On the Analytic Continuation of Schrödinger Equation

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Abstract

In resent 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:

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

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

$$\varepsilon_{\Theta} = \frac{E_0}{k_B \Theta_0} \tag{3}$$

The Schrödinger Equation on position basis for single particle is

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

in dimensionless ¹ variables this is:

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

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

$$\psi = \sqrt{\rho}e^{iS} \tag{6}$$

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

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

where the velocity field is given by

$$v^{l} = \frac{\varepsilon_{x}^{2}}{\varepsilon_{t}} \partial^{l} S \tag{8}$$

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

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

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

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.

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

From a numerical point of view Shcrödinger 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:

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

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

2 Grad-Log-Schrödinger Equation

Consider

$$\gamma = \log(\psi) \tag{13}$$

and use the effective inverse mass parameter

$$\sigma_m^2 = \frac{\varepsilon_x^2}{\varepsilon_t} \tag{14}$$

then Schrödinger Equation 5 becomes

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

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

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

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

but we have to assume a complex velocity

$$\frac{\partial z^k}{\partial t} = \eta^k \tag{18}$$

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

The Newtonian Grad Log Shcrödinger equation tells how an ensemble of identical particles moves on the complex plane, where the interaction between the particles comes from the velocitypotential $\frac{i\sigma_m^2}{2}\partial_l\partial^l\eta^k$. 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 Applications

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

$$\gamma = -x^2 f_2(t) - f_0(t) \tag{19}$$

using last equation on 15 we get:

$$i\left(-x^{2}\dot{f}_{2} - \dot{f}_{0}\right) = -\frac{\sigma_{m}^{2}}{2}\left(-2f_{2} + 4x^{2}f_{2}^{2}\right)$$

$$\dot{f}_{2} = -2i\sigma_{m}^{2}f_{2}^{2}$$

$$\dot{f}_{0} = i\sigma_{m}^{2}f_{2}$$
(20)
$$(21)$$

that gives the known solutions

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

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

$$\psi(x,t) = \left(\frac{4f_2}{2\pi \left(1 + 2i\sigma_m^2 f_2 t\right)^2}\right)^{1/4} e^{\frac{-x^2 f_2}{1 + 2i\sigma_m^2 f_2 t}}$$
(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 $f_2 - \infty$ on equation 22 we have a solution that resembles

the free particle propagator

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

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

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

The "moving" free particle has the ansatz:

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

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

$$i\left(-(x-x_t)^2\dot{f}_2 - (x-x_t)\dot{f}_1 - \dot{f}_0 + 2(x-x_t)f_2\dot{x}_t + f_1\dot{x}_t\right) = -\frac{\sigma_m^2}{2}\left(-2f_2 + 4(x-x_t)^2f_2^2 + f_1^2 + 4(x-x_t)f_1f_2\right)$$

$$\dot{f}_2 = -2i\sigma_m^2f_2^2$$

$$\dot{f}_1 = 2f_2\dot{x}_t - 2i\sigma_m^2f_1f_2$$
(2)

$$\dot{f}_2 = -2i\sigma_m^2 f_2^2$$
 (28)
 $\dot{f}_1 = 2f_2\dot{x}_t - 2i\sigma_m^2 f_1 f_2$ (29)

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

that gives the known solutions

$$f_2(t) = \frac{f_2}{1 + 2i\sigma_-^2 f_2 t} \tag{31}$$

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

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

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

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

Considering the ansatz:

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

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

$$\dot{f}_{2} = -2i\sigma_{m}^{2}f_{2}^{2} + \frac{i\omega^{2}}{2\sigma_{m}^{2}}$$
(37)

$$\dot{f}_1 = 2f_2\dot{x}_t - 2i\sigma_m^2 f_1 f_2 + x_t \frac{i\omega^2}{\sigma_m^2}$$
 (38)

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

that gives the solution known solution

$$\ddot{x}_t = -\omega^2 x_t \tag{40}$$

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

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

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

$$\ddot{x}_t = -\omega^2 x_t \tag{44}$$

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

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

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

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

3.3 Newton Grad Log Shcrödinger Equation on free particle

For the free particle in one dimension we have

$$\frac{d\eta}{dt} = \frac{i\sigma_m^2}{2} \partial_l \partial^l \eta \tag{49}$$

and then the cinematic equation for z is

$$z = z_0 + \int_0^t dt \eta(t) \tag{50}$$

If we start from the initial condition

$$\gamma(z,0) = -z^2 f_2 - f_0 \tag{51}$$

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

$$\eta_0 = 2i\sigma_m^2 f_2 z_0 \tag{52}$$

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

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

in this case the dispersion relation is given by

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

which is equal to the dispersion relation 26

The moving free particle has the initial condition

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

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

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

again this is constant, then the cinematic equation becomes

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

even though the mean value changes, we have the same dispersion 54.

3.4 Newton Grad Log Shcrödinger Equation on harmonic potential

For the particle in one dimensional harmonic potential we have

$$\frac{d\eta}{dt} = -\omega^2 z + \frac{i\sigma_m^2}{2} \partial_l \partial^l \eta \tag{58}$$

using the initial condition

$$\gamma(z,0) = -(z - a_0)^2 f_2 - (z - a_0) f_1 - f_0 \tag{59}$$

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

$$\eta_0 = 2i\sigma_m^2 f_2(z_0 - a_0) + i\sigma_m^2 f_1 \tag{60}$$

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

$$z(t) = z_0 \cos(wt) + \frac{\eta_0}{w} \sin(wt)$$

$$= z_0 \left(\cos(\omega t) + \frac{2i\sigma_m^2 f_2}{\omega} \sin(\omega t)\right) + \frac{i\sigma_m^2 (f_1 - 2f_2 a_0)}{\omega} \sin(\omega t) \quad (61)$$

and dispersion relation

$$\sigma^{2}(t) = \sigma_{0}^{2} \left(\left(\cos(\omega t) - \frac{2\sigma_{m}^{2} \operatorname{Im}(f_{2})}{\omega} \sin(\omega t) \right)^{2} + \left(\frac{2\sigma_{m}^{2} \operatorname{Re}(f_{2})}{\omega} \sin(\omega t) \right)^{2} \right)$$
(62)

which is equal to the relation 48 once that we recognize

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

$$Im(f_2) = \frac{\omega}{2\sigma_m^2} \frac{\cos(\operatorname{Re}(\phi_0)) \sin(\operatorname{Re}(\phi_0))}{\cos^2(\operatorname{Re}(\phi_0)) + \sinh^2(\operatorname{Im}(\phi_0))}$$
(63)

$$\operatorname{Im}(f_2) = \frac{\omega}{2\sigma_m^2} \frac{\cos(\operatorname{Re}(\phi_0))\sin(\operatorname{Re}(\phi_0))}{\cos^2(\operatorname{Re}(\phi_0)) + \sinh^2(\operatorname{Im}(\phi_0))}$$
(64)

References

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