Mathematical Modelling of Bloch NMR to Solve the Schrödinger Time Dependent Equation

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Solutions of the Schrödinger are not new in Physics. The Bloch NMR was mathematically modeled to solve the time dependent Schrödinger equation to investigate various problems in physics and chemistry. The solution was validated on the harmonic oscillator and two energies were consequently solved. The relationship between relaxation and energy was found to be negatively parabolic.

1. Introduction

Many solutions have been propounded for Schrödinger's equation. The application of these solutions is restricted to a few aspects of physics. One of the methods used for solving the Schrödinger equation is the Finite Difference Time Domain (FDTD) method [1]. It was used to solve numerically the Schrödinger equation for ground state and excited state eigenvalues, and eigenfunctions for a single particle in one-, two-, and three-dimensional potential wells. In the past, analytical methods which have been used to solve the Schrödinger equation are: supersymmetry [1], Nikiforov Uvarov method (NU) [3], asymptotic iteration method (AIM) [4,5], hyperviria perturbation [6], exact quantization rule (EQR) [7], perturbative formalism [8], wave function ansatz method [9], and path integral [10]. In all these methods highlighted above, none has been incorporated with the Bloch NMR to solve nuclear spin among other problems in physics and chemistry.

The solution of the Schrödinger equation using the mathematical modeling of Bloch NMR has wide range of applications in many fields of physics and chemistry. It can be used for checking and improving models developed to study quantum mechanical systems, improve on the effective analysis of biological systems, analyzing spin transport, nuclear spin dynamics, improvement of the numerical methods and so on.

In Sec. 2, the solution of the Schrödinger is given. In Sec. 3, the solution was validated by applying it to the harmonic solution. The energy

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levels were calculated and features of its simulations were explained. It was observed that the energy and relaxation shows a negative parabolic shape, which explains that $T_1 \rightarrow 0$ when the energy levels increases.

2. Derivation of Solution

The Schrödinger equation in its time dependent format is given as

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V\Psi(x,t) \qquad (1)$$

From the above expression, $-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$ is known as the kinetic expression of Eqn. (1). The idea of equalizing kinetic energy and magnetic energy was explained in [11] by calculating the theoretical magnetic energy of the spins of classical electrons. It was therefore concluded that the magnetic energy of a moving charge changes as the charge of the electron moves with a changed velocity i.e., kinetic energy. Magnetic field (H) is therefore related to the kinetic energy of the Schrödinger as shown below.

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} = -m \cdot H(r,t) \qquad (2)$$

Where, m is the magnetic moment and *H(r,t)* is the magnetic H- field. The magnetic H-field is defined in a macroscopic equation as

$$H(r,t) = \frac{1}{\mu_o} B(r,t) - M(r,t) \qquad (3)$$

Where, the μ_o is permeability of free space, $M(r,t)$ is the magnetization field and $B(r,t)$ is the

magnetic B-field, which is assumed in the above expression as

$$B(r,t) = M_o \quad \text{and} \quad M(r,t) = M_z$$

Where, M_o is the equilibrium magnetization.

From the Bloch NMR equations given as

$$\frac{dM_x}{dt} = \Delta\omega M_y - \frac{M_x}{T_2} \qquad (4)$$

$$\frac{dM_y}{dt} = -\Delta\omega M_x - \omega_1 M_z - \frac{M_y}{T_2} \qquad (5)$$

$$\frac{dM_z}{dt} = -\omega_1 M_y - \frac{(M_z - M_o)}{T_1} \qquad (6)$$

$$\frac{dM_x}{dt} = \gamma(M_y B_o); \quad \frac{dM_y}{dt} = -\gamma(M_x B_o); \quad \frac{dM_z}{dt} = 0$$

Where, $\Delta\omega = \omega_1 - \omega_o$ is the frequency difference between Larmor frequency and the frame of reference, $\omega_1 = -\gamma B_1$ is the Rabi frequency, $\omega_o = -\gamma B_O$ is the Larmor frequency, M_x, M_y are the transverse magnetization, M_z is the longitudinal magnetization, and M_o is the equilibrium magnetization

Inserting Eqns. (2) and (3) into Eqns. (6) and (1) yields

$$i\hbar \frac{\partial\Psi(x,t)}{\partial t} = -m \cdot \omega_1 M_y T_1 \Psi(x,t) + V\Psi(x,t) \quad (7)$$

Both sides must be equal to a constant called E. Therefore, Eqn. (7) yields

$$i\hbar \frac{\partial\Psi(x,t)}{\partial t} = E = -m \cdot \omega_1 M_y T_1 \Psi(x,t) + V\Psi(x,t)$$

By separating the variables, we have

$$\Psi(x,t) = X(x)T(t)$$

$$\frac{i\hbar}{T}\frac{\partial\Psi(x,t)}{\partial t} = E \qquad (8)$$

$$(-m \cdot \omega_1 M_y T_1 + V)X(x) = E \qquad (9)$$

The solution of Eqn. (8) is

$$T = \alpha(0)\exp\left(\frac{Et}{i\hbar}\right) = \alpha(0)\exp(i\omega t) \qquad (10)$$

The solution of Eqn. (9)

$$X(x) = \frac{E}{(-m \cdot \omega_1 M_y T_1 + V(x))} \qquad (11)$$

The full wave function must therefore be a linear combination of these fundamental solutions (Eqns. (10) and (11)). Thus, the wave function can be written as

$$\Psi(x,t) = \frac{E\alpha(0)\exp(i\omega t)}{(-m \cdot \omega_1 M_y T_1 + V(x))} \qquad (12)$$

The solution (Eqn. (12)) can be written in the following format

$$\Psi(x,t) = \frac{E\alpha(0)\exp\left(\frac{Et}{i\hbar}\right)}{(-m \cdot \omega_1 M_y T_1 + V(x))} \qquad (13)$$

$$\Psi(x,t) = \frac{E\alpha(0)\exp(i\omega t)}{(-m \cdot M_x \frac{T_1}{T_2} + V(x))} \qquad (14)$$

$$\Psi(x,t) = \frac{E\alpha(0)\exp\left(\frac{Et}{i\hbar}\right)}{(-m \cdot M_x \frac{T_1}{T_2} + V(x))} \qquad (15)$$

The solution (Eqns. (12) and (13)) was verified with $i\hbar \frac{\partial\Psi(x,t)}{\partial t} = H\Psi(x,t)$

$$\frac{\partial\Psi(x,t)}{\partial t} = \frac{E}{i\hbar}\left[\frac{E\alpha(0)\exp\left(\frac{Et}{i\hbar}\right)}{(-m \cdot \omega_1 M_y T_1 + V(x))}\right]$$

Multiplying both sides by $i\hbar$

$$i\hbar \frac{\partial\Psi(x,t)}{\partial t} = E\left[\frac{E\alpha(0)\exp\left(\frac{Et}{i\hbar}\right)}{(-m \cdot \omega_1 M_y T_1 + V(x))}\right]$$

$$i\hbar \frac{\partial\Psi(x,t)}{\partial t} = E\Psi(x,t)$$

The above gives us the following equation.

$$E\Psi(x,t) = H\Psi(x,t)$$

3. Application of Solution to the Harmonic Oscillator

The application of Eqn. (12) to harmonic oscillator, which is characterized by a quadratic potential, $V = \frac{kx^2}{2}$, yields the following Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + \frac{kx^2}{2}\Psi(x) = E_l\Psi(x)$$

The above equation was solved using

$$\Psi(x) = \frac{E\alpha(0)}{(-m \cdot \omega_1 M_y T_1 + \frac{kx^2}{2})}$$

Since, the probability of a particle being found anywhere on the x-axis is 1, the above equation was therefore normalized to know the value of $\alpha(0)$.

$$\alpha(0) = m \cdot \omega_1 M_y T_1$$

The energies obtained are

$$E = -\frac{\hbar^2}{2m}(1 - kx^2) = -\frac{\hbar^2}{2m}(1 - \frac{v(x)}{2}) \qquad (16)$$

$$E = -m \cdot \omega_1 M_y T_1 + V(x) = -m \cdot \omega_1 M_y T_1 + \frac{kx^2}{2} \qquad (17)$$

4.   Results and Discussion

Fig. 1 describes a different idea of a particle in the box. The energy levels of harmonic oscillator for potential (V) are listed in Table 1 (shown below)

Table 1: Harmonic Oscillator's energy levels

Potential (V)	Energy (Eqn. (16)) (J)	Energy (Eqn. (17)) (J)
1	$-\frac{\hbar^2}{4m}$	$1 - m \cdot \omega_1 M_y T_1$
2	0	$2 - m \cdot \omega_1 M_y T_1$
3	$\frac{\hbar^2}{4m}$	$3 - m \cdot \omega_1 M_y T_1$
4	$\frac{\hbar^2}{2m}$	$4 - m \cdot \omega_1 M_y T_1$
5	$\frac{3\hbar^2}{4m}$	$5 - m \cdot \omega_1 M_y T_1$

Fig. 2 shows the same effect as in Fig. 1. This means that by application the solution (Eqn. (17)) in operation is almost equal to the solutions in Eqn. (16). The effect of relaxation on both the Energy levels and potentials were shown in Fig. 3. The energy and relaxation shows a negative parabolic shape, which explains that $T_1 \to 0$ when the energy levels increase. The positive parabolic relation between energy levels and potentials is the usual relation as proven by former researchers. A solution was derived under the influence of two relaxations, T_1 & T_2 as can be seen in Eqns. (14) and (15), This has the potential of applying the solutions to magnetic resonance inference (MRI); analysis of dual spins (hole [12,13] and electron spins [14,16]) as present in semiconductors, spin

dependent hyperfine interaction (HFI), and anisotropic part of the Zeeman interaction (AZI) [16] amongst others. Also, figure 3 describes the relationship between potential and relaxation negatively linear.
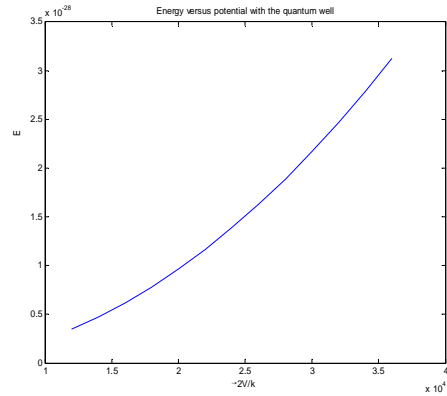

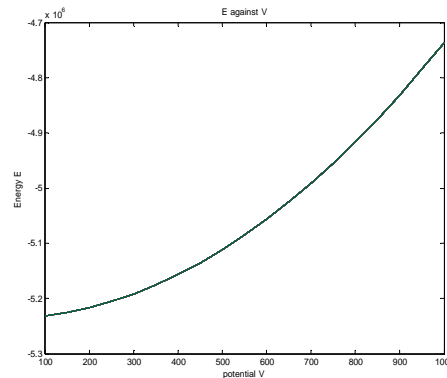Fig.1: The graph of Energy against (-2/k) potential. A graphical solution of Eqn. (16).

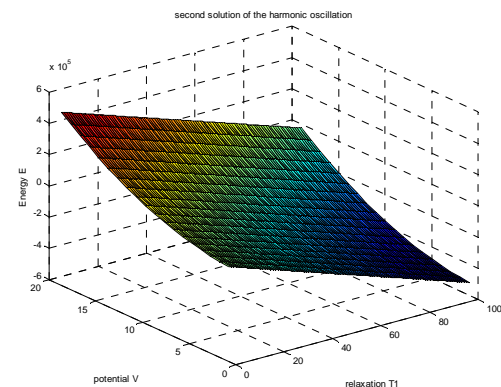Fig.2: The graph of energy against potential. A graphical solution of Eqn. (17).

Fig.3: A general solution of Eqn. (17) when $T_1 < 100$.

5. Conclusion

The introduction of the Bloch NMR equation into Schrödinger equation has shown success in predicting well established features of the harmonic oscillator. The concept of this paper is defining a clear research pathway towards investigating into spin dynamics, biological structure, and chemical bonding structure amongst other.

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