

On the Analytic Continuation of Schrödinger Equation

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Abstract

In recent papers [Yor24] [YH21] the wave function was analytically extended to the positions complex plane, arguing that Quantum Mechanics can be understood as a Complex Stochastic Optimal Control. In this work we study the analytical continuation of the Schrödinger Equation to the complex plane in position and time, how to perform numerical simulations, and the meaning of the results.

1 Dimensionless Schrödinger Equation

We write the Schrödinger Equation in dimensionless variables so we can understand better have a better numerical scheme.

First we choose some scales for our system:

- Length scale L_0 .
- Time scale T_0 .
- Mass scale M_0 .
- Temperature scale Θ_0

and a reference energy E_0 . Then we define the following dimensionless parameters:

$$\varepsilon_t = \frac{\hbar}{T_0 E_0} \tag{1}$$

$$\varepsilon_x^2 = \frac{\hbar^2}{L_0^2 E_0 M_0} \tag{2}$$

$$\varepsilon_\Theta = \frac{E_0}{k_B \Theta_0} \quad (3)$$

The Schrödinger Equation on position basis for single particle is

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi - V\psi \quad (4)$$

in dimensionless ¹ variables this is:

$$i \frac{\partial \psi}{\partial t} = -\frac{\varepsilon_x^2}{2\varepsilon_t} \nabla^2 \psi - \frac{V}{\varepsilon_t} \psi \quad (5)$$

Where we have chosen the mass scale M_0 to be the mass of the single particle. The polar decomposition of the wave function

$$\psi = \sqrt{\rho} e^{iS} \quad (6)$$

can be used on the Schrödinger Equation 5, from which the imaginary part gives a continuity equation:

$$\partial_t \rho + \frac{\varepsilon_x^2}{\varepsilon_t} \partial_l (\rho \partial^l S) = 0 \quad (7)$$

where the velocity field is given by

$$v^l = \frac{\varepsilon_x^2}{\varepsilon_t} \partial^l S \quad (8)$$

The real part of the polar decomposition of 5 gives a Hamilton-Jacobi equation:

$$\partial_t S = -\frac{\varepsilon_x^2}{2\varepsilon_t} (\partial_l S \partial^l S) - \frac{V}{\varepsilon_t} + \frac{\varepsilon_x^2}{2\varepsilon_t} \frac{\partial_l \partial^l \sqrt{\rho}}{\sqrt{\rho}} \quad (9)$$

where the last term is the denominated Quantum potential

As in Classical mechanics we can take the gradient of 9 to obtain the time derivative of the velocity field 8

$$\partial_t \left(\frac{\varepsilon_x^2}{\varepsilon_t} \partial^k S \right) + \frac{\varepsilon_x^2}{\varepsilon_t} (\partial^l S) (\partial_l \frac{\varepsilon_x^2}{\varepsilon_t} \partial^k S) = -\frac{\varepsilon_x^2}{\varepsilon_t} \partial^k \left(\frac{V}{\varepsilon_t} - \frac{\varepsilon_x^2}{2\varepsilon_t} \frac{\partial_l \partial^l \sqrt{\rho}}{\sqrt{\rho}} \right) \quad (10)$$

where we can use the material derivative $\frac{d}{dt} = \frac{\partial}{\partial t} + \frac{\partial x^l}{\partial t} \frac{\partial}{\partial x^l}$ and write the Newtonian equation:

¹Note that the wave function on position space also has units of $L_0^{-d/2}$, such that $\int dx^d |\psi|^2 = 1$ is dimensionless.

$$\frac{dv^k}{dt} = -\frac{\varepsilon_x^2}{\varepsilon_t} \partial^k U \quad (11)$$

From a numerical point of view Schrödinger Equation 5 is easier to solve than the polar form 7 and 9. In Classical Mechanics the Quantum potential does not exist, then it is easier to solve Newton equation 11 for an ensemble of positions and use a Monte Carlo simulation to evaluate mean values:

$$\int dx O \rho = \frac{1}{n} \sum_{i=1}^n O_i \quad (12)$$

where O_i is the observable evaluated on each element of the ensemble of n positions.

2 Grad-Log-Schrödinger Equation

Consider

$$\gamma = \log(\psi) \quad (13)$$

and use the effective inverse mass parameter

$$\sigma_m^2 = \frac{\varepsilon_x^2}{\varepsilon_t} \quad (14)$$

then Schrödinger Equation 5 becomes

$$i\partial_t \gamma = -\frac{\sigma_m^2}{2} (\partial_l \partial^l \gamma + \partial_l \gamma \partial^l \gamma) + \frac{V}{\varepsilon_t} \quad (15)$$

we call this the Log-Schrödinger Equation. Taking the gradient of last equation we obtain

$$\partial_t (\partial^k (-i\sigma_m^2 \gamma)) + \partial^l (-i\sigma_m^2 \gamma) \partial_l (\partial^k (-i\sigma_m^2 \gamma)) = -\sigma_m^2 \partial^k \left(\frac{V}{\varepsilon_t} - \frac{i}{2} \partial_l \partial^l (-i\sigma_m^2 \gamma) \right) \quad (16)$$

we call this the Grad-Log-Schrödinger Equation. Using $\eta^k = -i\sigma_m^2 \partial^k \gamma$ we obtain a Newtonian like equation

$$\frac{d\eta^k}{dt} = -\frac{\sigma_m^2}{\varepsilon_t} \partial^k V + \frac{i\sigma_m^2}{2} \partial_l \partial^l \eta^k \quad (17)$$

but we have to assume a complex velocity

$$\frac{\partial z^k}{\partial t} = \eta^k \quad (18)$$

and the analytical continuation of the potential V [Yor24].

The Newtonian Grad Log Schrödinger equation tells how an ensemble of identical particles moves on the complex plane, where the interaction between the particles comes from the velocity potential $\frac{i\sigma_m^2}{2}\partial_l\partial^l\eta^k$. It is clear that we recover classical mechanics on the complex plane if this interaction is zero, on other cases this is analogous to Bohm's quantum potential, with the difference that is linear, and does not depend on estimating the density of the particles, but directly uses the velocity. Before discussing more about this equation, let's study the Log-Schrödinger Equation 15.

3 Preliminars

3.1 Log-Schrödinger Equation on free particle

For the free particle we have $V = 0$. Let us study the dispersion of a Gaussian wave packet, we begin with the ansatz

$$\gamma = -x^2 f_2(t) - f_0(t) \quad (19)$$

using last equation on 15 we get:

$$\begin{aligned} i \left(-x^2 \dot{f}_2 - \dot{f}_0 \right) &= -\frac{\sigma_m^2}{2} (-2f_2 + 4x^2 f_2^2) \\ \dot{f}_2 &= -2i\sigma_m^2 f_2^2 \end{aligned} \quad (20)$$

$$\dot{f}_0 = i\sigma_m^2 f_2 \quad (21)$$

that gives the known solutions

$$f_2(t) = \frac{f_2}{1 + 2i\sigma_m^2 f_2 t} \quad (22)$$

$$f_0(t) = f_0 + \frac{1}{2} \log(1 + 2i\sigma_m^2 f_2 t) \quad (23)$$

$$\psi(x, t) = \left(\frac{4f_2}{2\pi(1 + 2i\sigma_m^2 f_2 t)^2} \right)^{1/4} e^{\frac{-x^2 f_2}{1 + 2i\sigma_m^2 f_2 t}} \quad (24)$$

where we used $f_0 = -\frac{1}{4} \log\left(\frac{4f_2}{2\pi}\right)$ to normalize the wave function. Note that considering the limit $f_2 \rightarrow \infty$ on equation 22 we have a solution that resembles

the free particle propagator

$$\psi(x, t) = \left(\frac{1}{2\pi (i\sigma_m^2 t)^2} \right)^{1/4} e^{\frac{-x^2}{2i\sigma_m^2 t}} \quad (25)$$

An important result of eq 22 is the wave packet dispersion relation:

$$\frac{1}{4 \operatorname{Re}(f_2(t))} = \frac{(1 - 2\sigma_m^2 \operatorname{Im}(f_2)t)^2 + (2\sigma_m^2 \operatorname{Re}(f_2)t)^2}{4 \operatorname{Re}(f_2)} \quad (26)$$

The "moving" free particle has the ansatz:

$$\gamma = -(x - x_t)^2 f_2(t) - (x - x_t) f_1(t) - f_0(t) \quad (27)$$

where x_t is a function of t alone and \dot{x}_t is a constant. Using last ansatz on 15 we get:

$$i \left(-(x - x_t)^2 \dot{f}_2 - (x - x_t) \dot{f}_1 - \dot{f}_0 + 2(x - x_t) f_2 \dot{x}_t + f_1 \dot{x}_t \right) = -\frac{\sigma_m^2}{2} \left(-2f_2 + 4(x - x_t)^2 f_2^2 + f_1^2 + 4(x - x_t) f_1 f_2 \right) \quad (28)$$

$$\dot{f}_2 = -2i\sigma_m^2 f_2^2 \quad (29)$$

$$\dot{f}_1 = 2f_2 \dot{x}_t - 2i\sigma_m^2 f_1 f_2 \quad (30)$$

$$\dot{f}_0 = -\frac{i\sigma_m^2}{2} (f_1^2 - 2f_2) + f_1 \dot{x}_t \quad (30)$$

that gives the known solutions

$$f_2(t) = \frac{f_2}{1 + 2i\sigma_m^2 f_2 t} \quad (31)$$

$$f_1(t) = \frac{-i}{\sigma_m^2} \dot{x}_t \quad (32)$$

$$f_0(t) = f_0 + \frac{1}{2} \log(1 + 2i\sigma_m^2 f_2 t) - \frac{i}{2\sigma_m^2} \dot{x}_t^2 t \quad (33)$$

$$\psi(x, t) = \left(\frac{4f_2}{2\pi (1 + 2i\sigma_m^2 f_2 t)^2} \right)^{1/4} e^{\frac{-(x-x_t)^2 f_2}{1 + 2i\sigma_m^2 f_2 t} + \frac{i}{\sigma_m^2} \left(\dot{x}_t (x - x_t) + \frac{1}{2} \dot{x}_t^2 t \right)} \quad (34)$$

which has the dispersion relation given by 26

3.2 Log-Schrödinger Equation on harmonic potential

For the harmonic potential we have $V = \frac{m\omega'^2}{2} x'^2$, in dimensionless variables is $V = \frac{x^2 \omega^2}{2} \frac{\varepsilon_t^2}{\varepsilon_x^2} = \frac{x^2 \omega^2 \varepsilon_t}{2\sigma_m^2}$. Which is convenient to rewrite like this:

$$V = \frac{\omega^2 \varepsilon_t}{2\sigma_m^2} \left((x - x_t)^2 + 2(x - x_t)x_t + x_t^2 \right) \quad (35)$$

Considering the ansatz:

$$\gamma = -(x - x_t)^2 f_2(t) - (x - x_t) f_1(t) - f_0(t) \quad (36)$$

where x_t is a function of t alone and \dot{x}_t is not a constant. Using last ansatz on 15 we get:

$$\begin{aligned} i \left(-(x - x_t)^2 \dot{f}_2 - (x - x_t) \dot{f}_1 - \dot{f}_0 + 2(x - x_t) f_2 \dot{x}_t + f_1 \dot{x}_t \right) &= -\frac{\sigma_m^2}{2} \left(-2f_2 + 4(x - x_t)^2 f_2^2 + f_1^2 + 4(x - x_t) f_1 f_2 \right) + \\ &\quad \frac{\omega^2}{2\sigma_m^2} \left((x - x_t)^2 + 2(x - x_t)x_t + x_t^2 \right) \\ f_2 &= -2i\sigma_m^2 f_2^2 + \frac{i\omega^2}{2\sigma_m^2} \end{aligned} \quad (37)$$

$$f_1 = 2f_2 \dot{x}_t - 2i\sigma_m^2 f_1 f_2 + x_t \frac{i\omega^2}{\sigma_m^2} \quad (38)$$

$$\dot{f}_0 = -\frac{i\sigma_m^2}{2} (f_1^2 - 2f_2) + f_1 \dot{x}_t + \frac{i\omega^2}{2\sigma_m^2} x_t^2 \quad (39)$$

that gives the solution known solution

$$\ddot{x}_t = -\omega^2 x_t \quad (40)$$

$$f_2(t) = \frac{\omega}{2\sigma_m^2} \quad (41)$$

$$f_1(t) = -i \frac{\dot{x}_t}{\sigma_m^2} \quad (42)$$

$$f_0(t) = i \frac{\omega t}{2} - i \int dt \left(\frac{\dot{x}_t^2}{2\sigma_m^2} - \frac{\omega^2 x_t^2}{2\sigma_m^2} \right) \quad (43)$$

that is the coherent state solution when $x_t(t) \neq 0$ and the ground state when $x_t = 0$

An alternative solution of eq 37 is given by:

$$\ddot{x}_t = -\omega^2 x_t \quad (44)$$

$$f_2(t) = i \frac{\omega}{2\sigma_m^2} \tan(\omega t + \phi_0) \quad (45)$$

$$f_1(t) = -i \frac{\dot{x}_t}{\sigma_m^2} \quad (46)$$

$$f_0(t) = \frac{1}{2} \log(\cos(\omega t + \phi_0)) - i \int dt \left(\frac{\dot{x}_t^2}{2\sigma_m^2} - \frac{\omega^2 x_t^2}{2\sigma_m^2} \right) \quad (47)$$

making $x_t(t) = 0$ and $\phi_0 = \pi/2$ we have the solution that resembles the harmonic propagator.

Considering ϕ_0 as a complex number, then dispersion relation of eq 44 is

$$\frac{1}{4 \operatorname{Re}(f_2(t))} = \frac{\sigma_m^2}{2\omega \tanh(\operatorname{Im}(\phi_0))} (\cos^2(\omega t + \operatorname{Re}(\phi_0)) + \tanh^2(\operatorname{Im}(\phi_0)) \sin^2(\omega t + \operatorname{Re}(\phi_0))) \quad (48)$$

3.3 Newton Grad Log Schrödinger Equation on free particle

For the free particle in one dimension we have

$$\frac{d\eta}{dt} = \frac{i\sigma_m^2}{2} \partial_t \partial^l \eta \quad (49)$$

and then the cinematic equation for z is

$$z = z_0 + \int_0^t dt \eta(t) \quad (50)$$

If we start from the initial condition

$$\gamma(z, 0) = -z^2 f_2 - f_0 \quad (51)$$

then for each initial position z_0 of the ensemble of particles on the complex plane, we have the initial velocity

$$\eta_0 = 2i\sigma_m^2 f_2 z_0 \quad (52)$$

even more, since $\partial_t \partial^l \eta = 0$, then η_0 is constant, then the cinematic equation becomes

$$z(t) = z_0(1 + 2i\sigma_m^2 f_2 t) \quad (53)$$

in this case the dispersion relation is given by

$$\begin{aligned} \langle z(t) \bar{z}(t) \rangle - \langle z(t) \rangle \langle \bar{z}(t) \rangle &= (\langle z_0 \bar{z}_0 \rangle - \langle z_0 \rangle \langle \bar{z}_0 \rangle) |1 + 2i\sigma_m^2 f_2 t|^2 \\ &= \sigma_0^2 \left((1 - 2\sigma_m^2 \operatorname{Im}(f_2) t)^2 + (2\sigma_m^2 \operatorname{Re}(f_2) t)^2 \right) \end{aligned} \quad (54)$$

which is equal to the dispersion relation [26](#)

The moving free particle has the initial condition

$$\gamma(z, 0) = -(z - a_0)^2 f_2 - (z - a_0) f_1 - f_0 \quad (55)$$

where we use a_0 to indicate a constant complex number, that indicates the center of the distribution, which is different from z_0 , that is the initial condition of each particle on the ensemble.

Then for each initial position z_0 of the ensemble of particles on the complex plane, we have the initial velocity

$$\eta_0 = 2i\sigma_m^2 f_2(z_0 - a_0) + i\sigma_m^2 f_1 \quad (56)$$

again this is constant, then the cinematic equation becomes

$$z(t) = z_0(1 + 2i\sigma_m^2 f_2 t) + i\sigma_m^2 (f_1 - 2f_2 a_0)t \quad (57)$$

even though the mean value changes, we have the same dispersion [54](#).

Note that the velocity

$$\eta = \frac{2i\sigma_m^2 f_2 t z - (i\sigma_m^2 (f_1 - 2f_2 a_0))(1 - 2i\sigma_m^2 f_2 t)}{1 + 2i\sigma_m^2 f_2 t} \quad (58)$$

always follows $\frac{i\sigma_m^2}{2} \partial_t \partial^l \eta = 0$. And the following energy relation holds for each particle

$$\frac{\eta^2}{2} = \frac{\eta_0^2}{2} \quad (59)$$

3.4 Newton Grad Log Schrödinger Equation on harmonic potential

For the particle in one dimensional harmonic potential we have

$$\frac{d\eta}{dt} = -\omega^2 z + \frac{i\sigma_m^2}{2} \partial_t \partial^l \eta \quad (60)$$

using the initial condition

$$\gamma(z, 0) = -(z - a_0)^2 f_2 - (z - a_0) f_1 - f_0 \quad (61)$$

then for each initial position z_0 of the ensemble of particles on the complex plane, we have the initial velocity

$$\eta_0 = 2i\sigma_m^2 f_2(z_0 - a_0) + i\sigma_m^2 f_1 \quad (62)$$

since again we have $\frac{i\sigma_m^2}{2} \partial_t \partial^l \eta = 0$ then the cinematic solution is given by

$$\begin{aligned}
z(t) &= z_0 \cos(\omega t) + \frac{\eta_0}{\omega} \sin(\omega t) \\
&= z_0 \left(\cos(\omega t) + \frac{2i\sigma_m^2 f_2}{\omega} \sin(\omega t) \right) + \frac{i\sigma_m^2 (f_1 - 2f_2 a_0)}{\omega} \sin(\omega t) \quad (63)
\end{aligned}$$

and dispersion relation

$$\sigma^2(t) = \sigma_0^2 \left(\left(\cos(\omega t) - \frac{2\sigma_m^2 \text{Im}(f_2)}{\omega} \sin(\omega t) \right)^2 + \left(\frac{2\sigma_m^2 \text{Re}(f_2)}{\omega} \sin(\omega t) \right)^2 \right) \quad (64)$$

which is equal to the relation 48 once that we recognize

$$\text{Re}(f_2) = \frac{\omega}{2\sigma_m^2} \frac{\cosh(\text{Im}(\phi_0)) \sinh(\text{Im}(\phi_0))}{\cos^2(\text{Re}(\phi_0)) + \sinh^2(\text{Im}(\phi_0))} \quad (65)$$

$$\text{Im}(f_2) = \frac{\omega}{2\sigma_m^2} \frac{\cos(\text{Re}(\phi_0)) \sin(\text{Re}(\phi_0))}{\cos^2(\text{Re}(\phi_0)) + \sinh^2(\text{Im}(\phi_0))} \quad (66)$$

An special case the dispersion relation is when $\text{Im}(f_2) = 0$ and $\text{Re}(f_2) = \frac{\omega}{2\sigma_m^2}$ where we recover the coherent state $\sigma^2(t) = \frac{\sigma_m^2}{2\omega}$, or the ground state when $a_0 = 0$.

As sanity check note the velocity:

$$\eta = \frac{\omega (z(2i\sigma_m^2 f_2 \cos(\omega t) - \omega \sin(\omega t)) + i\sigma_m^2 (f_1 - 2f_2 a_0))}{\omega \cos(\omega t) + 2i\sigma_m^2 f_2 \sin(\omega t)} \quad (67)$$

always follows $\frac{i\sigma_m^2}{2} \partial_t \partial^l \eta = 0$. And the following energy relation holds for each particle

$$\frac{\eta^2}{2} + \frac{\omega^2 z^2}{2} = \frac{\eta_0^2}{2} + \frac{\omega^2 z_0^2}{2} \quad (68)$$

An important result of the Schrödinger equation are the excited eigen states, the solutions are given by:

$$\phi_n(x) = H_n \left(\sqrt{\frac{\omega}{\sigma_m^2}} x \right) e^{-\frac{\omega}{2\sigma_m^2} x^2} \frac{1}{\sqrt{2^n n!}} \left(\frac{\omega}{\pi \sigma_m^2} \right)^{1/4} \quad (69)$$

where H_n are the Hermite polynomials, two important facts about them that we highlight is that have n real zeros and all are distinct, lets call $p_{n,j}$ the zeros of $H_n(x)$ for $j = 1, \dots, n$. Making the change of variable $z \rightarrow \sqrt{\frac{\omega}{\sigma_m^2}} z$, the eigen state of the harmonic oscillator has the velocity:

$$\eta_n = i\omega z - \sum_{j=1}^n \frac{i\omega}{z - p_{n,j}} \quad (70)$$

and acceleration:

$$\frac{d\eta_n}{dt} = -\omega^2 z + \sum_{j=1}^n \frac{\omega^2}{(z - p_{n,j})^3} \quad (71)$$

And the following energy relation holds for each particle

$$\frac{\eta_n^2}{2} + \frac{\omega^2 z^2}{2} + \frac{\omega^2}{2} \left(\sum_{j=1}^n \frac{1}{(z - p_{n,j})^2} \right) = \frac{\eta_0^2}{2} + \frac{\omega^2 z_0^2}{2} + \frac{\omega^2}{2} \left(\sum_{j=1}^n \frac{1}{(z_0 - p_{n,j})^2} \right) \quad (72)$$

We can observe that the nodal points of ϕ_n become poles of η_n , in the case of eigen states this poles are fixed, but in general they will move. Around simple poles we have the following wave function

$$\psi = (x - p(t))\varphi(x, t) \quad (73)$$

where $\varphi(x, t)$ is regular and different from zero in the vicinity of p .

4 Results

From our preliminar analysis we approximate the velocity in complex plane by the following function

$$\eta = \sum_{j=0}^m a_j(t) z^j + b \sum_{j=1}^n \frac{1}{z - p_j(t)} \quad (74)$$

with constant limits m and n . Some important assumptions on eq 74 are:

- The residue for all the poles is the same, and constant.
- The singularities of η can be approximated by simple poles (no branch cuts, poles of higher order, etc).
- The poles number n is constant, no creation or annihilation of them.
- The polynomial part also has a fixed number of elements, but for some times they can get the value 0 without any problem.

If we have an initial wave function $\psi(x, 0)$ from which we want to calculate some mean observables $\langle O(z, \eta) \rangle$, we can use Newton Grad Log Schrödinger equation 17 with the following proposed algorithm:

1. Select an ensemble of N initial positions $z_{0,l} = x_{0,l} + i0$, where $x_{0,l}$ are either random samples of $|\psi(x, 0)|^2$ and weight $w_l = \frac{1}{N}$, or regular grid of points on the domain of $\psi(x, 0)$ and weight it like $w_l = |\psi(x_{0,l}, 0)|^2 \Delta x$.
2. For the ensemble of points calculate the velocity $\eta_{0,l} = -i\sigma_m^2 \partial \log(\psi)$.
3. Make a fit of $\eta_{0,l}$ vs $z_{0,l}$ using a Rational Function approximation, with this is possible to find the poles of $\eta(z, 0)$ and determine the order n **check that all the residues are the same?**. Then write η in the form of eq 74, if wanted is possible to increase the order m at this initial state considering zero values for the extra added terms.
4. Use equation 17 to approximate the acceleration, we use analytical derivatives of our fitted η for the velocity potential.
5. With any integrator of your choice find new values of η and z after an small time step. Update the poles position $p_j(t)$ with equation ?? and calculate the new values of $a_j(t)$ using LSQ method (or other of choice).
6. Go to point 4 until the final time is reached.
7. The mean observable is given by $\langle O(z, \eta) \rangle = \sum_{l=1}^N O(z_{t,l}, \eta_{t,l}) w_l$

References

- [YH21] Ciann-Dong Yang and Shiang-Yi Han. “Extending quantum probability from real axis to complex plane”. In: *Entropy* 23.2 (2021), p. 210.
- [Yor24] Vasil Yordanov. “Complex stochastic optimal control foundation of quantum mechanics”. In: *Physica Scripta* 99.11 (2024), p. 115278.