

Schrödinger-Langevin Equation and Ion Transport at Nano Scale

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Abstract

Schrödinger-Langevin equation has been constructed for the ion-transport for K-ion channel. The stability of the solutions of this equation has been discussed under various physical situations. This will shed new light on the ion transport at nano-scale as well as the possibility of ion trapping and quantum information processing.

Keywords: Schrödinger-Langevin Equation, Stochastic Mechanics, Lyapunov Stability, Ion Transport at Nano Scale

1. Introduction

Quantum theory was developed to study the behaviour of isolated or closed dynamical system. Here, the time evolution of such a closed system is represented by a one-parameter unitary group in Hilbert space. The notion of Hamiltonian of the closed system is related with the infinitesimal generator of the group. However, if we consider the dynamics of an open quantum system where the energy exchange with the external world is relevant, the important issue is whether framework of quantum theory is adequate for the description of such open system. Several attempts [1-5] have been made to study the dynamics of open quantum system so as to understand diffusion, dissipation and other non-equilibrium phenomena. The framework of stochastic quantization as proposed by Nelson [6] and subsequently developed by other people [7-11] seem to be an attractive procedure to understand the forces which explicitly depend on velocities. Here, the dissipative potential term as well as a random potential term can be incorporated into Schrödinger equation which might incorporate the thermal and statistical influence of the environment or external world. Quantum mechanical version of classical Langevin equation has been developed known as Schrödinger-Langevin equation which describes the irreversible behavior of open quantum system based on Nelson stochastic quantization procedure. Recently, attempts have been made to study the stability of the solutions of S-L Equations [12].

One of the present authors [13] constructed S-L equation for ion transport through ion-channels using the framework of Nelson stochastic quantization. The stability of solutions of this type of S-L equation has been studied in this paper. This will shed new light on the ion transport at nano scale. To start with, we shall discuss general methods to solve non-linear Schrödinger equation in section 4.1. Then we shall apply this technique to find the stability of the solution of our S-L equation in Section 4.2. Finally, the possible implications are discussed in Section 5.

2. Schrödinger-Langevin Equation and its Construction

At first we will explore the idea and construction of Schrödinger-Langevin equation. Quantum mechanics for closed systems is well developed and based on firm footing. It has described so many sub-atomic phenomena in isolation with elegant ease. But in practise most of the systems are open, ie they interact with the environment. Several attempts have been made to incorporate these 'interactions' in the Schrödinger equation by means of some dissipative components. It has been suggested [9] that stochastic mechanics as developed by Nelson, can give us some understanding of how one should treat dissipative forces in terms of quantum dynamics. Here one considers the forces which explicitly depend on velocities. The simplest of those is the frictional force linearly

depending upon velocity. So we are in need for a theory which corresponds to quantized friction. First we will dwell upon the construction of Schrödinger equation in terms of Nelson's stochastic procedure. In this procedure, it is postulated that a kind of Brownian motion agitates all particles of matter. We shall assume that every particle performs a Markov process of the form

$$dx(t) = b(x(t), t)dt + d\omega(t) \tag{1}$$

where $\omega(t)$ is a Wiener process with $\omega(t) - \omega(s)$ independent of $x(r)$ whenever $r \leq s \leq t$. The diffusion coefficient is postulated as $v = \frac{\hbar}{2m}$, where \hbar is the reduced Planck's constant. b is the mean forward velocity and b_* is the mean backward velocity. $u = \frac{b - b_*}{2}$ and $v = \frac{b + b_*}{2}$ are referred to as osmotic velocity and current velocity respectively.

Studying the kinematics of this type of motion, we come to the 1st moment kind of equations

$$\frac{\partial u}{\partial t} = -\frac{\hbar}{2m} \nabla(\nabla \cdot v) - \nabla(v \cdot u) \tag{2}$$

$$\frac{\partial v}{\partial t} = -\frac{1}{m} \nabla V - v \cdot \nabla v + u \cdot \nabla u + \frac{\hbar}{2m} \nabla^2 u \tag{3}$$

where $F = -\nabla V$ is an external force acting on the particle and m is the mass of each particle. We now want to change the dependent variable as $\psi = \exp(R + iS)$. The osmotic velocity can be expressed in terms of a gradient [6]

$$u = v \frac{\nabla \rho}{\rho} = \frac{\hbar}{m} \nabla R \tag{4}$$

where ρ is the density.

Similarly we set the current velocity as a gradient

$$v = \frac{\hbar}{m} \nabla S \tag{5}$$

Keeping these assumptions, the Equations (2) and (3) can be changed into a linear partial differential equation, in fact the Schrödinger equation.

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{\hbar^2}{2m} \nabla^2 \psi + V\psi + \alpha(t)\psi \tag{6}$$

$\alpha(t)$ is an arbitrary constant over time.

To prove this, we can put the expression $\psi = \exp(R + iS)$ in the equation and get,

$$i\hbar \left(\frac{\partial R}{\partial t} + i \frac{\partial S}{\partial t} \right) = \frac{\hbar^2}{2m} \left(\nabla^2 R + i \nabla^2 S + (\nabla R + i \nabla S)^2 \right) + V + \alpha(t)$$

Now taking gradient on each side and separating the real and imaginary part, we come to the 1st moment Equations (2) and (3). Since we differentiate the energy equation over space and come to the force equations, it might not be unique. That is why the arbitrary function $\alpha(t)$ is taken into the equation. By choosing, for each t , the arbitrary constant in S appropriately we can arrange for $\alpha(t)$ to be zero.

Hence the conventional quantum mechanics can be formulated in terms of stochastic processes. We can then use either of the schemes in order to get the information about quantum dynamics.

We shall now see how can we extend stochastic mechanics so as to incorporate velocity dependent forces. Now let us consider the simplest possible velocity dependent frictional force $F_d = -\gamma v$.

Considering this force Equation (3) is modified into

$$\frac{\partial v}{\partial t} = -\frac{1}{m} \nabla V - \gamma v - v \cdot \nabla v + u \cdot \nabla u + \frac{\hbar}{2m} \nabla^2 u \tag{7}$$

Now putting the information $v = \frac{\hbar}{m} \nabla S$ in Equation (7)

we get

$$\frac{\partial v}{\partial t} = -\frac{1}{m} \nabla(V + \hbar \gamma S) - v \cdot \nabla v + u \cdot \nabla u + \frac{\hbar}{2m} \nabla^2 u \tag{8}$$

Now from Equations (2) and (8), by the similar procedure followed previously, we get the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{\hbar^2}{2m} \nabla^2 \psi + (V + \hbar \gamma S)\psi + \alpha(t)\psi \tag{9}$$

Here $S = \frac{1}{2i} \ln \left(\frac{\psi}{\psi^*} \right)$. So Equation (9) becomes

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{\hbar^2}{2m} \nabla^2 \psi + V\psi + \frac{\hbar \gamma}{2i} \ln \left(\frac{\psi}{\psi^*} \right) \psi + \alpha(t)\psi \tag{10}$$

This is one particular type of Schrödinger-Langevin (S-L) equation. One can also introduce other terms in the S-L equation. Here, we will concentrate on this particular S-L equation.

3. Mathematical Foundation of Stability of the Solution

We check the stability of the solution by the method of Lyapunov stability analysis. The solution of a linear equation (in our case linear in time t) is said to be stable if there exists a scalar function $L(x) > 0$ in the neighborhood of the origin such that $\frac{dL}{dt} \leq 0$ in that region. L is called the Lyapunov function. From a physicist's point of view Lyapunov function can be understood as the energy

of the system. We know that for stable equilibrium the potential energy is minimum. So if the total time derivative of the Lyapunov function is negative, it means that the the rate of change of energy is negative, i.e. the energy of the system is tending to it's minimum.

Van & Fülöp *et al.* [12] have taken a non-linear S-L equation of the form

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi + \frac{a_0 \hbar}{2i} \psi \ln \left(\frac{\psi}{\psi^*} \right) \quad (11)$$

Here V is the conservative potential contribution and the non-linear term is the contribution due to the dissipa-

$$\frac{dL}{dt} = -\oint \left[\rho \mathbf{v} \left(\frac{\mathbf{v}^2}{2} + V_q + V - E_s \right) + \frac{\nabla \ln \rho \cdot \nabla \cdot (\rho \mathbf{v})}{4} \right] \cdot dA + \int \rho \mathbf{v} \cdot F_d dV \quad (13)$$

V_q is the quantum potential. Now it is shown that $\frac{dL}{dt}$ is found to be negative providing the second term in the right hand side is negative. Since this term is the rate of change of energy due to the frictional force, it can be taken as negative.

Following Van & Fülöp *et al.*, we take the expectation value of the energy difference of the present and the stationary states as the Lyapunov function. Then we calculate the first variation of L and from that the total time

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi + \frac{a_0 \hbar}{2i} \left[\ln \frac{\psi}{\psi^*} \right] \psi + \frac{\hbar}{2i} \left[\left(\frac{a_1}{\tau_1} \right) \int_0^t \exp \left(-\frac{|t-t'|}{\tau_1} \right) dt' \left(\ln \left(\frac{\psi}{\psi^*} \right) \right) - \left(\frac{a_2}{\tau_2} \right) \int_0^t \exp \left(-\frac{|t-t'|}{\tau_2} \right) dt' \left(\ln \left(\frac{\psi}{\psi^*} \right) \right) \right] \psi \quad (14)$$

Here we will try to find the solution of Equation (14) and check the stability of it by the method of Lyapunov stability analysis.

4.1. Solution of the S-L Equation

We will try to find the solution of (14) following the method developed by Kostin [11] to find the solution of nonlinear Schrodinger-Langevin equation for the poten-

$$\frac{\partial \sigma}{\partial t} = -\frac{1}{2m} \left(\frac{\partial \sigma}{\partial x} \right)^2 - a_0 \sigma - \left[\frac{a_1}{\tau_1} \int_0^t \exp \left(-\frac{|t-t'|}{\tau_1} \right) \sigma dt' - \frac{a_2}{\tau_2} \int_0^t \exp \left(-\frac{|t-t'|}{\tau_2} \right) \sigma dt' \right] \quad (16)$$

From Equation (15) we get

$$\sigma(x, t) = \sigma_0(t)x + \sigma_1(t) \quad (17)$$

From Equation (16) we get

$$\frac{\partial \sigma}{\partial t} = -\frac{1}{2m} \sigma_0^2(t) - a_0 \sigma(x, t) - \left[\frac{a_1}{\tau_1} \int_0^t \exp \left(-\frac{|t-t'|}{\tau_1} \right) \sigma dt' - \frac{a_2}{\tau_2} \int_0^t \exp \left(-\frac{|t-t'|}{\tau_2} \right) \sigma dt' \right] \quad (18)$$

tive frictional force $F_d (= a_0 \mathbf{v})$ where $\mathbf{v} = -\frac{\hbar}{2i} \nabla \ln \left(\frac{\psi}{\psi^*} \right)$ is the velocity.

The Lyapunov function taken as the energy difference between present state and the stationary state, is expressed as

$$L(\rho, \mathbf{v}) = \int \rho \left[\frac{\mathbf{v}^2}{2} + \frac{1}{2} \left(\frac{\nabla \rho}{2\rho} \right)^2 + V - E_s \right] dV \quad (12)$$

where ρ is the probability density and E_s is the energy of the stationary state.

The total time derivative of L is found to be

derivative of L is calculated. The condition for stability can be derived by stating the total time derivative of L to be negative.

4. Schrödinger-Langevin Equation

It has been found that Schrodinger-Langevin equation can be constructed for the case of ionic diffusion along K ion channels [13]. The Schrodinger-Langevin equation describing the ionic diffusion is as follows

tial $V = 0$.

Let the solution be of the form

$$\psi(x, t) = \exp \left(\frac{i}{\hbar} \sigma(x, t) \right) \cdot [\sigma(x, t) \text{ is real}]$$

Putting in the Equation (14) we get

$$\frac{\partial^2 \sigma}{\partial x^2} = 0 \quad (15)$$

For weak non-markovian process, $[a_1, a_2 \ll a_0]$ neglecting the terms in the third bracket

$$\frac{\partial \sigma(x, t)}{\partial t} = -\frac{1}{2m} |\sigma_0|^2 - a_0 \sigma(x, t) \tag{19}$$

From Equation (19) we get

$$\sigma_0(t) = \sigma_0(0) \exp(-a_0 t) \tag{20.1}$$

$$\sigma_0(t) = \sigma_0(0) \exp(-a_0 t) - \exp(-a_0 t) \int_0^t \exp(a_0 s) A(s) ds \tag{21.1}$$

$$\sigma_1(t) = \sigma_1(0) \exp(-a_0 t) - \exp(-a_0 t) \int_0^t \frac{\exp(a_0 s)}{2m} |\sigma_0(s)|^2 ds - \exp(-a_0 t) \int_0^t \exp(a_0 s) B(s) ds \tag{21.2}$$

where A(s) and B(s) are defined as:

$$A(s) = \frac{a_1}{\tau_1} \int_0^s \exp\left(\frac{-|s-t'|}{\tau_1}\right) \sigma_0(t') dt' - \frac{a_2}{\tau_2} \int_0^s \exp\left(\frac{-|s-t'|}{\tau_2}\right) \sigma_0(t') dt' \tag{22.1}$$

$$B(s) = \frac{a_1}{\tau_1} \int_0^s \exp\left(\frac{-|s-t'|}{\tau_1}\right) \sigma_1(t') dt' - \frac{a_2}{\tau_2} \int_0^s \exp\left(\frac{-|s-t'|}{\tau_2}\right) \sigma_1(t') dt' \tag{22.2}$$

Since $\sigma(x, t)$ has linear spacial dependence, the velocity $v = -\frac{i\hbar}{2m} \frac{\partial}{\partial x} \ln\left(\frac{\psi}{\psi^*}\right) = -\frac{1}{m} \frac{\partial}{\partial x} \sigma(x, t)$ and hence the frictional force is independent of x. So we may conclude that frictional force is uniform all over the region and the flow is a steady one.

4.2. Stability Analysis of S-L Equation

In one dimension the S-L equation can be written as

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{\hbar a_0}{2i} \ln\left(\frac{\psi}{\psi^*}\right) \tag{23}$$

The stability condition of which is discussed in section III.

Following the above procedure of stability analysis, we find that the stability condition holds for our S-L equation if the following inequality is satisfied.

$$\int \rho v \cdot F_d dx + \frac{1}{a_0} \left[\frac{a_1}{\tau_1} \int_0^t \exp\left(\frac{-|t-t'|}{\tau_1}\right) \rho v' \cdot F'_d dx dt' - \frac{a_2}{\tau_2} \int_0^t \int_0^t \exp\left(\frac{-|t-t'|}{\tau_2}\right) \rho v' \cdot F'_d dx dt' \right] \leq 0 \tag{24}$$

where $F_d (= a_0 v)$ is the frictional force.

Now the first term is always negative. For weak non-Markovian limit $(a_1, a_2 \ll a_0)$, the term in the third bracket is very small compared to the first term. In this case the above inequality holds. So the equation has stable solution [12].

$$\sigma_1(t) = \sigma_1(0) \exp(-a_0 t) - \exp(-a_0 t) \int_0^t \frac{\exp(a_0 s)}{2m} |\sigma_0(s)|^2 ds \tag{20.2}$$

When the time constants (a_1, a_2) are considerable in comparison with a_0 , ie for strong non-markovian process we cannot neglect the terms in the third bracket. In that case, we find that the solution will be of the form

But for strong non-Markovian cases, there are two possibilities.

1) If the term in the third bracket is itself negative, then the inequality strictly holds.

$$\begin{aligned} & \frac{a_1}{\tau_1} \int_0^t \int_0^t \exp\left(\frac{-|t-t'|}{\tau_1}\right) \rho v' \cdot F'_d dx dt' \\ & \leq \frac{a_2}{\tau_2} \int_0^t \int_0^t \exp\left(\frac{-|t-t'|}{\tau_2}\right) \rho v' \cdot F'_d dx dt' \end{aligned} \tag{25}$$

2) If the term in the bracket is positive, then also the inequality can hold if the magnitude of the first term is greater than that of the term in the bracket.

$$\left| \int \rho v \cdot F_d dx \right| \geq \left| \frac{1}{a_0} \left[\frac{a_1}{\tau_1} \int_0^t \int_0^t \exp\left(\frac{-|t-t'|}{\tau_1}\right) \rho v' \cdot F'_d dx dt' - \frac{a_2}{\tau_2} \int_0^t \int_0^t \exp\left(\frac{-|t-t'|}{\tau_2}\right) \rho v' \cdot F'_d dx dt' \right] \right| \tag{26}$$

From Equation (25) we get the condition for stability as:

$$\frac{a_1}{a_2} \left(\frac{\tau_2}{\tau_1}\right)^2 \leq \frac{\int_0^{\tau_2} \exp(-|s|) \langle v'^2 \rangle ds}{\int_0^{\tau_1} \exp(-|s|) \langle v'^2 \rangle ds} \tag{27}$$

For the case of $\tau_1 = \tau_2$, the condition for stability is

$$a_1 \leq a_2 \tag{28}$$

Generally, let $\tau_2 = n\tau_1$. Where n is a positive real num-

ber. Then

$$\frac{a_1}{a_2} \cdot n^2 \leq \frac{\int_0^{\frac{t}{n\tau_1}} \exp(-|s|) \langle v'^2 \rangle ds}{\int_0^{\frac{t}{\tau_1}} \exp(-|s|) \langle v'^2 \rangle ds} \quad (29)$$

Now previously we have shown that

$v = -\frac{i\hbar}{2m} \frac{\partial}{\partial x} \ln \left(\frac{\psi}{\psi^*} \right) = -\frac{1}{m} \frac{\partial}{\partial x} \sigma(x, t)$. Again from the expression of σ we get $\langle v^2 \rangle = M \exp(-2a_0 S)$ where M is some constant over time. Then we get from the inequality

$$\frac{a_1}{a_2} \leq \frac{1-\beta}{n^2} \quad (30)$$

β is taken to be smaller than 1. where

$$\beta = \exp \left(-\frac{(1+2a_0)t}{n\tau_1} \right)$$

5. Conclusive Remarks

The above stability analysis of our S-L equation for ion transport at nano-scale clearly indicates the following:

- In the weak Non-Markovian limit *i.e.* $a_0 \gg a_1, a_2$, the S-L equation has a stable solution and the process is a reversible Markov process for certain duration of time τ_0 . This clearly shows that Nelson process is realizable in nature atleast in biological domain. This happens in the selectivity filter of K-ion channel.
- In strong Markovian limit where a_1 & a_2 can not be neglected, we can get also stable solutions under the condition given by Equation (30).

It is found from the recent experiments [14] that the ionic oscillations are found in the selectivity filter of K^+ ion channel for a certain duration of time. Real situation demands [15] a stable solution of S-L equation for a certain period. Our analysis confirms the stability of solutions in the weak non-Markovian limit. In the basket region of this channel it clearly shows diffusion of K^+ ions. It means that the S-L equation should also have a stable solution in the strong Markovian limit under a simple proportionality condition $\tau_2 = n\tau_1$. This kind of analysis will be helpful in understanding the behaviours of nano pores and it's applications in biological domain. Our proposal of building S-L equation for ion transport will shed new light not only in the context of nano-scale engineering but also in ion-trapping which is a challeng-

ing issue for quantum entanglement and build up quantum computer.

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