A Path Integral Approach to BOMCA

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Outline

1. Complex trajectory techniques and questions
   - Complex WKB
   - BOMCA
   - Questions
2. Path Integral Approaches and solutions
   - Don't ignore the form of the initial wave function
   - PI derivation of Complex WKB
   - Taylor series are not the only approximations
   - PI derivation of BOMCA
   - Solutions.

Trajectory techniques for the CQHJE

Start with the TDSE

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

Substitute

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

Get the CQHJE

$$S_t + \frac{1}{2m}S_x^2 + V(x) = \frac{i\hbar}{2m}S_{xx} \ .$$

Want to use a trajectory method for this as it's a perturbation of classical HJE.

Complex WKB

Method 1: Expand S in powers of $\hbar$:

$$S = S_0 + S_1\hbar + S_2\hbar^2 + \dots$$

(assume $S_0(x,0) = S(x,0)$ and $S_1(x,0) = S_2(x,0) = \dots = 0$). Can compute $S_0(X,T), S_1(X,T), S_2(X,T), \dots$ by integrating down *complex trajectories* $x(t)$ satisfying

$$m\ddot{x} + V'(x) = 0\ , \quad m\dot{x}(0) = S_0'(x,0)\ , \quad x(T) = X\ .$$

Complex WKB

Along the trajectory S_0' is identified with $m\dot{x}$. To get S_0:

$$\frac{dS_0}{dt} = \frac{1}{2}m\dot{x}^2 - V(x) \ .$$

To get S_1:

$$\begin{aligned}\frac{dS_1}{dt} &= \frac{i}{2m}S_0'' \ , \\ \frac{dS_0''}{dt} &= -V'' - \frac{1}{m}(S_0'')^2 \ .\end{aligned}$$

To get S_2:

Complex WKB

$$\begin{aligned}
\frac{dS_2}{dt} &= -\frac{1}{2m}(S_1')^2 + \frac{i}{2m}S_1'' \, , \\
\frac{dS_1'}{dt} &= \frac{i}{2m}S_0''' - \frac{1}{m}S_0''S_1' \, , \\
\frac{dS_1''}{dt} &= \frac{i}{2m}S_0'''' - \frac{1}{m}S_0'''S_1' - \frac{2}{m}S_0''S_1'' \, , \\
\frac{dS_0'''}{dt} &= -V''' - \frac{3}{m}S_0''S_0''' \, , \\
\frac{dS_0''''}{dt} &= -V'''' - \frac{4}{m}S_0''S_0''''' - \frac{3}{m}(S_0''')^2 \, .
\end{aligned}$$

etc.

Complex WKB

Numerical observations: This can work to get the wave function. Sometimes a single contributing trajectory, sometimes more than one, sometimes trajectories with very large contributions that must be discarded.

BOMCA

Method 2: Recall the CQHJE

$$S_t + \frac{1}{2m} S_x^2 + V(x) = \frac{i\hbar}{2m} S_{xx} \ .$$

Consider complex trajectories defined by

$$m \frac{dx}{dt} = S_x$$

BOMCA

Along these trajectories we have

$$
\begin{aligned}
\frac{dS}{dt} &= \frac{1}{2}m\dot{x}^2 - V(x) + \frac{i\hbar}{2m}S'' \ , \\
\frac{dS'}{dt} &= -V' + \frac{i\hbar}{2m}S''' \ , \\
\frac{dS''}{dt} &= -V'' - \frac{1}{m}(S')^2 + \frac{i\hbar}{2m}S'''', \\
\frac{dS'''}{dt} &= -V''' - \frac{3}{m}S''S''' + \frac{i\hbar}{2m}S''''' \ , \\
\frac{dS''''}{dt} &= -V'''' - \frac{4}{m}S''S'''' - \frac{3}{m}(S''')^2 + \frac{i\hbar}{2m}S'''''' \ .
\end{aligned}
$$

BOMCA

The BOMCA approximation: Choose some N and set $S^{(n)} = 0$ for all $n > N$. Get a closed system of equations for x, $S, S', S'', \ldots, S^{(N)}$. Trajectories are nonclassical and depend on N.

A complex analog of DPM.

Numerical observations: This also works, with same proviso about multiple trajectories.

Questions

- Why the need for multiple trajectories?
- Why the need for complex trajectories?
  Can you do just as well with real trajectories?
- What is the approximation scheme in BOMCA?
- What are the BOMCA trajectories?

The Path Integral

$$\psi(X,T) = \int_{-\infty}^{\infty} K(X,x_0,T)\psi(x_0,0)\, dx_0 \ ,$$

where

$$K(X,x_0,T) = \int \mathcal{D}x \ \ e^{iS[x]/\hbar} \ .$$

Integral is over all paths $x(t)$, $0 \le t \le T$, with $x(0) = x_0$, $x(T) = X$. $S[x]$ denotes classical action:

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

The Path Integral, Take 2

We're going to assume

$$\psi(x,0) = \exp\left(\frac{iS^{\text{init}}(x)}{\hbar}\right) , \quad S^{\text{init}} \in \mathbf{C} .$$

Merge the integration over x_0 into the path integral to get

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

Here integration over all paths with $x(T) = X$ — no initial condition.

First variation

Saddle points are points where first variation of exponent vanishes.

$$\begin{aligned} S[x] + S^{\mathrm{init}}(x(0)) &= \int_0^T \frac{1}{2} m\dot{x}^2 - V(x)\, dt + S^{\mathrm{init}}(x(0)) \\ \delta(S[x] + S^{\mathrm{init}}(x(0))) &= \int_0^T m\dot{x}\delta\dot{x} - V'(x)\delta x\, dt + S^{\mathrm{init}\prime}(x(0))\delta x(0) \\ &= \int_0^T \left(-m\ddot{x} - V'(x)\right)\delta x\, dt \\ &\quad + \left(S^{\mathrm{init}\prime}(x(0)) - m\dot{x}(0)\right)\delta x(0)\,. \end{aligned}$$

Need $m\ddot{x} + V'(x) = 0$ and $m\dot{x}(0) = S^{\mathrm{init}\prime}(x(0))$.

PI Derivation of Complex WKB

Expand the PI around saddle points, i.e. classical paths with $m\dot{x}(0) = S^{\text{init}\prime}(x(0))$ and $x(T) = X$. To leading order (keep quadratic terms):

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

$$\exp\left(\frac{i}{2h}\left(\int_0^T m\dot{\epsilon}^2 - V''(x(t))\epsilon^2 \, dt + S^{\text{init}\prime\prime}(x(0))\epsilon(0)^2\right)\right) \; .$$

PI Derivation of Complex WKB

Do the Gaussian integral (discretize): Get *classical wave function*

$$\psi(X,T) \approx \sum \frac{\exp\left(\frac{iS[x]}{\hbar}\right)\psi((x(0),0)}{\sqrt{D(T)}} \; .$$

Here

$$m\ddot{x} + V'(x(t)) = 0 \; , \quad m\dot{x}(0) = S^{\mathrm{init}\prime}(x(0)) \; , \quad x(T) = X \; .$$

$$m\ddot{D} + V''(x(t))D = 0 \; , \quad D(0) = 1 \; , \quad m\dot{D}(0) = S^{\mathrm{init}\prime\prime}(x(0)) \; .$$

PI Derivation of Complex WKB

Keep higher order terms in ϵ. Rescale $\epsilon = \sqrt{\frac{\hbar T}{m}}\delta$. To get first order in $\hbar$ correction need certain ϵ^3 and certain ϵ^4 terms. First order correction is to multiply classical wave function by

$$
\begin{aligned}
1 \quad &+ \quad \frac{i\hbar}{8m^2}\int_0^T dt\; V''''(x(t))\, D(t)^4 \left(\int_t^T \frac{du}{D(u)^2}\right)^2 \\
&+ \quad \frac{i\hbar}{24m^3}\int_0^T\int_0^T dt_1 dt_2\; V'''(x(t_1))\, V'''(x(t_2))\, D(t_1)^3 D(t_2)^3 \\
&\left(3\left(\int_{\max(t_1,t_2)}^T \frac{du}{D(u)^2}\right)\left(\int_{t_1}^T \frac{du}{D(u)^2}\right)\left(\int_{t_2}^T \frac{du}{D(u)^2}\right) + \right. \\
&\left. 2\left(\int_{\max(t_1,t_2)}^T \frac{du}{D(u)^2}\right)^3\right) \quad .
\end{aligned}
$$

PI Derivation of Complex WKB

Note quintuple integral. In fact, this expression is exactly $1 + i\hbar S_2 \approx e^{i\hbar S_2}$ in the complex WKB theory.

Conclusion — complex WKB is (to the appropriate order) equivalent to saddle point approximation of the PI around usual saddle points. Complex WKB is an efficient computation scheme avoiding multiple integrals for higher order terms.

A modification of usual asymptotic analysis

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

Usual approach: function $f(x) = n\log x - x$ has maximum at $x = n$. Expand around this to get

$$n\log x - x = (n\log n - n) - \frac{1}{2n}(x-n)^2 + \frac{1}{3n^2}(x-n)^3 + \ldots$$

For lowest order approx only retain quadratic terms:

$$n! \sim n^n e^{-n}\int_{-\infty}^{\infty} \exp\left(-\frac{1}{2n}(x-n)^2\right)dx = \sqrt{2\pi n}\,n^n e^{-n}\ .$$

A modification of usual asymptotic analysis

Instead of

$$n \log x - x \approx (n \log n - n) - \frac{1}{2n}(x-n)^2$$

use the quadratic approximation

$$n \log x - x \approx (n \log N - N) - \frac{1}{2S}(x-N)^2$$

where $N = n + O(1)$, $S = n + O(1)$. Gives leading order approximation

$$n! \sim N^n e^{-N} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{2S}(x-N)^2\right) dx = \sqrt{2\pi S} N^n e^{-N} .$$

This is just as good as Stirling.

A modification of usual asymptotic analysis

H.O.T.: We have approximated

$$n\log x - x \approx (n\log N - N) - \frac{1}{2S}(x-N)^2$$

But in fact

$$\begin{aligned} n\log x - x &= (n\log N - N) + \left(\frac{n}{N} - 1\right)(x-N) \\ &\quad - \frac{n}{2N^2}(x-N)^2 + \frac{n}{3N^3}(x-N)^3 \\ &\quad - \frac{n}{4N^4}(x-N)^4 + \dots \end{aligned}$$

A modification of usual asymptotic analysis

$$
\begin{aligned}
n! \quad \sim \quad & N^n e^{-N} \int_{-\infty}^{\infty} dx \; \exp\left(-\frac{1}{2S}(x-N)^2\right) \\
& \exp\left(\left(\frac{n}{N}-1\right)(x-N)+\frac{1}{2}\left(\frac{1}{S}-\frac{n}{N^2}\right)(x-N)^2\right. \\
& \left.+\frac{n}{3N^3}(x-N)^3-\frac{n}{4N^4}(x-N)^4+\dots\right) \\
= \quad & \sqrt{S}N^n e^{-N} \int_{-\infty}^{\infty} dy \; e^{-y^2/2} \exp\left(\frac{\sqrt{S}(n-N)}{N}y\right. \\
& \left.+\frac{N^2-Sn}{2N^2}y^2+\frac{nS^{3/2}}{3N^3}y^3-\frac{nS^2}{4N^4}y^4+\dots\right)
\end{aligned}
$$

and we can expand the last exponential in negative powers of n.

A modification of usual asymptotic analysis

First order correction term is

$$n! \sim \sqrt{2\pi S} N^n e^{-N} \left(1 + \frac{Z}{12N^6}\right) ,$$

$$\begin{aligned} Z &= 6N^6 + 10n^2S^3 - 6N^4nS + 6N^4Sn^2 - 12N^5Sn \\ &\quad +6N^6S - 9nS^2N^2 + 12n^2S^2N^2 - 12nS^2N^3 . \end{aligned}$$

Check: for *any* choice of $N = n + O(1)$ and $S = n + O(1)$ this gives first corrected Stirling

$$n! \sim \sqrt{2\pi n} N^n e^{-n} \left(1 + \frac{1}{12n} + \dots\right) .$$

So how to choose S, N? One idea — so that $Z = 0$.

A modification of usual asymptotic analysis

Summary: By replacing

$$n! \sim \sqrt{2\pi n}\; n^n e^{-n}$$

with

$$n! \sim \sqrt{2\pi S}\; N^n e^{-N}$$

where

$$N = n + O(1)\;, \quad S = n + O(1)\;,$$

chosen appropriately, we can make the leading order approximation to the factorial accurate to arbitrary (fixed) order in n^{-1}.

PI derivation of BOMCA

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

Here paths satisfy $x(T) = X$. Replace x by $x + \epsilon$ where x is going to be the path we expand around (analog of N). Quadratic approximation:

$$\begin{aligned} S[x+\epsilon] + S^{\mathrm{init}}(x(0)+\epsilon(0)) \; &= \; S[x] + S^{\mathrm{init}}(x(0)) \\ &+\frac{1}{2}\int_0^T m\dot{\epsilon}^2 - \left(V''(x(t)) + q(t)\right)\epsilon^2 \, dt \\ &+\frac{1}{2}\left(S^{\mathrm{init}\prime\prime}(x(0)) + q(0)\right)\epsilon(0)^2 \; . \end{aligned}$$

q is the analog of S in previous section.

PI derivation of BOMCA

Substantial simplification if we assume $m\dot{x}(0) = S^{\mathrm{init}\prime}(x(0))$ and $q(0) = 0$. Assume q is order $\hbar$ and also that $m\ddot{x} + V'(x)$ is of order $\hbar$. Leading order approximation:

$$\psi(X,T) \approx \sum \frac{\exp\left(\frac{iS[x]}{\hbar}\right)\psi((x(0),0)}{\sqrt{f(T)}} \; .$$

Here

$$m\ddot{x} + V'(x(t)) = O(\hbar)\;, \quad m\dot{x}(0) = S^{\mathrm{init}\prime}(x(0))\;, \quad x(T) = X\;.$$

$$m\ddot{f} + \big(V''(x(t)) + q(t)\big)\, f = 0\;, \quad f(0) = 1\;, \quad m\dot{f}(0) = S^{\mathrm{init}\prime\prime}(x(0))\;.$$

PI derivation of BOMCA

Claims:

- For correct choices of x and q this can be made exact to arbitrary order in $\hbar$.
- One such choice is BOMCA. To get order $\hbar^n$ accuracy here need to retain $S^{(2n+2)}$ in BOMCA.
- BOMCA is doing the calculations with remarkable efficiency.

PI derivation of BOMCA

Summary: Leading order is classical wave function

$$\psi(X,T) \approx \sum \frac{\exp\left(\frac{iS[x]}{\hbar}\right)\psi((x(0),0)}{\sqrt{D(T)}} .$$

$$m\ddot{x} + V'(x(t)) = 0 \ , \quad m\dot{x}(0) = S^{\mathrm{init}\prime}(x(0)) \ , \quad x(T) = X \ .$$

$$m\ddot{D} + V''(x(t))D = 0 \ , \quad D(0) = 1 \ , \quad m\dot{D}(0) = S^{\mathrm{init}\prime\prime}(x(0)) \ .$$

Don't forget $S^{\mathrm{init}}(x) = -i\hbar \ln \psi(x,0)$.

PI derivation of BOMCA

Complex WKB: Get higher accuracy by correcting the formula for the wave function:

$$\psi(X,T) \approx \sum \frac{\exp\left(\frac{iS[x]}{\hbar}\right)\psi((x(0),0)}{\sqrt{D(T)}} \exp\left(i(\hbar S_2 + \hbar^2 S_3 + \ldots)\right) \ .$$

$$m\ddot{x} + V'(x(t)) = 0 \ , \quad m\dot{x}(0) = S^{\mathrm{init}\prime}(x(0)) \ , \quad x(T) = X \ .$$

$$m\ddot{D} + V''(x(t))D = 0 \ , \quad D(0) = 1 \ , \quad m\dot{D}(0) = S^{\mathrm{init}\prime\prime}(x(0)) \ .$$

All the correction terms expressed in terms of x and D.

PI derivation of BOMCA

BOMCA: Get higher accuracy by correcting the definitions of x and D:

$$\psi(X,T) \approx \sum \frac{\exp\left(\frac{iS[x]}{\hbar}\right)\psi((x(0),0)}{\sqrt{D(T)}} \,.$$

$$m\ddot{x} + V'(x(t)) = N(t)\,, \quad m\dot{x}(0) = S^{\mathrm{init}\prime}(x(0))\,, \quad x(T) = X\,.$$

$$m\ddot{D} + \left(V''(x(t)) + q(t)\right) D = 0\,, \quad D(0) = 1\,, \quad m\dot{D}(0) = S^{\mathrm{init}\prime\prime}(x(0))\,.$$

Here $q(t), N(t) = O(\hbar)$, written in terms of x and D.

Why the need for multiple trajectories?

- Mathematically: The saddle point approximation sometimes needs more than one saddle point.
- Physically: To build $\psi(X, T)$ may require information about the initial wave function from different regions in space.
- Our trajectories are classical or near-classical (despite the initial Bohmian velocity). They cross.
- Our results have negative ramifications for those looking to construct Bohmian trajectories in the unipolar setting.

Why the need for complex trajectories? Can you do just as well with real trajectories?

- Mathematically: if you want to use the saddle point tecnnique you have to be willing to go off the real axis.
- The form of the initial wave function dictates real or complex: For WKB-type states $\psi_0(x) = A(x)e^{iS(x)/\hbar}$ with A and S real, can use real; for wave packet-type states $\psi_0(x) = e^{iS(x)/\hbar}$ with S complex, need to use complex states to apply saddle point techniques.

What is the approximation scheme in BOMCA?

- It's an $\hbar$ expansion. More precisely, the single dimensionless small parameter is $\frac{\hbar T}{mL^2}$ where L denotes the typical length scale of the potential (so each derivative of V is depressed by an extra power of L).
- The same appears to be true for DPM.
- Like any semiclassical scheme, BOMCA suffers from caustics associated with merging of trajectories. Details not worked out yet.

What are the BOMCA trajectories?

- Trajectories along which the classical wave function is *exact*. (But be careful — need both x and D.)
- A perturbation of a classical trajectory with built in quantum effects.
- So far only a perturbative definition, a nonperturbative definition would be a significant advance.
- Deep relations with central questions about bipolar/multipolar wave function decompositions (and the question of what PDE each component satisfies).

Thank you

Thank you for listening!