb{R}_q^n)$ wavefunction, which defines a rank one density matrix, $\hat{\rho}_0 = |\psi_0\rangle\langle\psi_0|$. The functions n, s are real. The Weyl symbol of $\hat{\rho}_0$ is given by the Wigner transform [2]

$$\rho_0(x; \hbar) = \int_{\mathbb{R}^n} dv n \left(q + \frac{1}{2}v \right) n \left(q - \frac{1}{2}v \right) \exp \frac{i}{\hbar} \phi(v, x) \quad (2.9)$$

$$\phi(v, x) = s \left(q + \frac{1}{2}v \right) - s \left(q - \frac{1}{2}v \right) - p \cdot v. \quad (2.10)$$

The $\hbar \rightarrow 0$ asymptotic form of ρ_0 may be calculated by a stationary phase approximation [7]. Let $\phi'(v, x) = \nabla_v \phi(v, x)$ and $\phi''(v, x) = \nabla_v \nabla_v \phi(v, x)$. The critical points of ϕ satisfy

$$2p = \nabla s \left(q - \frac{1}{2}v \right) + \nabla s \left(q + \frac{1}{2}v \right). \quad (2.11)$$

Suppose (v_0, x_0) is a solution set for this equation where $\det \phi''(v_0, x_0) \neq 0$, then the implicit function theorem defines a function $v = v(q, p) = v(x)$ obeying (2.11). Since $\phi'(v, x)$ is even in v , the roots occur in pairs. If $v = v(x)$ is a solution, then so is $v = -v(x)$. Incorporate this pairing behaviour via the notations $q_{\pm} = q \pm v(x)/2$, $p_{\pm} = \nabla s(q_{\pm})$, $x_{\pm} = (q_{\pm}, p_{\pm})$. In the non-singular region where $\det \phi''(v(x), x) \neq 0$, the Wigner transform above has asymptotic form

$$\rho_0(x; \hbar) \sim \hbar^{\frac{n}{2}} |\det \phi''(v(x), x)|^{-1/2} n(q_+) n(q_-) 2 \cos \left\{ \frac{1}{\hbar} S_0(x) + \frac{\pi}{4} \operatorname{sgn} \phi''(v(x), x) \right\}. \quad (2.12)$$

The phase $S_0(x) = \phi(v(x), x)$ and sgn denotes the signature of a symmetric matrix. If x is in the neighbourhood where (2.11) has no solutions, then $\rho_0(x)$ is $O(\hbar^\infty)$ small.

As Berry first noted [16] (in the $n = 1$ version of this problem), the phase S_0 is a symplectic area. To see this in the present context, define the χ_1 Lagrangian manifold $\lambda \equiv \{x \in \chi_1 | p = \nabla s(q)\}$. Construct two paths between the end points x_- and x_+ . Let the first path, $C(x_-, x_+)$, be a straight line from x_- to x_+ . As the second path, $\gamma_\lambda(x_+, x_-)$, choose any curve from x_+ to x_- lying on the surface λ . Then one finds

$$S_0(x) = \oint_{C(x_-, x_+) + \gamma_\lambda(x_+, x_-)} p \cdot dq. \quad (2.13)$$

The geometry of the loop in (2.13) is the well known chord mid-point construct [16, 17, 21–23]. The end points x_{\pm} of the directed chord $C(x_-, x_+)$ lie on λ , and x is the mid-point of this chord. By Stokes theorem, $S_0(x)$ is also the area of any membrane having boundary $C(x_-, x_+) + \gamma_\lambda(x_+, x_-)$.

3. Symplectic areas and WKB phases

This section shows how the secondary phase space WKB approximations for $U(t, x)$ or $\rho(t, x)$ can be reformulated in terms of primary phase space flows. This reduction process transforms all the χ_2 WKB phases into symplectic areas defined by closed loops in χ_1 . A key element of this analysis is the solvability of the appropriate two point boundary condition (BC) problem. We pose the BC problem in terms of Lagrangian manifolds and construct both short and long time solutions.

To begin with, we summarize Maslov’s WKB expansion for the extended Schrödinger problem (2.1). The $t = 0$ state for system (2.1) is assumed to have the generic form, $\Psi_0(x) = \alpha_0(x) e^{i\beta_0(x)/\hbar}$. The real functions α_0, β_0 have support on the domain $D_0 \subseteq \mathbb{R}_x^{2n}$. The phase β_0 defines a χ_2 Lagrangian manifold Λ_0 , via $y(x) = \nabla\beta_0(x), x \in D_0$. Let $\Pi_1(x, y) = x$ be the projection onto \mathbb{R}_x^{2n} . It is assumed that projection $\Pi_1 : \Lambda_0 \rightarrow D_0$ is a diffeomorphism.

The symbol $\mathcal{H}(x, y)$ in (2.1) is a pseudodifferential operator only if it is in a suitable class of functions. We employ Maslov’s notation for these spaces. The first is $T^m(\mathbb{R}_z^{4n})$. This space denotes those $C^\infty(\mathbb{R}_z^{4n})$ functions \mathcal{H} which satisfy the uniform growth estimates

$$|\nabla'_x \nabla'_y \mathcal{H}(x, y)| \leq C_{\gamma\rho} (1 + |x|)^m (1 + |y|)^m \quad |\gamma|, |\rho| \geq 0 \quad (x, y) \in \mathbb{R}_x^{2n} \times \mathbb{R}_y^{2n} = \mathbb{R}_z^{4n} \tag{3.1}$$

where integer $m \geq 0$ and the positive constants $C_{\gamma\rho}$ are independent of (x, y) . The symbols in the class $T^m(\mathbb{R}_z^{4n})$ are \hbar independent. Now widen this class so as to include the semiclassically admissible operators. These operators depend on \hbar and admit an asymptotic expansion about $\hbar = 0$. The function $\mathcal{H}(x, y; \hbar)$ belongs to the class $T^m_+(\mathbb{R}_z^{4n})$, if $\mathcal{H} \in C^\infty(\mathbb{R}_z^{4n} \times \mathbb{R}^+)$ and the small \hbar asymptotic expansion has coefficients and remainder term in $T^m(\mathbb{R}_z^{4n})$, cf [7].

To proceed three assumptions are required: (a) The function $\mathcal{H} \in T^m_+(\mathbb{R}_z^{4n}), m \geq 2$. (b) For arbitrary finite time intervals $[-T, T]$, the SPS Hamiltonian system (2.4) has unique smooth solutions, i.e. $G(t|x, y) \in C^\infty([-T, T], \mathbb{R}_z^{4n})$. (c) Let x be a non-focal point (cf definition 3) with respect to the Π_1 projection of the manifold $\Lambda_t = G(t)\Lambda_0$. Assume there are a finite number of points $x_0^j \in D_0, j = 1, \dots, N$, such that $\Pi_1 G(t|x_0^j, \nabla\beta_0(x_0^j)) = x$.

Each of these assumptions is required for an evident reason: (a) ensures that $\mathcal{H}(\overset{2}{X}, \overset{1}{Y})$ is a well defined Ψ DO, (b) prohibits finite time runaway trajectories and (c) assumes the existence of one or more solutions to the BC problem: which trajectories starting from Λ_0 have x as their final coordinate position? Locally varying (t, x) in (c) determines the initial x_0 as a function of (t, x) , namely $x_0^j = x_0^j(t, x)$.

Under the hypotheses (a)–(c) the $\hbar \rightarrow 0$ asymptotic solution of the Cauchy problem (2.1), with initial data Ψ_0 , is

$$\Psi(t, x) = \Psi^{sc}(t, x)[1 + O(\hbar)] \tag{3.2}$$

$$\Psi^{sc}(t, x) = \sum_{j=1}^N \frac{\phi_j(t, x)}{\sqrt{|J_j(t, x)|}} \exp \left\{ \frac{i}{\hbar} \beta_j(t, x) - \frac{i\pi}{2} m_j(t, x) \right\} \quad t \in [-T, T]. \tag{3.3}$$

Here $m_j(t, x)$ is the Maslov index for trajectory $\{G(\tau|z_0^j) : \tau \in [0, t]\}$, where $z_0^j = (x_0^j(t, x), \nabla\beta_0(x_0^j(t, x))) \in \Lambda_0$. The phase and amplitude functions are

$$\beta_j(t, x) = \beta_0(x_0^j) + \int_0^t \left[y(\tau|z_0^j) \cdot \dot{x}(\tau|z_0^j) - \mathcal{H}(G(\tau|z_0^j)) \right] d\tau \tag{3.4}$$

$$J_j(t, x) = \det \left(\frac{dx(t|x_0^j, \nabla \beta_0(x_0^j))}{dx_0^j} \right) \Big|_{x_0^j = x_0^j(t, x)} \quad (3.5)$$

$$\phi_j(t, x) = \left(\exp \int_0^t \text{Tr} \nabla_x \nabla_y \mathcal{H} \left(G(\tau|z_0^j) \right) d\tau \right) \alpha_0(x_0^j). \quad (3.6)$$

The family of operators $\mathcal{H}(\overset{2}{X}, \overset{1}{Y})$ consistent with the class $T_+^m(\mathbb{R}_z^{4n})$ is large. The growth index, m , must be 2 or greater to include kinetic energy in H . The operators $\mathcal{H}(\overset{2}{X}, \overset{1}{Y})$ need not have a polynomial dependence in momentum Y , nor do they need to be partial differential operators. This generality is essential to the SPS method we employ: normally, the Ψ DO defined by \mathcal{H}_1 and \mathcal{H}_2 will not be a finite order partial differential operator. The phases $\beta_j(t, x)$ have a geometric meaning. Define the \mathcal{H} flow transported Lagrangian manifold, $\Lambda_t \equiv G(t)\Lambda_0$. Then the surfaces $y_j(t, x) = \nabla \beta_j(t, x)$ describe the different sheets of Λ_t . Representation (3.2)–(3.6) is theorem 10.5 of [7].

In phase space quantum mechanics, the range of physical systems one may describe is controlled by the allowed functional form of the Weyl symbol Hamiltonian. For reasons of notational simplicity we presume H is static. Including time-dependent Hamiltonians, as a subsequent generalization, is a straightforward matter. The WKB summary above indicates that two restrictions on H are necessary.

Assumption A.

- (1) The Hamiltonian operator \hat{H} is semiclassically admissible, specifically $H \in T_+^m(\mathbb{R}_x^{2n})$, $m \geq 2$.
- (2) On finite time intervals $[-T, T]$, H generates a unique classical flow, $g(t|x) \in C^\infty([-T, T], \mathbb{R}_x^{2n})$.

Assumption A is common to all the propositions and theorems of this section and will not be explicitly cited in them.

Since l and r are linear functions of z , assumption A(1) implies that the composite functions $\mathcal{H}_1 = H \circ l$ and $\mathcal{H}_2 = H \circ l - H \circ r$ are in $T_+^m(\mathbb{R}_z^{4n})$, $m \geq 2$. Likewise, lemma 2 shows that assumption A(2) guarantees that $G(t|x, y) \in C^\infty([-T, T], \mathbb{R}_z^{4n})$ for both \mathcal{H}_1 and \mathcal{H}_2 flow. The requirement that $H \in T_+^m(\mathbb{R}_x^{2n})$ means that $H = H(x; \hbar)$ has the $\hbar \rightarrow 0$ uniform asymptotic expansion

$$H(x; \hbar) = H_0(x) + \sum_{j=1}^J \hbar^j H_j(x) + O(\hbar^{J+1}). \quad (3.7)$$

For many physical systems $H(x; \hbar) = H_0(x)$. For example, this occurs for a mass m charged particle moving in an external electromagnetic field. The higher order terms $H_j(x)$ have no effect on the leading order WKB approximation. So from here on we will identify H with H_0 and omit the subscript 0.

3.1. The boundary condition problem

Assumption A says nothing about the solvability of the BC problem. Rather than dealing with this by assumption, as was done in the Maslov representation (3.2)–(3.6), we will find existence proofs and explicit formulae for the BC solutions. We discuss the Schrödinger and Heisenberg problems in tandem. This allows us to compare how the chord mid-point structures are differently realized in these two BC solutions.

For the $U(t, x)$ and $\rho(t, x)$ evolutions, the initial state of the system is taken to be

$$U_0(x) = N_0(x) e^{i\Phi_0(x)/\hbar} \quad \rho_0(x) = \alpha_0(x) e^{iS_0(x)/\hbar} \quad x \in D_0 \subseteq \mathbb{R}^{2n} \tag{3.8}$$

where the domain D_0 is a simply connected open set. The phases Φ_0 and S_0 each define the single sheeted Lagrangian manifold, e.g. $\Lambda_0 = \{z \in \chi_2 | y(x) = \nabla S_0(x), x \in D_0\}$. The phases Φ_0 and S_0 are both assumed to be $C^\infty(\mathbb{R}^{2n})$.

BC problem. *Determine the trajectories $G(t|x_0, y_0)$ which begin on Λ_0 and have the final position $x \in D_t = \Pi_1 \Lambda_t$.*

(i) *The Schrödinger case: find the functions $x_0 = x_0(t, x)$ and $y_0 = y_0(t, x)$ from*

$$\frac{1}{2} [g(t|x_0 - \frac{1}{2}Jy_0) + (x_0 + \frac{1}{2}Jy_0)] = x \tag{3.9}$$

$$y_0 = \nabla \Phi_0(x_0) \quad x_0 \in D_0. \tag{3.10}$$

(ii) *The Heisenberg case: find the functions $x_0 = x_0(t, x)$ and $y_0 = y_0(t, x)$ from*

$$\frac{1}{2} [g(t|x_0 - \frac{1}{2}Jy_0) + g(t|x_0 + \frac{1}{2}Jy_0)] = x \tag{3.11}$$

$$y_0 = \nabla S_0(x_0) \quad x_0 \in D_0. \tag{3.12}$$

Lemma 2 justifies writing the left-hand sides of (3.9) and (3.11) as the weighted sum of the left and right flows. It is natural to interpret each of these equations as a mid-point condition. Conditions (3.10) and (3.12) ensure that (x_0, y_0) lies on Λ_0 . Observe that the initial density matrix ρ_0 is not real valued like approximation (2.12). However, by superposition with its complex conjugate the ρ_0 initial state can be made real.

We treat the small time and big time solutions to the BC problem with different methods and assumptions. The small time problem may be formulated as follows. Note that the mid-point and Λ_0 boundary conditions may be combined into a single statement, $\mathcal{M}_t(x') = x$.

Definition 1.

(i) *In the Schrödinger problem, set*

$$\mathcal{M}_t(x') = \tilde{M}_t(x') \equiv \frac{1}{2} [g(t|x' - \frac{1}{2}J\nabla\Phi_0(x')) + (x' + \frac{1}{2}J\nabla\Phi_0(x'))] = x. \tag{3.13}$$

(ii) *In the Heisenberg problem, set*

$$\mathcal{M}_t(x') = M_t(x') \equiv \frac{1}{2} [g(t|x' - \frac{1}{2}J\nabla S_0(x')) + g(t|x' + \frac{1}{2}J\nabla S_0(x'))] = x. \tag{3.14}$$

The initial phase $\beta_0(x)$ in the extended Schrödinger problem is equal to either $\Phi_0(x)$ or $S_0(x)$ depending on whether one has case (i) or (ii). Here it is assumed that the support of $\beta_0(x)$ is all of \mathbb{R}^{2n} , and that x is any point in \mathbb{R}^{2n} . If the non-linear function \mathcal{M}_t is invertible, then the BC problem has a single trajectory specified by the initial values, $x_0(t, x) = \mathcal{M}_t^{-1}(x)$ and $y_0(t, x) = \nabla\beta_0(x_0(t, x))$.

Proposition 1. *Let the Hessians $H''(x)$ and $\beta_0''(x)$ have x -uniform bounds*

$$\|H''(x)\| \leq c_1 < \infty \quad \|\beta_0''(x')\| \leq 2 \tag{3.15}$$

then there exists a $t_1 > 0$ such that the mid-point map $\mathcal{M}_t : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ is a diffeomorphism for $t \in [-t_1, t_1]$. Specifically, $x_0(t, x) = \mathcal{M}_t^{-1}(x)$ is a unique $C^1([-t_1, t_1], \mathbb{R}^{2n})$ solution of the BC problems (i) and (ii), respectively.

Proof. Consider the Heisenberg problem. For parameters $(t, x) \in ([-T, T], \mathbb{R}^{2n})$, define the family of maps $T_{t,x} : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$,

$$T_{t,x}(x') \equiv x + x' - M_t(x').$$

The idea of the proof is to show that $T_{t,x}$ is a contraction mapping. Its unique fixed point, $x^*(t, x)$, obeys $x = M_t(x^*(t, x))$ and establishes that M_t is invertible. Connect an arbitrary pair of points (x_1, x_2) by the linear path $x(\xi) = x_1 + \xi(x_2 - x_1)$. Integrate $dT_{t,x}(x(\xi))/d\xi$ on $\xi \in [0, 1]$ to show

$$|T_{t,x}(x_2) - T_{t,x}(x_1)| \leq |x_2 - x_1| \int_0^1 \|\nabla T_{t,x}(x(\xi))\| d\xi.$$

Whenever the integral above is less than one for all (x_1, x_2) , then $T_{t,x}$ is a contraction mapping. Taking the x' gradient of $T_{t,x}(x')$ it follows that

$$\begin{aligned} \|\nabla T_{t,x}(x')\| &\leq \frac{1}{2} [\|I - \nabla g(t|l')\| + \|I - \nabla g(t|r')\| + \frac{1}{2} \|\nabla g(t|l') - \nabla g(t|r')\| \|S_0''(x')\|] \\ &< 2(\exp c_1|t| - 1). \end{aligned}$$

To obtain the final inequality, $\|S_0''(x')\|$ was replaced by its bound 2, and the lemma 7 estimates of the Jacobi field ∇g were employed. Let $t_1 > 0$ satisfy $2(\exp(c_1 t_1) - 1) < 1$, then for times $|t| \leq t_1$ the rightmost combination above is less than one and $T_{t,x}$ is a contraction mapping for $(t, x) \in [-t_1, t_1] \times \mathbb{R}^{2n}$. An application of the implicit function theorem to $M_t(x_0(t, x)) = x$ establishes that $x_0 \in C^1([-t_1, t_1], \mathbb{R}^{2n})$. The same argument applies to the Schrödinger BC problem. \square

The merit of the short time BC solution given in proposition 1 is that it is global—applicable for all $(t, x) \in [-t_1, t_1] \times \mathbb{R}^{2n}$, and so in this time interval Λ_t has a diffeomorphic x -projection. Nevertheless, the results are restrictive. Typically only a small time interval $[-t_1, t_1]$ is allowed, and the Hamiltonian and initial phase must have no more than quadratic growth as $|x| \rightarrow \infty$.

The BC problem in the large time regime has a different geometry. Let Λ_0 have an x -projection, D_0 , that is contained within some compact set of \mathbb{R}^{2n} . As Λ_t evolves away from Λ_0 , it may develop into a multi-sheeted manifold. Here, it is helpful to recall some of the terminology related to caustic behaviour of Lagrangian manifolds, $\Lambda \subseteq \mathcal{X}_2$.

Definition 2. A point $m \in \Lambda$ is non-singular if it has a neighbourhood that is diffeomorphically projected onto \mathbb{R}^{2n} . If the opposite holds, it is singular. The set $\Sigma(\Lambda)$, of all singular points, is called the cycle of singularities. Its complement is the regular set, $\mathcal{R} = \Lambda / \Sigma(\Lambda)$.

Definition 3. The x projection of the cycle of singularities is the caustic or focal set, $\Pi_1(\Sigma(\Lambda)) = \mathcal{K}(\Lambda)$. Let $D_t = \Pi_1 \Lambda_t$ denote the x -image of Λ_t , and $\mathcal{K}(\Lambda_t)$ the associated caustic set. The non-focal set is defined as the complement of the caustic set, $\mathcal{N}_t = D_t / \mathcal{K}(\Lambda_t)$.

If Λ_t has more than one sheet, the inverse of projection $\Pi_1 : \Lambda_t \rightarrow D_t$ ceases to be single valued: there are $x \in \mathcal{N}_t$ with multiple pre-images, $\{m^j\}_1^N \subseteq \Lambda_t$, satisfying $\Pi_1 m^j = x$. The result below is stated for the Heisenberg BC problem, with obvious adjustment it applies to the Schrödinger problem.

Proposition 2. Let $\tilde{x} \in \mathcal{N}_t \subseteq D_t$ be a non-focal point with pre-images $\{m^j \in \Lambda_t\}_1^N$. Then the Heisenberg BC problem has solutions

$$M_t(x_0^j(t, x)) = x \quad j = 1, \dots, N.$$

The functions, $x_0^j(t, x)$, are smooth and have support in a neighbourhood, $\mathcal{N}_t \subseteq \tilde{U}_j \ni \tilde{x}$.

Proof. Let $F_t(x', x) = M_t(x') - x$, where F_t is smooth on the domain $(x', x) \in D_0 \times \mathcal{N}_t$. The implicit function theorem (IFT) solutions generated from $F_t(x', x) = 0$ will construct $x_0^j(t, x)$. In order to apply the IFT one must have a solution pair (x_0, x) , where $F_t(x_0, x) = 0$

and $\det \nabla_{x'} F_t(x_0, x) \neq 0$. Consider one pre-image m^j of \tilde{x} . Each $m^j \in \Lambda_t$ has a 1–1 association with a point in D_0 , via $x_0 = \Pi_1 G(-t|m^j)$. The set (x_0, \tilde{x}) is a solution pair of F_t . It remains to show that the determinant is non-zero. Since $\tilde{x} \in \mathcal{N}_t$, lemma 8 implies that $\det \nabla M_t(x_0) \neq 0$. Furthermore $\nabla_{x'} F_t(x', x) = \nabla M_t(x')$ shows that $\det \nabla_{x'} F_t(x_0, \tilde{x}) \neq 0$. The IFT then establishes the existence of $x_0^j(t, x)$ defined on a neighbourhood, $\tilde{U}_j \ni \tilde{x}$. If $F_t \in C^p$, $p \geq 1$, then $x_0^j \in C^p$. \square

Once Λ_t has become multi-sheeted, typically the regular set \mathcal{R}_t is divided by the cycle of singularities into disjoint subsets $\{\Lambda_t^j\}_1^N$. On $\Lambda_t^j \subset \mathcal{R}_t$, the restricted projection $\Pi_1^j \Lambda_t^j \equiv D_t^j \subset \mathcal{N}_t$ is diffeomorphic. In this circumstance, $x_0^j(t, x)$ has the explicit representation

$$x_0^j(t, x) = \Pi_1 G \left(-t | \left(\Pi_1^j \right)^{-1} x \right) \quad x \in D_t^j. \tag{3.16}$$

Identity (3.16) determines $x_0^j(t, x)$ directly without requiring an IFT construction.

As is evident from $J(x, t) = \det \nabla \mathcal{M}_t(x)$, cf (3.5), the gradient structures in the BC problem determine the WKB amplitudes as functions of the left and right Jacobi fields, $\nabla g(t|l')$ and $\nabla g(t|r')$. It is of interest to find a more geometric representation of these amplitudes. This is achieved by constructing a suitable χ_2 Poisson bracket related to the BC problem. First characterize the initial manifold Λ_0 by the (independent) constraint functions

$$\zeta(x', y') = y' - \nabla \Phi_0(x') \quad \eta(x', y') = y' - \nabla S_0(x').$$

The conditions $\zeta(x', y') = 0$ and $\eta(x', y') = 0$ define Λ_0 in our two problems. A second set of functions must necessarily carry information about the \mathcal{H} dynamics. Select the mid-point flow functions $x(t|x', y')$ for this role. Then one finds

Lemma 3. *In terms of the Λ_0 constraint functions, ζ and η , the \mathcal{H}_1 and \mathcal{H}_2 amplitudes have the χ_2 Poisson bracket representation*

$$\det \nabla \tilde{M}_t(x') = \det\{x(t), \zeta\}_2(x', \nabla \Phi_0(x')) \tag{3.17}$$

$$\det \nabla M_t(x') = \det\{x(t), \eta\}_2(x', \nabla S_0(x')). \tag{3.18}$$

Proof. Consider the \mathcal{H}_2 case, an elementary calculation shows that

$$\{x(t)_\alpha, \eta_\beta\}_2(x', \nabla S_0(x')) = \frac{1}{2} \left[\nabla g(t|l') \left(I - \frac{1}{2} J S_0''(x') \right) + \nabla g(t|r') \left(I + \frac{1}{2} J S_0''(x') \right) \right]_{\alpha\beta}.$$

The expression on the right is $\nabla M_t(x')$ and the determinant of this matrix is (3.18). \square

This type of bracket representation of the amplitudes is common [19, 22] in the SPS context. The components of constraint ζ (and η) are commutative with respect to the χ_2 bracket. This involution property is a necessary and sufficient condition [24] for the manifold Λ_0 to be Lagrangian. In addition, the mid-point variables $x(t)$ are commutative.

Our boundary condition analysis is concluded by identifying a χ_1 loop structure that is created by each BC solution. These loops are constructed from two types of χ_1 line segments—chords and trajectories. The quantity $C(x_1, x_2)$ denotes the chord (the \mathbb{R}^{2n} geodesic) from x_1 to x_2 . Trajectory line segments are specified by

$$\begin{aligned} T^+(x_1, x_2) &\equiv \{g(\tau|x_1); (\tau : 0 \rightarrow t)\} & x_2 &= g(t|x_1) \\ T^-(x_1, x_2) &\equiv \{g(\tau|x_1); (\tau : 0 \rightarrow -t)\} & x_2 &= g(-t|x_1). \end{aligned}$$

The \pm labelling distinguishes between forward and backward evolution.

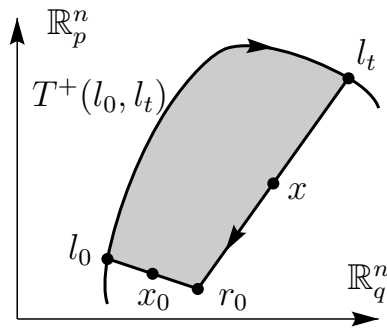


Figure 1. The Schrödinger loop.

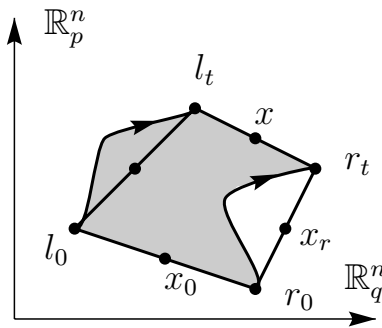


Figure 2. The Heisenberg BC solution.

Consider the Schrödinger problem with mid-point BC solution $x_0(x, t)$. The Λ_0 manifold requirement (3.10), when stated in the left–right variables, is

$$l_0(t, x) = x_0(t, x) - \frac{1}{2}J\nabla\Phi_0(x_0(t, x)) \quad r_0(t, x) = x_0(t, x) + \frac{1}{2}J\nabla\Phi_0(x_0(t, x)). \quad (3.19)$$

After time displacement t , the \mathcal{H}_1 flow moves $l_0 = l_0(t, x)$ and $r_0 = r_0(t, x)$ into the new positions $l_t = l_t(t, x) = g(t|l_0)$ and $r_t = r_t(t, x) = g(t|r_0)$, cf lemma 2(i).

The pair of points (l_t, r_0) defines the chord $C(l_t, r_0)$, having mid-point x . However, (l_t, r_0) are also the end points of the linked line segments, $C(r_0, l_0) + T^+(l_0, l_t)$. Altogether, for each $x \in \mathcal{N}_t$, one has (see figure 1) a three-sided oriented loop

$$\tilde{L}(t, x) = C(r_0, l_0) + T^+(l_0, l_t) + C(l_t, r_0).$$

Adjusting the notation above to cover the Heisenberg problem is easy. In this case, $l_0(t, x)$ and $r_0(t, x)$ are defined by (3.19) with S_0 replacing Φ_0 . The right point r_t is no longer the fixed point r_0 , but instead is $r_t = r_t(t, x) = g(t|r_0(t, x))$. The curve between r_t and r_0 is $T^-(r_t, r_0)$. The resultant BC loop is the four-segment structure (see figure 2)

$$W(t, x) \equiv C(r_0, l_0) + T^+(l_0, l_t) + C(l_t, r_t) + T^-(r_t, r_0).$$

The loop $W(t, x)$ is like the Schrödinger BC loop $\tilde{L}(t, x)$, but has an additional side $T^-(r_t, r_0)$ inserted at the point r_0 .

However, there is another simpler loop generated by the BC solution, denoted by $\gamma(t|C(r_0, l_0)) \equiv \{g(t|x') : x' \in C(r_0, l_0)\}$. This curve is the flow translated image of the chord $C(r_0, l_0)$. In general, it is no longer a straight line but it has end points (r_t, l_t) , so

$$L(t, x) \equiv C(l_t, r_t) + \gamma(t|C(r_0, l_0))$$

defines a two segment closed curve (see figure 3). We refer to $L(t, x)$ as the Heisenberg loop. Unlike the Schrödinger loop, it is localized in time and transports like a wavefront under the flow $g(t)$.

3.2. Evolution representations

Once the solution of the SPS boundary condition problem has been obtained in loop form, the induced WKB representations follow directly from Maslov’s expansion. Consider first the Heisenberg problem.

Theorem 1. *Suppose x is a non-focal point associated with the manifold Λ_t . Let $\{L^j(t, x)\}_1^N$ be the family of Heisenberg loops generated by the BC solutions $\{x_0^j(t, x)\}_1^N, x \in \mathcal{N}_t$. Then the $O(\hbar)$ approximation of $\rho(t, x)$ is*

$$\rho^{sc}(t, x) = \sum_{j=1}^N \alpha_j(t, x) \exp \left\{ \frac{i}{\hbar} S_j(t, x) - \frac{i\pi}{2} m_j(t, x) \right\} \tag{3.20}$$

$$S_j(t, x) = S_0(x_0^j(t, x)) + \oint_{L^j(t, x)} p \cdot dq \tag{3.21}$$

$$\alpha_j(t, x) = \left| \det \nabla M_t(x_0^j(t, x)) \right|^{-1/2} \alpha_0(x_0^j(t, x)). \tag{3.22}$$

Proof. Direct computation establishes this result. The $d\tau$ integral contribution to the χ_2 WKB phase in (3.4) has both a $y \cdot \dot{x}$ and a \mathcal{H}_2 contribution. The first of these is

$$\int_0^t y(\tau) \cdot \dot{x}(\tau) d\tau = \frac{1}{2} \int_0^t [\dot{g}(\tau|l_0) + \dot{g}(\tau|r_0)] \cdot J [g(\tau|l_0) - g(\tau|r_0)] d\tau \tag{3.23}$$

$$= \oint_{W(t, x)} p \cdot dq. \tag{3.24}$$

The top equality is the result of lemma 2(ii). The lower equality follows from an integration by parts. For example

$$\int_0^t \dot{g}(\tau|l_0) \cdot J g(\tau|l_0) d\tau = 2 \int_0^t p(\tau|l_0) \cdot \dot{q}(\tau|l_0) d\tau + (q_0^l \cdot p_0^l - q_t^l \cdot p_t^l)$$

where $(q_0^l, p_0^l) = l_0$ and $(q_t^l, p_t^l) = l_t$. The $d\tau$ integral is that of $p \cdot dq$ over the curve $T^+(l_0, l_t)$. The sum of all the surface terms from (3.23) is just the integral over the two chords, $C(r_0, l_0) + C(l_t, r_t)$. Thus one has that the time integral (3.23) is the loop integral (3.24).

The $\mathcal{H}_2 d\tau$ term may be rewritten in loop form by employing the Poincaré–Cartan identity in lemma 9. Setting the initial curve to be $\gamma_0 = C(r_0, l_0)$, identity (B.1) is

$$(H(l_0) - H(r_0))t = \oint_{C(r_0, l_0) + T^+(l_0, l_t) + g(t|C(l_0, r_0)) + T^-(r_t, r_0)} p \cdot dq.$$

Adding all the loop integrals gives (3.21).

The amplitude expressions result from $M_t(x_0^j(t, x)) = x$ and the fact that the exponentiated integral in (3.6) vanishes. This latter is a consequence of $\text{Tr} \nabla_x \nabla_y H \circ l = \text{Tr} H''(-\frac{1}{2}J) = 0$, etc. \square

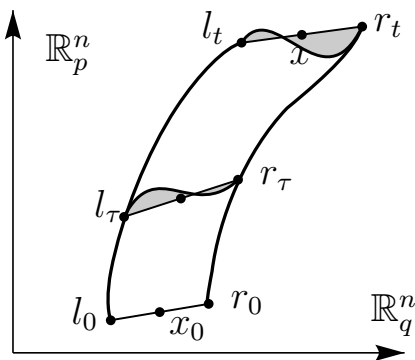


Figure 3. Heisenberg loop area $L(t, x)$.

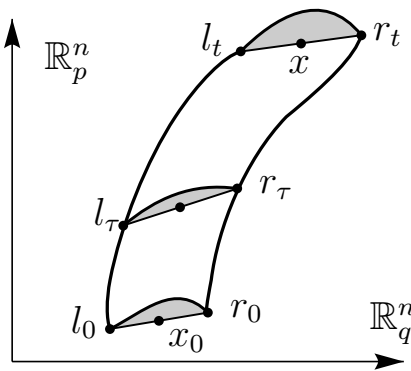


Figure 4. $S(t, x)$ as an evolving front.

The area representation of $S(t, x)$ (see figure 4) is a consequence of Stokes' theorem,

$$S(t, x) = S_0(x_0(t, x)) + \int_{\sigma(L(t, x))} dq \wedge dp. \quad (3.25)$$

Above, $\sigma(L(t, x))$ denotes any oriented surface with boundary $L(t, x)$. The specific form of (3.25) resulted from choosing the γ_0 curve to be $C(r_0, l_0)$. Other natural choices for the curve connecting r_0 and l_0 do occur. Consider the problem where $\rho_0(x)$ is given by the projection operator $\hat{\rho}_0 = |\psi_0\rangle\langle\psi_0|$. As was noted in section 2 the initial phase function $S_0(x)$ is the $C(l_0, r_0) + \gamma_\lambda(r_0, l_0)$ loop integral (2.13). By choosing $\gamma_0 = \gamma_\lambda(r_0, l_0)$ in identity (B.1) one can incorporate the initial phase into the final loop integral. So for this particular initial state, the entire Heisenberg phase has the form of a symplectic area

$$S(t, x) = \int_{\sigma(L'(t, x))} dq \wedge dp$$

where $L'(t, x) = g(t|\gamma_\lambda(r_0, l_0)) + C(l_t, r_t)$.

A symmetry that is specific to Heisenberg evolution is \hbar parity. Recall that, cf (2.9), the symbol $\rho_0(x; \hbar)$ for the initial state $\hat{\rho}_0 = |\psi_0\rangle\langle\psi_0|$ is an even function of \hbar . For most problems of physical interest, this \hbar -even property is maintained under time evolution. In detail, one has

Lemma 4 (Evolution \hbar -parity). *Suppose the real-valued $H(x; \hbar)$ and $\rho_0(x; \hbar)$ have even \hbar parity. Then the solution of (1.2), $\rho(t, x)$, is real and has even \hbar parity. The associated semiclassical expansion has the improved convergence*

$$\begin{aligned} \rho(t, x) &= \rho^{sc}(t, x)[1 + O(\hbar^2)] \\ \rho^{sc}(t, x) &= \sum_{j=1}^N \alpha_j(t, x) 2 \cos \left[S_j(t, x)/\hbar - \frac{\pi}{2} m_j(t, x) \right]. \end{aligned}$$

Proof. The function $\rho(t, x) = \rho(t, x; \hbar)$ is defined as the unique solution of (1.2). Since the Moyal bracket and $H(x; \hbar)$ are \hbar even, the equation of motion (1.2) is invariant under $\hbar \rightarrow -\hbar$. Because initial state $\rho_0(x; \hbar)$ is even it follows that $\rho(t, x; \hbar)$ is \hbar even. \square

The WKB representation for $U(t, x)$ is constructed by the same style of SPS argument employed for theorem 1.

Theorem 2. *Suppose x is a non-focal point associated with the manifold Λ_t . Let $\{\tilde{L}^j(t, x)\}_1^N$ be the family of loops generated by the Schrödinger BC solutions $\{x_0^j(t, x)\}_1^N$, $x \in \mathcal{N}_t$. Then the $O(\hbar)$ approximation of $U(t, x)$ is*

$$U^{sc}(t, x) = \sum_{j=1}^N N_j(t, x) \exp \left\{ \frac{i}{\hbar} \Phi_j(t, x) - \frac{i\pi}{2} m_j(t, x) \right\} \quad (3.26)$$

$$\Phi_j(t, x) = \Phi_0(x_0^j(t, x)) + \oint_{\tilde{L}^j(t, x)} p \cdot dq - H(l_0^j(t, x))t \quad (3.27)$$

$$N_j(t, x) = \left| \det \nabla \tilde{M}_t(x_0^j(t, x)) \right|^{-1/2} N_0(x_0^j(t, x)). \quad (3.28)$$

Lemma 8 establishes that the amplitudes $N_j(t, x)$ and $\alpha_j(t, x)$ are finite for all $x \in \mathcal{N}_t$. When $x \in \mathcal{K}(\Lambda_t)$ the amplitudes diverge and the representations of theorems 1 and 2 are not applicable at these caustic points. If x is not in D_t , it is classically forbidden. In this sector, $U(t, x)$ and $\rho(t, x)$ are $O(\hbar^\infty)$.

Let us clarify how theorem 2 matches the results derived by Marinov [17]. An important special case occurs in the problem where $U(0, x) = 1$. Here $\Phi_0 \equiv 0$ and $\Lambda_0 \subseteq \mathbb{R}_x^{2n}$. In particular, $l_0 = x_0 = r_0$, so the loop $\tilde{L}^j(t, x)$ simplifies into one chord $C(l_t, l_0)$ with mid-point x and one dynamical curve $T^+(l_0, l_t)$ connecting the chord end points, cf figure 7. If Λ_t has one sheet, then $N = 1$, and the theorem above gives the representation found in [17]. However, it should be noted that Marinov did not investigate the BC problem. Instead, his approach was to construct the phase $\Phi = \Phi_1(t, x)$ by solving the Hamilton–Jacobi (HJ) equation associated [15, 17, 25] with the evolution problem (1.1),

$$\partial_t \Phi(t, x) + H\left(x - \frac{1}{2} J \nabla \Phi(t, x)\right) = 0 \tag{3.29}$$

with the Cauchy initial data $\Phi(0, x) = 0$. Because of the highly non-linear character of $H(x)$ this HJ problem is much more difficult to solve than the BC problem (3.13) treated above. It is straightforward to verify that $\Phi(t, x)$ given by (3.27) is a solution of (3.29).

By way of contrast, the HJ equation associated with theorem 1 reads

$$\partial_t S(t, x) + H\left(x - \frac{1}{2} J \nabla S(t, x)\right) - H\left(x + \frac{1}{2} J \nabla S(t, x)\right) = 0.$$

All the $S_j(t, x)$ functions, provided by (3.21), are solutions of this Heisenberg HJ equation. As t nears 0, Λ_t will have one sheet. Its phase obeys $S(0, x) = S_0(x)$.

Marinov’s work established the central role of the symplectic phase $\Phi(t, x)$ in the semiclassical approximation of $U(t, x)$. However, knowledge of the HJ equation in the form (3.29), and the use of $\Phi(t, x)$ as the generator of a canonical transformation, cf (2.8), goes back to Poincaré [26].

The phases $\Phi(t, x)$ and $S(t, x)$ form representations of the χ_2 Lagrangian manifolds Λ_t , via $y = \nabla \Phi(t, x)$ and $y = \nabla S(t, x)$. In turn these phases define, cf (2.8), a canonical transformation between the dynamical left–right coordinates $l(t|l_0)$ and $r(t|r_0)$. The Λ_t phases also generate dynamical flow. In the Heisenberg case, one has

$$l(t|l_0) = g(t|l_0) = x - \frac{1}{2} J \nabla S(t, x) \quad r(t|r_0) = g(t|r_0) = x + \frac{1}{2} J \nabla S(t, x).$$

It is useful to review to what extent the use of the secondary phase space approach is critical in obtaining theorems 1 and 2. Marinov obtained the small time, $\Phi_0 = 0$, version of theorem 2 without using the embedding of χ_1 into χ_2 . In this approach (see [25] for related details) one starts with problem (1.1), and assumes a WKB representation for $U(t, x) \approx U^{sc}(t, x)$. After applying the definition of the $*$ product to $H * U^{sc}(t)$ the Hamilton–Jacobi equation (3.29) for $\Phi(t, x)$ is derived from the $\hbar \rightarrow 0$ limit. The transport equations for amplitudes $N(t, x)$ are obtained from (1.1) by extracting the ordinary differential equations generated by the higher order \hbar term identities. A similar approach would work for the $\rho(t, x)$ problem. What this strictly primary phase space approach misses is the recognition of the Lagrangian manifold Λ_t as the geometric structure that determines the Schrödinger and Heisenberg WKB expansions. Given the SPS setting, one can make the WKB representations global by following Maslov’s approach. In theorems 1 and 2 the base Lagrangian plane was always taken to be \mathbb{R}_x^{2n} with commutative coordinates $\{x_\alpha\}_1^{2n}$. The caustic and non-diffeomorphic behaviour of the Π_1 projection is avoided by replacing Π_1 by a different and non-singular projection: $\Pi^* \Lambda_t = \Lambda^*$. Here Λ^* is a new Lagrangian plane with mixed (but commuting) coordinates $\{x_{\alpha(i)}, y_{\beta(i)} : i = 1, \dots, 2n\}$. A related point concerns the amplitude representations. In the SPS setting, the amplitudes are determinants of a Poisson bracket formed from the constraints that define the initial Lagrangian manifold, Λ_0 .

4. Applications and examples

In this section, we collect various interpretations, extensions and applications of theorems 1 and 2. For example, in both the Schrödinger and Heisenberg pictures, the time evolution is

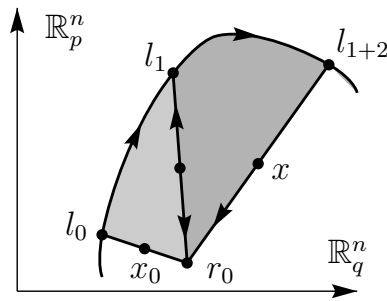


Figure 5. Schrödinger loop addition.

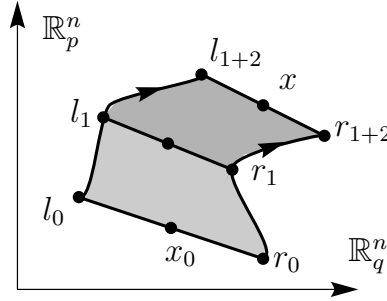


Figure 6. Heisenberg loop addition.

implemented by a one-parameter group. Define $\Gamma(t)\hat{\rho}_0 \equiv U(t)\hat{\rho}_0U(t)^\dagger$. These two group properties are $U(t_1 + t_2) = U(t_1)U(t_2)$ and $\Gamma(t_1 + t_2) = \Gamma(t_1) \circ \Gamma(t_2)$, respectively. What are the symplectic phase identities generated by these groups? Another question of interest is to establish the mutual consistency of the $U^{sc}(t, x)$ and $\rho^{sc}(t, x)$ approximations.

The systems (1.1) and (1.2) admit exact solutions if the Hamiltonians are quadratic. In this special case, the contrasting behaviour of $U(t, x)$ and $\rho(t, x)$ is explored. Finally, we show how the semiclassical solutions of (1.2) behave when $\rho_0(x)$ is not a rapidly oscillating function of \hbar .

4.1. Phase additivity identities

Phase additivity identities, mirroring the group properties of $U(t)$ and $\Gamma(t)$, are a direct consequence of the loop structure of the BC problem. Denote the BC loop integrals by

$$\varphi(t, x; \tilde{L}) = \oint_{\tilde{L}(t,x)} p \cdot dq \quad \mathcal{A}(t, x; W) = \oint_{W(t,x)} p \cdot dq.$$

First, consider the Schrödinger problem. Let t_1 and t_2 be successive time displacements. For $x \in \mathcal{N}_{t_1+t_2}$ the BC solution determines $x_0(t_1 + t_2, x)$ (where the j label is suppressed). The loop for the full time interval is

$$\tilde{L}_{1+2}(t_1 + t_2, x) \equiv T^+(l_0, l_{1+2}) + C(l_{1+2}, r_0) + C(r_0, l_0).$$

Here $l_{1+2} = g(t_1 + t_2|l_0)$. As figure 5 shows this loop can be decomposed into the sum of two (or more) sub-loops defined for t_1 and t_2 , e.g. $l_1 = g(t_1|l_0)$. Let \tilde{L}_1 and \tilde{L}_2 be the loops with end points (l_0, l_1, r_0) and (l_1, l_{1+2}, r_0) . It follows from their definitions that these loops are additive,

$$\tilde{L}_{1+2}(t_1 + t_2, x) = \tilde{L}_1(t_1, x_1) + \tilde{L}_2(t_2, x) \quad x_1 = \frac{1}{2}(l_1 + r_0).$$

As figure 6 makes clear there is a corresponding loop additivity in the Heisenberg BC problem. Using the phase definitions above, one obtains the following.

Proposition 3. *Let $x \in \mathcal{N}_{t_1+t_2}$ and suppose $\tilde{L}_{1+2}^j = \tilde{L}_1^j + \tilde{L}_2^j$; $W_{1+2}^j = W_1^j + W_2^j$ are loop decompositions consistent with the BC solutions $\tilde{M}_{t_1+t_2}^j(x_0^j(t_1 + t_2, x)) = x$ and $M_{t_1+t_2}^j(x_0^j(t_1 + t_2, x)) = x$, $j = 1, \dots, N$, then*

$$\varphi(t_1 + t_2, x; \tilde{L}_{1+2}^j) = \varphi(t_1, x_1^j; \tilde{L}_1^j) + \varphi(t_2, x; \tilde{L}_2^j) \tag{4.1}$$

$$\mathcal{A}(t_1 + t_2, x; W_{1+2}^j) = \mathcal{A}(t_1, x_1^j; W_1^j) + \mathcal{A}(t_2, x; W_2^j). \tag{4.2}$$

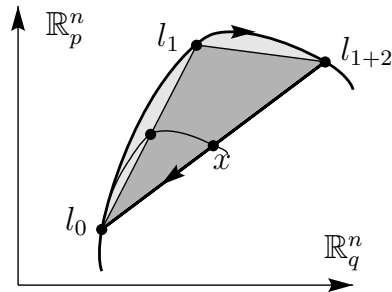


Figure 7. Marinov loop addition.

Consider the short time regime where proposition 1 holds. Let $\Phi_0 = 0$ and $x_0(\tau, x) = \tilde{M}_\tau^{-1}(x)$ be the BC solution. In this sector, it is possible to compare rule (4.1) with the phase addition formula established by Marinov [17].

First we need expressions for the area of polygons in $T^*\mathbb{R}^n_x$. Let the successive end points (l_1, l_2, \dots, l_N) define a loop L_N having midpoints (x_1, x_2, \dots, x_N) , then its area is

$$P_N(x_1, x_2, \dots, x_N) = 2 \sum_{i=1}^{N-1} \sum_{j>i}^N (-1)^{i+j+1} x_i \wedge x_j \quad x_i \wedge x_j = x_i \cdot Jx_j.$$

The triangle area P_3 appears in the Berezin integral representation [27] of $f_1 * f_2$, and the area P_N is the phase required for the higher order $*$ products [23]. The phase P_N is a cyclically invariant function of (x_1, x_2, \dots, x_N) .

Denote by $X(\tau, x)$ the two segment loops $T^+(x_0, g(\tau|x_0)) + C(g(\tau|x_0), x_0)$, where $x_0 = l_0 = \tilde{M}_\tau^{-1}(x)$. Suppose $\varphi(\tau, x; X)$ is the corresponding loop phase. In terms of these two-sided figures, see figure 7, the loop additivity is realized by

$$X_{1+2}(t_1 + t_2, x) = X_1(t_1, x_1) + X_2(t_2, x_2) + C(l_0, l_1) + C(l_1, l_2) + C(l_2, l_0).$$

The implied phase additivity now reads

$$\varphi(t_1 + t_2, x; X_{1+2}) = \varphi(t_1, x_1; X_1) + \varphi(t_2, x_2; X_2) + P_3(x, x_1, x_2). \tag{4.3}$$

Equation (4.3) is the version of additivity found by Marinov. The use of two-sided loops X , rather than the three-sided loops \tilde{L} , accounts for the extra triangular area P_3 .

A somewhat similar additivity links the Schrödinger and Heisenberg phases with each other. On the left branch of figure 2, $\varphi(t, x_l; X_l)$ is defined by a two-sided loop, $X_l(t, x_l) = T^+(l_0, l_t) + C(l_t, l_0)$. Similarly, $\varphi(t, x_r; X_r)$ is the right branch area defined by $X_r(t, x_r) = T^+(r_0, r_t) + C(r_t, r_0)$. Recall that the four-chord loop with midpoints (x, x_r, x_0, x_l) has symplectic area $P_4(x, x_r, x_0, x_l)$. With this notation, one has

Proposition 4. For $x \in \mathcal{N}_t$ let (x, x_r^j, x_0^j, x_l^j) be the midpoints of the Heisenberg BC loop solution $\{W^j(t, x)\}_1^N$. Then

$$\mathcal{A}(t, x; W^j) = \varphi(t, x_l^j; X_l^j) - \varphi(t, x_r^j; X_r^j) + P_4(x, x_r^j, x_0^j, x_l^j) \quad j = 1, \dots, N. \tag{4.4}$$

Proof. This follows directly from the loop decomposition

$$\begin{aligned} W(t, x) &= C(r_0, l_0) + T^+(l_0, l_t) + C(l_t, r_t) + T^-(r_t, r_0) \\ &= X(t, x_l) - X(t, x_r) + C(r_0, l_0) + C(l_0, l_t) + C(l_t, r_t) + C(r_t, l_0). \end{aligned}$$

□

4.2. Mutual consistency of $U^{sc}(t)$ and $\rho^{sc}(t)$

One may build the Heisenberg evolution $\rho(t, x)$ from its Schrödinger components, via $\rho(t, x) = U(t) * \rho_0 * \overline{U(t)}$. The goal of this subsection is to show that the use of the approximation $U(t, x) \approx U^{sc}(t, x)$ combined with the evaluation of the $*$ product by the stationary phase approximation constructs $\rho^{sc}(t, x)$. This calculation will be carried out using the single sheet BC solutions found in proposition 1. All the amplitudes and phases of $U^{sc}(t, x)$ and $\rho^{sc}(t, x)$ will be written without the multi-sheet subscript, j . This type of composition argument was used to construct $\rho^{sc}(t, x)$ in the one-dimensional case [28] and recently extended to \mathbb{R}_q^n in [29, 30].

First, observe that the required form of the $U^{sc}(t, x)$ is the Marinov version obeying the initial condition $U(t, x) = 1$. Since $\Phi_0 = 0$, the amplitude takes the simplified form

$$N(t, x) = \left[\det \frac{1}{2} (1 + \nabla g (t | \tilde{M}_t^{-1}(x))) \right]^{-1/2}. \quad (4.5)$$

Employing the three function $*$ product [23, 31], the approximate $\rho(t, x)$ is

$$\begin{aligned} \left[U^{sc}(t) * \rho_0 * \overline{U^{sc}(t)} \right] (x) &\equiv \mathcal{I}(t, x) \\ &= c \int U^{sc}(t, x_1) \rho_0(x_2) \overline{U^{sc}(t, x_3)} \delta(x_1 - x_2 + x_3 - x) e^{iP_3(x_1, x_2, x_3)/\hbar} dx_1 dx_2 dx_3 \\ &= c \int N(t, x_1) N(t, x_3) \alpha_0(x_2) e^{i[\varphi(t, x_1) - \varphi(t, x_3) + S_0(x_2) + P_3(x_1, x_2, x_3)]/\hbar} dx_1 dx_3 \end{aligned} \quad (4.6)$$

where $x_2 = x_1 + x_3 - x$ and $c = (\pi\hbar)^{-2n}$.

Denote the total phase in (4.6) by

$$\Theta(x_1, x_3; t, x) = \varphi(t, x_1) - \varphi(t, x_3) + S_0(x_1 + x_3 - x) + P_3(x_3, x, x_1). \quad (4.7)$$

Let $\xi = (x_1, x_3)$ and $\Theta''(\xi; t, x)$ be the Hessian of Θ with respect to the ξ variables. If $x_1 = x_1(t, x)$ and $x_3 = x_3(t, x)$ is an isolated non-degenerate critical point of Θ , i.e. the solution of $\nabla_\xi \Theta(\xi; t, x) = 0$, then the standard [7] stationary phase approximation to (4.6) states

$$\begin{aligned} \mathcal{I}^{sph}(t, x) &= 2^{2n} N(t, x_1) N(t, x_3) \alpha_0(x_2) |\det \Theta''(x_1, x_3; t, x)|^{-1/2} \\ &\quad \times \exp \left[\frac{i}{\hbar} \Theta(x_1, x_3; t, x) + \frac{i\pi}{4} \operatorname{sgn} \Theta''(x_1, x_3; t, x) \right]. \end{aligned} \quad (4.8)$$

Above, the functional form of the constraint condition is $x_2(t, x) = x_1(t, x) + x_3(t, x) - x$.

In component form, the critical point equation reads

$$x_1 = x + \frac{1}{2} J \nabla \varphi(t, x_3) - \frac{1}{2} J \nabla S_0(x_1 + x_3 - x) \quad (4.9)$$

$$x_3 = x + \frac{1}{2} J \nabla \varphi(t, x_1) + \frac{1}{2} J \nabla S_0(x_1 + x_3 - x). \quad (4.10)$$

For small times and under the same assumptions as proposition 1, one can show that the system above defines a contraction mapping and so has unique global solution $x_1 = x_1(t, x)$, $x_3 = x_3(t, x)$. In fact, the set of points $\{x_2(t, x), x_1(t, x), x, x_3(t, x)\}$ are exactly the four midpoints $\{x_0, x_l, x, x_r\}$ appearing in figure 2. The constraint condition for x_2 ensures that $P_3(x_3, x, x_1) = P_4(x_3, x, x_1, x_2)$. Substituting these critical point arguments into the total phase and using proposition 4, one has

$$\Theta(x_1(t, x), x_3(t, x); t, x) = S(t, x).$$

This demonstrates that the stationary phase produced by $U^{sc}(t) * \rho_0 * \overline{U^{sc}(t)}$ is the same as the Heisenberg WKB phase $S(t, x)$.

Verifying amplitude consistency is more elaborate. A non-trivial determinant identity for Θ'' in terms of the individual left–right flows is needed. Let $K_l = \nabla g(t|l)$, $l = x_2(t, x) - \frac{1}{2}\nabla JS_0(x_2(t, x))$ and $K_r = \nabla g(t|r)$, $r = x_2(t, x) + \frac{1}{2}\nabla JS_0(x_2(t, x))$. Using identities obtained from (4.9)–(4.10) one can establish [29]

$$\det \Theta''(x_1(t, x), x_3(t, x); t, x) = 2^{6n} (\det(1 + K_l)(1 + K_r))^{-1} \det \left[K_l \left(1 - \frac{1}{2}JS_0''(x_2) \right) + K_r \left(1 + \frac{1}{2}S_0''(x_2) \right) \right]. \tag{4.11}$$

Putting (4.11) into (4.8) recovers the Heisenberg amplitude $\alpha(t, x)$. In the small time sector, all the determinants above are positive and $\text{sgn}\Theta''(x_1, x_3; t, x) = 0$. Altogether, one has the identity

$$\left[U^{sc}(t) * \rho_0 * \overline{U^{sc}(t)} \right]^{stph} (t, x) = \rho^{sc}(t, x). \tag{4.12}$$

The approximate calculation of $\rho(t)$ based on $U^{sc}(t) * \rho_0 * \overline{U^{sc}(t)}$ can be utilized as a stand alone derivation of $\rho^{sc}(t)$. This is the approach adopted in [30]. Once the form of $U^{sc}(t)$ is given, this computation makes no use of the space χ_2 . In the regions where $U^{sc}(t, x)$ is multi-sheeted and the critical point equations (4.9), (4.10) do not define a contraction mapping, a rigorous implementation of the stationary phase analysis can be expected to be cumbersome.

4.3. Quadratic exactness

If the Hamiltonian is a quadratic function, then the semiclassical quantities $U^{sc}(t, x)$ and $\rho^{sc}(t, x)$ are exact solutions of (1.1) and (1.2). Thus it is of interest to obtain the explicit formulae for the phases and amplitudes which arise in this special case.

The general time-dependent Weyl symbol Hamiltonian of quadratic form is

$$H(t, x) = \frac{1}{2}x \cdot H''(t)x + H'(t) \cdot x$$

where $H''(t)$ is a $2n \times 2n$ symmetric matrix and $H'(t)$ is a $2n$ -component vector. Both $H''(t)$ and $H'(t)$ are real and t -continuous. The quantum Hamiltonian, $\hat{H}(t)$, results if x is replaced by \hat{x} in $H(t, x)$.

The classical trajectories $g(t, s|x)$ generated by a quadratic $H(t, x)$ are linear functions of x . Explicit representations of $g(t, s|x)$ are obtained as follows.

The dynamical equations for $g(t, s|x)$ and $\nabla g(t, s|x)$ are the linear ODEs,

$$\frac{d}{dt}g(t, s|x) = JH''(t)g(t, s|x) + JH'(t) \tag{4.13}$$

$$\frac{d}{dt}\nabla g(t, s|x) = JH''(t)\nabla g(t, s|x) \tag{4.14}$$

with initial conditions $g(s, s|x) = x$ and $\nabla g(s, s|x) = I$. Both (4.13) and (4.14) are Jacobi field equations, but (4.14) is homogeneous while (4.13) has an inhomogeneity $JH'(t)$. Let $K(t, s)$ be the $Sp(2n)$ solution of

$$\frac{d}{dt}K(t, s) = JH''(t)K(t, s) \quad K(s, s) = I. \tag{4.15}$$

The solution of the system (4.15) is unique, which implies that $\nabla g(t, s|x) = K(t, s)$. In terms of $K(t, s)$, the forward ($t > s$) and backward ($s < t$) flows are

$$g(t, s|x) = K(t, s)[x + F(t, s)] \tag{4.16}$$

$$g(s, t|x) = K(s, t)x - F(t, s) \tag{4.17}$$

$$F(t, s) = \int_s^t d\tau JK(\tau, s)^T H'(\tau) \quad t \geq s. \tag{4.18}$$

The solution (4.16) is verified by putting it into (4.13) and using the symplectic identity $K(t, s)JK(t, s)^T = J$. From (4.16) one obtains (4.17) by using the composition laws $g(t, s) \circ g(s, t) = Id$ and $K(s, t)K(t, s) = I$.

The behaviour of the Heisenberg evolution is summarized in the following lemma. Note that for time-dependent Hamiltonians the boundary condition problem needs to be stated in terms of $g(t, s)$. So the left-hand side of (3.14) has two times, e.g. $M_{t,s}(x')$.

Lemma 5. *For quadratic Hamiltonians the semiclassical density matrix is the exact solution of (1.2), $\rho^{sc}(t, x) = \rho(t, x)$. The structure of $\rho^{sc}(t, x)$ is given by*

(i) *the BC problem $M_{t,s}(x_0(t, x)) = x$ has a unique global solution given by the backward flow*

$$x_0(t, x) = K(s, t)x - F(t, s) \quad (4.19)$$

(ii)

$$S(t, x) = S_0(x_0(t, x)) \quad \det \nabla M_{t,s}(x') = 1 \quad (4.20)$$

(iii)

$$\rho^{sc}(t, x) = \rho_0(x_0(t, x)) e^{iS_0(x_0(t, x))/\hbar}. \quad (4.21)$$

Proof. The x -linearity of (4.16) combined with (3.14) implies $M_{t,s}(x') = g(t, s|x')$. Since $g(t, s)$ has inverse $g(s, t)$, (4.19) holds. The phase identity in (4.20) follows from the fact that chords evolve into chords, specifically $g(t, s|C(l_0, r_0)) = C(l_t, r_t)$. For this reason, the Heisenberg loop $L(t, x)$ collapses to zero, so that all the WKB phase resides in the S_0 term. The determinant identity is a consequence of $\nabla M_{t,s}(x')$ being a symplectic matrix. That $\rho^{sc}(t, x) = \rho(t, x)$ is verified by direct substitution into (1.2). \square

The x, y representation of the manifold Λ_t is

$$y(t, x) = \nabla S_0(K(s, t)x - F(t, s))K(s, t).$$

This formula shows that Λ_t is single sheeted. The determinant identity in (ii) establishes that Λ_t is non-singular for all t .

Next consider Schrödinger evolution. Let $\sigma(s) \equiv \{t \in \mathbb{R} | \det(K(t, s) - I) = 0\}$ denote the set of caustic times where the amplitude function of $U^{sc}(t, x)$ diverges. The behaviour of Schrödinger evolution is summarized below. These are known results [17, 32, 33] and their proof parallels that of lemma 5.

Lemma 6. *For quadratic Hamiltonian Schrödinger systems with initial data $U(0, x) = 1$, the semiclassical solution of (1.1) is exact at all non-caustic times. The structure of $U^{sc}(t, x) = U(t, x)$ for $t \in \mathbb{R}/\sigma(s)$ is given by*

(i) *the BC problem $\tilde{M}_{t,s}(x_0(t, x)) = x$ has a solution given by*

$$x_0(t, x) = (K(t, s) + I)^{-1}(2x - F(t, s)) \quad (4.22)$$

(ii)

$$N(t, x_0) = 2^n |\det[K(t, s) + I]|^{-1/2} \quad (4.23)$$

(iii)

$$\Phi(t, x) = -x \cdot J \frac{K(t, s) - I}{K(t, s) + I} x - 2J \frac{K(t, s)}{K(t, s) + I} F(t, s)x + C_0(t, s) \quad (4.24)$$

where $C_0(t, s)$ is an x -independent constant.

The manifold Λ_t is determined by the identity

$$y(t, x) = -2J \frac{1}{K(t, s) + I} [(K(t, s) - I)x + K(t, s)F(t, s)].$$

The x -linearity of $y(t, x)$ means that Λ_t is a hyperplane. For each $t_c \in \sigma(s)$, where $K(t_c, s)$ has a -1 eigenvalue, Λ_{t_c} is singular and $|y(t_c, x)| = \infty$. As $t \rightarrow t_c$, $U^{sc}(t, x)$ has a delta function behaviour.

In comparing these Heisenberg and Schrödinger solutions, it is evident that the main difference is that $\rho(t, x)$ is always caustic free, while $U(t, x)$ has singular behaviour at $t = t_c$.

4.4. Evolution of semiclassically admissible observables

An important special case of the Heisenberg evolution occurs when the initial operator $\hat{\rho}_0$ is semiclassically admissible, and as a result $S_0 = 0$. Most observables of physical interest (energy, momentum, angular momentum and their products) are semiclassically admissible.

How does theorem 1 simplify in this case? First, note that $S_0 = 0$ implies that the initial Lagrangian manifold $\Lambda_0 = \mathbb{R}^{2n}$. Furthermore, the BC equation (3.1) becomes $M_t(x') = g(t|x) = x$, and so $M_t^{-1}(x) = g(-t|x)$ for all t, x . From this it follows that $\det \nabla M_t(x') = 1$ and so there are no caustics. Since $S_0 = 0$, the left, right and mid-point BC solutions are the same $x_0(t, x) = l_0(t, x) = r_0(t, x)$. This means that the left, right and mid-point flows collapse to a common trajectory and as a result the Heisenberg loop $L(t, x)$ reduces to a point. As a consequence, $S(t, x) = 0$. Altogether one has

$$\rho^{sc}(t, x) = \rho_0(g(-t|x)). \quad (4.25)$$

This simple transport expression for $\rho^{sc}(t, x)$ is the point of departure [9–13] for higher order \hbar expansions of $\rho(t, x)$. Identity (4.25) is an example of Egorov's theorem [34].

The fact that $S(t, x)$ remains zero is in marked contrast to the behaviour of $U^{sc}(t, x)$ where the phase $\Phi(t, x)$ spontaneously becomes non-zero even if its $t = 0$ value vanishes. This Heisenberg null phase stability is a consequence of the symmetry $\mathcal{H}_2(x, y) = -\mathcal{H}_2(x, -y)$. In turn, this symmetry means that $y(t) = y_0$ is a constant of motion for χ_2 trajectories that have initial value $(x_0, y_0) = (x_0, 0)$. Equivalently, $\Lambda_t = \Lambda_0$.

5. Conclusions

The representations of operators by Weyl symbols give one a complete statement of quantum mechanics set in phase space. The Wigner transform is a Lie algebra isomorphism between operators (with commutator bracket) and symbols (with Moyal bracket). In this formalism, the Schrödinger and Heisenberg evolutions, $U(t, x)$ and $\rho(t, x)$, are generated by Hamiltonians that are pseudodifferential operators. These two problems are made amenable to semiclassical approximation by embedding them in an extended phase space $\chi_2 = T^*\chi_1$. Set in χ_2 , the two evolution problems become special cases of an extended Schrödinger evolution.

The geometry of the WKB approximation is controlled by Λ_t , the dynamical Lagrangian manifold in χ_2 . The associated BC problem is solved in terms of loops built from chords and trajectories in PPS. The symplectic area of these loops forms the WKB phase functions. The amplitudes are χ_2 Poisson brackets constructed from the family of constraints that define the initial BC Lagrangian manifold, Λ_0 .

An alternate characterization of Heisenberg evolution in symbol space is found in Marinov's [31] path integral representation of $\rho(t, x)$. This path integral has the following structure. Write the mapping $\rho_0(x) \mapsto \rho(t, x)$ in terms of an integral transform

$$\rho(t, x) = \int dx' K(t; x, x') \rho_0(x') \quad (5.1)$$

where the kernel K is $h^{-n} \text{Tr}[U(t)\Delta(x')U(t)^\dagger\Delta(x)]$. Define an action functional by

$$\mathcal{S}(t; \tilde{x}, \tilde{y}) = \int_0^t d\tau \left[\tilde{y}(\tau) \cdot \dot{\tilde{x}}(\tau) - \mathcal{H}(\tilde{x}(\tau) - \frac{1}{2}J\tilde{y}(\tau)) + \mathcal{H}(\tilde{x}(\tau) + \frac{1}{2}J\tilde{y}(\tau)) \right].$$

The path functions $\tilde{x}(\tau)$ obey the boundary conditions, $\tilde{x}(0) = x'$ and $\tilde{x}(t) = x$, while the functions $\tilde{y}(\tau)$ are unrestricted. Then K is the path integral,

$$K(t; x, x') = h^{-n} \iint D\tilde{x} D\tilde{y} e^{i\mathcal{S}(t; \tilde{x}, \tilde{y})/\hbar}. \quad (5.2)$$

Here $D\tilde{x} D\tilde{y}$ are infinite products of the dimensionless measures $h^{-n} dx$ and $h^{-n} dy$.

The points of contact between this path integral statement of $\rho(t, x)$ and the χ_2 WKB analysis are apparent. The sum of Hamiltonians in the functional $\mathcal{S}(t; \tilde{x}, \tilde{y})$ is just \mathcal{H}_2 . The stationary phase expansion of (5.1) will provide an alternate derivation of $\rho^{sc}(t, x)$.

The symplectic area WKB structure found for the evolutions $U(t)$ and $\rho(t)$ seems to be universal. For example, a gauge invariant generalization of theorem 2, suitable for quantum systems with external electromagnetic fields, has been recently published in [35] (theorem 6).

The extended phase space method developed here is expected to be a good platform for further study. Since the χ_2 Schrödinger evolution (2.1) is unitary in $L^2(\mathbb{R}_x^{2n})$, norm error bounds for $\|\rho(t) - \rho^{sc}(t)\|_2$ may be obtained with standard [7, 25] techniques. Higher order \hbar expansions, with $U^{sc}(t, x)$ and $\rho^{sc}(t, x)$ as first terms, are straightforward to derive using the known higher order transport equations. Similarly, the available globalization procedures [7, 15] readily apply in the χ_2 framework.

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Appendix A. Jacobi field applications

The Jacobi field of a classical system characterizes its stability. Given a trajectory $g(t|x)$, the $2n \times 2n$ matrix solution of the linear system

$$\frac{d}{dt} \nabla g(t|x) - JH''(g(t|x)) \nabla g(t|x) = 0 \quad (A.1)$$

$$\nabla g(0|x) = I \quad (A.2)$$

defines the associated Jacobi field. The solutions of (A.1) and (A.2) are symplectic matrices. For small times $\nabla g(t|x)$ will not differ greatly from its initial value I . This is made explicit in the following estimates. The norm $\|\cdot\|$ denotes the operator norm on \mathbb{R}^{2n} .

Lemma 7. *Let the Hessian of H have the x -uniform bound $\|H''(x)\| \leq c_1 < \infty$, then the Jacobi field has the growth estimates*

$$\|\nabla g(t|x)\| \leq e^{c_1 t} \quad \|\nabla g(t|x) - I\| \leq (e^{c_1 t} - 1). \quad (A.3)$$

Proof. Define $\xi(t|x) = \|\nabla g(t|x)\|$ and use $\frac{d}{dt}\|\nabla g(t|x)\| \leq \left\|\frac{d}{dt}\nabla g(t|x)\right\|$. Thus equation (A.1) and the Hessian bound imply

$$\begin{aligned} \frac{d}{dt}\xi(t|x) &\leq \|JH''(g(t|x))\|\xi(t|x) \leq c_1\xi(t|x) \\ \xi(t|x) &\leq e^{c_1 t}. \end{aligned}$$

Now estimate $\|\nabla g(t|x) - I\|$. The integral equation equivalent of (A.1) and (A.2) is

$$\nabla g(t|x) = I + \int_0^t JH''(g(\tau|x))\nabla g(\tau|x) d\tau.$$

Taking the norm of this relation gives

$$\|\nabla g(t|x) - I\| \leq \int_0^t \|JH''(g(\tau|x))\|\xi(\tau|x) d\tau \leq c_1 \int_0^t e^{c_1 \tau} d\tau = (e^{c_1 t} - 1). \quad \square$$

Next we consider the detailed linkage between the BC problem, finite WKB amplitudes and the non-singular set of Λ_t with respect to the projection Π_1 . Although this connection is implicit in the Maslov–Fedoriuk book [7], its precise statement is important for the BC solvability analysis and the interpretation of the WKB amplitude singularities.

First, let us collect several definitions and facts. Recall that D_0 is the support of S_0 or Φ_0 . Furthermore, the projection $\Pi_1 : \Lambda_0 \rightarrow D_0$ is diffeomorphic, with explicit inverse $\Pi_1^{-1}(x') = (x', \nabla S_0(x'))$, $x' \in D_0$. The regular subset of $\Lambda_t = G(t)\Lambda_0$ is $\mathcal{R}_t = \Lambda_t/\Sigma(\Lambda_t)$. Let $T_m(\Lambda_t)$ denote the tangent plane at $m \in \Lambda_t$. The statement, $m \in \mathcal{R}_t$, means that no vector in $T_m(\Lambda_t)$ has a zero Π_1 projection, i.e. $\dim \Pi_1 T_m(\Lambda_t) = 2n$. Since Λ_t is a Lagrangian manifold, $T_m(\Lambda_t)$ is a $2n$ -dimensional symplectic vector space for each m . With this notation, we have

Lemma 8. Let $x' \in D_0 = \Pi_1\Lambda_0$, then

$$\det \nabla M_t(x') \neq 0 \quad \Leftrightarrow \quad G(t|x', \nabla S_0(x')) \in \mathcal{R}_t. \quad (A.4)$$

Proof. The χ_2 Jacobi field $\nabla G(t|m')$ maps vectors on $T_{m'}(\Lambda_0)$ into vectors on $T_{G(t|m')}(\Lambda_t)$. The matrix $\nabla G(t|m')$ is symplectic, specifically $\det \nabla G(\tau|m') = 1$. Let $\{e_i\}_1^{2n}$ be a basis of $D_0 \subseteq \mathbb{R}^{2n}$ with origin at x' . Then $\{W_i = (e_i, S''_0(x')e_i)\}_1^{2n}$ is a basis of $T_{m'}(\Lambda_0)$, $m' = (x', \nabla S_0(x'))$. Since $\nabla G(t|m')$ is invertible, $\{\nabla G(t|m')W_i\}_1^{2n}$ is a basis of $T_{G(t|m')}(\Lambda_t)$. The Jacobi field for \mathcal{H}_2 flow is

$$\nabla G(\tau|x', y') = \begin{bmatrix} \frac{1}{2}[\nabla g(t|l') + \nabla g(t|r')] & \frac{1}{4}[-\nabla g(t|l') + \nabla g(t|r')]J \\ J[\nabla g(t|l') - \nabla g(t|r')] & -\frac{1}{2}J[\nabla g(t|l') + \nabla g(t|r')]J \end{bmatrix}.$$

Consider the conditions which ensure that $m \in \mathcal{R}_t$. Let $Z = (Z_x, Z_y)$ represent an arbitrary non-zero vector in $T_m(\Lambda_t)$. Since $\{\nabla G(\tau|m')W_i\}_1^{2n}$ is a basis, one has

$$Z = \sum_{i=1}^{2n} \lambda_i \nabla G(\tau|m')W_i = \sum_{i=1}^{2n} \lambda_i \nabla G(\tau|m') \begin{pmatrix} e_i \\ S''_0(x')e_i \end{pmatrix}$$

where at least one of the constants λ_i is non-zero. Projecting Z onto \mathbb{R}_x , gives

$$\Pi_1 Z = Z_x = \frac{1}{2} \frac{\partial}{\partial x'} \left[g(t|x' - \frac{1}{2}J\nabla S_0(x')) + g(t|x' + \frac{1}{2}J\nabla S_0(x')) \right] V$$

$$\Pi_1 Z = \nabla M_t(x')V \quad V = \sum_{i=1}^{2n} \lambda_i e_i \neq 0.$$

Thus a vector in $T_m(\Lambda_t)$ can have zero Π_1 projection iff $\det \nabla M_t(x') = 0$. □

With the replacement of S_0 by Φ_0 and M_t by \tilde{M}_t , the equivalence (A.4) holds for the Schrödinger problem.

Appendix B. A Poincaré–Cartan identity

The following identity is required in the proof of theorem 1.

Lemma 9. *Let γ_0 be an arbitrary smooth curve from x_1 to x_2 . Let $\sigma(t|\gamma_0)$ be the surface defined by the images of γ_0 under the flow $g(\tau, t_0)$, $t_0 \leq \tau \leq t$. Then*

$$\int_{\sigma(t|\gamma_0)} dp \wedge dq = \oint_{\partial\sigma(t|\gamma_0)} p \cdot dq = \int_{t_0}^t [H(\tau, g(\tau, t_0|x_2)) - H(\tau, g(\tau, t_0|x_1))] d\tau. \quad (\text{B.1})$$

Proof sketch. Decompose the curve γ_0 into segments that are singularity free with respect to some Lagrangian plane. For notational convenience, denote this plane by \mathbb{R}_q^n . Now locally embed this curve into a non-singular Lagrangian manifold λ_0 having phase $s_0(q)$. Denote by $\lambda_t = g(t, t_0|\lambda_0)$ the time evolution of λ_0 . Extend the original phase space χ_1 by adding time to the q -coordinate manifold, $(q, t; p, p_t) \in \chi_1^+ = T^*R^{n+1}$. Let $s(t, q)$ be the phase of λ_t , then the manifold

$$\lambda^+ \equiv \{(q, t; p, p_t) \in \chi_1^+ | (p, p_t) = (\nabla s(t, q), \partial_t s(t, q))\}$$

is Lagrangian. On λ^+ the 1-form $\omega^+ = p dq - H(t, q, p) dt$ is closed by virtue of the HJ equation. Closed loop integrals on λ^+ vanish and can be arranged to give (B.1). \square

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