J. Phys. A: Math. Gen. **38** (2005) 1977–2004 doi:10.1088/0305-4470/38/9/010

# Quantum normal forms, Moyal star product and Bohr–Sommerfeld approximation

**Matthew Cargo, Alfonso Gracia-Saz, R G Littlejohn, M W Reinsch and P de M Rios**

Departments of Physics and Mathematics, University of California, Berkeley, CA 94720, USA

E-mail: robert@wigner.berkeley.edu

Received 7 October 2004, in final form 9 November 2004
Published 16 February 2005
Online at stacks.iop.org/JPhysA/38/1977

**Abstract**

A normal form transformation is carried out on one-dimensional quantum Hamiltonians that transforms them into functions of the quantum harmonic oscillator. The method works with the Weyl transform (or 'symbol') of the Hamiltonian. The Moyal star product is used to carry out the normal form transformation at the level of symbols. Diagrammatic techniques are developed for handling the expressions that result from higher order terms in the Moyal series. Once the normal form is achieved, the Bohr–Sommerfeld formula for the eigenvalues, including higher order corrections, follows easily.

PACS numbers: 03.65.Sq, 02.40.Gh, 03.65.Vf, 02.20.Sv

## 1. Introduction

In this paper we carry out a normal form transformation for one-dimensional, quantum systems that transforms an original Hamiltonian by unitary conjugation into a function of the quantum harmonic oscillator. Operators are mapped by the Wigner–Weyl transform into their corresponding 'symbols', functions on phase space that can be thought of as the classical counterparts of the operators, and the Moyal star product is used to represent operator multiplication at the level of symbols. The $\hbar$ expansion of the Moyal star product provides a means of generating power series representations for the generators of the unitary operators that bring about the normal form transformation and for the normal form itself (the transformed Hamiltonian). The symbol of the original Hamiltonian (the classical Hamiltonian) is assumed to have a generic, stable fixed point in phase space, corresponding to bound states. The normal form transformation takes place in a neighbourhood of this fixed point, and produces a new Hamiltonian whose symbol is a function of the classical harmonic oscillator in this neighbourhood. This implies formally that the new quantum Hamiltonian is a function of the quantum harmonic oscillator.

Since the spectrum of an operator does not change under unitary conjugation, and since the eigenvalues of the harmonic oscillator are trivial, the normal form transformation also provides a power series in $\hbar$ for the eigenvalues of the original Hamiltonian. This series consists of the usual Bohr–Sommerfeld formula at lowest order plus higher order corrections. In this paper we use our normal form transformation to compute the first correction term (at order $\hbar^2$), a known result. In a subsequent paper we shall describe a similar normal form transformation for the multidimensional case of integrable quantum systems, including corrections to the torus or EBK quantization rule, where the corrections are apparently unknown.

One of our main accomplishments in this paper is the development of diagrammatic and other techniques for representing and manipulating expressions that result from the higher order terms in the Moyal star product. The expressions in question, which we represent as diagrams, are scalars under linear canonical transformations, constructed out of contractions of derivatives of functions on phase space, typically the symbols of operators, with the Poisson tensor. These can be thought of as generalizations of the Poisson bracket to objects with higher derivatives and any number of operands (not just two). The normal form transformation and the normal form itself are presented in terms of these diagrams. The diagrammatic notation is especially useful for representing higher order terms in various power series in $\hbar$, in which the leading term is some usual classical or semiclassical result.

Part of our motivation in this work was to develop (hopefully clean and elegant) methods for calculating higher order terms in $\hbar$ in semiclassical expansions. In this we were stimulated by several factors. One was the literature on deformation quantization, which reveals an interesting geometrical structure in higher order terms in generalizations of the Moyal star product to nontrivial phase spaces (symplectic or Poisson manifolds). The general idea is to deform the commutative algebra of multiplication of functions on the phase space into a noncommutative but associative algebra, where $\hbar$ is the deformation parameter and where the new multiplication rule is the generalized star product. It is also required that the order $\hbar$ term in the symbol representation of the commutator be proportional to the Poisson bracket. The new algebra is then interpreted as an algebra of operators on a quantum system, the 'quantized' version of the classical phase space. In one approach, the star product is represented as a formal power series in $\hbar$, a generalization of the Moyal formula, and one must work out the terms of the series subject to the constraint of associativity and the appearance of the Poisson bracket at first order. Basic references in this area include Bayen *et al* (1978), Fedosov (1994) and Kontsevich (2003). Although the phase space used in this paper, $\mathbb{R}^2$, upon which the Weyl symbol correspondence is based, is considered trivial, nevertheless throughout this work we have been thinking of generalizations to other (nonflat) phase spaces.

The Moyal star product is an attractive place to start looking for clean and efficient ways of generating quantum corrections to classical or semiclassical results, since it has an expansion in powers of $\hbar$ with a simple and explicit expression for the $n$th order term. Moreover, it represents the fundamental operation of operator multiplication, out of which other operations such as exponentiation, conjugation, etc, can be constructed. We have previously used the Moyal star product for normal form transformations in the theory of mode conversion (Littlejohn and Flynn 1991, 1992, 1993), and used it for developing perturbation expansions in quantum adiabatic theory (Littlejohn and Weigert 1993). Related work includes Braam and Duistermaat (1995), Emmrich and Weinstein (1996), Emmrich and Römer (1998), Colin de Verdière *et al* (1999) and Colin de Verdière and Parisse (1999). Our work on mode conversion only required near-identity transformations, that is, transformations that could be expanded in power series about the identity. In this paper, however, we must use transformations that are not near identity, a significantly complicating factor.

A practical motivation for looking at higher order terms derives from some recent work in the propagation of wave fields in optics (Forbes and Alonso 1998a, 1998b, 2001a, 2001b, 2001c, 2001d). Traditional WKB theory gives solutions for the problem of wave propagation, including prescriptions for what to do at caustics and for diffraction around obstacles (Maslov and Fedoriuk 1981, Keller 1962). But these prescriptions are awkward to implement in practice. It is possible to uniformize the approximate wave field by representing it as a linear combination of wave packets distributed along or near Lagrangian manifolds, but the simplest ways of doing this give results that in practice have poor accuracy compared to standard WKB methods, in spite of their formal equivalence at lowest order in the inverse wavelength. These circumstances limited our own ambitions along these lines some years ago (Littlejohn 1986). Forbes and Alonso, however, have developed variations on this idea that apparently are accurate numerically and reasonably simple algorithmically. A key element in their approach is a practical method of including higher order terms in the inverse wavelength. In other words, it may be that the problem of finding practical methods for dealing with caustics and diffraction and that of computing higher order terms go together. The method of Forbes and Alonso does not have any obvious invariance properties in phase space, but we wonder whether an approach based on the Moyal star product could simplify or perhaps improve on their ideas.

The quantum normal form transformation discussed in this paper, involving stable fixed points of the symbol of the Hamiltonian, is one of the simplest we could think of (hence one to be studied first), but there are a variety of other normal form problems, both classical and quantum, that occur in physical applications. For example, normal forms play an important role in transition state theory, where the real physical problems are usually quantum mechanical, but where often a classical model is adopted for simplicity. Then the transition state theory becomes related to problems of transport in classical Hamiltonian systems (Wiggins 1992, Uzer *et al* 2002, Mitchell *et al* 2003a, 2003b, 2004a, 2004b), in which classical normal form theory plays a part. Classical results produced in this way can be quantized to lowest order in $\hbar$ by semiclassical techniques (Creagh 2004), providing an account of quantum phenomena such as interference and tunnelling. It may be that quantum normal form methods such as those we develop in this paper could produce similar results in a more direct manner, including higher order corrections in $\hbar$.

Concerning the Bohr–Sommerfeld quantization rule and its higher order corrections, many methods for deriving these have been proposed over the years (Maslov and Fedoriuk 1981, Voros 1977, 1989, Kurchan *et al* 1989, to mention a few). There has also been some recent interest in generalizing these rules to nonflat phase spaces (Garg and Stone 2004), which however will not concern us in this paper. We distinguish between methods based on the WKB theory, applied to the Schrödinger equation (or other differential equations) and those that work with a symbols, such as the Weyl symbol. In the former class, we mention Heading (1962), Fröman and Fröman (1965, 1996, 2002) and Bender and Orszag (1978), the last of which presents higher order corrections to the Bohr–Sommerfeld rule for the one-dimensional Schrödinger equation. In this paper we are interested in methods that work with a symbol correspondence, which are more general in the class of operators they are capable of handling, and which lead to phase space geometry in a more direct manner. These are important in applications such as plasma physics where the WKB theory is applied to integral (as well as differential) equations (Berk and Pfirsch 1980). They also seem nearly essential in multidimensional problems.

In the framework of the Weyl symbol, references we are aware of that work out the one-dimensional Bohr–Sommerfeld rule and its corrections include Argyres (1965), Voros (1977) and Colin de Verdière (2004). Of these, the methods of Argyres and Colin de Verdière are similar, in that they work with traces of functions of the Hamiltonian, computed in symbol form by integrating over all of phase space. These methods work strictly with the spectrum of the operator, and do not attempt to find the eigenfunctions. These methods provide the simplest algorithms we are aware of for computing corrections to the one-dimensional Bohr–Sommerfeld rule, but as far as we can see they cannot be generalized to many dimensions. Voros has a more complicated formalism that in principle does produce eigenfunctions. In all three of these references, the corrections to the Bohr–Sommerfeld rule are presented in implicit form. The correction term of Argyres is equivalent to the sum of two diagrams, which can be combined into one as explained by Colin de Verdière (2004). The correction term presented by Voros is rather more complicated, and we have not attempted to show its equivalence to the others. Our method is more complicated than some of the others, but it does produce explicit representations of the transformations needed to find eigenfunctions and it can be generalized to the multidimensional case.

Our formula for the eigenvalues is an explicit one containing a single diagram in the order $\hbar^2$ correction. It is

$$E_n = \left[ H(A) + \frac{\hbar^2}{48}\frac{\mathrm{d}}{\mathrm{d}A}\left(\frac{1}{\omega(A)}\langle\{H, H\}_2\rangle_\phi\right) + O(\hbar^4)\right]\bigg|_{A=(n+1/2)\hbar}, \tag{1}$$

which uses the following notation. $E_n$ for $n = 0, 1, \ldots$ is the $n$th eigenvalue of the quantum Hamiltonian $\hat{H}$, which has Weyl symbol $H$. The latter is treated as a classical Hamiltonian with action-angle variables $(A, \phi)$, and is regarded as a function of the action $A$. The frequency of the classical motion is $\omega(A) = \mathrm{d}H/\mathrm{d}A$, and the notation $\{H, H\}_2$ refers to the second Moyal bracket, defined in (A.4*c*). This Moyal bracket is otherwise twice the Hessian determinant of the Hamiltonian,

$$\{H, H\}_2 = 2[H_{,xx}H_{,pp} - (H_{,xp})^2)]. \tag{2}$$

The angle brackets $\langle\cdots\rangle_\phi$ represent an average over the angle $\phi$. This result is discussed further in subsection 5.1.

This paper assumes some background in the Wigner–Weyl formalism and the Moyal star product. A sampling of references in this area includes Weyl (1927), Wigner (1932), Groenewold (1946), Moyal (1949), Voros (1977), Berry (1977), Balazs and Jennings (1984), Hillery *et al* (1984), Littlejohn (1986), McDonald (1988), Estrada *et al* (1989), Gracia-Bondía and Várilly (1995) and Ozorio de Almeida (1998). General physical references on semiclassical theory include Berry and Mount (1972), Guzwiller (1990) and Brack and Bhaduri (1997). Mathematical literature relevant to this paper includes Guillemin and Sternberg (1977), Leray (1981), Helffer and Robert (1981), Helffer and Sjöstrand (1983), Robert (1987) and Martinez (2002).

The basic idea of this paper can be motivated by starting with the usual, lowest order Bohr–Sommerfeld formula. This states that the eigenvalues of a quantum Hamiltonian are given approximately by setting $A = (n + 1/2)\hbar$ in the classical formula expressing the classical Hamiltonian $H$ as a function of its action $A$, $H = f(A)$. This formula suggests that the quantum Hamiltonian is a function of a quantum 'action operator', something like $\hat{H} = f(\hat{A})$, of which the classical formula is a lowest order representation by means of symbols, and that the eigenvalues of the action operator are $(n + 1/2)\hbar$. Since these are also the eigenvalues of the harmonic oscillator (of unit frequency), the suggestion is that the action operator is unitarily equivalent to the harmonic oscillator Hamiltonian. If this is so, then the quantum Hamiltonian is unitarily equivalent to a function of the harmonic oscillator. In this paper we find that these suggestions are borne out. We only require that the quantum Hamiltonian has a 'slowly varying' (defined in (5) Weyl symbol, and that the symbol has a generic extremum (fixed point) at some point in phase space. The classical analogue of the unitary transformation we construct is a canonical transformation that maps the level sets of the classical Hamiltonian around the extremum (which are topological circles) into exact circles about the origin. The latter, of course, are the level sets of the harmonic oscillator.

This paper is organized as follows. Section 2 explains the two stages of transformations that are applied to the original Hamiltonian $\hat{H}$, the first transforming it into a new Hamiltonian $\hat{K}$ whose symbol is a function of the harmonic oscillator at lowest order in $\hbar$, and the second transforming $\hat{K}$ to another new Hamiltonian $\hat{M}$ whose symbol is a function of the harmonic oscillator at all higher orders of $\hbar$. The first (or preparatory) transformation is explained in more detail in section 3. It is a quantized version of a classical normal form transformation, the latter being specified by a certain canonical transformation that maps the classical Hamiltonian into a function of the harmonic oscillator. The second transformation is further explained in section 4. It is based on Lie algebraic methods, like those used in classical perturbation theory. Then section 5 uses the normal form transformation plus some facts about symbols of functions of operators to compute the Bohr–Sommerfeld rule, including first corrections to the usual result. Finally, section 6 presents some conclusions and comments about the calculation. It should be possible to read the main body of this paper, skipping the appendices, to obtain an overview of our calculation. The appendices, however, are needed for the details, including notational conventions.

## 2. The setup

Let $\hat{H}$ be a Hermitian operator (the 'Hamiltonian') in a one-dimensional quantum system, that is, $\hat{H}$ acts on wavefunctions $\psi(x)$, $x \in \mathbb{R}$ (the Hilbert space is $L^2(\mathbb{R})$). We uniformly use hats ( $\hat{}$ ) over a letter to denote operators, whereas a letter without a hat represents the Weyl transform or symbol of the operator. For example,

$$H(x, p) = \int \mathrm{d}s\, \mathrm{e}^{-\mathrm{i}ps/\hbar} \langle x + s/2|\hat{H}|x - s/2\rangle \tag{3}$$

and

$$\hat{H} = \int \frac{\mathrm{d}x\, \mathrm{d}x'\, \mathrm{d}p}{2\pi\hbar}\, \mathrm{e}^{\mathrm{i}p(x-x')/\hbar} H\left(\frac{x+x'}{2}, p\right) |x\rangle\langle x'| \tag{4}$$

illustrate the Weyl transform and its inverse in the case of the Hamiltonian. We regard $H$ as the 'classical Hamiltonian', defined on the phase space $\mathbb{R}^2$, with coordinates $(x, p)$. We denote these coordinates collectively by $z^\mu = (x, p)$, $\mu = 1, 2$.

We assume that the symbol $H$ has an expansion in $\hbar$ beginning with the power $\hbar^0$,

$$H = H_0 + \hbar H_1 + \hbar^2 H_2 + \cdots, \tag{5}$$

where each $H_n$ is independent of $\hbar$. An operator whose symbol possesses this type of expansion will be called 'slowly varying' (also called àdmissible' or '$h$-admissible' (Voros 1977, Hellfer and Robert 1981)). Not all operators are slowly varying; for example, the unitary operator $\exp(-\mathrm{i}\hat{H}t/\hbar)$ is not. The leading term ($H_0$ in the example above) of the symbol of a slowly varying operator will be called the 'principal symbol'.

We assume $H$ is smooth and has a generic extremum (a fixed point) at some point of phase space. The fixed point need not be at $p = 0$, nor does $H$ need to be invariant under time-reversal ($p \to -p$). An extremum is considered generic if the Hessian matrix $H_{,\mu\nu}$ of the Hamiltonian is nonsingular at the extremum. Here and below we use comma notation for derivatives, for example,

$$H_{,\mu\nu} = \frac{\partial^2 H}{\partial z^\mu \partial z^\nu}. \tag{6}$$

For example, the fixed point $(x, p) = (0, 0)$ of the quartic oscillator ($V(x) = x^4$) is not generic, because the Hessian matrix has rank 1 at the fixed point.

It is convenient in what follows to assume that the extremum is a minimum (always the case for kinetic-plus-potential Hamiltonians). If not, we replace $\hat{H}$ by $-\hat{H}$ at the beginning of the calculation.

Radial equations (on which $x$ is the radial variable $r \geqslant 0$) are excluded from our formalism, because the Weyl symbol correspondence is not defined in the usual way on the half line, and because the centrifugal potential is singular. We believe the best way to handle such problems within a formalism like that presented in this paper is by reduction from a problem on a higher dimensional configuration space $\mathbb{R}^n$ under some symmetry, typically $SO(n)$. Nor are singular potentials such as the Coulomb potential covered by this formalism, because singularities generally invalidate the Moyal star product expansion in $\hbar$, itself an asymptotic expansion. The usual lowest order Bohr–Sommerfeld formula usually does give correct answers for singular potentials, at least to leading order in $\hbar$, but the structure of the higher order terms (in which powers of $\hbar$ occur, whether the corrections can be represented by powers of $\hbar$ at all, etc) presumably depends on the nature of the singularity.

In view of our assumptions, the classical Hamiltonian $H$ has level sets in some neighbourhood of the fixed point that are topological circles. We concentrate on this region of phase space, and ignore any separatrices and changes in the topology of the level sets of $H$ which may be encountered further away from the fixed point.

For convenience we perform a canonical scaling on the coordinates $(x, p)$ (or operators $(\hat{x}, \hat{p})$) to cause them both to have units of action$^{1/2}$. For example, in the case of the ordinary harmonic oscillator, we would write $x' = \sqrt{m\omega}x$, $p' = p/\sqrt{m\omega}$, and then drop the primes.

We shall perform a sequence of unitary operations that transform the original Hamiltonian $\hat{H}$ into a new Hamiltonian that is a function of the harmonic oscillator Hamiltonian, at least in the 'microlocal' sense of the symbols in the neighbourhood of the fixed point. The transformations will proceed in two stages. In the first stage, we perform a 'preparatory' transformation that maps $\hat{H}$ into a new Hamiltonian $\hat{K}$ that is a function of the harmonic oscillator Hamiltonian at lowest order in $\hbar$. We follow this by a sequence of near-identity unitary transformations that transform $\hat{K}$ into a new Hamiltonian $\hat{M}$ that is a function of the harmonic oscillator Hamiltonian to all higher orders in $\hbar$, at least formally. Thus, the stages are

$$\hat{H} \to \hat{K} \to \hat{M}. \tag{7}$$

What we mean by the harmonic oscillator Hamiltonian is really the action of the harmonic oscillator, given in operator and symbol form by

$$\hat{I} = \tfrac{1}{2}(\hat{x}^2 + \hat{p}^2), \qquad I = \tfrac{1}{2}(x^2 + p^2). \tag{8}$$

It turns out that an operator is a function $\hat{I}$ if and only if its symbol is a function of $I$, as is discussed more fully in appendix I, although the two functions are not the same beyond lowest order in $\hbar$. Thus, to ensure that the transformed Hamiltonian is a function of $\hat{I}$, we require that its symbol be a function of $I$.

## 3. The preparatory transformation

The preparatory transformation (the first arrow in (7)) is the most difficult, because it is not a near-identity transformation and cannot be handled by Lie algebraic (power series) methods. This transformation will transform $\hat{H}$ into another Hamiltonian $\hat{K}$ whose symbol is a function of $I$ plus terms of order $\hbar^2$ and higher. Thus, the principal symbol of $\hat{K}$ will be a function

**Table 1.** Notation for operators, symbols and functions depending on $\epsilon$.

| | | | | | | |
|---|---|---|---|---|---|---|
| $\epsilon = 0$ | $\hat{1}$ | $K$ | $K_n$ | $\mathrm{Id}^\mu$ | $\theta$ | $I$ |
| any $\epsilon$ | $\hat{U}_\epsilon$ | $H_\epsilon$ | $H_{n\epsilon}$ | $Z^\mu_\epsilon$ | $\phi_\epsilon$ | $A_\epsilon$ |
| $\epsilon = 1$ | $\hat{U}$ | $H$ | $\delta_{n0} H$ | $Z^\mu$ | $\phi$ | $A$ |

of $I$. The preparatory transformation only makes the leading order term in the symbol of $\hat{K}$ a function of $I$, not the higher order terms.

### 3.1. Imbedding $\hat{H}$ and $\hat{U}$ in a family

Let $\hat{H}$ be given. Ultimately, we shall seek a unitary transformation $\hat{U}$ such that the new Hamiltonian $\hat{K}$, defined by

$$\hat{K} = \hat{U}\hat{H}\hat{U}^\dagger, \qquad \hat{H} = \hat{U}^\dagger \hat{K}\hat{U}, \tag{9}$$

has a symbol $K$ that is a function of $I$ plus terms of order $\hbar^2$ and higher.

For the moment, however, it is conceptually simpler to imagine that $\hat{H}$ and $\hat{U}$ are given, and to seek a means based on Weyl symbols of computing $\hat{K}$, without regard to the functional form of $K$. We do this by imbedding $\hat{U}$ in a family, $0 \leqslant \epsilon \leqslant 1$, that is by assuming that there exists a smooth family of unitary operators $\hat{U}_\epsilon$, such that

$$\hat{U}_\epsilon = \begin{cases} 1 & \text{if} \quad \epsilon = 0, \\ \hat{U} & \text{if} \quad \epsilon = 1. \end{cases} \tag{10}$$

The family $\hat{U}_\epsilon$ can be seen as a path in the group of unitary transformations that act on Hilbert space, connecting the identity and the final $\hat{U}$. We do not assume $\epsilon$ is small, and do not carry out any power series expansion in $\epsilon$. We imbed $\hat{H}$ in a similar family, defining

$$\hat{H}_\epsilon = \hat{U}^\dagger_\epsilon \hat{K}\hat{U}_\epsilon, \tag{11}$$

so that

$$\hat{H}_\epsilon = \begin{cases} \hat{K} & \text{if} \quad \epsilon = 0, \\ \hat{H} & \text{if} \quad \epsilon = 1. \end{cases} \tag{12}$$

One might say that the $\epsilon$-evolution runs backwards, since $\hat{K}$ evolves into $\hat{H}$ as $\epsilon$ goes from 0 to 1. As always, Weyl symbols of the operators above are denoted without the hat, for example, $U, K, U_\epsilon, H_\epsilon$. There are several operators, symbols and functions in this paper that depend on $\epsilon$, the notation for which is summarized in table 1. We shall be interested in calculating $\hat{H}_\epsilon$, from which $\hat{K}$ follows by setting $\epsilon = 0$.

We obtain a differential equation for $\hat{H}_\epsilon$ by differentiating (11), which gives

$$\frac{\mathrm{d}\hat{H}_\epsilon}{\mathrm{d}\epsilon} = \frac{\mathrm{i}}{\hbar}[\hat{G}_\epsilon, \hat{H}_\epsilon], \tag{13}$$

where the Hermitian operator $\hat{G}_\epsilon$ (the 'generator') is defined by

$$\hat{G}_\epsilon = \mathrm{i}\hbar \hat{U}^\dagger_\epsilon \frac{\mathrm{d}\hat{U}_\epsilon}{\mathrm{d}\epsilon} = -\mathrm{i}\hbar \frac{\mathrm{d}\hat{U}^\dagger_\epsilon}{\mathrm{d}\epsilon}\hat{U}_\epsilon = \hat{G}^\dagger_\epsilon. \tag{14}$$

We assume that $\hat{G}_\epsilon$ is slowly varying. We shall solve (13) by converting operators to symbols and using the Moyal product formula. See appendix A for the Moyal star product and the diagrammatic notation we shall use for the functions and operations that arise from it.

### 3.2. Differential equations for $H_\epsilon$ and $H_{n\epsilon}$

We now transcribe (13) to symbols and substitute (A.6). This gives a differential equation for the symbol $H_\epsilon$,

$$\frac{\mathrm{d}H_\epsilon}{\mathrm{d}\epsilon} = -\{G_\epsilon, H_\epsilon\} + \frac{\hbar^2}{24}\{G_\epsilon, H_\epsilon\}_3 - \frac{\hbar^4}{1920}\{G_\epsilon, H_\epsilon\}_5 + \cdots, \tag{15}$$

which is subject to the boundary condition $H_\epsilon = H$ at $\epsilon = 1$. We express the solution of this equation in terms of a set of new functions or symbols, $H_{0\epsilon}$, $H_{2\epsilon}$, etc, which are required to satisfy the differential equations,

$$\frac{\mathrm{d}H_{0\epsilon}}{\mathrm{d}\epsilon} - \{H_{0\epsilon}, G_\epsilon\} = 0, \tag{16$a$}$$

$$\frac{\mathrm{d}H_{2\epsilon}}{\mathrm{d}\epsilon} - \{H_{2\epsilon}, G_\epsilon\} = \frac{1}{24}\{G_\epsilon, H_{0\epsilon}\}_3, \tag{16$b$}$$

$$\frac{\mathrm{d}H_{4\epsilon}}{\mathrm{d}\epsilon} - \{H_{4\epsilon}, G_\epsilon\} = \frac{1}{24}\{G_\epsilon, H_{2\epsilon}\}_3 - \frac{1}{1920}\{G_\epsilon, H_{0\epsilon}\}_5, \tag{16$c$}$$

etc, and the boundary condition $H_{n\epsilon} = \delta_{n0}\, H$ at $\epsilon = 1$. Then we have

$$H_\epsilon = H_{0\epsilon} + \hbar^2 H_{2\epsilon} + \hbar^4 H_{4\epsilon} + \cdots. \tag{17}$$

This is not an expansion of $H_\epsilon$ in powers of $\hbar$ as in (5), because the functions $H_{n\epsilon}$ are themselves allowed to have a dependence on $\hbar$. But each of these is slowly varying, so that if the series (17) is truncated, the order of the omitted term is given by the $\hbar$ coefficient. Finally, we define $K_n = H_{n\epsilon}$ evaluated at $\epsilon = 0$ (see table 1), so that we have an expansion of the symbol $K$ of $\hat{K}$,

$$K = K_0 + \hbar^2 K_2 + \hbar^4 K_4 + \cdots. \tag{18}$$

The solutions of (16*a*)–(16*c*) can be expressed in terms of a certain $\epsilon$-dependent, classical canonical transformation, $z'^\mu(\epsilon) = Z^\mu_\epsilon(z)$, where $z$ and $z'$ are the old and new variables, and $Z^\mu_\epsilon$ is the transformation function. The family of canonical transformations $Z^\mu_\epsilon$ reduces to the identity at $\epsilon = 0$, while at $\epsilon = 1$ we shall denote the transformation simply by $Z^\mu$ (without the $\epsilon$). See table 1. The transformation $Z^\mu_\epsilon$ will be defined in subsection 3.3, but it turns out that the left-hand sides of (16*a*)–(16*c*) are convective derivatives along the associated Hamiltonian flow. Equation (16*a*) is a homogeneous equation for the unknown $H_{0\epsilon}$, and the others are inhomogeneous equations with driving terms determined by lower order solutions. The structure of the system is that of a Dyson expansion, in which the canonical transformation $Z^\mu_\epsilon$ specifies a kind of interaction representation. The definition of $Z^\mu_\epsilon$ requires some notational understandings that are presented in appendix B.

### 3.3. The canonical transformations $Z$ and $Z_\epsilon$

The canonical transformation $Z^\mu_\epsilon$ is defined as the solution of the functional differential equation,

$$\frac{\mathrm{d}Z^\mu_\epsilon}{\mathrm{d}\epsilon} = \left\{Z^\mu_\epsilon, G_\epsilon\right\}, \tag{19}$$

subject to the initial conditions, $Z^\mu_\epsilon = \mathrm{Id}^\mu$ at $\epsilon = 0$, and we define $Z^\mu = Z^\mu_\epsilon$ at $\epsilon = 1$ (see table 1). The functions $Z^\mu_\epsilon$ so defined constitute a canonical transformation, for if we compute the $\epsilon$-derivative of their Poisson brackets among themselves, we find

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left\{Z^\mu_\epsilon, Z^\nu_\epsilon\right\} = \left\{\left\{Z^\mu_\epsilon, G_\epsilon\right\}, Z^\nu_\epsilon\right\} + \left\{Z^\mu_\epsilon, \left\{Z^\nu_\epsilon, G_\epsilon\right\}\right\} = -\left\{G_\epsilon, \left\{Z^\mu_\epsilon, Z^\nu_\epsilon\right\}\right\}, \tag{20}$$

where we have used the Jacobi identity. These are subject to the initial conditions $\left\{Z_\epsilon^\mu, Z_\epsilon^\nu\right\} = J^{\mu\nu}$ at $\epsilon = 0$. But since $J^{\mu\nu} = \text{const}$, the initial conditions are the solution for all $\epsilon$, as shown by direct substitution.

The canonical transformation $Z_\epsilon^\mu$ is not generated by $G_\epsilon$ regarded as an $\epsilon$-dependent Hamiltonian function, but rather by $G'_\epsilon = G_\epsilon \circ Z_\epsilon^{-1}$. That is, if we write $z^\mu(\epsilon) = Z_\epsilon^\mu(z_0)$ for the solution of Hamilton's equations,

$$\frac{\mathrm{d}z^\mu}{\mathrm{d}\epsilon} = J^{\mu\nu} G'_{\epsilon,\nu}(z), \tag{21}$$

then the functions $Z_\epsilon^\mu$ satisfy

$$\frac{\mathrm{d}Z_\epsilon^\mu}{\mathrm{d}\epsilon} = J^{\mu\nu} G'_{\epsilon,\nu} \circ Z_\epsilon = \{\mathrm{Id}^\mu, G'_\epsilon\} \circ Z_\epsilon = \left\{Z_\epsilon^\mu, G_\epsilon\right\}, \tag{22}$$

which agrees with (19). In the final step we have used an important property of the Poisson bracket, namely, that if $A$ and $B$ are any two functions and $Z$ is a canonical transformation (symplectic map), then

$$\{A, B\} \circ Z = \{A \circ Z, B \circ Z\}. \tag{23}$$

### 3.4. *Notation for $\epsilon$-derivatives*

The following notation will be useful for carrying out differentiations and integrations in the interaction representation, specified by composing a function with $Z_\epsilon^{-1}$.

For any function $F_\epsilon$ on phase space, possibly $\epsilon$-dependent, we define

$$\frac{DF_\epsilon}{D\epsilon} = \left[\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(F_\epsilon \circ Z_\epsilon^{-1}\right)\right] \circ Z_\epsilon, \tag{24}$$

for a kind of derivative operator in the interaction representation. This can be written in an alternative form,

$$\frac{DF_\epsilon}{D\epsilon} = \frac{\mathrm{d}F_\epsilon}{\mathrm{d}\epsilon} - \{F_\epsilon, G_\epsilon\}. \tag{25}$$

The proof of (25) is obtained by setting $F'_\epsilon = F_\epsilon \circ Z_\epsilon^{-1}$, so that

$$\frac{\mathrm{d}F_\epsilon}{\mathrm{d}\epsilon} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}(F'_\epsilon \circ Z_\epsilon) = \frac{\mathrm{d}F'_\epsilon}{\mathrm{d}\epsilon} \circ Z_\epsilon + (F'_{\epsilon,\mu} \circ Z_\epsilon)\frac{\mathrm{d}Z_\epsilon^\mu}{\mathrm{d}\epsilon}. \tag{26}$$

But by (19) and the chain rule for the Poisson bracket, the final term can be written as

$$(F'_{\epsilon,\mu} \circ Z_\epsilon)\left\{Z_\epsilon^\mu, G_\epsilon\right\} = \{F'_\epsilon \circ Z_\epsilon, G_\epsilon\} = \{F_\epsilon, G_\epsilon\}. \tag{27}$$

Rearranging the result gives (25).

### 3.5. *Solutions for $H_{n\epsilon}$ and $K_n$*

In view of (25), the left-hand sides of (16*a*)–(16*c*) can now be written $DH_{n\epsilon}/D\epsilon$. In particular, (16*a*) is simply $DH_{0\epsilon}/D\epsilon = 0$, which immediately gives $H_{0\epsilon} = C \circ Z_\epsilon$, where $C$ is a function independent of $\epsilon$. Substituting $\epsilon = 1$ and the boundary condition shown in table 1, we find $H = C \circ Z$. Then substituting $\epsilon = 0$, we find $C = K_0$. In summary,

$$H_{0\epsilon} = K_0 \circ Z_\epsilon. \tag{28}$$

In particular, substituting $\epsilon = 1$ we obtain

$$H = K_0 \circ Z, \qquad K_0 = H \circ Z^{-1}. \tag{29}$$

This completes the solution of $H_\epsilon$ and $K$ to lowest order.

The second-order equation (16*b*) can now be written as

$$\frac{DH_{2\epsilon}}{D\epsilon} = \frac{1}{24}\{G_\epsilon, H_{0\epsilon}\}_3. \tag{30}$$

We use (24) in this, compose both sides with $Z_\epsilon^{-1}$, integrate between $\epsilon$ and 1 and use the boundary condition $H_{2\epsilon} = 0$ at $\epsilon = 1$. The result is

$$H_{2\epsilon} = -\frac{1}{24}\int_\epsilon^1 \mathrm{d}\epsilon' \{G_{\epsilon'}, H_{0\epsilon'}\}_3 \circ Z_{\epsilon'}^{-1} \circ Z_\epsilon. \tag{31}$$

Finally, setting $\epsilon = 0$, we have

$$K_2 = -\frac{1}{24}\int_0^1 \mathrm{d}\epsilon \{G_\epsilon, H_{0\epsilon}\}_3 \circ Z_\epsilon^{-1}. \tag{32}$$

Similarly, we solve the fourth-order equation (16*c*), finding

$$K_4 = -\frac{1}{24}\int_0^1 \mathrm{d}\epsilon \{G_\epsilon, H_{2\epsilon}\}_3 \circ Z_\epsilon^{-1} + \frac{1}{1920}\int_0^1 \mathrm{d}\epsilon \{G_\epsilon, H_{0\epsilon}\}_5 \circ Z_\epsilon^{-1}. \tag{33}$$

Clearly the solutions for $H_{n\epsilon}$ and $K_n$ at any order $n$ can be written in terms of integrals over lower order solutions.

Let us now choose $\hat{U}$ so that $K$ will be a function of $I$ at lowest order in $\hbar$. We shall work backwards, first finding a canonical transformation $Z$ such that $K_0 = H \circ Z^{-1}$ is a function of $I$. We then imbed this in a one-parameter family $Z_\epsilon$, from which we compute $G_\epsilon$, $\hat{G}_\epsilon$, $\hat{U}_\epsilon$ and finally $\hat{U}$.

### *3.6. Construction of Z via action-angle variables*

The desired canonical transformation $Z$ can be specified in terms of the action-angle variables for the Hamiltonian $H$ and those of the harmonic oscillator, denoted by $(A, \phi)$ and $(I, \theta)$, respectively. All four of these variables are regarded as functions : $\mathbb{R}^2 \to \mathbb{R}$.

The action $A$ of the Hamiltonian $H$ is defined as a function of the energy by

$$A(E) = \frac{1}{2\pi}\int_{H<E} \mathrm{d}p\,\mathrm{d}x. \tag{34}$$

The integral is taken over the interior of the closed curve $H = E$ (a level set of $H$). The action vanishes at the fixed point, and is an increasing function of energy as we move away from it. Equation (34) is the standard way to write the definition of the action, but, keeping in mind the warnings of appendix B, if we wish to think of $A$ as a mapping : $\mathbb{R}^2 \to \mathbb{R}$, then we should not write $A(E)$ or $E(A)$, but rather

$$H = f_0 \circ A, \tag{35}$$

where $f_0 : \mathbb{R} \to \mathbb{R}$ is the function of a single variable expressing the relationship between energy and action. (The 0 subscript will be explained below.) The function $f_0$ is invertible in the region of interest, so $A = f_0^{-1} \circ H$. Then (34) can be written more properly by picking a point $z$ in the region of interest, writing $E = H(z)$, and then writing

$$A(z) = \big(f_0^{-1} \circ H\big)(z) = f_0^{-1}(E), \tag{36}$$

instead of the left-hand side of (34).

The easiest way to explain the canonical transformation $Z$ is to write down the equations,

$$A = I \circ Z, \qquad \phi = \theta \circ Z, \tag{37}$$

which presumes that some definition of the angles $\theta$ and $\phi$, conjugate to $I$ and $A$, respectively, has been made. (Angles $\theta$ and $\phi$ are defined relative to an arbitrary origin on each level set of

$I$ and $H$, respectively.) Then $Z$ maps the point with action-angle coordinates $(A, \phi) = (a, b)$ to the point with action-angle coordinates $(I, \theta) = (a, b)$ (the same coordinate values in two coordinate systems). $Z$ is canonical because it is the composition of one canonical transformation with the inverse of another (the transformations from $z = (x, p)$ to $(A, \phi)$ or $(I, \theta)$). This way of defining $Z$ makes it clear that $Z$ is defined over a domain that contains the fixed point and extends out to the first separatrix (but does not include it), otherwise what we are calling the 'region of interest'.

Unfortunately, this approach does not make it clear that $Z$ is smooth at the fixed point itself. This is important, because the series (A.1) employs derivatives of its operands of arbitrarily high order, and because the smoothness of functions is closely related to the form of asymptotic series involving them. In fact, for some problems, $Z$ and hence $A = I \circ Z$ are not smooth at the fixed point; the example of the quartic oscillator is discussed in appendix C. If, however, $H$ is smooth and its fixed point is generic, then it can be shown that there exists a smooth canonical transformation $Z$, defined over the region of interest, such that $A = I \circ Z$. Since $I$ is a smooth function on phase space, this implies that $A$ is smooth, too. The construction of $Z$ is discussed in appendix C, in which it is also shown that $f_0$ exists, is smooth and monotonic. This takes care of the first half of (37). As for the second half of (37), we define the harmonic oscillator angle $\theta$ by

$$x = \sqrt{2I}\sin\theta, \qquad p = \sqrt{2I}\cos\theta, \tag{38}$$

so the origin of $\theta$ is on the positive $p$-axis, and then we define $\phi = \theta \circ Z$, so that the origin of $\phi$ lies on the image of the positive $p$-axis under $Z^{-1}$.

Now using (37) and definition (29) of $K_0$, we have

$$K_0 = H \circ Z^{-1} = f_0 \circ A \circ Z^{-1} = f_0 \circ I, \tag{39}$$

that is, $K_0$ is the same function of the harmonic oscillator action $I$ as $H$ is of its own action $A$.

For reference we make some further remarks about the transformation $Z$. First, (38) was written without regard to the warnings of appendix B, but if we think of $z^\mu = (x, p)$ as values ($\in \mathbb{R}$) and $\theta$ and $I$ as functions, then the equation is put into proper notation by writing the left-hand side as $\mathrm{Id}^\mu(z)$ and $\theta$ and $I$ on the right-hand side as $\theta(z)$ and $I(z)$. Thus, (38) expresses the relation between the functions $\mathrm{Id}^\mu$ and functions $(\theta, I)$. Now composing this with $Z$ and using (37) gives

$$Z^\mu = \begin{pmatrix} \sqrt{2A}\sin\phi \\ \sqrt{2A}\cos\phi \end{pmatrix} \tag{40}$$

which gives an explicit representation of functions $Z^\mu$ in terms of functions $A$ and $\phi$.

The inverse transformation can be handled in a similar way. Let the transformation from $z^\mu = (x, p)$ to $(\phi, A)$ be expanded in a Fourier series in $\phi$,

$$z^\mu = \sum_n z_n^\mu(A)\, \mathrm{e}^{\mathrm{i}n\phi}, \tag{41}$$

where $z_n^\mu : \mathbb{R} \to \mathbb{C}$ are the expansion coefficients. This is subject to the same warnings about abuse of notation as (38). When these are straightened out and the result is composed with $Z^{-1}$, we obtain

$$(Z^{-1})^\mu = \sum_n \left(z_n^\mu \circ I\right) \mathrm{e}^{\mathrm{i}n\theta}, \tag{42}$$

an explicit representation of $Z^{-1}$.

### *3.7. Finding $Z_\epsilon$, $G_\epsilon$ and $\hat{U}_\epsilon$*

Now that we have Z, we imbed it in a smooth family $Z_\epsilon$ with the boundary values shown in table 1. Sjöstrand and Zworski (2002) show that this can be done in a neighbourhood of the fixed point, and Evans and Zworski (2004) give another proof that applies in the full domain. For later reference, we also define $\epsilon$-dependent versions of the action-angle variables,

$$A_\epsilon = I \circ Z_\epsilon, \tag{43a}$$

$$\phi_\epsilon = \theta \circ Z_\epsilon, \tag{43b}$$

with boundary values shown in table 1. Then we have

$$H_{0\epsilon} = f_0 \circ A_\epsilon. \tag{44}$$

All three Hamiltonians, $H$, $H_{0\epsilon}$ and $K$ are the same function ($f_0$) of their own actions ($A$, $A_\epsilon$ and $I$, respectively).

Next we wish to find a function $G_\epsilon$ such that (19) is satisfied for the given $Z_\epsilon$. This can always be done, since that equation can be solved for the derivatives $G_{\epsilon,\mu}$, the components of a closed 1-form (hence exact, since the region is contractible). This is a standard result in classical mechanics (Arnold 1989), which is summarized in component language in appendix E. The function $G_\epsilon$ is determined to within an $\epsilon$-dependent, additive constant. In the following we drop this constant, since its only effect is to introduce an $\epsilon$-dependent phase into $\hat{U}_\epsilon$, which has no effect on the transformed Hamiltonian.

Finally, given $G_\epsilon$, we transform it into the operator $\hat{G}_\epsilon$, and then define $\hat{U}_\epsilon$ as the solution of

$$\frac{\mathrm{d}\hat{U}_\epsilon}{\mathrm{d}\epsilon} = -\frac{\mathrm{i}}{\hbar}\hat{U}_\epsilon \hat{G}_\epsilon, \tag{45}$$

subject to the initial condition $\hat{U}_\epsilon = 1$ at $\epsilon = 0$. Then we set $\hat{U} = \hat{U}_\epsilon$ at $\epsilon = 1$. This completes the preparatory transformation (the construction of $\hat{U}$ such that $\hat{K}$ has a symbol that is a function of $I$ at lowest order). We do not need to solve (45) explicitly, since for the purposes of this paper we only need to calculate the effect on the symbol of a slowly varying operator when it is conjugated by $\hat{U}$. But it is important to know that $\hat{U}$ exists, as we have shown.

The preparatory transformation might have been carried out with oscillatory integrals coming from the integral representation of the Moyal star product, rather than in terms of a path $Z_\epsilon$ through the group of canonical transformations. Indeed, we tried this approach initially, but found that it led to complicated algebra beyond lowest order that we were not able to organize to our satisfaction. Perhaps with more effort that approach could be cast into suitable form.

The formalism we have presented is slightly simpler if we assume that the path through the group of canonical transformations, $Z_\epsilon$, $0 \leqslant \epsilon \leqslant 1$, is a one-parameter subgroup, that is, that $G_\epsilon$ is independent of $\epsilon$. This, however, is a special assumption that we did not want to make. Moreover, the use of an arbitrary path allows us to study what happens when we vary the path, which leads to interesting conclusions (see appendix H).

## 4. Second stage transformations

In the second stage (the second arrow in (7)) we transform $\hat{K}$ into a new Hamiltonian $\hat{M}$, such that the symbol $M$ is formally a function of $I$ to all orders in $\hbar$. We do this by Lie algebraic (power series) techniques that are similar to those used in classical perturbation theory (Dragt and Finn 1976, Cary 1981, Eckhardt 1986), although here there are higher order Moyal brackets appearing as well as Poisson brackets. See also Littlejohn and Weigert (1993) for an example of a Moyal-based perturbation calculation applied to an adiabatic problem in quantum mechanics.

### 4.1. The higher order transformations

We apply a sequence of near-identity unitary transformations, each of which is responsible for making the symbol of the Hamiltonian a function of $I$ at two successive orders of $\hbar$. Only even powers of $\hbar$ occur in this process. The sequence is defined by

$$\hat{M}^{(0)} = \hat{K}, \qquad \hat{M}^{(2)} = \hat{U}_2 \hat{M}^{(0)} \hat{U}_2^\dagger, \qquad \hat{M}^{(4)} = \hat{U}_4 \hat{M}^{(2)} \hat{U}_4^\dagger, \tag{46}$$

etc, where

$$\hat{U}_n = \exp(-\mathrm{i}\hbar^{n-1}\hat{G}_n), \tag{47}$$

and where $\hat{G}_n$ is the $n$th order generator, assumed to have a symbol $G_n$ that is slowly varying. Then, for example, the expression for $\hat{M}^{(2)}$ can be written as a series in $\hbar$ involving iterated commutators,

$$\hat{M}^{(2)} = \hat{K} - \mathrm{i}\hbar[\hat{G}_2, \hat{K}] - \frac{\hbar^2}{2}[\hat{G}_2, [\hat{G}_2, \hat{K}]] + \cdots, \tag{48}$$

and similarly for $\hat{M}^{(4)}$ etc. Transcribing (48) to symbols and using (A.6), we have

$$M^{(2)} = K + \hbar^2\{G_2, K\} + \hbar^4\left(-\tfrac{1}{24}\{G_2, K\}_3 + \tfrac{1}{2}\{G_2, \{G_2, K\}\}\right) + \cdots. \tag{49}$$

In a similar manner we write out commutator expansions for the higher order transformations in (46), transcribe them into symbols, compose the transformations together and substitute the expansion (18). We write the result in the form,

$$M = M_0 + \hbar^2 M_2 + \hbar^4 M_4 + \cdots, \tag{50}$$

where $M = M^{(\infty)}$, the symbol of the final Hamiltonian after all the second stage unitary transformations have been carried out, and where

$$M_0 = K_0, \tag{51$a$}$$

$$M_2 = K_2 + \{G_2, K_0\}, \tag{51$b$}$$

$$M_4 = K_4 + \{G_2, K_2\} - \tfrac{1}{24}\{G_2, K_0\}_3 + \tfrac{1}{2}\{G_2, \{G_2, K_0\}\} + \{G_4, K_0\}, \tag{51$c$}$$

etc. Each $M_n$ is slowly varying.

We want $M$ to be a function only of $I$. At lowest order we have this already,

$$M_0 = K_0 = f_0 \circ I = H \circ Z^{-1}. \tag{52}$$

At second order, we wish to choose $G_2$ in (51$b$) so that $M_2$ will be a function only of $I$, that is, independent of $\theta$. In the next few steps it is convenient to bring back the abuse of notation rejected in appendix B, and to think of functions like $K_2$, $M_2$, etc as functions of either $z = (x, p)$ or of the action-angle coordinates $(\theta, I)$, as convenient. Then the Poisson bracket in (51$b$) can be computed in action-angle variables, whereupon we have

$$M_2 = K_2 + \frac{\partial G_2}{\partial \theta}\omega(I), \tag{53}$$

where $\omega(I) = \mathrm{d}K_0/\mathrm{d}I$. Note that as a function, $\omega = f_0'$, since $K_0 = f_0 \circ I$, so $\omega(A) = \mathrm{d}H/\mathrm{d}A = f_0'(A)$. Thus, $\omega(A)$ is the frequency of the classical oscillator with Hamiltonian $H$. If we now average both sides of (53) over the angle $\theta$, we obtain

$$M_2 = \bar{K}_2, \tag{54}$$

where the overbar represents the $\theta$ average. The simple result is that $M_2$ is just the average of $K_2$, given by (32).

Then subtracting (54) from (53) and rearranging, we obtain

$$\frac{\partial G_2}{\partial \theta} = -\frac{1}{\omega(I)} \tilde{K}_2, \tag{55}$$

where the tilde represents the oscillatory part in $\theta$ of a function. Equation (55) always has a solution $G_2$ that is a periodic function of $\theta$, that is, it is a single-valued function of $(x, p)$, since $\tilde{K}_2$ has a Fourier series in $\theta$ without the constant term. Thus we have shown that it is possible to choose $G_2$ in (51*b*) such that $M_2$ is independent of $\theta$.

The same structure persists at all higher orders. For example, taking the averaged and oscillatory parts of the fourth-order equation (51*c*) yields an expression for $M_4$ that is independent of $\theta$ and a solvable equation for $G_4$. This shows that it is possible to transform the original Hamiltonian $\hat{H}$ into a function of the harmonic oscillator $\hat{I}$ to all orders in $\hbar$, at least in the sense of a formal power series for the symbol.

### 4.2. *Doing the $\epsilon$-integral*

The following steps require some notation and an important theorem regarding averaging operators that are explained in appendix D. The theorem in question is (D.8), which we apply to (54), using (32), to obtain a useful form of the expression for $M_2$:

$$\begin{aligned} M_2 &= -\frac{1}{24} \int_0^1 \mathrm{d}\epsilon \big\langle (G_\epsilon \Rrightarrow H_{0\epsilon}) \circ Z_\epsilon^{-1} \big\rangle_\theta \\ &= -\frac{1}{24} \int_0^1 \mathrm{d}\epsilon \, \langle G_\epsilon \Rrightarrow H_{0\epsilon} \rangle_{\phi_\epsilon} \circ Z_\epsilon^{-1}, \end{aligned} \tag{56}$$

where the diagrammatic notation is explained in appendix A. The $\epsilon$-integration in (56) can be done, yielding an expression independent of $\epsilon$, that is, independent of the path taken through the group of unitary or canonical transformations used in the preparatory transformation.

First we transform the integrand of (56) as described in appendix F, to obtain

$$\begin{aligned} M_2 &= \frac{1}{24} \int_0^1 \mathrm{d}\epsilon \left[ \frac{\mathrm{d}}{\mathrm{d}A_\epsilon} \left( \frac{1}{\omega \circ A_\epsilon} \langle H_{0\epsilon} \rightarrow G_\epsilon \rightrightarrows H_{0\epsilon} \rangle_{\phi_\epsilon} \right) \right] \circ Z_\epsilon^{-1} \\ &= \frac{1}{24} \frac{\mathrm{d}}{\mathrm{d}I} \left( \frac{1}{\omega \circ I} \int_0^1 \mathrm{d}\epsilon \, \langle H_{0\epsilon} \rightarrow G_\epsilon \rightrightarrows H_{0\epsilon} \rangle_{\phi_\epsilon} \circ Z_\epsilon^{-1} \right) \\ &= \frac{1}{24} \frac{\mathrm{d}}{\mathrm{d}I} \left( \frac{1}{\omega \circ I} \left\langle \int_0^1 \mathrm{d}\epsilon \, (H_{0\epsilon} \rightarrow G_\epsilon \rightrightarrows H_{0\epsilon}) \circ Z_\epsilon^{-1} \right\rangle_\theta \right), \end{aligned} \tag{57}$$

where once we have transformed $A_\epsilon$ into $I$ by composing with $Z_\epsilon^{-1}$ we can pull the factors depending on it out of the integral, since they are no longer $\epsilon$-dependent. Next we use the methods described in appendix G to guess and prove that

$$\frac{1}{2} \frac{D}{D\epsilon} (H_{0\epsilon} \rightrightarrows H_{0\epsilon}) = (H_{0\epsilon} \rightarrow G_\epsilon \rightrightarrows H_{0\epsilon}). \tag{58}$$

This makes the integral (57) easy to do, yielding,

$$M_2 = \frac{1}{48} \frac{\mathrm{d}}{\mathrm{d}I} \left( \frac{1}{\omega \circ I} \big\langle (H \rightrightarrows H) \circ Z^{-1} - (K_0 \rightrightarrows K_0) \big\rangle_\theta \right). \tag{59}$$

Let us call the two terms on the right-hand side of (59) the '$H$-term' and the '$K_0$-term'. Since $K_0 = f_0 \circ I$, the Moyal bracket in the $K_0$-term can be expanded out by the chain rule in terms of derivatives of $f_0$ and diagrams involving $I$. We find

$$(K_0 \rightrightarrows K_0) = 2 f_0' f_0'' (I \rightarrow I \leftarrow I) + f_0'^2 (I \rightrightarrows I), \tag{60}$$

where $f_0'$ means $f_0' \circ I$, etc, and where some diagrams have vanished since $(I \to I) = \{I, I\} = 0$. The nonvanishing diagrams can be calculated using (8), which gives

$$(I \rightarrow I \leftarrow I) = 2I, \qquad (I \rightrightarrows I) = 2, \tag{61}$$

so the $K_0$-term is a function only of $I$ and the angle average in (59) does nothing to this term. Finally we take the $I$-derivative and compute the $K_0$-term explicitly, finding,

$$K_0\text{-term} = -\frac{f_0''}{8} - \frac{f_0'''}{12} I. \tag{62}$$

The intermediate Hamiltonian $K$ is not unique, because of the choice of the path $Z_\epsilon$ through the group of canonical transformations that connects the identity at $\epsilon = 0$ and the given transformation $Z$ at $\epsilon = 1$. More precisely, $K_0 = H \circ Z^{-1}$ is unique because it is expressed purely in terms of $Z$, but $K_2$ and all higher order terms depend on $Z_\epsilon$ at intermediate values of $\epsilon$. Nevertheless, by (54), if we vary the path $Z_\epsilon$ while keeping the endpoints fixed, $K_2$ can change by at most a function whose $\theta$-average is zero, so that $M_2$ remains invariant. Such a function can be written as the $\theta$-derivative of some other function. These facts are proven in appendix H.

## 5. The eigenvalues

We have shown how to transform the original Hamiltonian $\hat{H}$ into a new Hamiltonian $\hat{M}$ whose symbol $M$ is a function of $I$ to any desired order in $\hbar$, and we have explicitly evaluated the first two terms $M_0$ and $M_2$ of the series for $M$. Let us write $M_n = g_n \circ I$, thereby defining the functions $g_n$, so that $= g \circ I$, where $g = g_0 + \hbar^2 g_2 + \hbar^4 g_4 + \cdots$. In view of (52) we have $g_0 = f_0$, and $g_2$ is given implicitly by (59).

As mentioned above, an operator is a function of $\hat{I}$ if and only if its symbol is a function of $I$. The two functions are the same at lowest order in $\hbar$, but it turns out that they differ at higher order. These facts are proved in appendix I. Thus, if we define a function $f$ by $\hat{M} = f(\hat{I})$ and expand it according to $f = f_0 + \hbar^2 f_2 + \hbar^4 f_4 + \cdots$, then we will have $f_0 = g_0$ but $f_2 \neq g_2$. Thus $f_0$ defined this way is the same function introduced above in (35), and we have $\hat{M} = f_0(\hat{I})$ at lowest order. This is just what we guessed in the introduction, and it implies the usual Bohr–Sommerfeld formula, since the eigenvalues of $\hat{I}$ are $(n + 1/2)\hbar$.

### 5.1. The Bohr–Sommerfeld rule to higher order

To carry the Bohr–Sommerfeld rule to higher order, it is necessary to find the relation between the symbol of an operator and the symbol of a function of that operator. This topic is discussed in appendix I. In the following we are interested in the case $\hat{M} = f(\hat{I})$ and $M = g \circ I$, so we will identify $\hat{M}$ and $\hat{I}$ with operators $\hat{B}$ and $\hat{A}$ of appendix I, respectively. Then (I.4) gives the relation between functions $f$ and $g$. Expanding $f$ and $g$ in even $\hbar$ series as above and using $M_n = g_n \circ I$, we can write (I.4) in the form,

$$\begin{aligned} M_0 + \hbar^2 M_2 + \cdots \\ &= f_0 + \hbar^2 \left[ f_2 - \frac{f_0''}{16}(I \rightrightarrows I) - \frac{f_0'''}{24}(I \rightarrow I \leftarrow I) \right] + \cdots \\ &= f_0 + \hbar^2 \left( f_2 - \frac{f_0''}{8} - \frac{f_0'''}{12} I \right) + \cdots, \end{aligned} \tag{63}$$

where $f_0$ means $f_0 \circ I$, etc, and where we use (61). This implies $M_0 = f_0 \circ I$, which we knew already, and allows us to solve for $f_2$ by equating the final quantity in the parentheses with $M_2$

in (59). We see that the second-order correction terms coming from (I.4) exactly cancel the $K_0$-term (62), so that $f_2 \circ I$ is just the $H$-term of (59),

$$f_2 \circ I = \frac{1}{48}\frac{\mathrm{d}}{\mathrm{d}I}\left(\frac{1}{\omega \circ I}\langle H \Rrightarrow H\rangle_\phi \circ Z^{-1}\right), \tag{64}$$

where we use (D.9).

The eigenvalues of $\hat{H}$ are the same as the eigenvalues of $\hat{M}$, which are given by $f \circ I$ evaluated at $I = (n+1/2)\hbar$, or as we shall prefer to write it, $f \circ A$ evaluated at $A = (n+1/2)\hbar$ (in this final step we are starting to confuse the functions $I$, $A$, with the values $I$, $A$). We compose $f \circ I = f_0 \circ I + \hbar^2 f_2 \circ I + \cdots$ with $Z$ and use (37), (52) and (64) to obtain (1), which is the Bohr–Sommerfeld formula including $O(\hbar^2)$ corrections.

Equation (1) is manifestly invariant under linear canonical transformations, since the matrix $J^{\mu\nu}$ is invariant under conjugation by a symplectic matrix. Therefore, although this equation was derived in coordinates $(x, p)$ with balanced units of action$^{1/2}$, the original units may be restored by a canonical scaling transformation, and the answer remains the same.

Equation (1) agrees with the result of Argyres (1965) and Colin de Verdière (2004), although their expressions for $E_n$ are expressed in implicit form. In the case $H = p^2/2m + V(x)$, we have $\{H, H\}_2 = 2V''(x)/m$, and (1) agrees with the second-order results of Bender and Orszag (1978), although we omit the details of the comparison.

### *5.2. Action operators*

The formalism presented naturally suggests a definition of an 'action operator'. Let $\hat{V}$ be the overall unitary transformation resulting from the composition of the preparatory and second stage transformations,

$$\hat{V} = \ldots \hat{U}_4 \hat{U}_2 \hat{U}, \tag{65}$$

so that

$$\hat{M} = \hat{V}\hat{H}\hat{V}^\dagger = f(\hat{I}). \tag{66}$$

We then define an action operator $\hat{B}$ by

$$\hat{B} = \hat{V}^\dagger \hat{I} \hat{V}, \tag{67}$$

so that

$$\hat{H} = \hat{V}^\dagger f(\hat{I})\hat{V} = f(\hat{B}). \tag{68}$$

This is the relation whose expression in terms of symbols is the Bohr–Sommerfeld formula. It is straightforward to write out the symbol $B$ of $\hat{B}$ in a power series in $\hbar$. Our analysis of the multidimensional Bohr–Sommerfeld formula involves action operators in a more intimate way than the one-dimensional case.

One can also transform creation and annihilation operators. Let $\hat{a} = (\hat{x} + \mathrm{i}\hat{p})/(\sqrt{2\hbar})$, $\hat{a}^\dagger = (\hat{x} - \mathrm{i}\hat{p})/(\sqrt{2\hbar})$, so that $\hat{I} = (\hat{a}^\dagger\hat{a} + 1/2)\hbar$, and define the unitarily equivalent operators $\hat{b} = \hat{V}^\dagger\hat{a}\hat{V}$, $\hat{b}^\dagger = \hat{V}^\dagger\hat{a}^\dagger\hat{V}$. In this way many of the algebraic relations involving creation and annihilation operators for the harmonic oscillator go over to more general oscillators, for example, $\hat{B} = (b^\dagger b + 1/2)\hbar$.

## 6. Conclusions

We conclude by presenting some comments on the present calculation.

We could have expanded $H$ in a power series in $\hbar$, as in (5), and used the boundary conditions $H_{n\epsilon} = H_n$ at $\epsilon = 1$, which would have made all the symbols of this paper,

$H_{n\epsilon}$, $K_n$, $M_n$, etc, independent of $\hbar$. We did not do this because the odd powers of $\hbar$ in the expansion of $H$ would complicate all subsequent formulae without otherwise raising any new, essential issues to be dealt with. The essence of the procedure we have given is one that operates only with even powers of $\hbar$.

In the calculation above there was a 'miraculous' cancellation of the $K_0$-term (62), where in one instance it arose as a consequence of doing the $\epsilon$-integral for $K_2$, and in the second as a consequence of working out the symbol of a function of an operator. One suspects that this cannot be accidental. We will provide a deeper insight into this cancellation in our subsequent work on the multidimensional problem.

One can imagine other normal form problems. The simplest is a quantized version of the classical transformation that maps the Hamiltonian in a simply connected region of phase space where $\mathrm{d}H \neq 0$ into the normal form $H = p$. This would provide a Moyal approach to ordinary WKB theory for wavefunctions. A more complicated example might be a transformation to a normal form with a separatrix, for example, a standard double well oscillator. A question would be what class of quantum operators whose principal symbols possess such a separatrix could be mapped into the standard normal form. Certainly the areas inside the separatrix would have to be the same for the classical transformation to exist, but whether this would be enough to guarantee the existence of the quantum normal form transformation is an open question, as far as we know.

The derivation of the multidimensional generalization of the Bohr–Sommerfeld formula (including order $\hbar^2$ corrections), also known as the Einstein–Brillouin–Keller or torus quantization rule, requires new diagrammatic methods not considered in this paper. The answer is not an obvious generalization of the one-dimensional formula, and it involves some new geometrical issues for its interpretation. These topics will be the subject of a companion paper.

## Acknowledgments

The authors would like to acknowledge stimulating and useful conversations with Yves Colin de Verdière, Jonathan Robbins, Alan Weinstein and Maciej Zworski. We would also like to thank the Mathematical Sciences Research Institute for their hospitality while part of this work was being carried out. Research at MSRI is supported in part by NSF grant DMS-9810361. Alfonso Gracia-Saz has been supported by fellowships from 'La Caixa' Foundation and la Secretaría de Estado de Universidades e Investigación del Ministerio Español de Educación y Ciencia. P de M Rios acknowledges support from a CNPq postdoctoral fellowship.

## Appendix A. Notation for Moyal star product

The Moyal star product $A * B$ of two symbols $A$, $B$ is the symbol of the operator product $\hat{A}\hat{B}$. We write the $\hbar$ expansion of this product in the following notation:

$$A * B = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{\mathrm{i}\hbar}{2}\right)^n \{A, B\}_n. \tag{A.1}$$

We call the bracket $\{,\}_n$ that occurs in this series the '$n$th order Moyal bracket' (other authors use this terminology to mean something else). This bracket is defined as follows. First, we define the Poisson tensor and its inverse by means of component matrices in the $z^\mu = (x, p)$ coordinates,

$$J^{\mu\nu} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \qquad J_{\mu\nu} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{A.2}$$

Note that $J_{\mu\nu}$ are the components of the symplectic form. We use $J^{\mu\nu}$ or $J_{\mu\nu}$ to raise and lower indices. This proceeds much as in metrical geometry, but one should note the sign change in

$$X^\mu Y_\mu = -X_\mu Y^\mu. \tag{A.3}$$

(In this paper we sum over repeated indices.) Next, we define

$$\{A, B\}_0 = AB, \tag{A.4a}$$
$$\{A, B\}_1 = A_{,\mu} J^{\mu\alpha} B_{,\alpha}, \tag{A.4b}$$
$$\{A, B\}_2 = A_{,\mu\nu} J^{\mu\alpha} J^{\nu\beta} B_{,\alpha\beta}, \tag{A.4c}$$
$$\{A, B\}_3 = A_{,\mu\nu\sigma} J^{\mu\alpha} J^{\nu\beta} J^{\sigma\gamma} B_{,\alpha\beta\gamma}, \tag{A.4d}$$

etc, as required for (A.1) to be the standard Moyal series for the star product. Note that $\{,\}_1$ is the usual Poisson bracket. In this paper a bracket $\{,\}$ without a subscript will be assumed to be a Poisson bracket. Note also that

$$\{A, B\}_n = (-1)^n \{B, A\}_n. \tag{A.5}$$

Finally, note that if $\hat{C} = [\hat{A}, \hat{B}]$, then the Moyal series for the symbol of the commutator is

$$\begin{aligned} C = [A, B]_* &= 2 \sum_{n=1,3,5,\ldots} \frac{1}{n!} \left(\frac{\mathrm{i}\hbar}{2}\right)^n \{A, B\}_n \\ &= \mathrm{i}\hbar \left( \{A, B\} - \frac{\hbar^2}{24}\{A, B\}_3 + \frac{\hbar^4}{1920}\{A, B\}_5 - \cdots \right), \end{aligned} \tag{A.6}$$

which defines the notation $[A, B]_*$.

In this paper we make use of an alternative, diagrammatic notation for $n$th order Moyal brackets and related expressions. For example, the ordinary Poisson bracket is written as

$$\{A, B\} = A \rightarrow B, \tag{A.7}$$

where the arrow indicates differentiations applied to the operands $A$ and $B$, connected by the $J^{\mu\nu}$ tensor. The base of the arrow is attached to the first index of $J^{\mu\nu}$ and the tip to the second index. The operands can be placed in any position, as long as the arrow goes in the right direction

$$A \rightarrow B = \begin{array}{c} A \\ \big\downarrow \\ B \end{array} = \begin{array}{c} B \\ \big\uparrow \\ A \end{array} = B \leftarrow A. \tag{A.8}$$

But if the direction of the arrow is reversed, then there is a sign change, due to the antisymmetry of $J^{\mu\nu}$

$$A \rightarrow B = -(A \leftarrow B), \tag{A.9}$$

which is the usual antisymmetry of the Poisson bracket. Similarly, the second Moyal bracket is given by

$$\{A, B\}_2 = A \rightrightarrows B = A \leftleftarrows B. \tag{A.10}$$

The two expressions on the right are equal because changing the direction of both arrows changes the sign twice. In this notation, the Jacobi identity is

$$[(A \rightarrow B) \rightarrow C] + [(B \rightarrow C) \rightarrow A] + [(C \rightarrow A) \rightarrow B] = 0, \tag{A.11}$$

where the square brackets are only for clarity. The first term can be expanded out by the chain rule, which in diagrammatic notation gives

$$(A \rightarrow B) \rightarrow C = (A \rightarrow B \rightarrow C) + (C \leftarrow A \rightarrow B). \tag{A.12}$$

Similarly expanding the other two terms gives the vanishing sum of six diagrams, providing a diagrammatic proof of the Jacobi identity.

## Appendix B. Notation for functions

In this paper it is convenient to use the (slightly nonstandard) notation $f : A \to B$ to mean that the domain of function $f$ is some suitably chosen subset of set $A$ (in the standard notation, $A$ itself is the domain).

For the calculations of this paper it is important to avoid the usual abuse of notation in physics in which a function is confused with the value of a function. (Actually it is practically impossible to avoid this everywhere, but we shall do so wherever it is likely to cause confusion.) A 'function' means a mapping, for example, $H, H_\epsilon, G_\epsilon, \ldots : \mathbb{R}^2 \to \mathbb{R}$, and a canonical transformation is another mapping, $Z_\epsilon, Z, \ldots : \mathbb{R}^2 \to \mathbb{R}^2$. The components $\mu = 1, 2$ of $Z$ or $Z_\epsilon$ will be denoted $Z^\mu$ or $Z^\mu_\epsilon$; each of these is a function : $\mathbb{R}^2 \to \mathbb{R}$. Functions will be denoted by bare symbols, $H$, $Z^\mu$, etc, whereas values of functions will involve the specification of an argument, $H(z)$, $Z^\mu(z_0)$, etc. It is also important to distinguish the identity map $\mathrm{Id} : \mathbb{R}^2 \to \mathbb{R}^2$ from its value, which are the coordinates themselves. The identity map is defined by

$$\mathrm{Id}^\mu(z) = z^\mu. \tag{B.1}$$

One must also be careful about notation for derivatives. We use comma notation for derivatives since notation such as $\partial A/\partial z^\mu$ prejudices the choice of symbol to be used for the argument of the function. For example, the notation

$$\frac{\partial A}{\partial z^\mu}(Z(z)) \tag{B.2}$$

is ambiguous; do we differentiate first and then substitute $Z(z)$ for the argument, or substitute first and then differentiate? To avoid this problem, we write $A,_\mu$ for the derivative of $A$, $A,_\mu \circ Z$ if we wish to differentiate first and then substitute, and $(A \circ Z),_\mu$ if we wish to substitute first and then differentiate, where $\circ$ represents the composition of two functions. The latter expression can be expanded by the chain rule,

$$(A \circ Z)_{,\mu} = (A_{,\nu} \circ Z) Z^\nu_{,\mu}. \tag{B.3}$$

Poisson and Moyal brackets defined in (A.4*a*)–(A.4*d*) always denote functions. For example, the notation $\{A(z), B(z)\}$ is meaningless, because it is only possible to take the Poisson bracket of functions, not numbers (the values of functions). On the other hand, $\{A, B\}(z)$ is meaningful.

## Appendix C. The existence and smoothness of *Z*

The notation of this appendix deviates somewhat from that of the main text.

In the following we assume that $H$ is smooth in the region of interest and that the fixed point is generic. We write $(q, p)$ for the coordinates on phase space. The differential $\mathrm{d}H$ vanishes at the fixed point, where the Hessian is positive definite, but nowhere else in the region of interest. We begin by showing that there exists a smooth canonical transformation $Z$ that maps the level sets of $H$ into circles about the origin. Since $Z$ is area preserving, this implies $A = I \circ Z$. The construction is based on the Morse lemma (Milnor 1969), a standard result that applies in this case because the fixed point is a nondegenerate critical point.

The Morse lemma states that there exists a smooth coordinate transformation, say, $(q, p) \mapsto (x, y)$, such that

$$H(x, y) = \tfrac{1}{2}(x^2 + y^2), \tag{C.1}$$

exactly. Here we abuse notation, writing $H$ for what is really the composition of $H$ with the mapping $(q, p) \mapsto (x, y)$.

The mapping $(q, p) \mapsto (x, y)$, which maps the levels sets of $H$ into circles about the origin of the $(x, y)$-plane, is not necessarily canonical, because it does not necessarily preserve area. But the Jacobian $J$, defined by

$$\mathrm{d}q\,\mathrm{d}p = J\,\mathrm{d}x\,\mathrm{d}y, \tag{C.2}$$

is smooth and nonvanishing in the region of interest. We shall take $J$ to be positive. We introduce polar coordinates $(r, \theta)$ in the $(x, y)$-plane, and write $J(x, y) = J(r, \theta)$. This is an abuse of notation which we shall also use for other functions defined on the $(x, y)$-plane, but it will be clear from context which set of coordinates is intended. Our strategy will be to perform two further smooth coordinate transformations, each of which maps circles about the origin into circles about the origin, the first of which eliminates the $\theta$-dependence of $J$, and the second, the $r$-dependence. See also Colin de Verdière and Vey (1979) for the first of these.

We write the first transformation in polar form,

$$r' = r, \qquad \theta' = \theta + f(r, \theta), \tag{C.3}$$

where we must have $\partial f/\partial\theta > -1$ in order for the transformation to be invertible. Then writing $Jr\,\mathrm{d}r\,\mathrm{d}\theta = J'r'\,\mathrm{d}r'\,\mathrm{d}\theta'$ to define the new Jacobian $J'$, we have

$$J' = \frac{J}{1 + \partial f/\partial\theta}. \tag{C.4}$$

We wish $J'$ to be independent of $\theta$. This is only consistent if $J' = \langle J\rangle$, where the angle brackets represent a $\theta$-average. Then we have

$$\frac{\partial f}{\partial\theta} = \frac{J(r,\theta)}{\langle J\rangle(r)} - 1 = g(r, \theta), \tag{C.5}$$

which defines the function $g$. We require a solution $f(r, \theta)$ of this equation such that $f(x, y)$ is smooth. It is convenient to express and solve this equation in $(r, \theta)$-coordinates, but we require smoothness in $(x, y)$-coordinates.

The function $g$ has the following properties. First, $g(x, y)$ is smooth, since both $J$ and $\langle J\rangle$ are smooth and positive. Second, $g > -1$, so any solution $f$ defines an invertible transformation. Third, $g(0) = 0$, where 0 is short for $(0, 0)$. Fourth, $\langle g\rangle = 0$.

We define the desired solution of (C.5) by

$$h(r, \theta) = \int_0^\theta g(r, \alpha)\,\mathrm{d}\alpha, \tag{C.6}$$

and

$$f(r, \theta) = h(r, \theta) - \langle h\rangle(r). \tag{C.7}$$

The first term alone on the right-hand side of (C.7) provides a solution of (C.5), but the second term is required for $f(x, y)$ to be smooth. In fact, the only question about the smoothness of $f(x, y)$ is at the origin, where the polar coordinates are singular.

The continuity of $f$ at the origin can be expressed in polar coordinates by requiring that the limit

$$\lim_{r\to 0} f(r, \theta) \tag{C.8}$$

exist for all $\theta$ and be independent of $\theta$. This holds for solution (C.7), in fact, $f(0) = h(0) = 0$.

Similarly, the differentiability of $f$ at the origin can be expressed in polar coordinates by requiring that the limit

$$\frac{\partial f}{\partial r}(0, \theta) = \lim_{r\to 0} \frac{1}{r}[f(r, \theta) - f(0, \theta)] \tag{C.9}$$

exist and have a $\theta$-dependence of the form $a\cos\theta + b\sin\theta$, where $a, b \in \mathbb{R}$. If this holds, then $a = (\partial f/\partial x)(0) = f_x(0)$ and $b = (\partial f/\partial y)(0) = f_y(0)$, where we use subscripts to indicate derivatives. This is because the limit in (C.9) is the directional derivative $(\hat{\mathbf{n}} \cdot \nabla f)(0)$, where $\hat{\mathbf{n}} = (\cos\theta, \sin\theta)$. In fact, we have

$$\begin{aligned}\frac{\partial h}{\partial r}(0,\theta) &= \int_0^\theta \frac{\partial g}{\partial r}(0,\alpha)\,\mathrm{d}\alpha = \int_0^\theta [g_x(0)\cos\alpha + g_y(0)\sin\alpha]\,\mathrm{d}\alpha \\ &= g_x(0)\sin\theta + g_y(0)[1-\cos\theta],\end{aligned} \tag{C.10}$$

since $g$ is smooth at 0. This shows that $h$ is not differentiable at 0, because of the 1 in the last term on the right-hand side. But subtracting $\langle h\rangle$ cancels this term, showing that $f$ is differentiable at 0, and, in fact,

$$f_x(0) = -g_y(0), \qquad f_y(0) = g_x(0). \tag{C.11}$$

Higher derivatives can be handled similarly. The derivative $(\partial^n f/\partial r^n)(0,\theta)$ is required to exist and be a polynomial of degree $n$ in $\cos\theta$ and $\sin\theta$ in order that $f(x, y)$ should possess all partial derivatives of degree $n$ at 0. The analysis is easier in the complex variables $z = x + \mathrm{i}y$, $\bar{z} = x - \mathrm{i}y$. Then the condition $\langle g\rangle = 0$ implies

$$\frac{\partial^{2n} g}{\partial^n z\,\partial^n \bar{z}}(0) = (\triangle^n g)(0) = 0, \tag{C.12}$$

where $\triangle = \partial^2/\partial x^2 + \partial^2/\partial y^2$ is the Laplacian. This can be used with (C.7) to show that $f$ possesses all partial derivatives of order $n$ at 0 (that is, $f$ is smooth at 0). Explicitly, we find

$$\frac{\partial^n f}{\partial^{n-m} z\,\partial^m \bar{z}}(0) = \frac{1}{\mathrm{i}(n-2m)}\frac{\partial^n g}{\partial^{n-m} z\,\partial^m \bar{z}}(0), \tag{C.13}$$

for $m = 0, \ldots, n$, excluding the case $n$ even and $m = n/2$. In the latter case the left-hand side of (C.13) vanishes ($f$ satisfies an equation like (C.12), as it must, since $\langle f\rangle = 0$). For example, at second order (reverting to rectangular coordinates) we find $f_{xx} = -g_{xy}/2$, $f_{yy} = +g_{xy}/2$, $f_{xy} = (g_{xx} - g_{yy})/4 = g_{xx}/2$.

Now transformation (C.3) can be written in the form,

$$x' = x\cos f - y\sin f, \qquad y' = x\sin f + y\cos f, \tag{C.14}$$

which, being the composition of smooth functions, is smooth. This leaves the functional form of $H$ invariant, that is, $H = (1/2)(x'^2 + y'^2)$.

We now drop the primes and return to (C.2), assuming that $J$ is a function only of $r$. For the second transformation the variable $w = r^2/2$ is convenient, so (C.2) can be written $\mathrm{d}q\,\mathrm{d}p = J(w)\,\mathrm{d}w\,\mathrm{d}\theta$, where $J$ is a smooth, positive function of $w$. Note that $w$ is just another notation for $H$ or $E$. Then we perform the coordinate transformation $w \mapsto w'$, where

$$w' = \int_0^w J(u)\,\mathrm{d}u, \tag{C.15}$$

so that $w'$ is a smooth and monotonic function of $w$. This implies

$$x' = \sqrt{w'/w}\,x, \qquad y' = \sqrt{w'/w}\,y, \tag{C.16}$$

which is smooth since $w'(w)/w$ is smooth and positive (including at $w = 0$, where $w' = J(0)$). Thus, $\mathrm{d}q\,\mathrm{d}p = \mathrm{d}w'\,\mathrm{d}\theta$, so $w'$ is another notation for the harmonic oscillator action $I$, and the function $w'(w)$ is the same as the function $f_0^{-1}(E)$ defined in (35). Since $w'(w)$ is smooth and monotonic, it is invertible and $f_0$ exists and is smooth and monotonic. Note also that the frequency $\omega = \mathrm{d}E/\mathrm{d}I$ in the present notation is $\mathrm{d}w/\mathrm{d}w' = 1/J$.

Finally, the desired canonical transformation $Z$ is the composition of the transformation of the Morse lemma composed with (C.3) and (C.15).

We note that if our conditions on $H$ are not met, then $Z$ need not be smooth at the fixed point. If $Z$ is not smooth, then neither is $A = I \circ Z$ nor $K_0 = H \circ Z^{-1}$. For example, the relation between action and energy for the quartic oscillator ($V(x) = x^4$) is given by $H = cA^{4/3}$, so $K_0 = c'(x^2 + p^2)^{4/3}$, where $c$ and $c'$ are constants. Thus, $K_0$ is not smooth at the fixed point, and neither is $Z$.

## Appendix D. Notation for averaging operators

This appendix develops an abuse-free notation for the averaging operator introduced in subsection 4.1. Let $Q : \mathbb{R}^2 \to \mathbb{R}$ be a function on phase space, treated as a Hamiltonian with evolution parameter $\alpha$,

$$\frac{\mathrm{d}z^\mu}{\mathrm{d}\alpha} = J^{\mu\nu} Q_{,\nu}(z), \tag{D.1}$$

where we assume $Q$ is independent of $\alpha$ so the equations are autonomous (unlike the case of $G_\epsilon$). Let $Y_\alpha^Q : \mathbb{R}^2 \to \mathbb{R}^2$ be the associated flow, with components $\left(Y_\alpha^Q\right)^\mu$. The superscript $Q$ indicates the Hamiltonian function generating the flow. The flow functions satisfy

$$\frac{\mathrm{d}\left(Y_\alpha^Q\right)^\mu}{\mathrm{d}\alpha} = J^{\mu\nu}\left(Q_{,\nu} \circ Y_\alpha^Q\right) = \left\{\left(Y_\alpha^Q\right)^\mu, Q\right\}. \tag{D.2}$$

We will be interested in the case that $Q$ is an action variable, $I$, $A_\epsilon$, or $A$.

For example, with $Q = I$, we have an advance map $Y_\alpha^I$ that advances the angle $\theta$ by $\alpha$. That is, if a point $z$ of phase space has action-angle coordinates $(\theta, I)$, then the point $Y_\alpha^I(z)$ has coordinates $(\theta + \alpha, I)$. Thus averaging over the angle $\theta$ can be written as

$$\bar{F} = \int_0^{2\pi} \frac{\mathrm{d}\alpha}{2\pi} F \circ Y_\alpha^I = \langle F \rangle_\theta, \tag{D.3}$$

which defines the notation $\langle F \rangle_\theta$. Similarly, we define $\langle F \rangle_{\phi_\epsilon}$ and $\langle F \rangle_\phi$, using the advance maps $Y_\alpha^{A_\epsilon}$ and $Y_\alpha^A$.

The advance maps $Z_\epsilon$ and $Y_\alpha$ are related by the following identity:

$$Z_\epsilon \circ Y_\alpha^{A_\epsilon} = Y_\alpha^I \circ Z_\epsilon. \tag{D.4}$$

In other words, angle evolution and $\epsilon$-evolution commute. We prove this by regarding both sides as functions of $\alpha$ at fixed $\epsilon$, and writing $X_\alpha$ and $X'_\alpha$ for the left- and right-hand sides, respectively. Note that $X_\alpha = X'_\alpha$ at $\alpha = 0$. The left-hand side satisfies the differential equation,

$$\begin{aligned}\frac{\mathrm{d}X_\alpha}{\mathrm{d}\alpha} &= \left(Z_{\epsilon,\nu} \circ Y_\alpha^{A_\epsilon}\right)\frac{\mathrm{d}\left(Y_\alpha^{A_\epsilon}\right)^\nu}{\mathrm{d}\alpha} = \left(Z_{\epsilon,\nu} \circ Y_\alpha^{A_\epsilon}\right)\left\{\left(Y_\alpha^{A_\epsilon}\right)^\nu, A_\epsilon\right\} \\ &= \left\{Z_\epsilon \circ Y_\alpha^{A_\epsilon}, A_\epsilon\right\} = \{X_\alpha, A_\epsilon\},\end{aligned} \tag{D.5}$$

where we have used the chain rule property of the Poisson bracket. The right-hand side satisfies

$$\frac{\mathrm{d}X'_\alpha}{\mathrm{d}\alpha} = \frac{\mathrm{d}Y_\alpha^I}{\mathrm{d}\alpha} \circ Z_\epsilon = \left\{Y_\alpha^I, I\right\} \circ Z_\epsilon = \{X'_\alpha, A_\epsilon\}, \tag{D.6}$$

where we have used (23) and (43*a*). Since $X_\alpha$ and $X'_\alpha$ satisfy the same differential equation and the same initial conditions, they are equal, $X_\alpha = X'_\alpha$, and identity (D.4) is proven. It can also be written in the form,

$$Y_\alpha^{A_\epsilon} \circ Z_\epsilon^{-1} = Z_\epsilon^{-1} \circ Y_\alpha^I. \tag{D.7}$$

It follows from this that for any function $F$ on phase space,

$$\left\langle F \circ Z_\epsilon^{-1} \right\rangle_\theta = \langle F \rangle_{\phi_\epsilon} \circ Z_\epsilon^{-1}. \tag{D.8}$$

In view of (43$b$) this is a plausible identity. In particular, at $\epsilon = 1$ we have

$$\langle F \circ Z^{-1} \rangle_\theta = \langle F \rangle_\phi \circ Z^{-1}. \tag{D.9}$$

To prove (D.8), we express the left-hand side as an integral, and then apply (D.7)

$$\int_0^{2\pi} \frac{\mathrm{d}\alpha}{2\pi} F \circ Z_\epsilon^{-1} \circ Y_\alpha^I = \int_0^{2\pi} \frac{\mathrm{d}\alpha}{2\pi} F \circ Y_\alpha^{A_\epsilon} \circ Z_\epsilon^{-1}. \tag{D.10}$$

## Appendix E. Function $G_\epsilon$ exists

Let $Z_\epsilon^\mu$ be an $\epsilon$-dependent canonical transformation, defined on a contractible region. We wish to show that there exists a function $G_\epsilon$ such that (19) is satisfied. Write $S^\mu{}_\nu = Z^\mu_{\epsilon,\nu}$ for the derivatives of $Z_\epsilon$, which form a symplectic matrix. Then

$$\frac{\mathrm{d}Z_\epsilon^\mu}{\mathrm{d}\epsilon} = S^\mu{}_\alpha J^{\alpha\beta} G_{\epsilon,\beta}, \tag{E.1}$$

or

$$G_{\epsilon,\beta} = J_{\beta\alpha} (S^{-1})^\alpha{}_\mu \frac{\mathrm{d}Z_\epsilon^\mu}{\mathrm{d}\epsilon} = S^\alpha{}_\beta J_{\alpha\mu} \frac{\mathrm{d}Z_\epsilon^\mu}{\mathrm{d}\epsilon} \tag{E.2}$$

where we use the property of symplectic matrices, $S^t J S = J$, where $J$ is the matrix with components $J_{\mu\nu}$. We must show that the second derivatives $G_{\epsilon,\beta\gamma}$ are symmetric. Differentiating, we find

$$G_{\epsilon,\beta\gamma} = S^\alpha{}_{\beta,\gamma} J_{\alpha\mu} \frac{\mathrm{d}Z_\epsilon^\mu}{\mathrm{d}\epsilon} + S^\alpha{}_\beta J_{\alpha\mu} \frac{\mathrm{d}S^\mu{}_\gamma}{\mathrm{d}\epsilon}. \tag{E.3}$$

The first term on the right-hand side is symmetric in $(\beta, \gamma)$, since

$$S^\alpha{}_{\beta,\gamma} = Z^\alpha_{\epsilon,\beta\gamma}, \tag{E.4}$$

and the second term is also, as we see by differentiating $S^t J S = J$ with respect to $\epsilon$ and juggling indices. Thus, the function $G_\epsilon$ exists.

## Appendix F. A transformation of the integrand of (56)

In this appendix to save writing we drop the $\epsilon$ subscripts on $H_{0\epsilon}$, $G_\epsilon$, $A_\epsilon$ and $\phi_\epsilon$, writing simply $H_0$, $G$, $A$ and $\phi$. The latter symbols, however, are not to be confused with the notation indicated in table 1 at $\epsilon = 1$. We have placed this part of the calculation in an appendix, to avoid confusion due to the notational change.

Let us pick out the $\phi$-average of the Moyal bracket in the integrand of (56) and write it in an obvious notation,

$$\langle G \overset{\rightarrow}{\underset{\rightarrow}{\Rrightarrow}} H_0 \rangle_\phi = \int_0^{2\pi} \frac{\mathrm{d}\phi}{2\pi} (G \overset{\rightarrow}{\underset{\rightarrow}{\Rrightarrow}} H_0), \tag{F.1}$$

where the parentheses are only for clarity. We now introduce a technique for 'breaking a bond' of an angle-averaged graph that is sometimes useful. The average of course depends only on $A$, if we think of it as a function of $(\phi, A)$. We imagine evaluating this average at constant action $A = a$, which we enforce by inserting a $\delta$-function and integrating over both $A$ and $\phi$. This transforms (F.1) into

$$\int \frac{\mathrm{d}A\, \mathrm{d}\phi}{2\pi} \delta(A - a)(G \overset{\rightarrow}{\underset{\rightarrow}{\Rrightarrow}} H_0), \tag{F.2}$$

where the integral is taken over a region of phase space that includes the level set $A = a$ (an orbit of $H_0$). We then transform variables of integration to $z = (x, p)$, we use $\mathrm{d}A\,\mathrm{d}\phi = \mathrm{d}^2z$ (since the transformation is canonical), we write out one of the bonds explicitly, and integrate by parts in the variable $z^\nu$:

$$\int \frac{\mathrm{d}^2z}{2\pi}\,\delta(A-a)(G_{,\mu} \rightrightarrows H_{0,\nu})J^{\mu\nu} = -\int \frac{\mathrm{d}^2z}{2\pi}[\delta'(A-a)A_{,\nu}(G_{,\mu} \rightrightarrows H_0) \\ +\delta(A-a)(G_{,\mu\nu} \rightrightarrows H_0)]J^{\mu\nu}. \tag{F.3}$$

The second term in the final integral vanishes, due to the symmetry of $G_{,\mu\nu}$ and the antisymmetry of $J^{\mu\nu}$. In the first term we switch variables of integration back to $(\phi, A)$ and do the $A$-integration, which gives

$$\int \frac{\mathrm{d}\phi}{2\pi}\frac{\partial}{\partial A}(A \leftarrow G \rightrightarrows H_0) = -\frac{\mathrm{d}}{\mathrm{d}A}\left(\frac{1}{\omega\circ A}\langle H_0 \rightarrow G \rightrightarrows H_0\rangle_\phi\right), \tag{F.4}$$

where we use $H_0 = f_0 \circ A$, that is, (44), and $\omega = f_0'$, and change the direction of an arrow in the final form.

## Appendix G. An antiderivative for the integral (57)

In this appendix we use the same notational simplifications as in appendix F.

In guessing an antiderivative that will allow us to do the integral (57), we must express the diagram $H_0 \rightarrow G \rightrightarrows H_0$, which contains one $G$ and three arrows, as $D/D\epsilon$ of some other diagram. We note by (25) that taking $D/D\epsilon$ of a diagram introduces both $G$ and an extra arrow. Therefore taking the antiderivative must remove $G$ and one arrow. The only diagram we can form from two copies of $H_0$ and two arrows is $H_0 \rightrightarrows H_0$, so we compute,

$$\frac{1}{2}\frac{D}{D\epsilon}(H_0 \rightrightarrows H_0) = \left(\frac{\mathrm{d}H_0}{\mathrm{d}\epsilon} \rightrightarrows H_0\right) - \frac{1}{2}(H_0 \rightrightarrows H_0) \rightarrow G. \tag{G.1}$$

The first term can be written as

$$(H_0 \rightarrow G) \rightrightarrows H_0 = (H_0 \leftleftarrows H_0 \rightarrow G) + 2\left(\begin{tikzcd}[column sep=small] & H_0 & \\ H_0 \arrow[ur] \arrow[rr] & & G \arrow[ul]\end{tikzcd}\right) + (H_0 \rightarrow G \rightrightarrows H_0), \tag{G.2}$$

where we use (16*a*) and the chain rule, while in the second term of (G.1) removing the parentheses provides a factor of 2, thereby cancelling the first term on the right-hand side of (G.2). As for the triangle diagram, it vanishes, as we note by writing,

$$\left(\begin{tikzcd}[column sep=small] & G \arrow[dr] & \\ H_0 \arrow[ur] \arrow[rr] & & H_0\end{tikzcd}\right) = \left(\begin{tikzcd}[column sep=small] & G \arrow[dl] \arrow[dr] & \\ H_0 & & H_0 \arrow[ll]\end{tikzcd}\right) = -\left(\begin{tikzcd}[column sep=small] & G \arrow[dr] & \\ H_0 \arrow[ur] \arrow[rr] & & H_0\end{tikzcd}\right), \tag{G.3}$$

where in the first step we reflect about the vertical line and in the second reverse the directions of all three arrows. The overall result is (58).

## Appendix H. The uniqueness of the intermediate Hamiltonian *K*

In this appendix we study how the intermediate Hamiltonian $K$ changes when the path $Z_\epsilon$ through the space of canonical transformations is varied. To do this we compose $Z_\epsilon$ with a near-identity, $\epsilon$-dependent canonical transformation that becomes the identity at $\epsilon = 0, 1$.

This is equivalent to replacing $Z_\epsilon^\mu$ with $Z_\epsilon^\mu + \delta Z_\epsilon^\mu$, where $\delta Z_\epsilon^\mu = \{Z_\epsilon^\mu, F_\epsilon\}$, where $F_\epsilon$ is a small, $\epsilon$-dependent function such that $F_\epsilon = 0$ at $\epsilon = 0, 1$. The corresponding variation in the inverse function $\left(Z_\epsilon^{-1}\right)^\mu$ can be found by varying $Z_\epsilon^{-1} \circ Z_\epsilon = \mathrm{Id}$, which gives

$$\delta\left(Z_\epsilon^{-1}\right)^\mu = -J^{\mu\nu} F_{\epsilon,\nu} \circ Z_\epsilon^{-1}. \tag{H.1}$$

Then we vary (28) to obtain,

$$\delta H_{0\epsilon} = \{H_{0\epsilon}, F_\epsilon\}. \tag{H.2}$$

Finally, to get $\delta G_\epsilon$, we vary (19) to obtain,

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left(\delta Z_\epsilon^\mu\right) = \left\{\delta Z_\epsilon^\mu, G_\epsilon\right\} + \left\{Z_\epsilon^\mu, \delta G_\epsilon\right\}. \tag{H.3}$$

The first term on the right-hand side is $\left\{\left\{Z_\epsilon^\mu, F_\epsilon\right\}, G_\epsilon\right\}$, while the left-hand side is

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left\{Z_\epsilon^\mu, F_\epsilon\right\} = \left\{\left\{Z_\epsilon^\mu, G_\epsilon\right\}, F_\epsilon\right\} + \left\{Z_\epsilon^\mu, \frac{\mathrm{d}F_\epsilon}{\mathrm{d}\epsilon}\right\}. \tag{H.4}$$

Rearranging this and using the Jacobi identity gives

$$\left\{Z_\epsilon^\mu, \delta G_\epsilon - \frac{DF_\epsilon}{D\epsilon}\right\} = 0, \tag{H.5}$$

where we use (25), or,

$$\delta G_\epsilon = \frac{DF_\epsilon}{D\epsilon}, \tag{H.6}$$

where we drop a possible $\epsilon$-dependent constant.

In the next few steps we adopt the same notational simplification mentioned at the beginning of appendix F, and in addition we drop the $\epsilon$ subscript on $F_\epsilon$ and $Z_\epsilon$. Then we combine (32), (H.1), (H.2) and (H.6) to obtain,

$$\delta K_2 = -\frac{1}{24}\int_0^1 \mathrm{d}\epsilon \left[\left\{\frac{\mathrm{d}F}{\mathrm{d}\epsilon}, H_0\right\}_3 - \{\{F, G\}, H_0\}_3 + \{G, \{H_0, F\}\}_3 - \{\{G, H_0\}_3, F\}\right] \circ Z^{-1}. \tag{H.7}$$

In this integral we perform an integration by parts, specified by

$$\begin{aligned}\frac{D}{D\epsilon}\{F, H_0\}_3 &= \left\{\frac{\mathrm{d}F}{\mathrm{d}\epsilon}, H_0\right\}_3 + \{F, \{H_0, G\}\}_3 - \{\{F, H_0\}_3, G\} \\ &= \left[\frac{\mathrm{d}}{\mathrm{d}\epsilon}(\{F, H_0\}_3 \circ Z^{-1})\right] \circ Z,\end{aligned} \tag{H.8}$$

which allows us to replace the first term of (H.7) with an exact $\epsilon$-derivative plus two more terms. The exact derivative can be integrated, giving zero because of the boundary conditions on $F$. What remains is

$$\begin{aligned}\delta K_2 = -\frac{1}{24}\int_0^1 \mathrm{d}\epsilon\, [&-\{F, \{H_0, G\}\}_3 + \{\{F, H_0\}_3, G\} - \{\{F, G\}, H_0\}_3 \\ &+ \{G, \{H_0, F\}\}_3 - \{\{G, H_0\}_3, F\}] \circ Z^{-1}.\end{aligned} \tag{H.9}$$

We now use an identity related to the Jacobi identity for operators, itself a consequence of the associativity of operator multiplication. Let $\hat{A}$, $\hat{B}$ and $\hat{C}$ be any three operators, and write out the Jacobi identity $[\hat{A}, [\hat{B}, \hat{C}]] + \text{cyclic} = 0$ in symbol form, expanding star commutators according to (A.6). The leading order term is the Jacobi identity for the Poisson bracket, and the next correction term is

$$\{A, \{B, C\}_3\} + \{A, \{B, C\}\}_3 + \text{cyclic} = 0. \tag{H.10}$$

Using this in (H.9) allows us to write the integrand as

$$\begin{aligned}\{H_0, \{G, F\}_3\} \circ Z^{-1} &= [(\omega \circ A)\{A, \{G, F\}_3\}] \circ Z^{-1} \\ &= -(\omega \circ I)\frac{\partial}{\partial\theta}(\{G, F\}_3 \circ Z^{-1}),\end{aligned} \tag{H.11}$$

where we have expanded the Poisson bracket with $H_0$ in action-angle variables. Finally, on restoring the $\epsilon$ we have

$$\delta K_2 = \frac{1}{24}(\omega \circ I)\frac{\partial}{\partial\theta}\int_0^1 \mathrm{d}\epsilon \{G_\epsilon, F_\epsilon\}_3 \circ Z_\epsilon^{-1}. \tag{H.12}$$

The variation in $K_2$ is an exact $\theta$-derivative, as claimed, and $M_2$ is invariant under variations in the path $Z_\epsilon$.

We do not know whether the space of symplectomorphisms we are considering is simply connected, but if not there arises the possibility of distinct paths $Z_\epsilon$ that are not homotopic. Since $M_2$ is unique, it must be that the difference in $K_2$ along such paths is still an exact $\theta$-derivative.

## Appendix I. Functions of operators versus functions of symbols

In this appendix we calculate the symbol of a function of an operator, in terms of the symbol of that operator, as a power series in $\hbar$. We briefly describe Green's function approach to this problem, which as far as we know was first presented by Voros (1977) and which is discussed further by Colin de Verdière (2004). In this appendix we adopt a general notation, in which $\hat{A}$ is any Hermitian operator, $f$ is any function : $\mathbb{R} \to \mathbb{R}$ and $\hat{B} = f(\hat{A})$. The problem will be to find the symbol $B$ in terms of the symbol $A$.

Let $a \in \mathbb{C}$ and let $\hat{G}_a = 1/(a - \hat{A})$ be Green's operator associated with $\hat{A}$. The symbol $G_a$ of $\hat{G}_a$ may be computed by demanding $G_a * (a - A) = (a - A) * G_a = 1$, expanding $G_a = G_{a0} + \hbar G_{a1} + \hbar^2 G_{a2} + \cdots$, expanding the Moyal star product, and collecting things by orders in $\hbar$. One finds that only even powers of $\hbar$ occur in the expansion of $G_a$, and that otherwise it is easy to solve for the leading terms. Through second order, the results are

$$G_{a0} = \frac{1}{a - A}, \tag{I.1$a$}$$

$$\begin{aligned}G_{a2} &= -\frac{1}{8}\frac{1}{a - A}\left\{\frac{1}{a - A}, A\right\}_2 \\ &= -\frac{1}{8}\left[\frac{(A \rightrightarrows A)}{(a - A)^3} + 2\frac{(A \rightarrow A \leftarrow A)}{(a - A)^4}\right].\end{aligned} \tag{I.1$b$}$$

This is a special case of the symbol of a function of an operator. For the general case, write $\hat{B} = f(\hat{A})$ in the form,

$$\hat{B} = \int_\Gamma \frac{\mathrm{d}a}{2\pi \mathrm{i}}\frac{f(a)}{a - \hat{A}}, \tag{I.2}$$

where the contour $\Gamma$ runs from $-\infty$ to $+\infty$ just below the real axis, and then returns just above it. This would appear to require that $f$ be analytic, but see Hellfer and Sjöstrand (1989), Davies (1995) and Dimasii and Sjötrand (1999) for extensions to smooth functions. (In some applications even nonsmooth functions $f$ are important, for example, Argyres (1965).) On taking symbols of both sides, this becomes

$$B = \int_\Gamma \frac{\mathrm{d}a}{2\pi \mathrm{i}} f(a) G_a, \tag{I.3}$$

or, on substituting the expansion for $G_a$ and doing the integrals,

$$B = f(A) - \hbar^2 \left[ \frac{f''(A)}{16}(A \rightrightarrows A) + \frac{f'''(A)}{24}(A \rightarrow A \leftarrow A) \right] + O(\hbar^4). \tag{I.4}$$

Green's function method becomes tedious at higher orders, but recently Gracia-Saz (2004) has found convenient methods for calculating the higher order terms, including the multidimensional case. It turns out that the fourth-order term in (I.4) contains 13 diagrams.

It was stated above that an operator is a function of $\hat{I}$ if and only if the symbol is a function of $I$. We prove this by noting that an operator is a function of $\hat{I}$ if and only if it commutes with the unitary operator $\hat{U}(t) = \exp(-\mathrm{i}t\hat{I}/\hbar)$ for all $t$. This follows since the spectrum of $\hat{I}$ is nondegenerate. But the unitary operator $\hat{U}(t)$ is a metaplectic operator (Littlejohn 1986), so when we conjugate an operator, $\hat{A} \mapsto \hat{U}(t)\hat{A}\hat{U}^{\dagger}(t)$, the symbol $A$ is rotated in phase space. Therefore an operator commutes with all $\hat{U}$ if and only if its symbol is rotationally invariant in phase space, that is, is a function of $I$.

The same thing can be proven at the level of $\hbar$ expansions. The general term of the series (I.4) involves diagrams composed of copies of $A$ connected by arrows. But if $A = I$, then all diagrams with three or more arrows attached to any $I$ vanish, since $I$ is a quadratic function of $z$. Therefore the only nonvanishing diagrams are linear ones and circular ones. A linear diagram with $n$ $I$ (two on the ends and $n-2$ in the middle) vanishes if $n$ is even, and is $2(-1)^{(n-1)/2} I$ if $n$ is odd. A circular diagram with $nI$ vanishes if $n$ is odd, and is $2(-1)^{n/2}$ if $n$ is even. Equation (61) is a special case of these rules. For now the point is that both these diagrams are functions of $I$. Thus the entire series (I.4) is a function of $I$, for any function $f$.

## References


Argyres P N 1965 *Physics* **2** 131

Arnold V I 1989 *Mathematical Methods of Classical Mechanics* (New York: Springer) appendix 6

Balazs N L and Jennings B K 1984 *Phys. Rep.* **104** 347

Bayen F, Flato M, Fronsdal C, Lichnerowicz A and Sternheimer D 1978 *Ann. Phys.* **111** 61

Bender C M and Orszag S A 1978 *Advanced Mathematical Methods for Scientists and Engineers* (New York: McGraw-Hill)

Berk H L and Pfirsch D 1980 *J. Math. Phys.* **21** 2054

Berry M V 1977 *Phil. Trans. R. Soc.* **287** 237

Berry M V and Mount K E 1972 *R. Prog. Phys.* **35** 315

Braam P J and Duistermaat J J 1995 *Panoramas of Mathematics, Banach Center Publications* v 34 (Warsaw: Institute of Mathematics, Polish Academy of Sciences) p 29

Brack Matthias and Bhaduri Rajat K 1997 *Semiclassical Physics* (Reading, MA: Addison-Wesley)

Cary J R 1981 *Phys. Rep.* **79** 131

Colin de Verdière Y 2004 Bohr–Sommerfeld rules to all orders *Preprint* http://www-fourier.ujf-grenoble.fr/ycolver/ebk.ps

Colin de Verdière Y, Lombardi M and Pollet J 1999 *Ann. Inst. H Poincaré* **71** 95

Colin de Verdière Y and Parisse B 1999 *Commun. Math. Phys.* **205** 459

Colin de Verdière Y and Vey J 1979 *Topology* **18** 283

Creagh S C 2004 *Nonlinearity* **17** 1261

Davies E 1995 *Cambridge Studies in Advanced Mathematics* vol 42 (Cambridge: Cambridge University Press)

Dimasii M and Sjöstrand J 1999 *Lecture Note Series* vol 268 (London Mathematical Society) chapter 8

Dragt A J and Finn J M 1976 *J. Math. Phys.* **17** 2215

Eckhardt B 1986 *J. Phys. A: Math. Gen.* **19** 2961

Emmrich C and Weinstein A 1996 *Commun. Math. Phys.* **176** 701

Emmrich C and Römer H 1988 *J. Math. Phys.* **39** 3530

Estrada R, Gracia-Bondía J M and Várilly J C 1989 *J. Math. Phys.* **30** 2789

Evans C and Zworski M 2004 *Book in preparation*

Fedosov B V 1994 *J. Diff. Geom.* **40** 213

Forbes G W and Alonso M A 1998a *J. Opt. Soc. Am.* A **15** 1329

Forbes G W and Alonso M A 1998b *J. Opt. Soc. Am.* A **15** 1341
Forbes G W and Alonso M A 2001a *J. Opt. Soc. Am.* A **18** 1132
Forbes G W and Alonso M A 2001b *J. Opt. Soc. Am.* A **18** 1146
Forbes G W and Alonso M A 2001c *J. Opt. Soc. Am.* A **18** 1357
Forbes G W and Alonso M A 2001d *J. Opt. Soc. Am.* A **18** 2557
Fröman N and Fröman P O 1965 *JWKB Approximation: Contributions to the Theory* (Amsterdam: North-Holland)
Fröman N and Fröman P O 1996 *Phase-Integral Method: Allowing Nearlying Transition Points* (New York: Springer)
Fröman N and Fröman P O 2002 *Physical Problems Solved by the Phase-Integral Method* (Cambridge: Cambridge University Press)
Garg A and Stone M 2004 *Phys. Rev. Lett.* **92** 010401
Gracia-Bondía J M and Várilly J C 1995 *J. Math. Phys.* **36** 2691
Gracia-Saz A 2004 The symbol of a function of an operator *Preprint* math.QA/0411163
Groenewold H J 1946 *Physica* **12** 405
Guillemin V and Sternberg S 1977 *Geometric Asymptotics* (Providence, RI: American Mathematical Society)
Gutzwiller Martin C 1990 *Chaos in Classical and Quantum Mechanics* (New York: Springer)
Heading J 1962 *An Introduction to Phase-Integral Methods* (New York: Wiley)
Helffer B and Robert D 1981 *Ann. Inst. Fourier* **26** 169
Helffer B and Sjöstrand J 1983 *J. Funct. Anal.* **53** 246
Helffer B and Sjöstrand J 1989 *Lecture Notes in Physics* vol 345 ed H Holder and A Jensen (New York: Springer)
Hillery M, O'Connell R F, Scully M O and Wigner E P 1984 *Phys. Rep.* **106** 123
Keller J B 1962 *J. Opt. Soc. Am.* **52** 116
Kontsevich M 2003 *Lett. Math. Phys.* **66** 157
Kurchan J, Leboeuf P and Saraceno M 1989 *Phys. Rev.* A **40** 6800
Leray J 1981 *Lagrangian Analysis and Quantum Mechanics* (Cambridge, MA: MIT Press)
Littlejohn R G 1986 *Phys. Rep.* **138** 193
Littlejohn R G and Flynn W G 1991 *Phys. Rev.* A **44** 5239
Littlejohn R G and Flynn W G 1992 *Chaos* **2** 149
Littlejohn R G and Flynn W G 1993 *Phys. Rev. Lett.* **70** 1799
Littlejohn R G and Weigert S 1993 *Phys. Rev.* A **48** 924
Martinez A 2002 *An Introduction to Semiclassical and Microlocal Analysis* (New York: Springer)
Maslov V P and Fedoriuk M V 1981 *Semi-Classical Approximations in Quantum Mechanics* (Dordrecht: Reidel)
McDonald S 1988 *Phys. Rep.* **158** 377
Milnor J 1969 *Morse Theory* (Princeton, NJ: Princeton University Press)
Mitchell K A, Handley J P, Tighe B, Knudson S K and Delos J B 2003a *Chaos* **13** 880
Mitchell K A, Handley J P, Knudson S K and Delos J B 2003b *Chaos* **13** 892
Mitchell K A, Handley J P, Tighe B, Flower A and Delos J B 2004a *Phys. Rev.* A **70** 043407
Mitchell K A, Handley J P, Tighe B, Flower A and Delos J B 2004b *Phys. Rev. Lett.* **92** 073001
Moyal J E 1949 *Proc. Camb. Phil. Soc.* **45** 99
Ozorio de Almeida Alfredo M 1998 *Phys. Rep.* **295** 265
Robert D 1987 *Autour de lápproximation Semi-Classique* (Boston, MA: Birkhaüser)
Sjöstrand J and Zworski M 2002 *J. Math. Pures Appl.* **81** 1
Uzer T, Jaffé C, Palacán J, Yanguas P and Wiggins S 2002 *Nonlinearity* **15** 957
Voros A 1977 *Ann. Inst. H Poincaré* **4** 343
Voros A 1989 *Phys. Rev.* A **40** 6814
Weyl H 1927 *Z. Phys.* **46** 1
Wiggins S 1992 *Chaotic Transport in Dynamical Systems* (New York: Springer)
Wigner E P 1932 *Phys. Rev.* **40** 749