Path integral derivations of novel complex trajectory methods

Jeremy Schiff[1], Yair Goldfarb[2] and David J. Tannor[2]

[1]Department of Mathematics, Bar-Ilan University, Ramat Gan, 52900 Israel

[2]Department of Chemical Physics, The Weizmann Institute of Science, Rehovot, 76100 Israel

July 29, 2008

Abstract

Path integral derivations are presented for two recently developed complex trajectory techniques for the propagation of wave packets, Complex WKB and BOMCA. Complex WKB is derived using a standard saddle point approximation of the path integral, but taking into account the $\hbar$ dependence of both the amplitude and the phase of the intial wave function, thus giving rise to the need for *complex* classical trajectories. BOMCA is derived using a modification of the saddle point technique, in which the path integral is approximated by expanding around a near-classical path, chosen so that up to some predetermined order there is no need to add any correction terms to the leading order approximation. Both Complex WKB and BOMCA give the same leading order approximation; in Complex WKB higher accuracy is achieved by adding correction terms, while in BOMCA no additional terms are ever added — higher accuracy is achieved by changing the path along which the original approximation is computed. The path integral derivation of the methods explains the need to incorporate contributions from more than one trajectory, as observed in previous numerical work. On the other hand, it emerges that the methods provide efficient schemes for computing the higher order terms in the asymptotic evaluation of path integrals. The understanding we develop of BOMCA suggests that there should exist near-classical trajectories that give *exact* quantum dynamical results when used in the computation of the path integral keeping just the leading order term. We also apply our path integral techniques to give a compact derivation of the semiclassical approximation to the coherent state propagator.

1 Introduction

In a recent series of papers [1, 2, 3] we have considered two complex trajectory techniques for solving the time-dependent Schrödinger equation (TDSE). By a "trajectory technique" we mean that we solve the TDSE for the wave function by integrating a system of ODEs along certain trajectories in configuration space. By a "complex trajectory technique" we mean that the relevant trajectories evolve in complex configuration space — i.e. we analytically continue the wave function and consider it as a function of complex space variables. (Note that the time variable remains real, so the trajectories are real curves in complex space.) The motivation for using complex trajectories comes from the substitution

$$\psi = \exp\left(\frac{iS}{\hbar}\right) \ , \quad S \in \mathbf{C} \ , \tag{1}$$

in the TDSE

$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{x})\psi \ . \tag{2}$$

This yields the *complex* quantum Hamilton Jacobi equation (CQHJE) [4, 5]

$$S_t + \frac{1}{2m}\left(\nabla S\right)^2 + V(\mathbf{x}) = \frac{i\hbar}{2m}\nabla^2 S \ . \tag{3}$$

Taking $\hbar$ as small, the CQHJE can be considered as a perturbation of the classical Hamilton Jacobi equation (HJE)

$$S_t + \frac{1}{2m}\left(\nabla S\right)^2 + V(\mathbf{x}) = 0 \ . \tag{4}$$

Since the classical HJE can be solved exactly by integration along trajectories in space defined by

$$\frac{d\mathbf{x}}{dt} = \frac{\nabla S}{m} \ , \tag{5}$$

it is natural to try a similar technique (at least as an approximation) for its perturbation, the CQHJE. Complex trajectories arise since S in equation (1), and hence ∇S in equation (5), are complex, leading to complex initial conditions for the evolution; furthermore the perturbation in (3) is complex.

In our earlier papers we observed that a reasonable approximation to the wave function may require taking into account contributions from more than one trajectory reaching a particular point in space. We gave no theoretical justification for this, and one of the purposes of the current paper is to fill this hole. More generally the aim of the current paper is to strengthen the theoretical basis of the techniques of our previous papers by showing how they can be derived by saddle point evaluation of the wave function in the path integral

representation. In this approach the need to (potentially) add the contributions of several trajectories emerges naturally.

In section 2 we give a detailed presentation of the two techniques under study here. In the first method, *Complex WKB* [3], the trajectories are solutions of the classical equations of motion. In the second method, which we call *BOMCA* [1, 2], (BOhmian Mechanics with Complex Action), the trajectories are order $\hbar$ perturbations of solutions of the classical equations. Indeed, in BOMCA the trajectories depend on the order in $\hbar$, while in complex WKB they remain the same; to increase the order in $\hbar$ in complex WKB we have to integrate a further system of ODEs along the trajectories.

In section 3 we present a path integral derivation of Complex WKB. Since the trajectories involved in Complex WKB are classical, this involves a standard saddle point approximation of the path integral. The approach, however, is still nonstandard in that the initial value of the wave function is taken into account, leading to complex classical trajectories. In this regard, our approach differs from standard time-dependent WKB theory [6]. Our approach is the appropriate one when the initial wave function has the form $\exp(iS^{\text{init}}(\mathbf{x})/\hbar)$, as implied by (1) (though note an interesting recent paper of Maia *et al.* [7]). The equivalence of Complex WKB to the saddle point approximation of the path integral gives rise to a potentially very useful result. While it has long been recognized that certain factors involved in the (leading order) saddle point approximation of path integrals, specifically elements of the so-called stability matrix, can be calculated efficiently by integrating certain ODEs along classical trajectories [8], it turns out that the same is true (at least in our situation) for all higher order correction terms. Within the path integral formulation, the expressions for higher order correction terms involve complicated multiple integrals; the Complex WKB method reformulates these expressions as solutions of a system of first order ODEs, which is much easier to handle computationally.

Before presenting the path integral derivation of BOMCA, in section 4 we present a slight modification to the standard method of asymptotic analysis of integrals with a large parameter. In section 5 we apply this modification to the path integral, and are led to BOMCA. The distinction between BOMCA and Complex WKB becomes extremely clear. Complex WKB and BOMCA give the same leading order approximation to the wave function $\psi(\mathbf{X}, T)$, determined as follows: First find complex classical trajectories $\mathbf{x}(t)$ satisfying appropriate initial and final conditions, specifically, solve the problem

$$m\ddot{\mathbf{x}}(t) + \nabla V(\mathbf{x}(t)) = 0 \ , \qquad \dot{\mathbf{x}}(0) = -\frac{i\hbar}{m}\nabla \log \psi_0(\mathbf{x}(0)) \ , \quad \mathbf{x}(T) = \mathbf{X} \ . \tag{6}$$

Here ψ_0 is the wave function at $t = 0$. Next, for each such trajectory, compute the matrix

U satisfying

$$m\ddot{U} + H(V)(\mathbf{x}(t))U = 0 \ , \qquad U(0) = I \ , \qquad \dot{U}(0) = -\frac{i\hbar}{m} H(\log \psi_0)(\mathbf{x}(0)) \ . \tag{7}$$

Here $H(V)$ denotes the matrix of second derivatives of V and $H(\log \psi_0)$ the matrix of second derivatives of $\log \psi_0$. Then the wave function is approximated by

$$\psi(\mathbf{X}, T) \approx \sum \frac{e^{iS[\mathbf{x}]/\hbar} \psi_0(\mathbf{x}(0))}{\sqrt{\det U(T)}} \ , \tag{8}$$

where $S[\mathbf{x}]$ denotes the classical action associated with the path $\mathbf{x}(t)$, i.e.

$$S[\mathbf{x}] = \int_0^T \left(\frac{1}{2} m \dot{\mathbf{x}}^2 - V(\mathbf{x}) \right) \, dt \ . \tag{9}$$

The sum in (8) is over contributing trajectories (possibly not all trajectories), as we will explain later. The distinction between Complex WKB and BOMCA lies in the manner in which higher order corrections are made to (8). In Complex WKB higher order corrections are made by multiplying the leading order contribution for each trajectory in (8) by a suitable factor of the form $1 + O(\hbar)$. In BOMCA, the formula (8) is never modified, but the paths $\mathbf{x}(t)$ and matrices $U(t)$ are no longer required to be classical. More explicitly, the differential equations in (6) and (7) are replaced by equations of the form

$$m\ddot{\mathbf{x}} + \nabla V(\mathbf{x}(t)) = O(\hbar) \ , \tag{10}$$

$$m\ddot{U} + H(V)(\mathbf{x}(t))U = O(\hbar) \ . \tag{11}$$

BOMCA gives explicit expressions for the terms to introduce on the right hand side of these equations, but, as we shall explain, they are not unique choices.

We call the quantity appearing on the right hand side of (8), with the classical choice of $\mathbf{x}$ and U, the *classical wave function*. Note that our use of the term "classical wave function" differs from previous uses, see for example Box 2.2 in [9]. We emphasize also that our classical wave function differs from the usual approximations made in time dependent WKB theory; the difference can be traced to different assumptions about the $\hbar$ dependence of the initial wave function, with our choice requiring the use of complex trajectories.

As we have explained, BOMCA provides a prescription for making the formula (8) more accurate, to any order in $\hbar$, by changing the equations that $\mathbf{x}$ and U satisfy. We are led to conjecture that there may exist choices of $\mathbf{x}$ and U, satisfying (10)-(11), such that formula (8) is *exact*. Unfortunately, at this stage we only know how to describe the right hand sides of equations (10) and (11) perturbatively in $\hbar$, and, as we have indicated above, there are many choices (one being associated with BOMCA). If there exist choices of $\mathbf{x}$ and U for which

(8) is exact, the relevant trajectories $\mathbf{x}$ would be an interesting intermediate object between classical and quantum trajectories. The usual notion of quantum trajectories (in Bohmian mechanics) are the paths in (real) configuration space satisfying $\dot{\mathbf{x}} = \frac{\hbar}{m}\mathrm{Im}\left(\nabla \log \psi(\mathbf{x}, t)\right)$ (see the books [10] and [9] for extensive discussion). One of the properties of these trajectories is that the velocity diverges at a node of the wave function, so near nodes quantum trajectories are qualitatively different from classical trajectories. In distinction to this, the non-classical trajectories that arise in BOMCA are always perturbations of classical trajectories. Certainly it is possible to express the wave function ψ in the form (8) only in certain regions of $\mathbf{X}, T$ space (like any other semiclassical formula, our formula suffers from problems related to caustics and Stokes' lines), but in these regions we conjecture that there exist non-classical trajectories which are perturbations of classical trajectories, which make the formula (8) exact.

After our derivation of BOMCA from the path integral, in section 6 we discuss the application of our ideas to the evaluation of other quantities in quantum mechanics. There is an extensive literature on the use of complex classical trajectories to compute the coherent state propagator, (see for example [11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21]), and we show how some relevant formulae can be derived using our techniques. Section 7 contains concluding comments. An appendix provides the multidimensional derivation of the classical wave function (8); in the most of the main text we present the path integral derivations just in the one dimensional case.

We conclude this introduction with a discussion of some relevant literature that has not yet been mentioned. The use of complex classical trajectories in semiclassical quantum mechanics goes back to Stine and Marcus [22] and Miller and George [23, 24, 25], and numerous different applications have been subsequently presented (see for example [26, 27]). As far as we know, the first attempt to use complex classical trajectories to propagate wave packets is in the works of Huber, Heller and Littlejohn [28, 29] (the superposition of contributions from more than one trajectory also appears in this work). Our work, however, is closer to the rather different viewpoint of Boiron and Lombardi [30]. Other developments in this area include the extensive work of de Aguiar and collaborators [31, 32, 33], and very recent contributions of Chou and Wyatt [34] and Sanz and Miret-Artes [35]. There are a number of papers on time dependent WKB that we also found illuminating: [36, 37, 38, 39]. Recent numerical work of Bender, Brody and Hook [40], suggesting strong connections between complex classical dynamics and quantum dynamics, is very encouraging; such connections also provided the motivation for the detailed studies of complex classical dynamics of Kay and Shnerb [41, 42]. Likewise, there are interesting connections between our current work

and a series of papers by Poirier and collaborators [43, 44, 45, 46, 47, 48]. Poirier considers a decomposition of the wave function as a sum of (nodeless) terms; we suspect this decomposition is strongly linked, if not identical to, the decomposition implied by (8) (at least in the time-dependent case [47]). Finally, we note that the hierarchy of ODEs in the BOMCA method can be viewed as a complex version of the DPM of Trahan, Hughes and Wyatt [49] which was originally developed for real trajectories (see the exposition in [9] and the comparison of BOMCA and DPM in [50]).

2 The Complex WKB and BOMCA methods

As explained in the introduction, the starting point for both the methods we consider in this paper is the substitution $\psi = e^{iS/\hbar}$ in the time-dependent Schrödinger equation to obtain the CQHJE (3). Here $S(\mathbf{x}, t)$ is complex. Both of our methods consist of approximating the CQHJE by a system of equations that can be solved by integrating along trajectories in complex configuration space. Both of our methods allow us to systematically improve the order of approximation in such a way that we might reasonably expect, in a suitable limit, to obtain exact results.

The first method, *complex WKB*, proceeds by an expansion of S in powers of $\hbar$. The relevant trajectories, irrespective of the order of approximation, are solutions of the complex classical equations of motion. Complex WKB is described in detail in subsection 2.1. The second method, *BOMCA*, involves a different approximation scheme that will be described in detail in section 2.2. The relevant trajectories depend on the order of approximation. The question arises as to whether these trajectories have a well-defined limit as the order of approximation is increased, and what this limit is. We will discuss this matter more in section 5.

In subsection 2.3 we summarize some of the findings of our previous work on complex WKB and BOMCA that are relevant for understanding the rest of this paper.

2.1 Complex WKB

Writing

$$S(\mathbf{x}, t) = \sum_{n=0}^{\infty} S_n(\mathbf{x}, t)\hbar^n \tag{12}$$

and substituting in the CQHJE we obtain the following PDEs for the component functions $S_n(\mathbf{x}, t)$:

$$S_{0t} + \frac{1}{2m} (\nabla S_0)^2 + V(\mathbf{x}) = 0 \ , \tag{13}$$

$$S_{nt} + \frac{\nabla S_0}{m} \cdot \nabla S_n = -\frac{1}{2m} \sum_{m=1}^{n-1} \nabla S_m \cdot \nabla S_{n-m} + \frac{i}{2m} \nabla^2 S_{n-1} \ , \quad n = 1, 2, \dots \ . \tag{14}$$

Along with the TDSE we assume we are provided with an initial wave function $\psi_0(\mathbf{x}) = \psi(\mathbf{x}, 0)$, and this provides us with an initial condition $S(\mathbf{x}, 0) = -i\hbar \log \psi_0(\mathbf{x})$ for the CQHJE. How are we to choose appropriate initial conditions for the component functions S_n? The archetypal form of the initial wave function we wish to consider is a nonnormalized Gaussian wave-packet, which in one spatial dimension takes the form

$$\psi_0(x) = \exp\left(-\frac{(a_0 + ia_1)(x - x_0)^2}{\hbar} + \frac{ip_0(x - x_0)}{\hbar} \right) \ . \tag{15}$$

Here a_0, a_1, x_0, x_1 are real constants, with $a_0 > 0$, related to the expectations and variance of position and momentum via

$$\langle x \rangle = x_0 \ , \qquad \langle p \rangle = p_0 \ , \tag{16}$$

$$\langle (x - x_0)^2 \rangle = \frac{\hbar}{2a_0} \ , \qquad \langle (p - p_0)^2 \rangle = \frac{\hbar(a_0^2 + a_1^2)}{2a_0} \ . \tag{17}$$

For this choice of ψ_0 we have

$$S(x, 0) = -i\hbar \log \psi_0(x) = i(a_0 + ia_1)(x - x_0)^2 + p_0(x - x_0) \ , \tag{18}$$

so it is natural to choose

$$S_0(x, 0) = i(a_0 + ia_1)(x - x_0)^2 + p_0(x - x_0) \ , \tag{19}$$

$$S_n(x, 0) = 0 \ , \qquad n = 1, 2, \dots . \tag{20}$$

In greater generality, we assume that we can write the initial wave function as $\psi_0(\mathbf{x}) = \exp(iS^{\text{init}}(\mathbf{x})/\hbar)$ and take $S_0(\mathbf{x}, 0) = S^{\text{init}}(\mathbf{x})$ and $S_n(\mathbf{x}, 0) = 0$ for $n \geq 1$. It is possible to generalize to the case that $S(\mathbf{x}, 0)$ can be expanded in a Taylor series in $\hbar$.

In complex WKB we opt to solve the system of equations (13)-(14) by integrating along trajectories defined by

$$\frac{d\mathbf{x}}{dt} = \frac{\nabla S_0}{m} \ . \tag{21}$$

Writing $\mathbf{v} = \frac{\nabla S_0}{m}$ and taking the gradient of (13) gives

$$\frac{\partial v_i}{\partial t} + (\mathbf{v} \cdot \nabla) v_i + \frac{1}{m} \frac{\partial V}{\partial x_i} = 0 \ . \tag{22}$$

Thus along the trajectories we have

$$\frac{d\mathbf{v}}{dt} = -\frac{1}{m}\nabla V(\mathbf{x}) \ . \tag{23}$$

(Here $\frac{d}{dt}$ denotes the Lagrangian derivative along the trajectories $\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla$.) We see the trajectories are simply classical trajectories. Note however that they are trajectories in *complexified* space. The initial condition for the TDSE gives the initial condition $S^{\rm init}(\mathbf{x})$ as a complex function of $\mathbf{x}$, and thus

$$\mathbf{v}(0) = \frac{1}{m}\nabla S^{\rm init}(\mathbf{x}(0)) \tag{24}$$

is in general complex.

To summarize to this stage: in complex WKB we choose to integrate along trajectories given by (21), and from (13) we deduce that these are actually classical trajectories, i.e. solutions of

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \ , \qquad \frac{d\mathbf{v}}{dt} = -\frac{1}{m}\nabla V(\mathbf{x}) \ , \tag{25}$$

with the complex initial condition (24). Also from (13) we deduce that the evolution of S_0 down these trajectories is given by

$$\frac{dS_0}{dt} = \frac{1}{2}m\mathbf{v}^2 - V(\mathbf{x}) \ . \tag{26}$$

To compute the evolution of $S_1, S_2, \ldots$ along the trajectories we need to use the equations (14). We have written these equations with precisely the Lagrangian derivative of S_n along the trajectories on the left hand side. Writing the first few equations out more explicitly we have

$$\frac{dS_1}{dt} = \frac{i}{2m}\nabla^2 S_0 \ , \tag{27}$$

$$\frac{dS_2}{dt} = -\frac{1}{2m}\left(\nabla S_1\right)^2 + \frac{i}{2m}\nabla^2 S_1 \ , \tag{28}$$

$$\frac{dS_3}{dt} = -\frac{1}{m}\nabla S_1\cdot\nabla S_2 + \frac{i}{2m}\nabla^2 S_2 \ . \tag{29}$$

We see that to find S_1 we need to follow the evolution of $\nabla^2 S_0$ along the trajectory, which may be found by calculating the second spatial derivatives of (13). To find S_2, we see from (28) that we need to follow the evolution of first and second spatial derivatives of S_1 along the trajectories. These are obtained by taking two spatial derivatives of (27), but to integrate the resulting equations we also need third and fourth derivatives of S_0, obtained by further differentiation of (13).

$D(n,d)$	$n=1$	$n=2$	$n=3$	general n
$d=1$	4	9	16	$(n+1)^2$
$d=2$	7	22	50	$\frac{1}{6}(n+1)(n+2)(4n+3)$
$d=3$	11	46	130	$\frac{1}{6}(n+1)(n+2)(2n^2+6n+3)$
general d	$\frac{1}{2}(d^2+3d+4)$	$\frac{1}{24}(d^4+\ldots)$	$\frac{1}{720}(d^6+\ldots)$	see (31)

Table 1: Total number of functions to be evolved along the trajectories as a function of dimensionality d and order n. The full expressions in the cases $n=2$ and $n=3$ with general d are $\frac{1}{24}(d^4+10d^3+47d^2+86d+72)$ and $\frac{1}{720}(d^6+21d^5+205d^4+1035d^3+3034d^2+4344d+2880)$ respectively. Note the numbers listed include a contribution of d for finding $\nabla S_0 = m\mathbf{v}$, which in practice is already determined when finding the trajectories.

Proceeding in this manner we see that to obtain $S_0, S_1, \ldots, S_n$ we need to follow up to the $2n$'th derivatives of S_0, up to the $2(n-1)$'th derivatives of S_1 etc. along the trajectory. The total number of derivatives of order up to i of a scalar function is

$$1 + d + \frac{d(d+1)}{2} + \frac{d(d+1)(d+2)}{6} + \ldots + \frac{d(d+1)\ldots(d+i-1)}{i!} = \frac{(d+i)!}{d!i!} \ , \qquad (30)$$

where d denotes the number of spatial dimensions. Thus the total number of functions we need to follow along the trajectories is given by

$$D(n,d) = \sum_{\substack{i=0 \\ i \text{ even}}}^{2n} \frac{(d+i)!}{d!i!} \ . \qquad (31)$$

We are not aware of a closed form expression for this sum, but tabulate it in Table 1 for some low values of d and n. For fixed n and large d we note that $D(n,d) \sim d^{2n}/(2n)!$, i.e. the number of functions we need to follow increases polynomially with the dimension.

At this juncture we write out in full the equations that we must integrate to obtain S_0, S_1, S_2: To find the trajectories we solve Newton's equations (25) with the required initial condition (24). The gradient of S_0 along the trajectories can be identified with $m\mathbf{v}$, and we do not need to recompute it. Higher derivatives of S_0 along the trajectories are determined by integrating the equations:

$$\frac{dS_{0,ik}}{dt} = -V_{ik} - \frac{1}{m}\sum_j S_{0,ij}S_{0,jk} \ , \qquad (32)$$

$$\frac{dS_{0,ikl}}{dt} = -V_{ikl} - \frac{1}{m}\sum_j \left(S_{0,ij}S_{0,jkl} + S_{0,kj}S_{0,jli} + S_{0,lj}S_{0,jik}\right) \ , \qquad (33)$$

$$\begin{aligned}\frac{dS_{0,iklm}}{dt} &= -V_{iklm} - \frac{1}{m}\sum_j \left(S_{0,ij}S_{0,jklm} + S_{0,kj}S_{0,jlmi} + S_{0,lj}S_{0,jmik} + S_{0,mj}S_{0,jikl}\right) \\ &\quad -\frac{1}{m}\sum_j \left(S_{0,jkl}S_{0,jim} + S_{0,jkm}S_{0,jil} + S_{0,jlm}S_{0,jik}\right) \ . \end{aligned} \qquad (34)$$

Here V_{ik} denotes $\frac{\partial^2 V}{\partial x_i \partial x_k}$ etc, and $S_{0,ik}$ denotes $\frac{\partial^2 S_0}{\partial x_i \partial x_k}$ etc. Derivatives of S_1 are determined by integrating the equations

$$\frac{dS_{1,i}}{dt} = \frac{i}{2m}\sum_j S_{0,jji} - \frac{1}{m}\sum_j S_{0,ij}S_{1,j} \ , \tag{35}$$

$$\frac{dS_{1,ik}}{dt} = \frac{i}{2m}\sum_j S_{0,jjik} - \frac{1}{m}\sum_j S_{0,ikj}S_{1,j} - \frac{1}{m}\sum_j \left(S_{0,kj}S_{1,ij} + S_{0,ij}S_{1,kj}\right) \ . \tag{36}$$

Finally S_0, S_1, S_2 are obtained by integrating the equations (26),(27) and (28) respectively. The initial conditions for all these equations are obtained from the initial condition for the TDSE via the function $S^{\text{init}}(\mathbf{x})$. Explicitly, we have

$$\begin{array}{ccccc} S_0(0) = S^{\text{init}}(\mathbf{x}(0)) & S_{0,i}(0) = S^{\text{init}}_i(\mathbf{x}(0)) & S_{0,ij}(0) = S^{\text{init}}_{ij}(\mathbf{x}(0)) & \dots \\ S_1(0) = 0 & S_{1,i}(0) = 0 & S_{1,ij}(0) = 0 & \dots \\ S_2(0) = 0 & S_{2,i}(0) = 0 & S_{2,ij}(0) = 0 & \dots \\ \vdots & \vdots & \vdots & \end{array} \tag{37}$$

Note that for an initial Gaussian wave packet (of the form (15) in one dimension) the function S^{init} is quadratic in the spatial variable, so only its first two derivatives will be nonzero.

A few final notes before leaving our description of the complex WKB method: First, observe that when computing to order n in complex WKB we use the derivatives of the potential up to order $2n$. We will see later how this emerges from the path integral approach. Second, observe that equation (32) is an example of a matrix Riccati equation [51], and in particular, it has solutions that become infinite in finite time. These singularities are a manifestation of the phenomenon of *caustics*, which appear in almost every application of the WKB method. We note however that the singularities in the matrix Riccati equation are pole-type singularities, and it is possible, in a suitable sense, to integrate through them [52]. This is reminiscent of the fact that it is often possible to "regularize" caustics [53, 54, 55, 56]. We are currently investigating the singularity structure of the full system of equations (27)-(28),(32)-(34),(35)-(36) [57]. Finally, we mention that although in this paper we work with the multidimensional Schrödinger equation in the form (2), assuming the mass matrix to be a multiple of the identity, there is no problem extending our formalism to work with a general positive definite mass matrix.

2.2 BOMCA

BOMCA is an alternate trajectory based approach for solving the CQHJE (3). Unlike complex WKB it does not involve an expansion in powers of $\hbar$. Another distinction is

that in complex WKB the trajectories are classical paths, and in BOMCA they are not. Furthermore, the trajectories in BOMCA depend on the order of the approximation.

In BOMCA we aim to integrate the CQHJE (3) by integrating along trajectories defined by

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \ , \quad \text{where} \quad \mathbf{v} = \frac{\nabla S}{m} \ . \tag{38}$$

Differentiating the CQHJE we see that along these trajectories the velocity field $\mathbf{v}$ satisfies

$$\frac{d\mathbf{v}}{dt} = -\frac{1}{m}\nabla V(\mathbf{x}) + \frac{i\hbar}{2m^2}\nabla^2\left(\nabla S\right) \ . \tag{39}$$

From the CQHJE we see that along such trajectories

$$\frac{dS}{dt} = \frac{1}{2m}\mathbf{v}^2 - V(\mathbf{x}) - \frac{i\hbar}{2m}\nabla^2 S \ . \tag{40}$$

The problem integrating (39) and (40) is that we have no information about the second and third derivatives of S that appear on the right hand sides. Borrowing an idea from complex WKB, we differentiate the CQHJE to find equations for the evolution of second and higher derivatives of S along the trajectories. At this stage we just write the equations for evolution of second, third and fourth derivatives:

$$\frac{dS_{ij}}{dt} = -V_{ij} - \frac{1}{m}\sum_p S_{ip}S_{pj} + \frac{i\hbar}{2m}\sum_p S_{ijpp} \ , \tag{41}$$

$$\frac{dS_{ijk}}{dt} = -V_{ijk} - \frac{1}{m}\sum_p (S_{ip}S_{pjk} + S_{jp}S_{pki} + S_{kp}S_{pij}) + \frac{i\hbar}{2m}\sum_p S_{ijkpp} \ , \tag{42}$$

$$\begin{aligned}\frac{dS_{ijkl}}{dt} &= -V_{ijkl} - \frac{1}{m}\sum_p (S_{ip}S_{pjkl} + S_{jp}S_{pkli} + S_{kp}S_{plij} + S_{lp}S_{pijk}) \\ &\quad -\frac{1}{m}\sum_p (S_{ijp}S_{pkl} + S_{ikp}S_{pjl} + S_{ilp}S_{pjk}) + \frac{i\hbar}{2m}\sum_p S_{ijklpp} \ .\end{aligned} \tag{43}$$

Apparently things have not improved: on the right hand sides of these equations fifth and sixth derivatives of S appear. Now we can state the procedure of the BOMCA approximation: *in nth order BOMCA ignore all terms involving derivatives of S of order exceeding $2n$.* Thus, in 1st order BOMCA the nonclassical term in (39) is taken to be zero and the trajectories are simply classical trajectories. The evolution (40) for S, however, involves a nonclassical term with second derivatives; but these second derivatives are computed by integrating (41) down the trajectories, after ignoring the term with 4th order derivatives in (41). A comparison with the equations of complex WKB establishes that *lowest order BOMCA is equivalent to lowest order complex WKB* (i.e. complex WKB where only the terms S_0 and S_1 are retained.)

Moving on to 2nd order BOMCA, a nonclassical term with third derivatives of S now remains in the equation for the trajectories (39), and fourth derivatives of S appear in (41). The evolution of the third and fourth derivatives of S is given by (42)-(43) after ignorning the higher derivative terms. We observe that the resulting equations are precisely the same as equations (33)-(34) that appeared in complex WKB. The trajectories, however, are different — thus 2nd order BOMCA is not equivalent to complex WKB of *any* order. The same is true for higher order BOMCA. Complex WKB and BOMCA however share the property that order n calculations involves derivatives of the potential V of order up to $2n$.

Note that ignoring the 5th and 6th derivative terms in (42)-(43) gives rise to order $\hbar$ errors in the 3rd and 4th derivatives of S. Through equations (39) and (41) this gives rise to order $\hbar^2$ errors in the trajectory $\mathbf{x}$ and the second derivative of S. At first glance it seems that the order $\hbar^2$ error in $\mathbf{x}$ should give rise to an order $\hbar^2$ error in S, as calculated from (40). But a careful calculation shows that the errors induced in S by both the error in $\mathbf{x}$ and the error in S_{ij} are of order $\hbar^3$, and thus we have achieved second order accuracy in S (and first order accuracy in $S/\hbar$, which is what determines the wave function). A similar calculation shows that in nth order BOMCA, as described above, we achieve nth order accuracy in S. There is no evident benefit to truncating the BOMCA equations, say, by ignoring 4th derivatives but not 3rd. This point was not adequately appreciated in [1, 2].

For clarity, we collect here the evolution equations for 2nd order BOMCA in the one dimensional case:

$$
\begin{aligned}
S_t &= \frac{1}{2}mv^2 - V(x) + \frac{i\hbar}{2m}S'' \ , && (44)\\
\frac{dx}{dt} &= v \ , && (45)\\
\frac{dv}{dt} &= -\frac{1}{m}V'(x) + \frac{i\hbar}{2m^2}S''' \ , && (46)\\
\frac{dS''}{dt} &= -V''(x) - \frac{1}{m}(S'')^2 + \frac{i\hbar}{2m}S'''' \ , && (47)\\
\frac{dS'''}{dt} &= -V'''(x) - \frac{3}{m}S''S''' \ , && (48)\\
\frac{dS''''}{dt} &= -V''''(x) - \frac{4}{m}S''S'''' - \frac{3}{m}(S''')^2 \ , && (49)
\end{aligned}
$$

This system is a singular perturbation of the Newton's equations. The system can be somewhat simplified. Introducing a new variable $f(t)$ defined (up to multiplication by a constant) by $S'' = \frac{m}{f}\frac{df}{dt}$, we can solve the S''' and S'''' evolution equations and find that the trajectories are determined by

$$
m\frac{d^2x}{dt^2} = -V'(x(t)) + \frac{i\hbar}{2m}S'''(t) \ , \qquad (50)
$$

$$m\frac{d^2f}{dt^2} = -V''(x(t))f(t) + \frac{i\hbar}{2mf(t)^3}\left(L - \int_0^t f(u)^4\left(V''''(x(u)) + \frac{3}{m}S'''(u)^2\right)du\right) \quad (51)$$

$$S'''(t) = \frac{1}{f(t)^3}\left(K - \int_0^t V'''(x(u))f(u)^3du\right) \ . \quad (52)$$

Here K, L are constants of integration related to $S'''(0), S''''(0)$.

We have not yet dealt with the question of initial conditions in BOMCA, but this is straightforward. Writing, as before,

$$S^{\rm init}(\mathbf{x}) = -i\hbar\log\psi(\mathbf{x},0) \ , \quad (53)$$

we take

$$S(0) = S^{\rm init}(\mathbf{x}(0)) \ , \quad (54)$$

$$v_i(0) = \frac{1}{m}S_i^{\rm init}(\mathbf{x}(0)) \ , \quad (55)$$

$$S_{ij}(0) = S_{ij}^{\rm init}(\mathbf{x}(0)) \qquad \text{etc.} \quad (56)$$

The number of equations is easier to discuss in BOMCA than in complex WKB. In nth order BOMCA we retain derivatives of S up to order $2n$, i.e. a total of $\begin{pmatrix} d+2n \\ d \end{pmatrix}$ functions. We also need to integrate to find $\mathbf{x}$; thus there are a total of

$$\begin{pmatrix} d+2n \\ d \end{pmatrix} + d \quad (57)$$

functions. But this number cannot be directly compared with the number in complex WKB. In complex WKB first the trajectories are computed using Newton's equations. If the aim is to determine the wave function at $\mathbf{X}$ at time T we solve (25), with boundary conditions (24) and $\mathbf{x}(T) = \mathbf{X}$. Once the trajectories are determined, the evolution of all the other functions along the trajectories is computed. In BOMCA it is necessary to solve for all the functions (admittedly a rather smaller number) in order to determine the trajectories; that is we look for a solution of the full BOMCA system satisfying initial conditions (54)-(56) and the final condition $\mathbf{x}(T) = \mathbf{X}$. At this stage we have not made a complete study of the relative efficiencies of the two approaches.

2.3 The need for multiple trajectories

We refer to our previous papers [1],[2],[3] for full details of the implementation of the methods and explicit numerical examples. In order to determine the wave function at position $\mathbf{X}$ and time T, it is necessary to find trajectories $\mathbf{x}(t)$ satisfying all the necessary initial conditions

and the condition $\mathbf{x}(T) = \mathbf{X}$. The missing initial data is simply the starting point of the trajectories, $\mathbf{x}(0)$. In every case we investigated we found there were multiple trajectories satisfying all the necessary conditions. That is, there are various possible choices of $\mathbf{x}(0)$, and we refer to the different possible choices as different "branches". In certain cases, the wave function associated with one branch gives an accurate result. In other cases, it is necessary to add the wave functions associated with more than one branch to get an accurate result. In still other cases, one branch gives an overwhelmingly large contribution and has to be discarded. For certain values of $\mathbf{X}$ and T there are transitions between the different behaviors, and in the neighborhoods of such transitions we could not get reasonable accuracy with our methods.

The upshot of all this is that our derivation of the complex WKB and BOMCA equations starting from the CQHJE (3) is apparently not telling us the whole story. In the following sections we will present derivations of complex WKB and BOMCA starting from the path integral formulation of quantum mechanics. In this approach the existence of multiple branches, and the need to sometimes incorporate one, sometimes more, is easily explained. We also find a non-technical explanation of what the trajectories in BOMCA are. At the same time, we see that the equations we have presented in detail for complex WKB and BOMCA actually provide an efficient way to perform certain higher order perturbative calculations with path integrals.

3 A path integral derivation of complex WKB

The aim of this section is to show how complex WKB emerges from the path integral formulation of quantum mechanics. In Feynman's path integral formulation the wave function (we work for now in one space dimension) is written

$$\psi(X,T) = \int_{-\infty}^{\infty} K(x_0, X, T)\psi_0(x_0)dx_0, \tag{58}$$

where $\psi_0(x_0) = \psi(x_0, 0)$ is the initial wavefunction and

$$K(x_0, X, T) = \int \mathcal{D}x \exp\left(\frac{iS[x]}{\hbar}\right) \tag{59}$$

is the propagator. The propagator is represented as a sum over all possible paths $x(t)$, $0 \le t \le T$, satisfying the boundary conditions $x(0) = x_0$ and $x(T) = X$. $S[x]$ denotes the classical action of the path x, given by

$$S[x] = \int_0^T \frac{1}{2}m\dot{x}^2(t) - V(x(t))\ dt. \tag{60}$$

Inserting eq.(59) into eq.(58), moving $\psi_0(x_0)$ into the argument of the exponent and incorporating the integration over x_0 into $\int \mathcal{D}x$ yields an alternate version of the path integral formulation

$$\psi(X,T) = \int \mathcal{D}x \exp\left(\frac{iS[x]}{\hbar} + \log\psi_0(x(0))\right) = \int \mathcal{D}x \exp\left(\frac{i\left(S[x] + S^{\rm init}(x(0))\right)}{\hbar}\right) \ , \quad (61)$$

where now $\int \mathcal{D}x$ represents now a sum over all possible paths satisfying the single boundary condition $x(T) = X$, and we have written, as before, $S^{\rm init}(x) = -i\hbar \log\psi_0(x)$.

The next step is to evaluate $\psi(X,T)$ using a saddle point approximation. To this end we consider the variation of the term in the exponential in the path integral, and in particular identify paths for which the first order variation vanishes. Replacing x by $x+\epsilon$ in the term in the exponential we have

$$\begin{aligned} S[x+\epsilon] + S^{\rm init}(x(0)+\epsilon(0)) &= \int_0^T \frac{1}{2}m\left(\dot{x}+\dot{\epsilon}\right)^2 - V(x(t)+\epsilon(t))\ dt + S^{\rm init}(x(0)+\epsilon(0)) \ , \\ &= S[x] + S^{\rm init}(x(0)) + \int_0^T \left(m\dot{x}\dot{\epsilon} - V'(x)\epsilon\right) dt + S^{\rm init\prime}(x(0))\epsilon(0) \\ &\quad + \int_0^T \left(\frac{1}{2}m\dot{\epsilon}^2 - \frac{1}{2}V''(x)\epsilon^2\right) dt + \frac{1}{2}S^{\rm init\prime\prime}(x(0))\epsilon(0)^2 \\ &\quad + \sum_{n=3}^{\infty}\frac{1}{n!}\left(S^{{\rm init}(n)}(x(0))\epsilon(0)^n - \int_0^T V^{(n)}(x)\epsilon^n dt\right) \ . \end{aligned} \quad (62)$$

After an integration by parts, and using the fact that $\epsilon(T) = 0$, as all paths have the same fixed end point, the linear terms in ϵ become

$$-\int_0^T \left(m\ddot{x} + V'(x)\right)\epsilon dt + \left(S^{\rm init\prime}(x(0)) - m\dot{x}(0)\right)\epsilon(0) \ . \quad (63)$$

Thus we deduce that *in a saddle point approximation of (61), the approximation will be a sum of contributions from classical paths satisfying the initial condition*

$$\dot{x}(0) = \frac{1}{m}S^{\rm init\prime}(x(0)) = -\frac{i\hbar}{m}\frac{\psi_0'(x(0))}{\psi_0(x(0))} \ . \quad (64)$$

These are exactly the complex classical paths that appear in complex WKB.

Proceeding to look at the quadratic terms in (62), we want the variable over which we integrate in the path integral to be dimensionless, so we rescale ϵ by writing

$$\epsilon(t) = \sqrt{\frac{\hbar T}{m}}\delta(t) \ . \quad (65)$$

After this change the quadratic terms in (62) become

$$\hbar T\left(\int_0^T \left(\frac{1}{2}\dot{\delta}^2 - \frac{1}{2m}V''(x(t))\delta^2\right) dt + \frac{1}{2m}S^{\rm init\prime\prime}(x(0))\delta(0)^2\right) \ . \quad (66)$$

We are now in a position to write the saddle-point approximation to (61):

$$\begin{aligned}\psi(X,T) &= \sum_{x(t)} \exp\left(\frac{i\left(S[x]+S^{\rm init}(x(0))\right)}{\hbar}\right) \\ &\int \mathcal{D}\delta \exp\left(iT\left(\int_0^T\left(\frac{1}{2}\dot\delta^2(t)-\frac{1}{2m}V''(x(t))\delta^2(t)\right)dt+\frac{S^{\rm init}{}''(x(0))}{2m}\delta(0)^2\right)\right) \\ &\exp\left(i\sum_{n=3}^{\infty}\frac{\hbar^{\frac{n}{2}-1}}{n!}\left(\frac{T}{m}\right)^{\frac{n}{2}}\left(S^{{\rm init}(n)}(x(0))\delta(0)^n-\int_0^T V^{(n)}(x)\delta^n(t)dt\right)\right)\ .\end{aligned} \tag{67}$$

Here the sum is over complex WKB paths, that is paths $x(t)$ obeying the classical equations of motion and the initial condition (64). However, as is usual in saddle-point approximations, more detailed calculations are necessary to decide which of these paths should be included in the sum. We will return to this point shortly.

3.1 The lowest order approximation

To compute the lowest order approximation we just need to evaluate the Gaussian integral

$$\int \mathcal{D}\delta \exp\left(iT\left(\int_0^T\left(\frac{1}{2}\dot\delta^2(t)-\frac{1}{2m}V''(x(t))\delta^2(t)\right)dt+\frac{S^{\rm init}{}''(x(0))}{2m}\delta(0)^2\right)\right)\ . \tag{68}$$

We recall that the integration here is over paths $\delta(t)$ obeying the single condition $\delta(T)=0$. As usual, we compute this integral by dividing the interval $[0,T]$ into N subintervals and discretizing. Appropriate (second order) discretization formulas for the various terms are

$$\int_0^T \dot\delta^2(t)dt \approx \frac{N}{T}\left(\delta_0^2+2\sum_{i=1}^{N-1}\delta_i^2-2\sum_{i=0}^{N-1}\delta_i\delta_{i+1}\right)\ , \tag{69}$$

$$\int_0^T V''(x(t))\delta^2(t)dt \approx \frac{T}{N}\left(\frac{1}{2}V''(x(0))\delta_0^2+\sum_{i=1}^{N-1}V''\left(x\left(\frac{iT}{N}\right)\right)\delta_i^2\right)\ , \tag{70}$$

where δ_i denotes $\delta(iT/N)$. Using these, the discretized version of the path integral is

$$\int d^N\Delta \exp\left(\frac{iN}{2}\Delta A\Delta^T\right) \tag{71}$$

where $\Delta = (\,\delta_0 \quad \delta_1 \quad \delta_2 \quad \dots \quad \delta_{N-1}\,)$, A denotes the tridiagonal $N\times N$ matrix

$$A=\begin{pmatrix} q & -1 & 0 & 0 & \dots \\ -1 & 2-\frac{T^2}{mN^2}V''\left(x\left(\frac{T}{N}\right)\right) & -1 & 0 & \dots \\ 0 & -1 & 2-\frac{T^2}{mN^2}V''\left(x\left(\frac{2T}{N}\right)\right) & -1 & \dots \\ 0 & 0 & -1 & 2-\frac{T^2}{mN^2}V''\left(x\left(\frac{3T}{N}\right)\right) & \dots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix} \tag{72}$$

and

$$q = 1 - \frac{T^2}{2mN^2} V''(x(0)) + \frac{T S^{\text{init}\,\prime\prime}(x(0))}{mN} \ . \tag{73}$$

(At this point it is maybe worthwhile noting that for an initial Gaussian wavefunction, $S^{\text{init}\,\prime\prime}(x(0))$ has a positive imaginary part.) The measure $d^N\Delta$ here includes a nontrivial N-dependent normalization; it turns out this should be chosen so that

$$\int d^N\Delta \exp\left(\frac{iN}{2}\Delta A \Delta^T\right) = \frac{1}{\sqrt{\det A}} \ . \tag{74}$$

(For the standard rules for Gaussian integrals see for example [60]; the correct choice of normalization is determined by checking that we get the correct result for a free particle.) The computation of the determinant $\det A$ proceeds as follows [61]: For $n = 1, 2, \ldots, N$, denote the determinant of the $n \times n$ matrix in the top left corner of A by D_n. Then we have

$$D_1 \ = \ q \ = \ 1 + \frac{T S^{\text{init}\,\prime\prime}(x(0))}{mN} + O\left(N^{-2}\right) \ , \tag{75}$$

$$D_2 \ = \ q\left(2 - \frac{T^2}{mN^2} V''\left(x\left(\frac{T}{N}\right)\right)\right) - 1 \ = \ 1 + \frac{2T S^{\text{init}\,\prime\prime}(x(0))}{mN} + O\left(N^{-2}\right) \ , \tag{76}$$

and for $3 \leq n \leq N$

$$D_n = \left(2 - \frac{T^2}{mN^2} V''\left(x\left(\frac{(n-1)T}{N}\right)\right)\right) D_{n-1} - D_{n-2} \ . \tag{77}$$

The recursion can be written in the equivalent form

$$\frac{D_n - 2D_{n-1} + D_{n-2}}{(T/N)^2} = -\frac{1}{m} V''\left(x\left(\frac{(n-1)T}{N}\right)\right) D_{n-1} \ . \tag{78}$$

We need to determine $\det A = D_N$. The recursion and the initial conditions are such that as $N \to \infty$, the D_n will tend to samples of a function $D(s)$, defined on the interval $0 \leq s \leq T$, obeying the differential equation $\ddot{D}(s) = -\frac{1}{m} V''(x(s)) D$ and initial conditions $D(0) = 1$ and $\dot{D}(0) = \frac{1}{m} S^{\text{init}\,\prime\prime}(x(0))$. The determinant we seek is simply $\det A = D(T)$.

To summarize, we have arrived at the lowest order approximation for the contribution of the path $x(t)$ in the sum (67): It is given by

$$\frac{1}{\sqrt{D(T)}} \exp\left(\frac{i\left(S[x] + S^{\text{init}}(x(0))\right)}{\hbar}\right) \ . \tag{79}$$

Here $S[x]$ denotes the classical action associated with the path $x(t)$, which is a solution of Newton's equations obeying the conditions $x(T) = X$ and $\dot{x}(0) = \frac{1}{m} S^{\text{init}\,\prime}(x(0))$. The function S^{init} is determined by the initial wave function via $S^{\text{init}}(x) = -i\hbar \log \psi(x, 0)$. The function $D(s)$ is the solution of the initial value problem

$$\ddot{D}(s) = -\frac{1}{m} V''(x(s)) D \ , \qquad D(0) = 1 \ , \ \dot{D}(0) = \frac{1}{m} S^{\text{init}\,\prime\prime}(x(0)) \ . \tag{80}$$

We check that the above gives an exact result in the case of the free particle ($V = 0$) and initial Gaussian wave function

$$\psi(x,0) = \exp\left(-\frac{a(x-x_0)^2}{\hbar} + \frac{ip_0(x-x_0)}{\hbar}\right) \ . \tag{81}$$

The initial wave function here has three parameters, x_0 and p_0 which are real and a which is complex, with positive real part. Classical paths take the form $x(t) = A + Bt$. The coefficients A, B should be determined by requiring

$$X = A + BT \ , \qquad B = \frac{1}{m}\left(p_0 + 2ia(A - x_0)\right) \ . \tag{82}$$

The classical action along the path $x(t)$ is then given by $S[x] = \frac{1}{2}mB^2T$ and $D(T) = 1 + \frac{1}{m}S^{\text{init}\,\prime\prime}(x(0))T = 1 + \frac{2iaT}{m}$. Putting everything together we obtain

$$\begin{aligned}\psi(X,T) &= \frac{1}{\sqrt{1+\frac{2iaT}{m}}}\exp\left(-\frac{a(A-x_0)^2}{\hbar} + \frac{ip_0(A-x_0)}{\hbar}\right)\exp\left(\frac{imB^2T}{2\hbar}\right) \\ &= \frac{1}{\sqrt{1+\frac{2iaT}{m}}}\exp\left(-\frac{a}{\hbar\left(1+\frac{2iaT}{m}\right)}\left(X - x_0 - \frac{p_0T}{m}\right)^2 + \frac{ip_0}{\hbar}\left(X - x_0 - \frac{p_0T}{m}\right) + \frac{ip_0^2T}{2\hbar m}\right) \ .\end{aligned} \tag{83}$$

It is straightforward to check that this is the exact solution of the Schrödinger equation for the given initial condition.

Having computed the lowest order approximation to the path integral in the one dimensional case, we now state the generalization to the multidimemsional case, leaving the proof to an appendix. Once again the saddle point paths are exactly the trajectories that appeared in the complex WKB method, specifcially they are classical paths $\mathbf{x}(t)$ obeying the initial condition

$$\dot{\mathbf{x}}(0) = \frac{1}{m}\nabla S^{\text{init}}(\mathbf{x}(0)) \ , \tag{84}$$

c.f. (24), as well as the final condition $\mathbf{x}(T) = \mathbf{X}$. The contribution from any such path to the wave function $\psi(\mathbf{X}, T)$ takes the form

$$\frac{1}{\sqrt{D(T)}}\exp\left(\frac{i\left(S[\mathbf{x}] + S^{\text{init}}(\mathbf{x}(0))\right)}{\hbar}\right) \ . \tag{85}$$

Here, as in the one-dimensional case, $S[\mathbf{x}]$ denotes the classicial action associated with the path $\mathbf{x}(t)$. The factor $D(T)$ is determined as follows: Denote by $U(s)$ the $d \times d$ matrix solution of the initial value problem

$$\ddot{U}(s) = -\frac{1}{m}H(V)(\mathbf{x}(s))U \ , \qquad U(0) = I \ , \ \dot{U}(0) = \frac{1}{m}H(S^{\text{init}})(\mathbf{x}(0)) \ , \tag{86}$$

where here $H(V)$ and $H(S^{\rm init})$ denote the $d \times d$ matrices of second derivatives of V and $S^{\rm init}$ respectively. Then $D(T) = \det(U(T))$.

We now wish to compare the lowest order path integral results with the lowest order approximation in complex WKB in the previous section. The path integral results all appear in the paragraph above. For ease, we assemble here all the necessary equations from complex WKB. The trajectories are determined from

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \ , \qquad \frac{d\mathbf{v}}{dt} = -\frac{1}{m}\nabla V(\mathbf{x}) \ , \tag{87}$$

with boundary conditions

$$\mathbf{v}(0) = \frac{1}{m}\nabla S_0^{\rm init}(\mathbf{x}(0)) \ , \qquad x(T) = \mathbf{X} \ . \tag{88}$$

The wave function is given by

$$\psi(\mathbf{X}, T) = \exp\left(\frac{iS_0(T)}{\hbar} + S_1(T)\right) \ . \tag{89}$$

The evolution equations of the necessary quantities along the trajectories are

$$\frac{dS_0}{dt} = \frac{1}{2}m\mathbf{v}^2 - V(\mathbf{x}) \ , \tag{90}$$

$$\frac{dS_1}{dt} = \frac{i}{2m}\sum_{i=1}^{d} S_{0,ii} \ , \tag{91}$$

$$\frac{dS_{0,ik}}{dt} = -V_{ik}\left(\mathbf{x}(t)\right) - \frac{1}{m}\sum_j S_{0,ij}S_{0,jk} \ , \tag{92}$$

with initial conditions

$$S_0(0) = S^{\rm init}(\mathbf{x}(0)) \ , \quad S_{0,ij}(0) = S_{ij}^{\rm init}(\mathbf{x}(0)) \ , \quad S_1(0) = 0 \ . \tag{93}$$

The correspondence is almost immediate. All that is necessary to do is to identify the matrix with entries $S_{0,ij}$ in complex WKB with the matrix product $m\dot{U}U^{-1}$ in the path integral approach. With this identification, the evolution equation (92) coincides with the second order evolution equation (86) for U. Also after this identification, the evolution equation for S_1, (91) reads $\frac{dS_1}{dt} = \frac{i}{2}{\rm Tr}(\dot{U}U^{-1})$, with solution (taking into account the appropriate initial conditions) $S_1(t) = \frac{i}{2}\log\det U(t)$, so $e^{iS_1} = 1/\sqrt{D(T)}$, giving the prefactor in (85). Finally, S_0 in complex WKB is identified with $S[\mathbf{x}] + S^{\rm init}(\mathbf{x}(0))$ in the path integral approach.

The path integral approach has added one significant piece of information over the direct complex WKB approach presented in the previous section. In the path integral approach we use the saddle point method for asymptotic evaluation of an integral. As is well known, when

there are multiple saddle points, it is sometimes necessary to take more than one into account to get an accurate approximation of the integral being studied. Deciding which saddle points contribute requires detailed analysis on a case-to-case basis. But at least we have found an explanation for the observations of our earlier work [2],[3] that for certain values of $\mathbf{X}$ and T it is necessary to include the contibutions of multiple trajectories. (It is interesting to compare this explanation for the origin of multiple trajectories with that given by Miller [58], based on the implicit nature of the equations that generate dynamical canonical transformations. We suspect that Miller's explanation may correlate with the existence of multiple solutions of the classical HJE, a connection that would bring us full circle to an understanding of the need for multiple trajectories in Complex WKB and BOMCA.) In future work [59] we hope to study the possible criteria for demarking different regions in $\mathbf{X}, T$ space in which different (numbers of) trajectories contribute. This is strongly interconnected with the existence of *caustics*. Caustics are points $\mathbf{X}, T$ at which the determinant $D(T)$ vanishes (on at least one trajectory, in fact such points are associated with coallescing trajectories). It is possible to study the dynamics of such points, and from this to deduce certain information about the dynamics of the regions in which different numbers of trajectories contribute. Unfortunately, however, at the moment deciding on which trajectories to include in a calculation is more of an art than a science.

3.2 The first order correction

We now consider the higher order terms in (67). We restrict ourselves in this section to the 1-dimensional case. The series in the exponential in the third line of (67) is an expansion in half-integer and integer powers of the dimensionless parameter $\frac{\hbar T}{mL^2}$ where L denotes a typical length scale of the functions $V(x)$ and $S^{\rm init}(x)$. We are assuming this parameter is small. All terms with half-integer powers multiply odd powers of δ and thus do not contribute to the value of the integral. The lowest order correction terms arise when we replace the exponential by

$$\begin{aligned} 1 \;+\; & \frac{i\hbar T^2}{24m^2}\left(S^{\rm init}{}''''(x(0))\delta(0)^4 - \int_0^T V''''(x)\delta^4(t)dt\right) \\ -\; & \frac{\hbar T^3}{72m^3}\left(S^{\rm init}{}'''(x(0))\delta(0)^3 - \int_0^T V'''(x)\delta^3(t)dt\right)^2 \ . \end{aligned} \tag{94}$$

After discretizing, in this approximation the integral (71) is replaced by an expression of the form

$$\int d^N\Delta \exp\left(\frac{iN}{2}\Delta A\Delta^T\right)\left(1+\sum_{i=0}^{N-1}\delta_i^4\mathcal{A}_i + \sum_{i=0}^{N-1}\sum_{j=0}^{N-1}\delta_i^3\delta_j^3\mathcal{B}_{ij}\right) \ , \tag{95}$$

where $\mathcal{A}_i$ and $\mathcal{B}_{ij}$, which do not depend on the components of δ, are

$$\mathcal{A}_i = \begin{cases} \frac{i\hbar T^2}{24m^2} S^{\text{init}\prime\prime\prime\prime}(x(0)) + O\left(\frac{1}{N}\right) & i = 0 \\ -\frac{i\hbar T^3}{24m^2 N} V^{\prime\prime\prime\prime}\left(x\left(\frac{iT}{N}\right)\right) & i > 0 \end{cases} , \tag{96}$$

$$\mathcal{B}_{ij} = \begin{cases} -\frac{\hbar T^3}{72m^3}\left(S^{\text{init}\prime\prime\prime}(x(0))\right)^2 + O\left(\frac{1}{N}\right) & i = j = 0 \\ \frac{\hbar T^4}{72m^3 N} S^{\text{init}\prime\prime\prime}(x(0)) V^{\prime\prime\prime}\left(x\left(\frac{iT}{N}\right)\right) + O\left(\frac{1}{N^2}\right) & i > 0, j = 0 \\ \frac{\hbar T^4}{72m^3 N} S^{\text{init}\prime\prime\prime}(x(0)) V^{\prime\prime\prime}\left(x\left(\frac{jT}{N}\right)\right) + O\left(\frac{1}{N^2}\right) & i = 0, j > 0 \\ -\frac{\hbar T^5}{72m^3 N^2} V^{\prime\prime\prime}\left(x\left(\frac{iT}{N}\right)\right) V^{\prime\prime\prime}\left(x\left(\frac{jT}{N}\right)\right) & i, j > 0 \end{cases} . \tag{97}$$

The Gaussian integrals in the above expression are standard. Taking into account our normalization of the measure $d^n\Delta$ we have

$$\int d^N\Delta \exp\left(\frac{iN}{2}\Delta A\Delta^T\right)\delta_i^4 = -\frac{3}{N^2\sqrt{\det A}}\left(A^{-1}_{ii}\right)^2 , \tag{98}$$

$$\int d^N\Delta \exp\left(\frac{iN}{2}\Delta A\Delta^T\right)\delta_i^3\delta_j^3 = -\frac{3i}{N^3\sqrt{\det A}}\left(3A^{-1}_{ii}A^{-1}_{jj}A^{-1}_{ij} + 2\left(A^{-1}_{ij}\right)^3\right) \tag{99}$$

(c.f. [60]). A calculation similar to the calculation of $\det A$ in the previous subsection shows that as $N \to \infty$

$$\frac{T}{N}A^{-1}_{ij} \to D(t_i)D(t_j)\int_{\max(t_i,t_j)}^T \frac{du}{D(u)^2} , \tag{100}$$

where $D(s)$ is the solution of (86). (This calculation uses the fact that a second, linearly independent, solution of the differential equation in (86) is given by $D(s)\int_0^s \frac{du}{D(u)^2}$.) In this manner we can write down the first order approximation to the path integral. For simplicity we restrict ourselves here to the case that $S^{\text{init}\prime\prime\prime}$ and $S^{\text{init}\prime\prime\prime\prime}$ vanish, as otherwise the relevant formulae are lengthy. Combining the formulae above we find that in this case the first order approximation is found by multiplying the leading order approximation by

$$\begin{aligned} 1 &+ \frac{i\hbar}{8m^2}\int_0^T V^{\prime\prime\prime\prime}(x(t))\,D(t)^4\left(\int_t^T \frac{du}{D(u)^2}\right)^2 dt \\ &+ \frac{i\hbar}{24m^3}\int_0^T\int_0^T V^{\prime\prime\prime}(x(t_1))\,V^{\prime\prime\prime}(x(t_2))\,D(t_1)^3D(t_2)^3 \\ &\left(3\left(\int_{\max(t_1,t_2)}^T \frac{du}{D(u)^2}\right)\left(\int_{t_1}^T \frac{du}{D(u)^2}\right)\left(\int_{t_2}^T \frac{du}{D(u)^2}\right) + 2\left(\int_{\max(t_1,t_2)}^T \frac{du}{D(u)^2}\right)^3\right) dt_1dt_2. \end{aligned} \tag{101}$$

We now need to compare this with a similar term arising in the complex WKB method. The first order approximation in complex WKB is obtained by multiplying the leading order approximation by $e^{i\hbar S_2(T)}$. To find S_2 it is necessary to integrate 5 new differential equations along the trajectories (in addition to those that have to be solved to find the lowest order approximation): the equations for $S_0^{\prime\prime\prime}, S_0^{\prime\prime\prime\prime}, S_1', S_1''$ and S_2, equations (33),(34),(35),(36) and

(28) respectively. All of these are linear equations, and an explicit formula can be written for the answer. To simplify matters we assume the initial conditions for all the 5 relevant quantities are zero, which is consistent with the assumption made in writing (101). In its most obvious form (without making any attempts to simplify the integrals that appear) the solution takes the form

$$\begin{aligned} S_2(T) &= \frac{1}{4m^2}\int_0^T \frac{1}{D^2(t)}\left(\int_0^t \frac{1}{D^2(u)}\left(\int_0^u V''''(x(v))D^4(v)dv\right)du\right)dt \qquad (102)\\ &+ \frac{1}{8m^3}\int_0^T \frac{1}{D^2(t)}\left(\int_0^t \frac{1}{D^2(u)}\left(\int_0^u V'''(x(v))D^3(v)dv\right)du\right)^2 dt \\ &+ \frac{3}{4m^3}\int_0^T \frac{1}{D^2(t)}\left(\int_0^t \frac{1}{D^2(u)}\left(\int_0^u \frac{1}{D^2(v)}\left(\int_0^v V'''(x(w))D^3(w)dw\right)^2 dv\right)du\right)dt \\ &+ \frac{1}{4m^3}\int_0^T \frac{1}{D^2(t)}\left(\int_0^t \frac{1}{D^2(u)}\left(\int_0^u V'''(x(v))D^3(v)dv\right)\right. \\ &\qquad \left.\left(\int_0^u \frac{1}{D^2(v)}\left(\int_0^v V'''(x(w))D^3(w)dw\right)dv\right)\ du\right)dt\ . \end{aligned}$$

It is a straightforward but tedious matter to check that the factor (101) is equal to $1 + i\hbar S_2$ (the first order approximation to $e^{i\hbar S_2}$).

Thus we see explicitly the equivalence of the first order approximation to the path integral and results from the complex WKB method retaining terms up to order S_2. For consistency, this equivalence must continue to higher orders. Note that if we keep terms up to order $\hbar^n$ in the path integral the resulting formulae will involve derivatives of V (and S^{init}) up to order $2n+2$, and the same is true if we retain terms up to S_{n+1} in complex WKB. We note that in practice, complex WKB is far easier to implement for higher order corrections. Although the number of differential equations that need to be integrated along the trajectories grows rapidly with the order, as described in the previous section, it remains relatively easy to write down the necessary differential equations, and integrating the relevant first order system along the trajectories is easily handled using standard computer packages. Direct application of path integral methods involves the calculation of iterated integrals, as in (102) or (101), which is a less standard procedure. The coefficients of the different iterated integrals (the number of which grows rapidly as order increases) also involve tricky combinatoric factors.

4 A modification of standard asymptotic analysis

In the previous section we have explained the connection of the complex WKB method as described in section 2 and the standard asymptotic evaluation of the path integral. We

would like to also understand BOMCA from this viewpoint. But there is a clear problem — whereas the trajectories in complex WKB are classical paths, corresponding to minima of the classical action, the paths in BOMCA are nonclassical. How can nonclassical paths possibly arise in the context of an asymptotic evaluation of the path integral? In this section we describe a modification of standard asymptotic analysis for Laplace-type integrals. In the next section we will apply what we have learn here to path integrals.

The usual approach to asymptotic evaluation of integrals such as $\int_{-\infty}^{\infty} g(x)e^{-\lambda f(x)}dx$, where λ is a large positive parameter, proceeds as follows: The integral is dominated by contributions from regions close to the minima of $f(x)$. Sufficiently near a minimum x_0 the function $f(x)$ is approximated by a quadratic Taylor polynomial $f(x_0) + \frac{1}{2}f''(x_0)(x-x_0)^2$. So we rewrite the integral in the form

$$\int_{-\infty}^{\infty} \tilde{g}(x)e^{-\lambda\left(f(x_0)+\frac{1}{2}f''(x_0)(x-x_0)^2\right)}dx \ , \tag{103}$$

where $\tilde{g}(x) = g(x)\exp\left(-\lambda\left(f(x) - f(x_0) - \frac{1}{2}f''(x_0)(x-x_0)^2\right)\right)$, and evaluate the contribution from the region near x_0 by expanding $\tilde{g}(x)$ in a Taylor series in $x - x_0$ and evaluating the resulting integrals exactly. This gives a series in negative powers of λ.

The modification to this procedure that we want to consider is as follows: The Taylor polynomial approximation to $f(x)$ at its minimum is only one of many ways to approximate $f(x)$ in the appropriate region by a quadratic function. Suppose we choose another quadratic approximant. How does this change the resulting asymptotic expansion?

For definiteness, we consider a specific example, asymptotic approximation of the factorial function for large n using the integral representation

$$n! = \int_0^{\infty} e^{n\log x - x}dx \ . \tag{104}$$

The function in the exponent has a minimum at $x = n$, and the usual asymptotic formula for $n!$ is obtained by approximating this function by the quadratic $n\log n - n - \frac{1}{2n}(x-n)^2$ and rewriting the integral

$$n! \sim n^n e^{-n}\int_{-\infty}^{\infty} e^{-(x-n)^2/2n}\tilde{g}(x)\ dx \ , \tag{105}$$

where

$$\begin{aligned}\tilde{g}(x) &= \exp\left(n\log x - x - (n\log n - n) + \frac{1}{2n}(x-n)^2\right) \\ &= 1 + \frac{1}{3n^2}(x-n)^3 - \frac{1}{4n^3}(x-n)^4 + \frac{1}{5n^4}(x-n)^5 + \frac{(n-3)}{18n^5}(x-n)^6 + \ldots\end{aligned} \tag{106}$$

Integrating gives the standard asymptotic series for $n!$

$$n! \sim \sqrt{2\pi} n^{n+\frac{1}{2}} e^{-n} \left(1 + \frac{1}{12n} + \frac{1}{288n^2} - \frac{139}{51840n^3} + \ldots\right) . \tag{107}$$

Note that to get the correct coefficient of n^{-r} it is necessary to keep certain terms of order up to $6r$ in the Taylor series (106).

Suppose now that instead of using the above quadratic approximant for the exponent we use the more general approximant $n \log N - N - \frac{1}{2S}(x-N)^2$. Here S and N are currently undetermined, but for definiteness we assume that $N = n + O(1)$ and $S = n + O(1)$. The integral now takes the form

$$n! \sim N^n e^{-N} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2S}(x-N)^2\right) \tilde{g}(x) dx \tag{108}$$

where

$$\begin{aligned} \tilde{g}(x) &= \exp\left(n \log x - x - (n \log N - N) + \frac{1}{2S}(x-N)^2\right) \qquad (109) \\ &= \exp\left(\left(\frac{n}{N} - 1\right)(x-N) + \frac{1}{2}\left(\frac{1}{S} - \frac{n}{N^2}\right)(x-N)^2 + \sum_{r=3}^{\infty} (-1)^{r-1} \frac{n}{rN^r} (x-N)^r\right) . \end{aligned}$$

Making the substitution $x - N = \sqrt{S} y$ this becomes

$$n! \sim N^n e^{-N} \sqrt{S} \int_{-\infty}^{\infty} e^{-y^2/2} \exp\left(\frac{(n-N)\sqrt{S}}{N} y + \frac{N^2 - nS}{2N^2} y^2 + \sum_{r=3}^{\infty} (-1)^{r-1} \frac{nS^{r/2}}{rN^r} y^r\right) dy . \tag{110}$$

Note that in the second exponent here the coefficients of y and y^3 behave as $n^{-1/2}$, the coefficients of y^2 and y^4 behaves as n^{-1}, and in general for $r \geq 3$ the coefficient of y^r behaves as $n^{1-r/2}$. We compute the integral by expanding the second exponential term in a power series in y and computing the resulting integrals exactly. The leading order approximation is $\sqrt{2\pi S} N^n e^{-N}$. The first order correction arises from replacing the second exponential by

$$1 + \left(\frac{N^2 - nS}{2N^2} y^2 - \frac{nS^2}{4N^4} y^4\right) + \frac{1}{2}\left(\left(\frac{(n-N)\sqrt{S}}{N}\right) y + \frac{nS^{3/2}}{3N^3} y^3\right)^2 \tag{111}$$

and integrating, to obtain

$$n! \sim \sqrt{2\pi S} N^n e^{-N} \left(1 + \frac{1}{12N^6} \left(\begin{array}{c} 6N^6 + 10n^2S^3 - 6N^4nS + 6N^4Sn^2 - 12N^5Sn + \\ 6N^6S - 9nS^2N^2 + 12n^2S^2N^2 - 12nS^2N^3 \end{array} \right)\right) . \tag{112}$$

It can be verified directly that provided $N = n + O(1)$ and $S = n + O(1)$ the correction term is $\frac{1}{12n} + O(n^{-2})$ for large n. Expanding the second exponential in (110) to suitable

higher order gives us higher correction terms, apparently depending on N and S as well as n, but in fact independent of the choice of N, S to the desired order.

Essentially what we have shown above is that Stirling's formula for $n!$ can be made to depend on two variables N and S while retaining all its properties. The obvious question that needs to be asked at this stage is whether N and S can be chosen usefully. A full investigation of this would take us off on a tangent to the main topic of this paper, so we limit ourselves here to the simple observation which will allow us to give a path integral derivation of BOMCA: *It is possible to choose N and S as functions of n in such a way that all correction terms to the leading order approximation $n! \sim \sqrt{2\pi S}N^n e^{-N}$ vanish.* Furthermore. at least in the case of the factorial function that we are looking at now, this is not simply a perturbative result; that is, we can find analytic functions N and S of n, with the correct asymptotic behavior for large $|n|$ and such that $\Gamma(n+1) = \sqrt{2\pi S}N^n e^{-N}$ at least in some region of the complex plane including the positive real axis. We will see in the next section how BOMCA is related to an analogous result for path integrals. Presumably there should be some way to select N and S "well" on the basis of properties of the integrand of (104), but we do not attempt to study this here.

5 A derivation of BOMCA from the path integral

The path integral is

$$\psi(X,T) = \int Dx \exp\left(\frac{i}{\hbar}(S[x] + S^{\text{init}}(x(0)))\right) \ , \tag{113}$$

where as before the integration is over all paths with $x(T) = X$. Applying the idea presented in the previous section means approximating $S[x] + S^{\text{init}}(x(0))$ with a quadratic, which we will take of the form

$$\begin{aligned} S[X] + S^{\text{init}}(X(0)) &+ \int_0^T \frac{1}{2}m(\dot{x}(t) - \dot{X}(t))^2 - \frac{1}{2}\left(V''(X(t)) + q(t)\right)(x(t) - X(t))^2 dt \\ &+ \frac{1}{2}(S^{\text{init}\prime\prime}(X(0)) + q(0))(x(0) - X(0))^2 \ . \end{aligned} \tag{114}$$

Here $X(t)$ is the path around which we are expanding, still to be fully determined, but assumed to be an order $\hbar$ perturbation of a classical path. Likewise the function $q(t)$ (which plays the role of S in the previous section) is currently undetermined, assumed of order $\hbar$. Using this quadratic as our leading order approximation in the path integral gives

$$\psi(X,T) = \exp\left(\frac{i}{\hbar}(S[X] + S^{\text{init}}(X(0)))\right) \int D\epsilon$$

$$\exp\left(\frac{i}{2\hbar}\left(\int_0^T m\dot{\epsilon}(t)^2 - \left(V''(X(t)) + q(t)\right)\epsilon(t)^2 dt + \left(S^{\text{init}\,\prime\prime}(X(0)) + q(0)\right)\epsilon(0)^2\right)\right)$$
$$\exp\left(\frac{i}{\hbar}\left(\int_0^T m\dot{X}(t)\dot{\epsilon}(t) - V'(X(t))\epsilon(t) + \frac{1}{2}q(t)\epsilon(t)^2 - \sum_{r=3}^{\infty}\frac{V^{(r)}(X(t))}{r!}\epsilon(t)^r\ dt\right.\right.$$
$$\left.\left. + S^{\text{init}\,\prime}(X(0))\epsilon(0) - q(0)\epsilon(0)^2 + \sum_{r=3}^{\infty}\frac{S^{\text{init}\,(r)}(X(0))}{r!}\epsilon(0)^r\right)\right)\ . \tag{115}$$

Here we have written $\epsilon(t) = x(t) - X(t)$. We can simplify the second exponential in the path integral in two ways. First, purely for ease of presentation we will assume that $S^{\text{init}\,(r)} = 0$ for $r > 3$, i.e. that the initial wave function is a Gaussian wave packet. There is no difficulty to restore the extra terms, but the calculations become extremely lengthy. Second, we make choices on the initial values of the currently unknown functions $X(t)$ and $q(t)$ to eliminate other terms in the second exponential as follows: First, we assume $q(0) = 0$. Second, integrating the term $\int_0^T m\dot{X}(t)\dot{\epsilon}(t)$ gives a boundary contribution $-m\dot{X}(0)\epsilon(0)$ and we can cancel this by requiring $m\dot{X}(0) = S^{\text{init}\,\prime}(X(0))$. Implementing all these simplifications gives us

$$\begin{aligned}\psi(X,T) &= \exp\left(\frac{i}{\hbar}(S[X] + S^{\text{init}}(X(0)))\right)\int D\epsilon \qquad (116)\\ &\exp\left(\frac{i}{2\hbar}\left(\int_0^T m\dot{\epsilon}(t)^2 - \left(V''(X(t)) + q(t)\right)\epsilon(t)^2 dt + S^{\text{init}\,\prime\prime}(X(0))\epsilon(0)^2\right)\right)\\ &\exp\left(\frac{i}{\hbar}\left(\int_0^T (-m\ddot{X}(t) - V'(X(t)))\epsilon(t) + \frac{1}{2}q(t)\epsilon(t)^2 - \sum_{r=3}^{\infty}\frac{V^{(r)}(X(t))}{r!}\epsilon(t)^r\ dt\right)\right)\ .\end{aligned}$$

Finally, we move to dimensionless quantities by substituting $\epsilon(t) = \sqrt{\frac{\hbar T}{m}}\delta(t)$, giving

$$\begin{aligned}\psi(X,T) &= \exp\left(\frac{i}{\hbar}(S[X] + S^{\text{init}}(X(0)))\right)\int D\delta\\ &\exp\left(\frac{iT}{2}\left(\int_0^T \dot{\delta}(t)^2 - \frac{1}{m}\left(V''(X(t)) + q(t)\right)\delta(t)^2 dt + \frac{1}{m}S^{\text{init}\,\prime\prime}(X(0))\delta(0)^2\right)\right)\\ &\exp\left(i\left(\int_0^T -\sqrt{\frac{mT}{\hbar}}\left(\ddot{X}(t) + \frac{1}{m}V'(X(t))\right)\delta(t) + \frac{T}{2m}q(t)\delta(t)^2\right.\right.\\ &\qquad\left.\left. - \sum_{r=3}^{\infty}\frac{\hbar^{r/2-1}T^{r/2}V^{(r)}(X(t))}{m^{r/2}r!}\delta(t)^r dt\right)\right)\ .\end{aligned} \tag{117}$$

Assuming that both $\ddot{X}(t) + \frac{1}{m}V'(X(t))$ and $q(t)$ are of order $\hbar$, we see that the coefficients of $\delta(t)$ and $\delta(t)^3$ in the second exponential are of order $\hbar^{-1/2}$, the coefficients of $\delta(t)^2$ and $\delta(t)^4$ are of order $\hbar^1$, and in general the coefficient of $\delta(t)^r$ is of order $\hbar^{r/2-1}$ for $r \geq 3$. (This is in direct analogy to the caclulations for the factorial function in section 4.) The leading order approximation to the path integral is obtained by simply discarding the second exponential

term. The remaining Gaussian integral is identical to one we have already computed (but with $V''(X(t))$ replaced by $V''(X(t))+q(t)$), and we obtain the leading order approximation

$$\psi(X,T) = \frac{\exp\left(\frac{i}{\hbar}(S[X] + S^{\rm init}(X(0)))\right)}{\sqrt{f(T)}} \tag{118}$$

where $f(s)$ is the solution of

$$\ddot{f}(s) = -\frac{1}{m}(V''(X(s)) + q(s))f(s)\ , \qquad f(0) = 1\ ,\ \dot{f}(0) = \frac{1}{m}S^{\rm init\,\prime\prime}(X(0))\ . \tag{119}$$

To obtain the first order correction to this, we need to replace the second exponential in the path integral by

$$\begin{aligned} 1 \ &+ \ \frac{i\hbar T}{2m}\left(\int_0^T \frac{q(t)}{\hbar}\delta(t)^2 - \frac{TV''''(X(t))}{12m}\delta(t)^4\ dt\right) \\ &- \ \frac{\hbar m T}{2}\left(\int_0^T \frac{\left(\ddot{X}(t) + \frac{1}{m}V'(X(t))\right)}{\hbar}\delta(t) + \frac{TV'''(X(t))}{6m^2}\delta(t)^3\ dt\right)^2\ . \end{aligned} \tag{120}$$

There are 5 terms here that we need to consider, as oppposed to 2 in the derivation of the first correction term in Complex WKB. In addition to the integration formulae (98)-(99) we need the formulae

$$\int d^N\Delta \exp\left(\frac{iN}{2}\Delta A\Delta^T\right)\delta_i\delta_j \ = \ \frac{i}{N\sqrt{\det A}}A^{-1}_{ij}\ , \tag{121}$$

$$\int d^N\Delta \exp\left(\frac{iN}{2}\Delta A\Delta^T\right)\delta_i^3\delta_j \ = \ -\frac{3}{N^2\sqrt{\det A}}A^{-1}_{ii}A^{-1}_{ij}\ . \tag{122}$$

Computing all the necessary integrals gives the following result for the first order correction: The leading order approximation should be multiplied by

$$\begin{aligned} 1 \ &- \ \frac{1}{2m}\int_0^T q(t)f(t)^2\left(\int_t^T \frac{du}{f(u)^2}\right)\ dt \\ &- \ \frac{im}{2\hbar}\int_0^T\int_0^T N(t_1)N(t_2)f(t_1)f(t_2)\left(\int_{\max(t_1,t_2)}^T \frac{du}{f(u)^2}\right)\ dt_1dt_2 \\ &+ \ \frac{1}{2m}\int_0^T\int_0^T N(t_1)V'''(X(t_2))f(t_1)f(t_2)^3\left(\int_{\max(t_1,t_2)}^T \frac{du}{f(u)^2}\right)\left(\int_{t_2}^T \frac{du}{f(u)^2}\right)\ dt_1dt_2 \\ &+ \ \frac{i\hbar}{8m^2}\int_0^T V''''\left(X(t)\right)f(t)^4\left(\int_t^T \frac{du}{f(u)^2}\right)^2\ dt \\ &+ \ \frac{i\hbar}{24m^3}\int_0^T\int_0^T V'''\left(X(t_1)\right)V'''\left(X(t_2)\right)f(t_1)^3f(t_2)^3 \\ &\quad \left(3\left(\int_{\max(t_1,t_2)}^T \frac{du}{f(u)^2}\right)\left(\int_{t_1}^T \frac{du}{f(u)^2}\right)\left(\int_{t_2}^T \frac{du}{f(u)^2}\right) + 2\left(\int_{\max(t_1,t_2)}^T \frac{du}{f(u)^2}\right)^3\right)\ dt_1dt_2. \end{aligned} \tag{123}$$

Here we have written $N(t) = \ddot{X}(t) + \frac{1}{m}V'(X(t))$. We have left the integrals here in the form they arise using the relevant rules for Gaussian integrals. To manipulate the integrals, though, it is more convenient to write them in terms of integrals in which all the variables are all ordered. Doing this gives:

$$
\begin{aligned}
1 \;-\; & \frac{1}{2m}\int_0^T dt_1 \int_{t_1}^T dt_2 \;\; q(t_1) f(t_1)^2 \frac{1}{f(t_2)^2} \\
- \; & \frac{im}{\hbar}\int_0^T dt_1 \int_{t_1}^T dt_2 \int_{t_2}^T dt_3 \;\; N(t_1) f(t_1) N(t_2) f(t_2) \frac{1}{f(t_3)^2} \\
+ \; & \frac{1}{m}\int_0^T dt_1 \int_{t_1}^T dt_2 \int_{t_2}^T dt_3 \int_{t_3}^T dt_4 \;\; N(t_1) f(t_1) V'''(t_2) f(t_2)^3 \frac{1}{f(t_3)^2}\frac{1}{f(t_4)^2} \\
+ \; & \frac{1}{2m}\int_0^T dt_1 \int_{t_1}^T dt_2 \int_{t_2}^T dt_3 \int_{t_3}^T dt_4 \;\; V'''(t_1) f(t_1)^3 \frac{1}{f(t_2)^2} N(t_3) f(t_3) \frac{1}{f(t_4)^2} \\
+ \; & \frac{1}{m}\int_0^T dt_1 \int_{t_1}^T dt_2 \int_{t_2}^T dt_3 \int_{t_3}^T dt_4 \;\; V'''(t_1) f(t_1)^3 N(t_2) f(t_2) \frac{1}{f(t_3)^2}\frac{1}{f(t_4)^2} \\
+ \; & \frac{i\hbar}{4m^2}\int_0^T dt_1 \int_{t_1}^T dt_2 \int_{t_2}^T dt_3 \;\; V''''(t_1) f(t_1)^4 \frac{1}{f(t_2)^2}\frac{1}{f(t_3)^2} \\
+ \; & \frac{i\hbar}{2m^3}\int_0^T dt_1 \int_{t_1}^T dt_2 \int_{t_2}^T dt_3 \int_{t_3}^T dt_4 \int_{t_4}^T dt_5 \;\; V'''(t_1) f(t_1)^3 \frac{1}{f(t_2)^2} V'''(t_3) f(t_3)^3 \frac{1}{f(t_4)^2}\frac{1}{f(t_5)^2} \\
+ \; & \frac{5i\hbar}{2m^3}\int_0^T dt_1 \int_{t_1}^T dt_2 \int_{t_2}^T dt_3 \int_{t_3}^T dt_4 \int_{t_4}^T dt_5 \;\; V'''(t_1) f(t_1)^3 V'''(t_2) f(t_2)^3 \frac{1}{f(t_3)^2}\frac{1}{f(t_4)^2}\frac{1}{f(t_5)^2}
\end{aligned}
\tag{124}
$$

Our intention now is to choose the functions $N(t)$ and $q(t)$ (both assumed to be of order $\hbar$) in such a way that there is no first order correction, i.e. so that the sum of the integrals in the above expression vanishes. From the above we see immediately that *for any choice of $N(t)$ it is possible to choose $q(t)$ such that the first order correction terms vanish.* One choice that suggests itself for $N(t)$ is simply to take $N(t) = 0$. Then the correct choice of $q(t)$ is

$$
\begin{aligned}
q(t) \;=\; & \frac{i\hbar}{mf(t)^4}\left(\frac{1}{2}\int_0^t du f(u)^4 V''''(X(u)) \right. \\
& + \frac{1}{m}\int_0^t du \int_0^u dv \int_0^v dw V'''(X(u)) f(u)^3 \frac{1}{f(v)^2} V'''(X(w)) f(w)^3 \\
& \left. + \frac{5}{m}\int_0^t du \int_0^u dv \int_0^v dw \frac{1}{f(u)^2} V'''(X(v)) f(v)^3 V'''(X(w)) f(w)^3 \right) .
\end{aligned}
\tag{125}
$$

The solution that is of main interest for us, however, is

$$
N(t) \;=\; -\frac{i\hbar}{2m^2 f(t)^3}\int_0^t V'''(X(u)) f(u)^3 du \tag{126}
$$

$$
\begin{aligned}
q(t) \;=\; & \frac{i\hbar}{mf(t)^4}\left(\frac{1}{2}\int_0^t du f(u)^4 V''''(X(u)) \right. \\
& \left. + \frac{3}{m}\int_0^t du \int_0^u dv \int_0^v dw \frac{1}{f(u)^2} V'''(X(v)) f(v)^3 V'''(X(w)) f(w)^3 \right)
\end{aligned}
\tag{127}
$$

We summarize what we have shown up to this point. For either of the choices of $N(t)$ and $q(t)$ given above (or for any other choice of $N(t)$ and the appropriate matching choice of $q(t)$) we have demonstrated that the leading order approximation to the path integral, (118), requires no first order correction. Here the path X and the function f are chosen to satisfy

$$\ddot{X}(t) + \frac{1}{m}V'(X(t)) = N(t) \ , \quad m\dot{X}(0) = S^{\text{init}\prime}(X(0)) \ , \ X(T) = X \ , \tag{128}$$

$$m\ddot{f}(s) + V''(X(s))f(s) = -q(s)f(s) \ , \quad f(0) = 1 \ , \ \dot{f}(0) = \frac{1}{m}S^{\text{init}\prime\prime}(X(0)) \ . \tag{129}$$

It is straightforward to check that the choice (126)-(127) describes BOMCA (compare equations (118),(126),(127),(128),(129) with (44),(50),(51),(52); the constants K, L should be chosen to be zero, and recall that in the discussion of BOMCA we wrote $S'' = \frac{m}{f}\frac{df}{dt}$). We have arrived at the understanding of BOMCA set out in the introduction — that it corresponds to an evaluation of the path integral around a near-classical path, chosen in such a way that the classical wave function remains accurate to any desired order in $\hbar$, with the path $\mathbf{x}$ and U being modified appropriately. We have found that in fact there are other ways to change $\mathbf{x}$ and U in such a way as to "correct" the classical wave function. In particular, we can continue to use classical paths, but replace the usual Jacobi equation with (129), where q is given by (125). (The existence of this option extends to higher dimensions.) In practice the direct derivation of BOMCA, as given in section 2, is clearly preferable over the path integral for determining higher order corrections. The path integral approach, however, is necessary to understand the need to add contributions from different (near-)classical trajectories can be justified.

Both the direct approach to BOMCA and the path integral approach only allow us to construct the relevant near-classical trajectories order-by-order in $\hbar$. The question arises as to whether it is possible to find pairs $\mathbf{x}$ and U for which the classical wave function is exact. As we have already explained in the introduction, the relevant paths would be an intermediate object between classical paths and the quantum trajectories of Bohmian mechanics — on the one hand the new paths would be order $\hbar$ perturbations of classical paths, but on the other hand they would enable permit the derivation of exact quantum dynamical results, at least in regions of configuration space where they exist. At this stage the existence of such paths remains just a conjecture.

6 The coherent state propagator

This section is a slight digression from the main point of this paper, but provides another illustration of our path integral methods, as well as the need for complex classical trajectories in "semiclassical" calculations. The so-called coherent state propagator has been studied extensively by many authors [11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21]. By the coherent state propagator we mean the overlap between the wave function $\psi(\mathbf{x}, T)$ evolving from an (initial) coherent state with another (final) coherent state. In fact our methods allow us to write down a rather more general object; we write down the leading order approximation for the overlap between the wave function $\psi(\mathbf{x}, T)$ evolving from an initial state of form $\exp(iS_i(\mathbf{x})/\hbar)$ with a final state of the form $\exp(iS_f(\mathbf{x})/\hbar)$. Using the Feynmann path integral representation of the (standard) propagator, the overlap takes the form

$$\mathcal{P} = \int_{-\infty}^{\infty} d\mathbf{x}_f \psi_f^*(\mathbf{x}_f) \int_{-\infty}^{\infty} d\mathbf{x}_i \psi_i(\mathbf{x}_i) \int \mathcal{D}\mathbf{x} \ \exp\left(\frac{iS[\mathbf{x}]}{\hbar}\right) \tag{130}$$

where the path integral is over all paths satisfying $\mathbf{x}(0) = \mathbf{x}_i$, $\mathbf{x}(T) = \mathbf{x}_f$. We can absorb the integrations over the initial and final position into the path integral to write this simply as

$$\mathcal{P} = \int \mathcal{D}\mathbf{x} \ \exp\left(\frac{i\left(S[\mathbf{x}] + S_i(\mathbf{x}(0)) - S_f^*(\mathbf{x}(T))\right)}{\hbar}\right) \tag{131}$$

where now the path integration is over all paths $\mathbf{x}(t)$, $0 \leq t \leq T$, with no specified boundary conditions.

To compute the semiclassical approximation to $\mathcal{P}$ we replace $\mathbf{x}$ in the exponent in the above expression by $\mathbf{x} + \varepsilon$ and expand to second order in ε. We choose $\mathbf{x}$ so that the linear term vanishes. Taking the action to be given by $\int_0^T \frac{1}{2}m\dot{\mathbf{x}}^2 - V(\mathbf{x})\ dt$ we find that the appropriate paths must satisfy

$$\begin{aligned} m\ddot{\mathbf{x}} + \nabla V(\mathbf{x}) &= 0 \ , & (132)\\ m\dot{\mathbf{x}}(0) &= \nabla S_i(\mathbf{x}(0)) \ , & (133)\\ m\dot{\mathbf{x}}(T) &= \nabla S_f^*(\mathbf{x}(T)) \ . & (134) \end{aligned}$$

The leading order approximation is thus a sum over such paths of the form

$$\mathcal{P} \approx \sum \psi_f^*(\mathbf{x}(T)) \exp(iS[\mathbf{x}]/\hbar)\psi_i(\mathbf{x}(0)) \int \mathcal{D}\varepsilon \ \exp(Q[\varepsilon]) \tag{135}$$

where

$$\begin{aligned} Q[\varepsilon] &= \frac{i}{2\hbar}\Bigg(\int_0^T m\dot{\varepsilon}^2 - \varepsilon(t)^T H(V)(\mathbf{x}(t))\varepsilon(t)\ dt \\ &\qquad + \varepsilon(0)^T H(S_i)(\mathbf{x}(0))\varepsilon(0) - \varepsilon(T)^T H(S_f^*)(\mathbf{x}(T))\varepsilon(T)\Bigg) \ . \end{aligned} \tag{136}$$

Following the method of the calculation in appendix A, the factor $\int \mathcal{D}\varepsilon \ \exp(Q[\varepsilon])$ can be replaced (modulo some normalization factor) by the large N limit of $1/\sqrt{\det V}$, where

$$V = \begin{pmatrix} I+G_0 & -I & 0 & 0 & 0 & \dots & \\ -I & 2I+G_1 & -I & 0 & 0 & \dots & \\ 0 & -I & 2I+G_2 & -I & 0 & & \\ 0 & 0 & -I & 2I+G_3 & -I & & \\ \vdots & \vdots & & \ddots & \ddots & & \\ & & & & -I & 2I+G_{N-1} & -I \\ & & & & & -I & I+G_N \end{pmatrix} . \tag{137}$$

Here

$$G_0 = \frac{T}{mN} H(S_i)(\mathbf{x}(0)) - \frac{T^2}{2mN^2} H(V)(\mathbf{x}(0)) \ , \tag{138}$$

$$G_r = -\frac{T^2}{mN^2} H(V)\left(\mathbf{x}\left(\frac{rT}{N}\right)\right) \ , \qquad r = 1, \dots, N-1 \ , \tag{139}$$

$$G_N = -\frac{T}{mN} H(S_f^*)(\mathbf{x}(T)) - \frac{T^2}{2mN^2} H(V)(\mathbf{x}(T)) \ . \tag{140}$$

The method for evaluating the determinant used in appendix A (with a slight addition to understand the nontrivial normalization) yields the final result

$$\mathcal{P} \approx \left(\frac{2\pi i\hbar}{m}\right)^{d/2} \sum \frac{\psi_f^*(\mathbf{x}(T)) \exp(iS[\mathbf{x}]/\hbar)\psi_i(\mathbf{x}(0))}{\sqrt{\det \begin{pmatrix} \dot{U}_1(T) + \frac{1}{m}\dot{U}_2(T) H(S_i)(\mathbf{x}(0)) - \frac{1}{m} H(S_f^*)(\mathbf{x}(T)) U_1(T) - \\ \frac{1}{m^2} H(S_f^*)(\mathbf{x}(T)) U_2(T) H(S_i)(\mathbf{x}(0)) \end{pmatrix}}} \tag{141}$$

Here U_1 and U_2 are two solutions of the equation

$$m\ddot{U}(t) = -H(V)U(t) \ , \tag{142}$$

satisfying initial conditions

$$\begin{cases} U_1(0) = I \\ \dot{U}_1(0) = 0 \end{cases} , \qquad \begin{cases} U_2(0) = 0 \\ \dot{U}_2(0) = I \end{cases} . \tag{143}$$

From equation (143) it follows that the entries of U_2 have dimensions of time, whereas those of U_1 are dimensionless.

Restricting to the case of Gaussian initial and final states, taken in the form

$$\psi_i(\mathbf{x}) = \exp\left(-\frac{m(\mathbf{x}-\mathbf{x}_{0i})^T \Omega_i (\mathbf{x}-\mathbf{x}_{0i})}{2\hbar} + \frac{i\mathbf{p}_{0i}\cdot(\mathbf{x}-\mathbf{x}_{0i})}{\hbar}\right) \ , \tag{144}$$

$$\psi_f(\mathbf{x}) = \exp\left(-\frac{m(\mathbf{x}-\mathbf{x}_{0f})^T \Omega_f (\mathbf{x}-\mathbf{x}_{0f})}{2\hbar} + \frac{i\mathbf{p}_{0f}\cdot(\mathbf{x}-\mathbf{x}_{0f})}{\hbar}\right) \ , \tag{145}$$

the above formula reduces to

$$\mathcal{P} \approx \left(\frac{2\pi i\hbar}{m}\right)^{d/2} \sum \frac{\psi_f^*(\mathbf{x}(T))\exp(iS[\mathbf{x}]/\hbar)\psi_i(\mathbf{x}(0))}{\sqrt{\det\left(\dot{U}_1(T) + i\dot{U}_2(T)\Omega_i + i\Omega_f^* U_1(T) + \Omega_f^* U_2(T)\Omega_i\right)}} \ . \tag{146}$$

Here $\mathbf{x}_{0i}, \mathbf{p}_{0i}$ are real parameters giving the expectation values of the position and momentum in the intial state, $\mathbf{x}_{0f}, \mathbf{p}_{0f}$ are real parameters giving the expectation of the position and momentum in the final state, and Ω_i, Ω_f are symmetric, complex matrices (with eigenvalues with positive real part). The relevant paths in the case of Gaussian initial states are those satisfying the boundary conditions

$$m\dot{\mathbf{x}}(0) = \mathbf{p}_{0i} + im\Omega_i(\mathbf{x}(0) - \mathbf{x}_{0i}) \ , \tag{147}$$

$$m\dot{\mathbf{x}}(T) = \mathbf{p}_{0f} - im\Omega_f^*(\mathbf{x}(T) - \mathbf{x}_{0f}) \ , \tag{148}$$

c.f. [11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21]. Note that the formula (146) is not dimensionless as for simplicity we have been working with nonnormalized Gaussian states.

We give one further simplifcation, just as an illustration of the use of this formula: In the scalar case for a free particle ($U_1(t) = 1, U_2(t) = t$) the formula gives the exact result

$$\mathcal{P} = \sqrt{\frac{2\pi\hbar}{m(\Omega_i + \Omega_f^* + iT\Omega_i\Omega_f^*)}} \tag{149}$$

$$\exp\left(-\frac{(p_i - p_f)^2 + m^2\Omega_i\Omega_f^*(x_i - x_f)^2 + iT(p_i^2\Omega_f^* + p_f^2\Omega_i) + 2im(x_i - x_f)(p_i\Omega_f^* + p_f\Omega_i)}{2\hbar m\left(\Omega_i + \Omega_f^* + iT\Omega_i\Omega_f^*\right)}\right) \ .$$

(Here we have slightly changed notation, dropping the "0" suffices on the position and momentum parameters.) It can be verified that the exponential is a pure phase if and only $p_f = p_i$, $x_f = x_i + p_i t/m$, in which case it becomes simply $\exp(itp_i^2/2m\hbar)$.

The initial and final conditions on the complex trajectories (147)-(148) are familiar from the literature, see in particular [20]. The semiclassical approximation (146) is presented somewhat differently from from formulae in the literature, but it would seem to be equivalent. Our derivation, while maybe not as careful as previous derivations, is a substantial simplification.

7 Concluding remarks

The main results of this paper are as follows: After a detailed presentation of the complex WKB and BOMCA methods we showed how complex WKB can be derived from a saddle

point approximation in the path integral formulation of quantum mechanics. The path integral approach to the method explains the need to incorporate the contributions from multiple trajectories; the original formulation however is much more useful for practical applications, avoiding the cumbersome multiple integrals that arise when computing higher order correction terms from the path integral. In terms of methodology, the novel aspect of our path integral derivation was incorporation of the initial wave function into the integrand prior to computing the saddle points and the relevant behavior near them: It is this that gives rise to complex trajectories. Complex and real trajectory methods in quantum mechanics are complementary, not contradictory — complex trajectories are needed to propagate wave packet-type states as considered in this paper, whereas real trajectories suffice for WKB-type states.

We then moved on to the path integral description of BOMCA. This required a further methodological innovation, the use of a general quadratic approximation in asymptotic analysis, as opposed to the standard Taylor approximation at the minimum. Using this more general asymptotic method we showed how to obtain BOMCA from the path integral (thus justifying the need for multiple trajectories in BOMCA too). In fact, from the path integral point of view at this stage BOMCA seems to be just one of many possible methods, a matter that merits further investigation. The overall picture of the relationship between complex WKB and BOMCA became clear. Both methods give rise to the same lowest order approximation to the wave function, the "classical wave function" (8). In complex WKB this approximation is refined by multiplying the wave function by suitable factors of the form $1 + O(\hbar)$, while keeping the same trajectories $\mathbf{x}$ and their variations U. In BOMCA, it is the formula (8) that remains the same, while $O(\hbar)$ corrections are made to the trajectories $\mathbf{x}$ and the matrices U; these are changed depending on the order of the approximation.

In section 6 we showed how our method of inserting the wave function into the path integral prior to making a saddle point approximation could be used to derive the coherent state propagator, measuring the overlap between an evolved Gaussian wave packet and another Gaussian state. Our derivation is a substantial simplifcation over previous ones. In the case of the coherent state propagator there is no alternative derivation to the path integral; for computations of the wave function, however, we emphasize that the derivation of the equations of complex WKB and BOMCA presented in section 2 is simpler than the path integral approach, which is only necessary to explain the need for multiple trajectories.

There are a number of areas in which further work is necessary. First and foremost, this paper was intended to provide the theoretical backing for the numerical studies in [1, 2, 3], and having done this, we hope that further numerical studies will be undertaken, especially

in multiple dimensions. There are several areas in which more theoretical developments would be welcome. First, we have almost completely avoided in this paper any discussion of caustics (points at which the denominator in (8) vanishes, rendering the approximation meaningless) and the related phenomenon of Stokes' lines. In the case of wave function approximations, the caustics and Stokes' lines are dependent on the time, and it is possible to write down equations describing their motion [59]. It is widely appreciated that the phenomena of caustics and Stokes' lines are "coordinate dependent", in the sense that they can be avoided (or moved) by working in momentum or phase space representations [53, 54, 55, 56]. However, not enough has been done yet to make these ideas into efficient techniques for calculations. Strongly related to these questions is the more mathematical question of the nature of the singularities in the system of ODEs arising in complex WKB at a caustic, which we are currently investigating [57].

Another matter requiring further investigation is a better understanding of the (linear) decomposition of the wave function implied in (8). Given an initial wave function is it possible (either abstractly or operationally) to write it as a sum of terms each of which evolves into one of the terms in the sum (8)? Is the evolution by the Schrödinger equation or some other equation? Many ideas in these directions have been discussed by Poirier and collaborators [43, 44, 45, 46, 47, 48].

Finally, we mention that we find the perturbed Newton's equations appearing in BOMCA to be fascinating. As mentioned above, from the path integral approach it emerges that the BOMCA equations are not unique, and we would like a way to select the version that emerges directly from the Schrödinger equation in section 2. We strongly suspect this to be related to some symmetry structure (recall that the underlying Newton's equations are Hamiltonian), but have not yet found this structure. Understanding this might give us clues as to how to find nonperturbative BOMCA trajectories, that is trajectories that when used in (8) give exact answers. In addition to these challenging, long-term goals, there is much to be done in seeking solutions of the first order BOMCA equations for specific systems and understanding, for example, the difference between the behavior of complex WKB and BOMCA near caustics.

Acknowledgements

J.S. wishes to thank David Kessler and Harry Dym for many useful discussions. Much of this work was done while J.S. was on sabbatical leave in the Departments of Mathematics

and Chemical Physics at the Weizmann Institute. This work was supported by the Israel Science Foundation (576/04).

Appendix A: Derivation of the classical wave function in the multidimensional case

In this appendix we derive the multidimensional form of the classical wave function as described in the introduction and in section 3, see equations (84),(85), (86) and the text around them. The result differs slightly from standard results, specifically in the initial conditions obeyed by the classical paths (84) and the function U (86), and in any case the relevant calculations in the multidimensional case do not seem to have made it into most of the existing texts on path integration techniques, so we see fit to give at least the key details of the derivation.

We start from the path integral in the form

$$\psi(\mathbf{X},T)=\int D\mathbf{x}\exp\left(\frac{i}{\hbar}(S[\mathbf{x}]+S^{\rm init}(\mathbf{x}(0)))\right)\ ,$$

where the integration is over all paths with $\mathbf{x}(T)=\mathbf{X}$. We use, in this appendix, an action of the form

$$S[\mathbf{x}]=\int_0^T\frac{1}{2}\sum_{i=1}^d m_i\dot{x}_i(t)^2-V(\mathbf{x}(t))\ dt\ ,$$

with a diagonal mass matrix; the case of a general mass matrix can be treated similarly. In the main text we quote results assuming all the masses m_i to be equal. We start by replacing $\mathbf{x}$ by $\mathbf{x}+\varepsilon$ in the exponent and expanding to second order. Requiring the linear terms in ε to vanish gives the classical equation of motion as well as the inital condition for $\mathbf{x}$ (84). The remaining terms give the approximation

$$\psi(\mathbf{X},T)\approx\sum e^{iS[\mathbf{x}]/\hbar}\psi_0(\mathbf{x}(0)\int D\varepsilon\ e^{Q[\varepsilon]}$$

where

$$\begin{aligned}Q[\varepsilon]\ &=\ \frac{i}{2\hbar}\left(\int_0^T\sum_{i=1}^d m_i\dot{\varepsilon}_i(t)^2-\sum_{i=1}^d\sum_{j=1}^d H(V)_{ij}(\mathbf{x}(t))\varepsilon_i(t)\varepsilon_j(t)dt\right.\\&\qquad\left.+\sum_{i=1}^d\sum_{j=1}^d H(S^{\rm init})_{ij}(\mathbf{x}(0))\varepsilon_i(0)\varepsilon_j(0)\right)\ .\end{aligned}$$

Here $H(V)$ and $H(S^{\rm init})$ denote the matrices of second derivatives of V and $S^{\rm init}$ respectively. We proceed by discretizing the integrals in $Q[\varepsilon]$. Bearing in mind that $\varepsilon(T)=0$ and using

the trapezium rule we have

$$\begin{aligned}\int_0^T H(V)_{ij}(\mathbf{x}(t))\varepsilon_i(t)\varepsilon_j(t)dt &\approx \frac{T}{2N}H(V)_{ij}(\mathbf{x}(0))\varepsilon_i(0)\varepsilon_j(0) \\ &\quad +\frac{T}{N}\sum_{r=1}^{N-1} H(V)_{ij}\left(\mathbf{x}\left(\frac{rT}{N}\right)\right)\varepsilon_i\left(\frac{rT}{N}\right)\varepsilon_j\left(\frac{rT}{N}\right) .\end{aligned}$$

Using a forward difference approximation for the derivative of $\varepsilon(t)$ and a "leftbox" type approximation for the relevant integral gives the approximation

$$\int_0^T \dot{\varepsilon}_i(t)^2 dt \approx \frac{N}{T}\left(\varepsilon_i(0)^2 + 2\sum_{r=1}^{N-1}\varepsilon_i\left(\frac{rT}{N}\right)^2 - 2\sum_{r=0}^{N-2}\varepsilon_i\left(\frac{rT}{N}\right)\varepsilon_i\left(\frac{(r+1)T}{N}\right)\right) .$$

(Although this would appear to be a first order approximation, since both the methods for constructing the derivative and computing the integral are first order, it is actually second order; the first order errors in the methods exactly cancel each other.) Putting this all together gives:

$$Q[\varepsilon] \approx \frac{iN}{2\hbar T}\Delta\begin{pmatrix} M+F_0 & -M & 0 & 0 & 0 & \dots \\ -M & 2M+F_1 & -M & 0 & 0 & \dots \\ 0 & -M & 2M+F_2 & -M & 0 & \\ 0 & 0 & -M & 2M+F_3 & -M & \\ \vdots & \vdots & & \ddots & \ddots & \\ & & & & -M & 2M+F_{N-1} \end{pmatrix}\Delta^T .$$

Here $\Delta = (\,\varepsilon(0) \quad \varepsilon(T/N) \quad \varepsilon(2T/N) \quad \dots\,)$. Each entry in the matrix in the previous equation is a $d \times d$ block matrix. M denotes the diagonal matrix with entries m_i, and the matrices F_r are defined by

$$\begin{aligned}(F_0)_{ij} &= \frac{T}{N}H(S^{\text{init}})_{ij}(\mathbf{x}(0)) - \frac{T^2}{2N^2}H(V)_{ij}(\mathbf{x}(0)) , \\ (F_r)_{ij} &= -\frac{T^2}{N^2}H(V)_{ij}\left(\mathbf{x}\left(\frac{rT}{N}\right)\right) , \qquad r = 1, \dots, N-1 .\end{aligned}$$

As a final step in the simplification of $Q[\varepsilon]$, we factor out factors of $\sqrt{M}$ on the right and the left from each block in the above matrix. In this way we obtain

$$Q[\varepsilon] \approx \frac{iN}{2\hbar T}\Delta\sqrt{\mathcal{M}}\begin{pmatrix} I+G_0 & -I & 0 & 0 & 0 & \dots \\ -I & 2I+G_1 & -I & 0 & 0 & \dots \\ 0 & -I & 2I+G_2 & -I & 0 & \\ 0 & 0 & -I & 2I+G_3 & -I & \\ \vdots & \vdots & & \ddots & \ddots & \\ & & & & -I & 2I+G_{N-1} \end{pmatrix}\sqrt{\mathcal{M}}\Delta^T . \tag{150}$$

where the matrix $\mathcal{M}$ is a diagonal matrix with N copies of M on its main diagonal, and the matrices G_r are defined by

$$\begin{aligned}(G_0)_{ij} &= \frac{1}{\sqrt{m_i m_j}}\left(\frac{T}{N}H(S^{\text{init}})_{ij}(\mathbf{x}(0)) - \frac{T^2}{2N^2}H(V)_{ij}(\mathbf{x}(0))\right) ,\\ (G_r)_{ij} &= -\frac{1}{\sqrt{m_i m_j}}\frac{T^2}{N^2}H(V)_{ij}\left(\mathbf{x}\left(\frac{rT}{N}\right)\right) , \qquad r = 1,\ldots,N-1 .\end{aligned}$$

It remains to compute the determinant of the matrix in (150). To do this, we first apply block Gaussian elimination [62] to eliminate the blocks under the leading block diagonal, a process that does not affect the determinant. This gives a matrix of the form

$$\begin{pmatrix} P_0 & -I & 0 & 0 & 0 & \ldots \\ 0 & P_1 & -I & 0 & 0 & \ldots \\ 0 & 0 & P_2 & -I & 0 & \\ 0 & 0 & 0 & P_3 & -I & \\ \vdots & \vdots & & \ddots & \ddots & \\ & & & & 0 & P_{N-1} \end{pmatrix}$$

where

$$\begin{aligned} P_0 &= I + G_0 ,\\ P_1 &= 2I + G_1 - P_0^{-1} ,\\ P_2 &= 2I + G_2 - P_1^{-1} ,\\ &\vdots \\ P_{N-1} &= 2I + G_{N-1} - P_{N-2}^{-1} .\end{aligned}$$

We wish to find $\det(P_0 P_1 P_2 \ldots P_{N-1})$. Define the matrices R_r, $r = 0,\ldots,N-1$, by $R_r = P_0 P_1 P_2 \ldots P_r$. Then we have

$$\begin{aligned} R_0 &= I + G_0 ,\\ R_1 &= (I+G_0)(2I+G_1) - I = I + 2G_0 + G_1 + G_0 G_1 \end{aligned}$$

and for $2 \le r \le N-1$:

$$R_r = R_{r-2}P_{r-1}P_r = R_{r-2}\left(P_{r-1}(2I+G_r) - I\right) = R_{r-1}(2I+G_r) - R_{r-2}$$

Rewriting the last equation, for $2 \le r \le N-1$ we have

$$\frac{R_r - 2R_{r-1} + R_{r-2}}{(T/N)^2} = R_{r-1}\frac{N^2}{T^2}G_r .$$

Taking the limit now as $N \to \infty$, we see that the sequence of matrices $R_0, R_1, \ldots, R_{N-1}$ is replaced by a function $R(t)$, defined by

$$\ddot{R}(t) = R(t)G(t) \ , \qquad \text{where} \ \ G_{ij}(t) = -\frac{1}{\sqrt{m_i m_j}} H(V)_{ij}(\mathbf{x}(t)) \ ,$$

supplemented with the initial conditions

$$R(0) = I \ , \qquad \dot{R}_{ij}(0) = \frac{1}{\sqrt{m_i m_j}} H(S^{\text{init}})_{ij}(\mathbf{x}(0)) \ .$$

Finally, we write $U(t) = R(t)^T$. Taking the transpose of all the equations above we see that $U(t)$ satisfies

$$\ddot{U}(t) = G(t)U(t) \ , \qquad U(0) = I, \ \ \dot{U}_{ij}(0) = \frac{1}{\sqrt{m_i m_j}} H(S^{\text{init}})_{ij}(\mathbf{x}(0)) \ .$$

The determinant of the matrix in (150) is simply $\det U(T)$, and (after checking the case of the free particle to fix the normalization) we deduce that

$$\psi(\mathbf{X}, T) \approx \sum \frac{e^{iS[\mathbf{x}]/\hbar} \psi_0(\mathbf{x}(0)}{\sqrt{\det U(T)}} \ .$$

as required.

References

[1] Y.Goldfarb, I.Degani and D.J.Tannor, J.Chem.Phys. **125** 231103 (2006). See also A.S.Sanz and S.Miret-Artés, J.Chem.Phys. **127** 197101 (2007); Y.Goldfarb, I.Degani and D.J.Tannor, J.Chem.Phys. **127** 197102 (2007).

[2] Y.Goldfarb and D.J.Tannor, J.Chem.Phys. **127** 161101 (2007).

[3] Y.Goldfarb, J.Schiff and D.J.Tannor, J.Chem.Phys. **128** 164114 (2008).

[4] R.A.Leacock and M.J.Padgett, Phys.Rev.D **28** (1983) 2491.

[5] M.V.John, Found.Phys.Lett. **15** (2002) 319.

[6] J.H.Van Vleck, Proc.Math.Acad.Sci.USA **14** (1928) 178.

[7] R.N.P.Maia, F.Nicacio, R.O.Vallejos and F.Toscano, Phys.Rev.Lett. **100** (2008) 184102.

[8] E.Kluk, M.F.Herman and H.L.Davis, J.Chem.Phys.**84** (1986) 326.

[9] R.E.Wyatt, *Quantum Dynamics with Trajectories*, Springer (2005).

[10] P.R.Holland, *The Quantum Theory of Motion: An Account of the de Broglie-Bohm Causal Interpretation of Quantum Mechanics*, Cambridge University Press (1993).

[11] J.R.Klauder, Phys.Rev.D **19** (1979) 2349.

[12] J.R.Klauder, Ann.Phys. **180** (1987) 108.

[13] Y.Weissman, J.Chem.Phys. **76** (1982) 4067.

[14] S.Adachi, Ann.Phys.**195** (1989) 45.

[15] A.L.Xavier Jr. and M.A.M.de Aguiar, Ann.Phys. **252** (1996) 458.

[16] A.L.Xavier Jr. and M.A.M.de Aguiar, Phys.Rev.A **54** (1996) 1808.

[17] A.L.Xavier Jr. and M.A.M.de Aguiar, Phys.Rev.Lett. **79** (1997) 3323.

[18] T.Van Voorhis and E.J.Heller, Phys.Rev.A **66** (2002) 050501.

[19] T.Van Voorhis and E.J.Heller, J.Chem.Phys. **199** (2003) 12153.

[20] A.D.Ribeiro, M.A.M.de Aguiar, and M.Baranger, Phys.Rev.E **69** (2004) 066204.

[21] M.Baranger, M.A.M.de Aguiar, F.Keck, H.J.Korsch and B.Schellhaaß, J.Phys.A: Math.Gen. **34** (2001) 7227-7286. See also F.Grossman and M.F.Herman, J.Phys.A: Math.Gen. **35** (2002) 9489; M.Baranger, M.A.M.de Aguiar, F.Keck, H.J.Korsch and B.Schellhaaß, J.Phys.A:Math.Gen. **35** (2002) 9493; M.Baranger, M.A.M.de Aguiar and H.J.Korsch, J.Phys.A:Math.Gen. **36** (2003) 9795.

[22] J. Stine, R.A. Marcus, Chem. Phys. Lett. **15** (1972) 536.

[23] W.H.Miller and T.F.George, J.Chem.Phys, **56** (1972) 5668.

[24] T.F.George and W.H.Miller, J.Chem.Phys, **56** (1972) 5722.

[25] T.F.George and W.H.Miller, J.Chem.Phys, **57** (1972) 2458.

[26] A.Shudo and K.S.Ikeda, Phys.Rev.Lett. **74** (1995) 682.

[27] M.Kuś, F.Haake and D.Delande, Phys.Rev.Lett. **71** (1993) 2167.

[28] D.Huber and E.J.Heller, J.Chem.Phys. **87** (1987) 5302.

[29] D.Huber, E.J.Heller and R.G.Littlejohn, J.Chem.Phys.**89** (1988) 2003.

[30] M.Boiron and M.Lombardi, J.Chem.Phys. **108** (1998) 3431.

[31] M.A.M de Aguiar, M.Baranger, L.Jaubert, F.Parisio and A.D.Ribeiro, J.Phys.A: Math.Gen. **38** (2005) 4645.

[32] F.Parisio and M.A.M. de Aguiar, J.Phys.A:Math.Gen. **38** (2005) 9317.

[33] M.Novaes and M.A.M. de Aguiar, Phys.Rev.A **72** (2005) 032105.

[34] C.C.Chou and R.E.Wyatt, Phys.Rev.A **76** (2007) 012115.

[35] A.S.Sanz and S.Miret-Artés, Chem.Phys.Lett. **445** (2007) 350.

[36] L.O'Raifeartaigh and A.Wipf, Found.Phys. **18** 307 (1988).

[37] P.Bracken, arXiv:math-ph/0608011 (2006).

[38] A.D.Gorman, Appl.Math.Lett **10** (1997) 33.

[39] I.M.Suarez Barnes, M.Nauenberg, M.Nockleby and S.Tomsovic Phys.Rev.Lett. **71** (1993) 1961.

[40] C.M.Bender, D.C.Brody and D.W.Hook, arXiv:0804.4169 (2008)

[41] T.Shnerb and K.G.Kay, Nonlinear Dyn. **42** (2005) 165.

[42] T.Shnerb and K.G.Kay, Phys.Rev.E **73** (2006) 046202.

[43] B.Poirier, J.Chem.Phys. **121** (2004) 4501.

[44] C.Trahan and B.Poirier, J.Chem.Phys. **124** (2006) 034115.

[45] C.Trahan and B.Poirier J.Chem.Phys. **124** (2006) 034116.

[46] B.Poirier and G.Parlant, J.Phys.Chem. **A 111** (2007) 10400.

[47] B.Poirier, arXiv:0803.0143 (2008).

[48] B.Poirier, *Reconciling semiclassical and Bohmian mechanics: VI. Multidimensional dynamics*, preprint (2008).

[49] C.J. Trahan, K.Hughes, R.E. Wyatt, J.Chem.Phys. **118** (2003) 9911.

[50] Y.Goldfarb, J.Schiff and D.J.Tannor, J.Phys.Chem.A **111** (2007) 10416.

[51] H.Abou-Kandil, G.Freiling, V.Ionescu and G.Jank, *Matrix Riccati Equations in Control and Systems Theory*, Birkhäuser Basel (2003).

[52] J.Schiff and S.Shnider, SIAM J.Numer.Anal. **36** (1999) 1392.

[53] M.S.Child, *Semiclassical Mechanics with Molecular Applications*, Clarendon Press, Oxford (1991).

[54] R.G.Littlejohn, Phys.Rev.Lett. **54** (1985) 1742.

[55] A.D.Ribeiro and M.A.M.de Aguiar, Ann.Phys. **323** (2008) 654.

[56] A.D.Ribeiro, M.Novaes and M.A.M.de Aguiar, Phys.Rev.Lett.**95** (2005) 050405.

[57] J.Schiff, in preparation.

[58] W.H.Miller, Adv.Chem.Phys. **25** (1974) 69.

[59] J.Schiff, Y.Goldfarb and D.Tannor, in preparation.

[60] `http://en.wikipedia.org/wiki/Gaussian_integral`

[61] I.M.Gelf'and, A.M.Yaglom, J.Math.Phys. **1** (1960) 48.

[62] H.Dym, *Linear Algebra in Action*, American Mathematical Society (1996).