Transition of Water Molecule Behavior from Sub-Atomic to Classic Scale

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Abstract
This article is based on the master thesis (Ciftci 2014) related to our invention which is published in World Intellectual Property Organization (WO/2011/048506) as microwave water heater and the theoretical part of whole project. In this article, heating water by microwave (with steady frequency, 2.45 GHz) is analyzed from sub-molecular to Classical Mechanic results of heating. As the aim of this study, we wanted to examine Quantum Mechanical base of heating water by microwave experiments. As a result, we derived a Semi-Quantum Mechanical equation for microwave-water interactions and thus, Wien displacement law can be derived to verify experimental observations by this equation.

Keywords: Microwave heating, semi-classic water molecule, water molecule behavior

1. Introduction
Quantum Mechanics also stands background of water heating by microwave, directly and indirectly. To examine Quantum Mechanical base of heating water by microwave, we need to start from a Quantum Mechanical phenomenon as photon. This approach also let us summarizing steps of heating water by microwaves. Observations started with photon production. Next step was creating phonons as a result of photon interaction with materials used. Then at the moment of interaction beginning between microwaves and water molecules, photon duality was witnessed. This is why we can define wave-water interactions. Also electric arc creation is a considerable situation about duality when microwave interacts with metals. Variety of water phases and thermodynamic cases followed these steps. It is also possible to prove these steps numerically.

2. Microwave Water Interactions
To learn what happens when water is heated by microwave, we should understand electromagnetic wave and its components' interactions with water molecule. For these interactions, dipole water molecules can be aligned by an electric field (Hayashi 1996; Ping et al. 2011). Those dipole molecules can be replaced in time depending on frequency and may not be affected by phase variation of electric field. Heating by phase delaying occurs twice in a dipole molecule and that can be commented as energy loose. Dipole molecules can move easily in an electric field. That motion is related with water viscosity and electron cloud mobility. It also depends on network of bonds between molecules (Schekunov & Vegiri 2002). For ice, we need very high field strengths (5.109 Vm-1) to prevent freezing (Kaatze et al. 2002). In low field strengths (105 Vm-1), hydrogen bonds become weak. Also aligned water molecules untie bonds with neighborhood molecules and re-orient to make new bonds (Wei et al. 2008).
An electric field can make hydrogen bonds longer (at 25.10^{9} \text{Vm}^{-1}, \pm 6\%) and the angle between bonds (at 25.10^{9} \text{Vm}^{-1}, \approx \%1-\%0.2) depends on alignment of the dipole molecule. In appropriate pressure conditions, there will be phase changes as freezing and melting. But it is up to electric field value. High field strengths cause anisotropic form of hydrogen bonds. These bonds are aligned along the field and little bit perpendicular to the field. In low field strengths, replacement and rotation occurs together (Vegiri 2004; Danielewicz-Ferchmin & Ferchmin 2006).

Liquid water is effected by magnetic field such that magnetic field is used to purify water. Water is diamagnetic and can have levitation ability (at 10 T, of world 50μT). Static magnetic field causes hydrogen bonds to extend (Ikezoe et al. 1998).

Electric field and magnetic fields have opposite effects on water, when applied separately. Electric and electromagnetic fields both re-orient water molecules and untie many hydrogen bonds (Symons 2001). Electromagnetic effects on water, show electric field effect more effectively rather than magnetic field effects (English & MacElroy 2003).

3. Quantum Mechanical View

In experiments we could see quantum mechanical effects and classical results together like photon duality and classic heating. We can explain water heating in Classic Mechanics. It is obvious that if you transport enough energy to water molecules, they will have kinetic energy and then break hydrogen bonds. Therefore, water physically will transform ice, liquid and steam phases. On the other hand, microwave as radiation of electron accelerating is a quantum mechanical phenomenon. Therefore, heating water by microwave is about electromagnetic wave - thermodynamic relations. According to the experiments, water heating and source energy have a mathematical response (1).

\[ h.\nu \propto M_{\text{H}_2\text{O}} \cdot C \cdot \Delta T \]  \hspace{1cm} (1)

Where \( \nu \) is a microwave photon frequency, \( C \) is specific heat capacity and total mass of water is \( M_{\text{water}} = N.M_{\text{H}_2\text{O}} \cdot \text{molecule} ; N \) is Avogadro Number. Thus equivalence becomes,

\[ N.\cdot h.\cdot \nu \propto M_{\text{water}} \cdot C \cdot \Delta T \]  \hspace{1cm} (2)

Another outlook to the equivalence will show the response of each symbol.

\[ \nu \propto \Delta T \quad , \quad h \propto C \quad \text{and} \quad N \propto M_{\text{water}} \]  \hspace{1cm} (3)

Each equivalence has signification in substance. The first equivalence shows that N molecules of water constitute \( M_{\text{water}} \) total mass of water used in the experiments. \( M_{\text{H}_2\text{O}} \cdot \text{molecule} \), \( M_{\text{water}} \) and \( N \) symbols are quantities of materials. The second equivalence of (3) includes nature constants. \( h \), Planck constant is the quantum of action in Quantum Mechanics and \( C \) is the heat capacity of water in Classic Mechanics. These constants are in universal constant category.

The most important equivalence is the third one as \( \nu \propto \Delta T \). We need to take attention that the frequencies we worked are fixed to 2.45 GHz. Phase changes are up to different frequency levels (kHz, MHz, GHz) (Kaatze et al. 2002). Thus, change in frequency results change in heat.

After that, for \( \Delta T = T - T_0 \) we can make \( \Delta T \approx T \) classic approach. Because in experiments \( C \) (bold
C), heat capacity of water, allows just low heat differences between $\Delta T$ and $T$. In the same way, $T_0 \approx 0$ approach is possible to show $T$ is total change of microwave heating effect. Let's perform verification of the equivalence (2). To do that, we need a proportional constant and then we will call it proportional constant $\phi$.

$$\phi. h. \nu = M_{H_2O \text{molecule}} \cdot C. \Delta T$$  \hspace{1cm} (4)

$$\phi. N. h. \nu = M_{water} \cdot C. \Delta T$$  \hspace{1cm} (5)

$$\lambda = \frac{\phi. N. c. h}{M_{water} \cdot C. T}$$  \hspace{1cm} (6)

Where $\lambda$ is a microwave photon wavelength and comes from $\nu = c/\lambda$. The value of proportional constant $\phi$ is 1,8243 and it is molecular rotational spectroscopic constant for $H_2$ in degrees K and Hz (Soures 1986). All constants together, defines $b$ (7, 8).

$$b = \frac{N. c. h}{M_{water} \cdot C}$$  \hspace{1cm} (7)

$$\lambda = b \cdot \frac{1}{T}$$  \hspace{1cm} (8)

The value $b$ is 0,298978 cmK and it is equal to Wien's displacement constant. Other constant values are: N as Avogadro Number, 6.022141 mol$^{-1}$; c, speed of light as 2.998$\times10^8$ m/s; h, Planck constant as 6.626$\times10^{-34}$ joule’s; C specific water heat capacity as 4.184 Joule.g$^{-1}$K$^{-1}$. 1 mol of water, $M_{water}$ is 18 g.

Equation (5) is indeed:

$$N. h. (\phi. \nu) = M_{water} \cdot C. \Delta T$$  \hspace{1cm} (5)

$\phi. \nu$ is vibration frequency for the equation. This comes from rotational action (Soures 1986). According to Wien, there is an inverse relation between the wavelength of the peak of the emission of a black body and its temperature when expressed as a function of wavelength. So these experiments are special kind of Wien displacement law.

### 4. Conclusion

Energy of photons, $E=nh\nu$, can be commented in two ways. The first one is energy of a light beam including $n$ photons vibrating with $\nu$ frequency. Second comment is that, $E=nh\nu$ is the energy of a photon vibrating with $n\nu$ frequency. Although both energy values are equal, there is a big difference physically. For example, a photon with 2.45 GHz frequency can heat a water molecule and has same energy value as 1000 photons which vibrate at 2.45 MHz frequency. But water molecule cannot be heated by 1000 photons with vibrating at 2.45 MHz frequency. Because 1000 photons are radio photons and the first photon is a microwave (millimeter wave) photon. They all have different effects and radio waves don’t affect water molecule. This
example is like key-lock relation and shows that water molecules can be rotated in different frequencies for each physical phase. The quantum-classic transition may starts from this phenomenon.

Considering \( \phi \) as molecular rotational spectroscopic constant for \( \text{H}_2 \) in degrees K and Hz, tells us (5) numeric equation is semi-classic. This equation (5) guides us to figure out water's quantum states - thermodynamic states - classical mechanic scale transitions. It is important not to make a general interference about other materials in the experiments. It is all about water nature.

5. Discussion

Deriving \( N \cdot h \cdot (\phi \cdot \nu) = M_{\text{water}} \cdot C \cdot \Delta T \) equation helped us to imply that left part of the equation is about microwave photon and provides energy for right part of the equation (to heat water). This is usual and right comment as cause and effect relation.

But \( \phi \) is about \( \text{H}_2 \) molecular vibration and thus equation (5) becomes spectroscopic motion equation for hydrogen bonds of water molecules in degrees K and Hz. Thus we could examine water molecular behavior from quantum mechanics to classic mechanics (as boiling, evaporating, phase changing and so on). So \( (\phi \cdot \nu) \) may not be about microwave photon energy directly.

In both comments, (5) shows the transitions of water molecule which is heated by microwave and this transition starts from Quantum Mechanical reasons (as vibrating, wave interaction) to its Classical Mechanics results (as phase variety).

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References


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