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**PROCEEDINGS OF THE FIRST  
INTERNATIONAL SEMINAR ON  
THEORETICAL PHYSICS &  
NATIONAL DEVELOPMENT**

*(A TRIBUTE TO PROFESSOR EMERITUS ALEX ANIMALU @70)*

Abuja, Nigeria      August 26-28, 2008

Editors

Godfrey E. Akpojotor

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## **Preface**

This volume contains papers presented at the First International Seminar on Theoretical Physics and National Development (ISOTPAND08) held at the Merit House (Abuja, Nigeria) from August 25- 29, 2008. This first meeting was to pay tribute to Emeritus Professor Alexander Obiefoka Eukora Animalu who joined the prestigious 'Age Club' of three scores and ten on August 28, 2008, The event recorded a huge success because it was seen by all as an opportunity to give honour to who it was due.

The opening ceremony on August 26 was under the chairmanship of the President of the Nigerian Academy of Science (represented by Professor Ephraim Okon, FAS). The highlights included an overview by Professor Animalu of a compendium of research output in physics in the past four decades (1965-2005) from 36 Nigerian Universities founded before 1999 and the presentation of a biography of Professor Animalu written by G.E. Akpojotor and J. Unaegbu. This was followed by the technical sessions which were richly informative and motivational as they were a combination of both pedagogical and advanced contents to cut across all the participants made up of senior and junior researchers, postdocs, graduate and undergraduate students. The closing ceremony was the birthday dinner on August 28, where encomiums rolled out from various groups including the foreign distinguished researchers who had read and were inspired in their graduate studies by both the English and Russian versions of Professor Animalu's 1977 Prentice-Hall-published book '*Intermediate Quantum Theory of Crystalline Solids.*' Indeed it was a great moment for Nigeria science in particular and scholarship in general.

The success of ISOTPAND08 motivated both the organizers (scientific committee) and the participants to reach the decision that ISOTPAND should become an annual event and should remain a forum for bringing senior researchers and eager beginners together. It was also decided that the proceedings of each event should be published after the papers contributed by participants have been peer-reviewed. It is hoped therefore that this first volume will be very useful to the scientific community.

We wish to acknowledge the main sponsor of ISOTPAND08 – the International Centre for Basic Research, Abuja – and the financial support of the following bodies: National Mathematical Centre, Raw Material and Research Development Council, National Office for Technology Acquisition and Promotion (NOTAP), National Universities Commission, Nigerian Energy Commission, and University of Nigeria, Nsukka, as well as other individual donors. We also acknowledge the commitment of all the participants to the success of the event. Finally, we express our appreciation to members of the local organizing committee and international scientific committee of the event for their various contributions.

Editors

Godfrey E. Akpojotor

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**TABLE OF CONTENTS**

<i>SPONSORING ORGANISATIONS.....</i>	<i>II</i>
<i>INTERNATIONAL SCIENTIFIC COMMITTEE OF ISOTPAND.....</i>	<i>III</i>
<i>PREFACE.....</i>	<i>IV</i>
<i>TABLE OF CONTENTS.....</i>	<i>VI</i>
<i>COMPENDIUM OF FOUR DECADES OF PHYSICS R &amp; D IN 36</i> <i>UNIVERSITIES IN NIGERIA.....</i>	<i>1</i>
A. O.E. Animalu .....	1
<i>A SOLUTION TO THE BAND GAP CATASTROPHE: PREDICTIVE</i> <i>CALCULATIONS OF PROPERTIES OF SEMICONDUCTORS AND OF</i> <i>NUCLEI.....</i>	<i>15</i>
Diola Bagayoko .....	15
<i>FULL POTENTIAL – LINEARIZED AUGMENTED PLANE WAVE (FP-LAPW)</i> <i>IN THE FRAMEWORK OF DENSITY FUNCTIONAL THEORY.....</i>	<i>36</i>
C.A. Madu and B.N Onwuagba.....	36
<i>A PHENOMENOLOGICAL APPROACH TO A MODEL OF SUPEREXCHANGE</i> <i>INTERACTIONS IN OPTICAL WELLS.....</i>	<i>43</i>
Godfrey E. Akpojotor and Weibin Li .....	43
<i>THE FEW-ELECTRON INTERACTION IN THE GROUND STATE OF</i> <i>STRONGLY CORRELATED ELECTRON SYSTEMS: A</i> <i>COMPUTATIONAL APPROACH.....</i>	<i>55</i>
J. O. A. Idiodi et al.....	55
<i>APPLICATION OF MATLAB IN AN EXACT COMPARATIVE NUMERICAL</i> <i>ANALYSIS OF THE 2-D ATTRACTIVE AND REPULSIVE HUBBARD</i> <i>MODEL.....</i>	<i>75</i>
PATRICK O. AKUSU .....	75
<i>SPECTROSCOPY STUDY OF THE LIGHT – HEAVY <math>\Lambda</math>-HYPERNUCLEI USING</i> <i>THE QUANTUM MECHANICAL HYPERVIRIAL THEOREMS.....</i>	<i>100</i>
OYEWUMI, K. J. ....	100
<i>REVIEW OF DEEP-INELASTIC ELECTRON-PROTON SCATTERING: A</i> <i>HADRONIC MECHANICS VIEWPOINT.....</i>	<i>133</i>

A.O.E. ANIMALU AND C.E. EKUMA.....	133
<i>RICCATI EQUATION IN BIOPHYSICS AND OTHER PHYSICAL PHENOMENA</i>	<i>154</i>
Tertsega Tivde and A.O.E. Animalu.....	154
<i>MATHEMATICAL ANALYSIS OF ADIABATIC MODEL OF BLOCH NMR FLOW EQUATIONS FOR FUNCTIONAL MAGNETIC RESONANCE IMAGING</i> .....	<i>177</i>
Awojoyogbe O. B <i>et al.</i> .....	177
<i>B-TRANSFORM AND APPLICATION TO THE SICKLE CELL MODELS</i> .....	<i>202</i>
Oyelami, B.O. <i>et al.</i> .....	202
<i>COMPARATIVE ANALYSES OF ATMOSPHERIC CO<sub>2</sub> AND CO CONCENTRATIONS OVER ISSYK-KUL, KYRGYZSTAN</i> .....	<i>221</i>
F.N. Okeke and E.A.Hanson.....	221
<i>AIR QUALITY MANAGEMENT IN NIGERIA – PROBLEMS AND CTS</i> .....	<i>229</i>
J. U. UGWUANYI.....	229
<i>SHALLOW WATER FLOW OVER A VARYING NON-UNIFORM BOTTOM REGION</i> .....	<i>238</i>
G C E Mbah.....	238
<i>LANGUAGE AND DIMENSIONALITY IN PHYSICS: THE PROSPECT OF AFRICAN RENASCENCE</i> .....	<i>255</i>
A.O.E. Animalu and A.O. Azali.....	255
<i>CLASSICAL FOUNDATIONS:TWO VERSIONS OF MAXWELL’S EQUATIONS</i>	<i>284</i>
Tepper L. Gill and Woodford W. Zachary.....	284
<i>THE AFRICAN SCIENTIFIC NETWORK AND PHYSICS EDUCATION IN AFRICA</i> .....	<i>321</i>
Abebe Kebede.....	321
<i>DEVELOPING COMPUTATIONAL PHYSICS IN SOUTH AFRICA</i> .....	<i>341</i>
Nithaya Chetty .....	341

## **MATHEMATICAL ANALYSIS OF ADIABATIC MODEL OF BLOCH NMR FLOW EQUATIONS FOR FUNCTIONAL MAGNETIC RESONANCE IMAGING**

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### **Abstract**

In this contribution, solutions to the Bloch NMR flow equations in the form of polynomials are presented. The polynomials are obtained in terms of trigonometric, algebraic, ordinary and special functions. By means of these polynomials, appropriate mathematical algorithms are developed to consider the motion of a blood molecule of mass  $m$  as a function of coordinate  $x$  alone. We derived the first integral (constant of the motion) and energy integral for the blood molecule. The energy integral gives us specific information about the motion of the blood molecule (oxyhemoglobin molecule or molecule of some other chemicals in the brain that take part in NMR signal production) depending on the energy required by neurons when subjected to various degree of excitation. This mathematical model and analysis may be very significant to explain the motion of the molecules of each fluid substance that is responsible for specific task performed by the brain. The dynamics of NMR signal as developed in terms of sine and cosine functions can be additional important tools that can help to see the direct relationship between changes in blood flow to the brain and neural communication.

**Keyword:** Bloch NMR flow equations, NMR transverse magnetization model polynomials, functional magnetic resonance imaging.



## **1. Introduction**

When there is an increased activity in the brain, blood is drawn faster through the flow system, this results in correspondence increase in signal intensity on the magnetic resonance (MRI) scan. Changes in blood flow and blood oxygenation in the brain (collectively known as hemodynamics) are closely linked to neural activity. When nerve cells are active they consume oxygen carried by hemoglobin in red blood cells from local capillaries. The local response to this oxygen utilization is an increase in blood flow to regions of increased neural activity. This hemodynamic response leads to local changes in the relative concentration of oxyhemoglobin and deoxyhemoglobin and changes in local cerebral blood volume in addition to this change in local cerebral blood flow. Functional MRI is based on the increase in blood flow to the local vasculature that accompanies neural activity in the brain. This result in a corresponding local reduction in deoxyhemoglobin because the increase in blood flow occurs without an increase of similar magnitude in oxygen extraction. Deoxyhemoglobin is paramagnetic therefore alters the  $T_2^*$  weighted magnetic resonance image signal [1-8]. Thus, deoxyhemoglobin is sometimes referred to as an endogenous contrast enhancing agent, and serves as the source of the signal for fMRI.

It is well known that when there is an increase in brain activity, oxygen is needed in the conversion of some substances into energy which the brain cells need to carry out specific tasks. However, It is not known whether the NMR signal observed in the brain fMRI is not a function of oxyhemoglobin alone but that some other chemicals in the brain take part in the signal production. It may be possible that other NMR sensitive chemicals are the source of the NMR signal that is observed. These other NMR sensitive chemicals may be the most important in brain metabolism. We know that an increase in blood flow to any part of the brain is caused by an increase in metabolic rate (or an increase in energy need of the excited neuron) in the area and thus a proportionate increase in the rate of neural communication. Solutions to the Bloch NMR flow equations in the form of polynomials which can be taken as the definitions of new NMR functions as presented in this paper can provide required mathematical algorithms and computational methods to reveal specific information needed to identify the NMR sensitive chemicals most important in brain metabolism.

## 2. Mathematical Method

We study the flow properties of the modified time independent Bloch NMR flow equation which describes the dynamics of blood flow under the influence of rF magnetic field as derived in the earlier studies [9].

For steady flow

$$\frac{\partial M_y}{\partial t} = 0 \quad (1)$$

$$V^2 T_1^2 \frac{d^2 M_y}{dx^2} + VT_1^2 \left( \frac{1}{T_1} + \frac{1}{T_2} \right) \frac{dM_y}{dx} + T_1^2 \left( \gamma^2 B_1^2(x) + \frac{1}{T_1 T_2} \right) M_y = T_1 M_o \gamma B_1(x) \quad (2)$$

Two reasonable initial boundary conditions which may conform to the real-time experimental arrangements were chosen. These are:

1.  $M_o \neq M_z$  a situation which holds good in general and in particular when the rF  $B_1(x)$  field is strong say of the order of 1.0G or more.

2. before entering signal detector coil, fluid particles has magnetization

$$M_x = 0, M_y = 0$$

If  $B_1(x)$  is large;  $B_1(x) \gg 1G$  or more so that  $M_y$  of the blood bolus changes appreciably from  $M_o$ .

Resonance condition exists at Larmor frequency

$$f_o = \gamma B - \omega = 0 \quad (4)$$

based on the following adiabatic condition

$$\gamma^2 B_1^2(x) \gg \left( \frac{1}{T_1 T_2} \right) \quad (5)$$

where  $\gamma$  denotes the gyromagnetic ratio of fluid spins;  $\omega/2\pi$  is the rF excitation frequency;  $f_o/\gamma$  is the off- resonance field in the rotating frame of reference.  $T_1$  and  $T_2$  are the spin-lattice and spin-spin relaxation times respectively. Equation (2) can be written as

$$V^2 T_1^2 \frac{d^2 M_y}{dx^2} + VT_1^2 \left( \frac{1}{T_1} + \frac{1}{T_2} \right) \frac{dM_y}{dx} + n^2 M_y = n T_1 M_o \quad (6)$$

where

$$VT_1 = \sqrt{1-x^2} \quad (7)$$

$$VT_1 = \frac{-4xT_2}{(T_1 + T_2)} \quad (8)$$

The parameter n is a real constant which completely defines the rF B<sub>1</sub> field of the NMR system.

$$n = \gamma B_1 \quad (9)$$

When the rF B<sub>1</sub> field is applied, M<sub>y</sub> has a maximum value when rF B<sub>1</sub> is maximum and M<sub>0</sub> = 0. At the point when the maximum NMR signal is received (maximum values of M<sub>y</sub> and rF B<sub>1</sub>, respectively), equation (6) becomes

$$V^2 T_1^2 \frac{d^2 M_y}{dx^2} + VT_1^2 \left( \frac{1}{T_1} + \frac{1}{T_2} \right) \frac{dM_y}{dx} + n^2 M_y = 0 \quad (10)$$

where n is a real constant. The solutions of equation (10) are obtained by power series:

$$M_y = \sum_{p=0}^{\infty} n_p x^p \quad (11)$$

The general recurrence relation can be written as

$$n_{p+2} = \frac{p^2 - n^2}{(p+1)(p+2)} n_p \quad (12)$$

From equation (12), we obtain for the even coefficients n = 2p

$$n_{even} = n_o \prod_{j=1}^{k/2} (k-2j)^2 - n^2 = \frac{2^{k-1} \pi n \csc\left(\frac{1}{2} \pi n\right)}{\Gamma\left(1 - \frac{1}{2}k - \frac{1}{2}n\right) \Gamma\left(1 - \frac{1}{2}k + \frac{1}{2}n\right)} \alpha_0 \quad (13)$$

and the odd coefficients n = 2p-1 as

$$n_{odd} = n_1 \prod_{j=1}^{(k-1)/2} (k-2j)^2 - n^2 = \frac{2^{k-1} \pi n \sec\left(\frac{1}{2} \pi n\right)}{\Gamma\left(1 - \frac{1}{2}k - \frac{1}{2}n\right) \Gamma\left(1 - \frac{1}{2}k + \frac{1}{2}n\right)} n_1 \quad (14)$$

The general solution is obtained in closed form as

$$M_y = n_0 \cos(n \sin^{-1} x) + \frac{n_1}{n} \sin(n \sin^{-1} x) \quad (15)$$

Performing a change of variables gives the equivalent form of the solution

$$M_y = c_1 \cos(n \sin^{-1} x) + c_2 \sin(n \sin^{-1} x) = c_3 M_n(x) + c_4 V_{real} M_{n-1}^*(x) \quad (16)$$

where

$$M_n(x) = \frac{n}{2} \sum_{k=0}^{n/2} (-1)^k \frac{(n-k-1)!}{k!(n-2k)!} (2x)^{n-2k} \quad (17)$$

and

$$M_n^*(x) = \sum_{k=0}^{n/2} (-1)^k \frac{(n-k)!}{k!(n-2k)!} (2x)^{n-2k} \quad (18)$$

Generally, whether an NMR transverse magnetization model Polynomial is an even or odd function depends on its degree n.

$$M_n(-x) = (-1)^n M_n(x) \quad (19)$$

$M_n(x)$  is an even function, when n is even and odd function, when n is odd.

$M_n(x)$  is the NMR transverse magnetization model polynomial of the first kind and  $M_n^*(x)$  is the NMR transverse magnetization model polynomial of the second kind. Another equivalent form of the solution is given by

$$M_y = c_5 \cosh[n \operatorname{In}(x + \sqrt{x^2 - 1})] + ic_6 \sinh[n \operatorname{In}(x + \sqrt{x^2 - 1})] \quad (20)$$

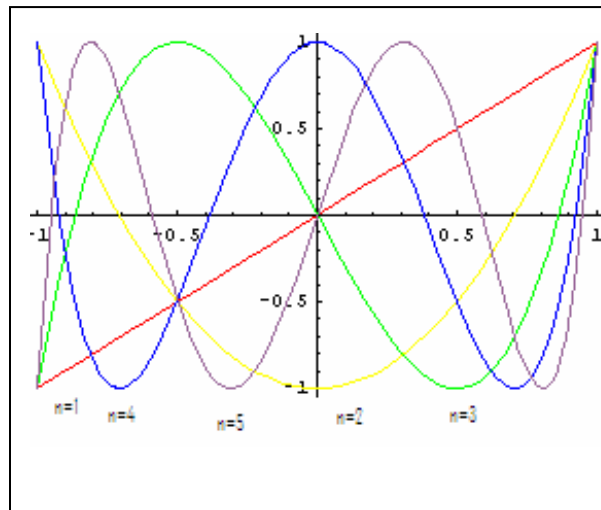
### 3. Generating Functions of the NMR Transverse Magnetization Model

The NMR transverse magnetization model polynomial of the first kind are a set of orthogonal polynomials defined as the solutions to the modified Bloch NMR flow equation and denoted by  $M_n(x)$ . They are used as an approximation to a least squares fit, and are intimately connected with trigonometric multiple-angle formulas. They are normalized such that  $M_n(x) = 1$ . The first few polynomials are illustrated in table 1 and figure 1 respectively for  $-1 < x < 1$  and  $n = 1, 2, 3, 4, 5$ .

The NMR transverse magnetization model polynomial of the first kind  $M_n(z)$  can be defined by the contour integral

$$M_n(z) = \frac{1}{4\pi i} \oint \frac{(1-t^2)t^{-n-1}}{(1-2tz+t^2)} dt \quad (21)$$

(n)	$M_n(x)$
1	$x$
2	$2x^2 - 1$
3	$4x^3 - 3x$
4	$8x^4 - 8x^2 + 1$
5	$16x^5 - 20x^3 + 5x$



*Table 1. The first few  $T_2^*$  weighted NMR transverse magnetization model polynomial of the first kind*

*Fig.1. The first few NMR transverse magnetization model polynomial of the first kind*

The NMR transverse magnetization model polynomials of the second kind are defined as

$$M_{n-1}(\cos t) = \frac{\sin(nt)}{\sin t} \quad (22)$$

Table 2. The first few NMR transverse magnetization model polynomials of the second kind.

N	$M_n^*(x)$
2	$4x^2 - 1$
3	$8x^3 - 4x$

The NMR transverse magnetization model polynomials of the first kind are defined through the identity

$$M_n(\cos \theta) = \cos(n\theta) \quad (23)$$

The NMR transverse magnetization model polynomials of the first kind can be obtained from the generating functions

$$h_1(t, x) \equiv \frac{1-t^2}{1-2xt+t^2} \quad (24)$$

and

$$h_2(t, x) \equiv \frac{1-xt}{1-2xt+t^2} \quad (25)$$

For  $|x| \leq 1$  and  $|t| < 1$

A closely related generating function is the basis for the definition of the NMR transverse magnetization model polynomials of the second kind.

The polynomials can also be defined in terms of the sums

$$M_n(x) = \cos(n \cos^{-1} x) = \sum_{q=0}^{\lfloor n/2 \rfloor} \binom{n}{2q} x^{n-2q} (x^2 - 1)^q \quad (26)$$

where  $\binom{n}{k=2q}$  is a binomial coefficient and  $\lfloor x \rfloor$  is the floor function or the product

$$M_n(x) = 2^{q-1} \prod_{k=1}^n \left\{ x - \cos \left[ \frac{(2k-1)\pi}{2n} \right] \right\} \quad (27)$$

The NMR transverse magnetization model polynomials are orthogonal polynomials with respect to the velocity weighting function  $(1-x^2)^{-1/2}$

$$\int_{-1}^1 \frac{M_n(x)M_m(x)}{V_{real}} dx = \begin{cases} \frac{1}{2}\pi\delta_{nm} & m \neq 0, n \neq 0 \\ \pi & n=m=0 \end{cases} \quad (28)$$

where  $\delta_{nm}$  is the Kronecker delta. The NMR transverse magnetization model polynomials of the first kind satisfy the additional discrete identity

$$\sum_{k=1}^m M_i(x)M_j(x)(x_k) = \begin{cases} \frac{1}{2}m\delta_{ij} & i \neq 0, j \neq 0 \\ m & i=j=0 \end{cases} \quad (29)$$

where  $x_k$  for  $k=1, \dots, m$  are the  $m$  zeros of  $M_n(x)$ .

By using this orthogonality, a piecewise continuous function  $f(x)$  in  $-1 \leq x \leq 1$  can be expressed in terms of NMR transverse magnetization model Polynomials:

$$\sum_{m=0}^{\infty} C_m P_m(x) = \begin{cases} f(x), & f(x) \text{ continuous} \\ \frac{f(x^-)+f(x^+)}{2} & \text{at discontinuous points} \end{cases} \quad (30)$$

where

$$C_m = \begin{cases} \frac{1}{\pi} \int_{-1}^1 \frac{1}{\sqrt{real}} f(x) M_n(x) dx & m=0 \\ \frac{2}{\pi} \int_{-1}^1 \frac{1}{\sqrt{real}} f(x) M_n(x) dx & m=1,2,3,4,\dots \end{cases} \quad (31)$$

This orthogonal series expansion is the Fourier-NMR series expansion or a Generalized Fourier Series expansion.

The NMR transverse magnetization model Polynomials also satisfy the recurrence relations

$$M_{n+1}(x) = 2xM_n(x) - M_{n-1}(x) \quad (32)$$

$$M_{n+1}(x) = xM_n(x) - \sqrt{VT_1} \{1 - [M_n(x)]^2\} \quad (33)$$

For  $n \geq 1$ , as well as

$$(x-1)[M_{2n+1}(x) - 1] = [M_{n+1}(x) - M_n(x)]^2 \quad (34)$$

$$2(x^2-1)[M_{2n}(x) - 1] = [M_{n+1}(x) - M_{n-1}(x)]^2 \quad (35)$$

They have a complex integral representation

$$M_n(x) = \frac{1}{4\pi i} \int_c \frac{(1-z^2)z^{-n-1}}{(1-2xz+z^2)} dz \quad (36)$$

and a Rodrigues representation

$$M_n(x) = \frac{(-1)^n VT_1 \sqrt{\pi}}{2^n (n - \frac{1}{2})!} \frac{d^n}{dx^n} [(1-x^2)^{n-1/2}] \quad (37)$$

The NMR transverse magnetization model polynomial of the first kind is related to the Bessel function of the first kind  $J_n(x)$  and modified Bessel function of the first kind  $I_n(x)$  by the relations



$$J_n(x) = i^n M_n \left( i \frac{d}{dx} \right) J_0(x) \quad (38)$$

$$I_n(x) = M_n \left( \frac{d}{dx} \right) I_0(x) \quad (39)$$

Putting  $x = \cos\phi$  allows the NMR transverse magnetization model polynomials of the first kind to be written as

$$M_n(x) = \cos(n\phi) = \cos(n \cos^{-1} x) \quad (40)$$

The second linearly dependent solution to the transformed differential equation

$$\frac{d^2 M_n}{d\phi^2} + n^2 M_n = 0 \quad (41)$$

is then given by

$$G_n(x) = \sin(n\phi) = \sin(n \cos^{-1} x) \quad (42)$$

which can also be written

$$G_n(x) = VT_1 M_{n-1}^*(x) \quad (43)$$

where  $G_n(x)$  is *not* a polynomial.

#### **4. The Signal Property of the NMR Transverse Magnetization Model Polynomials**

The signal property of the NMR transverse magnetization model polynomials is the trigonometric representation on  $[-1,1]$ . These celebrated NMR transverse magnetization approximation polynomial  $S_m(x)$  of degree  $\leq m$  for  $f(x)$  over  $[-1,1]$  can be written as a sum of  $\{M_n(x)\}$ :

$$f(x) \approx S_m(x) = \sum_{n=0}^m d_n M_n(x) \quad (44)$$

The coefficients  $\{d_n\}$  are computed with the formulas

$$d_n = \frac{2}{m+1} \sum_{k=0}^m f(x_k) M_n(x_k) = \frac{2}{m+1} \sum_{k=0}^m f(x_k) \cos\left(n \frac{2k+1}{2m+2} \pi\right) \quad (45)$$

for  $n = 2, 3, \dots, m$  where

$$x_k = \cos\left(\frac{2k+1}{2m+2} \pi\right) \text{ for } k = 0, 1, 2, 3, \dots, m \quad (46)$$

For illustration, several NMR transverse magnetization approximation polynomials of degree  $n = 1, 2, 3, 4,$  and  $5$  and their error analysis for trigonometric, algebraic, ordinary and special functions have been presented as chebyshev polynomials [10].

## 5. Dynamics of the NMR Transverse Magnetization

Based on equation (10), when the equilibrium magnetization  $M_0$  along the  $z$ -axis becomes zero, the transverse constant magnetization  $M_y$  with amplitude  $d = \frac{f_o}{\gamma}$  is maximum and there is no precession around  $z$ -axis.  $M_y(t)$  can be written as,

$$M_y(t) = M_{y0}(t) + M_{y1}(t)$$

where

$$M_{y0}(t) = g_o(0) \cos \frac{f_o t}{2} + i g_1(0) \sin \frac{f_o t}{2}$$

and

$$M_{y1}(t) = i g_o(0) \sin \frac{f_o t}{2} + g_1(0) \cos \frac{f_o t}{2} \quad (47)$$

The frequency  $f_o$  is called the Rabi frequency which describes transition between the states  $|0\rangle$  and  $|1\rangle$ , under the action of resonant rF  $B_1$  field. At  $t = 0$ , the spin is in the ground state,

$$g_o(0) = i \quad \text{and} \quad g_1(0) = 0 \quad (48)$$

From equation (47), we can write,

$$M_{y_o}(t) = \cos \frac{f_o t}{2}$$

and

$$M_{y_1}(t) = i \sin \frac{f_o t}{2} \quad (49)$$

If the rF  $B_1$  field is applied for a duration of  $\tau$  such that

$$\tau = \frac{\pi}{f_o} \quad (50)$$

then we can write from equation (49),

$$M_{y_o}(\tau) = 0 \quad \text{and} \quad M_{y_1}(\tau) = i \quad (51a)$$

and

$$|M_{y_o}(\tau)|^2 = 0 \quad \text{and} \quad |M_{y_1}(\tau)|^2 = 1 \quad (51b)$$

This mathematical analysis indicates that a pulse of a resonance rF field with duration given in equation (50) drives the spin system from the ground state to excited state. Such a pulse is called  $\pi$ -pulse. If the spin is already in the excited state,

$$g_o(0) = 0 \quad \text{and} \quad g_1(0) = 1 \quad (51c)$$

After the action of  $\pi$ -pulse we have

$$M_{y_o}(\tau) = i \quad \text{and} \quad M_{y_1}(\tau) = 0 \quad (51d)$$

Thus, a  $\pi$ -pulse drives the spin into the ground state. The  $\pi$ -pulse changes the state of the NMR system from  $|0\rangle$  to  $|1\rangle$  or from  $|1\rangle$  to  $|0\rangle$ . If a pulse of different duration is applied, we can drive the NMR system into a superpositional state, creating a one-qubit rotation. Following the same procedure, a  $\pi/2$ -pulse drives the system into a superposition with equal weights of the ground and the excited

states. The measurement of the state of the system gives the state  $|0\rangle$  or the state  $|1\rangle$  with equal probability,  $1/2$ . The same result is obtained when a  $\pi/2$ -pulse drives the system from a pure excited state as given in the initial conditions of equation (51c).

Considering the change of the average value of magnetization components under the action of resonant rF  $B_1$  field when the system is initially in the equilibrium (ground) state and its dynamics is described by equation (49), the evolution of the average values of the magnetization components is given by

$$M_x = 0$$

$$M_y(t) = \frac{1}{2} \sin f_o t \quad (52)$$

and

$$M_z(t) = \frac{1}{2} \cos f_o t \quad (53)$$

Equation (52) describes the precession of the average magnetization around the x-axis, in the rotating system of coordinates. At  $t = 0$ , the average magnetization points in the positive z- direction. The z-component of the average spin decreases, and the y-component increases. At any moment we have

$$M_y^2 + M_z^2 = \frac{1}{4} \quad (54)$$

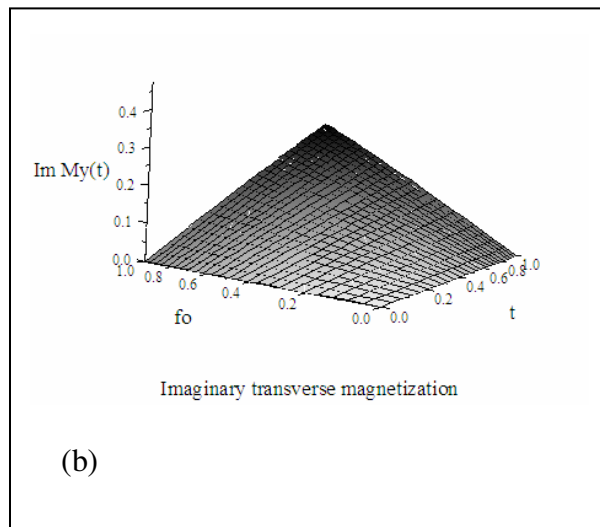
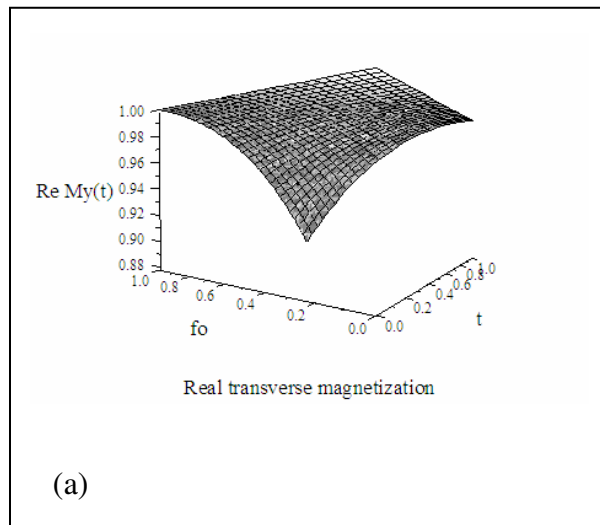
After the action of  $\pi/2$ -pulse, we have

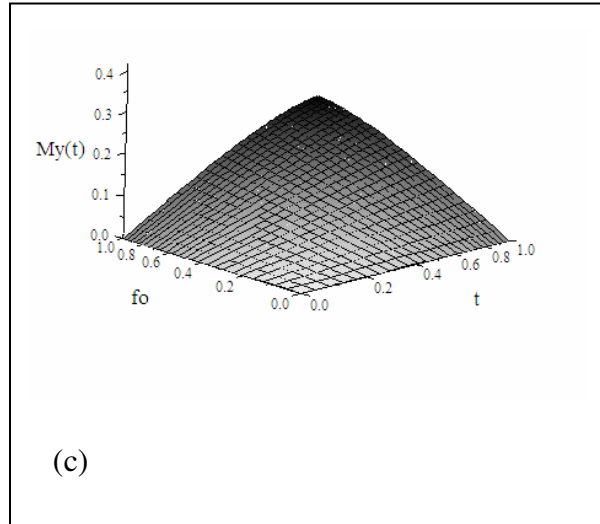
$$M_y = \frac{1}{2} \text{ and } M_z = M_o = 0 \quad (55)$$

This shows that the average magnetization points in the positive y-direction. A  $\pi$ -pulse, we obtain

$$M_y = 0 \text{ and } M_z = M_o = -\frac{1}{2} \text{ (negative z-direction)} \quad (56)$$

The graphical representation of the transverse magnetization derived in equation (49a), equation (49b) and equation (52) are shown in figure 2.





*Fig. 2 Graphics of the transverse magnetization derived in (a) equation (49a), (b) equation (49b) and (c) equation (52).*

## 6. Qualitative Description of the Position and Potential Energy of Blood Particles

Multiplying both sides of equations (7) and (8) by  $m/2$  gives

$$\frac{m}{2}V^2 = \frac{m}{2T_1^2} - \frac{m}{2T_1^2}x^2 \quad (57)$$

$$mV = \frac{-4xmT_2}{T_1(T_1 + T_2)} \quad (58a)$$

$$\frac{dx}{dt} = \frac{-4xT_2}{T_1(T_1 + T_2)} \quad (58b)$$

The solution of equation (58b) can be written as

$$x(t) = x_0 e^{-\frac{4T_2}{T_1(T_1 + T_2)}t} \quad (58c)$$

In equation (57) the quantity on the right depends only on the initial conditions and is therefore constant during the motion. It is called the *total energy*  $E = \frac{m}{2T_1^2}$ ,

and we have the law of conservation of kinetic  $E_k = \frac{m}{2}V^2$ , plus potential energy  $E_p(x) = \frac{k}{2}x^2$ , which holds, as we can see, only when the force is a function of  $x$  alone:

$$\frac{1}{2} mV^2 + E(x) = E_k + E_p(x) = E. \quad (59)$$

where  $k = \frac{m}{T_1^2}$ . Solving for  $V$ , we obtain

$$V = \frac{dx}{dt} = \sqrt{\frac{2}{m}[E - E(x)]^{1/2}} \quad (60)$$

The function  $x(t)$  is to be found by solving for  $x$  in the equation

$$\sqrt{\frac{m}{2}} \int_{x_0}^x [E - E(x)]^{-1/2} dx = t - t_0 \quad (61)$$

In this case, the initial conditions are expressed in terms of the constants  $E$  and  $x_0$ .

In applying equation (61), and in taking the indicated square root in the integrand, we must carefully use the proper sign, depending on whether the velocity  $V$  given by equation (60) is positive or negative. In cases where  $V$  is positive during some parts of the motion and negative during other parts, it may be necessary to carry out the integration in equation (61) separately for each part of the motion.

Equation (61) becomes, for this case, with  $t_0 = 0$ ,

$$\sqrt{\frac{m}{2}} \int_{x_0}^x \left( E - \frac{1}{2}kx^2 \right)^{-1/2} dx = t. \quad (62)$$

Making the substitutions

$$\sin \theta = x \sqrt{\frac{k}{2E}}, \quad (63)$$

$$\omega = \sqrt{\frac{k}{m}}, \quad (64)$$

so that

$$\sqrt{\frac{m}{2}} \int_{x_0}^x \left( E - \frac{1}{2} kx^2 \right)^{-1/2} dx = \frac{1}{\omega} \int_{\theta_0}^{\theta} d\theta = \frac{1}{\omega(\theta - \theta_0)}$$

by equation. (62),

$$\theta = \omega t + \theta_0$$

From equation (63):

$$x = \sqrt{\frac{2E}{k}} \sin \theta = A \sin(\omega t + \theta_0) \quad (65)$$

where

$$\sqrt{\frac{2E}{k}} = A \quad (66)$$

Thus the coordinate  $x$  oscillates harmonically in time, with amplitude  $A$  and frequency  $\omega/2$ . The initial conditions are determined by the constants  $A$  which are related to  $E$  and  $x_0$  by

$$E = \frac{1}{2} kA^2 \quad (67)$$

$$x_0 = \sin \theta_0 \quad (68a)$$

We can now determine the position function  $x(t)$  from equation (58c) as

$$x(t) = \sin \theta_0 e^{-\frac{4T_2}{T_1(T_1 + T_2)} t} \quad (68b)$$



It may be interesting to note that there is the sign difficulty in taking the square root in equation (62) by replacing  $(1-\sin^2 \theta)^{-1/2}$  by  $(\cos \theta)^{-1}$ , a quantity which can be made either positive or negative as required by choosing  $\theta$  in the proper quadrant.

The function in equations (57 and 59) is called the energy integral. The equation of motion is generally defined as

$$\frac{d^2x}{dt^2} + kx = 0 \quad (69)$$

An integral of the equations of motion of a mechanical system is called a *constant of the motion*. In general, any mechanical problem can be solved if we can find enough first integral, or constants of the motion. The general solution of equation (69) is given in equation (65).

Even in cases where the integral in equation (61) cannot easily be evaluated or the resulting equation solved to give an explicit solution  $x(t)$ , the energy integral in equation (59), gives us useful information about the solution. For a given energy  $E$ , we see from equation (60) that the blood molecule is confined to those regions on the  $x$ -axis where  $E(x) \leq E$ . Furthermore, the velocity is proportional to the square root of the difference between  $E$  and  $E(x)$ . Hence, if we plot  $E(x)$  versus  $x$ , we can give a good qualitative description of the kinds of motion that are possible. For the potential-energy function shown in Fig. 3 we note that the least energy possible is  $x_4E_0$ . At this energy, the blood molecule can only be at rest in  $x_0$ . With a slight higher energy  $E_1$ , the molecule can move between  $x_1$  and  $x_2$ ; its velocity decreases as it approaches  $x_1$  or  $x_2$ , it stops and reverses its direction when it reaches either  $x_1$  or  $x_2$ , which are called *turning points* of the motion. With energy  $E_2$ , the blood molecule may oscillate between turning points  $x_3$  and  $x_4$ , or remain at rest at  $x_5$ . With energy  $E_3$ , there are four turning points and the blood molecule may oscillate in either of the two potential valleys. With energy  $E_4$ , there is only one turning point; if the molecule is initially traveling to the left, it will turn at  $x_6$  and return to the right, speeding up over the valleys at  $x_0$  and  $x_5$ , and slowing down over the hill between. At energies above  $E_5$ , there are no turning points and the blood molecule will move in one direction only, varying its speed according to the depth of the potential at each point.

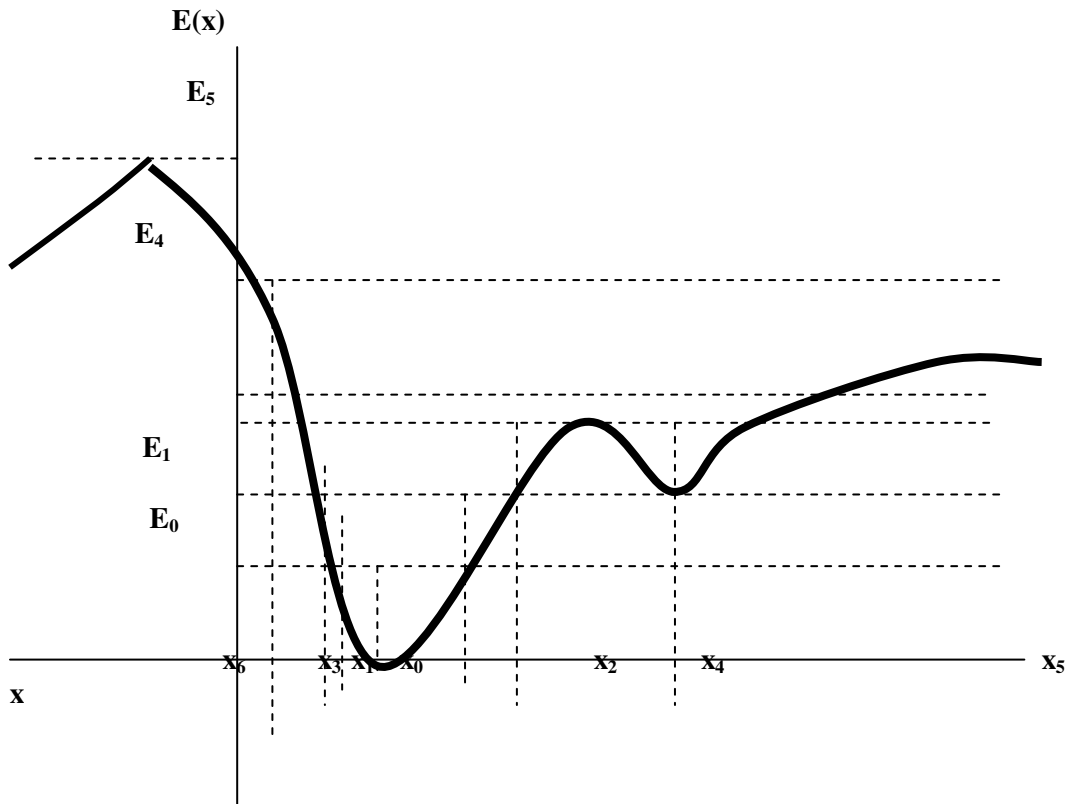


Fig. 3. A potential energy function for one-dimensional motion of blood particle when a blood particle is oscillating near a point of stable equilibrium we can find an approximate solution for its motion

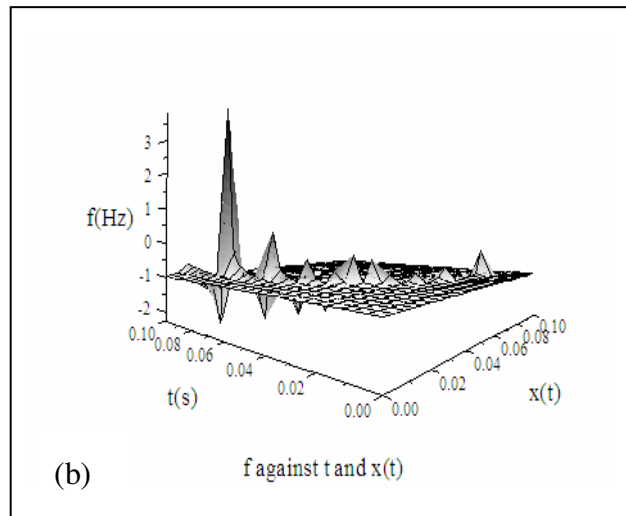
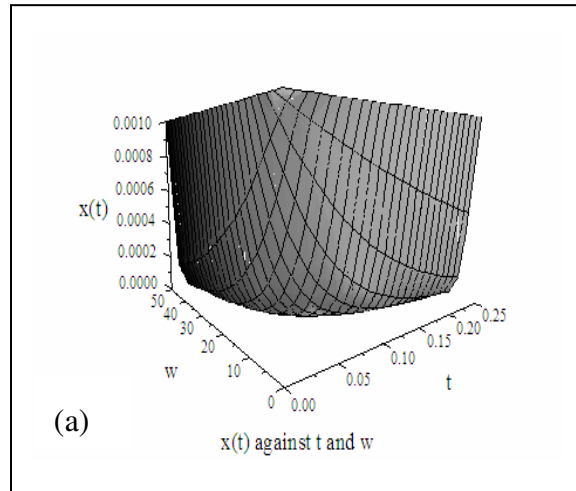


Fig. 4. Three dimensional graphics of equation (58c) when  $T_2 = 0.25\text{s}$  and  $x_o = 0.001\text{m}$

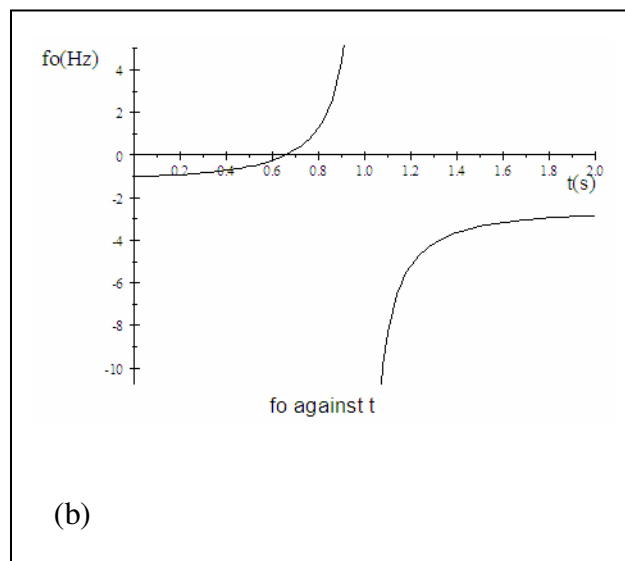
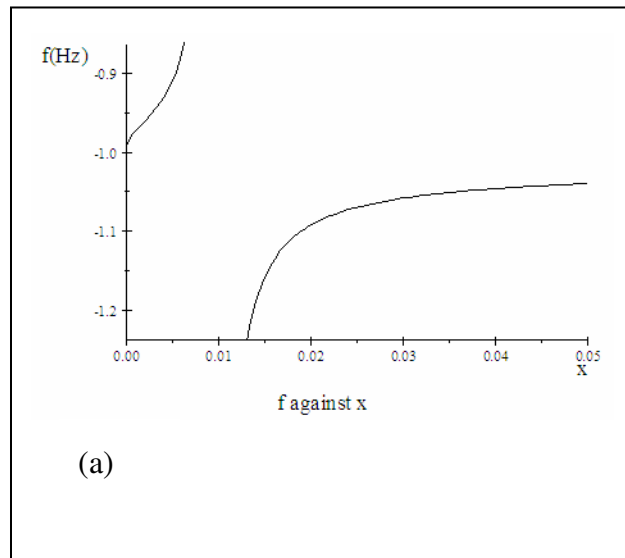


Fig. 5. Two dimensional graphics of equation (58c) when  $T_2 = 0.25s$  and  $x_o = 0.001m$

## 7. Conclusion

We have presented a theoretical model for the dynamics of blood molecules when there is a flush of blood to a region of the brain when becomes activated. As in classical mechanics, every blood molecule is assumed to follow a definite trajectory which specifies its position as a function of time. We consider a blood molecule moving in one dimension only. We take this as the  $x$  direction and that the trajectory is a function of  $x(t)$  which depends on  $T_1$  and  $T_2$  relaxation parameters of blood flow according to equation (68b). Graphics showing the position function  $x(t)$  from equation (58c) are presented in figures 4 and 5. Solutions to the Bloch NMR flow equations in the form of polynomials allow us to express the blood flow velocity of the blood molecule as the differential of position with respect to time, and the acceleration as the differential of the velocity. In this way we are able to specify the position and velocity of the blood molecule at a given time. Another important quantity derived as a result of the solution is momentum,  $p$ , defined as the product of the mass and the velocity in equation (58a).

The key to MRI is that the signal from hydrogen nuclei varies in strength depending on the surroundings. NMR relaxation is a consequence of local fluctuating magnetic fields within a molecule. Local fluctuating magnetic fields are generated by molecular motions. In this way measurement of relaxation times can provide functional information of motions within a molecule on the atomic level. This provides a means of discriminating between NMR sensitive chemicals that are the source of the NMR signal observed in the brain and those that are not.

A very important quantity derived in this study is the energy,  $E$  of the blood molecule. We distinguish between kinetic energy,  $E_k$ , which comes from the motion of the blood molecule, and the potential energy,  $E_p$ , which depends on its position. A point where  $E(x)$  has a minimum is called a point of stable equilibrium. A molecule at rest at such a point will remain at rest. If displaced a slight distance, it will experience a restoring force tending to return it, and it will oscillate about the equilibrium point. For a blood molecule moving without a force, both potential energy and kinetic energies are constant. Generally, they will vary during the motion, but in such a way that the total energy given by equation (59) remains constant.

A point where  $E(x)$  has a minimum is called a point of unstable equilibrium. In theory, a molecule at rest there can remain at rest, since the force is zero, but if it is displaced the slightest distance, the force acting on it will push it farther away from the unstable equilibrium position. A region where  $E(x)$  is consistent is called

a region of neutral equilibrium, since a molecule can be displaced slightly without suffering either a restoring or a repelling force.

This kind of qualitative discussion, based on the energy integral, is simple and very useful. It can be very interesting to study this model and understand it well enough to be able to see at a glance, for any potential energy curve, the types of motion that are possible. However, it may be only part of the force on a blood molecule is derivable from a potential function  $E(x)$ . If the remainder of the force is represent by  $F_R$ , we can write

$$F = \frac{dv}{dx} + F_R \quad (70)$$

In this case the energy ( $E_k+E_p$ ) is no longer constant. Since the motion of the blood molecule is governed by

$$F = ma = m \frac{d^2x}{dt^2} \quad (71)$$

If we substitute  $F$  from equation (70) in equation (71), and multiply by  $dx/dt$ , we have, after rearranging terms, the time rate of change of kinetic plus potential energy is equal to the power delivered by the additional force  $F_R$ .

From equations (57) and (67) the coordinate  $x$  oscillates harmonically in time, with amplitude  $A$  (equal to unity) and frequency  $\omega/2$  as one of the local response to an increase in blood flow to regions of increased neural activity. The difference in energy as shown in figure 2 in terms of  $T_1$  relaxation time is very significant because it can be accurately explored to identify the NMR sensitive chemicals that are the source of the NMR signal observed in the brain (Fig. 4 and 5). Since  $E_k \geq 0$ , we have  $E \geq E_p$ , which means that, classically, the blood molecule can be found only in the range  $-1 \leq x \leq 1$ . At the end of the interval, where  $E = E_p$ , its kinetic energy vanishes; the point  $x = \pm 1$  are called turning points.

It can be interesting to note that appropriate application of classical and quantum mechanics to equations (6, 59,& 69) can give valuable information about the physical quantities such as  $rF \gamma B_1 = n$ , position, velocity, energy and momentum of a blood molecule in terms of NMR parameters. We may be able to understand the *direct* relationship between change in blood flow to the brain and the increase in metabolic rate in this area of the brain and neural communication.

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## **8. References**

1. Belliveau, J. W., Kennedy D. N. Jr., McKinstry, R. C., Buchbinder, B. R., Weisskopf, R. M., Cohen, M. S., et al. (1991). Functional mapping of the human visual cortex by magnetic resonance imaging. *Science*, 254:716-719.
2. Cohen, M. S., Bookheimer, S. Y. (1994). Localization of brain function using magnetic resonance imaging. *Techniques in Neuroscience*, 17(7):268-277.
3. Heiken, J.P., Brown, J. J. (Eds.) (1991). *Manual of Clinical Magnetic Resonance Imaging* (2nd ed.). New York: Raven.
4. Horowitz, A. L. (1995). *MRI Physics for Radiologists: A Visual Approach* (3rd ed.). New York: Springer-Verlag.
5. Le Bihan, D. (moderator) (1995). NIH conference: Functional magnetic resonance imaging of the brain. *Annals of Internal Medicine*, 122:296-303.
6. Kwong, K. K., Belliveau, J. W., Chesler, D. A., Goldberg, I. E., Weisskopf, R. M., Poncelet, B. P., et al. (1992). Dynamic magnetic resonance imaging of human brain activity during primary sensory stimulation. *Proceedings of the National Academy of Sciences USA*, 89:5675-5679.
7. Ogawa, S., Lee, T. M., Kay, A. R., Tank, D. W. (1990). Brain magnetic resonance imaging with contrast dependent on blood oxygenation. *Proceedings of the National Academy of Sciences USA*, 87:9868-9872.
8. Rosen, B. R., Belliveau, J. W., Aronen, H. J., Kennedy, D., Buchbinder, B. R., Fischman, A., Gruber, M., Glas, J, Weisskopf, R. M., Cohen, M. S., et al., (1991). Susceptibility contrast imaging of cerebral blood volume: human experience. *Magnetic Resonance in Medicine*, 22(2):293-299.
9. Awojoyogbe, O. B. A Mathematical Model of Bloch NMR Equations for Quantitative Analysis of Blood Flow in Blood Vessels with Changing Cross-section **II**. *Physica A*, 323c, pp 534-550, (2003)

10. John H. Mathews (2004), Module for Chebychev polynomials  
[http://math.fullerton.edu/mathews/n2003/ChebyshevpolyMod/Links  
ChebyshevpolyMod link 25.html](http://math.fullerton.edu/mathews/n2003/ChebyshevpolyMod/LinksChebyshevpolyMod link 25.html).