A Gutzwiller trace formula for large hermitian matrices

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Abstract

We develop a semiclassical approximation for the dynamics of quantum systems in finite-dimensional Hilbert spaces whose classical counterparts are defined on a toroidal phase space. In contrast to previous models of quantum maps, the time evolution is in continuous time and, hence, is generated by a Schrödinger equation. In the framework of Weyl quantisation, we construct discrete, semiclassical Fourier integral operators approximating the unitary time evolution and use these to prove a Gutzwiller trace formula. We briefly discuss a semiclassical quantisation condition for eigenvalues as well as some simple examples.

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1 Introduction

Semiclassical analysis aims at approximating quantum dynamics in terms of suitable, corresponding classical dynamics in the semiclassical limit. Since the unitary quantum dynamics are generated by a self-adjoint Hamiltonian operator, a closely related problem for operators with a discrete spectrum is the semiclassical approximation of eigenvalues. Bohr-Sommerfeld quantisation conditions in one dimension were the first examples of such approximations. They were followed by the EBK conditions for integrable systems. A general approximation of quantum spectral functions in terms of classical quantities, however, was first given in terms of the Gutzwiller trace formula [Gut71]. The first rigorous proofs of a trace formula in a similar spirit were given by Colin de Verdière [CdV73a, CdV73b], and Duistermaat and Guillemin [DG75], for the case of a Laplacian on a closed manifold. The semiclassical case originally considered by Gutzwiller was proven by Meinrenken [Mei92].

Semiclassical methods have been successfully applied in a broad range of circumstances, from realistic models describing experiments to purely mathematical models. In many of those cases a classical configuration space is given. The classical phase space then is the cotangent bundle over the configuration space. The corresponding quantum systems are defined in an infinite dimensional Hilbert space, typically an L^2-space over the configuration space, and semiclassical methods are available that relate the quantum and the classical descriptions of the same physical system, see, e.g., [Zwo12]. In some situations (as, e.g., Toeplitz quantisation and quantum maps [Zel97, DEG03, Sch10]) the classical phase space, however, is a compact symplectic manifold, such as a sphere or a torus. There then exists no classical configuration space. The associated quantum Hilbert space is finite dimensional and the dimension of the Hilbert space tends to infinity in the semiclassical limit. A class of models of this type that have been studied intensively are quantised torus maps [DEG03], for which the dynamics take place in discrete time. Quantum maps are often studied as mathematical toy models, e.g. in the context of quantum chaos. However, phase spaces that are not cotangent bundles also have many applications in physics. For instance, toroidal phase spaces are relevant in solid state physics, see, e.g., [Har55], and more general symplectic manifolds play a role in molecular physics, see, e.g., [SZ06] and references therein.

Our goal in this article is to quantise Hamiltonian flows on tori and to approximate the resulting continuous-time quantum dynamics semiclassically, within the framework of Weyl quantisation. We then use the semiclassical approximation of the dynamics in order to prove a trace formula. As the quantum Hamiltonian acts in a finite dimensional Hilbert space, this is a Gutzwiller trace formula for hermitian matrices, with matrix size growing in the semiclassical limit. Since tori are special cases of compact Kähler manifolds, it may seem natural to apply results that were obtained in the context of Toeplitz quantisation [BdMG81] on compact Kähler manifolds. In this framework a Gutzwiller-type trace formula was proven by Borthwick, Paul and Uribe [BPU98], building on [BdMG81]. In a more recent approach, Paoletti uses the Szegö kernel of [BdMS76] in order to also prove local asymptotics [Pao11, Pao16]. Nevertheless, although the approach of the present article is not suitable for general compact Kähler manifolds we believe that proving a trace

formula for torus flows entirely within the framework of Weyl quantisation is useful for the following two reasons.

First, Weyl quantisation of observables on a torus is well known in the context of quantum maps. Furthermore, it allows us to outline the proof of the trace formula in close analogy to the classic proof in the case where the phase space is a cotangent bundle. The essential modification is a discretised ansatz for the semiclassical time evolution operator, see Eq. (2.12) below. Moreover, our main tool is a result that is essentially a stationary phase theorem for sums, see Appendix B.

Second, Weyl quantisation is particularly adapted to the case of Schrödinger operators in finite dimension including, e.g., discretisations of differential operators as in the Harper model [Har55] or in the case of Dirac operators in lattice field theory, see, e.g., [Rot12]. Toeplitz quantisation on tori [Zel97], however, is equivalent to anti-Wick quantisation as can be deduced from [BD96, BK01]. In representing Hamiltonian operators, anti-Wick quantisation, in turn, is not identical to Weyl quantisation but is the same to leading order [BD96, Lemma 3.9]. In particular, whereas Weyl symbols of Schrödinger operators (and similar types of difference operators) are $\hbar$-independent and, hence, identical to their principal symbols, anti-Wick symbols for the same operators are $\hbar$-dependent with the Weyl symbol providing only the principal part. We illustrate this statement in Appendix A; see also [Zel05, FT15] for a comparison of different quantisation schemes for symplectic maps.

The article is organised as follows. In Section 2 we introduce the general setting and present our main result, the trace formula in Theorem 1. In Section 3 we recall the Weyl quantisation of functions on a torus and develop some useful expressions for the action of a Weyl operator on a vector. In Section 4 we review relevant aspects of classical Hamiltonian dynamics on a torus phase space, with a particular emphasis on extending Hamilton-Jacobi dynamics beyond caustics and the construction of Maslov bundles. The main technical work is presented in Section 5, where the semiclassical approximation of the quantum time evolution is developed. The proof of our main Theorem 1 is given in Section 6. An application of the trace formula to derive semiclassical quantisation conditions can be found in Section 7. Finally, in Section 8 we discuss some simple examples.

2   Setting and main result

Let $\mathbb{T} = \mathbb{R}^2/(\ell_x\mathbb{Z} \oplus \ell_\xi\mathbb{Z})$ be a two dimensional torus, where $\ell_x, \ell_\xi > 0$ are two length parameters. The universal covering space of $\mathbb{T}$ is $\mathbb{R}^2$, and as a fundamental domain for the action of $\ell_x\mathbb{Z} \oplus \ell_\xi\mathbb{Z}$ on $\mathbb{R}^2$ we choose $\mathbb{F} = [0, \ell_x) \times [0, \ell_\xi)$. Weyl quantisation associates an N-dimensional Hilbert space $\mathbb{C}^N$, with inner product $\langle \psi, \phi \rangle_N := \frac{1}{N}\langle \phi, \psi \rangle_{\mathbb{C}^N}$, to the classical system, where

$$N = \frac{\ell_x\ell_\xi}{2\pi\hbar} \tag{2.1}$$

is a semiclassical parameter determined by the value of Planck's constant $\hbar$. In fact, one can view either $\hbar$ or N^{-1} as a semiclassical parameter. In the following we shall mainly use $\hbar$ for semiclassical asymptotic expansions, but one has to keep in mind that the relation

(2.1) allows one to rewrite expressions so as to hide $\hbar$. Also notice that since N is an integer $\hbar$ only takes values in a discrete set.

Vectors $\psi = (\psi_n) \in \mathbb{C}^N$ can be seen as 'wave functions' supported at the points

$$x_n = \frac{n\ell_x}{N}, \quad n = 0, \ldots, N-1, \tag{2.2}$$

in the interval $[0, \ell_x)$.

The Weyl quantisation of a classical observable $f \in C^\infty(\mathbb{T})$ is a linear operator $\mathrm{op}_N(f) : \mathbb{C}^N \to \mathbb{C}^N$ defined as

$$\mathrm{op}_N(f) := \sum_{m,n \in \mathbb{Z}} f_{mn} T^{mn}. \tag{2.3}$$

Here

$$f_{mn} = \frac{1}{\ell_x \ell_\xi} \int_{\mathbb{F}} f(x, \xi) \, \mathrm{e}^{-2\pi\mathrm{i}\left(\frac{m\xi}{\ell_\xi} - \frac{nx}{\ell_x}\right)} \mathrm{d}x \, \mathrm{d}\xi \tag{2.4}$$

are Fourier coefficients of the observable f, viewed as a smooth function on the fundamental domain $\mathbb{F}$, and the

$$T^{mn} = \mathrm{e}^{\mathrm{i}\pi \frac{nm}{N}} T^{m0} T^{0n} \tag{2.5}$$

are unitary operators in $\left(\mathbb{C}^N, \langle \cdot, \cdot \rangle_N\right)$ defined through

$$\left(T^{m0}\psi\right)_l := \psi_{(l+m) \bmod N} \quad \text{and} \quad \left(T^{0n}\psi\right)_l := \mathrm{e}^{-\frac{2\pi\mathrm{i}ln}{N}} \psi_l. \tag{2.6}$$

The latter represent translations in the x- and ξ-directions, respectively. This quantisation was introduced in [HB80], for details see, e.g., [BD96, DEG03].

A typical operator that one would want to represent in Weyl quantisation is a Schrödinger operator $-\hbar^2 \Delta + V$, where the Laplacian is a difference operator,

$$\begin{aligned}(-\Delta\psi)_l &:= -\frac{N^2}{\ell_x^2}\left(\psi_{(l+1) \bmod N} + \psi_{(l-1) \bmod N} - 2\psi_l\right) \\ &= -\frac{N^2}{\ell_x^2}\left((T^{1,0} + T^{-1,0} - 2\mathbb{1})\psi\right)_l.\end{aligned} \tag{2.7}$$

From the last expression one immediately identifies a symbol,

$$H(x, \xi) = \frac{\ell_\xi^2}{2\pi^2}\left(1 - \cos\left(\frac{2\pi\xi}{\ell_\xi}\right)\right) + V(x), \tag{2.8}$$

such that $\mathrm{op}_N(H) = -\hbar^2 \Delta + V$.

Given a classical Hamiltonian $H \in C^\infty(\mathbb{T})$ the Schrödinger equation is

$$\mathrm{i}\hbar \frac{\mathrm{d}\psi}{\mathrm{d}t}(t) = \mathrm{op}_N(H)\psi(t), \qquad \psi(0) = \psi_0 \in \mathbb{C}^N. \tag{2.9}$$

It generates a unitary one-parameter group $U(t)$, $t \in \mathbb{R}$, via $\psi(t) = U(t)\psi_0$. (See also [Lig16], where the corresponding Heisenberg equation is considered.)

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We remark that fixing the dimension N, every hermitian $N \times N$-matrix has a representation (2.3). This is not unique in the sense that one could provide alternative phase space representations of the same matrix. However, with varying N, the above construction yields a family of hermitian matrices associated with a fixed phase space and a fixed function f.

The first aim of this paper is to construct a semiclassical asymptotic expansion

$$U(t) \sim \sum_{k \geq 0} \left(\frac{\hbar}{\mathrm{i}} \right)^k U_k(t), \quad \hbar \to 0. \tag{2.10}$$

In a second step we use this expansion in order to evaluate the right-hand side of

$$\sum_n \rho \left(\frac{E_n - E}{\hbar} \right) = \frac{1}{2\pi} \int_{\mathbb{R}} \hat{\rho}(t) \, \mathrm{tr} \, U(t) \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} E t} \, \mathrm{d}t, \tag{2.11}$$

where $\rho \in C^\infty(\mathbb{R})$ with compactly supported Fourier transform $\hat{\rho}$. The sum on the left-hand side extends over all eigenvalues E_n of $\mathrm{op}_N(H)$, i.e., it is a spectral function of the Hamiltonian.

Evaluating the right-hand side of (2.11) using the semiclassical expansion (2.10) leads to an expression which we relate to the Hamiltonian flow on $\mathbb{T}$ generated by the classical Hamiltonian H. In order to achieve this we have to identify $U(t)$ as a suitable semiclassical Fourier integral operator (scFIO). Locally, the latter is given in terms of an oscillatory integral, whose phase function generates the Hamiltonian flow. In the present context of compact phase spaces this concept has to be amended appropriately, leading to the ansatz

$$U_k(t)_{nm} = \frac{1}{\ell_\xi} \int_{\mathbb{R}} a_k(t, x_n, x_m, \xi) \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} \phi(t, x_n, x_m, \xi)} \, \mathrm{d}\xi. \tag{2.12}$$

Since the quantum mechanical Hilbert space has finite dimension, the amplitude and the phase function of this 'position representation' of the time evolution operator are only evaluated at the points

$$x_n = \frac{n \ell_x}{N}, \quad n = 0, \ldots, N-1. \tag{2.13}$$

The amplitude and the phase function, however, are defined on the universal covering space $\mathbb{R}^2$, and not only on $\mathbb{F}$. They will have to be chosen such that $U(t)$ (approximately) satisfies the Schrödinger equation that follows from (2.9). If the phase function is chosen to be of the form

$$\phi(t, x, y, \xi) = S(t, x, \xi) - y\xi, \tag{2.14}$$

it will turn out that S is required to be a solution of the Hamilton-Jacobi equation,

$$H(x, \partial_x S) + \partial_t S = 0, \tag{2.15}$$

with initial condition $S(0, x, \xi) = x\xi$. Hence, S generates the canonical transformation

$$(x, \partial_x S(t, x, \xi)) \mapsto (\partial_\xi S(t, x, \xi), \xi) \tag{2.16}$$

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representing the Hamiltonian flow backwards in time (all lifted to the covering space $\mathbb{R}^2$). However, this is only true for sufficiently small times t, i.e., as long as no caustics occur. Beyond caustics one has to piece local, singularity free representations of the form (2.12) together. This requires a suitable Maslov bundle, eventually introducing Maslov phases into the resulting trace formula. We shall have to devote a sizeable portion of this work to solving this problem.

Assuming that E is a regular value for the classical Hamiltonian H, the energy surface

$$H^{-1}(E) := \{(x,\xi) \in \mathbb{T};\ H(x,\xi) = E\} \tag{2.17}$$

is a one-dimensional, not necessarily connected, submanifold of the two-dimensional torus. We denote by $\mathfrak{P}_E$ the set of periodic orbits of the Hamiltonian flow at energy E. The connected components of the energy surface $H^{-1}(E)$ are the primitive periodic orbits. Hence, the volume $\mathrm{vol}(H^{-1}(E))$ of the energy surface is the sum of the periods $t_{p\#}$ of all primitive periodic orbits $p^{\#} \in \mathfrak{P}_E$. Let W_p be the action of the orbit p and denote its Maslov phase by σ_p. Our main result then is the following.

Theorem 1. *Assume that E is a regular value for the classical Hamiltonian $H \in C^\infty(\mathbb{T})$, and let $\rho \in C^\infty(\mathbb{R})$ with Fourier transform $\hat{\rho} \in C_0^\infty(\mathbb{R})$ be a test function. Then, for every $p \in \mathfrak{P}_E$ there exists a function $a_p(\hbar)$ with a complete asymptotic expansion in powers of $\hbar$, such that*

$$\sum_n \rho\left(\frac{E_n - E}{\hbar}\right) = a_0(\hbar)\frac{\hat{\rho}(0)}{2\pi} + \sum_{p \in \mathfrak{P}_E} \frac{\hat{\rho}(t_p)\, a_p(\hbar)}{2\pi} e^{\frac{i}{\hbar}W_p - \frac{i\pi}{2}\sigma_p} + O(\hbar^\infty). \tag{2.18}$$

The leading asymptotic behaviour of the amplitude functions is

$$\begin{aligned} a_0(\hbar) &= \mathrm{vol}\left(H^{-1}(E)\right) + O(\hbar) \\ a_p(\hbar) &= t_{p\#} + O(\hbar), \end{aligned} \tag{2.19}$$

where $p^{\#}$ is the primitive periodic orbit associated with $p \in \mathfrak{P}_E$.

In the following we provide a self contained proof of this theorem using the explicit Weyl quantisation outlined above.

3 Weyl quantisation on the torus

Weyl quantisation of classical systems with toroidal phase space is based on irreducible unitary representations of the discrete Heisenberg group $H_3(\mathbb{Z})$, see [DEG03]. They are labelled by a positive integer N, the dimension of the representation. Similarly, Weyl quantisation of classical systems with phase space $\mathbb{R}^2$, the universal cover of $\mathbb{T}$, is based on the continuous Heisenberg group $H_3(\mathbb{R})$, whose irreducible unitary representations are labelled by the positive real parameter $\hbar$, physically Planck's constant divided by 2π, see [Fol89]. The representation of $H_3(\mathbb{Z})$ generated by the unitary operators (2.6) induces a

representation of $H_3(\mathbb{R})$ with $\hbar$ determined by (2.1). Consequently, the semiclassical limit $\hbar \to 0$ corresponds to $N \to \infty$, the limit of large matrices.

Using the definitions (2.5) and (2.6) in (2.3) we can rewrite the action of a Weyl-quantised observable $f \in C^\infty(\mathbb{T})$ on a vector $\psi = (\psi_k) \in \mathbb{C}^N$ as

$$
\begin{aligned}
(\mathrm{op}_N(f)\psi)_k &= \sum_{m \in \mathbb{Z}} \psi_{m \bmod N} \frac{1}{\ell_\xi} \int_0^{\ell_\xi} f\left(\ell_x \frac{k+m}{2N}, \xi\right) \mathrm{e}^{2\pi\mathrm{i}(k-m)\xi/\ell_\xi} \, \mathrm{d}\xi \\
&= \sum_{m \in \mathbb{Z}} \psi_{m \bmod N} \frac{1}{\ell_\xi} \int_0^{\ell_\xi} f\left(\frac{x_k + x_m}{2}, \xi\right) \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(x_k - x_m)\xi} \, \mathrm{d}\xi,
\end{aligned}
\tag{3.1}
$$

where $m \bmod N$ denotes the smallest non-negative integer m' such that N divides $m - m'$. The last line of (3.1) follows from (2.2) and (2.1) and the result is similar to the corresponding expression for the application of a Weyl operator in $L^2(\mathbb{R})$.

The infinite sum in (3.1) can be turned into a finite sum plus remainder using the following result.

Lemma 1. *Let $f \in C^\infty(\mathbb{T})$ and $\psi = (\psi_k) \in \mathbb{C}^N$. Then, for all $M \in \mathbb{N}$, we have*

$$
\begin{aligned}
(\mathrm{op}_N(f)\psi)_k = &\sum_{|k-m| \leq N^{\frac{1}{M}}} \psi_{m \bmod N} \frac{1}{\ell_\xi} \int_0^{\ell_\xi} f\left(\ell_x \frac{k+m}{2N}, \xi\right) \mathrm{e}^{2\pi\mathrm{i}(k-m)\xi/\ell_\xi} \, \mathrm{d}\xi \\
&+ O_M\left(\hbar^\infty\right).
\end{aligned}
\tag{3.2}
$$

In (3.2) the notation $g(\hbar) = O_M\left(\hbar^\infty\right)$ means that there exists a constant C_M, depending on M, such that $|g(\hbar)| \leq C_M \hbar^\alpha$ for all $\alpha > 0$.

Proof. The claim follows from integrating by parts, see e.g. [Gra08, Theorem 3.2.9], and only requires bounds on the derivatives of f with respect to ξ. $\qquad \square$

We remark that the restriction $|k-m| \leq N^{1/M}$ in the summation is equivalent to the condition

$$
|x_k - x_m| < N^{\frac{1}{M}-1} \ell_x.
\tag{3.3}
$$

The result can be rephrased as follows.

Lemma 2. *Let $f \in C^\infty(\mathbb{T})$ and $\psi = (\psi_k) \in \mathbb{C}^N$. Then, for all $L, M \in \mathbb{N}$,*

$$
\begin{aligned}
(\mathrm{op}_N(f)\psi)_k = &\sum_{|k-m| \leq N^{\frac{1}{M}}} \psi_{m \bmod N} \sum_{l=0}^{L-1} \frac{1}{l!} \left(\frac{\hbar}{2\mathrm{i}}\right)^l \frac{1}{\ell_\xi} \int_0^{\ell_\xi} \partial_\xi^l \partial_x^l f(x_k, \xi) \mathrm{e}^{2\pi\mathrm{i}(k-m)\xi/\ell_\xi} \, \mathrm{d}\xi \\
&+ O\left(N^{\frac{L}{M}-L}\right).
\end{aligned}
\tag{3.4}
$$

Proof. We first note that a Taylor expansion together with (3.3) gives

$$
f\left(\frac{x_k + x_m}{2}, \xi\right) = \sum_{l=0}^{L-1} \frac{1}{l!} \left(\frac{x_m - x_k}{2}\right)^l \partial_x^l f(x_k, \xi) + O\left(N^{\frac{L}{M}-L}\right).
\tag{3.5}
$$

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Using this identity on the right-hand side of (3.2), as well as (2.1) and the identity

$$(m - k)^l e^{2\pi i(k-m)\xi/\ell_\xi} = \left(\frac{i\ell_\xi}{2\pi}\right)^l \partial_\xi^l e^{2\pi i(k-m)\xi/\ell_\xi}, \qquad (3.6)$$

followed by an l-fold integration by parts, yields the desired result. $\qquad\square$

4 Classical dynamics on the torus

Before we can proceed to construct semiclassical approximations of the quantum time evolution we have to provide some classical input. Eventually we shall construct a suitable scFIO, and for that purpose we need equivalents to the classical data that are used in standard FIOs [Dui96, Hör85b] or their semiclassical counterparts [Mei92].

The general setting here is that of a Hamiltonian flow Φ_t on the phase space $\mathbb{T}$ generated by a Hamiltonian vector field X_H associated with a Hamiltonian function $H \in C^\infty(\mathbb{T})$. This flow is global since $\mathbb{T}$ is compact. Due to the covering of $\mathbb{T}$ by $\mathbb{R}^2$, $\pi : \mathbb{R}^2 \to \mathbb{T}$, most expressions given below hold on $\mathbb{R}^2$ as well as on $\mathbb{T}$ (at least locally). At some instances, however, we have to pay attention to differences, making use of that fact that the covering map provides the projection and the pull back for switching between covering space and base space.

Working on the covering space of the torus, the canonical one- and two-forms are given by $\theta := \xi \mathrm{d}x$ and $\omega := \mathrm{d}\theta = \mathrm{d}\xi \wedge \mathrm{d}x$. Here θ is not periodic in ξ, but ω can be regarded as a two-form on $\mathbb{T}$ as well.

For the purpose of semiclassical constructions it is convenient to work on the extended phase space $T^*\mathbb{R} \times \mathbb{T} \cong \mathbb{R}^2 \times \mathbb{T}$. Following an established convention, we denote points in that space as $(t, \tau, x, \xi) \in \mathbb{R}^2 \times \mathbb{T}$, where t is the time variable and $-\tau$ has the meaning of an energy. In these variables the canonical two-form is

$$\Omega := \mathrm{d}t \wedge \mathrm{d}\tau \oplus \omega, \qquad (4.1)$$

both on $\mathbb{R}^2 \times \mathbb{R}^2$ and on $\mathbb{R}^2 \times \mathbb{T}$. We then consider the extended classical Hamiltonian

$$H_{\mathrm{ext}}(t, \tau, x, \xi) = H(x, \xi) + \tau, \qquad (4.2)$$

generating the (extended) Hamiltonian flow

$$\Phi_\sigma^{\mathrm{ext}}(t, \tau, x, \xi) = \left(t + \sigma, \tau, \Phi_\sigma(x, \xi)\right). \qquad (4.3)$$

Standard FIOs require canonical relations. In the present context this is a twisted version of the graph of the extended Hamiltonian flow (4.3), which can be given as

$$\Lambda = \left\{(t, \tau, x, \xi, y, -\eta); \; (x, \xi) = \Phi_t(y, \eta), \; H_{\mathrm{ext}}(t, \tau, y, \eta) = 0\right\}, \qquad (4.4)$$

and which is a Lagrangian submanifold of $\mathbb{R}^2 \times \mathbb{T} \times \mathbb{T}$ or $\mathbb{R}^2 \times \mathbb{R}^2 \times \mathbb{R}^2$, equipped with the symplectic form

$$\tilde{\Omega} = \mathrm{d}t \wedge \mathrm{d}\tau \oplus \omega \oplus \omega. \qquad (4.5)$$

We also need local generating functions for Λ. These always exist in a neighbourhood of the initial manifold [GS94, Theorem 5.5]

$$\Lambda_0 = \{(0, \tau, x, \xi, y, -\eta);\ (x, \xi) = (y, \eta),\ H_{\text{ext}}(0, \tau, y, \eta) = 0\}, \tag{4.6}$$

in the form

$$\phi(t, x, y, \eta) = S(t, x, \eta) - \eta y, \tag{4.7}$$

where S satisfies the Hamilton-Jacobi equation

$$H\big(x, \partial_x S(t, x, \eta)\big) + \partial_t S(t, x, \eta) = 0 \quad \text{with initial condition} \quad S(x, \eta, 0) = x\eta. \tag{4.8}$$

A solution S exists when $|t|$ is sufficiently small, so as no caustic to occur. This solution defines a map $\phi : \mathfrak{V}_0 \to \mathbb{R}$, where $\mathfrak{V}_0$ is an open set in $\mathbb{R}^4$, such that

$$\begin{aligned}\big\{(t, \partial_t S(t, x, \eta), x, \partial_x S(t, x, \eta), \partial_\eta S(t, x, \eta), -\eta);\ (t, x, y, \eta) \in \mathfrak{V}_0, \\ (x, \xi) = \Phi^t(y, \eta),\ H_{\text{ext}}(t, \tau, y, \eta) = 0\},\end{aligned} \tag{4.9}$$

is a neighbourhood of Λ_0 in Λ. The above is formulated on the covering phase space. Working on the torus would result in the solution S of the Hamilton-Jacobi equation (4.8) to be discontinuous. In order to avoid this problem we shall use generating functions on the universal cover only.

Representations analogous to (4.9) can be given at any point of Λ where the map

$$(x, \xi, y, -\eta) \mapsto (x, \eta), \quad \text{with} \quad \Phi_t(y, \eta) = (x, \xi), \tag{4.10}$$

is locally surjective. On an open set $\mathfrak{V}_\alpha \subset \mathbb{R}^4$ one then finds a function

$$\phi_\alpha(t, x, y, \eta) = S_\alpha(t, x, \eta) - \eta y, \tag{4.11}$$

such that the analogue of (4.9) parametrises another piece of Λ. At points where local surjectivity of (4.10) is violated but where instead the map

$$(x, \xi, y, -\eta) \mapsto (\xi, \eta), \quad \text{with} \quad \Phi_t(y, \eta) = (x, \xi), \tag{4.12}$$

is locally surjective we may use an alternative generating function. Slightly abusing our notation, we introduce $\phi_\alpha : \mathfrak{V}_\alpha \to \mathbb{R}$, where now $\mathfrak{V}_\alpha$ is an open subset of $\mathbb{R}^5$, of the form

$$\phi_\alpha(t, x, y, \xi, \eta) = x\xi - y\eta - S_\alpha(t, \xi, \eta). \tag{4.13}$$

This gives a parametrisation

$$\begin{aligned}\big\{(t, \partial_t S_\alpha(t, \xi, \eta), \partial_\xi S_\alpha(t, \xi, \eta), \xi, -\partial_\eta S_\alpha(t, \xi, \eta), -\eta);\ (t, x, y, \xi, \eta) \in \mathfrak{V}_\alpha, \\ (x, \xi) = \Phi^t(y, \eta),\ H_{\text{ext}}(t, \tau, y, \eta) = 0\},\end{aligned} \tag{4.14}$$

of yet another piece of Λ. We denote by Λ_α the subset of Λ generated by the pair $\{\phi_\alpha, \mathfrak{V}_\alpha\}$, no matter whether it is parametrised in the sense of (4.9) or (4.14). In fact, all of Λ can

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be covered by local pieces of the above forms. This can be proven in analogy to [Zwo12, Lemma 10.5]; in the case (4.14) one only has to replace the one-form in [Zwo12, p. 230] by

$$\nu := \tau \mathrm{d}t - x\mathrm{d}\xi - y\mathrm{d}\eta. \tag{4.15}$$

Now let $\{\Psi_\alpha\}_\alpha$ be a partition of unity subordinate to the open cover $\{\Lambda_\alpha\}_\alpha$. We then call

$$\{\Gamma_\alpha\}_\alpha, \quad \text{where} \quad \Gamma_\alpha = \{\phi_\alpha, \mathfrak{V}_\alpha, \Psi_\alpha, \Lambda_\alpha\}, \tag{4.16}$$

a generating set of Λ.

We remark that if $\gamma(\sigma) = (\sigma, \Phi_\sigma(y, \eta))$ is a path in $\mathbb{R} \times \mathbb{R}^2$ connecting $(0, y, \eta)$ and $(t, \Phi_t(y, \eta))$ corresponding to $\lambda \in \Lambda$ then its action

$$W(\lambda) := \int_\gamma \theta + t\tau \tag{4.17}$$

generates Λ using suitable local coordinates [Mei92, Eq. (16)].

The pairs $\{\phi_\alpha, \mathfrak{V}_\alpha\}_\alpha$ generate a distinguished complex line bundle, the Maslov bundle, over Λ. This bundle is defined by the transition functions,

$$\kappa_{\alpha\beta} := \mathrm{e}^{\frac{\mathrm{i}\pi}{2}\sigma_{\alpha\beta}}, \tag{4.18}$$

where

$$\sigma_{\alpha\beta}(\lambda) := \frac{1}{2}\big(\mathrm{sgn}\,\mathrm{Hess}\,\phi_\alpha(\lambda) - \mathrm{sgn}\,\mathrm{Hess}\,\phi_\beta(\lambda)\big), \quad \lambda \in \Lambda_\alpha \cap \Lambda_\beta, \tag{4.19}$$

see [Mei92, Eq. (4)] and [Hör85a, Eq. (21.6.18)]. Note that here and throughout the article Hessians are defined only with respect to variables on the original phase space but not with respect to variables on the extended phase space. Now assume γ to be a continuous path in Λ defined on some compact parameter interval I. We choose a finite partition $t_0, \ldots, t_M$ of I such that $\gamma([t_{i-1}, t_i]) \subset \Lambda_{\alpha_i}$ for some α_i. Then we define the Maslov index of γ as

$$\mu(\gamma) := \sum_{i=1}^{M-1} \sigma_{\alpha_i \alpha_{i+1}}(\gamma(t_i)), \tag{4.20}$$

compare [Mei92, p. 288].

The constructions leading to (4.20) and (4.16) were performed in the covering space setting. However, they are also valid in the torus setting, since the constructions are essentially local. In particular, choosing $\mathfrak{V}_\alpha$, or rather Λ_α, small enough and fixing α one can uniquely identify the coordinates in the torus setting with those in the covering space setting. If (x, ξ) are coordinates of a point in $\mathbb{R}^2$, we shall denote coordinates of its projection to $\mathbb{T}$ by $(\check{x}^\alpha, \check{\xi}^\alpha)$. Conversely, if (x, ξ) are coordinates of a point on the torus we shall use $(\hat{x}^\alpha, \hat{\xi}^\alpha)$ to denote coordinates for this point lifted to $\mathbb{R}^2$ in the framework described above. We shall omit the dependence on α if it is clear from the context.

In order to achieve the above properties we choose a generating set (4.16) where the sets $\mathfrak{V}_\alpha$ are small enough to satisfy the following conditions: Let $\{z_1, \ldots, z_l\}$ be a subset of

the coordinates $\{x, y, \xi, \eta\}$ and define $\mathfrak{V}_\alpha^{z_1,\ldots,z_l}$ to be the image of $\mathfrak{V}_\alpha$ under the projection $(x, y, \xi, \eta) \mapsto (z_1, \ldots, z_l)$. Then we require

$$\operatorname{diam} \mathfrak{V}_\alpha^x, \operatorname{diam} \mathfrak{V}_\alpha^y < \frac{\ell_x}{2} \quad \text{and} \quad \operatorname{diam} \mathfrak{V}_\alpha^\xi, \operatorname{diam} \mathfrak{V}_\alpha^\eta < \frac{\ell_\xi}{2} \tag{4.21}$$

for every $t \in [0, T]$ with arbitrary but fixed T. Here $\operatorname{diam} M$ denotes the diameter of $M \subset \mathbb{R}^d$ measured in the euclidean metric.

We now develop a generating set for Λ that is adapted to the construction of discrete scFIOs which is carried out in Sec. 5. We start with an arbitrary subordinate partition of unity $\{\psi_\rho, V_\rho\}_\rho$ of $\mathbb{T}$. Translating this partition with $\ell_x \mathbb{Z} \oplus \ell_\xi \mathbb{Z}$ then gives a partition of unity of $\mathbb{R}^2$. Another related subordinate partition of unity, $\{\psi'_{\rho,t}, V'_{\rho,t}\}_\rho$, is given by

$$V'_{\rho,t} = \{(x, \xi), \ \Phi_t(y, \eta) = (x, \xi), \ (y, -\eta) \in V_\rho\} \quad \text{and} \quad \psi'_{\rho,t}(x, \xi) = \psi_\rho(y, -\eta). \tag{4.22}$$

Let further $\{\kappa_\beta, I_\beta\}_\beta$ be a subordinate partition of unity of the interval $[0, T]$ and set $\alpha = (\rho, \beta)$, as well as

$$\Lambda_\alpha = \left\{(t, \tau, x, \xi, y - \eta) \in \mathbb{R}^2 \times V'_{\rho,t} \times V_\rho; \ (t, \tau, x, \xi, y, -\eta) \in \Lambda\right\}, \tag{4.23}$$

and

$$\Psi_\alpha(t, \tau, x, \xi, y, -\eta) = \kappa_\beta(t)\psi'_{\rho,t}(x, \xi)\psi_\rho(y, -\eta). \tag{4.24}$$

Then $\{\Psi_\alpha, \Lambda_\alpha\}_\alpha$ is a subordinate partition of unity of Λ.

The above constructions also work on the covering space. There, translations by $\ell_x \mathbb{Z} \oplus \ell_\xi \mathbb{Z}$ introduce an equivalence relation on the collection of sets Λ_α. This generates equivalence classes $\Lambda_{\widetilde{\alpha}}, \mathfrak{V}_{\widetilde{\alpha}}$ and $\Psi_{\widetilde{\alpha}}$. In short, we also say that α, α' are in the equivalence class $\widetilde{\alpha}$.

Lemma 3. *Let $\Lambda_\alpha, \Lambda_{\alpha'}$ be in the same equivalence class $\Lambda_{\widetilde{\alpha}}$. Then*

$$\check{\Lambda}_{\alpha'} = \check{\Lambda}_\alpha \tag{4.25}$$

and the converse is also true. Moreover, assume that $\check{\lambda}_\alpha = \check{\lambda}_{\alpha'}$, where $\lambda_{\alpha'} \in \Lambda_{\alpha'}$ and $\lambda_\alpha \in \Lambda_\alpha$. Then

$$W(\lambda_\alpha) = W(\lambda_{\alpha'}) \tag{4.26}$$

If, in addition, $\mathfrak{V}_{\alpha'}, \mathfrak{V}_\alpha$ are in the same equivalence class $\mathfrak{V}_{\widetilde{\alpha}}$, then

$$\operatorname{Hess} \phi_\alpha(\lambda_\alpha) = \operatorname{Hess} \phi_{\alpha'}(\lambda_{\alpha'}). \tag{4.27}$$

Proof. Since the Hamiltonian is periodic the relation (4.26) follows for all λ_α and $\lambda_{\alpha'}$ in the set (4.25). This implies that ϕ_α and $\phi_{\alpha'}$ can be chosen of the same type and differ only by linear terms. Since the latter do not contribute to the Hessian this proves (4.27). $\qquad \square$

A consequence for the Maslov bundle with transition functions (4.18) follows immediately.

Corollary 1. *With the assumptions of Lemma 3, as well as $\alpha, \alpha' \in \widetilde{\alpha}$ and $\beta, \beta' \in \widetilde{\beta}$, it follows that*

$$\kappa_{\alpha\beta} = \kappa_{\alpha'\beta'}, \tag{4.28}$$

and

$$\partial_x \xi_\alpha(\lambda_\alpha) = \partial_x \xi_{\alpha'}(\lambda_{\alpha'}), \quad and \quad \partial_\xi x_\alpha(\lambda_\alpha) = \partial_\xi x_{\alpha'}(\lambda_{\alpha'}). \tag{4.29}$$

Another useful result is the following.

Lemma 4. *Assume the restrictions (4.21) on the size of the sets $\mathfrak{V}_\alpha$. If the projections $\check{\Lambda}_{\alpha'}$ and $\check{\Lambda}_\alpha$ have non-empty intersection then there exists a unique $\gamma \in \ell_x \mathbb{Z} \oplus \ell_\xi \mathbb{Z}$ such that*

$$\gamma(\Lambda_\alpha) \cap \Lambda_{\alpha'} \neq \emptyset, \tag{4.30}$$

where $\gamma(\Lambda_\alpha)$ is the γ-translate of Λ_α. The converse is also true.

Proof. Two points $\lambda \in \Lambda_\alpha$ and $\lambda' \in \Lambda_{\alpha'}$ satisfying $\check{\lambda}^\alpha = \check{\lambda}'^{\alpha'}$ can only differ by a torus translation $\gamma \in \ell_x \mathbb{Z} \oplus \ell_\xi \mathbb{Z}$. Suppose that there exists $\gamma' \neq \gamma$ in $\ell_x \mathbb{Z} \oplus \ell_\xi \mathbb{Z}$ as well as $\lambda, \tilde{\lambda} \in \Lambda_\alpha$ such that both $\gamma(\lambda)$ and $\gamma'(\tilde{\lambda})$ are in $\in \Lambda_{\alpha'}$. The distance in position and momentum coordinates, respectively, then is smaller than $\ell_x/2$ and $\ell_\xi/2$. As a consequence, the distance between $\gamma(\lambda)$ and $\gamma'(\tilde{\lambda})$ in the position and momentum coordinates contradicts the assumptions (4.21) since $\gamma' \neq \gamma$. $\square$

For the purpose of constructing discrete scFIOs we select exactly one representative $\Lambda_{\boldsymbol{\alpha}}$ in every equivalence class $\Lambda_{\widetilde{\alpha}}$ and denote the resulting generating set by

$$\{\Gamma_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}}, \quad \Gamma_{\boldsymbol{\alpha}} = \{\phi_{\boldsymbol{\alpha}}, \mathfrak{V}_{\boldsymbol{\alpha}}, \Psi_{\boldsymbol{\alpha}}, \Lambda_{\boldsymbol{\alpha}}\}. \tag{4.31}$$

We remark that $\{\Psi_{\boldsymbol{\alpha}}, \Lambda_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}}$ is not a partition of unity for the covering space, but we still have

$$\sum_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\lambda_{\boldsymbol{\alpha}}) = 1, \tag{4.32}$$

where the points $\lambda_{\boldsymbol{\alpha}}$ can be different for the different terms in the sum, but their projections $\check{\lambda}_{\boldsymbol{\alpha}}$ to the torus are identical.

5 Semiclassical approximation of time evolution

Before constructing a semiclassical approximation $U_{\mathrm{scl}}(t)$ of the unitary time evolution $U(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} \mathrm{op}_N(H)t}$ as in (2.10), we want to clarify in what sense such an approximation is to be understood. Since only the trace of $U(t)$ enters the trace formula (2.11), we need to estimate the difference $\mathrm{tr}(U_{\mathrm{scl}}(t) - U(t))$ in a suitable way. In the following we show that this difference can be estimated using the integrated Hilbert-Schmidt norm of an error term.

Lemma 5. *Let $T > 0$ and let $U_{\text{scl}}(t)$ be differentiable for $t \in (0, T)$, such that*

$$\int_0^T \left\| \left(\mathrm{i}\hbar\partial_t - \mathrm{op}_N(H) \right) U_{\text{scl}}(t) \right\|_{\text{HS}}^2 \mathrm{d}t = O\!\left(\hbar^\beta \right), \tag{5.1}$$

for some $\beta > 0$. Assume that the initial data satisfies

$$\left\| U_{\text{scl}}(0) - \mathbb{1} \right\|_{\text{HS}} = O(\hbar^\infty). \tag{5.2}$$

Then,

$$\left| \mathrm{tr}\, (U_{\text{scl}}(t) - U(t)) \right| = O\!\left(\hbar^{\frac{\beta-3}{2}} \right). \tag{5.3}$$

Proof. Let $t \in (0, T)$ and define

$$R(t) = \left(\mathrm{i}\hbar\partial_t - \mathrm{op}_N(H) \right) U_{\text{scl}}(t) \quad \text{and} \quad Z = U_{\text{scl}}(0) - \mathbb{1}. \tag{5.4}$$

We then have

$$\partial_t \left(U(-t) U_{\text{scl}}(t) \right) = -\frac{\mathrm{i}}{\hbar} U(-t) R(t). \tag{5.5}$$

Hence,

$$
\begin{aligned}
\left| \mathrm{tr}\left(U_{\text{scl}}(t) - U(t) \right) \right| &= \left| \mathrm{tr}\left[U(t) \left(U(-t) U_{\text{scl}}(t) - \mathbb{1} \right) \right] \right| \\
&= \left| \mathrm{tr}\left[U(t) \left(Z + \int_0^t \partial_\sigma \left(U(-\sigma) U_{\text{scl}}(\sigma) \right) \mathrm{d}\sigma \right) \right] \right| \\
&\leq \mathrm{tr}\left| U(t) Z \right| + \frac{1}{\hbar} \int_0^t \mathrm{tr}\left| U(t-\sigma) R(\sigma) \right| \mathrm{d}\sigma \\
&\leq \left\| U(t) \right\|_{\text{HS}} \left\| Z \right\|_{\text{HS}} + \frac{1}{\hbar} \int_0^t \left\| U(t-\sigma) \right\|_{\text{HS}} \left\| R(\sigma) \right\|_{\text{HS}} \mathrm{d}\sigma,
\end{aligned}
\tag{5.6}
$$

where in the last step we have used that trace norm and Hilbert-Schmidt norm satisfy $\mathrm{tr}\,|AB| \leq \|A\|_{\text{HS}} \|B\|_{\text{HS}}$, see e.g. [RS75, App. to IX.4, Prop. 5]. Recalling that $\|Z\|_{\text{HS}} = O(\hbar^\infty)$, keeping in mind that $\|U(t)\|_{\text{HS}} = \sqrt{N} = O(\hbar^{-1/2})$ and using

$$\int_0^t \left\| R(\sigma) \right\|_{\text{HS}} \mathrm{d}\sigma \leq \sqrt{t \int_0^t \left\| R(\sigma) \right\|_{\text{HS}}^2 \mathrm{d}\sigma} = O(\hbar^{\beta/2}) \tag{5.7}$$

establishes the desired estimate since $t \in (0, T)$. $\qquad\square$

The construction of a semiclassical approximation $U_{\text{scl}}(t)$ involves a quantisation of the Lagrangian manifold Λ (4.4). To this end we have to introduce a variant of scFIOs [Mei94] suitable for the present context.

Definition 1. *Let Λ be the Lagrangian submanifold of $\mathbb{R}^2 \times \mathbb{T} \times \mathbb{T}$ defined in (4.4) with generating set (4.31). An operator $U_{\text{scl}}(t) \in \mathrm{Mat}_N(\mathbb{C})$, $t \in (0, T)$, is then said to be a discrete scFIO associated with the Lagrangian manifold Λ, if*

$$U_{\text{scl}}(t) = \sum_{\boldsymbol{\alpha}} U_{\boldsymbol{\alpha}}(t), \tag{5.8}$$

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such that every $U_{\boldsymbol{\alpha}}$ has an asymptotic expansion in the Borel sense [Zwo12, Section 4.4.2.],

$$U_{\boldsymbol{\alpha}}(t) \sim \sum_{k \in \mathbb{N}_0} \left(\frac{\hbar}{\mathrm{i}}\right)^k U_{\boldsymbol{\alpha},k}(t), \tag{5.9}$$

where

$$U_{\boldsymbol{\alpha},k}(t)_{mn} = \left(\frac{1}{2\pi\hbar}\right)^{\frac{J+1}{2}} \frac{\ell_x}{N} \int_{\mathbb{R}^J} a_{\boldsymbol{\alpha},k}(t, \hat{x}_m, \hat{y}_n, \boldsymbol{\theta}) \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi_{\boldsymbol{\alpha}}(t,\hat{x}_m,\hat{y}_n,\boldsymbol{\theta})} \, \mathrm{d}\boldsymbol{\theta}. \tag{5.10}$$

Here $\phi_{\boldsymbol{\alpha}} \in C^\infty(\mathbb{R} \times \mathbb{R}^2 \times \mathbb{R}^J)$ are generating functions for the local pieces $\Lambda_{\boldsymbol{\alpha}}$ of Λ, and $a_{\boldsymbol{\alpha}} \in C_0^\infty(\mathbb{R} \times \mathbb{R}^2 \times \mathbb{R}^J)$.

As the only contribution to $U_{\boldsymbol{\alpha}}(t)$ that exceeds $O(\hbar^\infty)$ in magnitude derives from the Lagrangian manifold $\Lambda_{\boldsymbol{\alpha}}$, the integral in (5.10) can be converted into an integral over either $\mathfrak{V}_{\boldsymbol{\alpha}}^{\eta}$, when $J = 1$, or over $\mathfrak{V}_{\boldsymbol{\alpha}}^{\xi,\eta}$, when $J = 2$. In the first case the integration variable is $\theta = \eta$ and we denote the generating function by $\phi^I(t, x, y, \eta) = S^I(t, x, \eta) - y\eta$. In the second case we have that $\boldsymbol{\theta} = (\xi, \eta)$ and denote the generating function by $\phi^{II}(t, x, y, \xi, \eta) = x\xi - y\eta - S^{II}(t, \xi, \eta)$. Furthermore, we choose $\Lambda_{\boldsymbol{\alpha}}$ small enough such that if $\phi_{\boldsymbol{\alpha}}$ and $\phi_{\boldsymbol{\alpha}'}$ are not of the same form ϕ^I or ϕ^{II}, $\lambda \in \check{\Lambda}_{\boldsymbol{\alpha}} \cap \check{\Lambda}_{\boldsymbol{\alpha}'}$ implies that all derivatives $\partial_x \xi(\hat{\lambda}^{\boldsymbol{\alpha}'})$, $\partial_x \xi(\hat{\lambda}^{\boldsymbol{\alpha}})$, $\partial_\xi x(\hat{\lambda}^{\boldsymbol{\alpha}'})$ and $\partial_\xi x(\hat{\lambda}^{\boldsymbol{\alpha}})$ do not vanish.

In order to determine the discrete scFIO that satisfies the estimate (5.1) to a sufficient order in $\hbar$, we choose a partition $\{\phi_{\boldsymbol{\alpha}}, \mathfrak{V}_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}}$, insert (5.8) into the left-hand side of (5.1) and define

$$R_{\boldsymbol{\alpha},k}(t) = \big(\mathrm{i}\hbar\partial_t - \mathrm{op}_N(H)\big)U_{\boldsymbol{\alpha},k}(t) \tag{5.11}$$

for each coordinate patch $\boldsymbol{\alpha}$ and order $k \in \mathbb{N}_0$. Together with (5.4) this implies

$$R(t) = \sum_{\boldsymbol{\alpha},k} \left(\frac{\hbar}{\mathrm{i}}\right)^k R_{\boldsymbol{\alpha},k}(t). \tag{5.12}$$

With Lemma 5 in mind we then have to estimate

$$\mathrm{tr}\big(R(t)^*R(t)\big) = \sum_{\boldsymbol{\alpha}',k',\boldsymbol{\alpha},k} \left(\frac{\hbar}{\mathrm{i}}\right)^{k+k'} \mathrm{tr}\big(R_{\boldsymbol{\alpha}',k'}(t)^* R_{\boldsymbol{\alpha},k}(t)\big) \tag{5.13}$$

semiclassically. This will provide conditions to be satisified by the functions $a_{\boldsymbol{\alpha},k}$ in order for $R(t)$ to vanish to any finite order in $\hbar$.

As a first step we now determine representations of $R_{\boldsymbol{\alpha},k}(t)$ for the two cases (4.7) and (4.13) separately.

5.1 The case $\phi^I(t, x, y, \eta) = S^I(t, x, \eta) - y\eta$

In this case $\Lambda_{\boldsymbol{\alpha}}$ can locally be parametrised as in (4.9) using coordinates (t, x, η). We define a function $r_{\boldsymbol{\alpha}}$ through a Taylor expansion,

$$S_{\boldsymbol{\alpha}}^I(t, x, \xi) = S_{\boldsymbol{\alpha}}^I(t, y, \xi) + \partial_x S_{\boldsymbol{\alpha}}^I(t, y, \xi)(x - y) + r_{\boldsymbol{\alpha}}(t, y, x - y, \xi), \tag{5.14}$$

such that
$$r_{\boldsymbol{\alpha}}(t, y, 0, \xi) = \partial_x r_{\boldsymbol{\alpha}}(t, y, 0, \xi) = 0. \tag{5.15}$$

We also introduce the abbreviations
$$\xi_{t,x,\eta} := \partial_x S_{\boldsymbol{\alpha}}^I(t, x, \eta) \quad \text{and} \quad y_{t,x,\eta} := \partial_\eta S_{\boldsymbol{\alpha}}^I(t, x, \eta), \tag{5.16}$$

and define the set
$$\mathfrak{V}_{\boldsymbol{\alpha}}^I := \left\{ (t, x, y, \eta); \; (t, \tau, x, y_{t,x,\eta}, \xi_{t,x,\eta}, -\eta) \in \Lambda_{\boldsymbol{\alpha}}, |y - y_{t,x,\eta}| < \epsilon \right\}. \tag{5.17}$$

The following result determines the application of $\left(\mathrm{i}\hbar\partial_t - \mathrm{op}_N(H)\right)$ to an expression of the form (5.10) with $J = 1$.

Lemma 6. *Assume that $a_{\boldsymbol{\alpha},k}^I$ is smooth in $(t, x, y, \eta) \in \mathfrak{V}_{\boldsymbol{\alpha}}$. Then there exists a smooth function $b_{\boldsymbol{\alpha},k,\hbar}$ with an asymptotic expansion in $\hbar$ that is uniform in $\mathfrak{V}_{\boldsymbol{\alpha}}^I$,*
$$b_{\boldsymbol{\alpha},k,\hbar} \sim \sum_{n=0}^{\infty} \hbar^n b_{\boldsymbol{\alpha},k,n}, \tag{5.18}$$

such that the quantity (5.11) takes the form
$$R_{\boldsymbol{\alpha},k}(t)_{mn} = \frac{1}{2\pi\hbar} \frac{\ell_x}{N} \int_{\mathfrak{V}_{\boldsymbol{\alpha}}^\eta} c_{\boldsymbol{\alpha},k}^I(t, \hat{x}_m, \hat{y}_n, \eta) \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S_{\boldsymbol{\alpha}}^I(t,\hat{x}_m,\eta) - \hat{y}_m\eta)} \, \mathrm{d}\eta. \tag{5.19}$$

Here,
$$
\begin{aligned}
c_{\boldsymbol{\alpha},k}^I(t, x, y, \eta) :=\ & \mathrm{i}\hbar(\partial_t a_{\boldsymbol{\alpha},k}^I)(t, x, y, \eta) - \frac{\hbar}{2\mathrm{i}}(\partial_x \partial_\xi H)(x, \xi_{t,x,\eta}) a_{\boldsymbol{\alpha},k}^I(t, x, y, \eta) \\
& - \frac{\hbar}{\mathrm{i}}(\partial_\xi H)(x, \xi_{t,x,\eta})(\partial_x a_{\boldsymbol{\alpha},k}^I)(t, x, y, \eta) - \left(\frac{\hbar}{\mathrm{i}}\right)^2 b_{\boldsymbol{\alpha},k,\hbar}(t, x, y, \eta).
\end{aligned}
\tag{5.20}
$$

Proof. The proof follows the standard WKB-type strategy (see e.g. [Dui96, p. 105]). We use the representation (5.10) with $J = 1$, and the variable $\boldsymbol{\theta}$ is denoted as η. The first step in evaluating (5.4) is to use Lemma 1 for the application of $\mathrm{op}_N(H)$ to $U_{\boldsymbol{\alpha},k}$ with the matrix elements $(U_{\boldsymbol{\alpha},k})_{ln}$, where n is fixed, in place of ψ_l, as well as a summation over l with $|l - m| \leq N^{\frac{1}{M}}$ in (3.2). For the phase function in (5.10) we use (5.14), and then perform a Taylor expansion (3.5) of
$$H\left(\frac{x_m + x_l}{2}, \xi\right) a_{\boldsymbol{\alpha},k}^I(t, \hat{x}_l, \hat{y}_n, \eta) \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} r_{\boldsymbol{\alpha}}(t, \hat{x}_l, \hat{x}_m - \hat{x}_l, \eta)} \tag{5.21}$$

in $x_m - x_l$. We integrate by parts, use (3.6) and the periodicity of H, and obtain an asymptotic expansion in powers of $\hbar$ multiplied by $\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\xi - \partial_x S^I(t,\hat{x}_m,\eta))(x_m - x_l)}$. If the sum over l extended over all $l \in \mathbb{Z}$, it would be a Fourier series, with the ξ-integrals as Fourier coefficients. The latter, however, are of size $O(|m - l|^{-\infty})$. Hence, while adding an error of size $O(\hbar^\infty)$ one can indeed extend the restricted sum over l to all $l \in \mathbb{Z}$. The resulting Fourier series can be evaluated, thereby replacing the variable ξ with $\xi_{t,\hat{x}_m,\eta}$.

When applying $\mathrm{i}\hbar\partial_t$ to $U_{\boldsymbol{\alpha},k}$ we use the Hamilton-Jacobi equation (4.8) and evaluate the coefficients of the lowest powers in $\hbar$. This gives (5.20) by noting that $\mathrm{supp}\, a_{\boldsymbol{\alpha},k}^I \subset \mathfrak{V}_{\boldsymbol{\alpha}}$. $\square$

For later reference we note that the quantity (5.20), viewed as the coefficient function of a half-density, can be identified as a Lie-derivative along the Hamiltonian vector field generated by the (extended) classical Hamiltonian,

$$c_{\boldsymbol{\alpha},k}^{I}(\lambda)\mathrm{d}\lambda^{\frac{1}{2}} = \mathrm{i}\hbar\mathcal{L}_{X_{H_{\mathrm{ext}}}}\left(a_{\boldsymbol{\alpha},k}^{I}(\lambda)\mathrm{d}\lambda^{\frac{1}{2}}\right) + O(\hbar^{2}), \tag{5.22}$$

see [Zwo12, (10.2.22), (10.2.27)].

5.2 The case $\phi^{II}(t,x,y,\xi,\eta) = x\xi - y\eta - S^{II}(t,\xi,\eta)$

In the remaining case, a parametrisation of $\Lambda_{\boldsymbol{\alpha}}$ in the sense of (4.12) can be achieved with coordinates (t,ξ,η). We also introduce the abbreviations

$$x_{t,\xi,\eta} := \partial_{\xi}S_{\boldsymbol{\alpha}}^{II}(t,\xi,\eta) \quad \text{and} \quad y_{t,\xi,\eta} := -\partial_{\eta}S_{\boldsymbol{\alpha}}^{II}(t,\xi,\eta), \tag{5.23}$$

and choose a smooth function $\kappa_{\epsilon} : \mathbb{R} \to [0,1]$ satisfying

$$\kappa_{\epsilon}(x) = \begin{cases} 0, & |x| > \frac{2\epsilon}{3}, \\ 1, & |x| < \frac{\epsilon}{3}, \end{cases} \tag{5.24}$$

that is used to localise around initial and final points (5.23) of classical trajectories. We now assume that $A_{\boldsymbol{\alpha},k}$ is a function on $\Lambda_{\boldsymbol{\alpha}}$, therefore depending on the variables (t,ξ,η), and define

$$a_{\boldsymbol{\alpha},k}^{II}(t,\hat{x}_m,\hat{y}_n,\xi,\eta) = \kappa_{\epsilon}(\hat{x}_m - x_{t,\xi,\eta})\kappa_{\epsilon}(\hat{y}_n - y_{t,\xi,\eta})A_{\boldsymbol{\alpha},k}(t,\xi,\eta). \tag{5.25}$$

This function is localised on the set

$$\begin{aligned}\mathfrak{V}_{\boldsymbol{\alpha},\epsilon}^{II} :=\big\{&(t,x,y,\xi,\eta);\ (t,\tau,x_{t,\xi,\eta},\xi,y_{t,\xi,\eta},-\eta) \in \Lambda_{\boldsymbol{\alpha}},\\ &|x - x_{t,\xi,\eta}| < \epsilon,\ |y - y_{t,x,\eta}| < \epsilon\big\}.\end{aligned} \tag{5.26}$$

Note that here, in contrast to the previous case (5.17), we admit the variables x,y to be from a (small) neighbourhood of $\Lambda_{\boldsymbol{\alpha}}$.

In the present case, the application of $\mathrm{i}\hbar\partial_t - \mathrm{op}_N(H)$ to the respective expression of the form (5.10) gives the following results.

Lemma 7. *Using a function of the form* (5.25) *in* (5.10) *one gets*

$$R_{\boldsymbol{\alpha},k}(t)_{mn} = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\frac{\ell_x}{N}\int_{\mathfrak{V}_{\boldsymbol{\alpha}}^{\xi,\eta}} c_{\boldsymbol{\alpha},k}^{II}(t,\hat{x}_m,\hat{y}_n,\xi,\eta)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\hat{x}_m\xi-\hat{y}_n\eta-S_{\boldsymbol{\alpha}}^{II}(t,\xi,\eta))}\,\mathrm{d}\xi\mathrm{d}\eta, \tag{5.27}$$

where

$$\begin{aligned}c_{\boldsymbol{\alpha},k}^{II}(t,x,y,\xi,\eta) :=\ &\mathrm{i}\hbar\partial_t a_{\boldsymbol{\alpha},k}^{II}(t,x,y,\xi,\eta) + \frac{\hbar}{\mathrm{i}}(\partial_x H)(x_{t,\xi,\eta},\xi)(\partial_{\xi}a_{\boldsymbol{\alpha},k}^{II})(t,x,y,\xi,\eta)\\ &+ \frac{\hbar}{2\mathrm{i}}(\partial_x\partial_{\xi}H)(x_{t,\xi,\eta},\xi)a_{\boldsymbol{\alpha},k}^{II}(t,x,y,\xi,\eta) + O(\hbar^{2}).\end{aligned} \tag{5.28}$$

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Proof. Here the representation (5.10) requires $J = 2$ and the integration variables are $\boldsymbol{\theta} = (\xi, \eta)$. The first step in evaluating (5.4) consists of using Lemma 2 to evaluate the application of $\mathrm{op}_N(H)$ to $U_{\boldsymbol{\alpha},k}$. Here, again, the matrix elements $(U_{\boldsymbol{\alpha},k})_{ln}$ replace ψ_l and the summation extends over l with $|l - m| \le N^{\frac{1}{M}}$ such that n is fixed. This sum can be evaluated with Proposition 5. This gives (5.27), where

$$
\begin{aligned}
c_{\boldsymbol{\alpha},k}^{II}(t, \hat{x}_m, \hat{y}_n, \xi, \eta) = {}& \mathrm{i}\hbar \partial_t a_{\boldsymbol{\alpha},\hbar}^{II}(t, \hat{x}_m, \hat{y}_n, \xi, \eta) \\
& + \big(H(x_{t,\xi,\eta}, \xi) - H(\hat{x}_m, \xi)\big) a_{\boldsymbol{\alpha},k}^{II}(t, \hat{x}_m, \hat{y}_n, \xi, \eta) \\
& - \frac{\hbar}{2\mathrm{i}}(\partial_x \partial_\xi H)(\hat{x}_m, \xi) a_{\boldsymbol{\alpha},k}^{II}(t, \hat{x}_m, \hat{y}_n, \xi, \eta) + O\big(\hbar^2\big).
\end{aligned}
\tag{5.29}
$$

We now employ a Taylor expansion (see also [Hör85b, p. 23]),

$$
\begin{aligned}
\big(H(\hat{x}_m, \xi) - H(x_{t,\xi,\eta}, \xi)\big) \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi_{\boldsymbol{\alpha}}^{II}(t,\hat{x}_m,\hat{y}_n,\xi,\eta)} \\
= p_{\boldsymbol{\alpha}}(t, \hat{x}_m, \xi, \eta)\big(\hat{x}_m - x_{t,\xi,\eta}\big) \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi_{\boldsymbol{\alpha}}^{II}(t,\hat{x}_m,\hat{y}_n,\xi,\eta)} \\
= p_{\boldsymbol{\alpha}}(t, \hat{x}_m, \xi, \eta)\frac{\hbar}{\mathrm{i}}\partial_\xi \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi_{\boldsymbol{\alpha}}^{II}(t,\hat{x}_m,\hat{y}_n,\xi,\eta)},
\end{aligned}
\tag{5.30}
$$

use this in (5.29) and perform an integration by parts in the variable ξ. By [Hör85b, p. 24] one sees that this leads to (5.28). $\qquad\square$

We remark that, in analogy to (5.22), on $\Lambda_{\boldsymbol{\alpha}}$,

$$
c_{\boldsymbol{\alpha},k}^{II}(\lambda)\mathrm{d}\lambda^{\frac{1}{2}} = \mathrm{i}\hbar\mathcal{L}_{X_{H_{\mathrm{ext}}}}\left(A_{\boldsymbol{\alpha},k}(\lambda)\mathrm{d}\lambda^{\frac{1}{2}}\right) + O(\hbar^2),
\tag{5.31}
$$

see [Zwo12, (10.2.22), (10.2.27)].

5.3 Some auxiliary results

With (5.13) in mind we now estimate

$$
\int_0^T \sum_{n,m=0}^{N-1} \overline{R_{\boldsymbol{\alpha}',k'}(t)}_{nm} R_{\boldsymbol{\alpha},k}(t)_{nm}\ \mathrm{d}t
\tag{5.32}
$$

for all pairs $(\boldsymbol{\alpha}, \boldsymbol{\alpha}')$ and fixed $T > 0$. There are four cases, depending on whether Lemma 6 or Lemma 7 applies to $R_{\boldsymbol{\alpha},k}$ and $R_{\boldsymbol{\alpha}',k'}$, respectively. We use the notations introduced in Sections 5.1 and 5.2, in particular those for the various amplitude and phase functions.

We recall the definition (4.23) of the sets Λ_α, as well as the representatives $\Lambda_{\boldsymbol{\alpha}}$ of equivalence classes $\Lambda_{\widetilde{\alpha}}$ (with respect to translations by $\ell_x\mathbb{Z} \oplus \ell_\xi\mathbb{Z}$) as described around (4.31). We then define the set

$$
\Lambda_{\boldsymbol{\alpha}'\boldsymbol{\alpha}} := \left\{\hat{\lambda}^{\boldsymbol{\alpha}'};\ \lambda \in \check{\Lambda}_{\boldsymbol{\alpha}} \cap \check{\Lambda}_{\boldsymbol{\alpha}'}\right\}.
\tag{5.33}
$$

We also use the interval $I_\beta \subset [0, T]$ as defined in (4.22)-(4.24).

The four cases that occur are covered in the Lemmata 8–11, the first one being:

Lemma 8. *Let $R_{\boldsymbol{\alpha},k}$ be of the form* (5.19) *and $R_{\boldsymbol{\alpha}',k'}$ be of the form* (5.27), *then*

$$\frac{1}{(2\pi\hbar)^{\frac{5}{2}}}\left(\frac{\ell_x}{N}\right)^2 \sum_{m,n=0}^{N-1} \int_{I_\beta} \int_{\mathfrak{V}_{\boldsymbol{\alpha}'}^{\xi',\eta'}} \int_{\mathfrak{V}_{\boldsymbol{\alpha}}^{\eta}} \overline{c_{\boldsymbol{\alpha}',k'}^{II}(t,\hat{x}_m,\hat{y}_n,\xi',\eta')}\, c_{\boldsymbol{\alpha},k}^I(t,\hat{x}_m,\hat{y}_n,\eta)$$

$$e^{\frac{i}{\hbar}(\phi_{\boldsymbol{\alpha}}^I(t,\hat{x}_m,\hat{y}_n,\eta)-\phi_{\boldsymbol{\alpha}'}^{II}(t,\hat{x}_m,\hat{y}_n,\xi',\eta'))}\mathrm{d}\eta\mathrm{d}\xi'\mathrm{d}\eta'\mathrm{d}t \tag{5.34}$$

$$= \frac{1}{2\pi\hbar}\int_{\Lambda_{\boldsymbol{\alpha}'\boldsymbol{\alpha}}} g_{\boldsymbol{\alpha}',k',\hbar}\, e^{\frac{i\pi}{4}\operatorname{sgn}\operatorname{Hess}\phi_{\boldsymbol{\alpha}}^I}|\partial_x\xi|^{-\frac{1}{2}}e_{\boldsymbol{\alpha},k,\hbar}\mathrm{d}t\mathrm{d}\xi'\mathrm{d}\eta' + O(\hbar^\infty),$$

where $g_{\boldsymbol{\alpha}',k',\hbar}$ and $e_{\boldsymbol{\alpha},k,\hbar}$ are coefficients of half-densities on $\Lambda_{\boldsymbol{\alpha}'\boldsymbol{\alpha}}$ possessing asymptotic expansions in $\hbar$ that are uniform in $t \in [0,T]$. In particular,

$$e_{\boldsymbol{\alpha},k,\hbar}(\lambda) \sim \left(i\hbar\mathcal{L}_{X_{H_{\mathrm{ext}}}} a_{\boldsymbol{\alpha},k}(\lambda) + \sum_{n\geq 2}\hbar^n e_{\boldsymbol{\alpha},k,n}(\lambda)\right), \tag{5.35}$$

with $\lambda = (t,\xi',\eta') \in \Lambda_{\boldsymbol{\alpha}'\boldsymbol{\alpha}}$.

Proof. We first apply Lemma 15 to the sums over n and m on the left-hand side of (5.34). Up to an error term of size $O(\hbar^\infty)$ this gives two additional integrals,

$$\frac{1}{(2\pi\hbar)^{\frac{5}{2}}}\int_{I_\beta}\int_0^{\ell_x}\int_0^{\ell_x}\int_{\mathfrak{V}_{\boldsymbol{\alpha}'}^{\xi',\eta'}}\int_{\mathfrak{V}_{\boldsymbol{\alpha}}^{\eta}} \overline{c_{\boldsymbol{\alpha}',k'}^{II}}\, c_{\boldsymbol{\alpha},k}^I e^{\frac{i}{\hbar}(\phi_{\boldsymbol{\alpha}}^I-\phi_{\boldsymbol{\alpha}'}^{II}+sx\ell_\xi-sy\ell_\xi)}\mathrm{d}\eta\mathrm{d}\xi'\mathrm{d}\eta'\mathrm{d}x\mathrm{d}y\mathrm{d}t \tag{5.36}$$

where $s \in \mathbb{Z}$ is determined by Lemma 4 and Lemma 15. We then use the stationary phase theorem to evaluate the integrals over the variables (x,y,η). In order to determine the stationary points we use Lemma 4 and get

$$\begin{aligned}
\partial_y(\phi_{\boldsymbol{\alpha}}^I - \phi_{\boldsymbol{\alpha}'}^{II}) - s\ell_\xi = 0 &\quad\Leftrightarrow\quad \eta' = \eta + s\ell_\xi \\
\partial_x(\phi_{\boldsymbol{\alpha}}^I - \phi_{\boldsymbol{\alpha}'}^{II}) + s\ell_\xi = 0 &\quad\Leftrightarrow\quad \xi' = \partial_x S_{\boldsymbol{\alpha}}^I(t,x,\eta) + s\ell_\xi \\
\partial_\eta(\phi_{\boldsymbol{\alpha}}^I - \phi_{\boldsymbol{\alpha}'}^{II}) = 0 &\quad\Leftrightarrow\quad \hat{y}^{\boldsymbol{\alpha}} = \partial_\eta S_{\boldsymbol{\alpha}}^I(t,x,\eta).
\end{aligned} \tag{5.37}$$

With regard to the last equation we remark that the lifts $\hat{y}^{\boldsymbol{\alpha}}$ and $\hat{y}^{\boldsymbol{\alpha}'}$ to the covering space can only differ (locally) by a constant $r\ell_x$, $r \in \mathbb{Z}$.

The equations (5.37) can be solved to find $x(t,\xi',\eta')$ and $y(t,\xi',\eta')$. They determine the set of stationary points that can either be given in the form

$$\left(t, x(t,\xi',\eta') - r\ell_x, y(t,\xi',\eta') - r\ell_x, \eta' - s\ell_\xi\right) \in \mathfrak{V}_{\boldsymbol{\alpha}}^I, \tag{5.38}$$

or

$$\left(t, x(t,\xi',\eta'), y(t,\xi',\eta'), \xi',\eta'\right) \in \mathfrak{V}_{\boldsymbol{\alpha}'}^{II}. \tag{5.39}$$

Due to Lemma 3 the Hessian of the total phase, as a function of the variables (x,y,η), on the left-hand side of (5.34) is given by

$$\operatorname{Hess}_{x,y,\eta}(\phi_{\boldsymbol{\alpha}}^I - \phi_{\boldsymbol{\alpha}'}^{II}) = \operatorname{Hess}\phi_{\boldsymbol{\alpha}}^I = \begin{pmatrix} \partial_x^2 S_{\boldsymbol{\alpha}}^I & 0 & \partial_{x,\eta}S_{\boldsymbol{\alpha}}^I \\ 0 & 0 & -1 \\ \partial_{x,\eta}S_{\boldsymbol{\alpha}}^I & -1 & \partial_\eta^2 S_{\boldsymbol{\alpha}}^I \end{pmatrix}. \tag{5.40}$$

Recall that our definition of Hessians never involves derivatives with respect to t. Hence,

$$\det \operatorname{Hess}_{x,y,\eta}(\phi_{\boldsymbol{\alpha}}^I - \phi_{\boldsymbol{\alpha}'}^{II}) = -\partial_x^2 S_{\boldsymbol{\alpha}}^I = -\partial_x \xi. \tag{5.41}$$

We recall that we have chosen the partitions small enough so that this derivative does not vanish. Moreover,

$$(\phi_{\boldsymbol{\alpha}}^I - \phi_{\boldsymbol{\alpha}'}^{II})(\lambda) = W(\lambda) - W(\lambda) = 0, \tag{5.42}$$

and

$$\operatorname{sgn} \operatorname{Hess}_{x,y,\eta}(\phi_{\boldsymbol{\alpha}}^I - \phi_{\boldsymbol{\alpha}'}^{II})(\lambda) = \operatorname{sgn} \operatorname{Hess} \phi_{\boldsymbol{\alpha}}^I(\lambda). \tag{5.43}$$

An application of the stationary phase theorem then gives (5.34). The asymptotic expansion (5.35) follows from (5.22). $\square$

The next case is:

Lemma 9. *Let both $R_{\boldsymbol{\alpha},k}$ and $R_{\boldsymbol{\alpha}',k'}$ be of the form (5.27), then*

$$
\begin{aligned}
\frac{1}{(2\pi\hbar)^3} &\left(\frac{\ell_x}{N}\right)^2 \sum_{m,n=0}^{N-1} \int_{I_\beta} \int_{\mathfrak{Y}_{\boldsymbol{\alpha}'}^{\xi',\eta'}} \int_{\mathfrak{Y}_{\boldsymbol{\alpha}}^{\xi\eta}} \overline{c_{\boldsymbol{\alpha}',k'}^{II}(t,\hat{x}_m,\hat{y}_n,\xi',\eta')} \, c_{\boldsymbol{\alpha},k}^{II}(t,\hat{x}_m,\hat{y}_n,\xi,\eta) \\
&\qquad \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\phi_{\boldsymbol{\alpha}}^{II}(t,\hat{x}_m,\hat{y}_n,\xi,\eta) - \phi_{\boldsymbol{\alpha}'}^{II}(t,\hat{x}_m,\hat{y}_n,\xi',\eta'))} \mathrm{d}\xi \mathrm{d}\eta \mathrm{d}\xi' \mathrm{d}\eta' \mathrm{d}t \\
&= \frac{1}{2\pi\hbar} \int_{\Lambda_{\boldsymbol{\alpha}'\boldsymbol{\alpha}}} g_{\boldsymbol{\alpha}',k',\hbar} \mathrm{e}^{\frac{\mathrm{i}\pi}{4} \operatorname{sgn} \operatorname{Hess} \phi_{\boldsymbol{\alpha}}^{II}} e_{\boldsymbol{\alpha},k,\hbar} \mathrm{d}t \mathrm{d}\xi' \mathrm{d}\eta' + O(\hbar^\infty),
\end{aligned}
\tag{5.44}
$$

where $g_{\boldsymbol{\alpha}',k',\hbar}$ and $e_{\boldsymbol{\alpha},k,\hbar}$ are coefficients of half-densities on $\Lambda_{\boldsymbol{\alpha}'\boldsymbol{\alpha}}$ possessing asymptotic expansions in $\hbar$ that are uniform in $t \in [0,T]$. In particular,

$$e_{\boldsymbol{\alpha},k,\hbar}(\lambda) \sim \left(\mathrm{i}\hbar \mathcal{L}_{X_{H_{\mathrm{ext}}}} a_{\boldsymbol{\alpha},k}(\lambda) + \sum_{n\geq 2} \hbar^n e_{\boldsymbol{\alpha},k,n}(\lambda)\right), \tag{5.45}$$

with $\lambda = (t,\xi',\eta') \in \Lambda_{\boldsymbol{\alpha}'\boldsymbol{\alpha}}$.

Proof. We use a similar strategy as in the proof for Lemma 8, and first perform the sum over n and m by applying Lemma 15. With the appropriate modifications, including an additional integration over the variable ξ and a pre-factor $1/(2\pi\hbar)^3$, this gives a result similar to (5.36). We then apply the stationary phase theorem to the integrations over the variables (x,y,ξ,η). The conditions determining stationary points of the phase function are

$$
\begin{aligned}
\partial_x(\phi_{\boldsymbol{\alpha}}^{II} - \phi_{\boldsymbol{\alpha}'}^{II}) + s\ell_\xi = 0 &\quad\Leftrightarrow\quad \xi + s\ell_\xi = \xi' \\
\partial_y(\phi_{\boldsymbol{\alpha}}^{II} - \phi_{\boldsymbol{\alpha}'}^{II}) - s\ell_\xi = 0 &\quad\Leftrightarrow\quad \eta + s\ell_\xi = \eta' \\
\partial_\xi(\phi_{\boldsymbol{\alpha}}^{II} - \phi_{\boldsymbol{\alpha}'}^{II}) = 0 &\quad\Leftrightarrow\quad \partial_\xi S_{\boldsymbol{\alpha}}^{II}(t,\xi,\eta) = \hat{x}^{\boldsymbol{\alpha}} \\
\partial_\eta(\phi_{\boldsymbol{\alpha}}^{II} - \phi_{\boldsymbol{\alpha}'}^{II}) = 0 &\quad\Leftrightarrow\quad -\partial_\eta S_{\boldsymbol{\alpha}}^{II}(t,\xi,\eta) = \hat{y}^{\boldsymbol{\alpha}}.
\end{aligned}
\tag{5.46}
$$

These equations can be solved for $x(t, \xi', \eta')$ and $y(t, \xi', \eta')$. The set of stationary points can be either given as

$$\big(t, x(t, \xi', \eta') - r\ell_x, y(t, \xi', \eta') - r\ell_x, \xi' - s\ell_\xi, \eta' - s\ell_\xi\big) \in \mathfrak{V}_{\boldsymbol{\alpha}}^{II}, \tag{5.47}$$

or as

$$\big(t, x(t, \xi', \eta'), y(t, \xi', \eta'), \xi', \eta'\big) \in \mathfrak{V}_{\boldsymbol{\alpha}'}^{II}. \tag{5.48}$$

The Hessian of the phase function is

$$\mathrm{Hess}_{x,y,\xi,\eta}(\phi_{\boldsymbol{\alpha}}^{II} - \phi_{\boldsymbol{\alpha}'}^{II}) = \mathrm{Hess}\,\phi_{\boldsymbol{\alpha}}^{II} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & -\partial_\xi^2 S_{\boldsymbol{\alpha}}^{II} & -\partial_{\eta\xi} S_{\boldsymbol{\alpha}}^{II} \\ 0 & -1 & -\partial_{\xi\eta} S_{\boldsymbol{\alpha}}^{II} & -\partial_\eta^2 S_{\boldsymbol{\alpha}}^{II} \end{pmatrix}, \tag{5.49}$$

so that

$$\det \mathrm{Hess}_{x,y,\xi,\eta}(\phi_{\boldsymbol{\alpha}}^{II} - \phi_{\boldsymbol{\alpha}'}^{II}) = 1. \tag{5.50}$$

The stationary phase theorem, together with (5.31), now gives the result. $\qquad\square$

The third case is:

Lemma 10. *Let both $R_{\boldsymbol{\alpha},k}$ and $R_{\boldsymbol{\alpha}',k'}$ be of the form (5.19), then*

$$\frac{1}{(2\pi\hbar)^2} \left(\frac{\ell_x}{N}\right)^2 \sum_{m,n=0}^{N-1} \int_{I_\beta} \int_{\mathfrak{V}_{\boldsymbol{\alpha}'}^{\eta'}} \int_{\mathfrak{V}_{\boldsymbol{\alpha}}^{\eta}} \overline{c_{\boldsymbol{\alpha}',k'}^I(t, \hat{x}_m, \hat{y}_n, \eta')}\, c_{\boldsymbol{\alpha},k}^I(t, \hat{x}_m, \hat{y}_n, \eta)$$
$$e^{\frac{i}{\hbar}(\phi_{\boldsymbol{\alpha}}^I(t,\hat{x}_m,\hat{y}_n,\eta) - \phi_{\boldsymbol{\alpha}'}^I(t,\hat{x}_m,\hat{y}_n,\eta'))}\mathrm{d}\eta\mathrm{d}\eta'\mathrm{d}t \tag{5.51}$$
$$= \frac{1}{2\pi\hbar} \int_{\Lambda_{\boldsymbol{\alpha}'\boldsymbol{\alpha}}} g_{\boldsymbol{\alpha}',k',\hbar} e^{\frac{i\pi}{4} f_{\boldsymbol{\alpha}}} e_{\boldsymbol{\alpha},k,\hbar}\mathrm{d}t\mathrm{d}x'\mathrm{d}\eta' + O(\hbar^\infty),$$

where $g_{\boldsymbol{\alpha}',k',\hbar}$ and $e_{\boldsymbol{\alpha},k,\hbar}$ are coefficients of half-densities on $\Lambda_{\boldsymbol{\alpha}'\boldsymbol{\alpha}}$ possessing asymptotic expansions in $\hbar$ that are uniform in $t \in [0,T]$. In particular,

$$e_{\boldsymbol{\alpha},k,\hbar}(\lambda) \sim \left(i\hbar \mathcal{L}_{X_{H_{\mathrm{ext}}}} a_{\boldsymbol{\alpha},k}(\lambda) + \sum_{n\geq 2} \hbar^n e_{\boldsymbol{\alpha},k,n}(\lambda)\right), \tag{5.52}$$

with $\lambda = (t, x', \eta') \in \Lambda_{\boldsymbol{\alpha}'\boldsymbol{\alpha}}$. Moreover,

$$f_{\boldsymbol{\alpha}} := \mathrm{sgn}\,\mathrm{Hess}_{y,\eta}\,\phi_{\boldsymbol{\alpha}}^I = \mathrm{sgn}\begin{pmatrix} 0 & -1 \\ -1 & \partial_\eta^2 S_{\boldsymbol{\alpha}}^I(\lambda) \end{pmatrix}. \tag{5.53}$$

Proof. We again employ the same strategy as in the proofs of Lemmata 8 and 9. The sums over n and m are evaluated with the help of Lemma 15 and, with some modifications, this gives a result similar to (5.36). There is integration over the variable ξ' and, for convenience, we name the integration variables introduced by Lemma 15 as x' and y. Next

we apply the stationary phase theorem to the integrations over the variables (y, η). The conditions determining stationary points of the phase function are

$$
\begin{aligned}
\partial_y(\phi_{\boldsymbol{\alpha}}^I - \phi_{\boldsymbol{\alpha}'}^I) - s\ell_\xi = 0 &\quad \Leftrightarrow \quad \eta' = \eta + s\ell_\xi \\
\partial_\eta(\phi_{\boldsymbol{\alpha}}^I - \phi_{\boldsymbol{\alpha}'}^I) = 0 &\quad \Leftrightarrow \quad \hat{y}^{\boldsymbol{\alpha}} = \partial_\eta S_{\boldsymbol{\alpha}}^I(t, x', \eta),
\end{aligned}
\tag{5.54}
$$

and can be solved for $y(t, x', \eta')$. The stationary points can therefore be given either in the form

$$
\left(t, x - r\ell_x, y(t, x', \eta') - r\ell_x, \eta' - s\ell_\xi\right) \in \mathfrak{V}_{\boldsymbol{\alpha}}^I
\tag{5.55}
$$

or as

$$
\left(t, x', y\left(t, x', \eta'\right), \eta'\right) \in \mathfrak{V}_{\boldsymbol{\alpha}'}^I.
\tag{5.56}
$$

The Hessian that is required by the stationary phase theorem is the one given in (5.53), hence

$$
\det \operatorname{Hess}_{y,\eta}(\phi_{\boldsymbol{\alpha}}^I - \phi_{\boldsymbol{\alpha}'}^I) = -1.
\tag{5.57}
$$

$\square$

Finally, the last case is:

Lemma 11. *Let $R_{\boldsymbol{\alpha},k}$ be of the form (5.27) and $R_{\boldsymbol{\alpha}',k'}$ be of the form (5.19), then*

$$
\frac{1}{(2\pi\hbar)^{\frac{5}{2}}} \left(\frac{\ell_x}{N}\right)^2 \sum_{m,n=0}^{N-1} \int_{I_\beta} \int_{\mathfrak{V}_{\boldsymbol{\alpha}'}^{\eta'}} \int_{\mathfrak{V}_{\boldsymbol{\alpha}}^{\xi,\eta}} \overline{c_{\boldsymbol{\alpha}',k'}^I(t, \hat{x}_m, \hat{y}_n, \eta')} \, c_{\boldsymbol{\alpha},k}^{II}(t, \hat{x}_m, \hat{y}_n, \xi, \eta)
$$

$$
\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\phi_{\boldsymbol{\alpha}}^{II}(t, \hat{x}_m, \hat{y}_n, \xi, \eta) - \phi_{\boldsymbol{\alpha}'}^I(t, \hat{x}_m, \hat{y}_n, \eta'))} \mathrm{d}\xi \mathrm{d}\eta \mathrm{d}\eta' \mathrm{d}t
\tag{5.58}
$$

$$
= \frac{1}{2\pi\hbar} \int_{\Lambda_{\boldsymbol{\alpha}'\boldsymbol{\alpha}}} g_{\boldsymbol{\alpha}',k',\hbar} \mathrm{e}^{\frac{\mathrm{i}\pi}{4} f_{\boldsymbol{\alpha}}'} |\partial_\xi x|^{-\frac{1}{2}} e_{\boldsymbol{\alpha},k,\hbar} \mathrm{d}t\mathrm{d}\xi'\mathrm{d}\eta' + O(\hbar^\infty),
$$

where $g_{\boldsymbol{\alpha}',k',\hbar}$ and $e_{\boldsymbol{\alpha},k,\hbar}$ are coefficients of half-densities on $\Lambda_{\boldsymbol{\alpha}'\boldsymbol{\alpha}}$ possessing asymptotic expansions in $\hbar$ that are uniform in $t \in [0, T]$. In particular,

$$
e_{\boldsymbol{\alpha},k,\hbar}(\lambda) \sim \left(\mathrm{i}\hbar \mathcal{L}_{X_{H_{\mathrm{ext}}}} a_{\boldsymbol{\alpha},k}(\lambda) + \sum_{n \geq 2} \hbar^n e_{\boldsymbol{\alpha},k,n}(\lambda)\right),
\tag{5.59}
$$

with $\lambda = (t, \xi', \eta') \in \Lambda_{\boldsymbol{\alpha}'\boldsymbol{\alpha}}$. Moreover,

$$
f_{\boldsymbol{\alpha}}' := \operatorname{sgn} \operatorname{Hess}_{y,\xi,\eta} \phi_{\boldsymbol{\alpha}}^{II} = \operatorname{sgn} \begin{pmatrix} 0 & 0 & -1 \\ 0 & -\partial_\xi^2 S_{\boldsymbol{\alpha}}^{II} & -\partial_{\xi\eta} S_{\boldsymbol{\alpha}}^{II} \\ -1 & -\partial_{\xi\eta} S_{\boldsymbol{\alpha}}^{II} & -\partial_\eta^2 S_{\boldsymbol{\alpha}}^{II} \end{pmatrix}.
\tag{5.60}
$$

Proof. We again employ the same strategy as in the proofs of Lemmata 8–10. The sums over n and m are evaluated with the help of Lemma 15 and, with some modifications, this gives a result similar to (5.36). Here we apply the stationary phase theorem to the

integrations over the variables (y, ξ, η). The conditions determining stationary points of the phase function are

$$
\begin{aligned}
\partial_y(\phi_{\boldsymbol{\alpha}}^{II} - \phi_{\boldsymbol{\alpha}'}^{II}) = 0 &\quad \Leftrightarrow \quad \eta' = \eta + s\ell_\xi \\
\partial_\eta(\phi_{\boldsymbol{\alpha}}^{II} - \phi_{\boldsymbol{\alpha}'}^{II}) = 0 &\quad \Leftrightarrow \quad \hat{y}^{\boldsymbol{\alpha}} = \partial_\eta S_{\boldsymbol{\alpha}}^{II}(t, \xi, \eta) \\
\partial_\xi(\phi_{\boldsymbol{\alpha}}^{II} - \phi_{\boldsymbol{\alpha}'}^{II}) = 0 &\quad \Leftrightarrow \quad \hat{x}^{\boldsymbol{\alpha}} = \partial_\xi S_{\boldsymbol{\alpha}}^{II}(t, \xi, \eta).
\end{aligned}
\tag{5.61}
$$

These equations can be solved for $x(t, \xi', \eta')$ and $y(t, \xi', \eta')$. They determine the set of stationary points that can either be given in the form

$$
\left(t, x(t, \xi', \eta') - r\ell_x, y(t, \xi', \eta') - r\ell_x, \xi' - s\ell_\xi, \eta' - s\ell_\xi \right) \in \mathfrak{V}_{\boldsymbol{\alpha}}^{II},
\tag{5.62}
$$

or

$$
\left(t, x(t, \xi', \eta'), y(t, \xi', \eta'), \eta' \right) \in \mathfrak{V}_{\boldsymbol{\alpha}'}^{I}.
\tag{5.63}
$$

In order to apply the stationary phase theorem we still need the determinant of the Hessian as given in (5.60), i.e.

$$
\det \mathrm{Hess}_{y, \xi, \eta}(\phi_{\boldsymbol{\alpha}}^{II} - \phi_{\boldsymbol{\alpha}'}^{II}) = \partial_\xi^2 S_{\boldsymbol{\alpha}}^{II} = \partial_\xi x.
\tag{5.64}
$$

We recall that we have chosen the partitions such that $\partial_\xi x \neq 0$. $\qquad\square$

5.4 Semiclassical construction

We now have all the means necessary for the construction of a discrete scFIO as in Definition 1 that satisfies the estimate (5.3) to any desired (positive) power in $\hbar$. In order to achieve this, Lemma 5 implies that we need an estimate

$$
\int_0^T \mathrm{tr}\, R(t)^* R(t) \mathrm{d}t = O(\hbar^\beta)
\tag{5.65}
$$

with $\beta > 3$. To get this estimate, we perform the double sum over $\boldsymbol{\alpha}$ and $\boldsymbol{\alpha}'$ in (5.13) by first fixing $\boldsymbol{\alpha}'$ and summing over $\boldsymbol{\alpha}$, and subsequently summing over $\boldsymbol{\alpha}'$.

In the following approach the Lemmata 8–11 will be used for the summation over $\boldsymbol{\alpha}$, and this should only involve the densities $e_{\boldsymbol{\alpha}, k, \hbar}$. However, the Lemmata 10 and 11 show that for fixed $\boldsymbol{\alpha}'$ this is not necessarily possible as the phases have to be chosen correctly. In order to make such an approach feasible we therefore require that $a_{\boldsymbol{\alpha}, k}^I$ is of the form

$$
a_{\boldsymbol{\alpha}, k}^I(t, x, y, \eta) = \kappa_\epsilon(y - y_{t, x, \eta}) A_{\boldsymbol{\alpha}, k}^I(t, x, \eta),
\tag{5.66}
$$

with $A_{\boldsymbol{\alpha}, k}^I$ defined locally on Λ. Moreover, we require that the phases of the amplitude functions $a_{\boldsymbol{\alpha}, k}^{I/II}$ are given by $\pi/2$ times the Maslov index (4.20), such that

$$
a_{\boldsymbol{\alpha}, k}^{I/II} e^{-\frac{i\pi}{2} \mu(\gamma(\lambda))} \in \mathbb{R}.
\tag{5.67}
$$

For this to be possible we need to investigate the phases $f_{\boldsymbol{\alpha}}$ and $f_{\boldsymbol{\alpha}}'$ in (5.51) and (5.58) in combination with an additional phase coming from the Maslov bundle contribution.

Lemma 12. *Let $\lambda \in \Lambda_{\boldsymbol{\alpha'\alpha_1}} \cap \Lambda_{\boldsymbol{\alpha'\alpha_2}}$, and let $f_{\boldsymbol{\alpha_1}}$ and $f'_{\boldsymbol{\alpha_2}}$ be as defined in (5.51) and (5.58), respectively. Then*

$$- \operatorname{sgn} \operatorname{Hess} \phi^I_{\boldsymbol{\alpha_1}}(\lambda) + f_{\boldsymbol{\alpha_1}}(\lambda) = - \operatorname{sgn} \operatorname{Hess} \phi^{II}_{\boldsymbol{\alpha_2}}(\lambda) + f'_{\boldsymbol{\alpha_2}}(\lambda). \tag{5.68}$$

Proof. We have to prove that

$$- \operatorname{sgn} \operatorname{Hess} \phi^I_{\boldsymbol{\alpha_1}} + \operatorname{sgn} \operatorname{Hess}_{y,\eta} \phi^I_{\boldsymbol{\alpha_1}} = - \operatorname{sgn} \operatorname{Hess} \phi^{II}_{\boldsymbol{\alpha_2}} + \operatorname{sgn} \operatorname{Hess}_{y,\xi,\eta} \phi^{II}_{\boldsymbol{\alpha_2}}. \tag{5.69}$$

$\operatorname{Hess} \phi_{\boldsymbol{\alpha_2}}$ is given by (5.49), and using (5.53) a simple calculation shows that

$$\operatorname{sgn} \operatorname{Hess} \phi^{II}_{\boldsymbol{\alpha_2}} = 0 = \operatorname{sgn} \operatorname{Hess}_{y,\eta} \phi^I_{\boldsymbol{\alpha_1}}. \tag{5.70}$$

We now compare (5.40) in the proof of Lemma 8 with (5.60) in the proof of Lemma 11. Since $\lambda \in \Lambda_{\boldsymbol{\alpha'\alpha}}$, in a neighbourhood of λ there is a bijection between ∂_ξ and ∂_x given by

$$\partial_\xi = (\partial_\xi x)\, \partial_x. \tag{5.71}$$

In combination with Lemma 3 this shows that there exists a hermitian matrix P that is a product of a permutation matrix and a diagonal matrix with diagonal entries 1 and (5.71), such that

$$- \operatorname{Hess}_{y,\xi,\eta} \phi^{II}_{\boldsymbol{\alpha_2}}(\lambda) = \left(P^* \operatorname{Hess} \phi^I_{\boldsymbol{\alpha_1}} P\right)(\lambda), \tag{5.72}$$

where $\operatorname{Hess} \phi^I_{\boldsymbol{\alpha_1}}$ is given in (5.40). Thus, [Lan69, Theorem 3, p. 187] shows that

$$- \operatorname{sgn} \operatorname{Hess} \phi^I_{\boldsymbol{\alpha_1}}(\lambda) = \operatorname{sgn} \operatorname{Hess}_{y,\xi,\eta} \phi^{II}_{\boldsymbol{\alpha_2}}(\lambda), \quad \lambda \in \Lambda_{\boldsymbol{\alpha'\alpha}}, \tag{5.73}$$

which proves the claim. $\qquad\square$

We note that an application of Lemma 12 to the right-hand sides of (5.51) and (5.58) establishes the desired property that the phases appearing in these expressions only depend on $\boldsymbol{\alpha'}$, but not on $\boldsymbol{\alpha}$.

In order to facilitate the construction of the semiclassical time evolution we introduce the globally defined half-density $|A_0| \mathrm{d}\lambda^{\frac{1}{2}}$ as the solution of the the initial value problem

$$\begin{cases} (\mathcal{L}_{X_{\text{ext}}} |A_0|)(\lambda) \mathrm{d}\lambda^{\frac{1}{2}} = 0, & \lambda \in \Lambda, \\ |A_0|(\lambda) \mathrm{d}\lambda^{\frac{1}{2}} = |\mathrm{d}t \wedge \mathrm{d}y \wedge \mathrm{d}\eta|^{\frac{1}{2}}, & \lambda \in \Lambda_0. \end{cases} \tag{5.74}$$

Here $|\mathrm{d}t \wedge \mathrm{d}y \wedge \mathrm{d}\eta|$ is the canonical density of the conormal bundle Λ_0, see (4.6). The unique solution of (5.74) is

$$|A_0| \mathrm{d}\lambda^{\frac{1}{2}} = \pi^* \left(|\mathrm{d}t \wedge \mathrm{d}y \wedge \mathrm{d}\eta|^{\frac{1}{2}}\right), \tag{5.75}$$

where π^* is the pull-back of the projection

$$\pi(t, \tau, x, \xi, y, -\eta) = (t, y, -\eta), \quad (t, \tau, x, \xi, y, -\eta) \in \Lambda, \tag{5.76}$$

see [DG75, Lemma 6.1]. The quantity $A_0 \mathrm{d}\lambda^{\frac{1}{2}}$ then involves the Maslov-factor (5.67) in addition to $|A_0|\mathrm{d}\lambda^{\frac{1}{2}}$.

We also define a shifted nearest neighbourhood $N(\lambda)$ of $\lambda \in \Lambda$ using the partition $\{\Lambda_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}}$,

$$\lambda' \in N(\lambda) \quad \Leftrightarrow \quad \lambda' \in \Lambda_{\boldsymbol{\alpha'\alpha}} \quad \text{and} \quad \lambda \in \Lambda_{\boldsymbol{\alpha\alpha'}}. \tag{5.77}$$

Then

$$\lambda' \sim \lambda \quad \Leftrightarrow \quad \lambda', \lambda \in N(\lambda), \tag{5.78}$$

defines an equivalence relation on

$$\tilde{\Lambda} := \bigcup_{\boldsymbol{\alpha}} \Lambda_{\boldsymbol{\alpha}} \setminus \bigcup_{\boldsymbol{\alpha}} \partial\Lambda_{\boldsymbol{\alpha}}, \tag{5.79}$$

and thus yields a disjoint decomposition

$$\left\{\tilde{\Lambda}_{\boldsymbol{\beta}}\right\}_{\boldsymbol{\beta}} \tag{5.80}$$

of $\tilde{\Lambda}$. The boundaries in (5.78) can be neglected since they do not contribute to the integral estimates in the following.

Proposition 1. *For every $\beta > 0$ there exists a discrete scFIO $U_{\mathrm{scl}}(t)$ in the sense of Definition 1 that satisfies the assumptions of Lemma 5. Away from caustics it has the following Van Vleck form*

$$U_{\mathrm{scl}}(t)_{m_N n_N} = \frac{1}{\sqrt{2\pi\hbar}} \frac{\ell_x}{N} \sum_{\alpha_N} \left| \det\left(\frac{\partial^2 W}{\partial x \partial y}(\lambda_{\alpha_N})\right) \right|^{\frac{1}{2}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}W(\lambda_{\alpha_N}) + \frac{\mathrm{i}\pi}{2}\tilde{\mu}(\gamma_{\alpha_N})} + O(\hbar). \tag{5.81}$$

Here $\lambda_{\alpha_N} = (t, \tau, x_{m_N}, \xi_{\alpha_N}, y_{n_N}, -\eta_{\alpha_N})$ is in a suitable neighbourhood of the non-caustic point, the sum extends over all trajectories γ_{α_N} connecting $(y_{n_N}, \eta_{\alpha_N})$ with $(x_{m_N}, \xi_{\alpha_N})$, and

$$\tilde{\mu}(\gamma_{\alpha_N}) = \mu(\gamma_{\alpha_N}) + \frac{1}{2} \operatorname{sgn} \operatorname{Hess} \phi_\alpha(\lambda_{\alpha_N}). \tag{5.82}$$

In order to emphasise that matrix indices range from 0 to $N-1$, with a direct implication on the points x_n and, therefore, on classical quantities, we added an index N. Note that the functions ϕ_α in (5.82) are independent of N.

Proof. We have to prove that Lemma 5 is satisfied up to an arbitrary but fixed $T > 0$. We fix T and choose $\mathfrak{V}_{\boldsymbol{\alpha}}$ sufficiently small so as to fulfill the assumptions made previously in this section.

The first step is to prove the condition (5.2) imposed on the initial value $U_{\mathrm{scl}}(0)$. We recall that the initial Lagrangian manifold Λ_0, see (4.6), is generated by a function $\phi^I(t, x, y, \eta)$, see (4.7). In agreement with (5.75) we choose for the amplitude function in (5.10),

$$|A_k^I|(0, x, \eta) = \begin{cases} 1, & k = 0 \\ 0, & k \geq 1, \end{cases} \tag{5.83}$$

and localise

$$|A_{\boldsymbol{\alpha},k}|\mathrm{d}\lambda^{\frac{1}{2}} := \Psi_{\boldsymbol{\alpha}}|A_k^I|\mathrm{d}\lambda^{\frac{1}{2}}, \tag{5.84}$$

where Ψ_α is given in (4.24).

In order to evaluate $U_{\mathrm{scl}}(0)$ we recall that

$$\phi^I(0,x,y,\eta) = (x-y)\eta \tag{5.85}$$

holds. With Lemma 15 we then obtain

$$\int_{\mathfrak{V}_{\boldsymbol{\alpha}}^\eta} \Psi_{\boldsymbol{\alpha}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\phi_{\boldsymbol{\alpha}}} \mathrm{d}\eta = \sum_{j=0}^{N-1} \Psi_{\boldsymbol{\alpha}}(0,\tau,\hat{x},\eta_j,\hat{y}_n,-\eta_j) \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\hat{x}_m - \hat{y}_n)\eta_j} + O(\hbar^\infty) \tag{5.86}$$

where $\eta_j = j\ell_\xi/N + r\ell_\xi$ with some $r \in \mathbb{Z}$. The condition (4.32) hence implies

$$U_{\mathrm{scl}}(0)_{mm} = 1 + O(\hbar^\infty). \tag{5.87}$$

Off the diagonal, for $U(0)_{mn}$ with $m \neq n$, we note that

$$\frac{1}{\hbar}(\hat{x}_m - \hat{y}_n)\eta_j = \frac{2\pi(m-n)j}{N} + 2\pi l \quad \text{for some} \quad l \in \mathbb{Z}. \tag{5.88}$$

Therefore,

$$\sum_{j=0}^{N-1} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\hat{x}_m - \hat{y}_n)\eta_j} = 0, \tag{5.89}$$

which implies that

$$U_{\mathrm{scl}}(0)_{mn} = O(\hbar^\infty). \tag{5.90}$$

Hence, the initial condition (5.2) is fulfilled.

The main task in this proof is to obtain the estimate (5.1). Every term $\operatorname{tr} R_{\boldsymbol{\alpha}',k'}(t)^* R_{\boldsymbol{\alpha},k}(t)$ can be written as one of the four cases described by the Lemmata 8–11. We evaluate the integrals ocurring in these Lemmata recursively in their orders k on every set $\tilde{\Lambda}_{\boldsymbol{\beta}}$, and note that in each of the four cases the half-densities $e_{\boldsymbol{\alpha},k,\hbar}$ possess complete asymptotic expansions in powers of $\hbar$ with similar leading terms, see (5.35), (5.45), (5.52) and (5.59). Since $\partial_x \xi = (\partial_\xi x)^{-1}$, the additional factors in (5.34) and (5.58) reflect the choice of coordinates for the respective half-densities $e_{\boldsymbol{\alpha},k,\hbar}$.

Suppose a global half-density $|A_k|\mathrm{d}\lambda^{\frac{1}{2}}$ on Λ is given. It can be localised in the covering space using the partition of unity $\{\Psi_{\boldsymbol{\alpha}}, \Lambda_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha}}$ of (4.31), as

$$|A_{\boldsymbol{\alpha},k}|\mathrm{d}\lambda^{\frac{1}{2}} := \Psi_{\boldsymbol{\alpha}}|A_k|\mathrm{d}\lambda^{\frac{1}{2}}. \tag{5.91}$$

Due to (4.32) we then have

$$\sum_{\boldsymbol{\alpha}} \left(\mathcal{L}_{X_{H_{\mathrm{ext}}}} |A_{\boldsymbol{\alpha},k}|\mathrm{d}\lambda_{\boldsymbol{\alpha}}^{\frac{1}{2}} \right)(\lambda_{\boldsymbol{\alpha}}) = \sum_{\boldsymbol{\alpha}} \left(\Psi_{\boldsymbol{\alpha}} \left(\mathcal{L}_{X_{H_{\mathrm{ext}}}} |A_k|\mathrm{d}\lambda_{\boldsymbol{\alpha}}^{\frac{1}{2}} \right) \right)(\lambda_{\boldsymbol{\alpha}}) \tag{5.92}$$

in a neighbourhood of the points $\lambda_{\boldsymbol{\alpha}}$, where the sum in (5.92), respectively (4.32), extends over all $\boldsymbol{\alpha}$ with $\lambda_{\boldsymbol{\alpha}} \in \Lambda_{\boldsymbol{\alpha}}$ corresponding to the same point λ in the extended torus phase space, i.e., where $\check{\lambda}_{\boldsymbol{\alpha}} = \lambda$.

Hence, combining the Lemmata 8–11 with Lemma 12 shows that for fixed $\boldsymbol{\alpha}'$ in (5.13) we can extract the coefficient depending on $\boldsymbol{\alpha}'$ and perform the $\boldsymbol{\alpha}'$-summation. This shows that if we start with the globally defined half-density $A_0 \mathrm{d}\lambda^{\frac{1}{2}}$ of (5.75), using (5.92) we see that when $k = 0$,

$$\sum_{\boldsymbol{\alpha}} \mathcal{L}_{X_{H_{\mathrm{ext}}}} \left(|A_{\boldsymbol{\alpha},0}| \mathrm{d}\lambda^{\frac{1}{2}} \right) = 0. \tag{5.93}$$

Then, for fixed $\boldsymbol{\alpha}'$, we sum all half-densities of the next order in $\hbar$, except the term coming from the Lie derivatives, and denote the resulting half-density on Λ by $r_1 \mathrm{d}\lambda^{\frac{1}{2}}$. The next step then is to solve the inhomogeneous Cauchy problem,

$$-\left(\mathcal{L}_{H_{\mathrm{ext}}} |A_k| \mathrm{d}\lambda^{\frac{1}{2}} \right) + r_k \mathrm{d}\lambda^{\frac{1}{2}} = 0, \tag{5.94}$$

for $k = 1$ by the method of characteristics in analogy to [Dui74, Theorem 1.4.1]. This can be done since the extended Hamiltonian flow is complete and tangential to Λ. Again, (5.91) and (5.92), as well as an application of Lemma 4, show that in (5.13) the next order in $\hbar$ (with $\boldsymbol{\alpha}'$ fixed) also vanishes. We proceed in this recursive manner by solving (5.94) with the method of characteristics. The emerging half-density r_k is composed of the half-densities of order k in $\hbar$ in the asymptotic expansions of $e_{\boldsymbol{\alpha},k,\hbar}$. Again (5.91) and (5.92) together with the Lemmata 8–11 show that every term of a given order in $\hbar$ is recursively canceled. An application of Borel's theorem [Zwo12, Theorem 4.15] then shows that U_{scl} exists and satisfies the claim.

The Van Vleck expression follows from an application of the stationary phase theorem to the η-integration in (5.10), see, e.g., [Mei92, p. 288]. $\qquad\square$

6 Trace formula

In this section we prove Theorem 1. We recall that the starting point is the relation (2.11) where on the left-hand side the sum extends over all eigenvalues E_n of the quantum Hamiltonian $\mathrm{op}_N(H)$ (counted with their multiplicities), and $\rho \in C^\infty(\mathbb{R})$ is a test function with compactly supported Fourier transform

$$\hat{\rho}(E) := \int_{\mathbb{R}} \rho(x) \mathrm{e}^{-\mathrm{i}Ex} \mathrm{d}x. \tag{6.1}$$

The trace formula (2.18) is derived from (2.11) by using the semiclassical expression for $\mathrm{tr}\, U(t)$, developed in Section 5, on the right-hand side.

We assume E to be a regular value of the classical Hamiltonian $H \in C^\infty(\mathbb{T})$ so that the energy surface $H^{-1}(E)$ (2.17) is a submanifold of the phase space $\mathbb{T}$. In this setting the sets $\mathcal{O}_T$ of fixed points of Φ^T always satisfy the clean intersection property [GS13, p. 280]. In particular, $\mathcal{O}_0 \cap H^{-1}(E) = H^{-1}(E)$. The set $\mathfrak{P}_E$ of periodic orbits of the Hamiltonian

flow with energy E consists of primitive periodic orbits, $p^{\#}$, and their m-fold repetitions, p, with periods $t_p = m t_{p^{\#}}$.

Since the energy surface is one dimensional a simple calculation shows that when every point on $H^{-1}(E)$ is non-stationary one has

$$\text{vol}\big(H^{-1}(E)\big) = \sum_{p^{\#}} t_{p^{\#}}, \tag{6.2}$$

where the sum is over all primitive periodic orbits in $H^{-1}(E)$.

Now let $p \in \mathfrak{P}_E$ and denote its lift to the covering space by $\hat{p}$. Then, with some obvious abuse of the notation in (4.17), we set for the action of p,

$$W_p := W + E t_p + s \ell_\xi x, \tag{6.3}$$

with

$$t = t_p, \ (y, \eta) = \hat{p}(0) \text{ and } (x, \xi) = \hat{p}(t_p) \tag{6.4}$$

in (4.17). The integer s is determined by $\xi - \eta = s\ell_\xi$. It turns out that W_p is independent of the choice $(t_p, -E, x, \xi, y, -\eta)$ satisfying (6.4).

The trace formula also requires the Conley-Zehnder index σ_p of periodic orbits $p \in \mathfrak{P}_E$. For its definition we refer to Appendix C.

With this information we are ready to prove our main result.

Proof of Theorem 1. Our first observation is that due to Proposition 1 we can approximate the unitary time evolution $U(t)$ semiclassically by some $U_{\text{scl}}(t)$ to any desired order $\beta > 0$ in the sense of Lemma 5. Hence $|\operatorname{tr}(U(t) - U_{\text{scl}}(t))| = O(\hbar^{\infty})$, and we therefore now study $\operatorname{tr} U_{\text{scl}}(t)$. In order to obtain an asymptotic expansion in powers of $\hbar$ we have to calculate the asymptotic expansions of $\operatorname{tr} U_{\boldsymbol{\alpha}, k}$ for every $k \in \mathbb{N}_0$.

We first consider the case where $\Lambda_{\boldsymbol{\alpha}}$ is generated by a function ϕ_{α}^I, see Section 5.1. With $U_{\boldsymbol{\alpha}, k}$ of the form (5.10) one finds

$$\frac{1}{2\pi} \int_{\mathbb{R}} \operatorname{tr} U_{\boldsymbol{\alpha}, k}(t) \hat{\rho}(t) \ \mathrm{e}^{\frac{\mathrm{i}}{\hbar} E t} \mathrm{d}t$$

$$= \frac{1}{(2\pi)^2 \hbar} \frac{\ell_x}{N} \sum_{m=0}^{N-1} \int_{\mathbb{R}} \int_{\mathbb{R}} a_{\boldsymbol{\alpha}, k}^I(t, \hat{x}_m, \hat{x}_m, \eta) \hat{\rho}(t) \mathrm{e}^{\frac{\mathrm{i}}{\hbar} [\phi_{\boldsymbol{\alpha}}^I(t, \hat{x}_m, \hat{x}_m, \eta) + E t]} \mathrm{d}\eta \mathrm{d}t \tag{6.5}$$

$$= \frac{1}{(2\pi)^2 \hbar} \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} a_{\boldsymbol{\alpha}, k}^I(t, \hat{x}, \hat{x}, \eta) \hat{\rho}(t) \mathrm{e}^{\frac{\mathrm{i}}{\hbar} [\phi_{\boldsymbol{\alpha}}^I(t, \hat{x}, \hat{x}, \eta) + s \ell_\xi x + E t]} \mathrm{d}\eta \mathrm{d}x \mathrm{d}t + O(\hbar^{\infty}),$$

where the last line follows from an application of Lemma 15. It turns out that the integer s arising from Lemma 15 is the same as in (6.3). We apply the stationary phase theorem and identify as the conditions of stationary phase,

$$\begin{aligned} \partial_t \phi_{\boldsymbol{\alpha}}^I &= -E \\ \partial_x \phi_{\boldsymbol{\alpha}}^I + s \ell_\xi &= \eta \\ \partial_\eta \phi_{\boldsymbol{\alpha}}^I + r \ell_x &= x. \end{aligned} \tag{6.6}$$

Here the last identity follows from $\hat{y}|_{y=x} = \hat{x} + r\ell_x$. These conditions imply that x and η are on a periodic orbit of period t and energy E. When $t = 0$ the set of such periodic points is given by the energy surface $H^{-1}(E)$. When $t \neq 0$, the points are on a non-trivial periodic orbit $p \in \mathfrak{P}_E$. We define $p_{\boldsymbol{\alpha}} := \Lambda_{\boldsymbol{\alpha}} \cap p$ and choose $\Lambda_{\boldsymbol{\alpha}}$ small enough such that $p_{\boldsymbol{\alpha}}$ is connected.

Upon applying the stationary phase theorem we are left with an integral over $p_{\boldsymbol{\alpha}}$, which we parametrise with the variable ν, leading to

$$\frac{1}{2\pi} \int_{\mathbb{R}} \operatorname{tr} U_{\boldsymbol{\alpha},k}(t)\, \hat{\rho}(t) \mathrm{e}^{\frac{\mathrm{i}}{\hbar} Et} \mathrm{d}t \sim \sum_{p_{\boldsymbol{\alpha}}} \frac{\hat{\rho}(t)}{2\pi} \int_{p_{\boldsymbol{\alpha}}} \psi_{\boldsymbol{\rho}}(\nu) a_{\hbar,k}(\nu) \mathrm{e}^{\frac{\mathrm{i}}{\hbar} W_p - \mathrm{i}\frac{\pi}{2}\sigma_p} \mathrm{d}\nu. \tag{6.7}$$

Here $a_{\hbar,k}$ is a smooth function on $p_{\boldsymbol{\alpha}}$ with a complete asymptotic expansion in $\hbar$, and $\psi_{\boldsymbol{\rho}}$ is determined by $\Psi_{\boldsymbol{\alpha}}$, see (4.24). The Maslov contribution σ_p was derived in [Mei94, Theorem 13] by means of the identification outlined in [GS13, p. 137] and is independent of $\nu \in p_{\boldsymbol{\alpha}}$; the same is true for the action W_p.

In order to find the leading semiclassical contribution it suffices to study $\operatorname{tr} U_{\boldsymbol{\alpha},0}$ in (5.10). The rest contributes terms of at least $O(\hbar)$ to (2.19). Since there are only finitely many contributions labelled by $\boldsymbol{\alpha}$ the errors can be uniformly bounded with respect to $\hbar$. For a two dimensional phase space the condition of regular periodic orbits amounts to the identity $\det|\mathbb{1} - \mathrm{d}f_p| = 1$ in [GS13, Eq. (11.23)], where f_p denotes the Poincaré map along p. Using this, as well as [GS13, pp. 279 & 282], we conclude that the right-hand side of (6.7) is equal to

$$\begin{aligned}
&\frac{\hat{\rho}(0)}{2\pi} \int_{H^{-1}(E)} \psi_{\rho}(\nu) \mathrm{d}\nu \left(1 + O(\hbar)\right) \\
&+ \sum_{p_{\boldsymbol{\alpha}}} \frac{\hat{\rho}(t_p)}{2\pi} \int_{p_{\boldsymbol{\alpha}}} \psi_{\boldsymbol{\rho}}(t) \mathrm{e}^{\frac{\mathrm{i}}{\hbar} W_p - \mathrm{i}\frac{\pi}{2}\sigma_p} \mathrm{d}t \left(1 + O(\hbar)\right),
\end{aligned} \tag{6.8}$$

where the path $p_{\boldsymbol{\alpha}}$ is parametrised by time.

The same calculations can be done in the case (4.13). We again have to solve (6.6) together with $\partial_\xi \phi_{\boldsymbol{\alpha}}^{II} = x$. The sum over all $\boldsymbol{\alpha}$ can be performed as $\psi_{\boldsymbol{\rho}}$ satisfies the relation (4.32). This finally proves the theorem. $\qquad\square$

7   A semiclassical quantisation condition

In this section our intention is to explore to what extent the trace formula of Theorem 1 allows us to characterise individual eigenvalues of the quantum Hamiltonian $\operatorname{op}_N(H)$.

The first step is to observe that Theorem 1 can be rewritten as follows.

Lemma 13. *With the assumptions of Theorem 1, one has, locally uniformly in $r \in \mathbb{R}$,*

$$\begin{aligned}
\sum_n \rho\left(\frac{E_n - E - r\hbar}{\hbar}\right) \\
= \sum_{k \in \mathbb{Z}} \sum_{p \in \mathfrak{P}_E^{\#}} \rho\left(t_{p^{\#}}^{-1}\left(\frac{W_{p^{\#}}}{\hbar} + r t_{p^{\#}} - \frac{\pi}{2}\sigma_{p^{\#}} - 2\pi k\right)\right) + O(\hbar).
\end{aligned} \tag{7.1}$$

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Proof. We note that $W_p = kW_{p\#}$, $t_p = kt_{p\#}$ and $\sigma_p = k\sigma_{p\#}$ (see (C.4)) if p is a k-fold repetition of $p^{\#}$. This allows us to write the periodic-orbit sum in (2.18) as a double sum over the (finitely many) primitive periodic orbits and their repetitions.

Furthermore, a comparison of the left-hand sides of (2.18) and (7.1) reveals that the latter requires the 'classical' energy to be $E + r\hbar$. We therefore need to evaluate the right-hand side of (2.18) at this energy. Using

$$W_p(E + r\hbar) = W_p(E) + r\hbar t_p(E) + O(\hbar^2) \tag{7.2}$$

we obtain

$$\sum_{k \in \mathbb{Z}} \sum_{p\#} \hat{\rho}\left(kt_{p\#}\right) t_{p\#} \mathrm{e}^{\mathrm{i}k\left(\frac{W_{p\#}}{\hbar} + rt_{p\#} - \frac{\pi}{2}\sigma_{p\#}\right)} + O(\hbar). \tag{7.3}$$

The remainder estimate depends on ρ but is locally uniform in r. Applying Poisson summation to the sum over k proves the claim. $\qquad\square$

The right-hand side of (7.1) suggests that in the vicinity of E one finds an eigenvalue of $\mathrm{op}_N(H)$, iff

$$\frac{W_{p\#}}{\hbar} + rt_p - \frac{\pi}{2}\sigma_{p\#} \approx 2\pi k \tag{7.4}$$

In other words, together with (7.2) this would be some form of a Bohr-Sommerfeld quantisation condition: $E + r\hbar$ is an approximate eigenvalue, iff

$$\frac{1}{2\pi\hbar}W_{p\#}(E + r\hbar) = k + \frac{1}{4}\sigma_{p\#}(E + r\hbar) + O(\hbar) \tag{7.5}$$

holds. In the following we want to explore to what extent such a relation can be derived from the trace formula. Our approach uses the tools developed in [PP98] to estimate eigenvalue clustering.

In order to determine the cases where (7.4) is fulfilled we now introduce some counting measures. We assume that E is regular value of H. Then the energy surface $H^{-1}(E)$ consists of a finite and disjoint set of periodic orbits. In analogy to [PP98, p. 23] we introduce the function

$$Q(r; E, \hbar) := \frac{1}{2\pi} \sum_{p\# \in \mathfrak{P}_E} \left[\pi - \frac{W_{p\#}}{\hbar} + \frac{\pi}{2}\sigma_{p\#} - rt_{p\#}\right]_{2\pi}, \tag{7.6}$$

where $[z]_{2\pi} = z \bmod 2\pi$ such that $-\pi < [z]_{2\pi} \leq \pi$. We remark that, as a function of r, each term in (7.6) jumps in value by one at the points in the set

$$\Omega_{p\#}(\hbar) := \left\{r \in \mathbb{R}; \ \left[\frac{W_{p\#}}{\hbar} - \frac{\pi}{2}\sigma_{p\#} + rt_{p\#}\right]_{2\pi} = 0\right\}. \tag{7.7}$$

We now define

$$\begin{aligned} N_{\min}(\hbar, E, r) &:= \left|\left\{p^{\#} \in \mathfrak{P}_E^{\#}; \ \Omega_{p\#}(\hbar) \cap \left[-\frac{r}{2}, \frac{r}{2}\right] \neq \emptyset\right\}\right|, \\ N_{\max}(\hbar, E, r) &:= \left|\left\{p^{\#} \in \mathfrak{P}_E^{\#}; \ \Omega_{p\#}(\hbar) \cap \left[-\frac{3r}{2}, \frac{3r}{2}\right] \neq \emptyset\right\}\right|, \end{aligned} \tag{7.8}$$

and relate these cardinalities to the function (7.6).

Lemma 14. *If $r > 0$ is sufficiently small, then*

$$N_{\min}(\hbar, E, r) = Q\left(\frac{r}{2}; E, \hbar\right) - Q\left(-\frac{r}{2}; E, \hbar\right) + O(r)$$

$$N_{\max}(\hbar, E, r) = Q\left(\frac{3r}{2}; E, \hbar\right) - Q\left(-\frac{3r}{2}; E, \hbar\right) + O(r). \tag{7.9}$$

Proof. We recall that $|\mathfrak{P}_E^{\#}|$ is finite since E is a regular value. Furthermore, r sufficiently small means that $\Omega_{p\#}(\hbar) \cap [-3r/2, 3r/2]$ has at most one element. We then set $N_{\min,p\#} = 1$ if $[-r/2, r/2] \cap \Omega(\hbar, p^{\#}) \neq \emptyset$ and $N_{\max,p\#} = 1$ if $[-3r/2, 3r/2] \cap \Omega(\hbar, p^{\#}) \neq \emptyset$. This gives

$$Q\left(\frac{r}{2}; E, \hbar\right) - Q\left(-\frac{r}{2}; E, \hbar\right) + O(r) = \sum_{p\# \in \mathfrak{P}_E^{\#}} N_{\min,p\#},$$

$$Q\left(\frac{3r}{2}; E, \hbar\right) - Q\left(-\frac{3r}{2}; E, \hbar\right) + O(r) = \sum_{p\# \in \mathfrak{P}_E^{\#}} N_{\max,p\#}, \tag{7.10}$$

which proves the claim. $\qquad\square$

Since the number of primitive periodic orbits is finite we can always find $\omega_0 > 0$ and $r_0 > 0$ such that for all $r \in [-r_0, r_0]$, $0 < \hbar < \hbar_0$ and $p^{\#} \in \mathfrak{P}_E^{\#}$,

$$\left|\frac{W_{p\#}}{\hbar} - \frac{\pi}{2}\sigma_{p\#} + rt_{p\#}\right| > \omega_0. \tag{7.11}$$

We remark that, in contrast to [PP98, Eq. (1.9)], in (7.11) an absolute value is taken.

We now define a local eigenvalue counting function as

$$N_{E,r}(\hbar) := |\{E_n \in \sigma(\mathrm{op}_N(H)); \ |E_n - E| < r\hbar\}|. \tag{7.12}$$

Here the eigenvalues in (7.12) are counted with their multiplicities. In view of the Bohr-Sommerfeld condition (7.4) our aim therefore is to identify situations where, for small r, one has $N_{E,r}(\hbar) \geq 1$. To this end we establish an upper and a lower bound for the local eigenvalue counting function.

Proposition 2. *There exist $\hbar_0 > 0$ and $r_0 > 0$ such that for all $0 < r < r_0$ and $0 < \hbar < \hbar_0$,*

$$N_{\min}(\hbar, E, r) \leq N_{E,r}(\hbar) \leq N_{\max}(\hbar, E, r). \tag{7.13}$$

Proof. In a first step we prove the bounds

$$N_{\min}(\hbar, E, r) - C_0 r + O_r(\hbar)$$

$$\leq N_{E,r}(\hbar) - \frac{r}{\pi} \mathrm{vol}\left(H^{-1}(E)\right) \tag{7.14}$$

$$\leq N_{\max}(\hbar, E, r) + C_0 r + O_r(\hbar)$$

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with some $C_0 > 0$. In view of Lemma 14 this can be done very much in analogy to the proof of [PP98, Theorem 1.1]. We note that in the present case the integrals over the energy surface in [PP98] can be carried out since the Liouville measure of a periodic orbit is known explicitly; it is dt when t is the time coordinate. We also note that in the present case the analogue of [PP98, Theorem 5.1] is given by our Theorem 1, and even includes an improved error term.

In order to prove (7.13) we note that the first terms in the first and third line of (7.14) are monotonously increasing in r. Since the first terms in each line of (7.14) are integers we can neglect the terms with C_0, $\mathrm{vol}(H^{-1}(E))$ and $O_r(\hbar)$ when $\hbar$ and r are sufficiently small. $\qquad\square$

Obviously, when under the conditions of Proposition 2 we have that $N_{\min}(\hbar, E, r) = N_{\max}(\hbar, E, r) := N$ then $N_{E,r} = N$. Moreover, the upper bound for $N_{E,r}$ is easily obtained by a combination of Proposition 2 and Eq. (7.8).

Corollary 2. *With the assumptions of Proposition 2 we have $N_{E,r} \leq \left|\mathfrak{P}_E^{\#}\right|$.*

We obtain the following consequence of Proposition 2:

Proposition 3. *In addition to the assumption of Proposition 2, suppose that the exact Bohr-Sommerfeld condition*

$$\frac{W_{p\#}}{\hbar} - \frac{\pi}{2}\sigma_{p\#} = 2\pi k. \tag{7.15}$$

holds. Then for every $\hbar < \hbar_0$ we have $N_{E,r} \geq 1$.

Proof. We have to show that $N_{\min}(\hbar, E, r) \geq 1$ for every $\hbar < \hbar_0$. But this follows if we insert the Bohr-Sommerfeld condition (7.15) in (7.8) resp. (7.7). $\qquad\square$

This proposition is the closest one can get towards a Bohr-Sommerfeld quantisation condition on the basis of the trace formula only. Notice that our approach never makes use of any eigenfunctions. Therefore, we have not relied on constructing quasi-modes, which is the usual approach to Bohr-Sommerfeld conditions, see, e.g., [Cha03] for the case of Toeplitz operators on compact Kähler manifolds.

8 Examples

In this section we discuss some simple examples. We begin with classical Hamiltonians that are either of the form $H(x, \xi) = H(x)$, or of the form $H(x, \xi) = H(\xi)$.

When the classical Hamiltonian is of the form $H(x)$ the equations of motion are

$$\dot{\xi} = -\partial_x H = -H', \quad \dot{x} = \partial_\xi H = 0. \tag{8.1}$$

The solutions of (8.1) are given by $x(t) = x_0$ and $\xi(t) = \xi_0 - tH'$. We assume that the energy $E = H(x_0)$ is not critical. A (primitive) periodic orbit is given when $\xi(t_{p\#}) = \xi_0 \pm \ell_\xi$.

Hence the primitive period is $t_{p\#} = |\ell_\xi/H'(x_0)|$. Moreover, the action is $W_p = \ell_\xi x$ and originates from the third term in (6.3).

The set $\mathfrak{P}_E$ of periodic orbits of energy E is discrete, as E is non-critical. Periodic orbits $p \in \mathfrak{P}_E$ can be labelled by the points $x_0 \in [0, \ell_x)$ such that $H(x_0) = E$.

On the classical side it remains to determine the Conley-Zehnder index of a periodic orbit. A short calculation shows that $T\Phi_t V_M(H^{-1}(E)) = V_M(\Phi_t(H^{-1}(E)))$ for every t (see Appendix C). Therefore, we have the extremal case that every point in the extended phase space belongs to a caustic [Mei92, p. 280]. From (C.3) we hence conclude that the Conley-Zehnder index is equal to zero. A somewhat lengthy but straightforward calculation using [Mei00, Lemma 8.3] indeed shows that the third and second term in [Mei94, Proposition 12] cancel each other in complete agreement with assumption (A2) in [Mei94, p. 9].

With this input one can set up the trace formula (2.18) in the form

$$
\sum_m \rho\left(\frac{E - E_m}{\hbar}\right) = \sum_{x_0 \in H^{-1}([0,\ell_x))} \frac{\ell_\xi}{2\pi|H'(x_0)|} \hat\rho(0)\big(1 + O(\hbar)\big)
$$
$$
+ \sum_{x_0 \in H^{-1}([0,\ell_x))} \sum_{k \in \mathbb{Z}\setminus\{0\}} \frac{\ell_\xi}{2\pi|H'(x_0)|} \hat\rho\left(\frac{k\ell_\xi}{|H'(x_0)|}\right) e^{\frac{i}{\hbar}k\ell_\xi x_0}\big(1 + O(\hbar)\big).
$$
$$(8.2)$$

This trace formula can also be proved directly, making use of the explicit knowledge of the eigenvalues,

$$
E_m = H\left(\frac{\ell_x m}{N}\right), \quad m = 1, \dots, N,
$$
$$(8.3)$$

and rewriting

$$
\sum_{m=1}^N \rho\left(\frac{E - E_m}{\hbar}\right) = \frac{1}{2\pi}\int_{\mathbb{R}} \hat\rho(t) \sum_{m=1}^N e^{\frac{it}{\hbar}\left[E - H\left(\frac{\ell_x m}{N}\right)\right]} dt.
$$
$$(8.4)$$

We apply [DF37, Theorem 4] to the sum on the right-hand side, and use the stationary phase theorem for the emerging integrals over a variable x in addition to the integral over t. The phase functions are $\phi(t, x) = t(E - H(x)) \pm nx\ell_\xi$, so that the condition of stationary phase gives $E = H(x)$ in the variable t, and $-tH'(x) = \mp n\ell_\xi$ in the varibale x. The first condition determines the points x_0 labelling (primitive) periodic orbits of energy E, and the second condition provides the periods of the orbits. Carrying out the stationary phase theorem eventually gives (8.2).

The case of a classical Hamiltonian $H(x, \xi) = H(\xi)$ is very similar. A particular example of this leads to a discretised version of the negative Laplacian. As the Weyl symbol of the Laplacian on $\mathbb{R}$, i.e., the negative second derivative, is $H_{\mathbb{R}}(x, \xi) = \xi^2$, a naive guess of the classical Hamiltonian leading to a discretised Laplacian would be to restrict this function to $\mathbb{F}$. However, on $\mathbb{T}$ this would correspond to a non-continuous function. Continuity could be restored by choosing $H(x, \xi) = (\xi - \ell_\xi/2)^2$ for $(x, \xi) \in \mathbb{F}$. Although this function is not smooth on $\mathbb{T}$, an operator $\mathrm{op}_N(H)$ could still be defined using (2.3) or [Lig16, Theorem

2.3]. Its eigenvalues are

$$E_m = H\left(\frac{\ell_\xi m}{N}\right) = \left(\frac{m}{N} - \frac{1}{2}\right)^2 \ell_\xi^2, \quad m = 1, \ldots, N, \tag{8.5}$$

and one could use this explicit expression to set up a trace formula.

A reverse approach would be to start with the 'natural' discretised Laplacian as a difference operator, e.g., defined on $\ell_2(\mathbb{Z})$ as

$$(-\Delta f)_n := -(f_{n+1} + f_{n-1} - 2f_n), \qquad (f_n) \in \ell_2(\mathbb{Z}). \tag{8.6}$$

In the present context, where $\mathrm{op}_N(H)$ is an operator on $\mathbb{C}^N$ expressed in terms of the phase-space translations (2.6), the closest analogue to (8.6) would be (2.7), see also [dFdM10, p. 160]. It then follows from (2.8) that in order to realise this operator as $\mathrm{op}_N(H)$ one has to choose

$$H(x, \xi) = \frac{\ell_\xi^2}{2\pi^2}\left(1 - \cos\left(\frac{2\pi\xi}{\ell_\xi}\right)\right), \tag{8.7}$$

which is independent of x. Hence, in analogy to (8.5) the eigenvalues of the discretised Laplacian $-\hbar^2 \Delta$ are

$$E_m := \frac{\ell_\xi^2}{2\pi^2}\left(1 - \cos\left(\frac{2\pi m}{N}\right)\right), \quad m = 1, \ldots, N. \tag{8.8}$$

Zero is always a non-degenerate eigenvalue. If N is even, the largest possible value $\frac{\ell_\xi^2}{\pi^2}$ is also a non-degenerate eigenvalue. Every other eigenvalue is two-fold degenerate.

As a final example we mention (a variant of) the Harper model [Har55] with classical Hamiltonian

$$H(x, \xi) = \cos\left(\frac{2\pi x}{\ell_x}\right) + \cos\left(\frac{2\pi\xi}{\ell_\xi}\right). \tag{8.9}$$

In $\mathbb{F}$ the critical points of this function are given by $(0, 0)$, $(\ell_x/2, \ell_\xi/2)$, $(0, \ell_\xi/2)$ and $(\ell_x/2, 0)$. At the first point H takes a maximum, at the second a minimum and the other two are saddle points. The energy surface $H^{-1}(0)$, as seen in $\mathbb{F}$, is the straight line connecting the two saddle points plus its continuation connecting the points $(\ell_x/2, \ell_\xi)$ and $(\ell_x, \ell_\xi/2)$. Therefore, every periodic orbit on the torus is a projection of a periodic orbit in the covering space. Hence, its action (6.3) has $s = 0$ and, in absolute value, is the phase space area enclosed by the orbit. The Conley-Zehnder index is $\sigma_p = 2$ for a (primitive) orbit at positive energy, and $\sigma_p = -2$ at negative energy.

With all this input one can then evaluate the trace formula (2.18), as well as the quantisation conditions discussed in Section 7. The latter are rigorous versions of the condition (1.9) in [Har55], or (2) in [GA03].

Acknowledgements

A   Explicit comparison of anti-Wick and Weyl quantisations

Anti-Wick quantisation is an alternative to the Weyl quantisation (2.3)–(2.6), and in this appendix we provide explicit expressions for the matrix elements of anti-Wick operators; for details see [BD96].

If $f \in C^\infty(\mathbb{T})$ is a classical observable, its anti-Wick quantisation is the operator

$$\mathrm{op}_N^{AW}(f) := \frac{1}{2\pi\hbar} \int_{\mathbb{F}} f(x,\xi)\, P(x,\xi)\, \mathrm{d}x\, \mathrm{d}\xi, \tag{A.1}$$

in $\mathbb{C}^N$, where

$$P(x,\xi)_{jk} = \sqrt{\frac{1}{\pi\hbar}} \frac{\ell_x}{N} \sum_{n,m\in\mathbb{Z}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\xi\left(\frac{j-k}{N}-(n-m)\right)\ell_x} \mathrm{e}^{-\frac{1}{2\hbar}\left[\left(\frac{j\ell_x}{N}-n\ell_x-x\right)^2 + \left(\frac{k\ell_x}{N}-m\ell_x-x\right)^2\right]} \tag{A.2}$$

is a projector on a coherent state localised at $(x,\xi) \in \mathbb{T}$. (Here we used the definitions of [BD96] with the choices $\kappa = (0,0)$, $z = \mathrm{i}$ and $(a,b) = (\ell_x, \ell_\xi)$.)

Proposition 4. *Let $f \in C^\infty(\mathbb{T})$, then the matrix elements of the anti-Wick operator $\mathrm{op}_N^{AW}(f)$ are*

$$\mathrm{op}_N^{AW}(f)_{jk}$$
$$= \sqrt{\frac{1}{\pi\hbar}} \sum_{n\in\mathbb{Z}} \mathrm{e}^{-\frac{1}{4\hbar}\left(\frac{j-k}{N}-n\right)^2\ell_x^2} \int_{-\infty}^{\infty} \frac{1}{\ell_\xi} \int_0^{\ell_\xi} f(x,\xi)\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\xi\left(\frac{j-k}{N}-n\right)\ell_x}\, \mathrm{e}^{-\frac{1}{\hbar}\left[x-\left(\frac{j+k}{2N}\ell_x-\frac{n}{2}x\right)\right]^2}\, \mathrm{d}\xi\, \mathrm{d}x. \tag{A.3}$$

Proof. We use (A.2) in (A.1) and interchange integration and summation, exploiting the exponential damping term. We then use the identity

$$\mathrm{e}^{-\frac{1}{2\hbar}\left[\left(\frac{j\ell_x}{N}-n\ell_x-x\right)^2 + \left(\frac{k\ell_x}{N}-m\ell_x-x\right)^2\right]} = \mathrm{e}^{-\frac{1}{\hbar}\left[x-\left(\frac{j+k}{2N}\ell_x-\frac{n+m}{2}\ell_x\right)\right]^2} \mathrm{e}^{-\frac{1}{4\hbar}\left(\frac{j-k}{N}-(n-m)\right)^2\ell_x^2}, \tag{A.4}$$

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shift the summation index, $n - m = \mu$, and change variables in the x-integration, $x \mapsto x + ml_x$. Hence we obtain

$$\mathrm{op}_N^{AW}(f)_{jk} =$$
$$\frac{1}{\ell_\xi} \sqrt{\frac{1}{\pi\hbar}} \sum_{\mu \in \mathbb{Z}} \mathrm{e}^{-\frac{1}{4\hbar}\left(\frac{j-k}{N}-\mu\right)^2 \ell_x^2} \int_0^{\ell_\xi} \sum_{m \in \mathbb{Z}} \int_{m\ell_x}^{(m+1)\ell_x} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\xi\left(\frac{j-k}{N}-\mu\right)\ell_x} \mathrm{e}^{-\frac{1}{\hbar}\left[x-\left(\frac{j+k}{2N}\ell_x-\frac{n}{2}\ell_x\right)\right]^2} f(x,\xi) \,\mathrm{d}x \,\mathrm{d}\xi,$$
$$(\mathrm{A.5})$$

where in the last step we used $f(x + l_x, \xi) = f(x, \xi)$. The summation over m can now be carried out, proving the claim. $\qquad\square$

More explicit expressions can be obtained when f depends either on only x or ξ. First assume that $f(x,\xi) = \varphi(x)$, then the ξ-integration can be performed, yielding

$$\mathrm{op}_N^{AW}(f)_{jk} = \delta_{jk} \sqrt{\frac{1}{\pi\hbar}} \int_{-\infty}^\infty \varphi(x) \, \mathrm{e}^{-\frac{1}{\hbar}\left(x-\frac{j\ell_x}{N}\right)^2} \,\mathrm{d}x. \qquad (\mathrm{A.6})$$

With the Fourier expansion

$$\varphi(x) = \sum_{n \in \mathbb{Z}} \varphi_n \, \mathrm{e}^{2\pi\mathrm{i}n\frac{x}{\ell_x}} \qquad (\mathrm{A.7})$$

this becomes

$$\mathrm{op}_N^{AW}(f)_{jk} = \delta_{jk} \sum_{n \in \mathbb{Z}} \varphi_n \, \mathrm{e}^{2\pi\mathrm{i}\frac{jn}{N}} \, \mathrm{e}^{-\hbar\frac{\pi^2 n^2}{\ell_x^2}}. \qquad (\mathrm{A.8})$$

If, however, $f(x,\xi) = \phi(\xi)$, then the x-integration can be performed,

$$\mathrm{op}_N^{AW}(f)_{jk} = \sum_{n \in \mathbb{Z}} \mathrm{e}^{-\frac{1}{4\hbar}\left(\frac{j-k}{N}-n\right)^2 \ell_x^2} \frac{1}{\ell_\xi} \int_0^{\ell_\xi} \phi(\xi) \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\xi\left(\frac{j-k}{N}-n\right)\ell_x} \,\mathrm{d}\xi. \qquad (\mathrm{A.9})$$

With the Fourier series

$$\phi(\xi) = \sum_{m \in \mathbb{Z}} \phi_m \, \mathrm{e}^{2\pi\mathrm{i}m\frac{\xi}{\ell_\xi}} \qquad (\mathrm{A.10})$$

this simplifies to

$$\mathrm{op}_N^{AW}(f)_{jk} = \sum_{n \in \mathbb{Z}} \phi_{k-j+nN} \, \mathrm{e}^{-\hbar\frac{\pi^2 (k-j+nN)^2}{\ell_\xi^2}}. \qquad (\mathrm{A.11})$$

As an example, the anti-Wick quantisation of the classical Hamiltonian (2.8) with potential $V(x) = \cos(\frac{2\pi x}{\ell_x})$, as in the Harper Hamiltonian (8.9), is

$$\mathrm{op}_N^{AW}(H)_{jk} = -\frac{N^2}{\ell_x^2} \left(\delta_{j,k-1} + \delta_{j,k+1} - 2\right) \mathrm{e}^{-\hbar\frac{\pi^2}{\ell_\xi^2}} + \delta_{jk} \cos\left(\frac{2\pi j}{N}\right) \mathrm{e}^{-\hbar\frac{\pi^2}{\ell_x^2}}. \qquad (\mathrm{A.12})$$

We contrast this with the Weyl quantisation of the same symbol,

$$\mathrm{op}_N(H)_{jk} = -\frac{N^2}{\ell_x^2} \left(\delta_{j,k-1} + \delta_{j,k+1} - 2\right) + \delta_{jk} \cos\left(\frac{2\pi j}{N}\right), \qquad (\mathrm{A.13})$$

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which is a discretised Schrödinger operator in the usual sense.

From this example one concludes that Weyl quantisation allows one to represent discretised Schrödinger operators, or indeed other difference operators, using an $\hbar$-independent symbol. If one were to represent the same operator in the framework of anti-Wick quantisation one would have to use a symbol with an $\hbar$-expansion in all orders.

B   A semiclassical summation formula

In this appendix we prove a technical statement which is applied in the main part in several places. For that purpose we need the following preparation where, for simplicity we denote either of the ordered pairs (ℓ_x, ℓ_ξ) or (ℓ_ξ, ℓ_x) by (ℓ, ℓ^*).

Lemma 15. *Let $a \in C_0^\infty(0, \ell)$, and let $\phi \in C^\infty(\mathbb{R})$ be such that there exists $\nu \in \mathbb{Z}$ with*

$$(\nu - 1)\ell^* < \phi'(t) < (\nu + 1)\ell^*. \tag{B.1}$$

Then

$$\frac{\ell}{N} \sum_{n=0}^{N-1} a\left(\tfrac{n\ell}{N}\right) e^{\frac{i}{\hbar}\phi\left(\frac{n\ell}{N}\right)} = \int_0^\ell a(t) e^{\frac{i}{\hbar}(\phi(t) - \nu\ell^* t)} dt + O(\hbar^\infty). \tag{B.2}$$

Proof. Taking into account that

$$\frac{2\pi N}{\ell} = \frac{\ell^*}{\hbar}, \tag{B.3}$$

and applying the Poisson summation formula, see e.g. [DF37, Theorem 4], gives

$$\frac{\ell}{N} \sum_{n=0}^{N-1} a\left(\tfrac{n\ell}{N}\right) e^{\frac{i}{\hbar}\phi\left(\frac{n\ell}{N}\right)} = \int_0^\ell a(t) e^{\frac{i}{\hbar}\phi(t)} \, dt + 2 \sum_{n=1}^\infty \int_0^\ell a(t) e^{\frac{i}{\hbar}\phi(t)} \cos\left(\tfrac{n\ell^* t}{\hbar}\right) dt. \tag{B.4}$$

The phase ϕ in the first integral has no stationary points in supp a, whereas the stationary points in the second integral are determined by $\phi'(t) = \pm n\ell^*$. Due to (B.1) this gives $n = |\nu|$, and therefore only one term in the sum over n exceeds $O(\hbar^\infty)$. Hence (B.2) follows. □

This Lemma is an essential ingredient needed to prove the following statement.

Proposition 5. *Let $H \in C^\infty(\mathbb{R}^2)$ be periodic with respect to $\ell_x \mathbb{Z} \oplus \ell_\xi \mathbb{Z}$, and let $h \in C^\infty(\mu\ell_\xi, (\mu + 1)\ell_\xi)$, where $\mu \in \mathbb{Z}$. Define*

$$\varphi(x, \xi) = x\xi - h(\xi), \tag{B.5}$$

and assume that $A \in C^\infty(\mathbb{R})$ is compactly supported in $(\mu\ell_\xi, (\mu + 1)\ell_\xi)$. Moreover, let κ_ϵ be of the form (5.24) and define

$$a(x, \xi) = \kappa_\epsilon(x - h'(\xi))a(\xi). \tag{B.6}$$

One then obtains for every fixed $l \in \mathbb{Z}$

$$\sum_{\substack{m, \\ |l-m| \leq N^{\frac{1}{M}}}} \frac{\ell_x}{N} \frac{1}{\ell_\xi} \int_0^{\ell_\xi} H(x_l, \eta) e^{\frac{i}{\hbar}(x_l - x_m)\eta} d\eta \int_{\mu\ell_\xi}^{(\mu+1)\ell_\xi} a(x_m, \xi) e^{\frac{i}{\hbar}\varphi(x_m, \xi)} d\xi$$

$$= \frac{\ell_x}{N} \int_0^{\ell_\xi} H(x_l, \xi) A(\xi) e^{\frac{i}{\hbar}\varphi(x_l, \xi)} d\xi + O(\hbar^\infty). \tag{B.7}$$

where the error estimate depends uniformly on l.

Proof. We first notice that the support of $\kappa_\epsilon(x - h'(\xi))$ is compact, and therefore the function is bounded. Thus the second integral on the left-hand side in (B.7) is uniformly bounded with respect to x_m and $\hbar$. The first integral is a Fourier integral, and since H is smooth, it is of size $O(|l-m|^{-\infty})$. Hence, we can add further terms to the series such that it includes exactly N consecutive integers $m_0, \ldots, m_0 + N - 1$ centered around l, causing an error of size $O(\hbar^\infty)$.

Since $\eta \in [0, \ell_\xi]$ and $(\mu-1)\ell_\xi < \xi < (\mu+1)\ell_\xi$, we have $(\mu-2)\ell_\xi < \xi - \eta < \mu\ell_\xi$. Thus we can apply Lemma 15 with $\nu = \mu - 1$ and obtain

$$\sum_{\substack{m, \\ |l-m| \leq N^{\frac{1}{M}}}} \frac{\ell_x}{N} \int_0^{\ell_\xi} H(x_l, \eta) e^{\frac{i}{\hbar}(x_l - x_m)\eta} d\eta \int_{\mu\ell_\xi}^{(\mu+1)\ell_\xi} a(x_m, \xi) e^{\frac{i}{\hbar}\varphi(x_m, \xi)} d\xi$$

$$= \int_{\mathbb{R}} \int_0^{\ell_\xi} \int_{\mu\ell_\xi}^{(\mu+1)\ell_\xi} a(x, \xi) H(x_l, \eta) e^{\frac{i}{\hbar}\phi_l(x, \xi, \eta)} dx d\xi d\eta + O(\hbar^\infty), \tag{B.8}$$

where

$$\phi_l(x, \xi, \eta) = x\big(\xi - \eta - (\mu - 1)\ell_\xi\big) - h(\xi) + x_l\eta. \tag{B.9}$$

Regarding ξ as a parameter, we can approximate the integral over x and η with the stationary phase theorem. The Hessian of the phase function satisfies $|\det \text{Hess}\,\phi_l| = 1$ and $\text{sgn}\,\text{Hess}\,\phi_l = 0$, and the stationary points are given by $x = x_l$ and $\eta = \xi - (\mu - 1)\ell_\xi$. Since by (B.6) the function a is constant with respect to x in an ϵ-neighbourhood of $\{(h'(\xi), \xi); \xi_0 \leq \xi \leq \xi_0 + \lambda_\xi\}$, all subleading terms of finite order in $\hbar$ vanish. Therefore,

$$\int_{\mathbb{R}} \int_0^{\ell_\xi} \int_{\mu\ell_\xi}^{(\mu+1)\ell_\xi} a(x, \xi) H(x_l, \eta) e^{\frac{i}{\hbar}\phi_l(x, \xi, \eta)} dx d\xi d\eta$$

$$= 2\pi\hbar \int_0^{\ell_\xi} a(x_l, \xi) H(x_l, \xi - \mu\ell_\xi) e^{\frac{i}{\hbar}\phi_l(x_l, \xi, \xi - \mu\ell_\xi)} d\xi + O(\hbar^\infty) \tag{B.10}$$

$$= \frac{\ell_\xi \ell_x}{N} \int_0^{\ell_\xi} a(\xi) H(x_l, \xi) e^{\frac{i}{\hbar}[x_l\xi - h(\xi)]} d\xi + O(\hbar^\infty).$$

$\square$

C The Conley-Zehnder index

We outline the definition of the Conley-Zehnder index using results and notations of [Dui76, Mei94].

Let (E, ω) be a symplectic vector space. Its Lagrangian Grassmannian $\Lambda(E)$ is the set of all Lagrangian subspaces of E. Given $L_1, L_2, L_3 \in \Lambda(E)$, we define on $L_1 \oplus L_2 \oplus L_3$ the quadratic form $Q(x_1, x_2, x_3) = \omega(x_1, x_2) + \omega(x_2, x_3) + \omega(x_3, x_1)$, as well as its signature $s(L_1, L_2, L_3) := \operatorname{sgn} Q$

Suppose now that L_1 and L_2 depend on $t \in [a, b]$, and that L_3 is transversal (see [Lee13, p. 143]) to L_1 and L_2 for all $t \in [a, b]$. We then define [Mei94, (5)]

$$[L_1 : L_2]_a^b = \frac{1}{2}[s(L_1(a), L_2(a), L_3) - s(L_1(b), L_2(b), L_3)]. \tag{C.1}$$

Let $0 = t_0 < t_1 < \ldots < t_\nu < \ldots < t_k = T$ be a partition of $[0, T]$ and assume that for every subinterval $[t_{\nu-1}, t_\nu]$ there exists $L_{3,\nu} \in \Lambda(E)$ such that L_1, L_2 and $L_{3,\nu}$ satisfy the above requirements. We then set

$$[L_1 : L_2]_0^T = \sum_{\nu=1}^{k} [L_1 : L_2]_{t_{\nu-1}}^{t_\nu}. \tag{C.2}$$

Now let (M, ω) be a symplectic manifold, with cotangent bundle $\pi : T^*M \to M$. The vertical bundle V_M is defined by $V_M(p) = \ker \mathrm{T}\,\pi|_p$, $p \in M$, where $\mathrm{T}\,\pi$ is the differential of the projection π, and is a Lagrangian submanifold. We assume that a Hamiltonian $H \in C^\infty(M)$ is given that generates a Hamiltonian flow Φ_t. We also assume that $\lambda \in \mathbb{R}$ is a regular value of H and that p is a periodic orbit of Φ_t in $H^{-1}(\lambda) \subset M$ with period t_p.

We now assume that $\dim M = 2$. Then a periodic orbit p itself is a Lagrangian submanifold. Using [Mei94, (A2) p. 9] we now define the Conley-Zehnder index of a periodic orbit p by [Mei94, p. 10],

$$\sigma_p = \left[\mathrm{T}\, \Phi_{t_p}^{-1} V_M(q) : V_M(\Phi_{t_p}^{-1}(q)) \right]_0^{t_p}, \tag{C.3}$$

where q is an arbitrary point on p; the expression (C.3) is independent of the choice of q. In a two dimensional phase space the Conley-Zehnder index is additive, i.e.,

$$\sigma_p = k\sigma_{p^\#}, \tag{C.4}$$

if p is a k-fold repetition of a primitive periodic orbit $p^\#$, see [Mei94, p. 10].

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