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Quantum Dynamics for Ion Channel Transport, Poisson-Schrödinger Modell

Abstract. *This paper deals with the mathematical model of the ion permeation in potassium channels of biomembrane. Based on the Hamiltons, variational principle was led out to the set of compiling equations describing quantum dynamics of the potassium ion transport; Poisson-Schrödinger equation for electric potential $\varphi(r,t)$, and Schrödinger equation for wave function $\psi(r,t)$. Received the set of equations was formulated in the form of two variational identities. A numerical algorithm of the solution, was proposed, based on the meshles Galerkin approximation.*

Streszczenie. *W pracy przedstawiono model matematyczny przepływu jonów sodu, potasu w kanałach biomembrany komórki żywej. Podano kryterium funkcji działania Lagrange'a dla kompatybilności kwantowego opisu układu. W oparciu o zasadę najmniejszego działania Hamiltona, wyprowadzono sprzężony układ równań opisujący dynamikę transportu jonów; równanie Poissona dla potencjału elektrycznego $\varphi(r,t)$ oraz równanie Shrödingera dla funkcji falowej $\psi(r,t)$. Otrzymany układ równań sformułowano w postaci dwóch tożsamości wariacyjnych Galerkina. Zaproponowano algorytm numeryczny rozwiązania otrzymanych równań oparty o metodę bez siatkowej aproksymacji Galerkina. (**Model Poissona-Schrödinger'a transportu jonów w kanałach biomembrany żywej komórki**)*

Keywords: ion transport, multiscale model, quantum dynamics, Poisson-Shrödinger equation, Hamilton's principle, meshles Galerkin approximation
Słowa kluczowe: transport jonów, model wieloskalowy, dynamika kwantowa, równanie Poissona, równanie Shrödingera, wariacyjne tożsamości całkowe Galerkina, bezsiatkowa aproksymacja Galerkina

Introduction

All living cells are surrounded by a thin cell membrane, which is composed of two layers of phospholipid molecules. The cell membrane acts as a hydrophobic, low dielectric barrier that is impermeable to charged particles such as Na^+,K^+,Cl^+ ions [1]. The transport of ions across the

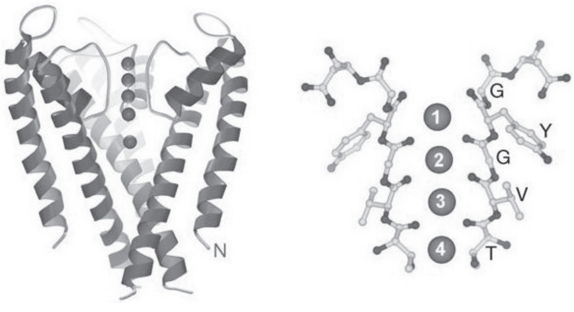

Fig. 1. Schematic representation of the KcsA K^+ channel

cell membrane is regulated by specialized water filled conduits call ion channels. Ion channels are biological subnanotubes formed by protein molecules across the cell membrane, through which ions can freely move in and out when the gates are open and have the character of quantum dynamics [4]. In this paper the Hamilton principle whies the Euler Lagrange theory to the quantum dynamics of ionic transport will be introduced.

Variational Derivation of the Linear Schrödinger Equation

The quantum dynamics of ionic transport is described by the wave function $\psi(x,t)$ satisfying the Schrödinger equation [5] Let $\mathcal{H}$ be complex Hilbert space, the space of complex-valued function $\psi(x,t)$ described on $\mathcal{R}^3$ with the Hermitian inner product $<\cdot,\cdot>$,

$$<\psi_1,\psi_2>=\int \psi_1(x)\overline{\psi_2(x)}dx \tag{1}$$

where the overbear denotes complex conjunction. Consider the Lagrangian density $\mathcal{L}(\psi)$ given by

$$\mathcal{L}(\psi,\overline{\psi})=\frac{i\hbar}{2}\{\frac{\partial\psi}{\partial t}\overline{\psi}-\psi\frac{\partial\overline{\psi}}{\partial t}\}-\overline{\mathcal{H}}\psi\overline{\psi} \tag{2}$$

where $\overline{\mathcal{H}}$ is the Hamiltonian which have following form

$$\overline{\mathcal{H}}\psi=-\frac{\hbar^2}{2m}\nabla^2\psi+V\psi \tag{3}$$

The function $\psi(\mathbf{x},t)=u(\mathbf{x},t)+iv(\mathbf{x},t)$ is a wave function of ions, and m, q the are a mass and the charge of the ions, h is the Planck constant, $\hbar=h/2\pi$. After all, the lagrangian

$$\mathcal{L}(\psi,\overline{\psi})=\frac{i\hbar}{2}\left(\frac{\partial\psi}{\partial t}\overline{\psi}-\psi\frac{\partial\overline{\psi}}{\partial t}\right)- -\frac{\hbar^2}{2m}(\nabla\otimes\psi)\circ(\nabla\otimes\overline{\psi})-V\psi\overline{\psi} \tag{4}$$

The action functional, $S(\psi,\overline{\psi})$ where $\psi,\overline{\psi})$ are taken as independent variables, have a form

$$\begin{aligned} S(\psi,\overline{\psi}) &= \int\int \mathcal{L}(\psi,\overline{\psi})dxdt = \\ &= \int\int\left\{\frac{i\hbar}{2}\left(\frac{\partial\psi}{\partial t}\overline{\psi}-\psi\frac{\partial\overline{\psi}}{\partial t}\right)-\right. \\ &\quad \left.-\frac{\hbar^2}{2m}(\nabla\otimes\psi)\circ(\nabla\otimes\overline{\psi})-V\psi\overline{\psi}\right\}dxdt \end{aligned} \tag{5}$$

Hamiltonian principle states that first variation of the action functional $\delta S(\psi,\overline{\psi})$,

$$\delta S(\psi,\overline{\psi})=0 \tag{6}$$

Now we compute the first variation $\delta S(\psi,\overline{\psi})$,

$$\begin{aligned} \delta S = \int\int\Bigg\{&\left(\frac{\partial\mathcal{L}}{\partial\overline{\psi}}\delta\overline{\psi}+\frac{\partial\mathcal{L}}{\partial\dot{\overline{\psi}}}\delta\dot{\overline{\psi}}+\frac{\partial\mathcal{L}}{\partial(\nabla\otimes\overline{\psi})}\delta(\nabla\otimes\overline{\psi})\right)+ \\ &+\left(\frac{\partial\mathcal{L}}{\partial\overline{\psi}}\delta\overline{\psi}+\frac{\partial\mathcal{L}}{\partial\dot{\overline{\psi}}}\delta\dot{\overline{\psi}}+\frac{\partial\mathcal{L}}{\partial(\nabla\otimes\psi)}\delta(\nabla\otimes\psi)\right)\Bigg\}dxdt \end{aligned} \tag{7}$$

The next step involves the use of integration by parts to second, third, fifth and sixth terms in (7)

$$\begin{aligned} &\int\int\frac{\partial\mathcal{L}}{\partial\dot{\overline{\psi}}}\delta\dot{\overline{\psi}}dxdt=\int\int\frac{\partial\mathcal{L}}{\partial\dot{\overline{\psi}}}\delta\left(\frac{\partial\overline{\psi}}{\partial t}\right)dxdt= \\ &=\int\int\frac{\partial\mathcal{L}}{\partial\dot{\overline{\psi}}}\frac{\partial}{\partial t}\left(\delta\overline{\psi}\right)dxdt=-\int\int\frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\dot{\overline{\psi}}}\right)\delta\overline{\psi}dxdt \end{aligned} \tag{8}$$

For the third and sixth terms we will use the divergence theorem and obtain the following form One should explain that at the integration by parts they omitted boundary therm as the variation $\delta\psi, \delta\overline{\psi}$ vanish at the boundary of the space-time region. Next linking results of integrating we noting that all of the terms are of the form $F_1(\overline{\psi})\delta\overline{\psi} + F_2(\psi)\delta\psi$, where

$$\delta S(\psi, \overline{\psi}) = \int\int\Big\{\Big(\frac{\partial\mathcal{L}}{\partial\overline{\psi}} - \frac{\partial}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{\overline{\psi}}} - \nabla\circ\Big(\frac{\partial\mathcal{L}}{\partial(\nabla\otimes\overline{\psi})}\Big)\Big)\delta\overline{\psi} +$$

$$+\Big(\frac{\partial\mathcal{L}}{\partial\psi} - \frac{\partial}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{\psi}} - \nabla\circ\Big(\frac{\partial\mathcal{L}}{\partial(\nabla\otimes\psi)}\Big)\Big)\delta\psi\Big\}dxdt = 0 \tag{9}$$

According to the fundamental lemma of variational calculus, condition (6) implies the following coupled system of two Euler-Lagrange equations

$$\frac{\partial\mathcal{L}}{\partial\overline{\psi}} - \frac{\partial}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{\overline{\psi}}} - \nabla\circ\Big(\frac{\partial\mathcal{L}}{\partial(\nabla\otimes\overline{\psi})}\Big) = 0 \tag{10}$$

$$\frac{\partial\mathcal{L}}{\partial\psi} - \frac{\partial}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{\psi}} - \nabla\circ\Big(\frac{\partial\mathcal{L}}{\partial(\nabla\otimes\psi)}\Big) = 0 \tag{11}$$

Which after calculate the successive derivatives of the Lagrangian (4), we receive a conjugate set of the Schrödinger equations.

$$i\hbar\frac{\partial\overline{\psi}}{\partial t} = \frac{\hbar^2}{2m}\nabla^2\overline{\psi} - V\overline{\psi}, \quad i\hbar\frac{\partial\psi}{\partial t} = \frac{\hbar^2}{2m}\nabla^2\psi - V\psi \tag{12}$$

The above procedure of the variational scheme we will apply in further analysis to create system of Maxwell-Schödinger equations, describing the interaction of the outside electromagnetic field with quantum dynamics of ionic transport in biomembrane channels [1],[2] .

Lagrangian Structure of Schrödinger-Maxwell's Equations

In this section we will derive a system of Schrodinger Maxwell's equations describing the interacting of ions flux in the channels of lipid bilayers, under interaction of outside electromagnetic field $\mathbf{E}, \mathbf{B}$.

$$\mathbf{E} = -\nabla\otimes\varphi - \frac{\partial\mathbf{A}}{\partial\mathbf{t}}, \quad \mathbf{B} = \nabla\times\mathbf{A} \tag{13}$$

The ions flux will be to take as the quantum particles describing by the wave functions $\Psi(x,t)$. The interaction of the wave function with the electromagnetic field is described by the minimal coupling rule; formally in the Lagrangian density $\mathcal{L}(\psi, \varphi, \mathbf{A})$ the ordinary derivatives, $\frac{\partial}{\partial t}$ and $\nabla\otimes$ are substituted by Weyl covariant derivatives[4] ,[7],

$$\frac{\partial}{\partial t} : \longrightarrow \frac{\partial}{\partial t} + \frac{jq}{\hbar}\varphi; \quad \nabla\otimes : \longrightarrow \nabla\otimes - \frac{jq}{\hbar}\mathbf{A} \tag{14}$$

where $\otimes$ is a symbol of tensor product and q, is the electrical charge. For the complex-valued wave functions $\Psi(x,t) = u(x,t) + jv(x,t)$ belonging to Hilbert space with the Hermitian inner product, (1) the Lagrangian density of the Schrödinger equation (2) for a stream of ions becomes following form,

$$\mathcal{L}_1(\psi, \varphi, \mathbf{A}) = \frac{i\hbar}{2}\Big(\frac{\partial\psi}{\partial t}\overline{\psi} - \psi\frac{\partial\overline{\psi}}{\partial t}\Big) - \frac{\hbar^2}{2m}(\nabla\otimes\psi)\circ(\nabla\otimes\overline{\psi}) -$$

$$-\frac{\hbar^2}{2m}\Big(\nabla\otimes\psi - \frac{jq}{\hbar}\mathbf{A}\psi\Big)\circ\Big(\nabla\otimes\overline{\psi} - \frac{jq}{\hbar}\mathbf{A}\overline{\psi}\Big) - q\psi\overline{\psi} \tag{15}$$

Assuming, that outside field, $\mathbf{E}$ and $\mathbf{A}$ that are not fixed,they aren't determined openly, then to the lagrangian density $\mathcal{L}_1$ we need to add to the lagrangian density of the electromagnetic field $\mathcal{L}_2$, where

$$\mathcal{L}_2(\varphi, \mathbf{A}) = \frac{1}{2}(\mathbf{D}^2 - \mathbf{B}^2) = \tag{16}$$

$$= \frac{1}{2}\Big(\varepsilon(\frac{\partial\mathbf{A}}{\partial t} + \nabla\otimes\varphi)\Big)^2 - \frac{1}{2}\Big(\nabla\otimes\mathbf{A}\Big)^2$$

The total action $\mathcal{S}(\varphi, \psi, \overline{\psi}, \mathbf{A})$ in this case, is a integral from the sum of (15) and (16) $\mathcal{L}_1(\varphi, \psi, \overline{\psi}, \mathbf{A}) + \mathcal{L}_2(\varphi, \psi, \overline{\psi}, \mathbf{A})$.

$$\mathcal{S}(\varphi, \psi, \overline{\psi}, \mathbf{A}) = \int\int\mathcal{L}(\varphi, \psi, \overline{\psi}, \mathbf{A})dxdt = \tag{17}$$

$$= \int\int\Big\{\frac{i\hbar}{2}\Big(\frac{\partial\psi}{\partial t}\overline{\psi} - \psi\frac{\partial\overline{\psi}}{\partial t}\Big) - \frac{\hbar^2}{2m}(\nabla\otimes\psi)\circ(\nabla\otimes\overline{\psi}) -$$

$$-\frac{\hbar^2}{2m}\Big(\nabla\otimes\psi - \frac{jq}{\hbar}\mathbf{A}\psi\Big)\circ\Big(\nabla\otimes\overline{\psi} - \frac{jq}{\hbar}\mathbf{A}\overline{\psi}\Big) - q\psi\overline{\psi}$$

$$+\frac{1}{2}\Big(\varepsilon(\frac{\partial\mathbf{A}}{\partial t} + \nabla\otimes\varphi)\Big)^2 - \frac{1}{2}(\nabla\otimes\mathbf{A})^2\Big\}dxdt$$

The Hamiltonian's principle states that first variation of the action $\delta\mathcal{S}(\phi, \psi, \overline{\psi}, \mathbf{A})$ vaschis,

$$\delta\mathcal{S}(\varphi, \psi, \overline{\psi}, \mathbf{A}) = 0 \tag{18}$$

Taking one by one the first variation of the total action integral $\mathcal{S}(\phi, \psi, \overline{\psi}, \mathbf{A})$ (17) respect to $\delta\varphi$,$\delta\psi$, $\delta\overline{\psi}$ and $\delta_{\mathbf{A}}$ we obtain

$$\delta\mathcal{S} = \int\int\Big\{\Big(\frac{\partial\mathcal{L}}{\partial\psi} - \frac{\partial}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{\psi}} - \nabla\circ\Big(\frac{\partial\mathcal{L}}{\partial(\nabla\otimes\psi)}\Big)\Big)\delta\psi +$$

$$+\Big(\Big(\frac{\partial\mathcal{L}}{\partial\overline{\psi}} - \frac{\partial}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{\overline{\psi}}} - \nabla\circ\Big(\frac{\partial\mathcal{L}}{\partial(\nabla\otimes\overline{\psi})}\Big)\Big)\delta\overline{\psi} +$$

$$+\Big(\frac{\partial\mathcal{L}}{\partial\mathbf{A}} - \frac{\partial}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{\mathbf{A}}} - \nabla\times\frac{\partial\mathcal{L}}{\partial\nabla\times\mathbf{A}}\Big)\circ\delta\mathbf{A} +$$

$$+\Big(\frac{\partial\mathcal{L}}{\partial\varphi} - \nabla\circ\frac{\partial\mathcal{L}}{\partial\nabla\otimes\varphi}\Big)\delta\varphi\Big\}dxdt \tag{19}$$

the set of Eulerabc Lagrange equations, which are the Schrödinger-Maxwell equations.

$$\frac{\partial\mathcal{L}}{\partial\psi} - \frac{\partial}{\partial t}\Big(\frac{\partial\mathcal{L}}{\partial\dot{\psi}}\Big) - \nabla\circ\Big(\frac{\partial\mathcal{L}}{\partial(\nabla\otimes\psi}\Big) = 0 \tag{20}$$

$$\frac{\partial\mathcal{L}}{\partial\overline{\psi}} - \frac{\partial}{\partial t}\Big(\frac{\partial\mathcal{L}}{\partial\dot{\overline{\psi}}}\Big) - \nabla\circ\Big(\frac{\partial\mathcal{L}}{\partial(\nabla\otimes\overline{\psi})}\Big) = 0 \tag{21}$$

$$\frac{\partial\mathcal{L}}{\partial\mathbf{A}} - \frac{\partial}{\partial t}\Big(\frac{\partial\mathcal{L}}{\partial\dot{\mathbf{A}}}\Big) - \nabla\times\Big(\frac{\partial\mathcal{L}}{\partial(\nabla\times\mathbf{A})}\Big) = 0 \tag{22}$$

$$\frac{\partial\mathcal{L}}{\partial\varphi} - \nabla\circ\Big(\frac{\partial\mathcal{L}}{\partial(\nabla\otimes\varphi)}\Big) = 0 \tag{23}$$

Equations (19) and (20) they are the Schrödingers equations for waves function ψ, $\overline{\psi}$; and (21) is the equation for magnetic potential $\mathbf{A}$. Equation (23) is the conection equations of Poisson-Schrödinger type.

After calculation of the respective derivatives for Lagrange density $\mathcal{L}(\varphi, \psi, \overline{\psi}, \mathbf{A})$ we obtain the equations (20)-(23) in the modified form

$$(24)\quad i\hbar\frac{\partial\psi}{\partial t} = \frac{\hbar^2}{2m}\nabla^2\psi + \frac{iq\hbar}{2m}\left(\nabla\otimes\psi - \frac{iq}{\hbar}\mathbf{A}\psi\right)\circ\mathbf{A} - q\varphi\psi$$

$$(25)\quad i\hbar\frac{\partial\overline{\psi}}{\partial t} = \frac{\hbar^2}{2m}\nabla^2\overline{\psi} + \frac{iq\hbar}{2m}\left(\nabla\otimes\overline{\psi} - \frac{iq}{\hbar}\mathbf{A}\overline{\psi}\right)\circ\mathbf{A} - q\varphi\overline{\psi}$$

$$(26)\quad \varepsilon\frac{\partial^2\mathbf{A}}{\partial t^2} = \nabla\times\Big(\nabla\times\mathbf{A}\Big) +$$

$$+\frac{iq\hbar}{2m}\Big((\nabla\otimes\psi)\overline{\psi} + (\nabla\otimes\overline{\psi})\psi\Big) + \frac{q^2}{m}\mathbf{A}\psi\overline{\psi}$$

$$(27)\quad \nabla\circ\Big(\varepsilon\nabla\otimes\varphi\Big) = q\psi\overline{\psi}$$

Exponential Form of Wave Functions

For the exponential form of the wave functions ψ and $\overline{\psi}$

$$(28)\quad \psi(x,t) = u(x,t)e^{jS(x,t)},\ \overline{\psi}(x,t) = u(x,t)e^{-jS(x,t)}$$

where $(u, S) : \mathbf{R^3}\times\mathbf{R}$, and $S(x,t)$ is a function describing the phase angle of the wave function $\psi(x,t)$, Lagrangian density (15), takes the form

$$(29)\quad \mathcal{L}_1(u,\varphi,S,\mathbf{A}) = \frac{1}{2}\bigg\{i\hbar\frac{\partial u}{\partial t}u - \frac{\hbar^2}{2m}(\nabla\otimes u)^2 -$$

$$-\left(\frac{\partial S}{\partial t} + q\varphi + \frac{1}{2m}(\nabla\otimes S - q\mathbf{A})^2\right)u^2\bigg\}$$

The electromagnetic part $\mathcal{L}_2(\varphi, \mathbf{A})$ has the same form as (16) . In this case the function of action $\mathcal{S}(u,\varphi,S,\mathbf{A})$ is given by the expression

$$\mathcal{S}(u,\varphi,S,\mathbf{A}) = \int\int\Big\{\mathcal{L}_1(u,\varphi,S,\mathbf{A}) + \mathcal{L}_2(\varphi,\mathbf{A})\Big\}dxdt$$

Let now compute the first variational of the action function $\delta\mathcal{S}$

$$\delta\mathcal{S} = \int\int\bigg\{\frac{\partial\mathcal{L}}{\partial u}\delta u + \frac{\partial\mathcal{L}}{\partial\dot{u}}\delta\dot{u} + \frac{\partial\mathcal{L}}{\partial(\nabla\otimes u)}\circ\delta(\nabla\otimes u) +$$

$$+\frac{\partial\mathcal{L}}{\partial\dot{S}}\delta\dot{S} + \frac{\partial\mathcal{L}}{\partial(\nabla\otimes S)}\circ\delta(\nabla\otimes S) + \frac{\partial\mathcal{L}}{\partial\mathbf{A}}\circ\delta\mathbf{A} +$$

$$+\frac{\partial\mathcal{L}}{\partial(\nabla\times\mathbf{A})}\circ\delta(\nabla\times\mathbf{A}) + \frac{\partial\mathcal{L}}{\partial\dot{\mathbf{A}}}\circ\delta\dot{\mathbf{A}} +$$

$$(30)\quad +\frac{\partial\mathcal{L}}{\partial\varphi}\delta\varphi + \frac{\partial\mathcal{L}}{\partial(\nabla\otimes\varphi)}\circ\delta(\nabla\otimes\varphi)\bigg\}dxdt$$

Using the divergent theorem and principles of integration by parts, we obtain the following system of equations

$$(31)\quad -\frac{\hbar^2}{2m}\nabla^2 u + \left(\frac{\partial S}{\partial t} + q\varphi + \frac{1}{2m}(\nabla\otimes S) - q\mathbf{A})^2\right)u = 0$$

$$(32)\quad \frac{\partial}{\partial t}(u^2) + \frac{1}{m}\nabla\circ\Big((\nabla\otimes S - q\mathbf{A})u^2\Big) = 0$$

$$(33)\quad \nabla\circ\left(\varepsilon(\frac{\partial\mathbf{A}}{\partial t} + \nabla\otimes\varphi)\right) = -qu^2$$

(34)

$$\nabla\times(\nabla\times\mathbf{A}) = -\frac{\partial}{\partial t}\left(\frac{\partial\mathbf{A}}{\partial t} + \nabla\otimes\varphi\right) + \frac{q}{2m}(\nabla\otimes S - q\mathbf{A})u^2$$

For the static analyze and without external magnetic field we take $u = u(x), \varphi = \varphi(x), \mathbf{A} = 0, S = \omega t = 0,$.

Stationary System of Poisson-Schrödinger Equations

For geometric scheme of ion channel (Fig. 2) system of equations (31)-(34) determine the system boundary conditions of Dirichlet-Neuman type.

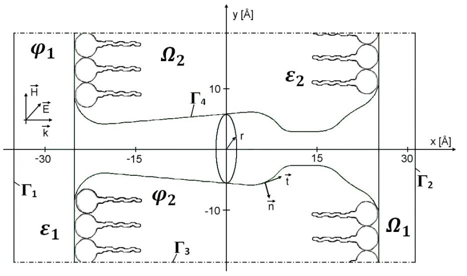

Fig. 2. Schematic representation of border surface of the KcsA K^+ channel

$$(35)\quad -\frac{h^2}{2m}\nabla^2 u + q\varphi u = 0$$

$$(36)\quad \nabla\circ(\varepsilon\nabla\otimes\varphi) = -qu^2$$

It should be noted that equation (35) is static Shrödinger equation and (36) is Poisson equation. Right side of this equation is volume density of electric charge $\rho(x)$, where

$$(37)\quad \rho(x) = -qu^2(x)$$

and q is the charge of ion transport.

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