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Analytical Solutions of a Three Dimensional Time-Dependent Schrödinger Equation Using the Bloch NMR Approach for NMR Studies

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Abstract

The three dimensional time dependent Schrödinger equation was solved using the Bloch NMR approach with the help of the hermit differential polynomial. Its solution shed more light on the nature of the transverse magnetization. It was discovered that the transverse and longitudinal magnetization is the same mathematical but may vary with respect of the speed of the particles. This gives the theory wide range application in semiconductors, superconductivity and spintronics.

Keywords: Bloch NMR, Schrodinger Equation, Characteristics Energy, Wave function, Potential

1. INTRODUCTION

Solutions of the one dimensional Schrodinger equation has been discussed in many literatures in mathematics and physics[1- 9] with few objections and modifications [10]. Its application was limited to solving known quantum problems in physics. The emergence of the three dimensional Schrödinger equation and its acceptability is most widely discussed because of its applicability in versed fields of physics, chemistry and material science. The quantum dot among other applications of three dimensional Schrödinger equation has been widely discussed e.g. material analysis [11],light emitting diode [12,13],biological systems[14,15], Chemical composition gradient [16],Computation[17], chemical and biological sensors[18] e.t.c.

Like the one dimensional Schrödinger equation, the three dimensional time-dependent Schrödinger equation have also been solved using different methods i.e. Symplectic splitting operator methods [19]; Exact solutions [20]; Multiconfiguration Time-Dependent Hartree (MCTDH) Method [21, 22]; finite difference methods [23]. Fundamentally, solving a known problem in physics should follow basic principle, though there is room for improvements.

The application of the three dimensional Schrödinger equation in nuclear magnetic resonance(NMR) and magnetic resonance imaging(MRI) have not been so much explored to solve problems in medical imaging, crystallography, ultra short strong laser pulses, biological systems (e.g molecular sensing), chemical structures and composition, spin dynamics of superconductors and semiconductors. The idea of this paper is to introduce a new perspective into analyzing the above mentioned problems.

2. DERIVATION OF THEORY

The three dimensional time-dependent Schrödinger equation is given as

$$-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}+V(x,y,z,t)\right)\Psi(\mathrm{x,y,z,t})=\mathrm{i}\frac{\partial\Psi(\mathrm{x,y,z,t})}{\partial \mathrm{t}} \qquad (1)$$

From the above expression, the first task is to equalize the kinetic energy of equation (1) to the magnetic energy which has been calculated by Togt (23). The first derivations are

$$\frac{\partial^2}{\partial x^2}=\frac{m}{\hbar}\left(\mu.H(\mathrm{x,y,z,t})\right)$$

$$\frac{\partial^2}{\partial y^2} = \frac{m}{\hbar}\left(\mu . H(\mathrm{x, y, z, t})\right)$$

$$\frac{\partial^2}{\partial z^2} = \frac{m}{\hbar}\left(\mu . H(\mathrm{x, y, z, t})\right)$$

Where μ is the magnetic moment and H(r,t) is the magnetic H field.

The assumption of Togt [24] was that the magnetic energy emerged as the charge of the electron moves with a changing velocity i.e kinetic energy. Magnetic field ($H(\mathrm{x, y, z, t})$) is further analyzed macroscopically as

$$H(\mathrm{x, y, z, t}) = \frac{1}{\mu_o}\mathrm{B}(\mathrm{x, y, z, t}) - M(\mathrm{x, y, z, t})$$

Since an external magnetization is not applied in this experiment, $B(\mathrm{x, y, z, t}) = 0$

Therefore

$$H(\mathrm{x, y, z, t}) = -M(\mathrm{x, y, z, t})$$

The magnetic field $M(\mathrm{x, y, z, t})$ is further analyzed as

$$M(\mathrm{x, y, z, t}) = \frac{\mathrm{dM_x}}{\mathrm{dx}} + \frac{\mathrm{dM_y}}{\mathrm{dy}} + \frac{\mathrm{dM_z}}{\mathrm{dz}}$$

$$M(\mathrm{x, y, z, t}) = \frac{\mathrm{dM_x}}{\mathrm{dt}}.\frac{\mathrm{dt}}{\mathrm{dx}} + \frac{\mathrm{dM_y}}{\mathrm{dt}}.\frac{\mathrm{dt}}{\mathrm{dy}} + \frac{\mathrm{dM_z}}{\mathrm{dt}}.\frac{\mathrm{dt}}{\mathrm{dz}}$$

Where $\frac{\mathrm{dt}}{\mathrm{dx}} = \frac{1}{\mathrm{v_x}}$, $\frac{\mathrm{dt}}{\mathrm{dy}} = \frac{1}{\mathrm{v_y}}$, $\frac{\mathrm{dt}}{\mathrm{dz}} = \frac{1}{\mathrm{v_z}}$

Equation [1] transforms to

$$-\frac{1}{2}\left(\frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}} + \frac{m\mu}{\hbar v_y}\frac{\mathrm{dM_y}}{\mathrm{dt}} + \frac{m\mu}{\hbar v_z}\frac{\mathrm{dM_z}}{\mathrm{dt}} + V(x, y, z, t)\right)\Psi(\mathrm{x, y, z, t}) = \mathrm{i}\frac{\partial\Psi(\mathrm{x,y,z,t})}{\partial \mathrm{t}} \tag{2}$$

Equation [2] yields the following set of equations

$$-\frac{1}{2}\left(\frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}} + V(x)\right)\Psi(\mathrm{x, t}) = \mathrm{i}\frac{\partial\Psi(\mathrm{x,t})}{\partial \mathrm{t}} \tag{3}$$

$$-\frac{1}{2}\left(\frac{m\mu}{\hbar v_y}\frac{\mathrm{dM_y}}{\mathrm{dt}}+V(y)\right)\Psi(\mathrm{y,t})=\mathrm{i}\frac{\partial\Psi(\mathrm{y,t})}{\partial\mathrm{t}} \tag{4}$$

$$-\frac{1}{2}\left(\frac{m\mu}{\hbar v_z}\frac{\mathrm{dM_z}}{\mathrm{dt}}+V(z)\right)\Psi(\mathrm{z,t})=\mathrm{i}\frac{\partial\Psi(\mathrm{z,t})}{\partial\mathrm{t}} \tag{5}$$

Both sides of the equations [3-5] are equated to a constant E.

$$-\frac{1}{2}\left(\frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}}+V(x)\right)\Psi(\mathrm{x,t})=\mathrm{E}=\mathrm{i}\frac{\partial\Psi(\mathrm{x,t})}{\partial\mathrm{t}} \tag{6}$$

$$-\frac{1}{2}\left(\frac{m\mu}{\hbar v_y}\frac{\mathrm{dM_y}}{\mathrm{dt}}+V(y)\right)\Psi(\mathrm{y,t})=\mathrm{E}=\mathrm{i}\frac{\partial\Psi(\mathrm{y,t})}{\partial\mathrm{t}} \tag{7}$$

$$-\frac{1}{2}\left(\frac{m\mu}{\hbar v_z}\frac{\mathrm{dM_z}}{\mathrm{dt}}+V(z)\right)\Psi(\mathrm{z,t})=\mathrm{E}=\mathrm{i}\frac{\partial\Psi(\mathrm{z,t})}{\partial\mathrm{t}} \tag{8}$$

Using separation of variables

$$\Psi(\mathrm{x,t})=\mathrm{X(x)T(t)},\ \ \Psi(\mathrm{y,t})=\mathrm{Y(y)T(t)},\ \ \Psi(\mathrm{z,t})=\mathrm{Z(z)T(t)}, V(x)=V(y)=V(z)=0$$

$$\mathrm{T(t)}=\alpha(0)\exp(-\mathrm{i}\omega\mathrm{t})$$

The constant $\alpha(0)$ was calculated as $\alpha(0)=\frac{1}{(2\mathrm{i}\omega\mathrm{t})^{\frac{1}{2}}\pi^{\frac{1}{4}}}$ to give

$$\mathrm{T(t)}=\frac{1}{(2\mathrm{i}\omega\mathrm{t})^{\frac{1}{2}}\pi^{\frac{1}{4}}}\exp(-\mathrm{i}\omega\mathrm{t})$$

The second term of the variables is written as

$$\left(\frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}}\right)\mathrm{X}=\mathrm{EX}$$

$$\frac{m\mu}{\hbar v_x}\left(X\frac{\mathrm{dM_x}}{\mathrm{dt}}+\mathrm{M_x}\frac{\mathrm{dX}}{\mathrm{dt}}\right)=EX$$

$$X'=\frac{1}{\mathrm{M_x}}\left(E-\frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}}\right)X \tag{9}$$

Since the solution of equation [9] is paramount, the differential equation of the hermit polynomial is applied to simplify it. The differential equation of the hermit polynomial is given as

$$y''(x) - 2xy'(x) + 2\varepsilon y(x) = 0 \tag{10}$$

Equations [10] fits into equation (9) where $y''(x) = 0$, $y'(x) = X'$, $y(x) = X$,

$$\varepsilon = \frac{1}{2M_x}\left(E - \frac{m\mu}{\hbar v_y}\frac{\mathrm{dM_x}}{\mathrm{dt}}\right)$$

Therefore the hermit differential polynomial takes the new form

$$-2xX' - 2\varepsilon X = 0 \tag{11}$$

Let $p = \sum_{n=0}^{\infty} c_n\, x^n$. This generated a relationship as shown

$$c_{n+1} = -\frac{\varepsilon}{n(n+1)}c_n$$

Where $c_1 = -\varepsilon c_0$

The solution of the first part of equation[11] is

$$X_1 = c_0\left[-\frac{\left(\frac{1}{2M_x}\left(E-\frac{m\mu\mathrm{dM_x}}{\hbar v_x\ \mathrm{dt}}\right)\right)}{2} - \frac{\left(\frac{1}{2M_x}\left(E-\frac{m\mu\mathrm{dM_x}}{\hbar v_x\ \mathrm{dt}}\right)\right)^3}{12} - \frac{\left(\frac{1}{2M_x}\left(E-\frac{m\mu\mathrm{dM_x}}{\hbar v_x\ \mathrm{dt}}\right)\right)^5}{2880}\right]$$

$$X_2 = c_1\left[-\frac{\left(\frac{1}{2M_x}\left(E-\frac{m\mu\mathrm{dM_x}}{\hbar v_x\ \mathrm{dt}}\right)\right)}{2} - \frac{\left(\frac{1}{2M_x}\left(E-\frac{m\mu\mathrm{dM_x}}{\hbar v_x\ \mathrm{dt}}\right)\right)^3}{144} - \frac{\left(\frac{1}{2M_x}\left(E-\frac{m\mu\mathrm{dM_x}}{\hbar v_x\ \mathrm{dt}}\right)\right)^5}{86400}\right]$$

On the assumption that $c_0 = \exp(ikx)$ and $c_1 = \exp(-ikx)$. The second term was considered (the first term was discarded because they are equal and the third term was discarded due to complexities). Applying an assumed general solution of $X(x) = X_1 + X_2$, therefore

$$X(x) = \frac{1}{24M_x}\left(E - \frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}}\right)\exp(ikx) + \frac{1}{144M_x}\left(E - \frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}}\right)\exp(-ikx) \tag{12}$$

Equation [12] can be written in the format $X(x) = A\sin(kx) + B\cos(kx)$

Where $A = \frac{1}{24M_x}\left(E - \frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}}\right)$, $B = \frac{1}{144M_x}\left(E - \frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}}\right)$, $k = \frac{n\pi}{L}$

Applying the boundary conditions $x = 0$ and $x = L$, the constant E was calculated as shown below

$E = \frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}}$ or $144M_x\sqrt{\frac{2}{L}} - \frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}}$

Therefore,

$$X(x) = \frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}}\sin\left(\frac{n\pi}{L}x\right) \quad \text{or} \quad X(x) = \left(144M_x\sqrt{\frac{2}{L}} - \frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}}\right)\sin\left(\frac{n\pi}{L}x\right) \tag{13}$$

Likewise,

$$Y(y) = \frac{m\mu}{\hbar v_y}\frac{\mathrm{dM_y}}{\mathrm{dt}}\sin\left(\frac{n\pi}{L}y\right) \tag{14}$$

or

$$Y(y) = \left(144M_y\sqrt{\frac{2}{L}} - \frac{m\mu}{\hbar v_y}\frac{\mathrm{dM_y}}{\mathrm{dt}}\right)\sin\left(\frac{n\pi}{L}y\right) \tag{15}$$

$$Z(z) = \frac{m\mu}{\hbar v_z}\frac{\mathrm{dM_z}}{\mathrm{dt}}\sin\left(\frac{n\pi}{L}z\right) \tag{16}$$

or

$$Z(z) = \left(144M_z\sqrt{\frac{2}{L}} - \frac{m\mu}{\hbar v_z}\frac{\mathrm{dM_z}}{\mathrm{dt}}\right)\sin\left(\frac{n\pi}{L}z\right) \tag{17}$$

The validity of equations[12-17] was tested using $\frac{X(x)''}{X(x)} - \frac{Y(y)''}{Y(y)} - \frac{Z(z)''}{Z(z)}$

$$\frac{X(x)''}{X(x)} - \frac{Y(y)''}{Y(y)} - \frac{Z(z)''}{Z(z)} = -\frac{{n_x}^2\pi^2}{L^2} - \frac{{n_y}^2\pi^2}{L^2} - \frac{{n_z}^2\pi^2}{L^2} = -\frac{2ME}{\hbar^2} \tag{18}$$

The solution of equation [18] gave $-\frac{2ME}{\hbar^2}$ which gave an allowed energy (as shown below)

$$E = \frac{\pi^2\hbar^2}{2ML^2}\left({n_x}^2 + {n_y}^2 + {n_z}^2\right)$$

The wave function can be resolved as follows

$$\Psi(\mathrm{x},\mathrm{t}) = \frac{1}{(2\mathrm{i}\omega\mathrm{t})^{\frac{1}{2}}\pi^{\frac{1}{4}}}\cos(\omega\mathrm{t})\,\frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}}\sin\left(\frac{n\pi}{L}x\right)$$

$$\Psi(\mathrm{x},\mathrm{t}) = \frac{1}{(2\mathrm{i}\omega\mathrm{t})^{\frac{1}{2}}\pi^{\frac{1}{4}}}\cos(\omega\mathrm{t})\sin\left(\frac{n\pi}{L}x\right)\left(144M_x\sqrt{\frac{2}{L}} - \frac{m\mu}{\hbar v_x}\frac{\mathrm{dM_x}}{\mathrm{dt}}\right) \tag{19}$$

$$\Psi(\mathrm{y},\mathrm{t}) = \frac{1}{(2\mathrm{i}\omega\mathrm{t})^{\frac{1}{2}}\pi^{\frac{1}{4}}}\cos(\omega\mathrm{t})\,\frac{m\mu}{\hbar v_y}\frac{\mathrm{dM_y}}{\mathrm{dt}}\sin\left(\frac{n\pi}{L}x\right)$$

$$\Psi(\mathrm{y},\mathrm{t}) = \frac{1}{(2\mathrm{i}\omega\mathrm{t})^{\frac{1}{2}}\pi^{\frac{1}{4}}}\cos(\omega\mathrm{t})\sin\left(\frac{n\pi}{L}x\right)\left(144M_y\sqrt{\frac{2}{L}} - \frac{m\mu}{\hbar v_y}\frac{\mathrm{dM_y}}{\mathrm{dt}}\right) \tag{20}$$

$$\Psi(\mathrm{z},\mathrm{t}) = 0 \tag{21}$$

Applying the boundary conditions $x = 0$ and $x = L$, the wave function is equal to zero and takes the format

$$\frac{n\pi}{a} = bM_x + c\dot{M}_x$$

$a = \frac{1}{(2\mathrm{i}\omega\mathrm{t})^{\frac{1}{2}}\pi^{\frac{1}{4}}}\cos(\omega\mathrm{t})\sin\left(\frac{n\pi}{L}x\right)$, $b = 144\sqrt{\frac{2}{L}}$, $c = \frac{m\mu}{\hbar v_x}$,

$$\mathrm{M_y} = \frac{\sin\left(\frac{n\pi}{L}x\right)}{(2\mathrm{i}\omega)^{\frac{1}{2}}\pi^{\frac{1}{4}}}\left(\exp\left(\frac{144\sqrt{\frac{2}{L}}\hbar v_x}{m\mu}\right)\right)\left(-\frac{\mathrm{t}^{1/2}\cos(\omega\mathrm{t})}{2\omega^2} + \frac{\omega^2\mathrm{t}^{-1/2}-2}{\omega^3}\sin(\omega\mathrm{t})\right) + \mathrm{C}\exp\left(\frac{144\sqrt{\frac{2}{L}}\hbar v_x}{m\mu}\right) \tag{22}$$

Assuming $\exp\left(\frac{144\sqrt{\frac{2}{L}}\hbar v_x}{m\mu}\right) \ll \left(-\frac{\mathrm{t}^{1/2}\cos(\omega\mathrm{t})}{2\omega^2} + \frac{\omega^2\mathrm{t}^{-1/2}-2}{\omega^3}\sin(\omega\mathrm{t})\right)$ and $\frac{\sin\left(\frac{n\pi}{L}x\right)}{(2\mathrm{i}\omega)^{\frac{1}{2}}\pi^{\frac{1}{4}}} = 1$

Equation [22] reduces to

$$\mathrm{M_y} = \mathrm{A}\sin(\omega\mathrm{t}) - \mathrm{B}\cos(\omega\mathrm{t}) \tag{23}$$

Where $A = \frac{\omega^2 t^{-1/2} - 2}{\omega^3}$ and $B = \frac{t^{1/2}}{2\omega^2}$ are constants which generates infinitely many solutions. The physical interpretations of equations (24) is its applicability to resolving NMR, MRI and MQ NMR problems with respect to time and frequency. The transverse magnetization is therefore obtained.

RESULTS AND DISCUSSION

The introduction of the Bloch NMR had no effect on the basics of the Schrödinger solutions. For example, equations (12-17) yielded the allowed energy equations without any additional term. This validated the basic quantum mechanics and certified the solutions of the wave functions valid-to solving problems relating to spintronics, biophysics, chemical reaction analysis semiconductors and superconductivity. A general solution (equation[23]) for the transverse magnetizations was obtained which must be true in all cases the time should be almost equal to quadro-inverse of the larmour frequency. At this condition, equation (23) is written as

$$M_y = A\sin(\omega t) \tag{24}$$

This is solution expected to open up the dynamics of NMR, MRI and MQ NMR .

CONCLUSION

The theory of the three dimensional time–dependent Schrödinger-Bloch solution satisfied the basic concept of quantum physics. Thereby giving the solutions as stated in equation (19-21) a fundamental prospect towards expanding past research done in various field of physics, chemistry, material science etc.

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