Protons in Water as a Fermi Gas

P. R. Silva – Retired associate professor – Departamento de Física – ICEx – Universidade Federal de Minas Gerais – email: prsilvafis@gmail.com

Abstract- Hydrogen-bond kinetics plays an important role in the establishment of the transport properties of water. In this paper we propose to consider protons in water as a Fermi gas. We use Fermi statistics to determine the Fermi energy, the averaged time between collisions of the protons, and the speed of sound in liquid water. This time is also used to interpret the response in frequency of the cytoplasm to an applied external electric field.

1 – Introduction

Water is one of the most important substances of nature. Therefore the study of its microscopic structure seems to play a fundamental role in understanding its place in the physical and life sciences [1,2,3]. An isolated molecule of water appears to be a very simple system, once it consists of two hydrogen atoms attached to an atom of oxygen. However, when in contact with other identical molecules in the liquid and solid phases, the water substance displays a rich variety of phenomena [3]. For instance, the dipole moment of water goes from 1.86 D in the gas phase to approximately 3.0 D in the condensed phase (liquid or solid) [4].

An important feature associated to water in its condensed phase is the hydrogen bonding. Appropriate treatment of the kinetics of these bonds requires the use of the quantum mechanics and appears to account for various anomalies presented by the physical properties of water [5].

But, what is a hydrogen bond? As was pointed out by Pauling [6],"Under certain conditions an atom of hydrogen is attracted by rather strong forces to two atoms instead of only one, so that it may be considered to be acting as a bond between them."

Meanwhile, Pimentel and McClellan [7] advanced an equivalent definition of hydrogen bond, namely: "A hydrogen bond is said to exist when (1) there is a evidence of a bond, and (2) there is a evidence that this bond sterically involves an hydrogen atom already bonded to another atom."

Besides this, in the case of water, Chaplin [8] has pointed out that: "Typically hydrogen bonding occurs where the partially positive charged hydrogen atom lies between partially charged oxygen atoms, for instance."

2 – A bold hypothesis

Hydrogen-bond kinetics seems to play an important role in the establishment of the transport properties of water [9]. We may think the proton-current as a bean of particles which travels freely until to suffer a collision. Therefore it is possible to consider an average time τ between collisions and a proton mean free path ℓ, such that $\ell = v_F\tau$, being v_F a characteristic speed of the protons.

A bold hypothesis to be introduced here is to take the protons associated to the hydrogen-bond kinetics in water [9] behaving as a Fermi gas. An immediate consequence of this conjecture is to write the Fermi energy of this gas [10]

$$E_F = [\, h^{2}/(8\, M)]\, (\, 3/\pi)^{2/3}\, n^{2/3}, \qquad (1)$$

where h is the Planck's constant, M the proton mass and n the number density of "free" protons in the liquid water. Next we show that the knowledge of E_F permit us to determine the characteristic time τ associated to the proton motion as well to its mean free path.

3 – Average collision time as a particle lifetime

There are two characteristics linear momenta that we can associate to the free protons associated to the kinetic of the hydrogen bonds in water. They are the Fermi momentum Mv_F and the Compton momentum Mc. By taking into account the fermionic character of the proton, we will write a non-linear Dirac-like equation describing the "motion" of this particle. We have [7]

$$\partial\Psi/\partial x - (1/c)\, \partial\Psi/\partial t = [(M\, v_F)/\hbar]\, \Psi - [(Mc)/\hbar]\, |\, \Psi^{*}\Psi|\Psi. \qquad (2)$$

We see that eq. (2) contains only first order derivatives of the field Ψ. Besides this, the field Ψ exhibits not a spinorial character. Taking the zero of (2) and solving for $|\Psi^{*}\Psi|$, we get

$$|\Psi^{*}\Psi| = v_F/c. \qquad (3)$$

On the other hand in the collision process, the free proton loss its memory. We may think that this feature looks similar to the annihilation of a particle-anti particle pair, each of mass-energy equal to E_F. Putting this in a form of the uncertainty principle yields

$$2\, E_F\, \Delta t = h/2 \qquad \text{or} \qquad h\, \upsilon/2 = 2\, E_F. \tag{4}$$

Solving equation (4) for υ, we get

$$\upsilon = 1/\Delta t = 4\, E_F/h. \tag{5}$$

By combining the results of (3) and (5) we obtain the line width Γ tied to the "particle" decay

$$\Gamma = (1/3)\, \upsilon\, |\Psi^*\Psi| = 4\, E_F\, v_F/(\, 3h\, c\,). \tag{6}$$

We have introduced the factor one third in relation (6), thinking that equation (2) refers to a case of spherical symmetry, whereas in the presence of an electrical field we have an explicit brake of symmetry , conferring a linear character to the problem.

The averaged time between collisions τ is then given by

$$\tau = 1/\Gamma = (3\, h\, c\,)/(\, 4\, E_F\, v_F\,). \tag{7}$$

Taking in account that

$$v_F = (2E_F/M)^{1/2} = [h/(2M)]\,(3n/\pi)^{1/3}, \qquad (8)$$

and by using relations (8) and (1) into (7), we obtain

$$\tau = (M^2\, c)/(n\, \pi\, \hbar^2). \qquad (9)$$

The proton mean free path is given by

$$\ell = v_F\tau = (Mc/\hbar)\,(3/\pi)^{1/3}\, n^{-2/3}. \qquad (10)$$

The Fermi length of the proton gas reads

$$\lambda_F = h/(Mv_F) = 2\,[\pi/(3n)]^{1/3}. \qquad (11)$$

4 – Numerical evaluation of the quantities related to the proton gas

As is well known that 18 cubic centimeters of liquid water contains two times the Avogadro's number of protons, by inserting this information jointly with the other constants in relations (8) to (11), we get:

$$\lambda_F = 5.67\ x10^{-10}\ m; \quad v_F = 793\ m/s; \quad \tau = 3.57\ x10^{-7}\ s; \quad \ell = 2.83\ x10^{-4}\ m. \qquad (12)$$

Luzar and Chandler [9] pointed out that: "In the hydrogen-bond definition employed by them, two water molecules separated by less than 3.5 Å can be either bond or not bonded, depending upon their relative orientations. At large separations, a bond cannot form." This information comes from the first

coordination shell of water, as measured by its oxygen-oxygen radial distribution function.

In a previous paper [11], we have identified this length of 3.5 Å as the Fermi length of protons in water, but the present calculations shows a somewhat great value for it, namely $\lambda_F = 5.67$ Å as can be verified in (12).

5 – Application to biology

In a letter to Physics Today [12], Francis X. Hart advanced a model accounting for the effect of an external electric field on a cell. According to Hart [12], the interior of a cell is filled with a substance which is gel-like and good ionic conductor named cytoplasm. As was pointed by him: "When an external electric field is applied, the ions quickly redistribute themselves to produce a field that essentially cancels the field inside the cytoplasm. The resulting potential difference must then appear almost entirely across the membrane. The time scale for that process is on the order of a microsecond." Yet according hart [12], applied fields with frequency less than 1MHz, does not significantly affects the molecules of the cytoplasm.

In this section we wish to tie the ionic current above mentioned to the motion of the proton gas. Thinking the protonic current, as a current in the process of charging a capacitor, we can write

$$E = \rho\, j_{max} \exp[-t/(RC)] = E_{max} \exp(-t/\tau). \qquad (13)$$

In (13), ρ is the resistivity and j_{max}, and E_{max} are maximum of the current density and of the electric field, respectively. We also have identified in (13), τ with the characteristic time of a RC circuit.

It is possible to verify in (13), that if the external electric field is turned on at t=0, after a time elapsed of $T = 4\tau$, the resultant electric field inside the cytoplasm effectively vanishes. Let us evaluate T, we have

$$T = 4\tau = 4 \text{ x } 3.57\text{x}10^{-7} \text{ s} \cong 1.4\text{x}10^{-6} \text{ s}. \qquad (14)$$

As the cell is constituted in a great portion by liquid water, it seems that the time T here estimated is in agreement with the experimental findings reported by Hart [12].

6 – The sound velocity in liquid water

In the previous section we have proposed that: protons in water behave in a certain sense as the free electrons in metals. Meanwhile, the speed of sound in metals is basically dictated by the fermionic character of the free electrons. Therefore we think that the analogous role of the protons, performing hydrogen-bonding in water, may be relevant as a means to evaluate the sound velocity in this liquid.

The propagation of a sound wave involves only transport of energy:-not matter. Thinking in this way we assume that which is relevant for the propagation of the sound in water is the relative motion of the two protons, both belonging to the same water molecule. In treating this relative motion we consider that the reduced mass of the proton, $\mu = M/2$, plays an important role.

Here we propose another bold hypothesis, namely: The speed of sound in water, v_{sound}, can be computed by substituting in the relation for the Fermi velocity, the mass of the proton by its reduced mass $\mu = M/2$. Doing this, we get

$$v_{sound} = [h/(2\mu)] (3n/\pi)^{1/3} = (h/M) (3n/\pi)^{1/3} = 2\, v_F. \qquad (15)$$

In obtaining (15), we have used (8). Numerical estimate of (15) gives

$$v_{sound} \cong 1586 \text{ m/s}. \qquad (16)$$

This value must be compared with

$$v_{sound}(\text{measured}) \cong 1555 \text{ m/s}, \qquad (17)$$

which is the maximum speed of sound in water, measured at 74,0°C (please see reference [13]).

References

[1] J. A. Morrone and R. Car, in: "Nuclear quantum effects in water", arXiv:0803.3635v1, 25 Mar 2008.

[2] M. F. Chaplin, in: "Water: its importance to life", Biochemistry and Molecular Biology Education **29**, pp.54-59(2001).

[3] D. S. Eisenberg and W. Kauzmann, "The structure and properties of water", Clarendon Press, Oxford, 2005.

[4] P. L. Silvestrelli and M. Parrinelo, in: "Water Molecule Dipole in the Gas and in the Liquid Phase", Phys. Rev. Lett. **82**, pp. 3308-3311(1999).

[5] D. Flamini, M. A. Ricci, and F. Bruni, in: "A new water anomaly: the temperature dependence of the proton mean kinetic energy", arXiv:0901.4273v2, 28 Jan 2009.

[6] L. Pauling, "The Nature of Chemical Bond", 2nd ed., Cornell University press, N. York, 1948.

[7] G. C. Pimentel and A. L. McClellan, "The hydrogen bond", Freeman, San Francisco, 1960.

[8] M. Chaplin, in: "Water's Hydrogen Bond Strength", arXiv:0706.1355v1, 2007.

[9] Alenka Luzar and David Chandler, "Hydrogen-bond kinetics in liquid water", Nature 379,p.55-57, 4 January 1996.

[10] C. Kittel, Introduction to Solid State Physics, 5th Edition, Wiley, 1976- Ch. 6.

[11] P. R. Silva, in: “Memory of Living Beings and Its Three Characteristic Times”, Progress in Physics **10**, pp. 79-81(2014).

[12] F. X. Hart, in: “Modeling a cell in an external electric field”, Physics Today **67**(10), 11(2014).

[13] www1.lsbu.ac.uk /water/data.html