

# Spin physics and biological membranes

**Yury Kiselev**

Joint Institute for Nuclear Research, VBLHEP, Dubna, 141980, Russia

E-mail: [yury.kiselev@cern.ch](mailto:yury.kiselev@cern.ch)

**Abstract.** Formula for calculating the concentration profile of ions in biological membranes has been obtained. It is assumed that ions are moving in a viscous medium under the action of the electric field and a concentration gradient. The problem is that ions are coated with shells consisting of water dipoles. These dipoles copy the form of the ions and in a strong electric field they can acquire the shape of an ellipsoid which changes the effective ion radius in the membrane. Calculation of the  $\text{Na}^{+1}$  and  $\text{K}^{+1}$  profiles leads to a conclusion that active and passive transport of ions is closely associated with the shape of the hydrated shells. The work was performed at the Veksler and Baldin Laboratory of High Energy Physics, JINR, Dubna.

## 1. Introduction

In solid, liquid and gaseous media the force of the electric field acting on ions is balanced by the friction force proportional to the velocity of particle motion. At equality of forces, the drift velocity of charges is to be proportional to the electric field intensity. In a membrane, this velocity also depends on the concentration gradient, and on a specific membrane feature allowing the so-called active or passive transport of ions. Hereafter, we calculate the profiles of the  $\text{Na}^{+1}$  and  $\text{K}^{+1}$  concentration in a membrane and show that the active or passive transport is determined by the shape of the hydrate shells. The work was performed at the Laboratory of High Energy Physics, JINR, Dubna.

## 2. Concentration profile of ions in a membrane

Before considering the ion motion in a biological membrane we recall the classical scheme of these calculations using the electron gas in metal [1]. At the collision with the ion lattice of metals the electrons give up, on the average, a momentum  $mv$  during the mean interval of the free motion  $\tau$ /(s), where  $m$ /(kg) is the mass, and  $v$ /(m·s<sup>-1</sup>) is the mean drift velocity of electrons. On equating the momentum transfer velocity  $mv/\tau$ /(N) to the electric force  $eE$ /(N) of the electric field  $E$ /(V·m<sup>-1</sup>) acting on the elementary charge  $e$ /(C), results [1] to the equation (1) which is one of the forms of the Ohm law

$$mv/\tau = -eE, \quad (1)$$

from where it follows that the drift velocity  $v$  is proportional to the field intensity  $E$ .

A physical analogy is also preserved in the case when the ions are moving under the action of the electric field in liquid solutions. For a spherical particle of radius  $r$  in a solvent of viscosity  $\eta$ /(kg·m<sup>-1</sup>s<sup>-1</sup>), the friction force is given by Stokes' law  $F_S = 6\pi\eta rv$ , where  $v$  is the velocity of the ion. This time, as in (1), equating of forces gives

$$6\pi\eta rv = zeE, \quad (2)$$



where  $z$  is the ion valence. The velocity  $v$  should be again proportional to the field in a membrane but, in solutions, there is also the thermodynamic force  $F_x/(\text{J}\cdot\text{m}^{-1})$  depending on the gradient of the normalized concentration of ions  $C(x)$  [2]

$$F_x = -kT \left( \frac{\partial \ln C}{\partial x} \right), \quad (3)$$

where  $k = 1.38 \cdot 10^{-23}/(\text{J}\cdot\text{K}^{-1})$  is the Boltzmann constant,  $T/(\text{K})$  is the absolute temperature,  $x/(\text{m})$  is the ion coordinate along the channel;  $0 < x \leq d$ ,  $d$  is the membrane thickness. Adding  $F_x$  and  $v = u \cdot E$  to equation (2), where  $u/(\text{m}^2 \cdot \text{s}^{-1} \cdot \text{V}^{-1})$  is the mobility of the ion, we have

$$6\pi\eta ruE = zeE - kT \left( \frac{\partial \ln C}{\partial x} \right), \quad (4)$$

The electric field is equal to the potential gradient  $E = -\partial\varphi/\partial x$ . Let  $\varphi(x=0) = 0$  be the electrical potential of the solution, then  $\varphi(x=d) = V_r = -(0.05 \div 0.15)$ , where  $V_r/(\text{V})$  is the rest potential of the membrane, and integrating (4) over  $x$  we obtain:

$$\ln C(x) - \ln C(0) = \frac{1}{kT}(ze - 6\pi\eta ru) \int_0^x -d\varphi = \frac{-1}{kT}(ze - 6\pi\eta ru) \left( V_r \frac{x}{d} - 0 \right). \quad (5)$$

The function  $V_r \cdot x/d$ , describes a linear voltage distribution over  $x$ . The mobility  $u$  in (5) is conveniently expressed in terms of the diffusion coefficient  $D/(\text{m}^2 \cdot \text{s}^{-1})$ , since the latter does not depend on the molecular weight of ions. Using the Einstein relation [2]

$$u = \frac{zeD}{kT}, \quad (6)$$

substituting equation (6) into (5), and replacing  $(-(-V_r) = |V_r|)$  we obtain the following formula to calculate the ratio of concentrations

$$\frac{C(x)}{C(0)} = \exp\left\{ \frac{ze|V_r|}{kT} \frac{x}{d} \left( 1 - \frac{6\pi\eta D}{kT} r \right) \right\}. \quad (7)$$

Let the radius  $r$  of the ion at which the expression in the brackets is equal to zero be denoted as  $r_0$ . Without a membrane,  $C(x) = C(0)$ , the ion radius  $r = r_0$  is fixed and it is determined by the Stokes - Einstein formulae [2]

$$r_0 = \frac{kT_0}{6\pi\eta_0 D_0}. \quad (8)$$

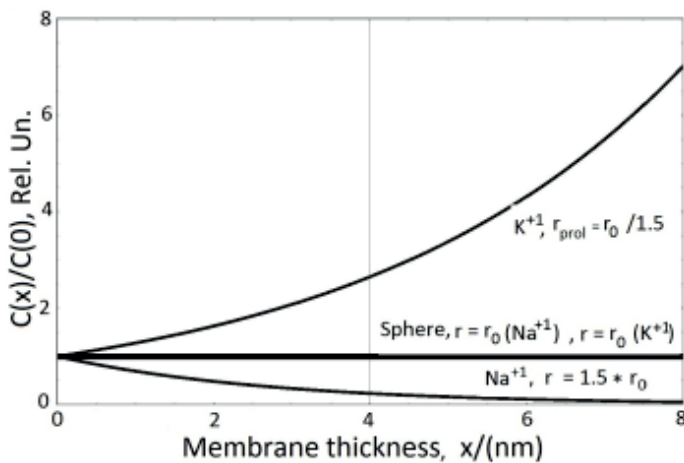
Hence, the ion profile in a solution is the straight line  $C(x)/C(0) = 1$ , shown in Fig 1. Combining formulas (7) and (8) we get the concentration profile in the common case:

$$C(x)/C(0) = \exp\left\{ \frac{ze|V_r|}{kT} \frac{x}{d} \left( 1 - \frac{\eta D T_0}{\eta_0 D_0 T} \frac{r}{r_0} \right) \right\} = \exp\left\{ \frac{ze|V_r|}{kT} \frac{x}{d} \left( 1 - \xi \frac{r}{r_0} \right) \right\}, \quad (9)$$

where  $r$  is the actual radius of an ion in the membrane. In a solution of different viscosity and temperature  $\xi = \eta D T_0 / (\eta_0 D_0 T) = 1$  since the ion radius in (8) is fixed. Assume, for example, that the  $\text{Na}^{+1}$  ions are in the water at  $T_0 = 298/(\text{K})$ . In this case  $\eta_0 = 0.891 \cdot 10^{-3}$ , the diffusion coefficient is  $D_0(\text{Na}^{+1}) = 1.33 \cdot 10^{-9}$  [2]. At the temperature  $T = 309/(\text{K})$ ,  $\eta = 0.699 \cdot 10^{-3}$  [2], and since  $\xi = 1$  we have  $T_0/\eta_0 D_0 = T/\eta D$  and the diffusion coefficient is changed to  $D(\text{Na}^{+1}) = 1.76 \cdot 10^{-9}$ ; however at both temperatures the radius of  $\text{Na}^{+1}$  ions stays the same:  $r = r_0 = 184 \cdot 10^{-12}/(\text{m})$ .

Nevertheless, it is known [3] that the calculation by (8) coincides with the experimentally measured radius with the accuracy up to 2. The problem is that the ions are coated with shells consisting of water dipoles. We illustrate the importance of such complication by the following examples. Let us imagine that the radius of  $\text{Na}^{+1}(z = +1)$  in a membrane is enlarged due to hydration up to  $r = 1.5 \cdot r_0 = 1.5 \times 184 \cdot 10^{-12}$ . The new profile calculated by (9) is presented in Fig. 1. The ion concentration decays along the membrane. This example demonstrates the concentration profile at the passive transport of ions.

In the next example, we consider the  $\text{K}^{+1}(z = +1)$  ion having a larger dipole polarizability compared with the  $\text{Na}^{+1}$  one. Note that dipole and quadrupole interactions of ions with an electric field in membranes are small one to influence any ion motion. The important reason to consider these interactions follows by the fact that the water dipoles copy the shape of the ions. Such complex charge structures are considered in physics of nuclear moments.



**Figure 1.** Concentration profiles of ions. The line is a profile in a solution without a membrane at  $r = r_0$ ; the  $\text{Na}^{+1}$  shows the passive transport at  $r = 1.5 \cdot r_0$ ; the active transport of  $\text{K}^{+1}$  at  $r_p = r_0/1.5$ .

In a strong electric field, these objects can acquire an elliptical shape, and the hydrated shell around an ion has to repeat this shape. Because hydrated shells are ingredients of the solvent, the ellipsoidal objects in a solution have a different friction and therefore the different effective radius compared with the spherical one. This means that the concentration profile, in accordance with (9), is changed. Suppose now that  $r_0 = (a+b)/2$ , where  $2a$  are the length of the major and  $2b$  of minor ellipse axes, respectively. Let  $\text{K}^{+1}$  ion be in the water at  $T_0 = 298/(\text{K})$  then  $\eta_0 = 0.891 \cdot 10^{-3}$ , and since  $D_0(\text{K}^{+1}) = 1.96 \cdot 10^{-9}$  [2] then (8) gives  $r_0 = 125 \cdot 10^{-12}/(\text{m})$ . Assuming that  $a = 195 \cdot 10^{-12}$  and  $b = 55 \cdot 10^{-12}$ , the effective radius of the prolate ellipsoids in a solution is  $r_p \cong (a \cdot b^2)^{1/3} \cong 84 \cdot 10^{-12}$  [2]. Substituting of  $r_p/r_0 = 84/125 \cong 0.67$  and  $\xi = 1$  in (9) gives the concentration profile of  $\text{K}^{+1}$  ion, shown in Fig. 1. This profile displays the active transport of the  $\text{K}^{+1}$  ions. For numeric estimations, it is conveniently to simplify (9) assuming  $\xi = 1$ ,  $x = d$ , which yields

$$\frac{C(x=d)}{C(x=0)} = \exp\left\{\frac{ze|V_r|}{kT} \left(1 - \frac{r}{r_0}\right)\right\}, \quad (10)$$

where  $e/k = 11594/[C/(\text{J} \cdot \text{K}^{-1})]$ ,  $T$  (K). Hence, for the above  $\text{Na}^{+1}$  ions  $r/r_0 = 1.5$  and at  $|V_r| = 0.15/(\text{V})$ , and (10) gives  $C(d) \cong C(0)/25$ . Thus, the  $\text{Na}^{+1}$  intracellular concentration is decreased by 25 times compared with extracellular one; like approximately it does in the cells

of a squid. This is the passive transport of ions. For the  $K^{+1}$  ion with the shape of a prolate ellipsoid  $r_{prol}/r_0 = 84/125 = 0.67$  and  $C(d) \cong 7 \cdot C(0)$ ; hence, the  $K^{+1}$  will increase their concentration on passing the membrane. The case of  $K^{+1}$  illustrates a mechanism of the active transport by changing the shape of hydration shells of the ions.

### 3. Conclusion

Equations (9) and (10) have been obtained to calculate the concentration profile of ions in biological membranes. It is shown that the friction forces and effective ion radius in membranes depends on the shape of shells covering ions. Analysis of the  $Na^{+1}$  and  $K^{+1}$  profiles lead to a conclusion that a possible mechanism of active and passive transport can be closely associated with changing of hydrated shells of ions by membranes.

#### 3.1. References

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