THE SCHRÖDINGER EQUATION FOR GROUND STATE OF THE DEUTERON: EXAMPLE OF TRANSITION FROM CLASSICAL MECHANICS TO QUANTUM MECHANICS

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Abstract. In this paper I start with the studying of a system of two interacting particles, with the same mass $M$, using the framework of classical mechanics, subsequently, I derive the equation of Schrödinger for such system, finally, I update such differential equation, adding the binding energy of the deuteron in its ground state and setting $M$ equals to the nucleon mass, namely $M \approx 940 \text{ MeV}$.

Really, it is an advanced tutorial, since for its fully comprehension, it is required the knowledge of the Analytical Mechanics and the basics of the Quantum Mechanics as well.

1. Introduction

Let’s consider a system composed by two particles, of the same mass $M$ and which are interacting with a spring which connects one particle to the other (see figure 1 below).

![Two-particles system](image)

**Figure 1.** Two-particles system

Within certain limits, we can say that our mechanical system possesses six degrees of freedom, so in order to identify, uniquely, its position, it is suffice to know the six coordinates $(x, y, z)$ of both points.

Then, we can conclude that the total kinetic energy $T$ of such system, is given by the subsequent formula:

$$T = \frac{1}{2} M \left( \dot{x}_1^2 + \dot{y}_1^2 + \dot{z}_1^2 \right) + \frac{1}{2} M \left( \dot{x}_2^2 + \dot{y}_2^2 + \dot{z}_2^2 \right)$$
whereas the corresponding Lagrangian function $\mathcal{L}$, is:

\begin{equation}
\mathcal{L} = T - V = \frac{1}{2} M \left( \dot{x}_1^2 + \dot{y}_1^2 + \dot{z}_1^2 \right) + \frac{1}{2} M \left( \dot{x}_2^2 + \dot{y}_2^2 + \dot{z}_2^2 \right) - V \left( |r_2 - r_1| \right)
\end{equation}

wherein the function $V \left( |r_2 - r_1| \right)$ takes account of the potential energy of interaction between the two particles of our mechanical system, as a function of the distance between them.

Next we compute the so called conjugate momentum for each degree of freedom, for example, if we consider the coordinate $x_1$, then the corresponding conjugate momentum $p_{x_1}$, is:

\begin{equation}
p_{x_1} = \frac{\partial L}{\partial \dot{x}_1} = M \ddot{x}_1 \Rightarrow \ddot{x}_1 = \frac{p_{x_1}}{M}
\end{equation}

and similarly for other Lagrangian coordinates: $y_1$, $z_1$, $x_2$, $y_2$, $z_2$.

Next I write the Hamiltonian function of our mechanical system, which is defined by the subsequent formula:

\begin{equation}
\mathcal{H} = \sum_i q_i p_i - \hat{\mathcal{L}}
\end{equation}

where $q_i$ are the Lagrangian coordinates, namely $x_i$, $y_i$, $z_i$, and $p_i$ are the corresponding conjugate momentum, furthermore, the index $i$ of summation, runs over all the degrees of freedom. Finally the function $\hat{\mathcal{L}}$ is the same Lagrangian function, which is rewritten using the substitutions (1.2).

After a simple computation, we get the subsequent formula for the Hamiltonian of our mechanical system:

\begin{equation}
\mathcal{H} = \sum_i q_i p_i - \hat{\mathcal{L}} = \frac{p_{x_1}^2 + p_{y_1}^2 + p_{z_1}^2}{2M} + \frac{p_{x_2}^2 + p_{y_2}^2 + p_{z_2}^2}{2M} + V \left( |r_2 - r_1| \right)
\end{equation}

At this point, we are ready to give a Quantum Mechanical version of that Hamiltonian function, simply substituting each conjugate momentum with its corresponding operator, according to the principles of the same Quantum Mechanics. Nevertheless, before that, we want to give a more convenient form to our Hamiltonian function.

In order to do such proposal, I introduce two new coordinates:

$$r_G = \frac{Mr_1 + Mr_2}{2M}, \quad r = r_1 - r_2$$

which are the coordinate of the center of mass of the system, and the relative coordinate of the two points, respectively.

From the definitions above, we can write the position vectors $r_1$, $r_2$, like below:

$$r_1 = r_G + \frac{r}{2}, \quad r_2 = r_G - \frac{r}{2}$$

As we can see such equations are vector equations, so if we rewrite them using the components of their respective vectors, we get:
\begin{align*}
  x_1 &= x_G + \frac{x}{2}, \quad y_1 = y_G + \frac{y}{2}, \quad z_1 = z_G + \frac{z}{2}, \\
  x_2 &= x_G - \frac{x}{2}, \quad y_2 = y_G - \frac{y}{2}, \quad z_2 = z_G - \frac{z}{2}.
\end{align*}

Now, let’s consider the first scalar equation, and let’s multiply both sides by the mass $M$, here is what we get:

$$
Mx_1 = Mx_G + \frac{Mx}{2}
$$

which can be rewritten as follows:

$$
(1.4) \quad Mx_1 = \frac{M_{TOT}}{2}x_G + \mu x
$$

where $M_{TOT}$ is the total mass of our mechanical system, and $\mu$ is the reduced mass of such system, which, in turn, is defined as follows:

$$
\frac{1}{\mu} = \frac{1}{M} + \frac{1}{M}
$$

Of course, with the aid of the same procedure, we can write similar equations for the remaining degrees of freedom.

If we compute the first derivative of equation (1.4), we get:

$$
(1.5) \quad p_{x_1} = \frac{px_G}{2} + p
$$

As we can see, equation (1.5) expresses the momentum of particle $\#1$, along the $x-$axis, as a sum between the momentum $p_G$ of the center of mass of the system, and the momentum $p$ of the relative motion along the same $x-$axis. Again, similar equations can be written for the remaining degrees of freedom.

Finally, I substitute the equations (1.5) into the Hamiltonian (1.3), so I can write this:

$$
(1.6) \quad H = \frac{p_G^2}{2M_{TOT}} + \frac{p^2}{2\mu} + V(r) = H_G + H_{rel}
$$

where:

$$
H_G = \frac{p_G^2}{2M_{TOT}}, \quad H_{rel} = \frac{p^2}{2\mu} + V(r)
$$

As we can see, we have broken the full Hamiltonian function in two parts, the former $H_G$, which describes the motion of the center of mass of the system, and the latter $H_{rel}$, which describes the relative motion of the two particles.

2. The Ground State of the Deuteron

The deuteron is a bound state of the pair proton-neutron, with a binding energy $\epsilon = 2.226 \, \text{MeV}$ and a potential well of a square shape, defined as below:

$$
V(r) = \begin{cases} 
-V_0 = -35 \, \text{MeV}, & r \leq r_0 = 1.7 \cdot 10^{-13} \, \text{cm} \\
0, & r > r_0
\end{cases}
$$

In order to describe the relative motion of the pair neutron-proton, we can consider only the part $H_{rel}$ of the full Hamiltonian function:

$$
(2.1) \quad H_{rel} = \frac{p^2}{2\mu} + V(r)
$$
Subsequently I write the square of the momentum $p^2$ of the relative motion, using its Cartesian components:

$$p^2 = p_x^2 + p_y^2 + p_z^2$$

and after a substitution into the formula of $H_{rel}$, we can write this:

$$H_{rel} = \frac{1}{2\mu} \left( p_x^2 + p_y^2 + p_z^2 \right) + V(r)$$

The transition to Quantum Mechanics, can be made simply replacing $p_x$, $p_y$, $p_z$ with their corresponding operators:

$$p_x = -i\hbar \frac{\partial}{\partial x}, \quad p_y = -i\hbar \frac{\partial}{\partial y}, \quad p_z = -i\hbar \frac{\partial}{\partial z}$$

in doing so, I get the corresponding Hamiltonian operator $\hat{H}_{rel}$:

$$\hat{H}_{rel} = -\frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(r)$$

Such operator, can be used in order to write the Schrödinger Equation for relative motion of the neutron-proton system:

$$\left\{ -\frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(r) \right\} \psi = -\epsilon \psi$$

or in a more symbolic form:

$$\left\{ -\frac{\hbar^2}{2\mu} \Delta^2 + V(r) \right\} \psi = -\epsilon \psi$$

where the operator $\Delta^2$ is the Laplace operator.

We can simplify such equation, recalling that, the angular moment $l$ of the ground state of the deuteron is zero: $l = 0$. So the Schrödinger equation can be rewritten, like below:
\begin{equation}
\left\{ -\frac{\hbar^2}{2\mu} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + V(r) \right\} \psi = -\epsilon \psi
\end{equation}

Of course, the function $V(r)$ which appears in equation (2.4), can be replaced by the square potential well, defined at beginning of this section.

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