A MOLECULAR STRUCTURE OF AN ATOMIC NUCLEUS

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Abstract: In this work we extend our work on a quantum dynamics of beta decay to show that an atomic nucleus can be described as a molecule which is supposed to be formed by bonding atoms as described in molecular physics. However, there is only one type of atom in our formulation and that atom is the neutron which has been shown to possess the physical structure of a dwarf hydrogen-like atom under the influence of a generalised Yukawa MGESCP potential rather than the Coulomb potential as in the case of the normal hydrogen atom. We construct Schrödinger wave equation to describe the deuteron as a molecular ion which has similar physical structure to the molecular ion of the hydrogen molecule. We also construct Schrödinger wave equation to describe the deuterium and obtain the corresponding energy spectrum, by showing that the deuterium has a similar physical structure to that of a helium atom. As a further discussion, we suggest possible structures for nuclei with high numbers of protons and neutrons and show that these nuclei may form narrow lattices therefore they could fold to form three-dimensional spherical structures by layers of shells by bonding similar to hydrogen bonding.

In our previous work on a quantum dynamics of beta decay we showed that a neutron may have the structure of a dwarf hydrogen-like atom and the beta decay is a physical event that requires a sophisticated form of potential for its description, such as a generalised Yukawa MGESCP potential. We also showed that this complicated process could be broken down into various consecutive stages of physical processes that require different forms of potentials to describe the physical process at each stage [1]. From this view of the neutrons as dwarf atoms we naturally arrive at the conclusion that a nucleus of an atomic atom should also have the structure of a molecule which is defined as a collection of atoms bonding together and the bonding can be described using the form of a potential that is used to describe the strong force. However, in an atomic nucleus we have both protons and neutrons and a proton only has a positive charge without an electron orbiting it therefore nuclei are not neutral nuclear molecules but nuclear molecular ions. For a comparison, let us consider the normal hydrogen molecule H_2 which is composed of two hydrogen atoms each of which has one proton and one electron. Despite the neutral atomic molecule H_2 has two protons and two electrons, the pair electrons are shared between the two protons to form the covalent bonding and orbit both protons. Now if one electron is removed from the neutral atomic molecule H_2 then we have the molecular ion H_2^+ which has only one electron which orbits both protons. This is the representation that we will apply to the deuteron which is the nucleus of a deuterium, which is formed by one proton and one neutron that are assumed to attract each other by a strong

force which can be derived from a generalised Yukawa MGESCP potential. We have two different views that can be applied to the physical structure of the deuterium described as follows. If the Coulomb potential is applied, then a deuterium is an isotope of the normal hydrogen atom with a neutron in the nucleus besides the proton, as shown in Figure 1. However, if a generalised Yukawa MGESCP potential is applied then a deuterium can be viewed as an isotope of the normal helium atom without neutrons at the nucleus but only two protons and two electrons one of which can be supposed to be orbiting very close to the two protons, as shown in Figure 2.

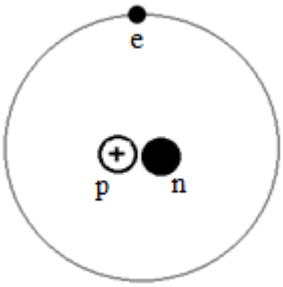

Figure 1: A deuterium with Coulomb potential

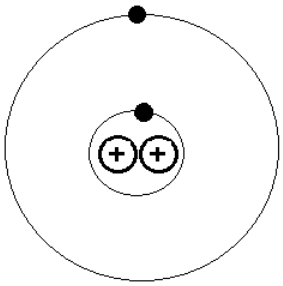

Figure 2: A deuterium with generalised Yukawa potential

In the following we will examine how the two different views of the deuteron and the deuterium, as depicted above, and their corresponding quantum dynamics can be described using the Schrödinger wave equation in quantum mechanics. For the case of the deuteron, it has been shown from experiments that the bound state of the deuteron exists in a triplet state that can be described by the Schrödinger equation in the centre-of-mass system as

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(r) - E\right)\psi(\mathbf{r}) = 0 \tag{1}$$

where $\mu = M_p M_n/(M_p + M_n)$ and the potential $V(r)$ can be taken as a square well potential $\{V(r) = -V_0$ for $r < a$ and $V(r) = 0$ for $r > a\}$, or a Yukawa potential $\{V(r) = -V0r-1\exp-ra$, or an exponential potential $Vr=-V0\exp-ra$ [2]. However, if the deuteron has a physical structure as shown in Figure 2 then it can also be viewed as a molecular ion which is composed of two protons and one electron, and the physical system is described by using a generalised Yukawa potential rather than the usual Coulomb potential as for the case of the hydrogen molecular ion H_2^+. If we assume the generalised Yukawa potential to be the MGESCP potential given as [3] [4]

$$V(r) = -\frac{V_0 e^{-2\alpha r}}{r} - \frac{V_0}{r} - V_0 \alpha e^{-2\alpha r} \tag{2}$$

where V_0 is the potential depth and the parameter $\alpha \in (0, \infty)$ and using the centre-of-mass coordinates for the deuteron molecular ion, as shown in Figure 3, where **R** is the relative position vector of the two protons positioned at A and B; **r** is the position vector of the electron at C; r_A and $r_B$are the distances of the electron from the protons,

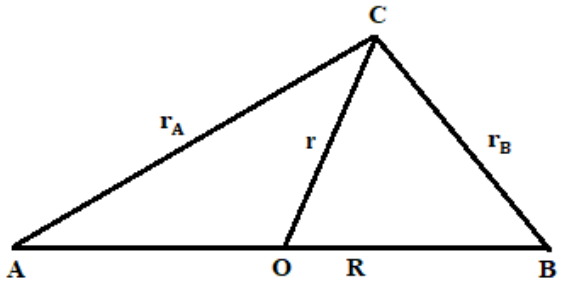

Figure 3: The centre-of-mass coordinate system for deuteron molecular ion

then the Schrödinger wave equation for the deuteron molecular ion can be written as

$$\left(-\frac{\hbar^2}{2\mu_{AB}}\nabla_R^2-\frac{\hbar^2}{2\mu_e}\nabla_r^2-\frac{V_0e^{-2\alpha r_A}}{r_A}-\frac{V_0}{r_A}-V_0\alpha e^{-2\alpha r_A}-\frac{V_0e^{-2\alpha r_B}}{r_B}-\frac{V_0}{r_B}-V_0\alpha e^{-2\alpha r_B}+\frac{q^2}{4\pi\varepsilon_0 R}-E\right)\psi(\mathbf{r},\mathbf{R})=0 \tag{3}$$

where $\mu_{AB}=M_p/2$ where M_p is the mass of the proton; and the reduced mass μ_e of the electron is given as $\mu_e=2mM_p/(m+2M_p)\approx m$ where m is the mass of the electron [2]. In the Born-Oppenheimer approximation the wave motion of the electron described by a new wavefunction $\chi_j(\mathbf{r},\mathbf{R})$ that satisfies the following equation [5]

$$\left(-\frac{\hbar^2}{2\mu_e}\nabla_r^2-\frac{V_0e^{-2\alpha r_A}}{r_A}-\frac{V_0}{r_A}-V_0\alpha e^{-2\alpha r_A}-\frac{V_0e^{-2\alpha r_B}}{r_B}-\frac{V_0}{r_B}-V_0\alpha e^{-2\alpha r_B}+\frac{q^2}{4\pi\varepsilon_0 R}-E\right)\chi_j(\mathbf{r},\mathbf{R})=0 \tag{4}$$

If the wave equation given in Equation (4) could be solved exactly then the wavefunctions $\chi_j(\mathbf{r},\mathbf{R})$ would become the molecular orbitals of the deuteron in analogy with the atomic orbitals. In this case the eigenenergies $E_j(R)$ that correspond to the wavefunction $\chi_j(\mathbf{r},\mathbf{R})$ would be found for each value of the distance R.

Now, it is also seen from Figure 2 that the physical structure of a deuterium is similar to that of a helium except there are no neutrons inside the nucleus and the quantum dynamics of the two electrons are described by two different potentials in which the inner electron is described by a generalised Yukawa MGESCP potential and the outer electron simply by the Coulomb potential. In the following we will formulate this atomic structure of the deuterium using also the Schrödinger wave equation in quantum mechanics.

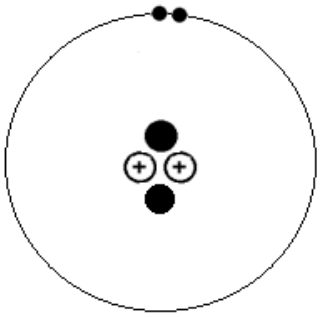

Figure 4: A Helium with Coulomb potential

As shown in Figure 4, the Hamiltonian for a helium atom in which the two electrons are on the same orbit under the influence of the Coulomb potential due to the two protons in the nucleus can be found to be of the form

$$H = -\frac{\hbar^2}{2\mu_e}(\nabla_1^2 + \nabla_2^2) - \frac{2q^2}{4\pi\varepsilon_0 r_1} - \frac{2q^2}{4\pi\varepsilon_0 r_2} + \frac{q^2}{4\pi\varepsilon_0 r_{12}} \tag{5}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the positions of the two electrons and $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. Since the distance r_{12} between the two electrons in assumed to be short therefore the term $q^2/4\pi\varepsilon_0 r_{12}$ is not negligible and the Schrödinger wave equation that is obtained from the Hamiltonian given in Equation (5) cannot be solved to obtain exact solutions. On the other hand, if we refer again to Figure 2 for the case of the deuterium in which the neutron is instead regarded as a dwarf hydrogen-like atom then the deuterium also has the atomic structure similar to the helium given in Figure 4, except the quantum dynamics of the outer electron is described by the Coulomb potential but the inner electron by the a generalised Yukawa MGESCP potential given in Equation (2). The Hamiltonian in this case takes the form

$$H = -\frac{\hbar^2}{2\mu_e}(\nabla_1^2 + \nabla_2^2) - \frac{2q^2}{4\pi\varepsilon_0 r_1} - \frac{2V_0 e^{-2\alpha r_2}}{r_2} - \frac{2V_0}{r_2} - 2V_0\alpha e^{-2\alpha r_2} + \frac{q^2}{4\pi\varepsilon_0 r_{12}} \tag{6}$$

As mentioned above for the case of the normal helium atom the two electrons are in the same orbit and they are supposed to be close to each other therefore the last term that involves the interaction between two electrons as given in Equations (5) is not neglected, however, for the case to the deuterium as shown in Figure 2, the two electrons are on different orbits which are far away from each other therefore the last term in the Hamiltonian given in Equation (6) that involves the interaction between them is negligible due to large distance. In this case the Hamiltonian is reduced to

$$H = -\frac{\hbar^2}{2\mu_e}\nabla_1^2 - \frac{2q^2}{4\pi\varepsilon_0 r_1} - \frac{\hbar^2}{2\mu_e}\nabla_2^2 - \frac{2V_0 e^{-2\alpha r_2}}{r_2} - \frac{2V_0}{r_2} - 2V_0\alpha e^{-2\alpha r_2} \tag{7}$$

Since the Hamiltonian given in Equation (7) is the sum of two separate Hamiltonians therefore the corresponding wavefuntion that describes the system is separable and can be

written as $\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_1(\mathbf{r}_1)\psi_2(\mathbf{r}_2)$. The corresponding Schrödinger wave equation applied to the system is written as

$$\left(-\frac{\hbar^2}{2\mu_e}\nabla_1^2 - \frac{2q^2}{4\pi\varepsilon_0 r_1} - \frac{\hbar^2}{2\mu_e}\nabla_2^2 - \frac{2V_0 e^{-2\alpha r_2}}{r_2} - \frac{2V_0}{r_2} - 2V_0\alpha e^{-2\alpha r_2} - E\right)\psi(\mathbf{r}_1, \mathbf{r}_2) = 0 \qquad (8)$$

Using the separable wavefunction $\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_1(\mathbf{r}_1)\psi_2(\mathbf{r}_2)$ the Schrödinger wave equation given in Equation (8) can now be written as a system of two separate Schrödinger wave equations as follows

$$\left(-\frac{\hbar^2}{2\mu_e}\nabla_1^2 - \frac{2q^2}{4\pi\varepsilon_0 r_1}\right)\psi_1(\mathbf{r}_1) = E_1\psi_1(\mathbf{r}_1) \qquad (9)$$

$$\left(-\frac{\hbar^2}{2\mu_e}\nabla_2^2 - \frac{2V_0 e^{-2\alpha r_2}}{r_2} - \frac{2V_0}{r_2} - 2V_0\alpha e^{-2\alpha r_2}\right)\psi_2(\mathbf{r}_2) = E_2\psi_2(\mathbf{r}_2) \qquad (10)$$

where $E = E_1 + E_2$.

Solutions to Equation (9) are the normalised radial eigenfunctions of the bound states that can be found and given as

$$R_{nl}(r) = -\left(\left(\frac{2kmq^2}{\hbar^2 n}\right)^3 \frac{(n-l-1)!}{2n\big((n+l)!\big)^3}\right)^{1/2} e^{-\rho/2}\rho^l L_{n+l}^{2l+1}(\rho) \qquad (11)$$

where $\rho = (-8\mu_e E/\hbar^2)^{1/2} r$ and $L_{n+l}^{2l+1}(\rho)$ is the associated Laguerre polynomial. The bound state energy eigenvalues are given by

$$E_n = -\frac{\mu_e k^2 q^4}{2\hbar^2}\frac{1}{n^2} \qquad (12)$$

On the other hand, solutions to Equation (10) are the radial eigenfunctions of the bound states which can also be obtained as

$$R_{nl}(r) = N_{nl} r^{\left(-1+\sqrt{4l(l+1)+1}\right)/2} e^{-\beta r} L_n^{1+\sqrt{4l(l+1)+1}}(2\beta r) \qquad (13)$$

where $\beta^2 = \left(2\mu_e(V_0 + V_0 e^{-2\alpha r})/\hbar^2\left(2n + 1 + \sqrt{4l(l+1)+1}\right)\right)^2$ [4]. The corresponding energy spectrum E_{nl} is given by

$$E_{nl} = -V_0\alpha e^{-2\alpha r} - \frac{\mu_e}{2\hbar^2}\left(\frac{(V_0 + V_0 e^{-2\alpha r})}{n+l+1}\right)^2 \qquad (14)$$

Although this energy spectrum is discrete with respect to the quantum numbers n and l, it depends continuously on the radial distance r. In particular, we showed in our work on a quantum dynamics of beta decay that if the Yukawa potential remains constant, i.e., $e^{-mr}/r = -(ikJ/2a)$, where m and kJ are parameters in the generalised Dirac equation given in the form [6] [7]

$$\gamma^{\mu}\partial_{\mu}\psi = -im\psi + kJ \tag{15}$$

then the generalised Yukawa MGESCP potential given in Equation (2) is reduced to the potential that is used to describe the strong force.

$$V(r) = -\frac{V_0}{r}(1 + (1 + \alpha r)e^{-2\alpha r}) = -\frac{V_0}{r} + \frac{ikJ}{2\alpha}(1 + \alpha r) = -\frac{V_0}{r} + \frac{ikJ}{2}r + \frac{ikJ}{2\alpha} \tag{16}$$

And from the energy spectrum given in Equation (14) we also obtain

$$E_{nl} = \frac{ikJ}{2}r - \frac{\mu_e}{2\hbar^2}\left(\frac{(V_0 - (ikJ\alpha/2)r)}{n + l + 1}\right)^2 \tag{17}$$

As a further extension, we now discuss how a nucleus which is composed of many protons and many neutrons can be formed if the neutrons are regarded as dwarf hydrogen-like atoms. In order to be able construct possible nuclear structures as molecules from the assumption of the structure of the neutrons as dwarf hydrogen-like atoms we now assume further that the protons and the neutrons are arranged so that they will have the physical structure similar to that of a hydrogen molecule H_2 or that of a hydrogen molecular ion H_2^+. This means that they are arranged so that they can share electrons so that each of the nucleons is seen to have one or two electrons orbiting around it. As an illustration, in the following we give such possible structures for the first few nuclei, where ⊕ represents a neutron and ⊕ represents a proton. For nuclei with even numbers of protons and neutrons, we have the following figures

Figure 5: A nucleus with two protons and two neutrons

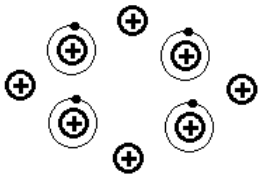

Figure 6: A nucleus with four protons and four neutrons

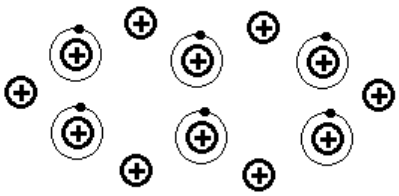

Figure 7: A nucleus with six protons and six neutrons

In the above figures, each pair of neutrons next to each other share a pair of electrons and each proton shares a pair of electrons given by the two neutrons next to it.

For the case of nuclei with odd numbers of protons and neutrons, we suggest that they would have the molecular structures given in the following figures in which it is assumed that each nucleus is a coupling of a deuteron and other nuclei. For example, in Figure 8 the nucleus is a coupling of the nucleus of a helium and a deuteron. In Figure 9 the nucleus is a coupling of the nucleus of a beryllium and a deuteron. In Figure 10 the nucleus is a coupling of the nucleus of a carbon and a deuteron. Therefore in the case of odd numbers of protons and neutrons, besides atomic bonding we also have molecular bonding between the nuclei which are now have molecular structures.

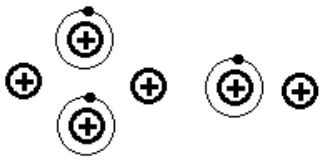

Figure 8: A nucleus with three protons and three neutrons

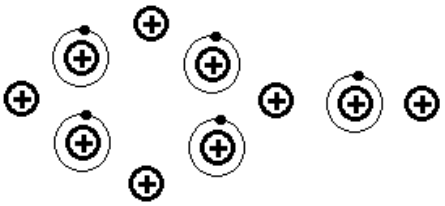

Figure 9: A nucleus with five protons and five neutrons

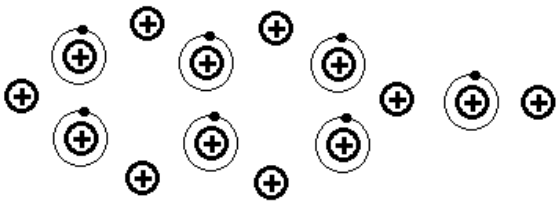

Figure 10: A nucleus with seven protons and seven neutrons

The molecular structures of nuclei that are depicted in the above suggestive figures are long and narrow lattices therefore in order to form the spherical shapes that they are assumed to possess, they should fold to form three-dimensional spherical structures by internal bonding similar to hydrogen bonding. In particular, the three-dimensional structures may also form layers of shells with the characteristics that have been observed in nuclear physics. It is remarkable to mention here that the molecular structure of an atomic nucleus may also be determined topologically by moduli spaces of circle packings [8]. As a further speculation, we would like to make a note here that the above depicted figures are just a few possible arrangements that can be formed from the protons and the neutrons and whether they should be arranged according to particular patterns, for example like DNA patterns in biology, to

form the basis for the creation of all physical objects is an interesting question that needs further investigation.

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