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# Intriguing Peculiarities of the Hydrogen and Lithium Hydride Molecules Including the Entanglement

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In the first part of this communication, we will consider the homopolar diatomic hydrogen molecule ($H_2$) and in the second part the heteronuclear diatomic lithium hydride molecule (LiH). De Broglie's equation can be used to describe the wave nature of a particle in motion

$$\lambda = h/m\upsilon \quad \ldots (1).$$

where h (= $6.63 \times 10^{-34}$ *J sec*)[1] is Planck's constant, λ and m are the wavelength and the mass of a particle moving at a speed υ. For the sake of simplicity, we will consider $H_2$ and LiH are moving at a non-relativistic speed υ.

We also want to remind you here that, by definition, two particles are entangled when any change in one particle causes a change in the other no matter how far apart, they are.

***The first peculiarity.*** $H_2$ exists in two nuclear isomeric forms: ortho $H_2$ with the parallel proton's spins (a triplet state) and para $H_2$ with antiparallel spins (a single state). Ortho isomer is less stable than para one but at STP., due to thermal excitation, the ratio of these isomers is 3:1 (ortho $H_2$: para $H_2$).

The experimental equilibrium bond length of $H_2$ is about $7.4 \times 10^{-11}$ *m* or about 43500 diameters of the proton (its diameter is approximately $1.7 \times 10^{-15}$ *m*). This is the distance between two protons of $H_2$. These protons are spin-coupled though they are vastly apart in terms of their diameter. This implies that they are entangled sharing two quantum states. Moreover, the two electrons of $H_2$ are also spin-coupled forming the spin-singlet ground state (total spin is zero). This coupling also occurs at this huge distance. Therefore, it implies that these electrons are also entangled.

***The second peculiarity.*** Premović [1] calculated the most probable/average speed of $H_2$ occupying 22.1 $dm^3$ at STP is about 1500 *m* $sec^{-1}$.[2] Employing eqn. (1) and the mass of $H_2$ [ m ($H_2$) = $3.4 \times 10^{-27}$ *kg*], he estimated that de Broglie's average wavelength is approximately $1.3 \times 10^{-10}$ *m*. Since the proton (hereinafter $H^+$) is a component of $H_2$ its most probable/ average speed would be also about

[1] To avoid confusion in further text, the SI units are given in italics.
[2] The mean free path of $H_2$ under normal conditions is $1.3 \times 10^{-7}$ *m*.

1500 $m\ sec^{-1}$. Using the same equation, he estimated that de Broglie's average wavelength of $H^+$ is about $0.65 \times 10^{-10}$ $m$. However, now the following questions arise: does a quantum mechanical model of $H_2$ in non-relativistic motion consist of a single wave packet (with an "average de Broglie wavelength" of about $1.3 \times 10^{-10}$ $m$) or does it consist of two vastly separated identical $H^+$ wave packets (with an "average de Broglie wavelength" of about $0.65 \times 10^{-10}$ $m$)? If de Broglie's model is right, then the wave packets of these protons interact with each other giving the single wave packet. But now this wave packet should have the $H^+$ an "average wavelength" of about $0.65 \times 10^{-10}$ $m$ but not about $1.3 \times 10^{-10}$ $m$ as the above single wave packet based on de Broglie's approach. Moreover, if these two H wave packets interact with each other then they must be entangled since the distance between them is enormous: 43500 $H^+$ diameters.

***The third peculiarity.*** In one of our previous communications [2], we proposed that Broglie's waves of the protons of $H_2$ interact with each other. The superposition of these waves can result in two types of interference depending on whether their waves are in phase or out of phase: constructive or destructive interference. As the distance between the $H_2$ protons is so large the superposition is possible only if these two protons are entangled.

In their constructive interference, the resultant wave would have twice large the $H^+$ amplitude but its wavelength would be the same as the $H^+$ wavelength. Now we would deal with a single $H_2$ wave packet. In the destructive interference, the two $H^+$ waves would cancel each other so there would be no resultant wave. Does this mean there would be no $H_2$ wave packet in this case?

**The peculiarities of LiH**. LiH consists of two independent species: partly positive $Li^{+\delta}$ and partly negative $H^{-\delta}$. They are linked by an ionic-covalent bond.[3] The diameter of its nucleus $Li^{3+}$ (hereinafter $Li^{3+}$) is about $10^{-14}$ $m$ and the diameter of its $H^+$ nucleus is approximately $1.7 \times 10^{-15}$ $m$; the experimental bond length of gaseous LiH is about $1.6 \times 10^{-8}$ $m$. Thus, the distance between Li (or $Li^{3+}$) and H (or $H^+$) in this molecule is about $3 \times 10^6$ $Li^{3+}$ diameters and about $10^7$ $H^+$ diameters.

Let us assume that the de Broglie's $Li^{3+}$ wave of LiH interacts with its de Broglie's $H^+$ wave. The (constructive or destructive) superposition of these dissimilar waves can result in rather complex two but quite different de Broglie's waves and the wave packets. As the bond length of LiH is so large in terms of the $Li^{3+}$ diameter or the $H^+$ diameter then their superposition is possible only if the $Li^{3+}$ and $H^+$ nuclei are entangled.

However, now the following question arises: does a quantum mechanical model of LiH in non-relativistic motion consist of a single wave packet or does it consist of two vastly separated $Li^{3+}$ and $H^+$ wave packets? If de Broglie's model is right, then the wave packets of these nuclei interact with each other giving the above single wave packet. But now this packet should be rather complicated. Moreover, if these two packets interact with each other then they have to be entangled since the distance between them is immense: about $3 \times 10^6$ $Li^{3+}$ diameters and about $10^7$ $H^+$ diameters.

[3] The bond in LiH is about 76 % ionic or $\delta \approx 0.76$.

## References

[1] P. I. Premović, *Hydrogen molecule in the light of the de Broglie theory*. The General Science Journal, May 2023.
[2] P. I. Premović, *The hydrogen molecule and deuterium atom in the light of de Broglie's theory.* The General Science Journal, May 2023.