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Using Gravitational Waves to Put Limits on Primordial Magnetic Fields

By David Garrison

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Abstract- We describe a technique for using simulated tensor perturbations in order to place upper limits on the intensity of magnetic fields in the early universe. As an example, we apply this technique to the beginning of primordial nucleosynthesis. We determined that any magnetic seed fields that existed before that time were still in the process of being amplified. In the future, we plan to apply this technique to a wider range of initial magnetic fields and cosmological epochs.

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Using Gravitational Waves to Put Limits on Primordial Magnetic Fields

David Garrison

Abstract- We describe a technique for using simulated tensor perturbations in order to place upper limits on the intensity of magnetic fields in the early universe. As an example, we apply this technique to the beginning of primordial nucleosynthesis. We determined that any magnetic seed fields that existed before that time were still in the process of being amplified. In the future, we plan to apply this technique to a wider range of initial magnetic fields and cosmological epochs.

I. INTRODUCTION

Magnetic fields are believed to have played a large part in the dynamics of the evolution of our universe. However, little is known about the existence of magnetic fields when the universe was very young. There are no direct observations of primordial magnetic fields. Theories also disagree on the amplitude of primordial magnetic fields. There are currently several dozen theories about the origin of cosmic magnetic fields [2, 18]. The main reason that we believe that primordial magnetic fields existed is because they may have been needed to seed the large magnetic fields observed today. Most theories of cosmic magnetic field generation fall into one of three categories [2, 12, 18]: 1) magnetic fields generated by phase transitions; 2) electromagnetic perturbations expanded by inflation; and 3) turbulent magnetofluid resulting in charge and current asymmetries. Once generated, these seed magnetic fields were amplified by a dynamo however, we don't know when or how this dynamo did it's work.

Most models calculate the magnitude of primordial magnetic fields by starting with the observed strength of galactic or intergalactic magnetic fields and calculating how this field should have been amplified or diffused by external effects such as the magnetic dynamo and expansion of the universe [2, 18]. A major problem is that there doesn't appear to be a universal agreement of how efficiently a dynamo could have strengthened seed magnetic fields or when the strengthening occurred. Estimates of the strength of these seed fields can vary by tens of orders of magnitude. In the absence of amplification mechanisms, the frozen-in condition of magnetic field lines tells us that [2, 18].

$$\vec{B}_0 = \vec{B}a^2. \quad (1)$$

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Here \vec{B}_0 is the present magnetic field where the scale factor is unity and \vec{B} is the magnetic field when the scale factor was a . Once amplification and diffusion are taken into account, this relationship can be used to calculate the amplitude of magnetic seed fields. Seed magnetic fields produced during Inflation are predicted to have a current strength somewhere between 10^{-11} G and 10^{-9} G on a scale of a few Mpc [2, 18, 26]. Magnetic seed fields generated by phase transitions are believed to be less than 10^{-23} G at galactic scales [2, 18]. Some turbulence theories imply that magnetic fields were not generated until after the first stars were formed therefore requiring no magnetic seed fields [2].

Given how little is understood about primordial magnetic fields and the general lack of agreement among theoretical predictions, it seems clear that the existence of primordial magnetic fields can neither be confirmed or ruled out. It seems that the best we can do is set an upper limit on the strength of primordial magnetic fields and utilize this limit as a starting point in developing models of cosmic turbulence. Observations of the CMB limit the intensity of the magnetic seed fields to a current upper limit of 10^{-9} G [2, 18, 26, 38].

It is well known that gravitational waves can interact with a magnetofluid in the presence of a magnetic field. Work by Duez et al [15] showed how gravitational waves can induce oscillatory modes in a plasma field if magnetic fields are present. Work by Kahniashvili and others [30, 31, 32, 34, 35, 36] have shown how a turbulent plasma can yield gravitational waves. The result may be a highly nonlinear interaction as energy is transferred from the fluid to the gravitational waves and back resulting in potentially significant density perturbations. Magnetic fields are the glue that bind the gravitational waves to the plasma field. The objective of this work is to utilize the interaction between gravitational waves and the primordial magnetofluid in order to put limits on the strength of magnetic fields that could have existed in the early universe.

II. PRIMORDIAL GRAVITATIONAL WAVE AMPLITUDES

According to Boyle, Primordial Gravitational Waves develop primarily from tensor perturbations expanded by the inflation event [3, 4]. The process is similar to that of scalar perturbations and the two are related by a tensor/scalar ratio

$$r = \Delta_t^2 / \Delta_s^2. \tag{2}$$

Here the Δ terms refer to the primordial power spectrums. As a function of horizon exit time, τ_{out} and wavenumber, k ,

$$\Delta_t^2(k, \tau_{out}) = 64\pi G \frac{k^3}{2\pi^2} |h_k(\tau_{out})|^2 \approx 8 \left(\frac{H_*}{2\pi M_{pl}} \right)^2, \tag{3}$$

$$\Delta_s^2(k, \tau_{out}) \approx \frac{1}{2\epsilon_*} \left(\frac{H_*}{2\pi M_{pl}} \right)^2, \tag{4}$$

$$r(k) \equiv \Delta_t^2(k, \tau_{out}) / \Delta_s^2(k, \tau_{out}) \approx 16\epsilon_*. \tag{5}$$

$M_{pl} = (8\pi G)^{-1/2}$ is the "reduced Planck mass" and ϵ is the slow roll parameter. Also the asterisk (*) terms denote the value of the parameters when the tensor perturbation exits the horizon. The wavenumber is commonly defined as $k = a_* H_*$ at the horizon exit.

$$\langle 0 | \hat{\Omega} | 0 \rangle = \langle 0 | h_{ij}(n, \eta) h^{ij}(n, \eta) | 0 \rangle = \frac{\mathcal{C}^2}{2\pi^2} \int_0^\infty n^2 \sum_{p=1,2} |h_p(\eta)|^2 \frac{dn}{n}. \tag{7}$$

Here, n refers to a dimensionless angular wave number, p refers to the left and right handed polarizations of the gravitational waves and $\eta = \int \frac{dt}{a(t)}$ is the conformal time.

The constant \mathcal{C} should be taken as $\mathcal{C} = \sqrt{16\pi} l_{pl}$. It can be shown that the mean-square amplitude of the gravitational wave is

$$h^2(n, \eta) = \left[\frac{4l_{pl}}{\sqrt{\pi}} n \right]^2 \sum_{p=1,2} |h_p(\eta)|^2. \tag{8}$$

The square root of the equation above will provide a root-mean squared (RMS) amplitude of a gravitational wave for a specific wave number. To complete the power spectrum, we show that the amplitude of gravitational waves can be expressed as

$$h(n, \eta) = \left[\frac{4l_{pl}}{\sqrt{\pi}} n \right] |h(\eta)|. \tag{9}$$

Using the relation $n_H = 4\pi$, which corresponds to the current Hubble radius [19, 20],

$$h(n, \eta) = 16\sqrt{\pi} l_{pl} \frac{n}{n_H} |h(\eta)|. \tag{10}$$

Grishchuk shows that this can be expressed in a convenient form as

$$h(n) = 16\sqrt{\pi} l_{pl} \frac{b}{l_0} \left(\frac{n}{n_H} \right)^{2+\beta}. \tag{11}$$

The variable β is the power-law inflation parameter with -2 corresponding to the de Sitter universe and b is a constant defined in terms of β as

$$b = \frac{2^{|2+\beta|}}{|1+\beta|^{|1+\beta|}} \tag{12}$$

Once the tensor mode enters the horizon, $k \gg aH$, the strain amplitude of the gravitational waves can be defined as

$$h_k = \frac{1}{a\sqrt{2k}}. \tag{6}$$

Unfortunately, because there is not a consistent dimensionless definition of the Hubble Parameter, this method does not allow for an easy way to calculate the amplitude of gravitational waves in the early universe. We therefore turn to Grishchuk's work [19, 20]. Grishchuk believed that gravitational waves were generated by inflation and amplified by a process called parametric amplification. Starting with the idea that the gravitational wave power spectrum is deduced by treating contracted tensor perturbations as eigenvalues of a quantum mechanical operator that works on the vacuum state we see that

l_0 is a constant that denotes an arbitrary Hubble radius during inflation, it is on the order of $10^6 l_{pl}$ according to Grishchuk.

$$a(\eta) = l_0 |\eta|^{1+\beta} - \infty \leq \eta ; -2 \leq \beta \leq -1 \tag{13}$$

Since Grishchuk's solution effectively varies by wavenumber, n_H , to some power between 0 and -1, we can see that Boyle and Grishchuk's solutions may be equivalent for $\beta = -1.5$. By setting n_H to reflect a Hubble parameter earlier than the current epoch, we can calculate the spectrum of gravitational waves at any time in the history of the universe post inflation.

III. OVERVIEW OF THE SOFTWARE

As described in the article, Numerical Relativity as a Tool for Studying the Early Universe [17], the code used here was specifically developed to study relativistic plasma physics in the early universe. This code is based on the Cactus Framework (www.cactuscode.org). Cactus was originally developed to perform numerical relativistic simulations of colliding black holes but its modular design has since allowed it to be used for a variety of Physics, Engineering and Computer Science applications. It is currently being maintained by the Center for Computation and Technology at Louisiana State University. Cactus codes are composed of a mesh (which provides the framework) and the thorns (which provide the physics). The code used within this work, SpecCosmo, is a collection of cactus thorns written in a combination of Fortran 90, C and C++.

The code uses the relativistic MHD evolution equations proposed by Duez [14]. It is also designed to utilize a variety of different differencing schemes including 2nd order Finite Differencing, 4th order Finite

Differencing and Spectral Methods. This work uses Fourier Spectral Methods and periodic boundary conditions exclusively. These involve treating the functions as generic periodic functions and calculating the derivatives using FFTs and inverse FFTs. The code is capable of solving Einstein's Equations directly (through a modified BSSN formulation) as well as the relativistic MHD equations. The code was thoroughly tested [17] and found to accurately model known GRMHD dynamics. These tests included MHD waves induced by gravitational waves test, the consistency of cosmological expansion test and shock tests.

The initial data used was derived from work done by several projects involving primordial magnetic fields, phase transitions and early universe cosmology in general [16, 28, 34, 36, 37]. This study models a high energy epoch of the universe after inflation and the Electroweak phase transition when the universe was about 3 minutes old. The author chose this as the starting point for our study because it was the beginning of the Primordial Nucleosynthesis in the early universe.

IV. EVOLUTION EQUATIONS

The MHD equations used here are based on Duez's evolution equations [14].

$$\bar{\partial}_0 K = \alpha \left(\tilde{A}^{ij} \tilde{A}_{ij} + \frac{1}{3} K^2 \right) + 4\pi\alpha(\rho + S) . \tag{18}$$

$$\bar{\partial}_0 \phi = -\frac{\alpha}{6} K , \tag{19}$$

$$\bar{\partial}_0 \phi_i = -\frac{1}{6} \alpha \bar{D}_i K - \kappa^\phi \mathcal{C}_i , \tag{20}$$

$$\bar{\partial}_0 \tilde{\gamma}_{ij} = -2\alpha \tilde{A}_{ij} , \tag{21}$$

$$\begin{aligned} \bar{\partial}_0 \tilde{A}_{ij} = e^{-4\phi} \left[\alpha (\tilde{R}_{ij} - 8\pi S_{ij}) - 2\alpha \bar{D}_{(i} \phi_{j)} + 4\alpha \phi_i \phi_j + \Delta \tilde{\Gamma}^k_{ij} (2\alpha \phi_k) \right]^{TF} \\ + \alpha K \tilde{A}_{ij} - 2\alpha \tilde{A}_{ik} \tilde{A}^k_j , \end{aligned} \tag{22}$$

$$\bar{\partial}_0 \tilde{\gamma}_{kij} = -2\alpha \bar{D}_k \tilde{A}_{ij} - \kappa^\gamma \mathcal{D}_{kij} , \tag{23}$$

$$\bar{\partial}_0 \tilde{\Lambda}^i = -\frac{4}{3} \alpha \tilde{D}^i K + 2\alpha \left(\Delta \tilde{\Gamma}^i_{kl} \tilde{A}^{kl} + 6\tilde{A}^{ij} \phi_j - 8\pi \tilde{\gamma}^{ij} S_j \right) . \tag{24}$$

The bar denotes a derivative taken with respect to the fiducial metric and the tilde again denotes a derivative taken with respect to the conformal metric. Also, \mathcal{C}_i and \mathcal{D}_{kij} are constraint equations and κ^ϕ and κ^γ

$$\partial_t \rho_* + \partial_j (\rho_* v^j) = 0, \tag{14}$$

$$\partial_t \tilde{\tau} + \partial_i (\alpha^2 \sqrt{\gamma} T^{0i} - \rho_* v^i) = s, \tag{15}$$

$$\partial_t \tilde{S}_i + \partial_j (\alpha \sqrt{\gamma} T_i^j) = \frac{1}{2} \alpha \sqrt{\gamma} T^{\alpha\beta} g_{\alpha\beta,i}, \tag{16}$$

$$\partial_t \tilde{B}^i + \partial_j (v^j \tilde{B}^i - v^i \tilde{B}^j) = 0. \tag{17}$$

Here ρ_* is conserved density, v^j is velocity, $\tilde{\tau}$ is the energy variable, \tilde{S}_i is the momentum variable, s is the source term, α is the lapse term, γ is the determinate of the three metric and T^{ij} is the stress-energy tensor. The tilde denotes that the term was calculated with respect to the conformal metric. The first equation comes from conservation of baryon number, the second derives from conservation of energy, the third is conservation of momentum and the fourth is the magnetic induction equation. For this simulation we use Geodesic Slicing, $\alpha = 1.0$, $\beta_i = 0.0$.

The code utilizes a first order version of the BSSN equations to simulate the background space-time. For fixed gauge conditions, the modified BSSN equations as defined by Brown [6] are:

are proportionality constants. ρ , S , S_j and S_{ij} are source terms as found in the standard version of the BSSN equations. Brown et al also defined:

$$\mathcal{C}_i = \phi_i - \bar{D}_i \phi = 0,$$

$$\mathcal{D}_{kij} = \tilde{\gamma}_{kij} - \bar{D}_k \tilde{\gamma}_{ij} = 0,$$

$$\Delta \tilde{\Gamma}^i_{kl} = \frac{1}{2} \tilde{\gamma}^{ij} (\tilde{\gamma}_{klj} + \tilde{\gamma}_{lkj} - \tilde{\gamma}_{jkl}) ,$$

$$\tilde{R}_{ij} = -\frac{1}{2} \tilde{\gamma}^{kl} \bar{D}_k \tilde{\gamma}_{lij} + \tilde{\gamma}_{k(i} \bar{D}_{j)} \tilde{\Lambda}^k + \tilde{\gamma}^{\ell m} \Delta \tilde{\Gamma}^k_{\ell m} \Delta \tilde{\Gamma}_{(ij)k}$$

$$+ \tilde{\gamma}^{k\ell} [2\Delta\tilde{\Gamma}^m_{k(i}\Delta\tilde{\Gamma}_{j)ml} + \Delta\tilde{\Gamma}^m_{ik}\Delta\tilde{\Gamma}_{mj\ell}] ,$$

V. EXPERIMENTAL SET-UP AND ASSUMPTIONS

In order to determine the upper limit of primordial magnetic fields that existed at a particular stage in the evolution of our universe, we inject a broad spectrum of gravitational waves into a homogenous relativistic plasma field with a constant magnetic field and study the results. This is similar to what Duez did in the second of two papers [15]. The basic idea of the Duez paper was to calculate the effect that standing gravitational plane waves would have on a homogenous plasma field with a constant magnetic field. The result was to excite magnetosonic and Alfen waves in the

plasma based on the polarization of the gravitational waves and other parameters such as the density, temperature and magnetic field of the plasma. This was done as a test of their GRMHD code but we use it here to probe what magnetic fields may have been physically allowable in the early universe. We choose to perform this study 180s after the big bang although such a study could have been performed anytime after electro-weak symmetry breaking. For the results to be relevant, we must assume that magnetogenesis and any dynamo effects had already created and strengthened a primordial magnetic fields

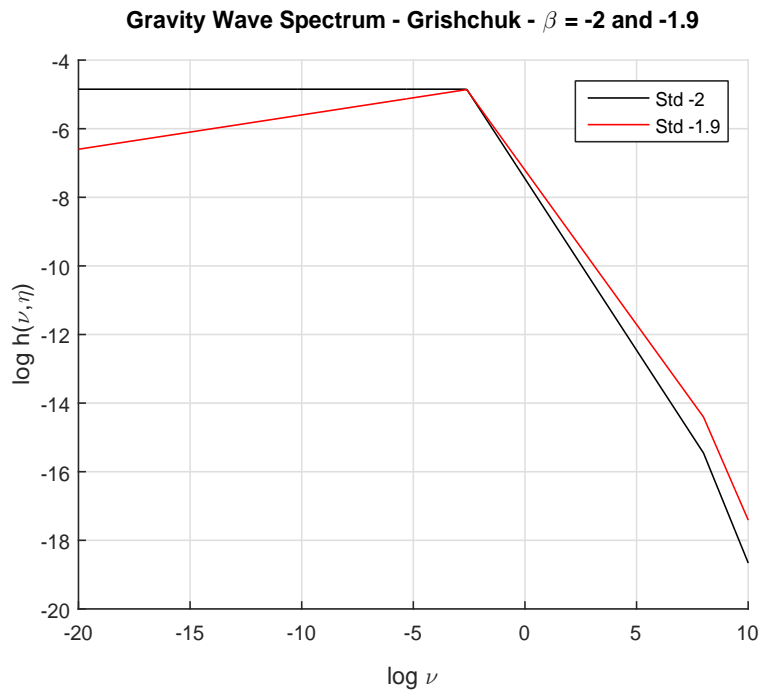


Figure 1: Primordial Gravitational Wave spectrum as calculated by Grishchuk's method for $t = 180$ s.

that would gradually be weakened by the expansion of the universe. The temperature, density, Hubble parameter, scale factor and mass contribution of the universe at this stage are all well known [28]. We utilized an initial temperature of 1.0×10^9 K. The scale factor and Hubble Parameter are $a = 2.81 \times 10^{-9}$ and $H = 2.46 \times 10^{-3} s^{-1}$ respectively. The mass/energy density at the time was $1.08 \times 10^4 \frac{kg}{m^3}$. Our study assumes that 80% of the mass density of the universe was composed of "dark matter". This was chosen to be consistent with our current dark matter to baryonic matter ratio. This "dark matter" was simulated using a pressureless, non-magnetic fluid with no internal energy, in addition to the magnetofluid used to simulation regular matter. This was done to keep us from over estimating the effects of magnetic fields on the matter field. The amplitude of the gravitational waves at this epoch was determined using Grishchuk's solution described in a previous section.

We ran 6 simulations with different values of a fixed magnetic fields along the z-axis, $0 G, 10^2 G, 10^4 G, 10^5 G, 10^6 G$ and $10^8 G$. Each run used random tensor perturbations with amplitudes up to 10^{-19} . We utilized a three dimensional computational grid with 64^3 internal grid points corresponding to 4^3 meters with a courant factor of 0.1. The domain size of 4^3 meters was chosen to allow for multiple light crossing times during the course of the simulation. Geodesic slicing conditions and periodic boundary conditions were used for all simulation runs. We also used a 3rd order iterative Crank Nicolson time scheme for time integration. A spectral differencing method was used and the simulations ran for over 1,000 iterations. There were no shocks or discontinuities in the system so we did not utilize our HRSC routines.

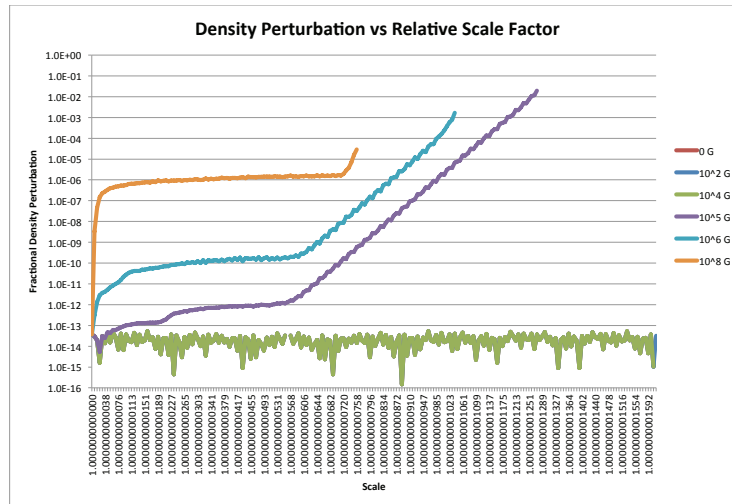


Figure 2: Density perturbations as the result of different initial magnetic fields

VI. RESULTS

As one can see from Figure 2, the density perturbations appear larger as the intensity of the initial magnetic field increases. There appears to be no difference between the 0 G magnetic field and the 10^4 G magnetic field. However, the 10^5 G magnetic field seems to have a much larger effect on the plasma field with density perturbations on the order of a part in 10^{12} result. When the magnetic fields are near or above 10^5 G the perturbations continue to grow until the system becomes unstable. This is clearly an unphysical result. It should be noted that a primordial magnetic field of 10^8 would correspond to a current cosmological magnetic field of 10^{-9} G which is the established upper limit.

VII. DISCUSSION

The goal of this project was to develop a technique for testing the upper limit of cosmological magnetic fields throughout different epochs of universal evolution. We did this using the beginning of Primordial Nucleosynthesis as an example. We observed that the relative amplitude of density perturbations varied according to the strength of the initial magnetic fields. Our observed instabilities for magnetic fields greater than 10^4 G imply that such strong magnetic fields should not have been physically possible during the Primordial Nucleosynthesis epoch. We saw that the maximum possible magnetic field as determined by observation, is not physically viable. From this we conclude that the amplification of the seed magnetic fields either did not finish until much later or current cosmological magnetic fields should have amplitudes below 10^{-13} G. Future work will involve applying this technique to later epochs over a wider range of initial magnetic fields in order to more accurately determine upper limits for magnetic field intensities.

VIII. CONFLICTS OF INTERESTS

The author declares that there are no conflict of interests regarding the publication of this article.

IX. ACKNOWLEDGEMENT

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Biocosmological Role of Gauge Particles in the Origin of Chiral Life and the Inflationary Origin of Matter-Antimatter Asymmetry in Semiclosed Friedman Universe

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Abstract- The biocosmological role of CP-symmetry-violating chiral Z^0 boson in the origin of the chiral life and the cosmological role of CP-symmetric Higgs boson H^0 in the inflationary origin of the matter-antimatter asymmetry in the semiclosed Friedman universe are discussed.

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I. INTRODUCTION

In 1860 L. Pasteur¹ wrote: "Life as manifested to us is a function of the asymmetry of the Universe. I can even imagine that all living species are primordially in their structure, in their external forms (like left-right chiral asymmetry) of a function of the Universe." A. Salam² later wrote that Pasteur was prophetic in the unification of biology and cosmology. We here discuss the biocosmological role of the chiral Z^0 boson predicted in 1968 in the origin of chiral life, and the cosmological role of the Higgs boson H^0 discovered in 2014 in the inflationary origin of matter-antimatter symmetry in the semiclosed Friedman universe.

II. BIOCOSMOLOGY

A. Salam² summarized the presently accepted view of the origin of life as occurring in three stages: cosmic, prebiotic chemical, and biological:

- 1) The cosmic stage concerns itself with the early history of the universe, where electroweak forces made a phase transition into electromagnetic and weak forces 10^{-12} s after the universe was born. The radius of the universe was then extended from Planck scale $\sim 10^{-33}$ cm to 10^{-2} cm; the temperature was $250\text{Gev} \sim 10^{12}\text{K}$; and the carriers of the neutral weak force of Z^0 boson acquired the mass by Higgs mechanism.
- 2) Chemistry became important after the planets were formed, some 10 billions years later, though it may have played a role in the presolar epochs as well (long after the quarks of the early cosmic era had condensed into protons and neutrons and much after the recombination with electrons, taking place

some 10^5 years following Big Bang). Molecules of future life could thus have formed before the origin of the Earth.³

- 3) The biological era concerns itself with the replication of nucleic acid polymers and protein synthesis. The biological era may have started some 4 billion years ago.

III. Z^0 BOSON AND CHIRAL LIFE

It is known that all amino acids and proteins utilized in living systems are of the L (left-handed) type. Salam emphasized the role of the chiral Z^0 interaction as its weak interaction works as a contact interaction in biochemical process (zwitterionic process).² Then, starting from Z^0 interactions,⁴ the quantum mechanical cooperative and condensation phenomena^{5,6} could give rise to second order phase transitions from D (right-handed) to L type occurring generally at low temperatures below a critical point T_C , known as $T_C \ll T_B = 3\text{K} \ll T_E \sim 300\text{K}$, where T_B is the ambient cosmic background radiation temperature at the present epoch of the expanding universe. T_E is the Earth's present surface temperature. There the crucial problem is that of amplification of the electroweak advantage over the course of time so that, for example, the 20 amino acids convert almost entirely from L to D type.

We are thus led to look for the origin of the chiral life in more distant and cooler parts of the universe,^{7,8,9} arriving at the semiclosed Friedman model of the extragalactic radio source where the evolutionarily earlier upper hemisphere of the universe is filled with negative dark energy causing large mass defect.^{10,11}

IV. PLANCKEON- H^0 BOSON COMPOSITE

In his 1963 paper: Semiclosed Worlds in the General Theory of Relativity Zel'dovich¹² wrote: "A class of Friedman solutions of general relativity equation is found in which, as we approach the matter from infinity, we reach a singularity at the gravitational radius. But beyond this point the metric is continued in an unusual way—the radius decreases again and goes to zero only after passing through a maximum" (Novikov's similar work¹³ noted in proof). Andreev, Stanyukovich and

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others^{14,15} found related solutions showing the possible existence of a gravitationary closed point particle with Planck mass m_{pl} and radius l_{pl} moving with light vlocity which they called maximon or Planckeon. These particles can emit radiation only if they collide with massive object, but the radiation is unobservable by the Doppler effect.

We here propose a gravitationally bound Planckeon-Higgs boson composite^{10,11} creating negative attractive potential and positive rest mass energy:

$$-Gm_H m_{pl}/l_{pl} = -G(m_H/m_{pl})m_{pl}^2/l_{pl} = -10^{-17} Gm_{pl}^2/l_{pl} < 0, \quad (1)$$

$$10^{-17} m_{pl} c^2 = 10^{-17} (\hbar c/l_{pl}) > 0, \quad (2)$$

filling the evolutionarily earlier upper hemisphere as dark energy and evolutionarily later lower hemisphere as dark matter of the closed Friedman universe. Here we have used $m_H = 10^{-17} m_{pl} = 10^{-22} g$. On the equator separating the two hemispheres we have

$$10^{-17} (m_{pl} c^2 - Gm_{pl}^2/l_{pl}) = 0, \quad (3)$$

where the mass energy is absorbed by the attractive potential.

V. EVOLUTIONARY HISTORY OF FRIEDMAN UNIVERSE

We extend the Friedman metric in Lorentz-Friedman-Reissner-Nordström form^{10,11}:

$$ds^2 = c^2 g_{tt} dt^2 - g_{rr} dr^2, \quad g_{tt} = g_{rr}^{-1} = 1 - r^2/r_g^2 + L_\theta^2 l_{pl}^2/r^2 \quad (4)$$

Here $r_g = 2GM/c^2$ is the gravitational radius of the universe having Newtonian mass M and radius $R \geq r_g$, and

$$L_\theta = \hbar l_\theta / 2\pi, \quad l_\theta = \text{integer}. \quad (5)$$

is the quantized angular momentum.

The evolutionary history of the Lorentz-Friedman black hole is contained in the integral

$$l_{pl} = \int^R g_{rr} r dr = \int^R r dr (1 - r^2/r_g^2 + L_\theta^2 l_{pl}^2/r^2)^{-1}. \quad (6)$$

giving the unitary and holographic information content (entropy)¹⁶ of the black hole acquired by an observer approaching the matter distribution through empty space from infinity:

$$(R/l_{pl})^2 = (10^{28}/10^{-33})^2 = 10^{120}. \quad (7)$$

VI. SUPERLUMINAL INFLATION AND SUBLUMINAL EVOLUTION

The light velocity is obtained by solving $ds^2 = 0$ as:

$$\begin{aligned} dr/dt &= c(g_{tt}/g_{rr}) = c(1 - r^2/r_g^2 + L_\theta^2 l_{pl}^2/r^2) \\ &> c \text{ at } r \sim l_{pl} \text{ and } r \sim r_g - l_{pl} \\ &= c \text{ at } r = r_C = (r_g/l_{pl})^{1/2} \\ &= c \text{ in between } r_C < r < r_C = c \text{ and } r \sim r_g - l_{pl} \end{aligned} \quad (8)$$

Eqs.(8) show that, starting from quantum fluctuations of preexisting metric for $0 < r < l_{pl}$, the light velocity is superluminal at $r \sim l_{pl}$ and $r_g - l_{pl}$. After Big Bang at temperature $T_B = 10^{27} K$, dr/dt decreases with the increase of r towards $r = r_C = (r_g/l_{pl})^{1/2} = L_\theta^2 10^{-2} \text{ cm}$ for $r_g = R = 10^{28} \text{ cm}$.

During the superluminal and inflationary epoch of electroweak and grand unification of gauge fields by Higgs mechanism, a causally related small region extends from $r \sim 10^{-25} \text{ cm}$ to $r \sim 10 \text{ cm}$, followed by a brief interlude of reheating, retuning to the pre-inflationary temperature of the universe. Further evolution is described by standard Friedman universe starting the radiation dominated phase of Hubble's evolutionary history expanding with subluminal velocity. Hubble constant H relates the velocity v of a massive extragalactic object to its distance d from the Earth:

$$H = v/d \quad (9)$$

The COBE astronomical observations of the large-scale homogeneity of the distribution of matter and galaxy formation on the scale of 10^{10} cm light years can be explained by the superluminal and bi-directional EPR causal connection between radius $r = l_{pl}$ and $r = r_C$, while stars, clusters of galaxies, voids and other structures larger than 10^8 light years seem to indicate the angular momentum (5) $l_\theta \sim 10^3$ so that $r_C = l_\theta 10^{-2} \sim 10 \text{ cm}$, the high l_θ value indicating the multi-directional inflation.

VII. H⁰ BOSON AND INFLATION

H⁰ boson has non-vanishing vacuum expectation value which spontaneously breaks electroweak gauge symmetry and which, in turn, gives rise to the Higgs mechanism capable of giving mass to the gauge bosons.

The PC and T symmetric Klein-Gordon equation

$$[\partial^2/\partial^2(ct)^2 - \partial^2/\partial^2r^2 + (\hbar/mc)^2]\psi = 0 \quad (10)$$

obeyed by the Higgs boson wave function $\psi(r, t)$ can be decomposed into two-component Dirac form:

$$\begin{aligned} (\partial/\partial ct - \partial/\partial r + \hbar/mc)\psi_+ &= 0, \\ (\partial/\partial ct + \partial/\partial r + \hbar/mc)\psi_- &= 0, \end{aligned} \quad (11)$$

where ψ_{\pm} represent the positive and negative energy states of the Higgs boson going forward and backward in time.

During the inflation, starting at $r = l_{pi}$ and ending at $r = r_c$, the light velocities $(dr/dt)_{\pm}$ are given by

$$\begin{aligned} (dr/dt)_{+} &= c[(1 - r/r_g + L_{\theta}l_{pi}/r)], \\ &> c \text{ at } r = l_{pi} \\ &= c \text{ for } r = r_c = (L_{\theta}l_{pi}r_g)^{1/2} \end{aligned} \quad (12)$$

and

$$\begin{aligned} (dr/dt)_{-} &= c[(1 + r/r_g + L_{\theta}l_{pi}) \\ &> c \text{ at } r = r_g - l_{pi} \\ &= c \text{ for } r = r_c = (L_{\theta}l_{pi}r_g)^{1/2}. \end{aligned} \quad (13)$$

The CERN high energy proton-proton collision experiment creating H^0 boson, immediately decaying into a counter-propagating pair of photons, seems to tell the preference of H^0 boson, going forward in time, to its antiboson, going backward in time, by the present universe expanding forward in time.

VIII. MATTER-ANTIMATTER ASYMMETRY

Matter-antimatter symmetry required by quantum theory and relativity is largely violated in cosmic scale outside high energy laboratory experiments. As there were equal amount of gauge matter and antimatter, immediately after the moment of the hot Big Bang at $r = r_c$, we here propose to consider that the probability of collision between H^0 boson and the gauge matter, comoving forward in time, dominates over the collision between H^0 boson and antimatter, counter-propagating backward in time during inflation expanding forward in time.

IX. COSMOLOGICAL DOUBLE-SLIT EXPERIMENT

In his positron theory Feynman extended Jordan-Paulil propagator

$$\begin{aligned} D(\mathbf{r}, t) &= t/|t|\delta(c^2t^2 - r^2) \\ &= D_{ret} - D_{adv} \end{aligned} \quad (14)$$

To

$$\begin{aligned} D &= D_{ret} + D_{-} \\ &= D_{adv} + D_{+}. \end{aligned} \quad (15)$$

Here D_{ret} and D_{adv} are the retarded and advanced propagators. D_{\pm} are the Fourier contributions from positive and negative frequency sheets. At the Chicago meeting Pauli criticized Feynman's D_F by applying it to the single electron double-slit experiment. Feynman¹⁷ replied Pauli by showing a delayed-choice double-slit equipped with time-dependent shutters

creating $\Lambda + V = N$ shaped electron-positron pairs, zigzagging in time.

A matter-antimatter symmetric cosmology is conceivable by replacing the shutter by the Big Bang and the slit by the 3-dimensional Lorentz sphere: $(ct)^2 - r^2 = l_{pi}^2$ filled with point-like Planckons and joined onto Friedman universe at $r = r_c$, allowing a topological (non-Hausdorff) worm hole where the timelike 3-vectors is undefined.

X. EARLY COMMENT ON GAUGE THEORY

After C. N. Yang's keynote address: "Gauge Fields, Electromagnetism and the Bohm-Aharonov Effect" at the 1983 Tokyo symposium on the Foundations of Quantum Mechanics (ISQM),^{10,11} Greenberger asked: Why is that we do not have a gauge theory of gravity that works in this simple and beautiful way in the Bohm-Aharonov experiment using electron holography? Yang¹⁸ answered: "All gauge theories are related to connection on fibre bundles. In the case of gravity the bundle is a special one, the tangent bundle. That is why, in the final analysis, gravity is different from other gauge theories."

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By F. I. Bashirov & N. K. Gaisin

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Keywords: crystallographic point symmetry; hindered molecular motion; nuclear magnetic resonance; second moment; single crystal; symmetry distortion.

I. INTRODUCTION

The use of spectroscopy techniques such as neutron, Raman, infrared, dielectric, electron, nuclear magnetic and electric quadrupole resonance spectroscopy to study condensed state physics problems has several advantages. This includes the detailed nature of the information, which can be obtained on structural and dynamical properties, and the definiteness of the interpretation, which can be given to the data. The theoretical studying of hindered molecular motion (HMM) dynamics is normally carried out by examining the time depended auto-correlation function (ACF) of a physical quantity of the molecule. A notable progress has been made in the theory of HMM by using the properties of continuous [1] and point [2, 3] symmetry groups.

The second moment of NMR spectral line broadened owing to the magnetic dipole-dipole interaction of nuclear spins is serving as one of main probes of HMM in crystalline substances [4-7]. Measuring the second moment allows one to testing various models of HMM taking place in condensed matter.

The basic statements of the well-known HMM models have been carefully discussed in [2, 8]. The

most recent developed model, the so-called extended angular jump model (EAJM), is well appropriate to exploring HMM of symmetrical molecules in single crystals, powders, and liquids. It was successfully applied to examine the rates of nuclear magnetic relaxation [9-11], the relative intensities of Raman light scattering [11, 13], dielectric [14, 15] and infrared [13] absorption, and the incoherent neutron scattering function [7, 8, and 16] in mono- and polycrystalline molecular media.

Recently, EAJM-approach was used by describing the intramolecular contribution to the second moment of NMR line shape [17]. This time, we decided to expand this application up to ability of simulating whole NMR spectral line second moment in molecular crystals without any restriction on the temperature region. So, this paper is devoted to add EAJM-approach to simulating the second moment of NMR absorption line broadened owing to the magnetic dipole-dipole interaction of homo- and hetero-nuclear spins in perfect and symmetry distorted crystals. We shall consider the contributions of both intra- and inter-molecular dipole-dipole interactions to the 2nd moment. The validity of the application will be verified by approximating the known experimental data on the 2nd moment of the proton NMR spectral line measured for two main directions of the external magnetic field in the single crystal of ammonium chloride at large temperature region [18].

II. BASICS OF THE THEORY OF NMR 2ND MOMENT M_2 IN MOLECULAR CRYSTALS

The second moment of NMR spectral line M_2 broadened owing to magnetic dipole-dipole interaction of identical resonant nuclear spins in molecular crystals can be simulated by using the following basic expression [3-6]:

$$M_2 = \frac{1}{N_i} \sum_{i=1}^{N_i} \sum_{j \neq i} \frac{3}{4} \hbar^2 \gamma_j^2 r_{ji}^{-6} I_j (I_j + 1) (3 \cos^2 \theta_{ji} - 1)^2, \quad (1)$$

where the subscript i labels the resonant nuclear spins of a molecule and the symbol N_i designates the number of such spins, the subscript j labels all resonant nuclear spins of the crystal; the symbols γ and I denote respectively

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the gyromagnetic ratio and the quantum number of the nuclei; $\hbar = 1.0544 \cdot 10^{-34}$ J-s is Planck's constant, θ_{ji} is the polar angle that forms the internuclear vector $\mathbf{r}_{ji} = r_{ji} (r_{ji}, \varphi_{ji}, \theta_{ji})$ with respect to the intensity vector of stationary magnetic field \mathbf{B}_0 allocating the laboratory reference frame (LRF). The azimuthal angle φ_{ji} can be any.

In the case of the direction of intramolecular vector $\mathbf{r}_{ji} (r_{ji}, \varphi_{ji}, \theta_{ji})$ changes accidentally, its spherical angles ($\varphi_{ji}, \theta_{ji}$) as well as some intermolecular vectors present random functions of time. As a result, spectral distribution of NMR signal is modified. However, the intramolecular and intermolecular vectors effect on NMR signal by different way. Consequently, simulating the NMR second moment M_2 is to be performed by accounting for two additive contributions – intramolecular $M_2^{(intra)}$ and intermolecular $M_2^{(inter)}$:

$$M_2 = M_2^{(intra)} + M_2^{(inter)}. \quad (2)$$

a) *Intramolecular contribution – $M_2^{(intra)}$*

The intramolecular contribution $M_2^{(intra)}$ to the total second moment M_2 accounting for the hindered motion of intramolecular vectors can be presented in the form [19]:

$$M_2^{(intra)} = \frac{1}{N_i} \sum_{i=1}^{N_i} \sum_{j \neq i} \left[\frac{3}{4} \hbar^2 \gamma_j^2 I_j (I_j + 1) \cdot \int_{-\delta v_i}^{\delta v_i} J_{ji}^{(0)}(\omega_i) dv_i \right], \quad (3)$$

where

$$J_{ji}^{(0)}(\omega_i) = \int_{-\infty}^{+\infty} K_{ji}^{(0)}(t) \exp(i\omega_i t) dt \quad (4)$$

is the no normalized spectral density function (SDF) of the autocorrelation function

$$K_{ji}^{(0)}(t) = \langle F_{ji}^{(0)}(t) F_{ji}^{(0)*}(t + \tau) \rangle \quad (5)$$

of the lattice part of spin-spin interaction Hamiltonian

$$F_{ji}^{(0)}(t) = r_{ji}^{-3} (3 \cos^2 \theta_{ji}(t) - 1) = \left(\frac{16\pi}{5} \right)^{1/2} r_{ji}^{-3} Y_0^{(2)}[\varphi_{ji}, \theta_{ji}(t)]. \quad (6)$$

The quantity $Y_0^{(2)}[\varphi_{ji}, \theta_{ji}(t)]$ is the zero component of the 2nd rank normalized spherical function. In Equation (3), the integration has to be performed within the limits of the double line width from $-\delta v_i$ up to $+\delta v_i$, where $v_i = \omega_i / 2\pi = \gamma_i B_0$ is the resonance frequency of i -th spins, B_0 – the module of induction vector of the static magnetic field, γ_i – the gyromagnetic ratio of resonant nuclei, $\delta v_i = 1/T_{2i}$ (T_{2i} is the spin-spin relaxation time).

The outcomes of simulating Equation (3) depend on the physical model of molecular motion. With respect to the goal of the present studying, EAJM-approach will be used as the model of HMM [2, 8]. Within the framework of that model, the analytical expression of normalized SDF $J_0^{(2)}(\omega_i)$ of the tensor component $Y_0^{(2)}[\phi(t), \vartheta(t)]$ is presented for a single crystal sample by

$$J_0^{(2)}(\omega) = J_0^{(2)}(q_\alpha, \phi, \vartheta, \omega) = \frac{5}{2\pi} \sum_{\alpha} \sum_{l=0}^2 \frac{q_\alpha \tau_\alpha}{1 + (\omega \tau_\alpha)^2} a_{\alpha l 0}(\phi) \cos^{2l} \vartheta. \quad (7)$$

It is noted that the angles φ_{ji} and θ_{ji} of the internuclear vector \mathbf{r}_{ji} do not present explicitly in Equation (7). Instead, there are two spherical angles ϕ and ϑ , by which orientation of the crystallographic reference frame sets up in the axial laboratory one. The subscript α labels irreducible representations (IR) Γ_α of the HMM point symmetry group G.

By accounting for Equation (7), the no normalized SDF $J_{ji}^{(0)}(\omega_i)$ takes the form:

$$J_{ji}^{(0)}(\omega_i) = J_{ji}^{(0)}(q_\alpha, \phi, \vartheta, \omega_i) = \frac{16\pi}{5} r_{ji}^{-6} J_0^{(2)}(q_\alpha, \phi, \vartheta, \omega_i) =$$

$$8 r_{ji}^{-6} \sum_{\alpha} \sum_{l=0}^2 \frac{q_{\alpha} \tau_{\alpha}}{1 + (\omega_i \tau_{\alpha})^2} a_{\alpha l 0}(\phi) \cos^{2l} \vartheta. \quad (8)$$

The rated expressions of the factors $a_{\alpha l 0}(\phi)$ are tabulated explicitly as functions of azimuthal angle ϕ for all crystallographic point symmetry groups of pure rotation in [2,8]. A quantity q_{α} , the dynamic weight of IR Γ_{α} of the group G, is playing a role of adjustable parameter of the theory that has to be experimentally determined. It satisfies the normalization condition: $\sum q_{\alpha} = 1$. For ideal symmetry of HMM, a dynamic weight q_{α} reduces its static value value equals to the dimension of IR Γ_{α} of the group G. The parameter τ_{α} , the HMM correlation time adapted to Γ_{α} , relates the expression:

$$\tau_{\alpha} = (1 - \chi_{\alpha E}^{-1} \sum_i p_i \chi_{\alpha i})^{-1} \tau, \quad (9)$$

where $\chi_{\alpha i}$ and $\chi_{\alpha E}$ are the characters of i -th and identical classes, respectively, p_i – the probability of the fundamental act of motion appropriate to i -th class of the group G, and τ – a mean time between two successive steps of motion. The time τ is ordered to Arrhenius low:

$$\tau = \tau_0 \exp(E_a/RT), \quad (10)$$

where E_a is the height of activation energy barrier averaged on the HMM symmetry group, τ_0 is a mean time between two sequential attempts to overlap the barrier.

By substituting Equation (8) in Equation (3), we shall obtain the 2nd moment expression specified by the intramolecular action of resonant spins j to target resonant spins i in analytical form by

$$M_2^{(\text{intra})} = \frac{6}{N_i} \sum_{i=1}^{N_i} \sum_{j \neq i} \hbar^2 \gamma_j^2 r_{ji}^{-6} I_j(I_j + 1) \int_{-\delta v_i}^{\delta v_i} \left[\sum_{\alpha} \sum_{l=0}^2 \frac{q_{\alpha} \tau_{\alpha}}{1 + (2\pi v_i \tau_{\alpha})^2} a_{\alpha l 0}(\phi) \cos^{2l} \vartheta \right] dv_i. \quad (11)$$

By performing the prescribed integration, we are obtaining:

$$M_2^{(\text{intra})} = \frac{6}{\pi N_i} \sum_{i=1}^{N_i} \sum_{j \neq i} \hbar^2 \gamma_j^2 r_{ji}^{-6} I_j(I_j + 1) \sum_{\alpha} \sum_{l=0}^2 q_{\alpha} a_{\alpha l 0}(\phi) \cos^{2l} \vartheta \arctg(2\pi \cdot \delta v_i \cdot \tau_{\alpha}). \quad (12)$$

For a powder, by averaging over the angles ϕ and ϑ , Equation (12) reduces to:

$$M_2^{(\text{intra|pow})} = \frac{6}{5\pi N_i} \sum_{i=1}^{N_i} \sum_{j \neq i} \hbar^2 \gamma_j^2 r_{ji}^{-6} I_j(I_j + 1) \sum_{\alpha} q_{\alpha} \arctg(2\pi \cdot \delta v_i \cdot \tau_{\alpha}). \quad (13)$$

In a regime of a fast molecular motion, the inequality $(2\pi \cdot \delta v_i \cdot \tau_{\alpha}) \ll 1$ is valid that follows the equality $\arctg(2\pi \cdot v_i \cdot \tau_{\alpha}) = 0$. In this case the dipole-dipole contribution to the second moment vanishes, that is, $M_2^{(\text{intra})} = 0$, and so-called phenomenon of "spectral line narrowing" or "bandwidth narrowing" is observed.

Alternatively, in the case of a slow motion regime, inequality $(2\pi \cdot v_i \cdot \tau_{\alpha}) \gg 1$ followed by equality $\arctg(2\pi \cdot v_i \cdot \tau_{\alpha}) \pi/2$ is valid. Furthermore, taking into account the normalization condition $\sum_{\alpha} q_{\alpha} = 1$, Equation (13) reduces down to a permanent value:

$$M_2^{(\text{intra|pow})} = \frac{3}{5N_i} \sum_{i=1}^{N_i} \sum_{j \neq i} \hbar^2 \gamma_j^2 r_{ji}^{-6} I_j(I_j + 1) \quad (14)$$

presented earlier by Abraham and Lösche [5, 6].

For single crystals, Equation (12) reduces to an expression retaining the angular dependence of the 2nd moment produced by homonuclear dipole-dipole interaction in the slow molecular motion regime:

$$M_{2ji}^{(\text{intra})} = \frac{3}{N_i} \sum_{i=1}^{N_i} \sum_{j \neq i} \hbar^2 \gamma_j^2 r_{ji}^{-6} I_j(I_j + 1) \sum_{\alpha} \sum_{l=0}^2 q_{\alpha} a_{\alpha l 0}(\phi) \cos^{2l} \vartheta. \quad (15)$$

As to the second moment contribution produced by the heteronuclear dipole-dipole interaction, the respective formula differs from that above presented by the factor 4/9 [20]. In this case, Equation (15) has to be replaced by

$$M_{2si}^{(\text{intra})} = \frac{4}{3N_i} \sum_{i=1}^{N_i} \sum_s \hbar^2 \gamma_s^2 r_{si}^{-6} I_s(I_s + 1) \sum_{\alpha} \sum_{l=0}^2 q_{\alpha} a_{\alpha l 0}(\phi) \cos^{2l} \vartheta, \quad (16)$$

where the subscript s labels no resonant nuclear spins of the molecule and N_s is the number of such spins.

b) *Intermolecular contribution* $-M_2^{(\text{inter})}$

The expression of intermolecular contribution to the 2nd moment $M_2^{(\text{inter})}$ associated with homonuclear interaction will be derived by modifying the basic Equation (1) to a form involving the spherical harmonics. We shall replace the angular dependent multiplier $(3 \cos^2 \theta_{ji} - 1)^2$ by its equivalent doublet $\frac{16\pi}{5} |Y_0^{(2)}(\varphi_{ji}, \theta_{ji})|^2$, where $Y_0^{(2)}(\varphi_{ji}, \theta_{ji})$ is a normalized spherical harmonic (function) of the 2nd order, a unit spherical tensor of the 2nd rank. Notice: (2) $Y_0^{(2)}(\varphi_{ji}, \theta_{ji})$ has no dependence of the azimuthal angle φ_{ji} in this particular case of the zero component of unit spherical tensor of the 2nd rank. Thus, we are rewriting expression (1) in terms of spherical tensors as:

$$M_2^{(\text{inter})} = \frac{12\pi}{5N_i} \sum_{i=1}^{N_i} \sum_{j=1}^{N_j} \hbar^2 \gamma_i^2 r_{ji}^{-6} I_i(I_i + 1) |Y_0^{(2)}(\varphi_{ji}, \theta_{ji})|^2, \quad (17)$$

where N_i is the number of intramolecular resonant spins and N_j is outer (relative to the target molecule) resonant spins. The angles θ_{ji} and φ_{ji} are determined in the LRF.

Nevertheless, it is helpful to assign the internuclear vectors in the crystallographic reference frame (CRF). To produce this change, we shall transform spherical tensors from CRF to LRF by rotation to the three-dimensional Euler angles (ϕ, ϑ, ξ) according to the rule [21]:

$$Y_0^{(2)}(\varphi', \theta') = \sum_{m=-2}^2 D_{0m}^{(2)}(\phi, \vartheta, \xi) Y_m^{(2)}(\varphi, \theta), \quad (18)$$

where (2) $D_{0m}^{(2)}(\phi, \vartheta, \xi)$ is an element of Wigner matrix. Now, we can rewrite Equation (17) as:

$$M_2^{(\text{inter})} = \frac{12\pi}{5N_i} \sum_{i=1}^{N_i} \sum_{j=1}^{N_j} \hbar^2 \gamma_i^2 r_{ji}^{-6} I_i(I_i + 1) \left[\sum_{m=-2}^2 D_{0m}^{(2)}(\phi, \vartheta, \xi) Y_m^{(2)}(\varphi_{ji}, \theta_{ji}) \right]^2. \quad (19)$$

By replacing $D_{0m}^{(2)}(\phi, \vartheta, \xi) = \sqrt{(4\pi/5)} Y_m^{(2)}(\vartheta, \phi)$ and renaming $M_2^{(\text{inter})} = M_{2ji}^{(\text{inter})}(\phi, \vartheta)$ we shall transform Equation (19) to

$$M_{2ji}^{(\text{inter})}(\phi, \vartheta) = \frac{48\pi^2}{25N_i} \sum_{i=1}^{N_i} \sum_{j=1}^{N_j} \hbar^2 \gamma_i^2 r_{ji}^{-6} I_i(I_i + 1) \left[\sum_{m=-2}^2 Y_m^{(2)}(\phi, \vartheta) Y_m^{(2)}(\varphi_{ji}, \theta_{ji}) \right]^2, \quad (20)$$

where ϕ and ϑ are the spherical angles of the vector \mathbf{B}_0 assigned in LRF, and φ_{ji} and θ_{ji} are those of the internuclear vector \mathbf{r}_{ji} determined in CRF, the subscripts i and j label the resonant homonuclear spins.

By multiplying Equation (20) by the factor 4/9 and replacing subscript j by v to label no resonant nuclear spins, we shall get the heteronuclear analog of the intermolecular contribution to the 2nd moment $M_{2vi}^{(\text{inter})}$

$$M_{2vi}^{(\text{inter})}(\phi, \vartheta) = \frac{64\pi^2}{75N_i} \sum_{i=1}^{N_i} \sum_{v=1}^{N_v} \hbar^2 \gamma_v^2 r_{vi}^{-6} I_v(I_v + 1) \left[\sum_{m=-2}^2 Y_m^{(2)}(\phi, \vartheta) Y_m^{(2)}(\phi_{vi}, \theta_{vi}) \right]^2. \quad (21)$$

c) Total expression of the 2nd moment – M_2

Taking into account above presented Equations (2), (12), (15), (16), (20), and (21), we are able to write the total expression of the NMR 2nd moment $M_2^{(T)}(\phi, \vartheta)$:

$$M_2^{(T)}(\phi, \vartheta) = \frac{2\hbar^2}{N_i\pi} \sum_{i=1}^{N_i} \left[3 \sum_{\substack{j=1 \\ j \neq i}}^{N_i-1} \gamma_i^2 I_i(I_i + 1) r_{ji}^{-6} + \frac{4}{3} \sum_{s=1}^{N_s} \gamma_s^2 I_s(I_s + 1) r_{si}^{-6} \right] \cdot \\ \sum_{\alpha} \sum_{l=0}^2 q_{\alpha} \arctg(2\pi \cdot \delta v_i \cdot \tau_{\alpha}) a_{\alpha l 0}(\phi) \cos^{2l} \vartheta + \\ \frac{48\pi^2 \hbar^2}{25N_i} \sum_{i=1}^{N_i} \sum_{j'=1}^{N_{j'}} \gamma_i^2 I_i(I_i + 1) r_{j'i}^{-6} \left[\sum_{m=-2}^2 Y_m^{(2)}(\phi, \vartheta) Y_m^{(2)}(\phi_{j'i}, \theta_{j'i}) \right]^2 + \\ \frac{64\pi^2 \hbar^2}{75N_i} \sum_{i=1}^{N_i} \sum_{v=1}^{N_v} \gamma_v^2 I_v(I_v + 1) r_{vi}^{-6} \left[\sum_{m=-2}^2 Y_m^{(2)}(\phi, \vartheta) Y_m^{(2)}(\phi_{vi}, \theta_{vi}) \right]^2. \quad (22)$$

The temperature dependence of Equation (22) takes place implicitly by means of the dynamical variable τ_{α} included in intramolecular part of the 2nd moment. Besides, owing to the temperature dependence of the components r_{ji} , r_{vi} , ϕ_{ji} , θ_{ji} , ϕ_{vi} and θ_{vi} of the internuclear vectors \mathbf{r}_{ji} , \mathbf{r}_{vi} , the intermolecular part of the 2nd moment has to be also temperature depended. Meanwhile, it is reasonable to assume that small fluctuations of angles $\phi_{j'i}$, $\theta_{j'i}$ and ϕ_{vi} , θ_{vi} about their equilibrium values can't give notable change of local magnetic field on the sites of target protons. Therefore, by evaluating the 2nd moment in the fast motion regime, we shall take into account only the dependence of internuclear distances r_{ji} and r_{vi} of temperature.

It is timely to remind the meaning of some quantities and labels displayed in Equation (22):

N_i is the number of identical resonant nuclear spins of a target molecule,

i and j label intramolecular resonant nuclear spins,

j' labels resonant spins outer relative to the target molecule,

s – intramolecular no resonant heteronuclear spins,

v – no resonant heteronuclear spins outer relative to the target molecule,

ϕ and ϑ designate the spherical angles of the axial magnetic field direction with respect to CRF,

ϕ_{ji} and θ_{ji} – the spherical angles of \mathbf{r}_{ji} - internuclear vector fixed in the CRF,

q_{α} and $a_{\alpha l 0}$ – the quantities of the EAJM-approach theory [2, 8].

III. APPLICATION TO THE SINGLE CRYSTAL OF AMMONIUM CHLORIDE NH_4Cl

a) Overview

Ammonium chloride being one of the most studied substances is frequently used as a touchstone of the validity of various theories on the structure and physical properties of crystals. It is an ionic crystal, which ammonium ions exhibit random reorientation and consequently they have no permanent orientation ordering. Unit cell of NH_4Cl is a body-centered cube of CsCl type. At center of a cubic cell, a tetrahedron of ammonium cation NH_4^+ is placed, and its corners are occupied by chlorine anions Cl^- . The lattice parameter is $r_{\text{Cl-Cl}} = r_{\text{N-N}} = (3.844 \pm 0.024) \cdot 10^{-10}$ m, four nearest protons of NH_4^+ - cation are displaced at the distance $r_{\text{N-H}} = (1.038 \pm 0.04) \cdot 10^{-10}$ m from a nitrogen nucleus, and the neighboring protons are spaced from each other to the distance $r_{\text{H-H}} = (1.695 \pm 0.04) \cdot 10^{-10}$ m [22].

Below 242.9 K, the crystal is in its ordered phase. The equilibrium disposition of atoms is shown in Figure 1. The random local motion of ammonium ions does not change the ordered structure of the crystal. It means that the reorientation symmetry group of any ammonium ion vector is the point symmetry group of tetrahedron T.

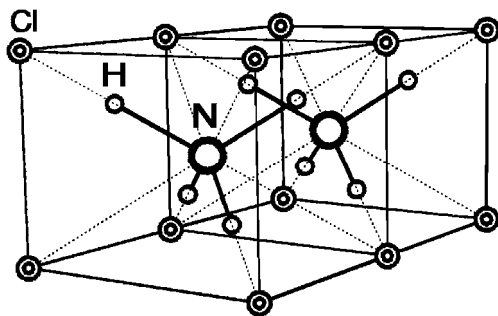


Figure 1: Schematic of the NH_4Cl crystal structure in the ordered phase ($T < 242.9$ K).

In the single crystal of NH_4Cl , Bersohn and Gutowsky have investigated the proton resonance spectra [18] and we have measured the proton spin-lattice relaxation times [10]. It was found that both the shape of spectral line and the relaxation times are anisotropic and show temperature dependence. To discuss the continuous wave data the quantum mechanical calculation were applied, but no extra knowledge was added about crystal structure [18]. The proton relaxation data were discussed in the framework of classical mechanical EAJM-approach taken as the model of NH_4^+ cation HMM [2, 8]. As a result of such simulation, a phenomenon of the site symmetry distortion was discovered in the ordered phase of NH_4Cl .

In the following description, we shall simulate particular contributions to the proton NMR 2nd moment in the single crystal of NH_4Cl for slow and fast motion regimes of NH_4^+ cation (low and high temperature regions) by using Equations (15), (16), (20), and (21), first. Then, we shall approximate the experimental curves of temperature dependence ($-200^\circ\text{C} < T < 25^\circ\text{C}$) of the total 2nd moment M_2 [18] by general Equation (22) for two orientations of the NH_4Cl single crystal in the static magnetic field: $[1,0,0] \parallel \mathbf{B}_0$ and $[1,1,0] \parallel \mathbf{B}_0$.

We shall calculate the particular contributions to the angular dependent second moment of proton NMR spectral line stimulated by

- interaction between the inner four proton spins, which gives rise intraionic proton-proton contribution – $M_{2,\text{HH}}^{(\text{intra})}$
- action of the unique inner nitrogen nuclear spin to 4 proton spins, which produces the intraionic nitrogen-proton contribution – $M_{2,\text{NH}}^{(\text{intra})}$
- action of 104 nearest adjacent proton spins to 4 proton spins of target NH_4^+ cation giving rise the interionic proton-proton contribution – $M_{2,\text{HH}}^{(\text{inter})}$
- action of 8 nearest adjacent chlorine spins to 4 proton spins of the target NH_4^+ cation giving rise the interionic chlorine-proton contribution $M_{2,\text{ClH}}^{(\text{inter})}$, and
- action of 6 nearest adjacent nitrogen spins to 4 proton spins of the target NH_4^+ cation giving rise the interionic nitrogen-proton contribution – $M_{2,\text{NH}}^{(\text{inter})}$

All actions of other nuclear spins to the target proton spins are neglected here. Due to their remoteness, they give a small effect in the studied 2nd moment.

- Slow motion regime of NH_4^+ -cation
 - Intraionic proton-proton contribution – $M_{2,\text{HH}}^{(\text{intra})}(\phi, \vartheta)$

Accounting for the values of proton spin $I_j = I_{\text{H}} = 1/2$ and the number of protons $N_i = N_{\text{H}} = 4$ in Equation (15), we shall get the rated expression of $M_{2,\text{HH}}^{(\text{intra})}(\phi, \vartheta)$ by:

$$M_{2,\text{HH}}^{(\text{intra})}(\phi, \vartheta) = \frac{27}{4} \gamma_{\text{H}}^2 \hbar^2 r_{\text{HH}}^{-6} \sum_{\alpha=1,2} \left(\sum_{l=0}^2 q_{\alpha} a_{\alpha l 0}(\phi) \cos^{2l} \vartheta \right). \quad (23)$$

Substituting in Equation (23) 1) table data: $\gamma_H = 26753 \text{ s}^{-1}\text{Gs}^{-1}$ and $\hbar = 1.0544 \cdot 10^{-27} \text{ erg}\cdot\text{s}$; 2) experimental values: $q_1 = 0.25$, $q_2 = 0.73$ [10, 11], $r_{\text{HH}} = 1.695 \cdot 10^{-8} \text{ cm}$ [22], and 3) expressions of the factors $a_{\omega 0}(\phi)$ [2, 8]: $a_{100}(\phi) = (1/8)(1+3\cos^2 2\phi)$, $a_{110}(\phi) = -(3/4)(1+\cos^2 2\phi)$, $a_{120}(\phi) = (3/8)(3+\cos^2 2\phi)$, $a_{200}(\phi) = (1/4)(1-\cos^2 2\phi)$, $a_{210}(\phi) = (1/2)(1+\cos^2 2\phi)$, and $a_{200}(\phi) = -(1/4)(3+\cos^2 2\phi)$ allows us to obtain the explicit expression of $M_{2,\text{HH}}^{(\text{intra})}(\phi, \vartheta)$ by

$$M_{2,\text{HH}}^{(\text{intra})}(\phi, \vartheta) = 48.39 - 20.09[\cos^2 2\phi + 2(1+\cos^2 2\phi)\cos^2 \vartheta - (3+\cos^2 2\phi)\cos^4 \vartheta]. \quad (24)$$

The surface-plot graph of $M_{2,\text{HH}}^{(\text{intra})}(\phi, \vartheta)$, the HH-intraionic part of the proton NMR 2nd moment, drawn according to Equation (24) as a function of spherical angles ϕ and ϑ of the crystal orientation in the static magnetic field for a slow motion regime of NH_4^+ cation in NH_4Cl single crystal is presented in Figure 2a. The graph of $M_{2,\text{HH}}^{(\text{intra})}(\vartheta)$, abridged dependence $M_{2,\text{HH}}^{(\text{intra})}$ of the polar angle ϑ , while the azimuthal angle ϕ is fixed by $\pi/4$, is shown in Figure 2b.

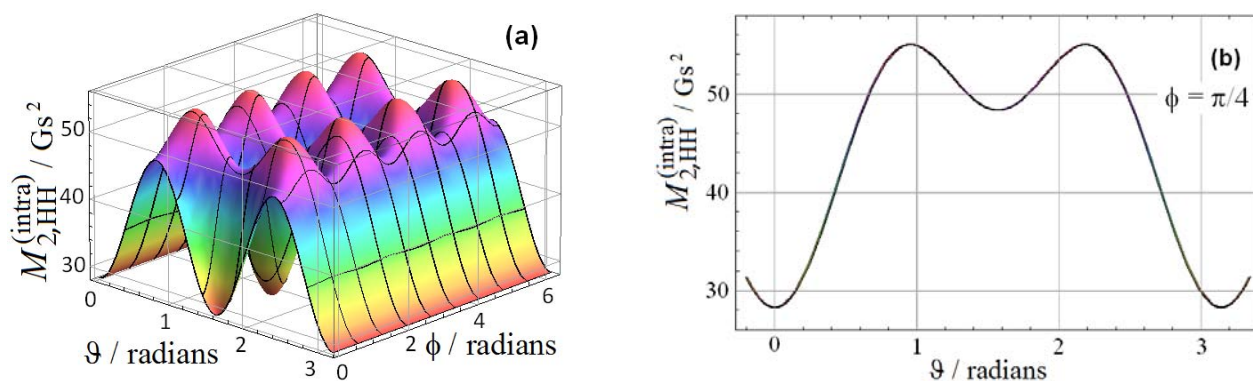


Figure 2: The graphs of the theoretical angular dependence of HH-intraionic contribution $M_{2,\text{HH}}^{(\text{intra})}$ to the proton NMR 2nd moment in NH_4Cl single crystal drawn for a slow motion regime of NH_4^+ cation according to Equation (24) as a function: a) of spherical angles ϕ and ϑ , b) of polar angle ϑ for $\phi = \pi/4$.

ii. Intraionic nitrogen-proton contribution – $M_{2,\text{NH}}^{(\text{intra})}(\phi, \vartheta)$

By substituting the number of protons $N_i = 4$, the number of nitrogen spins $N_s = 1$, Plank constant $\hbar = 1.054 \cdot 10^{-27} \text{ erg}\cdot\text{s}$, the nitrogen spin value $I_s = I_N = 1$ and gyromagnetic ratio $\gamma_N = 1933.3 \text{ s}^{-1}\text{Gs}^{-1}$, and experimental values of dynamic weights: $q_1 = 0.25$, $q_2 = 0.73$ [10, 11], $r_{\text{NH}} = 1.038 \cdot 10^{-8} \text{ cm}$ [22], and expressions of the factors $a_{\omega 0}(\phi)$: $a_{100}(\phi) = (1/8)(1+3\cos^2 2\phi)$, $a_{110}(\phi) = -(3/4)(1+\cos^2 2\phi)$, $a_{120}(\phi) = (3/8)(3+\cos^2 2\phi)$, $a_{200}(\phi) = (1/4)(1-\cos^2 2\phi)$, $a_{210}(\phi) = (1/2)(1+\cos^2 2\phi)$, and $a_{200}(\phi) = (1/4)(3+\cos^2 2\phi)$ [2, 8] in Equation (16), we are obtaining the expression of $M_{2,\text{NH}}^{(\text{intra})}(\phi, \vartheta)$ in the explicit form by

$$M_{2,\text{NH}}^{(\text{intra})}(\phi, \vartheta) = 0.786263 [\cos^2 2\phi + 2(1+\cos^2 2\phi)\cos^2 \vartheta - (3+\cos^2 2\phi)\cos^4 \vartheta]. \quad (25)$$

The surface-plot graph $M_{2,\text{NH}}^{(\text{intra})}(\phi, \vartheta)$, the intraionic NH-contribution to the proton NMR 2nd moment, drawn according to Equation (25) as a function of spherical angles ϕ and ϑ of the crystal orientation in the static magnetic field for a slow motion regime of NH_4^+ cation in NH_4Cl single crystal is presented in Figure 3a. The plane graph $M_{2,\text{NH}}^{(\text{intra})}(\vartheta)$ drawn according to Equation (25) as a function of solely polar angle ϑ is presented in Figure 3b, whereas azimuth angle is fixed by $\phi = \pi/4$.

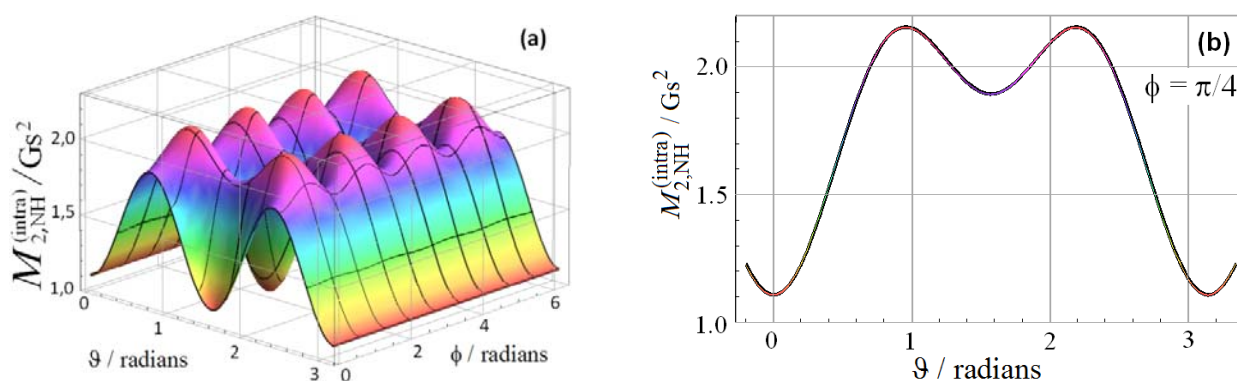


Figure 3: The graphs $M_{2,NH}^{(intra)}(\phi, \vartheta)$ and $M_{2,NH}^{(intra)}(\vartheta)$ of NH-intraionic contribution to the proton NMR second moment in NH_4Cl single crystal drawn according to Equation (25) for a slow motion regime of NH_4^+ -cation as functions of: a) spherical angles ϕ and ϑ and b) polar angle ϑ for $\phi = \pi/4$, respectively.

iii. Interionic proton-proton contribution – $M_{2,HH}^{(inter)}(\phi, \vartheta)$

The schematic of target NH_4^+ -ion with inner protons numerated by 1, 2, 3, and 4 is shown in Figure 4. Besides, 26 neighboring NH_4^+ -ions are presented therein. During this simulation, we shall assume that all protons are immobile and confine ourselves to 104 nearest outer protons, from which only four protons numerated by 5, 6, 7, and 8 are shown in Figure 4. Now, we shall write an expression describing interionic HH-contribution of only 104 nearest protons to inner 4 protons $M_{2,HH}^{(inter)}(\phi, \vartheta)$:

$$M_{2ji}^{(inter)}(\phi, \vartheta) = \frac{48\pi^2}{25N_i} \sum_{i=1}^{N_i} \sum_{j'=5}^{108} \hbar^2 \gamma_i^2 r_{ji}^{-6} I_i(I_i + 1) \left[\sum_{m=-2}^2 Y_m^{(2)}(\phi, \vartheta) Y_m^{(2)}(\varphi_{j'i}, \theta_{j'i}) \right]^2, \quad (26)$$

where for commodity the outer protons are labeled by j' ($5 \leq j' \leq 108$). By substituting the numbering values of constants γ_{HH} and \hbar , just presented, $I_i = I_H = 1/2$, $N_i = 4$, Equation (26) takes the following semi explicit form:

$$M_{2,HH}^{(inter)}(\phi, \vartheta) = 2.82721 \cdot 10^{-45} \sum_{j'=5}^{108} \sum_{i=1}^4 \left| \sum_{m=-2}^2 Y_m^{(2)}(\phi, \vartheta) Y_m^{(2)}(\varphi_{j'i}, \theta_{j'i}) \right|^2 r_{ji}^{-6}, \quad (27)$$

where the values of proton-proton distances r_{ji} and angles $\varphi_{j'i}$ and $\theta_{j'i}$ are to be estimated by using the structure data [22]: $r_{ClCl} = r_{NN} = 3.844 \cdot 10^{-10}$ m, $r_{NH} = 1.038 \cdot 10^{-10}$ m, $r_{HH} = 1.695 \cdot 10^{-10}$ m.

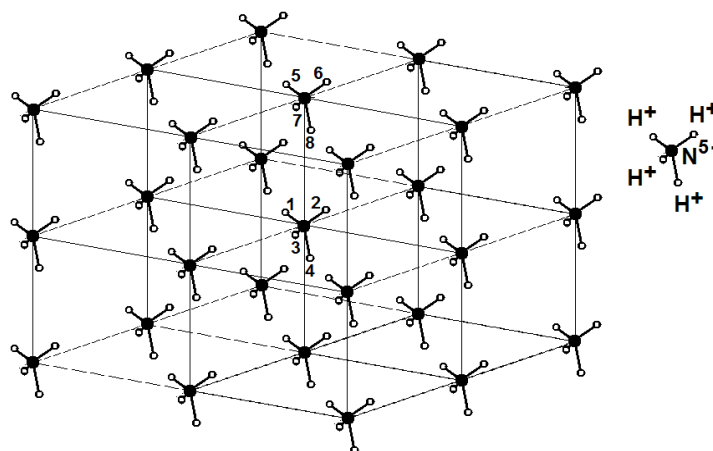


Figure 4: The disposition of hydrogen and nitrogen nuclei in NH_4Cl single crystal taken into account by evaluating the interionic contributions to the 2nd moment of proton NMR spectral line. The numbers counted from 1 to 4 numerates the target protons and the numbers from 5 to 8 label the protons of an adjacent arbitrary chosen NH_4^+ -cation. The chlorine ions are not displayed in Figure 4. They are presented in Figure 1

The surface plot graph of $M_{2,HH}^{(inter)}(\phi, \vartheta)$, the HH-interionic contribution to the proton NMR 2nd moment of ammonium chloride single crystal drawn according to Equation (27) as a function of spherical angles ϕ and ϑ of the crystal orientation in the static magnetic field for a slow motion regime of NH_4^+ -cations is shown in Figure 5a. The plan graph of $M_{2,HH}^{(inter)}(\vartheta)$, the graph $M_{2,HH}^{(inter)}(\phi, \vartheta)$ for $\phi = \pi/4$, is shown in Figure 5b.

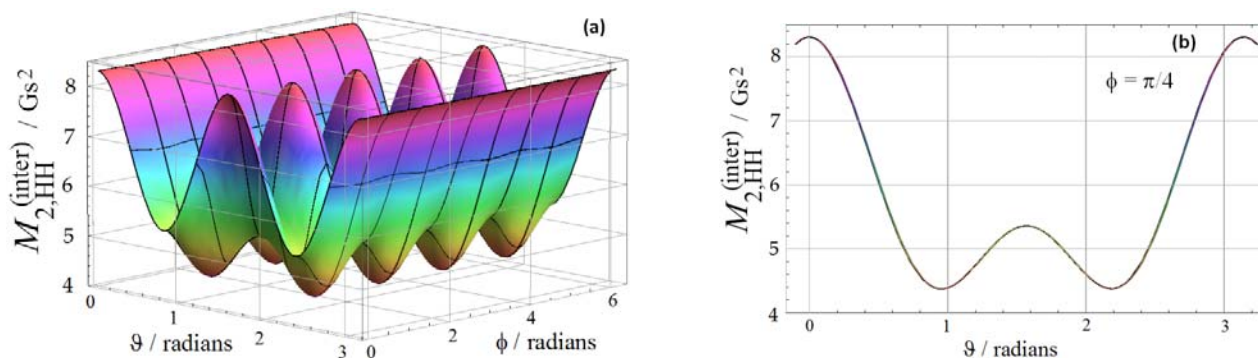


Figure 5: The graphs of $M_{2,HH}^{(inter)}(\phi, \vartheta)$ and $M_{2,HH}^{(inter)}(\vartheta)$, the HH-interionic contribution to the proton NMR 2nd moment in ammonium chloride single crystal, drawn according to Equation (27) as functions of spherical angles ϕ and ϑ (Figure 5a) and polar angle ϑ for $\phi = \pi/4$ (Figure 5b) of the crystal orientation in the static magnetic field for a slow motion regime of NH_4^+ -cations.

iv. *Interionic nitrogen-proton contribution – $M_{2,NH}^{(inter)}(\phi, \vartheta)$*

By substituting constant values $\hbar = 1.0544 \cdot 10^{-27}$ erg.s, $\gamma_v = \gamma_N = 1933.3$ s⁻¹Gs⁻¹, $I_v = I_N = 1$, the numbers of protons $N_i = 4$ and nitrogen nuclei $N_v = N_N = 6$ in Equation (21), we are getting the rated expression of interionic contribution created by 6 nearest nitrogen nuclear spins for a slow motion regime of NH_4^+ -cations:

$$M_{2,NH}^{(inter)}(\phi, \vartheta) = 1.75 \cdot 10^{-47} \sum_{v=1}^6 \sum_{i=1}^4 \left| \sum_{n=-2}^2 Y_n^{(2)}(\phi, \vartheta) Y_n^{(2)}(\varphi_{vi}, \theta_{vi}) \right|^2 r_{vi}^{-6}. \quad (28)$$

The graphs of $M_{2,NH}^{(inter)}(\phi, \vartheta)$ and $M_{2,NH}^{(inter)}(\vartheta)$ similar to those of $M_{2,HH}^{(inter)}(\phi, \vartheta)$ and $M_{2,HH}^{(inter)}(\vartheta)$ displayed in Figure 5 are shown in Figure 6:

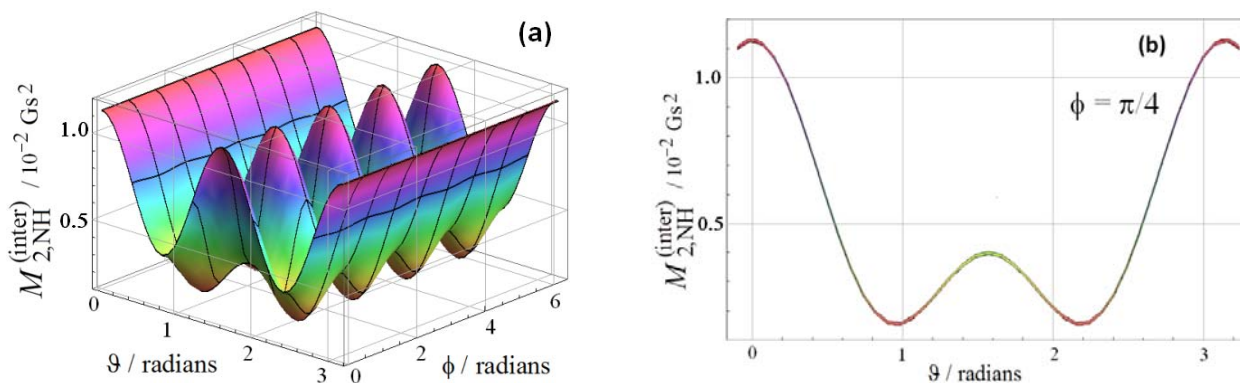


Figure 6: The graphs of $M_{2,NH}^{(inter)}(\phi, \vartheta)$ and $M_{2,NH}^{(inter)}(\vartheta)$, the interionic NH-contribution to the proton NMR 2nd moment in ammonium chloride single crystal drawn according to Equation (28) as functions of spherical angles ϕ and ϑ (Figure 6a) and ϑ for $\phi = \pi/4$ (Figure 6b) of the crystal orientation in the static magnetic field for a slow motion regime of NH_4^+ -cations.

v. *Interionic chlorine-proton contribution – $M_{2,ClH}^{(inter)}(\phi, \vartheta)$*

By substituting constant values $\hbar = 1.0544 \cdot 10^{-27}$ erg.s, $\gamma_v = \gamma_{Cl} = 2557.3$ s⁻¹Gs⁻¹, $I_v = I_{Cl} = 3/2$, the number of protons $N_i = N_H = 4$ and the number of chlorine spins $N_v = N_{Cl} = 8$, the rated expression of the heteronuclear interionic ClH-contribution $M_{2,ClH}^{(inter)}(\phi, \vartheta)$ follows from Equation (21):

$$M_{2,\text{ClH}}^{(\text{inter})}(\phi, \vartheta) = 5.42 \cdot 10^{-47} \sum_{v=1}^8 \sum_{i=1}^4 \left| \sum_{n=-2}^2 Y_n^{(2)}(\phi, \vartheta) Y_n^{(2)}(\varphi_{vi}, \theta_{vi}) \right|^2 r_{vi}^{-6}. \quad (29)$$

The graphs of $M_{2,\text{ClH}}^{(\text{inter})}(\phi, \vartheta)$ and $M_{2,\text{ClH}}^{(\text{inter})}(\vartheta)$, similar to those of $M_{2,\text{HH}}^{(\text{inter})}(\phi, \vartheta)$ and $M_{2,\text{HH}}^{(\text{inter})}(\vartheta)$ presented in Figure 5, are shown in Figure 7.

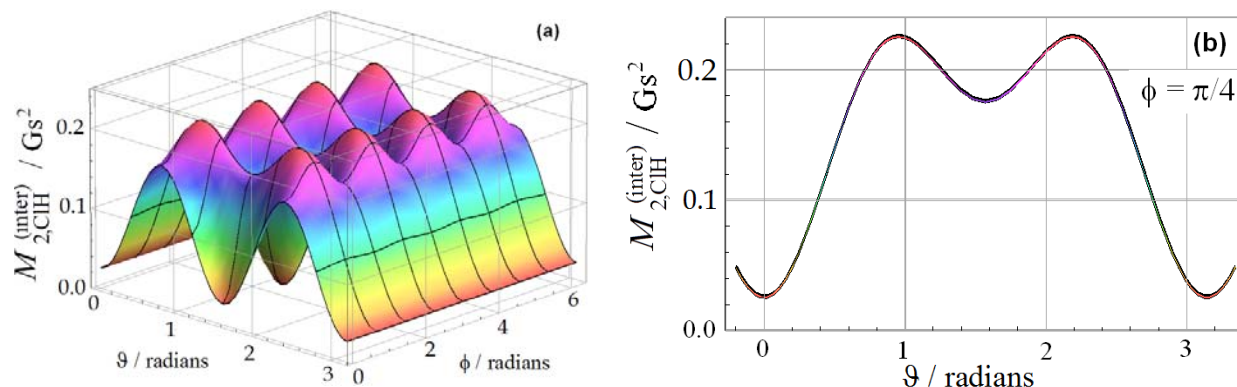


Figure 7: The graphs of $M_{2,\text{ClH}}^{(\text{inter})}(\phi, \vartheta)$ and $M_{2,\text{ClH}}^{(\text{inter})}(\vartheta)$, the interionic ClH-contribution to the proton NMR 2nd moment in ammonium chloride single crystal, drawn according to Equation (29) as functions of a) spherical angles ϕ and ϑ and b) polar angle ϑ ($\phi = \pi/4$) of the crystal orientation in the static magnetic field for a slow motion regime of NH_4^+ -cations.

vi. Total proton 2nd moment for the slow motion regime of NH_4^+ -cation – $M(\phi, \vartheta)$

Summing the partial contributions to M_2 given by Equations (24), (25), (27), (28), and (29), we are getting the expression of the total proton 2nd moment $M_2(\phi, \vartheta)$ in the semiexplicit form as a function of polar ϑ and azimuthal ϕ angles of the NH_4Cl crystal orientation in the static magnetic field for the slow motion regime of NH_4^+ -cation:

$$\begin{aligned} M_2(\phi, \vartheta) = & 50.28 - 20.88 \cdot \cos^2 2\phi + 41.76 \cdot (1 + \cos^2 2\phi) \cdot \cos^2 \vartheta - 20.88 \cdot (3 + \cos^2 2\phi) \cdot \cos^4 \vartheta \\ & + 2.83 \cdot 10^{-45} \cdot \sum_{i=1}^4 \sum_{j'=5}^{108} \left| \sum_{m=-2}^2 Y_m^{(2)}(\phi, \vartheta) Y_m^{(2)}(\varphi_{vi}, \theta_{vi}) \right|^2 r_{j'i}^{-6} + \\ & 1.75 \cdot 10^{-47} \sum_{v=1}^6 \sum_{i=1}^4 \left| \sum_{n=-2}^2 Y_n^{(2)}(\phi, \vartheta) Y_n^{(2)}(\varphi_{vi}, \theta_{vi}) \right|^2 r_{vi}^{-6} \\ & 5.42 \cdot 10^{-47} \sum_{v=1}^8 \sum_{i=1}^4 \left| \sum_{n=-2}^2 Y_n^{(2)}(\phi, \vartheta) Y_n^{(2)}(\varphi_{vi}, \theta_{vi}) \right|^2 r_{vi}^{-6} +, \end{aligned} \quad (30)$$

where the distances $r_{j'i}$ and r_{vi} are indicated in cm ($1\text{cm} = 10^{-2}\text{m}$) and the 2nd moment – in Gs^2 ($1\text{Gs} = 10^{-4}\text{T}$). The spherical harmonics $Y_n^{(2)}(\phi, \vartheta)$, $Y_m^{(2)}(\varphi_{vi}, \theta_{vi})$ and $Y_m^{(2)}(\varphi_{vi}, \theta_{vi})$ are defined as built-in functions of the software Wolfram Mathematica™. The graph of the theoretical angular dependence of the total proton 2nd moment $M_2(\phi, \vartheta)$ drawn by Equation (30) are presented in Figure 8a.

In Figure 8b, the graph of the theoretical dependence of the total proton 2nd moment is shown as a function of polar angle ϑ for the azimuthal angle fixed by $\phi = \pi/4$. At that orientation of the crystal, the values of the 2nd moment can be determined along all principal axes of the cubic unit cell. The experimental values of the second moment at low temperature (-195°C), that is in the ordered phase, has been found equal to $36.5\text{Gs}^2 \pm 0.7\text{Gs}^2$ for the direction of static magnetic field vector oriented alongside the fourfold symmetry axis $\mathbf{B}_0 || [1,0,0]$, and $54.6\text{Gs}^2 \pm 0.6\text{Gs}^2$ – alongside the twofold symmetry axis $\mathbf{B}_0 || [1,1,0]$ [18]. These values calculated by using our theoretical formula given by Equation (30) are equal to $37.75\text{Gs}^2 \pm 1.5\text{Gs}^2$ and $55.82\text{Gs}^2 \pm 2.5\text{Gs}^2$, respectively, which agree satisfactorily with those experimentally determined.

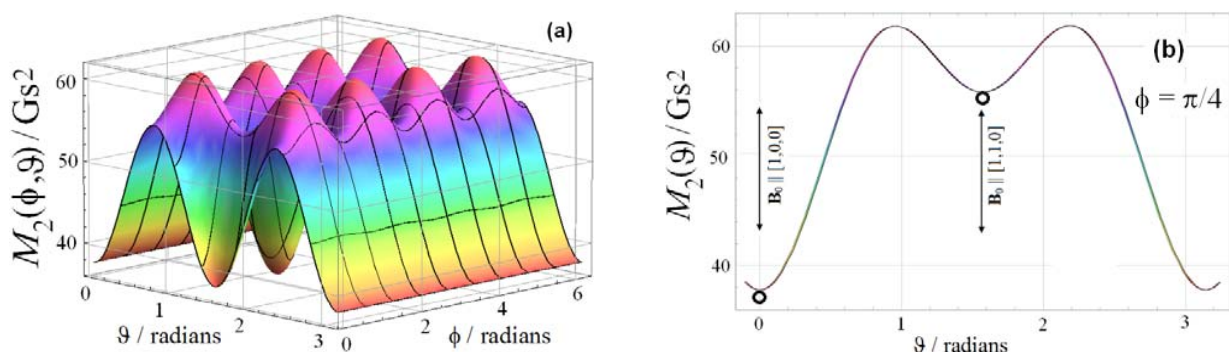


Figure 8: The graphs of the theoretical angular dependence of the proton NMR total 2nd moment in ammonium chloride single crystal for a slow motion regime of NH₄⁺ cation:

a) $M_2(\phi, \theta)$ and b) $M_2(\theta)$. The graph of $M_2(\theta)$ is drawn for $\phi = \pi/4$. Experimental values of $M_2(\theta)$ mapped by open circles are given for two directions of the static magnetic field in the unit cell of NH₄Cl [18]: $\mathbf{B}_0 || [1,0,0]$ and $\mathbf{B}_0 || [1,1,0]$.

c) *Fast motion regime of NH₄⁺ -cation*

i. *Overview*

Fast motion of ammoniums taking place at high temperatures follows decreasing the intraionic contributions down to zero: $M_{2,HH}^{(intra)}(\phi, \theta) = 0$ and $M_{2,NH}^{(intra)}(\phi, \theta) = 0$, whereas interionic ones decrease partially. Therefore, the residual proton 2nd moment in the fast motion regime of NH₄Cl reduces down to 3 additive residual interionic contributions: $M_{2,HH}^{(inter-res)}(\phi, \theta)$, $M_{2,NH}^{(inter-res)}(\phi, \theta)$, and $M_{2,ClH}^{(inter-res)}(\phi, \theta)$.

Hindered rotation of ammoniums averages the internuclear vectors of relevant dipole-dipole interactions. Hence, in order to compute the terms $M_{2,HH}^{(inter-res)}(\phi, \theta)$, $M_{2,NH}^{(inter-res)}(\phi, \theta)$ and $M_{2,ClH}^{(inter-res)}(\phi, \theta)$ in the fast motion regime of NH₄⁺-cations, the spin-spin distances have to be replaced by those dynamically averaged, in the formulae (27), (28), and (29). We shall assume that the average proton-proton distances $\langle r_{HH} \rangle$ between the protons of adjacent NH₄⁺-cations in the first coordinate sphere will be taken equal to the lattice parameter $\langle r_{HH} \rangle_1 = r_{NN} = 3.844 \cdot 10^{-8}$ cm. Relative distances in the second and third coordinate spheres will respectively equal to $\langle r_{HH} \rangle_2 = \sqrt{2} \cdot r_{NN}$ and $\langle r_{HH} \rangle_3 = \sqrt{3} \cdot r_{NN}$. In agreement with crystal structure, the distances $r_{vi} = \langle r_{NH} \rangle$ and $r_{vi} = \langle r_{ClH} \rangle$ cited in Equations (28) and (29) have to be replaced by relative average values $\langle r_{NH} \rangle = r_{NN}$ and $\langle r_{ClH} \rangle = \sqrt{3}/2 \cdot r_{NN}$.

The three- and two-dimensional theoretical graphs of the partial interionic 2nd moment $M_{2,HH}^{(inter-res)}(\phi, \theta)$, $M_{2,NH}^{(inter-res)}(\phi, \theta)$, and $M_{2,ClH}^{(inter-res)}(\phi, \theta)$ are presented for the NH₄⁺-cation fast motion regime as functions of polar angle θ and azimuth angle ϕ in Figures 9-11 (a) and as a function of polar angle θ , whereas the azimuth angle ϕ is fixed by $\phi = \pi/4$, in Figures 9-11 (b). The graphs of Figures 12 display the total 2nd moment in the fast motion regime.

ii. *Interionic proton-proton contribution – $M_{2,HH}^{(inter-res)}(\phi, \theta)$*

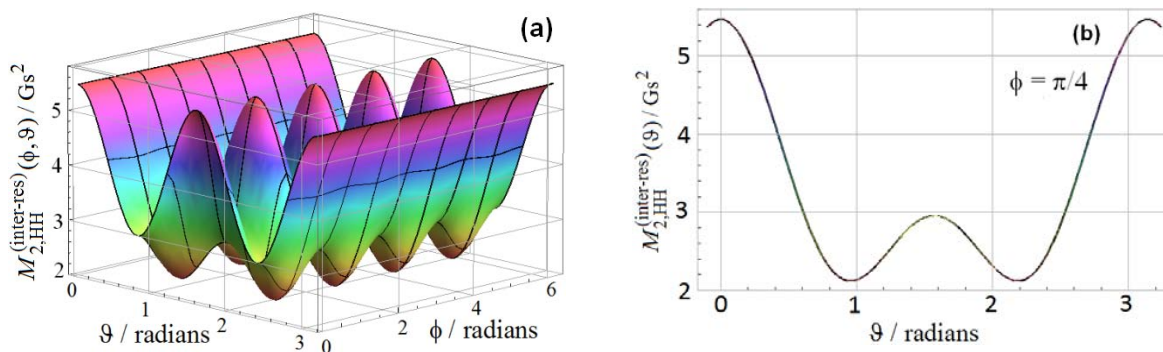


Figure 9: The graphs of $M_{2,HH}^{(inter-res)}(\phi, \theta)$ and $M_{2,HH}^{(inter-res)}(\theta)$, the HH-interionic contribution to the proton NMR 2nd moment in ammonium chloride single crystal, drawn according to Equation (27) as functions of spherical angles ϕ and θ (Figure 9a) and polar angle θ for $\phi = \pi/4$ (Figure 9b) of the crystal orientation in the static magnetic field for a fast motion regime of NH₄⁺-cations. The HH-distances were taken as average values by $\langle r_{HH} \rangle_1 = r_{NN}$, $\langle r_{HH} \rangle_2 = \sqrt{2} \cdot r_{NN}$, and $\langle r_{HH} \rangle_3 = \sqrt{3} \cdot r_{NN}$ ($r_{NN} = 3.844 \cdot 10^{-8}$ cm).

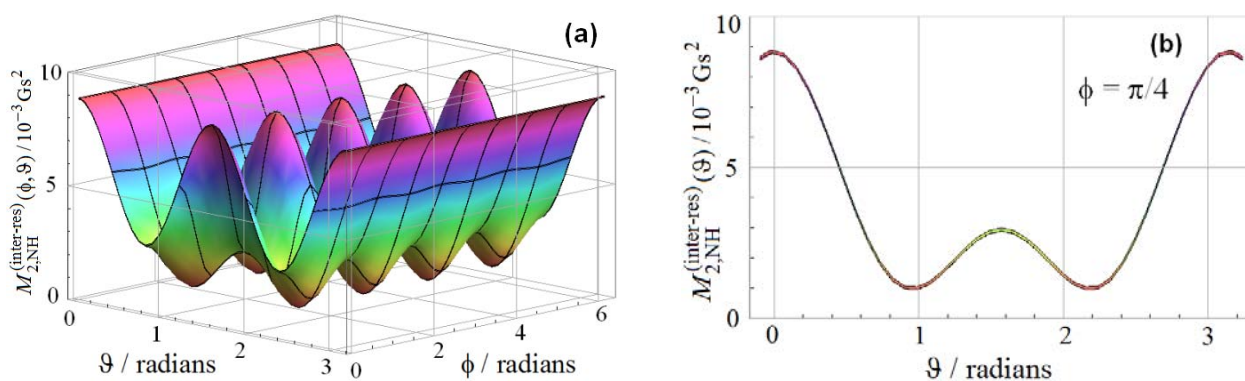
iii. Interionic nitrogen-proton contribution – $M_{2,\text{NH}}^{(\text{inter-res})}(\phi, \vartheta)$ 

Figure 10: The graphs of $M_{2,\text{NH}}^{(\text{inter-res})}(\phi, \vartheta)$ and $M_{2,\text{NH}}^{(\text{inter-res})}(\vartheta)$, the NH-interionic contribution to the proton NMR 2nd moment in ammonium chloride single crystal, drawn according to Equation (28) as functions of spherical angles ϕ and ϑ (Figure 10a) and polar angle ϑ for $\phi = \pi/4$ (Figure 10b) of the crystal orientation in the static magnetic field for a fast motion regime of NH_4^+ -cations. The NH-distances were taken as average values by $\langle r_{\text{NH}} \rangle = r_{\text{NN}}$ ($r_{\text{NN}} = 3.844 \cdot 10^{-8}$ cm).

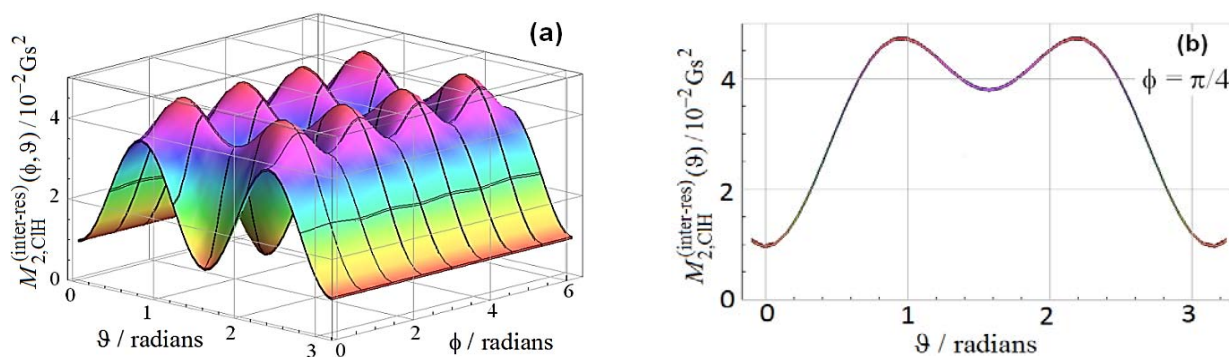
iv. Interionic chlorine-proton contribution – $M_{2,\text{ClH}}^{(\text{inter-res})}(\phi, \vartheta)$ 

Figure 11: The graphs of $M_{2,\text{ClH}}^{(\text{inter-res})}(\phi, \vartheta)$ and $M_{2,\text{ClH}}^{(\text{inter-res})}(\vartheta)$, the ClH-interionic contribution to the proton NMR 2nd moment in ammonium chloride single crystal, drawn according to Equation (29) as functions of spherical angles ϕ and ϑ (Figure 11a) and polar angle ϑ for $\phi = \pi/4$ (Figure 11b) of the crystal orientation in the static magnetic field for a fast motion regime of NH_4^+ -cations. The ClH-distances were taken as average values by $\langle r_{\text{ClH}} \rangle = 3/2 \cdot r_{\text{NN}}$ ($r_{\text{NN}} = 3.844 \cdot 10^{-8}$ cm).

v. Total proton 2nd moment for the fast motion regime of NH₄⁺ -cation – $M_2^{(res)}(\phi, \vartheta)$

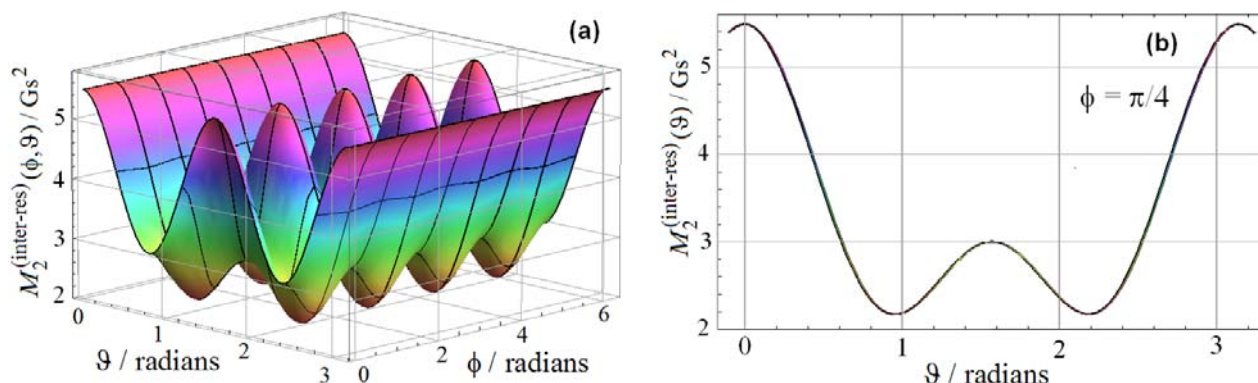


Figure 12: The graphs of $M_2^{(inter-res)}(\phi, \vartheta)$ and $M_2^{(inter-res)}(\vartheta)$, the total residual proton NMR 2nd moment in ammonium chloride single crystal, drawn according to Equation (30) as functions of spherical angles ϕ and ϑ (Figure 12a) and polar angle ϑ for $\phi = \pi/4$ (Figure 12b) of the crystal orientation in the static magnetic field for a fast motion regime of NH₄⁺-cations.

vi. Temperature dependence of the total proton 2nd moment $M_2(\phi, \vartheta)$ for 2 selected directions in NH₄Cl

To describe $M_2^{(T)}(0, 0)$ and $M_2^{(T)}(\pi/4, \pi/2)$, the experimental temperature dependences of the total proton NMR 2nd moment for 2 directions of NH₄Cl in the external magnetic field: $[1, 0, 0] \uparrow \uparrow \mathbf{B}_0$ (e.g. $\phi = 0, \vartheta = 0$) and $[1, 1, 0] \uparrow \uparrow \mathbf{B}_0$ (e.g. $\phi = \pi/4, \vartheta = \pi/2$) [21], we shall use Equations (9)-(10) reduced to $\tau_a = \tau = \tau_0 \exp(E_a/RT)$ and Equations (24, 25, 27-29). Performing necessary calculations, we are obtaining the rated expression of $M_2^{(T)}(0, 0)$ by

$$M_2^{(T)}(0, 0) = 5.50 + 32.25 \cdot \frac{2}{\pi} \cdot \arctg[4257 \cdot \delta B_H(0, 0) \cdot \tau_0 \cdot \exp\left(\frac{E_a}{RT}\right)] \quad (31)$$

and the rated expression of $M_2^{(T)}(\pi/4, \pi/2)$ by

$$M_2^{(T)}(\pi/4, \pi/2) = 3.00 + 52.8 \cdot \frac{2}{\pi} \cdot \arctg[4257 \cdot \delta B_H(\pi/4, \pi/2) \cdot \tau_0 \cdot \exp\left(\frac{E_a}{RT}\right)]. \quad (32)$$

Here, $\delta B_H(0, 0)$ and $\delta B_H(\pi/4, \pi/2)$ are the proton NMR line widths expressed in Gauss for directions $[1, 0, 0] \uparrow \uparrow \mathbf{B}_0$ and $[1, 1, 0] \uparrow \uparrow \mathbf{B}_0$ in the slow motion regime, τ_0 is the time interval between two successive attempts to overlap the reorientation barrier, and E_a is the HMM activation energy. By using Equations (31) and (32) and the constant values $\delta B_H(0, 0) = 19.5$ Gs, $\delta B_H(\pi/4, \pi/2) = 23.3$ Gs [21] and $E_a = 4.83$ kcal/mol [2], we approximated the proton NMR experimental data of $M_2[1, 0, 0]$ and $M_2[1, 1, 0]$ with the help of computer program "Origin Lab-Origin 2016™". The corresponding graphical results are shown in Figure 13. The present approximation allowed us to determine the time constant τ_0 to be equal to $6.09 \cdot 10^{-14}$ s and $5.01 \cdot 10^{-14}$ s for crystal orientations $[1, 0, 0] \uparrow \uparrow \mathbf{B}_0$ and $[1, 1, 0] \uparrow \uparrow \mathbf{B}_0$, respectively. From relaxation measurements performed in rotating reference frame, the corresponding values of τ_0 were extrapolated to $8.4 \cdot 10^{-14}$ s and $9.4 \cdot 10^{-14}$ s [2]. For the reason that the quantity τ_0 has a meaning of adjustable parameters in NMR-spectroscopy, we are concluding that the agreement found under the order of greatness amongst the experimental data of τ_0 is satisfactorily.

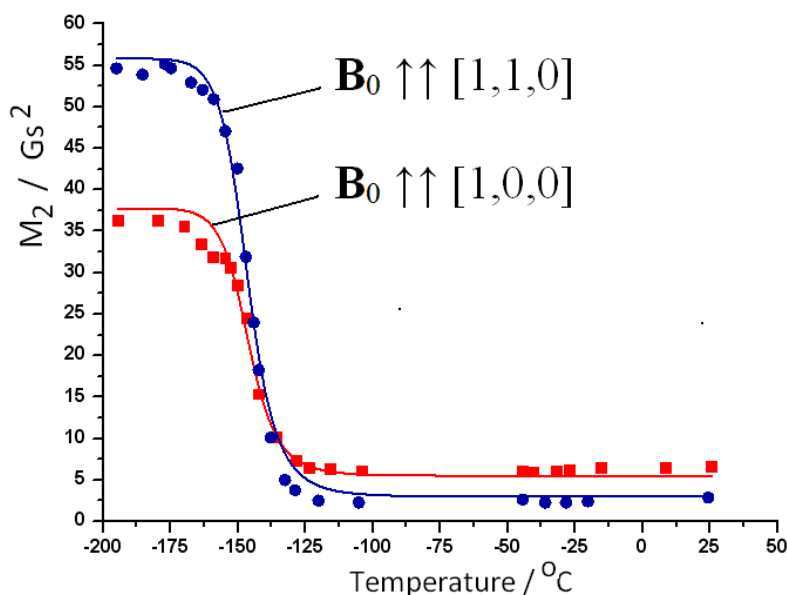


Figure 13: Temperature dependence of the 2nd moment of proton NMR absorption spectral line in the single crystal of ammonium chloride. Experimental data mapped for direction $[1,0,0]\uparrow\uparrow B_0$ are shown by square symbols "■" and for direction $[1,1,0]\uparrow\uparrow B_0$ – by round symbols "●" [21]. Theoretical lines are drawn by using Equations (31) and (32), constant values $\delta B_H(0,0) = 19.5$ Gs ($[1,0,0]\uparrow\uparrow B_0$) and $\delta B_H(\pi/4,\pi/2) = 23.3$ Gs ($[1,1,0]\uparrow\uparrow B_0$) [21] and $E_a = 4.83$ kcal/mol [2].

IV. DISCUSSION

The presented approach to simulating the NMR 2nd moment in molecular crystals, in general, and particularly, the angular and temperature dependence of the proton NMR 2nd moment in ammonium chloride allowed us to take new quantitative knowledge on the structure and molecular dynamics herein. In the Table, the theoretical values of different contributions to the 2nd moment are exposed for main orientations of the NH_4Cl crystal at slow and fast hindered motion regimes. NH_4^+ -cation slow motion regime is observed at low temperatures, lower 175°C (98 K), and dominant contribution to M_2 is $M_{2,HH}^{(intra)}$, which is due to intraionic proton-proton interaction. At high temperatures, higher 100°C (173 K), NH_4^+ -cation fast motion regime is observed and major contribution to M_2 is also defined by proton-proton interaction, but, this time, it is due to interionic one, $M_{2,HH}^{(inter)}$.

Table 1: The theoretical values of the 2nd moment contributions to the proton magnetic resonance spectral line in the single crystal of NH_4Cl at different orientation and motion regimes of NH_4^+ -cation

ORIENTATION	$B_0 \uparrow\uparrow [100]$	$B_0 \uparrow\uparrow [111]$	$B_0 \uparrow\uparrow [110]$
Slow motion regime ($\omega_0\tau_\alpha \gg 0$)			
$M_{2,HH}^{(intra)}, Gs^2$	28.30	55.09	48.39
$M_{2,NH}^{(intra)}, Gs^2$	1.11	2.16	1.89
$M_{2,HH}^{(inter)}, Gs^2$	8.31	4.38	5.35
$M_{2,CH}^{(inter)}, 10^{-2} Gs^2$	2.56	22.66	17.56
$M_{2,NH}^{(inter)}, 10^{-2} Gs^2$	1.13	0.16	0.40
Fast motion regime ($\omega_0\tau_\alpha \ll 0$)			
$M_{2,HH}^{(inter)}, Gs^2$	5.47	2.12	2.96
$M_{2,CH}^{(inter)}, 10^{-2} Gs^2$	0.97	4.73	3.79
$M_{2,NH}^{(inter)}, 10^{-2} Gs^2$	0.88	0.10	0.29

V. CONCLUSIONS

NMR investigation of structure and motion in single-crystals is one of the most powerful analytical methods. While simple approach for understanding of non-standard structures did not exist, this article describes and demonstrates a technique that can be used to cope with the challenges of crystallography. Together with the relaxation measurements, simulating the second moment of spectral lines allows one to perform an accurate analysis of dynamics and geometry of internal motion as well as crystal structure.

In this article, the analytical expressions describing overall angular dependence of the NMR 2nd moment were derived in a simplest and smart way. The theoretical results are expressed in comprehensible analytical form, easy to use. Application to the model crystal of NH₄Cl allowed us to prove the evidence of the tetragonal distortion of crystal structure that takes place in the ordered phase of ammonium chloride. Analyses of the 2nd moment temperature data for two orientations have shown that all parameters associated with the motion can be obtained. These parameters are in satisfactory agreement with those taken from NMR-relaxation and other spectroscopic studies.

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Modulus of Elasticity of LaB_6 - MeB_2 (Me - Ti, Zr, Hf) Composite at High Temperatures based on the Interfacial Interactions

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D. Zakarian^α & A. Khachatryan^σ

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I. INTRODUCTION

A quasi-binary eutectic composite is a system of two components in the absence of their mutual solubility. In eutectic systems, the boundary contact between the components may be coherent, semicoherent or amorphous depending on the types and structures ratio parameters of their crystal lattices.

If you know the general principle of calculating of the theoretical strength under uniaxial tension through the energy of pure components, the problem of the same calculation for composite is rather ambiguous and complex, which is associated with the influence of the boundaries of the components.

This paper discusses the mechanical properties such as strength, elastic modulus, maximum strain, as well as the surface energy of components contacts in composite as a function of temperature. All of these characteristics are determined by the energy of interaction between the elements in composite. The object of study is Quasi-binary eutectic composites LaB_6

– MeB_2 (Me - Ti, Zr, Hf). Mutual insolubility components of these systems is confirmed by quantum-mechanical calculations and is presented in [1].

II. RESEARCH METHODS, NUMERICAL SIMULATION AND DISCUSSION OF RESULTS

The method of determining the total energy of the alloy per molecule within the pseudopotential method is based on the summation of the potentials of paired intermolecular interactions [2]. If the concentration of component A is denoted C, the energy of system from two components can be written

$$U = U_{AA}C^2 + U_{BB}(1-C)^2 + 2C(1-C)U_{AB}. \quad (1)$$

Here

$$U_{AA}C^2 = \frac{1}{2N} \sum_{i \neq j} \Phi_{AA}(R_{ij}), \quad (2)$$

$$U_{BB}(1-C)^2 = \frac{1}{2N} \sum_{i \neq j} \Phi_{BB}(R_{ij}), \quad (3)$$

$$U_{AB} \cdot 2C(1-C) = \frac{1}{2N} \sum_{i \neq j} \Phi_{AB}(R_{ij}), \quad (4)$$

where Φ_{AA} , Φ_{BB} , Φ_{AB} - potentials of interactions between these components [2], and U_{AA} , U_{BB} , U_{AB} - the energy of interaction between the components A - A, B - B and A - B.

The first component has a connection of A - A type, and the second component connection B - B, at the interface - only A - B connection. Equation (1) can be written as

$$U = U_{AA}C^2 + U_{BB}(1-C)^2 + 2C(1-C)U_{AB} = C^2U_{AA}^* + (1-C)^2U_{BB}^*, \quad (5)$$

where

$$U_{AA}^* = U_{AA} + U_{AB} \frac{1-C}{C}, \quad U_{BB}^* = U_{BB} + U_{AB} \frac{C}{1-C}. \quad (6)$$

Tension along the z axis is determined from the relation [3]

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$$\sigma_z = \frac{1}{S_i \cdot d} \cdot \frac{\partial U_{ii}(d)}{\partial e_z}, \quad (7)$$

where e_z - relative deformation, and U_{ii} is a U_{AA} or U_{BB} ,
 d - lattice parameter in the direction of the axis of

deformation, S_i - atomic plane area in a crystal lattice that is perpendicular to the axis of strain. For calculating the formulas based on strength (6, 7) there is the following relationship:

$$\sigma_A^* = \left[\frac{1}{d_A \cdot S_A} \frac{\partial U_{AA}(d_A)}{\partial e_z} + \frac{1-C}{C} \frac{1}{d_V \cdot S_V} \frac{\partial U_{AB}(d_V)}{\partial e_z} \right] = \sigma_A + \frac{1-C}{C} \sigma_{AB}, \quad (8)$$

$$\sigma_B^* = \left[\frac{1}{d_B \cdot S_B} \frac{\partial U_{BB}(d_B)}{\partial e_z} + \frac{C}{1-C} \frac{1}{d_V \cdot S_V} \frac{\partial U_{AB}(d_V)}{\partial e_z} \right] = \sigma_B + \frac{C}{1-C} \sigma_{AB} \quad (9)$$

The paper considers in equal deformed state condition in which the permissible deformation of the composite in tension coincides with the maximum deformation of the reinforcing fibers. In equal deformed state, according to the rule of mixtures, excluding the impact of joining the borders of the two components, the maximum strength of the quasi-binary system will be

$$(\sigma_c)_{\max} = \delta \Omega_A \cdot \sigma_A + \delta \Omega_B \cdot \sigma_B^{\max}. \quad (10)$$

Here, $\delta \Omega_A$, $\delta \Omega_B$ the volume fractions of LaB_6 and MeB_2 , σ_B^{\max} - maximum strength of MeB_2 and σ_A - strength of LaB_6 or resistance of the matrix at the maximum deformation of hardener (i.e. when $\varepsilon = \varepsilon_{\max}$), which is called "temporary resistance."
 With the impact of borders joining have

$$(\sigma_c^*)_{\max} = \delta \Omega_A \cdot \sigma_A^* + \delta \Omega_B \cdot \sigma_B^{*(\max)}. \quad (11)$$

With a very small strain the curve stress - strain is close to a linear law, and then:

$$\sigma_c = \delta \Omega_A \sigma_A + \delta \Omega_B \sigma_B = E_A \varepsilon_A \delta \Omega_A + E_B \varepsilon_B \delta \Omega_B, \quad (12)$$

and taking into account the phase of interaction (Figure 1.)

$$\sigma_c^* = \delta \Omega_A \sigma_A^* + \delta \Omega_B \sigma_B^* = E_A^* \varepsilon_A \delta \Omega_A + E_B^* \varepsilon_B \delta \Omega_B, \quad (13)$$

where σ_c ; σ_A ; σ_B stresses in composite and in components A and B,

E_i , E_i^* , ε_i - elastic modulus and the strain of the components (and without taking into account the interfacial interaction).

In equal deformed state ($\varepsilon_c = \varepsilon_A = \varepsilon_B$)

$$E_c = \sigma_c / \varepsilon_c; \quad E_c^* = \sigma_c^* / \varepsilon_c. \quad (14)$$

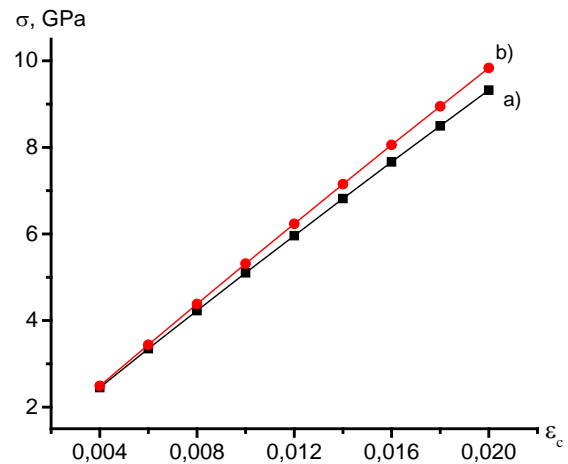


Fig. 1: The linear dependence of the composite stress from small strain ε_c : a) $\sigma = \sigma_c$, b) $\sigma = \sigma_c^*$.

For small values of deformation the calculated values of the stress and the elastic modulus of $\text{LaB}_6 - \text{TiB}_2$ composite (at zero temperature) are shown (Table 1.).

Table 1: The calculated values of the stress and the average value of elastic modulus (in GPa) of $\text{LaB}_6 - \text{TiB}_2$ composite with and without interfacial interaction

ε_c	σ_c	σ_c^*	\bar{E}_c	\bar{E}_c^*
0,004	2,041	2,121	510	530
0,006	3,063	3,185		
0,008	4,081	4,252		
0,010	5,101	5,312		

To identify the mechanical characteristics depending on the temperature, it is necessary to be able to calculate the energy of the electron-ion system of the materials at different temperatures. In the method of pseudopotentials, it means to find a change in the volume of the unit cells, at temperatures different from zero, ie, obtain the explicit dependence of the total energy of the lattice parameters and volume at nonzero temperature.

Note that the calculation of the energy of the electron - ion system in the second-order of perturbation theory in the pseudopotential means using the harmonic approximation. But application of this approach in the lattice dynamics enough to calculate certain physical characteristics that are associated with a change in crystal lattice volume with increasing temperature. This problem can be avoided if use [5] "quasi-harmonic model" (developed by the authors), which allows to

identify the temperature dependence of the unit cell volume in the harmonic approximation. The result is a dependence of the energy of the electron-ion system on temperature through the unit cell volume

$$U_{i,j}(T) = U_{i,j}(\Omega_{i,j}(T)) \quad (15)$$

The final formula for calculating the theoretical strength at uniaxial tensile versus temperature are presented in the form:

$$\sigma_A^*(T) = \sigma_A(T) + \frac{1-C}{C} \sigma_{AB}(T); \quad \sigma_B^*(T) = \sigma_B(T) + \frac{1-C}{C} \sigma_{AB}(T) . \quad (16)$$

In borides with a high content of boron, the boron atoms form stable complexes structures (B_6), their influence on the physico-mechanical characteristics of the material occurs at high temperatures, which leads to the appearance of peaks or abrupt changes in the physical and mechanical characteristics [6].

It was found that for uniaxial deformation in the temperature range from 0 to 2750 K the characteristic exponential dependence of strength on temperature disrupted in a temperature range (1300 - 2200K) in the case of LaB_6 . In this interval an increase in temperature leads to higher theoretical strength. The same dependence is observed for eutectic systems $LaB_6 - MeB_2$ (Me - Ti, Zr, Hf), which constitutes mainly from the LaB_6 [1].

Accounting for the interaction energy between heterogeneous elements A and B at the interface of the two phases results in a change of its value and the

maximum deformation and hence the maximum strength in the composite. Note that at $T = 0K$ for MeB_2 maximum deformation (Me -Ti, Zr, Hf) is approximately $\epsilon_{max} \approx 0,099$ [6]. In the calculation of the effective strength the extension member results in an increase of maximum deformation (at $T = 0 K$ $\epsilon_{Bmax}^* = 0,11$, and $\epsilon_{Bmax}^* = 0,1161$ for in case of TiB_2 and ZrB_2 , for HfB_2 $\epsilon_{Bmax}^* = 0,1158$. The increase in the maximum deformation of hardener - the result of interactions of the components (phases), which entails an increase in the temporary matrix resistance, tending to its maximum value, and, in general, increases the strength of the composite.

Results of computational experiment on the calculation of the elastic modulus for composite and components, as well as their temperature dependence are presented in Table. II-III.

Table. II: The elastic moduli of composite materials and components in the system $LaB_6 - MeB_2$ and experimental value in Gpa

Phase	E (Calculation)	E (Experiment)
LaB_6	495,05	478,73 [7] 320 [9]
TiB_2	600,06	540,53 [7] 545[9]
HfB_2	523,97	479,71 [7]
ZrB_2	534,67	495,80 [8] 430[9]
$LaB_6 - TiB_2$	506,28	-
$LaB_6 - HfB_2$	507,63	-
$LaB_6 - ZrB_2$	507,46	- 430-450[9]

The values obtained for the Young's modulus are close to their experimental values within acceptable limits (the maximum relative error of ~ 7%), given that

the calculations considered only perfect single crystals, real crystals always have a lower value.

Table III: Dependence of the Young's modulus (GPa) of components LaB_6 , TiB_2 and composite $LaB_6 - TiB_2$ on temperature

T, K	E_A	E_B	E_c
0	495,05	600,06	506,28
300	487,50	593,35	498,86
500	478,19	580,28	489,11
750	466,25	571,09	477,41
1000	450,76	548,67	461,24
1500	430,09	530,29	440,81
2000	400,15	500,07	410,84
2500	360,23	476,13	372,63
2750	330,18	440,06	341,94

If a crystal is subjected to deformation and simultaneously the temperature rises, then in parallel with deformation thermal expansion will operate. Quantum-mechanical calculations show that the interaction between the boron atoms is much stronger than between metal and boron, and even more than metal-metal bond [2]; i.e. B_6 complex expansion requires higher temperatures. This is confirmed by results of calculating the dependence of deformation on the temperature.

At temperatures $T > 1300$ K expansion of B_6 complex on the plane [200] counteracts the uniaxial strain (stretch) of the complex in the perpendicular direction, as a result of which there appear anomalies in the graph of the strength – temperature dependence. At relatively small deformations, in which the elastic modulus is determined, this effect is not observed (Figure II). Figure III shows the dependence of the modulus of elasticity- maximum strength ratio of the composite on the temperature. In the temperature range of 1000-2500 K, an area of the characteristic hardening of a composite is marked out.

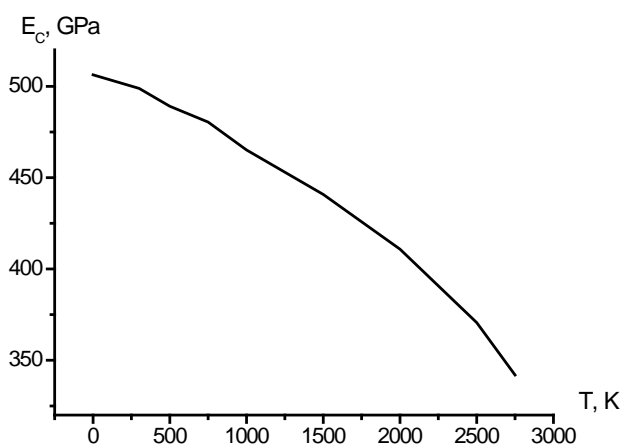


Fig. II: The dependence of the elastic modulus on temperature of the $\text{LaB}_6 - \text{MeB}_2$ composite

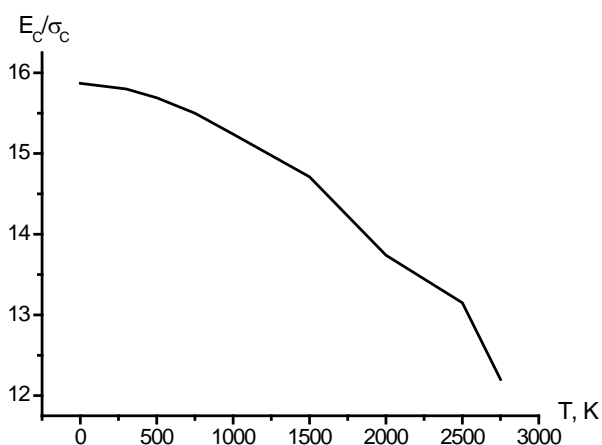


Fig. III: Temperature dependence of the ratio of the modulus of elasticity and ultimate strength of the $\text{LaB}_6 - \text{MeB}_2$ composite

Accounting components interaction in composites at the interface connections increases the value of composite modulus of elasticity.

The boundary of the two phases in the composite serves as a redistribution of property area: increasing the plasticity of refractory component and the theoretical strength and elastic modulus of the composite as a whole. Up to the melting temperature composites $\text{LaB}_6 - \text{MeB}_2$ have high strength and elastic modulus.

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Inflationary Origin of Matter-Antimatter Asymmetry in Semiclosed Friedman Universe

By Noboru Hokkyo

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Abstract- The cosmological role of the Higgs boson in the inflationary origin of the matter-antimatter asymmetry in the semiclosed Friedman universe is discussed.

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I. INTRODUCTION

In 2014 the CERN high energy proton-proton collision experiment detected the Higgs boson with mass m_H of about 100 proton mass:

$$m_H \sim 10^2 m_p \sim 10^{-17} m_{pl}, \quad (1)$$

where $m_{pl} \sim 10^{-5}g$ is the Planck mass. Being a scalar the Higgs boson has no electric and color charge. It has its own antiparticle and CP-symmetry.

The cosmological implication of the graviton-Higgs boson composite was discussed¹ in curved spacetime as it may generate huge cosmological constant Λ in negative sense, while its anti-boson composite may flatten the curve in positive sense.

II. PLANCKEON ORIGIN OF DARK ENERGY

In 1963 paper: Semiclosed Worlds in the General Theory of Relativity Zel'dovich¹ wrote: "A class of Friedman solutions of general relativity equation is found in which, as we approach the matter from infinity, we reach a singularity at the gravitational radius. But beyond this point the metric is continued in an unusual way—the radius decreases again and goes to zero only after passing through a maximum" (Novikov's similar work² noted in proof). Andreev, Stanyukovich and others^{3,4} found related solutions showing the possible existence of a gravitational closed point particle with Planck mass m_{pl} and radius l_{pl} moving with light velocity which they called maximon or Planckeon. These particles can emit radiation only if they collide with massive object, but the radiation is unobservable by the Doppler effect.

We here propose a gravitationally bound Planckeon-Higgs boson composite^{10,11} creating negative attractive potential and positive rest mass energy:

$$\begin{aligned} -Gm_H m_{pl}/l_{pl} &= -G(m_H/m_{pl})m_{pl}^2/l_{pl} \\ &= -10^{-17} Gm_{pl}^2/l_{pl} < 0, \quad (2) \\ 10^{-17} m_{pl} c^2 &= 10^{-17} (\hbar c/l_{pl}) \end{aligned}$$

$$\sim 10^{15} kT > 0, \quad (3)$$

filling the evolutionarily earlier upper hemisphere as dark energy and evolutionarily later hemisphere as dark matter of the closed Friedman universe. On the equator separating the two hemispheres we have

$$10^{-17} (m_{pl} c^2 - Gm_{pl}^2/l_{pl}) = 0, \quad (4)$$

where the rest mass energy is absorbed by the attractive potential.

III. H⁰ BOSON AND FRIEDMAN UNIVERSE

We extend the Friedman metric to Lorentz-Friedman-Reissner-Nordström form:

$$\begin{aligned} ds^2 &= c^2 g_{tt} dt^2 - g_{rr} dr^2, \\ g_{tt} &= g_{rr}^{-1} = 1 - r^2/r_g^2 + L_0^2 l_{pl}^2/r^2, \quad (5) \end{aligned}$$

Here $r_g = 2GM/c^2$ is the gravitational radius of the universe having Newtonian mass M and radius $R \geq r_g$, and

$$L_0 = \hbar l_0 / 2\pi, \quad l_0 = \text{integer}. \quad (6)$$

is the quantized angular momentum.

The evolutionary history of the Lorentz-Friedman black hole is contained in the integral

$$\begin{aligned} l_{pl} &= \int^R g_{rr} r dr \\ &= \int^R r dr (1 - r^2/r_g^2 + L_0^2 l_{pl}^2/r^2)^{-1}. \quad (7) \end{aligned}$$

giving the unitary and holographic information content (entropy)⁵ of the black hole acquired by an observer approaching the matter distribution through empty space from infinity:

$$(R/l_{pl})^2 = (10^{28}/10^{33})^2 = 10^{120}. \quad (8)$$

IV. SUPERLUMINAL INFLATION AND SUBLUMINAL EVOLUTION

The light velocity is obtained by solving $ds^2 = 0$ as:

$$\begin{aligned} dr/dt &= c(g_{tt}/g_{rr}) = c(1 - r^2/r_g^2 + L_0^2 l_{pl}^2/r^2) \\ &> c \text{ at } r \sim l_{pl} \text{ and } r \sim r_g - l_{pl} \\ &= c \text{ at } r = r_c = (r_g/l_{pl})^{1/2} \end{aligned}$$

$$= c \text{ in between } r_c < r < r_c = c \text{ and } r \sim r_g - l_{pl} \quad (9)$$

Eqs.(9) show that, starting from quantum fluctuations of preexisting metric for $0 < r < l_{pl}$, the light

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velocity is superluminal at $r \sim l_{pl}$ and $r_g - l_{pl}$. After Big Bang at temperature $T_B = 10^{27}K$, dr/dt decreases with the increase of r towards $r = r_C = (r_g/l_{pl})^{1/2} = L_\theta^2 10^{-2}cm$ for $r_g = R = 10^{28}cm$.

During the superluminal and inflationary epoch of electroweak and grand unification of gauge fields by Higgs mechanism, a causally related small region extends from $r \sim 10^{-25}cm$ to $r \sim 10cm$, followed by a brief interlude of reheating, returning to the pre-inflationary temperature of the universe. Further evolution is described by standard Friedman universe starting the radiation dominated phase of Hubble's evolutionary history expanding with subluminal velocity. Hubble constant H relates the the velocity v of a massive extragalactic object to its distance d from the Earth:

$$H = v/d \tag{10}$$

The COBE astronomical observations of the large-scale homogeneity of the distribution of matter and galaxy formation on the scale of $10^{10}cm$ light years can be explained by the superluminal and bi-directional EPR causal connection between radius $r = l_{pl}$ and $r = r_C$, while stars, clusters of galaxies, voids and other structures larger than 10^8 light years seem to indicate the angular momentum (5) $l_\theta \sim 10^3$ so that $r_C = l_\theta 10^{-2} \sim 10cm$, the high l_θ value indicating the multi-directional inflation.

V. INFLATION AS ULTRAVIOLET ANOMALY

The Klein-Gordon amplitude of transition (propagator) $D(s^2)$ for the Higgs boson between two points separated by a 4-dimensional squared distance $s^2 = (ct)^2 - r^2$, is given by⁶

$$D(s^2) = -\delta(s^2)/4\pi + (\lambda/4\pi s)H_1^{(2)}(s/\lambda), \tag{11}$$

where $H_1^{(2)}$ is the Hankel function of the second kind and $\lambda = \hbar/mc$ is the particle wavelength. We find:

$$D(s^2) \sim \delta(s^2) \text{ on the light cone } ds^2 = 0, \tag{12}$$

$$\sim (1/s^{3/2}) \exp(-is/\lambda) \text{ within the light cone } ds^2 > 0, \tag{13}$$

$$\sim (1/|s|^{3/2}) \exp(\pm |s|/\lambda) \text{ outside the light cone } ds^2 < 0, \tag{14}$$

The \pm sign in eq.(14) allows the ultraviolet anomaly of the Higgs boson:

$$(1/|s|^{3/2}) \exp(|s|/\lambda) \rightarrow \exp(l_{pl}/\lambda)/l_{pl}^{3/2} \rightarrow 1/l_{pl}^{3/2}, \tag{15}$$

to be compared to De-Sitter solution of general relativity equation:

$$r(t) \sim \exp(\pm \sqrt{\Lambda} ct) \rightarrow \exp(ct/l_{pl}), \tag{16}$$

where $\Lambda = 1/l_{pl}^2$.

VI. HIGGS BOSON IN GRAVITATIONAL FIELD

The PC and T symmetric Klein-Gordon equation

$$[\partial^2/\partial^2(ct)^2 - \partial^2/\partial^2r^2 + (\hbar/mc)^2]\psi = 0 \tag{17}$$

obeyed by the Higgs boson wave function $\psi(r, t)$ can be decomposed into two-component Dirac form:

$$\begin{aligned} (\partial/\partial ct - \partial/\partial r + \hbar/mc)\psi_+ &= 0, \\ (\partial/\partial ct + \partial/\partial r + \hbar/mc)\psi_- &= 0, \end{aligned} \tag{18}$$

where ψ_\pm represent the positive and negative energy states of the Higgs boson going forward and backward in time.

During the inflation, starting at $r = l_{pl}$ and ending at $r = r_C$, the light velocities $(dr/dt)_\pm$ are given by

$$\begin{aligned} (dr/dt)_+ &= c[(1 - r/r_g + L_\theta l_{pl}/r], \\ &> c \text{ at } r = l_{pl} \\ &= c \text{ for } r = r_C = (L_\theta l_{pl} r_g)^{1/2} \end{aligned} \tag{19}$$

and

$$\begin{aligned} (dr/dt)_- &= c[(1 + r/r_g + L_\theta l_{pl}/r] \\ &> c \text{ at } r = r_g - l_{pl} \\ &= c \text{ for } r = r_C = (L_\theta l_{pl} r_g)^{1/2}. \end{aligned} \tag{20}$$

The CERN high energy proton-proton collision experiment creating H^0 boson, immediately decaying into a counter-propagating pair of photons, seems to tell the preference of H^0 boson, going forward in time, to its antiboson, going backward in time, by the present universe expanding forward in time.

VII. MATTER-ANTIMATTER ASYMMETRY

Matter-antimatter symmetry required by quantum theory and relativity is largely violated in cosmic scale outside high energy laboratory experiments. As there were equal amount of gauge matter and antimatter, immediately after the moment of the hot Big Bang at $r = r_C$, we here propose to consider that the probability of collision between H^0 boson and the gauge matter, comoving forward in time, dominates over the collision between H^0 boson and antimatter, counter-propagating backward in time during inflation expanding forward in time.

VIII. COSMOLOGICAL DOUBLE-SLIT EXPERIMENT

In his positron theory Feynman⁶ extended Jordan-Pauli propagator

$$\begin{aligned} D(r, t) &= t/|t| \delta(c^2t^2 - r^2) \\ &= D_{ret} - D_{adv} \end{aligned} \tag{21}$$

to

$$\begin{aligned} D_F &= D_{ret} + D_- \\ &= D_{adv} + D_+. \end{aligned} \tag{22}$$

Here D_{ret} and D_{adv} are the retarded and advanced propagators. D_\pm are the Fourier contributions from positive and negative frequency sheets. At the

Chicago meeting Pauli criticized Feynman's D_F by applying it to the single electron double-slit experiment. Feynman¹⁷ replied Pauli by showing a delayed-choice double-slit equipped with time-dependent shutters creating $\Lambda + V = N$ shaped electron-positron pairs, zigzagging in time.

A matter-antimatter symmetric cosmology is conceivable by replacing the shutter by the Big Bang and the slit by the 3-dimensional Lorentz sphere: $(ct)^2 - r^2 = |p_i|^2$ filled with point-like Planckons and joined onto Friedman universe at $r = r_c$, allowing a topological (non-Hausdorff) worm hole where the timelike 3-vectors is undefined.

IX. EPR CORRELATION ON INSECT

In 1903 Oudemans⁸ discovered a phenomenon of pattern integration on the wings of the insect. When a moth or butterfly settles to assume its natural resting posture fragmental patterns appearing on the exposed but not necessarily visible surface of forewings, hindwings, head, throx, abdomen, and some of legs are integrated to form a composite but unified and scale invariant spatial pattern. Since the phenomenon is observable for both diurnal and nocturnal insects, and since a single mutation seems to be able to transform as a correlated whole, not aquired by adaptation and selection in which independent biochemical processes occurring in spatially distant parts of organisms are organized to form a predetermined patterns at the final stage of development. O. Costa de Beauregard⁹ took the phenomenon as a manifestation of the Leibnizian notion "Preharmony" or the Lamarckian slogan "The function creates the organ." We here propose to call it as the biological EPR correlation between spatially separated pattern elements, zigzagging in time.

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The Cosmic Web, the Seed of Galaxies- Are Also Made of Warm Intergalactic Medium(WHIM) and Dark Energy?

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Abstract- Universe consisted of mysterious Dark energy (70%), Dark matter(25%) and that make up now 95% of matter in the universe which reveal it self as gravity. Enormous filaments and blobs of dark matter in early universe condensed as universe condensed. Within the cosmic webs, all galaxies, stars, planets were next created. Galaxies are not dotted randomly throughout universe but are generally either concentrated in groups or in clusters, which are connected again by multitude of filaments and voids. These filamentary distributions of galaxies explained by vast quantities of dark matter enveloping galaxies and filamentary cold gas flowing within them, responsible for star formation within them and the dark matter ISM is the dominant mass in the universe. Galaxies over passing time, clumped itself in a filamentary networks.

Keywords: *large scale structure of universe; galaxies: clusters, cosmic webs WIMPs.*

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The Cosmic Web, the Seed of Galaxies- are also Made of Warm Intergalactic Medium(WHIM) and Dark Energy?

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Abstract- Universe consisted of mysterious Dark energy (70%), Dark matter(25%) and that make up now 95% of matter in the universe which reveal it self as gravity. Enormous filaments and blobs of dark matter in early universe condensed as universe condensed. Within the cosmic webs, all galaxies, stars, planets were next created. Galaxies are not dotted randomly throughout universe but are generally either concentrated in groups or in clusters, which are connected again by multitude of filaments and voids. These filamentary distributions of galaxies explained by vast quantities of dark matter enveloping galaxies and filamentary cold gas flowing within them ,responsible for star formation within them and the dark matter ISM is the dominant mass in the universe. Galaxies over passing time , clumped itself in a filamentary networks . In the cosmic web hypothesis, all spherical structures appeared probably first within filaments, growing in between them, followed by the great walls [planar structures] connecting the filaments of cosmic Web. Massive filamentary structures observed at relatively small distances from us. These filaments located about 6.7 billion light-years away from us and extends over at least 60 million light-years even. 'Superclusters' are also filamentary cluster-cluster bridges. Computerized numerical simulations shows balance between dark matter and dark energy, determines both how universe expands and how regions of unusually high or low matter density evolved with time. Most of baryons in the local universe are also missing in that they are not in galaxies or in the previously

detected gaseous phases. Rupak Bhattacharya and Pranab Bhattacharya [here are authors] suggest that these missing baryons are so predicted may be in a moderately hot phase, 1E5 to 1E7 K, largely in form of giant cosmic filaments that connect the denser virialized clusters and groups of galaxies. These filaments can be detected through absorption lines they produce in the spectra of background Active Galactic Nucleus. Models show that the highest covering fraction of such filaments occurs in super clusters and the archive has two AGNs projected behind super clusters, both of which show absorption systems (in Lyalpha LybetaOVI) at the super cluster red shift

The universe is so permeated by a network of filaments, sheets, and knots collectively forming a "cosmic web." The discovery of the cosmic web, especially through its signature of absorption of light from distant sources by neutral hydrogen in the intervening intergalactic medium, exemplifies the interplay between theory and experiment that drives science and is one of the great examples in which numerical simulations have played a key and decisive role. We authors in this article recount the milestones in our understanding of cosmic structures; summarizing its impact on astronomy, cosmology, and physics; and look ahead by outlining the challenges faced as we prepare to probe the cosmic web at new wavelengths.

Keywords: large scale structure of universe; galaxies: clusters, cosmic webs WIMPs.

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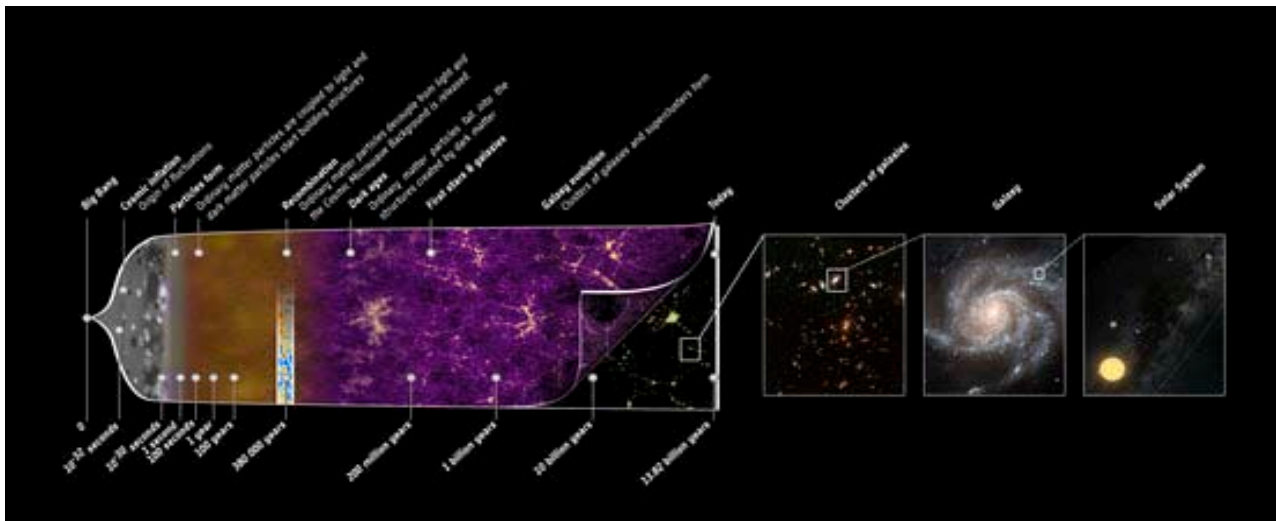


Figure 1

I. THE COSMIC WEB

The web is the frame work on which our universe was built, if at all it was once created. It consisted primarily of “dark matter,” a mysterious stuff that makes up 85% of the matter in observable universe but has revealed itself only through its gravity. Enormous amount of filaments and blobs of the stuff was condensed as the universe gradually matured and expanded. Within them seeds of galaxies and their stars, planets creating streams of light stretching between inky large voids. Voids are empty spaces filled with dark energies. Dark energy pervades everything, stretching space time and affecting the evolution of the cosmic webs.

So our universe is made of voids, filaments, knots and sheets known as cosmic webs. Each point in space time may be classified in one of four possible cosmic web types: voids, sheets, filaments and knots. Voids co-exist with a net of interconnected filaments. The entire observable universe is tangled in a web like structure, the frame work, on which universe was once built up. We all today know it also that universe consisted of mysterious *Dark energy* (70%), *Dark matter*(25%) and that make up now 95% of the matter in universe and which reveal it self as gravity. Enormous filaments and blobs of dark matter in early universe condensed as universe condensed. Within these cosmic webs, all galaxies, stars, planets, planetismals, asteroids were actually created. Our universe consists of billions and billions numbers of galaxies, some are larger, some smaller, some are spiral disc shaped, like our Milky way, some non spiral, elliptical, some dwarf galaxies, some dark galaxies, some as say first galaxies some are in clusters. More than 700,000 galaxies, whose observed Doppler colors indicated a significant red shift and are therefore presumed to be at large cosmological distances. Galaxies are however not dotted randomly through out universe but are generally

either concentrated in groups or in clusters, which are connected again by multitude of filaments. These filamentary distributions of galaxies can be explained by vast quantities of dark matter enveloping galaxies and filamentary cold gas flowing within them, responsible for stars formation within them and the dark matter ISM is the dominant mass in universe.

The observed large scale structure of universe is thought to be due to gravitational growth of density fluctuations in post-inflation era. In this model, the evolving cosmic web is governed by non-linear gravitational growth of the initially by weak density fluctuations in the dark energy dominated cosmology. The cosmic web can be now traced by a tiny fraction of luminous baryonic matter.

[Red shift - what is red shift? What is its relation with expansion of our universe? The red shift termed as z , of any kind of luminous sources is increase of measured radiations wavelength with respect to emitted one. It can be defined with mathematical equation as $z \equiv \lambda_o - \lambda_e / \lambda_e$ where λ_e is wavelength of the radiation emitted by the luminous source and λ_o is the observed person one’s position in the earth measuring red shift of distant luminous objects. The physical explanation of the red shift, of course, is a direct consequence of expansion of our universe from Big Bang. In fact, one can demonstrate that expansion of space time caused also an increase of wavelength of emitted photons from the luminous source towards the observer person in the earth. One can demonstrate that the expansion of space time causes also an increase of the wavelength of the emitted photons from the source towards the observer. Using equation when applied to light rays in space time that travels along a geodesic of the space-time, which may be defined by $ds^2 = 0$, if one can fix t_e and t_o as times when the radiation was emitted and observed, respectively, we have equations like $\int_{t_e}^{t_o} c dt / a(t) = \int_{r_e}^{r_o} dr / (1-Kr^2)^{1/2} = fK(r)$. The light emitted from the source at the time $t_e + \delta t_e$ is then seen by the observer

at $t_0 + \delta t_0$ and since the two objects are following the cosmological expansion we have equation that $fK(r) = \int_0^{t_0 + \delta t_0} \frac{cdt}{a(t)}$, we obtain then $\delta t_0 / a_0 = \delta te / a(te)$ or when $a_0 = a(t_0)$, or equivalently $a(te) / \lambda e = a_0 / \lambda_0$. From this relation it is also clear that the red shift and the expansion parameter of our universe are always interconnected. For a generic instant t we have, in fact, $1 + z = a_0 / a(t)$ shows that the objects at the present time in observable universe have red shift $z = 0$ and that the red shift (z) grows at lower expansion factors]

At very high red shifts ($z > 1100$) the pre-galactic medium was very hot, was relatively dense, ionised, with a substantial pressure of radiations. The cosmic microwave background (CMB) observations constrain the amplitudes of density in homogeneities to be very small at the last scattering red shift $z \sim 1000$. The universe then expanded, the matter cooled, and eventually recombined, being mostly in neutral phase during the "Dark ages" of the universe. At some red shift, $6 < z < 14$, hydrogen in the universe was re-ionised, likely due to UV radiation from the first luminous objects, leaving the intergalactic medium (IGM) highly re-ionised state. The re-ionisation indicated the formation of the first luminous objects at the end of the "Dark ages", either by star forming galaxies or as Active Galactic Nuclei (AGN). At the same evolution stage, formation of strong density in homogeneities in the cosmic structure occurs. Since then the non-linear dynamical flows in the vicinity of density in homogeneities would have created large scale cosmic structure shocks of modest strength, thus heating up the baryonic matter and simultaneously producing highly non-equilibrium energetic particle distributions, magnetic fields and electromagnetic emission.

The most current theory of structures formation in the observable universe aims to explain, the structures were mostly homogeneous but slightly inhomogeneous too, Universe that we observe around us, 13.7 Gyr after the Big bang, as the outcome of the growth of the primordial density fluctuations of quark gluon plasma that are observed as the temperature variations in the CMB. The formations of galaxies were possibly the most prominent visual aspect of the formation of cosmic structures that were shaped by the interplay next between the pull of the gravity and the expansion of space under influence of Dark energy. Baryonic gas condensed in the gravitational wells that had already been established by the gravitational contraction of dark matter density perturbations. This condensation was followed by the formation of stars as filamentary cold gas flowed within them, responsible for star formation within galaxies and thus the emission of photons. All galactic structures [galaxies over passing time, clumped itself in a filamentary network] through the gravitational instability, eventually formed a cosmic net work of voids, filaments, knots and sheets, because gravity was purely then attractive force, and regions of

slightly higher density in the early universe accreted matter from their surroundings and grew more over dense, with time. In the cosmic web hypothesis, spherical structures appeared probably first within filaments, growing in between them, followed by the great walls [planar structures] connecting the filaments of cosmic Web. These filaments were spreaded millions of light years long and did constitute the skeleton of the early Universe: Galaxies gathered around them, and immense galaxy clusters were formed at their intersections, lurking like giant spiders waiting for more matter to accreted. Scientists and physicists are today struggling to determine how they swirl into existence. Although massive filamentary structures have been often observed at relatively small distances from us. The filament is located about 6.7 billion light-years away from us and extends over at least 60 million light-years even. As our early universe evolved, the cosmic web gradually sharpened more & more, under dense regions known as voids, empty material known as filaments and these materials subsequently flowed into over dense knots.[In the cosmic web, under dense, almost empty regions of the universe, the voids, are delimited by great wall-like sheets and very elongated filaments of matter, which sporadically intersected each other, gave rise to very high-density regions, the clusters. Galaxies, including the most massive ones, are found in large concentrations at such 'nodes' of the web, the clusters; less massive galaxies are prominent in filaments; only very few galaxies inhabit the voids. Large scale structures in the distribution of galaxies were thought to have evolved through gravitational instabilities from small density fluctuations in the (largely homogeneous) early Universe. These structure of galaxies consisted of rich and poor clusters, were connected by filaments and sheets, with regions largely devoid of galaxies (voids) in between. Numerical simulations of the growth of initial density fluctuations through a nonlinear regime, motivated by the likely physics of the early Universe, also show a network of filaments and voids, but the origin of this picture of filaments as the dominant structure was not well understood. J. Richard Bond, Lev Kofman & Dmitry Pogosyan^[1] showed in 1996 that the 'web' of filaments that defined the final state in these simulations was present also in the initial density fluctuations; the pattern of the web was defined largely by the rare density peaks in the initial fluctuations, with the subsequent nonlinear evolution of the structure bringing the filamentary network into sharper relief. Applying these results to the observed galaxy distribution, they suggested that 'superclusters' were filamentary cluster-cluster bridges, and we predict that the most pronounced filaments will be found between clusters of galaxies that are aligned with each other and close together.

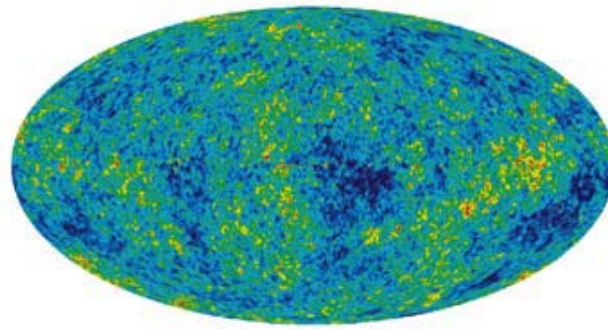


Figure 2

[All sky high resolution map of the microwave light emitted only 380'000 years after the big bang and detected by the WMAP satellite. Colors correspond to temperature variations with amplitude of 10⁻⁵ around the 2.7K black body spectrum. (Image courtesy of the NASA / WMAP Science Team)]

a) *Between inflation and the release of the cosmic microwave background ($t < 1$ sec to $t = 380,000$ years)*

After the end of inflation, the universe so consisted of more or less uniform bath of fundamental particles, like zero rest mass particles (as it was told by Rupak Bhattacharya), Higgs particles (many kinds of Higgs particles are there), quarks, electrons and their all their anti-particles. There were also neutrinos, photons, dark energies, gravitons and dark matter particles- an unknown type of massive particle that did not interacted with photons and is therefore called as dark (as it does not emit light). At this time there was slightly more matter than anti-matter, but as the particles collided with their anti-particles they were annihilated, leaving the universe dominated by particles, and by some unsown mechanisms all anti-matter disappeared. Where and why all antimatters disappeared not known to us very well. Quarks then teamed up in trios, forming protons or neutrons – the constituents of atomic nuclei as we know them today. This all happened within the first second after the Big Bang epoch. About three minutes after the Big Bang, protons and neutrons had combined to form the nuclei of hydrogen and helium.

The density and temperature of particles in early universe were so extremely high, and collisions between the particles were then very frequent. Cosmologists refer to this by saying that ordinary matter (such as electrons, protons, neutrons and the few atomic nuclei that had formed by then) was tightly coupled to the photons. Because of these frequent interactions, photons could not travel freely: the universe was then opaque. Besides, ordinary matter is subject to gravity (by a particle called Gravitons) and ideally any denser region – such as the seed fluctuations that were present at the end of inflation – would draw more matter from their surroundings, growing denser and more massive. However, ordinary matter at this epoch was coupled to photons, and radiation pressure of photons pushed away any concentration of matter that may be created under the effect of gravity. This phenomenon prevented any fluctuations in the distribution of ordinary matter to grow denser as long as matter is coupled to

the photons. At the same time, dark matter particles were not bound to the photons, since the two species do not interact with one another. This type of dark matter particle is also referred to as cold dark matter (CDM) because the velocity of these particles is much lower than the speed of light. Hence, fluctuations in the distribution of cold dark matter can grow denser and more massive even before the release of the cosmic microwave background. Astronomers also refer to hot dark matter (HDM), or they are neutrinos – particles with a very small mass and no electric charge that travel almost nearly at the speed of light. In the first second of the universe, neutrinos were coupled to photons, but these two types of particles decoupled immediately after. Since they do not interact with light during most of the universe's history, neutrinos considered as a type of dark matter, and since their velocity is close to the speed of light, they are regarded also as hot dark matter. Fluctuations in the distribution of hot dark matter grew denser and more massive, but due to their high velocity, these particles tend to dissipate and their fluctuations are damped on small scales so, effectively, only fluctuations on intermediate and large scales can grow. The growth of primordial fluctuations in hot and cold dark matter give rise to two completely different distributions of cosmic structure. In hot dark matter models, the first structures to form are the most massive, that subsequently fragmented into smaller and smaller structures. This has been discarded on the basis of observations of galaxies in the early universe: since the first objects that are seen to emerge in cosmic history had low mass, and they gradually evolved into more massive structures, cosmologists have established that the bulk of dark matter in the universe was enough cold. However, a small fraction of hot dark matter is present in the universe as neutrinos. Depending on the mass of neutrinos (which has not been determined yet but has mass) the effect of hot dark matter could be more or less evident in distribution of cosmic structure on different scales, since neutrinos tend to smooth out the formation of small-scale structures.

b) *Between the release of the cosmic microwave background and the formation of the first stars and galaxies ($t = 380,000$ years to $t =$ a few hundred million years)*

About 380,000 years after the Big Bang epoch, the universe had expanded enough so that its density was much lower than at earlier epochs. Likewise, the temperature of the universe had also cooled down from the billions of Kelvin of the first few minutes and had reached about 3000 Kelvin. Protons and electrons could finally combine to form atoms of neutral hydrogen. Electrons disappeared from the view of photons and these two species decoupled from one another. This marked the beginning of the period known as the Dark Ages – a name arising from the fact that there were no individual sources of light, like stars, only clouds of neutral hydrogen was there.

The decoupling had two effects: photons became free to propagate across the universe, which was then largely transparent, and which we now can observe as the cosmic microwave background (CMB); on the other hand, ordinary matter particles were free to assemble under the effect of gravity. From this moment on, ordinary and dark matter could both react to gravity: denser concentrations of matter (both ordinary and dark) grew denser and more massive. Since dark matter particles were already created a network of dense and empty structures (voids), ordinary matter particles could feel the gravitational attraction from the densest concentrations of dark matter and fall toward them. But ordinary matter could also get rid of energy quite effectively by heating up and emitting radiation, which caused it to sink even further into the already existing regions of high matter density. These processes gave rise to a highly sub-structured network of sheets and filaments of ordinary and dark matter known as the cosmic web, which constitutes the skeleton supporting the later emergence of stars and galaxies. Eventually the densest concentrations gave rise to the first stars, leading to the end of the Dark Ages. The Light appeared from the first stars

c) *After the formation of the first stars and galaxies ($t =$ a few hundred million years to $t =$ now)*

A few hundred million years after the Big Bang, distribution of matter in the universe produced very dense knots at the intersections of the sheets and filaments that made up the cosmic webs. In these knots, the density of ordinary matter was so high that the formation of stars and galaxies became possible. Eventually the first stars and galaxies sparked into existence and light could escape from them, revealing the distant universe to telescopes today. The first stars were formed almost exclusively out of hydrogen and helium and are believed to have been extremely massive (about 100 times the mass of the Sun or more) and to have lived very short lives, exploding soon after their formation as supernovae and releasing their

material in the surroundings, triggering the birth of new stellar generations. Later generations included other elements formed in the nuclear furnace of previous stars, and their masses were typically smaller. The first generation of stars formed in relatively low-mass galaxies. Massive galaxies, and even more massive structures such as galaxy clusters, formed later.

d) *How did the formation of structure affect the cosmic microwave background?*

The birth of first stars and galaxies had an interesting effect on the cosmic microwave background (CMB) photons. Ultraviolet radiation released by these objects ionised hydrogen atoms, turning them back into protons and electrons. This created a series of expanding bubbles of ionised gas – a bit like the holes in Swiss cheese – and within a few hundred million years these bubbles had merged and the entire Universe was ionised again, a period of time termed re-ionisation according to late Prof Meghnad Saha.

The CMB photons were affected by the re-ionisation; they were scattered off the free electrons in the re-ionised universe, washing out some of the primordial fluctuations in the CMB as we observe it today. Since this happened when the universe was already matured and had reached a substantial size, the effect of re-ionisation can be detected in the fluctuations of the CMB on large scales. This effect is expressed in terms of the 'opacity', which describes the average density of free electrons that are present along the line of sight between an observer (in this case, the telescope on board Planck) and the CMB. This parameter also provides a tool to estimate when the first stars formed.

e) *How is the history of cosmic structure encoded in the cosmic microwave background and power spectrum?*

The variations in the density of matter at the time when the cosmic microwave background (CMB) formed derive from the seed fluctuations that were produced at the end of inflation and can be deciphered by looking at the power spectrum for cosmic structure in the universe at a range of scales. At scales smaller than about one degree – or twice the size of the full Moon on the sky – the graph shows the imprint and oscillation pattern of sound waves that were present in the fluid of ordinary matter and radiation in the very early universe, before the CMB was released. The sound is like Hissss and ever fantastic rhythmic musical one of finest tunes. At this epoch, ordinary matter was tightly coupled to the photons, and the radiation pressure of photons pushed away any concentration of matter that might have been created under the effect of gravity. The interplay between gravity, which pulled together the fluid of matter and radiation, and the radiation pressure, which pushed it away, caused a series of rhythmic compressions and rarefactions everywhere in the fluid. This results in the pattern of fantastic sound waves that

is visible in the central part of the power spectrum graph. Since gravity is caused by both dark and ordinary matter particles, but the radiation pressure of photons is only experienced by ordinary matter (because dark matter particles are not coupled to photons), the shape of these oscillations contains information about the amount of ordinary matter relative to the amount of dark matter. As dark matter was not bound to the photons, any concentration of dark matter could grow denser and denser even before the release of the CMB. The relative contribution of ordinary matter particles (also referred to as baryons) to the overall cosmic budget is expressed in terms of the 'Omega_b' parameter, where b stands for baryons, and the relative contribution of cold dark matter particles is expressed in terms of the 'Omega_c' parameter, where c stands for cold. The 'cold' in cold dark matter refers to the low speed of these particles ('warm' dark matter particles move at higher speed and 'hot' dark matter particles move at the speed of light).

While gravity pulls matter together to form structures, the expansion of the universe may counteract this effect and hamper the formation of cosmic structure. For this reason, the amount of fluctuations in the universe depended also on the speed of cosmic expansion, and that quantity can be extracted from the shape of the oscillations in the power spectrum of the CMB. The speed of the universe expansion is expressed in terms of the Hubble constant, H_0, which quantifies the expansion of the Universe at present time.

f) *What does the cosmic microwave background tell us about the overall 'shape' of the Universe?*

The CMB holds clues to the nature and distribution of structure in the universe, and the average density of this matter played a key role in determining the geometry of the universe. The geometry of the universe could take on one of three shapes: it can be curved like the surface of a ball and finite in extent (positively curved); ii) curved like a saddle and infinite in extent (negatively curved), or iii) it can be flat and infinite. The geometry and density of the universe are related in such a way that, if the average density of matter in universe is found to be less than the so-called critical density (roughly equal to 6 hydrogen atoms per cubic metre) the universe will be open and infinite. If the density is greater than the critical density the universe will be closed and finite. If the density just equals the critical density, the universe is flat.

Cosmologists studied the relative sizes of the oscillations of the fluid of matter and radiation at the time the CMB was released to learn more about the shape of the universe. The oscillations translated into regions of higher and lower temperature on the CMB map, and contain information about the amount of particles present. More specifically, the shape of the universe can be determined by looking at where the first

of these oscillations appears in the power spectrum. The location of the first oscillation corresponded to a specific size in the early universe called the sound horizon – the maximum distance that a sound wave could have crossed from the Big Bang until the time of the CMB release. To cosmologists, the sound horizon works like a standard measure of known length. By measuring its length in the temperature fluctuations of the CMB, it is possible to determine if the universe is flat or curved. This is expressed in terms of the parameter 'Omega_K' and is equal to zero for exactly flat space

II. THE FORMATION OF STRUCTURES IN THE UNIVERSE

One of the main goal of today's cosmology is understanding of formation of the structures that we observe in the universe nowadays as various types of galaxies, super clusters, all stars and planets, satellites, asteroids. The Jeans theory of *gravitational instability*, is able to explain mechanism of formation of stars from a quasi homogeneous gas/or fluid, can also be used in the framework of the expanding universe in order to describe, at first order, the formation of galaxies. The standard model predicts the existence of small fluctuations in density field, originated in first instants after the Big Bang by quantum oscillations of the scalar field driving the expansion in the inflationary epoch. The CMB observations measured the amplitude of fluctuations of the primordial universe and it is possible to show how their gravitational amplification could explain formation of large scale structures of universe. As and according to the standard model the scenario of formation predicted that galaxies which were first objects to form, while the structures on larger scale (e.g. clusters and super clusters) were generated via merging of smaller objects: therefore, this picture is called hierarchical clustering. We authors of this article let now describe the basis of the Jeans theory that is able to explain the growth of small density fluctuations: the basic concept is that the perturbations of a uniform fluid are able to grow if self-gravity is able to dominate the stabilizing effect of pressure. The basic laws that describe the dynamics of a self-gravitating fluid are the continuity, the Euler and the Poisson equations

$$\partial \rho / \partial t + \nabla \cdot (\rho \vec{u}) = 0$$

$$\partial \vec{u} / \partial t + (\vec{u} \cdot \nabla) \vec{u} = -1/\rho \nabla p - \nabla \Phi$$

$$\nabla^2 \Phi = 4\pi G \rho$$

where ρ , \vec{u} and p are the density, the velocity and the pressure of the fluid element and Φ is the gravitational potential. In this analysis we neglected the effects of thermal conduction and viscosity. This means that we are assuming the conservation of entropy per unit of mass S, described by the following equation

$$\partial S^{\vec{r}}/\partial t + u^{\vec{r}} \cdot \nabla^{\vec{r}} S = 0$$

The system composed by the last 4 equations admits a static solution of the kind $\rho = \rho_0$, $u^{\vec{r}} = 0$, $S = S_0$, $p = p_0$, $\nabla^{\vec{r}} \Phi = 0$. However this is not compatible with the cosmological principle, because from the Poisson equation a uniform density implies that Φ varies spatially. In other words this means that a fluid with homogeneous density distribution cannot be stationary and must be globally expanding or contracting. For what concerns cosmology, we must consider the solution corresponding to the expansion (or contraction) of a homogeneous and isotropic distribution of matter:

$$\rho(t) = [\alpha_0/\alpha(t)]^3 \rho(t_0)$$

$$u^{\vec{r}} = \alpha^{\cdot}(t)/\alpha(t) r^{\vec{r}}$$

$$\Phi = 2\pi G/3 \rho r^2$$

$$p = p(\rho, S)$$

$$S = const$$

This solution also has the problem that both u and Φ diverge for $r \rightarrow \infty$ that can be solved adopting the more accurate relativistic solution, If now we introduce small perturbations δ , $v^{\vec{r}}$, φ , $d\rho$ and dS to all the physical variables, so that

$$\rho = \rho_0 + \delta\rho_0 = \rho_0(1 + \delta)$$

$$u^{\vec{r}} = u^{\vec{r}}_0 + v^{\vec{r}}, \quad \Phi = \Phi_0 + \varphi, \quad p = p_0 + dp, \quad S = S_0 + dS$$

where the index '0' represents the zeroth-order solutions, and put these new values into the system, neglecting the second-order terms, we obtain the new system of equations:

$$\delta \cdot + 3a/\alpha \delta + \dot{a}/\alpha (r^{\vec{r}} \cdot \nabla^{\vec{r}}) \delta + (\nabla^{\vec{r}} \cdot v^{\vec{r}}) = 0$$

$$\dot{v}^{\vec{r}} + \dot{a}/\alpha v^{\vec{r}} + \dot{a}/\alpha (r^{\vec{r}} \cdot \nabla^{\vec{r}}) v^{\vec{r}} = -1/\rho \nabla dp - \nabla \varphi$$

$$\nabla^2 \varphi - 4\pi G \rho_0 \delta = 0$$

$$\dot{dS} + \dot{a}/\alpha (r^{\vec{r}} \cdot \nabla^{\vec{r}}) dS = 0$$

perturbations in the form of small plane-wave departures by the unperturbed one:

$$du_i = u_i(t) e^{i\vec{k} \cdot \vec{r} - t},$$

where the variables u_i ($i=1, 2, 3, 4, 5$) correspond to the small perturbations in the different variables and the wave vector $k^{\vec{r}}$ corresponds to a wavelength λ that varies with time following the Hubble expansion:

$$k = 2\pi/\lambda = 2\pi/\lambda_0 \times a_0/a = k_0 \times a_0/a.$$

These primordial perturbations are considered that constituted the "seeds" for the formation of the structures in the early universe. But The Jeans theory is valid only for $|\delta| \ll 1$, while the structures observed nowadays correspond to over densities $|\delta| \gg 1$, for

example a cluster of galaxies correspond to a value of δ of several hundred.

III. CURRENT RESULTS ON COSMOLOGY THE CDM MODEL

Current observational data suggest as a favourite scenario the so-called "concordance" *Cold Dark Matter* (Λ CDM) model. In this picture the Universe remains flat with the energy density at the present epoch dominated by a cosmological constant and the remaining fraction mainly due to non-baryonic, non-collisional dark matter (DM) with low primordial velocity dispersion. The fraction of density due to standard baryonic matter Ω_b is only of few percent. After the radiation epoch ($z \sim > 104$), the DM component starts to dominates driving the growth of the density fluctuations up to the epoch of recombination when they become observable as gas temperature fluctuations imprinted in the CMB anisotropies. Since the CDM particles have a low velocity dispersion, the typical perturbations that survive to the effect of free-streaming correspond to masses of the order of $M \approx M_J(z_{rec}) \approx 10^5 M_\odot$, thus to the typical scales of proto galaxies.

Therefore, in this scenario galaxies form first while clusters are created via merging of smaller objects: this picture is called *hierarchical clustering* of structure formation. The dark energy component starts to dominate the expansion at $z \leq 0.5$ and, it has the effect of accelerating the expansion of the Universe. The main problem with the existence of this energy component, its physical origin is still unknown: the most natural explanation is the vacuum energy but the energy density ρ_Λ currently estimated is of the order of

a) Cosmic web even in dwarf and local group galaxies

The near by filaments of the cosmic web connected also our local group of galaxies to large scale cosmic web and computer simulation model reveal that these filaments should channel a steady rain of pristine dwarf galaxies which are too composed of dark matter into the local environment. Because filaments fall into them, also in firm large distances and accrete over a large fraction of the age of universe. These dwarf galaxies that are in process of arriving today can be expected to exhibit very large speed gas is also conveyed into galaxies along the filaments but because of presence of gravitational forces this is rapidly slowed down, first shock heating and then condensing into clouds that fall into the center of gravitational well and contribute to build up gaseous disk component of galaxies. Cloud of active hydrogen known as high velocity cloud surround so our milky way and andromeda galaxies. Hence both large galaxies within local group appear to be continuously accreting gas fed to them from the cosmic web. The question still to be solved as per authors, is how the large-scale cosmic environment of a CDM universe affected the

internal properties of dark matter haloes and of the baryonic galaxies, they hosted during their formation and the subsequent billion years of cosmic evolution in 2003, NASA's Wilkinson Microwave Anisotropy Probe (WMAP) spacecraft mapped the afterglow of the big bang, the cosmic microwave background (CMB), to produce, in essence, the universe's baby picture. The universe supposedly sprang into existence infinitely dense and hot and immediately doubled its size 100 times over. After about 10–32 seconds of such "inflation," the expansion slowed, and 400,000 years later, the universe cooled enough to allow free-flying protons and electrons to form hydrogen atoms. That transformation freed light trapped by the particles, which has since stretched into microwaves and cooled to 2.725 kelvin. The CMB is not exactly uniform. Inflation magnified infinitesimal quantum fluctuations in the newborn universe, which eventually seeded the filaments in the cosmic web. The fluctuations also caused the temperature of the CMB to vary across the sky by about 0.001%.

The COBE (Cosmic Background Explorer Study) could detect small anisotropy, subsequently mapped in sharp detail by WMAP (Wilkinson Microwave Anisotropy Probe) imprinted on the cosmic Microwave Background (CMB) when universe was 3, 80,000 years old. COBE study fueled the model of growth structure universe and mini scale fluctuations in very early universe. The fact, very little is known about the energy and Mass of the Universe, within the framework of Standard cosmological model. 95% of the universe (Ω the mass density of the universe divided by the Critical density for closed universe) is composed primarily of Dark energy (72%) and Dark Matter (23%) and only 5% is the detectable matter. As baryons [most of which is hydrogen and helium], - the protons, atomic nuclei that constitute ordinary matter, galaxies, Stars, planets, Planetismals, all comets, all planets, all living and dead trees, all animals and ourselves and all the materials we see, The remaining 95% matter is mysterious in nature. The dark energy is assumed to be uniform, but the normal and dark matter are not. The balance between dark matter and dark energy determines both how the universe expands and how regions of unusually high or low matter density evolved with time. We can, should detect and measure it in physical state. From studies of Quasars we know that clouds of baryons were present in the early universe about 4 billion years ago (red shift $Z > 2$) in the form of Photo Ionized diffuse high speed intergalactic gas as told just in previous paragraph and that accounted 3/4th of total baryonic mass in the universe. When nucleon synthesis happened with observed light elements at $Z > 2$, $\Omega_b > 3.5\%$, 75% estimated baryons mass were involved. These clouds of Photo ionized intergalactic gas became more and more sparse as time moved towards present and structures like galaxies, galaxy

groups, galaxy clusters started to be assembled, only a small fraction of the baryons that were present in Intergalactic medium (ISM) at red shift $Z > 2$ are found in stars, cold or warm ISM hot inter cluster gas and residual photo ionized inter galactic medium and it is estimated that 50% of baryon mass is still missing. Most of the baryons in the local universe are also missing in that they are not in galaxies or in the previously detected gaseous phases. Rupak Bhattacharya and Pranab Bhattacharya suggested that these missing baryons are so predicted may be in a moderately hot phase, $1E5$ to $1E7$ K, largely in the form of giant cosmic filaments that connect the denser virialized clusters and groups of galaxies. These filaments can be detected through absorption lines they produce in the spectra of background AGNs. Models show that the highest covering fraction of such filaments occurs in super clusters and the archive has two AGNs projected behind superclusters, both of which show absorption systems (in Ly α Ly β OVI) at the super cluster red shift.

b) Question to be solved yet

The question still to be solved as per authors are what are the properties of dark matter and dark energy? Precisely how is the web organized? Exactly how do galaxies form in it? The web spans size scales from individual galaxies to the breadth of the observable universe. In its evolution, it traces the complexity we see today back through time to the big bang how the large-scale cosmic environment of a CDM universe affected the internal properties of dark matter haloes and of the baryonic galaxies, they hosted during their formation and the subsequent billion years of cosmic evolution?

Unlike the "baryonic" matter (neglecting the real fact that there are also leptons that, however, contributed very negligible mass of universe), dark matter does not interact appreciably in any other way than through gravity —the weakest but only real long-range force among the four fundamental forces that govern the laws of universe. The best candidates for dark matter is probably till date so far is Cold Dark Matter (CDM), a kind of dark matter that has non-relativistic energies already at very early times and thus led to a bottom-up theory of galaxy structures formation in the early universe in COBE. Dark energy is on the other hand required to explain the observed accelerated expansion of space time (or in other way, equivalently, the weakening of gravity on very large scales and responsible for the expansion of the universe). Baryonic matter thus appeared to be a subdominant component that, while making up all the visible objects in the Universe, is not the most important ingredient in the attempt to understand the structure of the Universe.

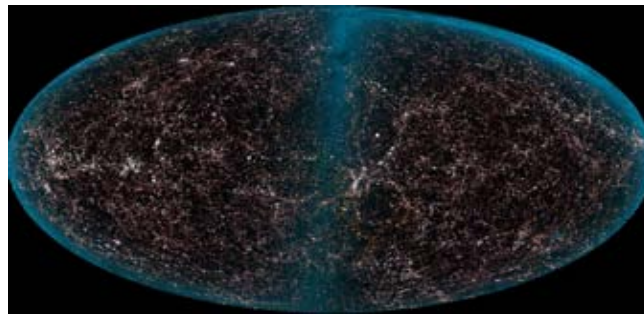


Figure 3

[The highly inhomogeneous universe in 13.7 Gyr, all sky distribution of infrared sources (mostly galaxies) from the Two Micron All Sky Survey (2MASS) in the nearby Universe. The filamentary nature of the cosmic web is clearly visible. (Atlas Image courtesy of 2MASS/UMass/IPAC-Caltech/NASA/NSF).]

c) N body Simulations study of Cosmic Web

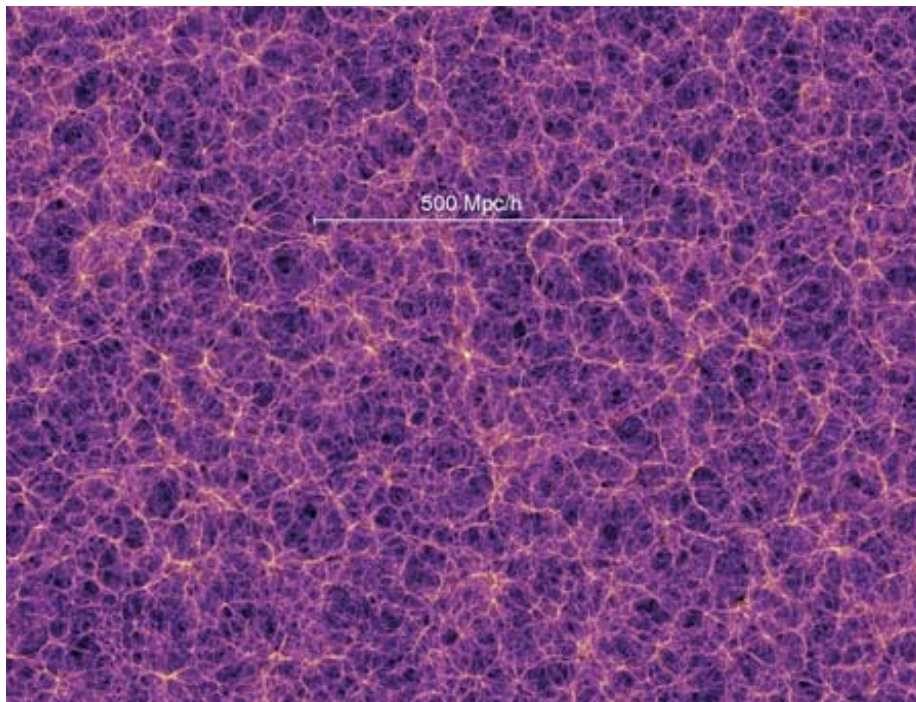
This cosmic web is the large-scale environment, in which galaxies formed and evolved and its existence had been established in large red shift surveys ($z > 2$) of many hundred thousand galaxies over the last decades. Since dark matter interacts only gravitationally, it is thus relatively easy to model and computationally affordable. For many years, the numerical study of cosmic structures formation had therefore been focused on the realm of N-body simulations [Simulations that use a particle discretisation of the phase-space are known as N-body simulations. In these simulations, the phase-space density $f(x, p, t)$ is discretized with massive particles and evolved according to the collisionless limit of the Boltzmann equation, Thus, in the N-body method, the initial phase space is sampled with particles representing a small sub volume of the full 6-dimensional phase space. Each one of these particles is then evolved in a self-consistent way, fulfilling Liouville's theorem (cf. e.g. Hockney & Eastwood, 1981). The numerical evolution thus requires two steps: (1) a gravity solver, to compute the particle accelerations, and (2) a time integrator, to update particle positions and momentum.]i.e. the Vlasov equation, under self-gravity]: which have had a huge success in showing that the spatial distribution of gravitationally collapsed structures — the dark matter haloes — is highly compatible with the observed distribution of galaxies. Dark matter haloes are connected to each other by large-scale filamentary structures. Cold gas flowing within this 'cosmic web' is believed to be an important source of fuel for galaxy and star formation at high red shift. These simulations are still giving important insights into the detailed aspects of spatial clustering, mass distribution and even internal properties of galaxies through additional semi-analytic models that attempt to relate the properties of galaxies to those of the dark matter haloes in which they are embedded. The physics of baryonic matter is in contrast very complex and computationally expensive. However, it is baryonic galaxies that we see and use to constrain our cosmological theories to reproduce the one Universe in which we live. Including baryonic matter in

our simulations of the universe is a challenging necessity to bring our understanding of structure formation to the next level. Only rather recently, the huge growth in available computer power has opened the spectacular possibility to study the condensation of the baryonic gas component into galaxies in cosmological simulations. Gas is able to radiatively cool and thus settles in the centers of the dark matter haloes. 'Sub-grid' models capture the collapse of gas clumps below the resolution limit, making it possible to simulate the formation of stars. The simulated disk galaxies thus consist of a dark matter halo filled with hot gas, a cold gaseous disk and a stellar disk. The quest has indeed started to use such hydrodynamic cosmological simulations to further our detailed understanding of the formation and evolution of galaxies and structure in the universe.

From the point of view of cosmology, the vacuum or voids appears to have an energy density, which may be called "dark energy" or the "cosmological constant" From a particle physics viewpoint, the vacuum is also permeated by a "Higgs Field" - named after physicist Peter Higgs,

Since 2010, many important studies across the world, showed that the main constituents of the universe, across 90 percent of its history, from the formation and evolution of structures such as galaxies, clusters of galaxies, and the "cosmic web" of intergalactic matter, to the stars, gas, dust, super massive black holes, and dark matter of which they are composed. These elements are coupled in a complicated evolutionary progression as matter accreted into galaxies, stars form and evolve, black holes grew, supernovae and active galactic nuclei expelled matter and energy into the intergalactic medium (IGM), and galaxies collide and merge. There remained four questions to be solved yet, form the focus for research in the coming decade. The questions are: (1) How do cosmic structures form and evolve? (2) How do baryons cycle in and out of galaxies, and what do they do while they are there? (3) How do black holes grow, radiate, and influence their surroundings? (4)

What were the first objects to light up the universe and when did they do it?



[Caption -: Simulations based on the standard cosmological model, as shown here, indicate that on very large distance scales, galaxies should be uniformly distributed. But observations show a clumpier distribution than expected, (The length bar represents about 2.3 billion light years)

Figure 4

[Caption -: Simulations based on the standard cosmological model, as shown here, indicate that on very large distance scales, galaxies should be uniformly distributed. But observations show a clumpier distribution than expected. (The length bar represents about 2.3 billion light years.)]

In the modern hierarchical theories of galaxies structure formation, It is considered that rich clusters of galaxies formed at the vertices of a web like distribution of matter, with filaments emanating from them to large distances and with smaller objects forming and draining in along these filaments. The amount of mass contained in structures near the clusters can be comparable to the collapsed mass of the cluster itself. As the lensing kernel is quite broad along the line of sight around cluster lenses with typical red shifts $z_l=0.5$, structures many mega parsecs away from the cluster are essentially at the same location as the cluster itself, when considering their effect on the cluster's weak lensing signal. When large-scale numerical simulations of structure formation in a Λ -dominated cold dark matter model was used to quantify the effect that large-scale structure near clusters has upon the cluster masses deduced from weak lensing analysis. A correction for the scatter in possible observed lensing masses should be included when interpreting mass functions from weak lensing surveys.

It was in fact Jerome Drexler, an applied armature physicist who hypothesized and discovered the relativistic-baryon dark matter in early part of 2002 and the dark matters was considered to be engaged in galaxy formation. But Drexler's hypothesis of relativistic dark baryons, would imply that the Dark matter cannot clump on galaxy scales since they are relativistic. The alternate hypothesis might be that Relativistic-baryons entered the universe at the time of the Big bang as a radial outward dispersion of very high energy relativistic charged particles, having low entropy. Because of their very low entropy, the big bang could satisfy the Second Law of Thermodynamics. The initial very high energies of the big-bang relativistic baryons would correspond to the estimated initial temperatures in the current big bang theories. Actually, relativistic-baryon dark matter forms into long large filaments that can create galaxy clusters, galaxies, and stars, but only after those dark matter filaments collide with other similar long large dark matter filaments (http://www.nature.com/nature/journal/v435/n7042/fig_tab/435572a_F1.html what drexler recently told^[2] New Releases from website from NASA/Harvard, entitled "Motions in nearby galaxy cluster reveal presence of hidden superstructure," regarding Chandra x-ray images of the Fornax cluster makes the significant statement: "Astronomers think that most of the matter in the universe is concentrated in long large filaments of

dark matter [now called the “cosmic web”] and galaxy clusters are formed where these filaments intersect/collide.” [2]

<http://www.nasa.gov/centers/marshall/news/news/releases/2004/04-231.html>) according to the 2004 NASA/Harvard/Columbia University team, relativistic-baryon dark matter does not form galaxy clusters or galaxies until after the dark matter filaments intersect/collide. These collisions slow the relativistic protons and helium nuclei and also create pions and muons, which decay into electrons. The created electrons then transform the slowed protons and helium nuclei into hydrogen and helium atoms, the basic ingredients of galaxies and stars. Thus, these remnants of the dark-matter-filament collisions are ideal for forming galaxies, galaxy clusters, and stars.

d) *Warm matter in formation of galaxies and cosmic Web?*

The most accepted model of cosmology structure formation is so till date CDM model including the dark energy, or from that particle universe evolved as baryons in diffuse intergalactic medium accelerated towards the site of formation of such structures under influence of gravity and shocks and that heats trillions of Kelvin temperature. The question then remains What is that Dark energy? If from dark matter, What is dark matter? It is distinct from Dark energy? How that matter organized and how is cosmic web organized? How galaxies formed in it? Are the dark energy the zero rest mass particles in Higgs fields and photon that was emitted later with formation of stars is condensation of zero mass (mass less particles), Rupak Bhattacharya and Professor Pranab kumar Bhattacharya suggested? Are they missing baryons? Is it possible that the missing baryons may be concentrated into those filamentary cosmic web structures and they are hot intergalactic medium(WHIM)?The distribution of baryons beyond galaxies thus may be described. The majority of the baryons, which represent 4% of the cosmic mass and energy budget, lie far from individual galaxies in the diffuse intergalactic medium (IGM). Many of these baryons may be in a warm phase that can be probed by quasar absorption in the Lyman- α line of hydrogen. The mature field of quasar spectroscopy can diagnose the location, physical state, metallicity, and general geometry of this gas, which is called the “cosmic web.” The remainder of the gas is kept very hot by in fall and shocks and is mostly in higher density regions such as filaments, groups and clusters. The hot gas is only detectable via X-rays and the absorption of highly ionized species of heavy elements. The baryons in low density regions of space are excellent tracers of underlying dark matter. The evolution of the cosmic web indicates where to look for the baryons in collapsed objects but the overall inefficiency of galaxy formation has conspired to keep most baryons dark.

Scientists think dark energy is a form of repulsive gravity that now dominates the universe, although they have no clear picture of what it actually is. Understanding the nature of dark energy is one of the biggest problems in science. Possibilities include the cosmological constant, which is equivalent to the energy of empty space. Other possibilities include a modification in general relativity on the largest scales, or a more general physical field. Vikhlinin and his colleagues used Chandra to observe the hot gas in dozens of galaxy clusters, which are the largest collapsed objects in the universe. Some of these clusters are relatively close and others are more than halfway across the universe. increase in mass of the galaxy clusters over time aligns with a universe dominated by dark energy The study strengthens the evidence that dark energy is the cosmological constant. Although it is the leading candidate to explain dark energy, theoretical work suggests it should be about 10 raised to the power of 120 times larger than observed. Therefore, alternatives to general relativity, such as theories involving hidden dimensions, are being explored. These results have consequences for predicting the ultimate fate of the universe. If dark energy is explained by the cosmological constant, the expansion of the universe will continue to accelerate, and the Milky Way and its neighbor galaxy, Andromeda, never will merge with the Virgo cluster. In that case, about a hundred billion years from now, all other galaxies ultimately would disappear from the Milky Way's view and, eventually, the local super clusters of galaxies also would disintegrate.

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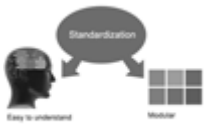
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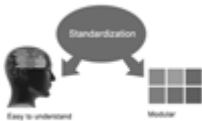
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Abstract:

The summary should be two hundred words or less. It should briefly and clearly explain the key findings reported in the manuscript-- must have precise statistics. It should not have abnormal acronyms or abbreviations. It should be logical in itself. Shun citing references at this point.

An abstract is a brief distinct paragraph summary of finished work or work in development. In a minute or less a reviewer can be taught the foundation behind the study, common approach to the problem, relevant results, and significant conclusions or new questions.

Write your summary when your paper is completed because how can you write the summary of anything which is not yet written? Wealth of terminology is very essential in abstract. Yet, use comprehensive sentences and do not let go readability for brevity. You can maintain it succinct by phrasing sentences so that they provide more than lone rationale. The author can at this moment go straight to shortening the outcome. Sum up the study, with the subsequent elements in any summary. Try to maintain the initial two items to no more than one ruling each.

- Reason of the study - theory, overall issue, purpose
- Fundamental goal
- To the point depiction of the research
- Consequences, including definite statistics - if the consequences are quantitative in nature, account quantitative data; results of any numerical analysis should be reported
- Significant conclusions or questions that track from the research(es)

Approach:

- Single section, and succinct
- As an outline of job done, it is always written in past tense
- A conceptual should situate on its own, and not submit to any other part of the paper such as a form or table
- Center on shortening results - bound background information to a verdict or two, if completely necessary
- What you account in an abstract must be regular with what you reported in the manuscript
- Exact spelling, clearness of sentences and phrases, and appropriate reporting of quantities (proper units, important statistics) are just as significant in an abstract as they are anywhere else

Introduction:

The **Introduction** should "introduce" the manuscript. The reviewer should be presented with sufficient background information to be capable to comprehend and calculate the purpose of your study without having to submit to other works. The basis for the study should be offered. Give most important references but shun difficult to make a comprehensive appraisal of the topic. In the introduction, describe the problem visibly. If the problem is not acknowledged in a logical, reasonable way, the reviewer will have no attention in your result. Speak in common terms about techniques used to explain the problem, if needed, but do not present any particulars about the protocols here. Following approach can create a valuable beginning:

- Explain the value (significance) of the study
- Shield the model - why did you employ this particular system or method? What is its compensation? You strength remark on its appropriateness from a abstract point of vision as well as point out sensible reasons for using it.
- Present a justification. Status your particular theory (es) or aim(s), and describe the logic that led you to choose them.
- Very for a short time explain the tentative propose and how it skilled the declared objectives.

Approach:

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- Explain materials individually only if the study is so complex that it saves liberty this way.
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- Do not take in frequently found.
- If use of a definite type of tools.
- Materials may be reported in a part section or else they may be recognized along with your measures.

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- Report the method (not particulars of each process that engaged the same methodology)
- Describe the method entirely
- To be succinct, present methods under headings dedicated to specific dealings or groups of measures
- Simplify - details how procedures were completed not how they were exclusively performed on a particular day.
- If well known procedures were used, account the procedure by name, possibly with reference, and that's all.

Approach:

- It is embarrassed or not possible to use vigorous voice when documenting methods with no using first person, which would focus the reviewer's interest on the researcher rather than the job. As a result when script up the methods most authors use third person passive voice.
- Use standard style in this and in every other part of the paper - avoid familiar lists, and use full sentences.

What to keep away from

- Resources and methods are not a set of information.
- Skip all descriptive information and surroundings - save it for the argument.
- Leave out information that is immaterial to a third party.

Results:

The principle of a results segment is to present and demonstrate your conclusion. Create this part a entirely objective details of the outcome, and save all understanding for the discussion.

The page length of this segment is set by the sum and types of data to be reported. Carry on to be to the point, by means of statistics and tables, if suitable, to present consequences most efficiently. You must obviously differentiate material that would usually be incorporated in a study editorial from any unprocessed data or additional appendix matter that would not be available. In fact, such matter should not be submitted at all except requested by the instructor.



Content

- Sum up your conclusion in text and demonstrate them, if suitable, with figures and tables.
- In manuscript, explain each of your consequences, point the reader to remarks that are most appropriate.
- Present a background, such as by describing the question that was addressed by creation an exacting study.
- Explain results of control experiments and comprise remarks that are not accessible in a prescribed figure or table, if appropriate.
- Examine your data, then prepare the analyzed (transformed) data in the form of a figure (graph), table, or in manuscript form.

What to stay away from

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- Never confuse figures with tables - there is a difference.

Approach

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- If you desire, you may place your figures and tables properly within the text of your results part.

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- You may propose future guidelines, such as how the experiment might be personalized to accomplish a new idea.
- Give details all of your remarks as much as possible, focus on mechanisms.
- Make a decision if the tentative design sufficiently addressed the theory, and whether or not it was correctly restricted.
- Try to present substitute explanations if sensible alternatives be present.
- One research will not counter an overall question, so maintain the large picture in mind, where do you go next? The best studies unlock new avenues of study. What questions remain?
- Recommendations for detailed papers will offer supplementary suggestions.

Approach:

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<i>References</i>	Complete and correct format, well organized	Beside the point, Incomplete	Wrong format and structuring



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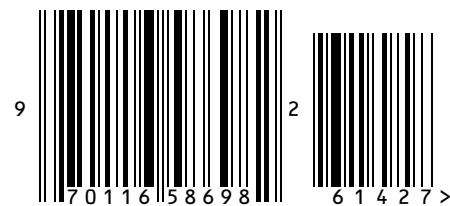
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