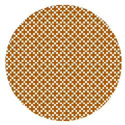
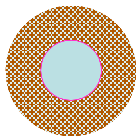
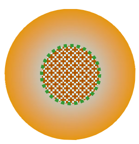
The typical NMR Experiment the results of which required a consideration of this nature: the bulk susceptibility and contributions to induced field distribution. "COMMENT" on the procedure



1. Experimental determination of Shielding tensors by HR PMR techniques in single crystalline solid state, require Spherically Shaped Specimen. The bulk susceptibility contributions to induced fields is zero inside spherically shaped specimen.

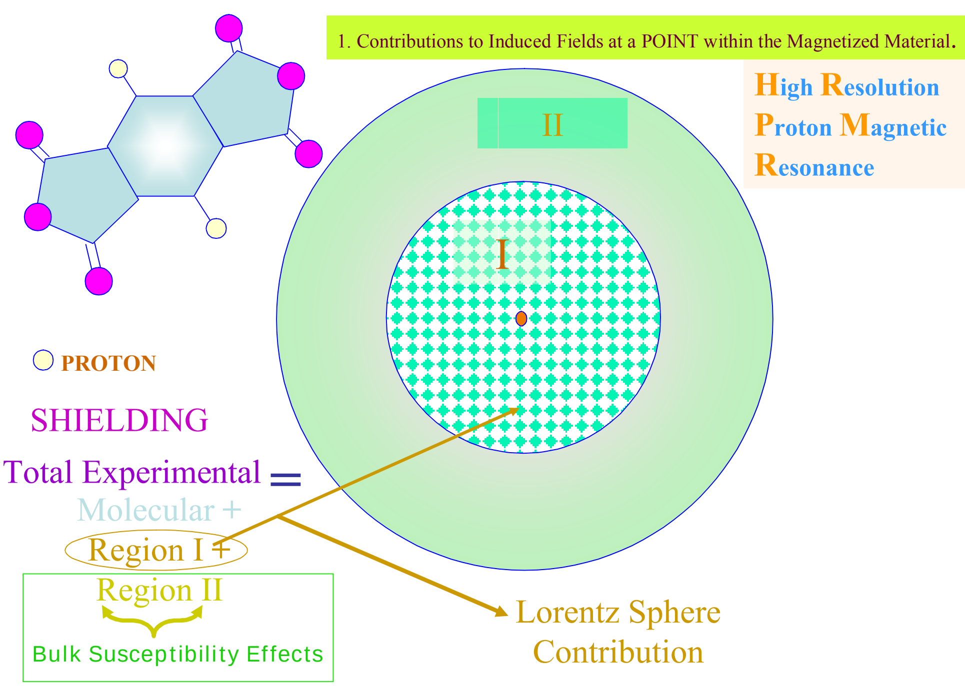


2. The above criterion requires that a semi micro **spherical volume element is carved out** around the site within the specimen and around the specified site this carved out region is a cavity which is called the Lorentz Cavity. Provided the Lorentz cavity is spherical and the outer specimen shape is also spherical, then the criterion 1 is valid.



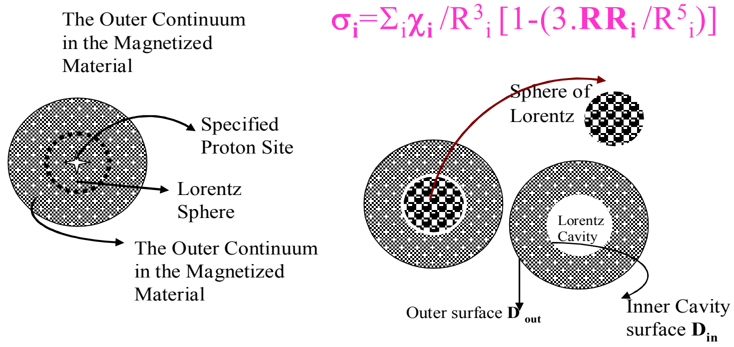
3. In actuality the carving out of a *cavity is only hypothetical* and the carved out portion contains the atoms/molecules at the lattice sites in this region as well. The distinction made by this hypothetical boundary is that all the materials outside the boundary is treated as a continuum. For matters of induced field contributions the materials inside the Lorentz sphere must be considered as making discrete contributions.

Illustration in next slide depicts pictorially the above sequence



1. Contributions to Induced Fields at a POINT within the Magnetized Material.

$$\sigma_i=\Sigma_i\chi_i/R^3_i[1-(3.\mathbf{RR_i}/R^5_i)]$$



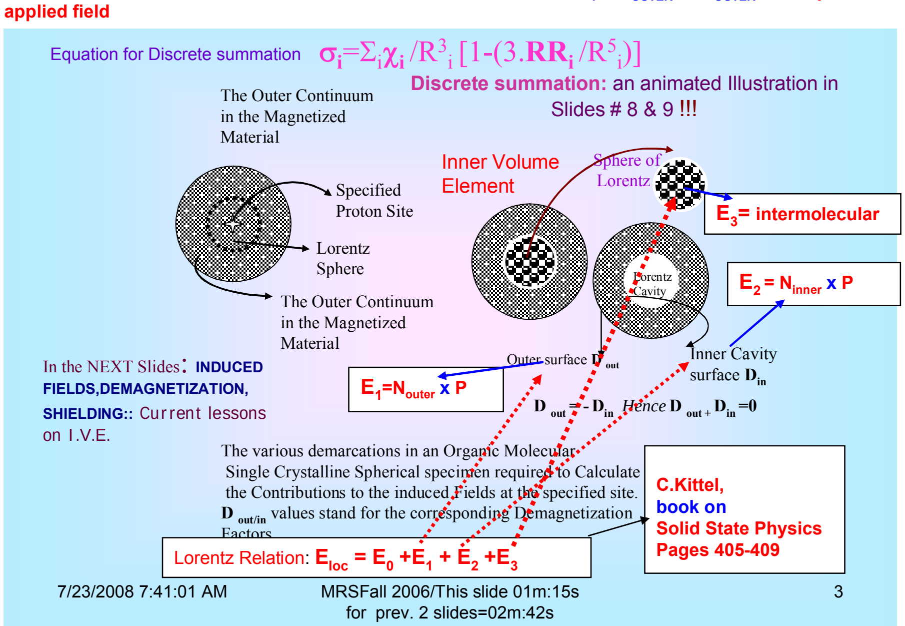
$\mathbf{D}_{out} = -\mathbf{D}_{in}$ *Hence* $\mathbf{D}_{out} + \mathbf{D}_{in} = 0$

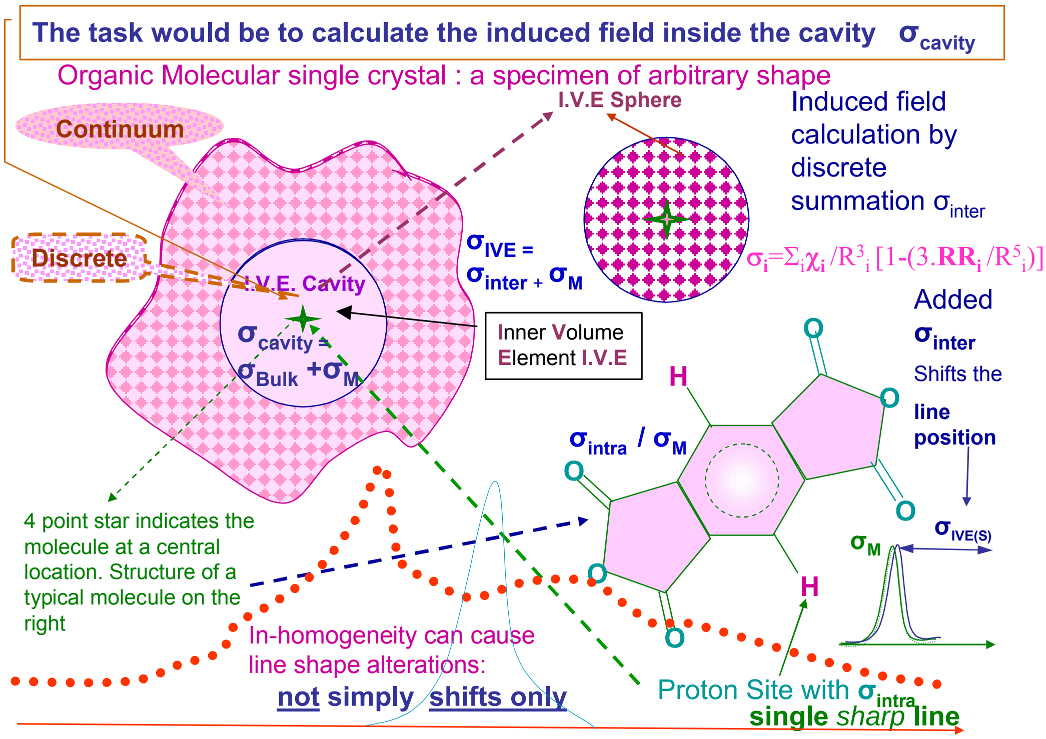
The various demarcations in an Organic Molecular Single Crystalline Spherical specimen required to Calculate the Contributions to the induced Fields at the specified site. $\mathbf{D}_{out/in}$ values stand for the corresponding Demagnetization Factors

For the first time, the quantitative criteria could be concretized for demarcating the Lorentz sphere within the Specimen. --"REMARK"

"CLARIFICATION"-Reproducing the Standard Values of the Demagnetization factors is a test for the validity of the Mathematical procedure used for estimating induced field distributions.

E_3 is the discrete sum at the center of the spherical cavity; does not depend upon macroscopic specimen shape. (Lorentz field) E_2 is usually for only a spherical Inner Cavity; with Demagnetization factor=*0.33* ; E_2 = [N_{INNER} or D_{INNER}] P E_1 is the contribution assuming the uniform bulk susceptibility and depend upon outer shape E_1 =[N_{OUTER} or D_{OUTER}]P **E_0 is the externally applied field**

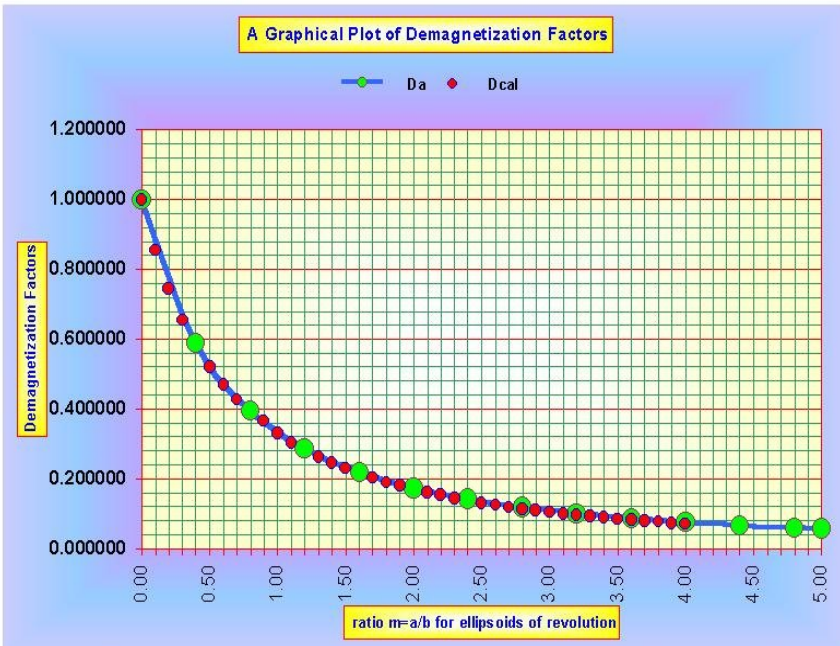




"COMMENT" on surface charges & a"consolidated" depiction

Referring to the above Scheme it may be evident that, if the Cavity field, that is the field from the external bulk, at the centre of the Spherical Void, the **"INNER VOLUME ELEMENT"** is calculated by the appropriate convenient summation procedure with a magnetic dipole model, then there would be no necessity to define infinitesimal current densities and consequent dipole moments to envisage a convenient integration procedure. It is this preoccupation with a method of integration, which required reformulating the equations by defining surface charges, by which the original elegant point dipole and the magnetic dipole model for the induced get smeared out of the grasp and the physical picture does not remain as much vivid as visualized at the start. As has been shown, this summation on the basis of a magnetic dipole model could be retained all through and the demagnetization factor could be obtained. Consequently an apparent contradiction which confronts the visualization in the Solid State Physics could get an easy and convincing way out. The points of view regarding the Lorentz ellipsoids are the topic of contributions in *"3rd Alpine Conference on SSNMR (2003)"*. ***http://saravamudhan.tripod.com/id12.html*** An indication on how to extend this summation procedure (described in Sheet 8, 9 & 10) for calculating line shapes has been included in the materials for the **"MRSFall2006".** **http://nehuacin.tripod.com/id4.html.** The case inhomogeneous **specimen is an exclusive topic covered in the presentation at EENC-Ampere conference at Lille, France and at EUROMAR2006 (York, UK)**

COMPARISON of standard results of Demagnetization factor and the values obtained by a more convenient procedure for accounting for the Induced Fields within Magnetized Materials. **Equivalence of the two methods evidenced---- "COMMENT"**



		DEMAGNETIZATION FACTORS	
a / b	**= m**	**CALCULATED**	**STANDARD**
0 / 3.0	= 0.0	1.000 000	1.000 000
0.3/ 3.0	0.1	0.854 914	0.860 804
0.6/ 3.0	0.2	0.744 581	0.750 484
1.2/ 3.0	0.4	0.582 239	0.588 154
1.8/ 3.0	0.6	0.469 904	0.475 826
2.4/ 3.0	0.8	0.388 514	0.394 440
3.0/ 3.0	1.0	0.328 862	0.333 333
4.2/ 3.0	1.4	0.244 325	0.248 803
5.4/ 3.0	1.8	0.189 575	0.194 056
6.6/ 3.0	2.2	0.151 841	0.156 326
7.8/ 3.0	2.6	0.124 602	0.129 090
9.0/ 3.0	3.0	0.104 220	0.108 709
10.5/ 3.0	3.5	0.085 159	0.089 651
12.0/ 3.0	4.0	0.070 912	0.075 407

Demagnetization factors Under the column CALCULATED are the values from present work and those under the column STANDARD are from earlier values obtained using elliptic integrals and those analytical expressions are given as functions of '**m**' values without the explicit mention of '**a**' and '**b**' values. The 'a'&'b' values corresponding to a/b are typical values used in the present calculations.

To describe a Paradoxical Situation: begin with the excerpt as below copied from the Reference:

"COMMENT"

Reviews of Modern Physics, Vol. 64, No. 2, April 1992

The most familiar treatment of the local-field problem is due to Lorentz. Consider a dielectric in an applied electric field $\mathbf{E}_{mac}$, which induces a polarization field $\mathbf{P}$. Now imagine a fictitious spherical cavity within the sample and examine the field at a point near the center of the sphere. The radius of the cavity must be large compared with the nearest-neighbor spacing. The total field at this point can then be expressed

$$\mathbf{E}_{loc}=\mathbf{E}_{mac}+\mathbf{E}_{in}+\frac{4\pi}{3}\mathbf{P} \ , \longrightarrow \text{Equation 1}$$

where E_{in} is the field due to the dipole moments induced on the molecules within the cavity. Lorentz showed that this contribution is zero for cubic or random structures. Using $\mathbf{P}=n\alpha\mathbf{E}_{loc}$, where n is the molecular density and α the molecular polarizability, leads to the Clausius-Mossotti (CM) or Lorentz-Lorenz result:

$$\frac{E_{loc}}{E_{mac}}=\frac{1}{1-\frac{4\pi}{3}n\alpha} \ . \qquad (1)$$

Equation 2

In **equation 1** above $\mathbf{E}_{Loc}$ on the Left Hand Side of the equation, obviously depends on the value of $\mathbf{P}$ for estimation. And, in equation 2, the value for to is to be estimated from the value of $\mathbf{E}_{Loc}$.

If $\mathbf{P}$ is related to $\mathbf{E}_{mac}$ (instead of to $\mathbf{E}_{Loc}$ in equation-2) which is the applied field, then the paradoxical situation would not be posed. The paradox is that $\mathbf{E}_{Loc}$ is a field which is a value including the effect of $\mathbf{P}$, and hence to know $\mathbf{E}_{Loc}$ for equation 2 the value of $\mathbf{P}$ must have been known already. **--------Remark**

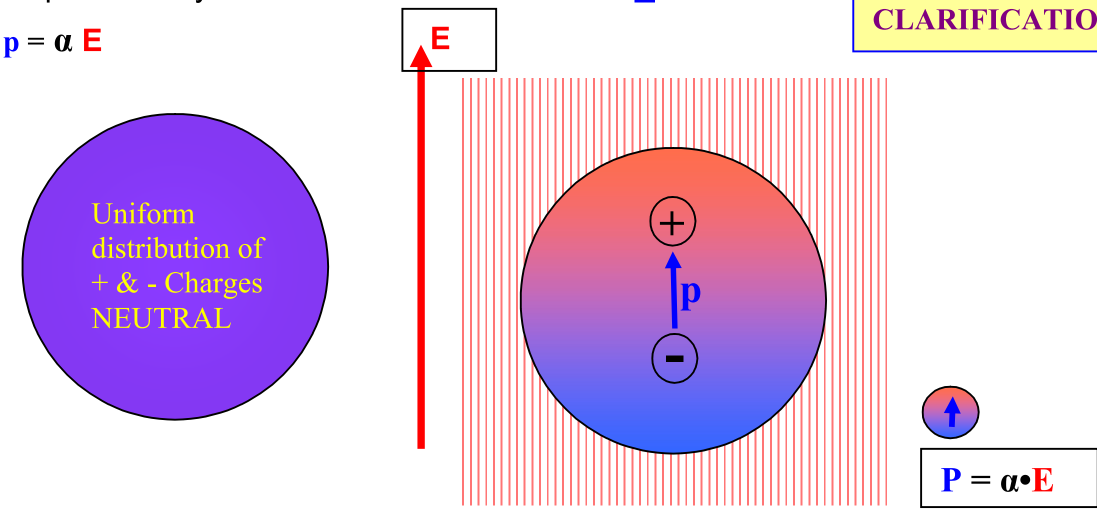
Polarizability is the relative tendency of a charge distribution, like the electron cloud of an atom or molecule, to be distorted from its normal shape by an external electric field, which may be caused by the presence of a nearby ion or dipole.

The electronic polarizability **α** is defined as the ratio of the induced dipole moment **p** of an atom to the electric field **E** that produces this dipole moment.

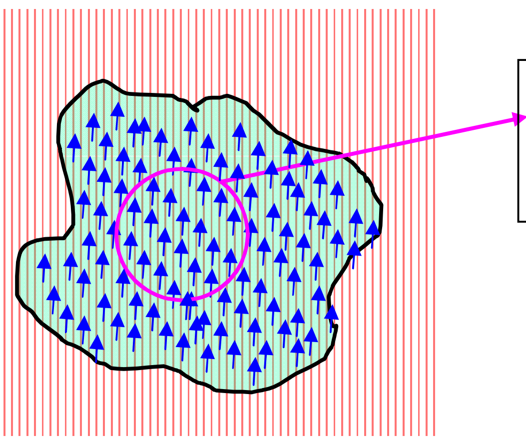
Polarizability has the SI units of $C \cdot m^2 \cdot V^{-1} = A^2 \cdot s^4 \cdot kg^{-1}$ but is more often expressed as polarizabilty volume with units of cm^3 or in $Å^3 = 10^{-24}\ cm^3$.

CLARIFICATION

$\mathbf{p} = \alpha\ \mathbf{E}$



α is the molecular Polarizability for a single molecule



Polarization density = **P**
(*number of dipoles per unit volume*)

$P = n \bullet p = n \bullet \alpha \bullet E$
'n' is the number of polarized molecules per unit volume

P gets modified if **E is modified internally, but α is unalterable if electronic structure of the molecule is not changed.**

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$p_{mod} = \alpha \,.\, E_{mod}$

$E_{mod} = E_{APP} + E_{INTERNAL}$

CLARIFICATION

$E_{INTERNAL} = \Sigma_{near}\, p.\, (1-3.\cos^2\theta)/(r_i)^3 + \Sigma_{distant}\, p.\, (1-3.\cos^2\theta)/(r_i)^3$

$E_{INTERNAL} = E_{DISCRETE} + E_{CONTINUUM}$

$E_{DISCRETE}$ is calculated as an exactly summed value
$E_{CONTINUUM}$ is calculated by integrals invoking surface charges

ZEROTH ORDER:

Under the influence of $E_{APP} = E_0$ $p^0 = \alpha \,.\, E_0$

$p^1 = \alpha \,.\, (E_0 + (E_{DISCRETE})^0 + (E_{CONTINUUM})^0)$ the second & third terms are calculated using p^0 values, and the sum is are the first order correction E^1 to E_0

FIRST ORDER

Under the influence of $E_0 + E^1$

$p^1 = \alpha \,.\, (E_0 + E^1)$

$p^2 = \alpha \,.\, (E_0 + (E_{DISCRETE})^1 + (E_{CONTINUUM})^1)$ the second & third terms are calculated using p^1 values, and the sum is the second order correction E^2 to E_0

$p^n = \alpha \,.\, (E_0 + (E_{DISCRETE})^{n-1} + (E_{CONTINUUM})^{n-1})$

$p^n = \alpha \,.\, (E_0 + (E_{inter}(p^{n-1})) + (E_{bulk}(p^{n-1})))$

$p^n = \alpha \,.\, (E_0 + (E_{inter}(p^{n-1})) + (E_{bulk}(p^{n-1})))$

The last two terms in the above equation are functions of the polarizability calculated to the extent of same order 'n'.

Repeat iteration until the condition $(p^n - p^{n-1}) < \varepsilon$ is valid, where ε is the tolerance limit for the difference.

But in the ideal limit,

would p^n be ever equal to p^{n-1} ?

Within the experimental accuracies, the factor p can be determined experimentally. By a convenient procedure, a value for p can be calculated using mathematical techniques and the procedures can be standardized so as to be able to arrive at a Value for p so that this iterated result is the within tolerance limits the same as the experimentally obtained tolerable value. The tolerance values (experimental and by evaluation) may be same in favorable cases.

In an equation to use a same value on the left and right would mean that one claims an ideal situation.

This rationale as above could be deduced as the consequence of the confidence which resulted from the interpretations required in context of HR PMR in solids.

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2. Calculation of induced field with the Magnetic Dipole Model using point dipole approximations

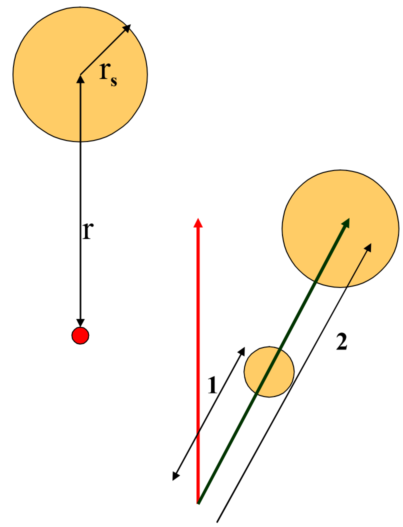
$$\sigma_{zz} = \frac{\chi}{r^3} - \frac{3 \bullet r^2 \bullet \cos^2(\theta) \bullet \chi}{r^5} = \sigma$$

$$\sigma_N = \frac{\chi_v \bullet V}{r^3} \bullet \left(1 - 3 \bullet \cos^2(\theta)\right)$$

χ_v = Volume Susceptibility

V = Volume = (4/3) π r_s^3

$$\sigma_N = \frac{\chi_v \bullet \frac{4}{3} \bullet \pi \bullet r_s^3}{r^3} \left[1 - 3 \bullet \cos^2(\theta)\right]$$

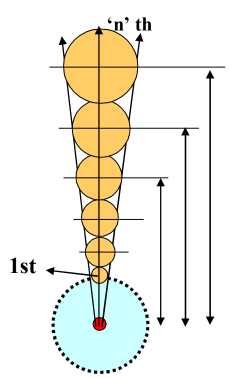


χ_v = -2.855 x 10^{-7} r_s/r = 45.8602='C'

$\sigma_1 = \sigma_2 = 2.4 \times 10^{-11}$ for θ=0

2. Calculation of induced field with the Magnetic Dipole Model using point dipole approximations

For the Point Dipole Approximation to be valid practical criteria had been that the ratio $r : r_S$ = **10:1**



R_i : r_i = 10 : 1 or even better and the ratio R_i / r_i = 'C' can be kept constant for all the 'n' spheres along the line (radial vector)

$$\sigma^i{}_N = \frac{\chi_v \bullet \frac{4}{3} \bullet \pi \bullet r_i^3}{R_i^3} \left[1 - 3 \bullet \cos^2(\theta)\right] = \sigma_i$$

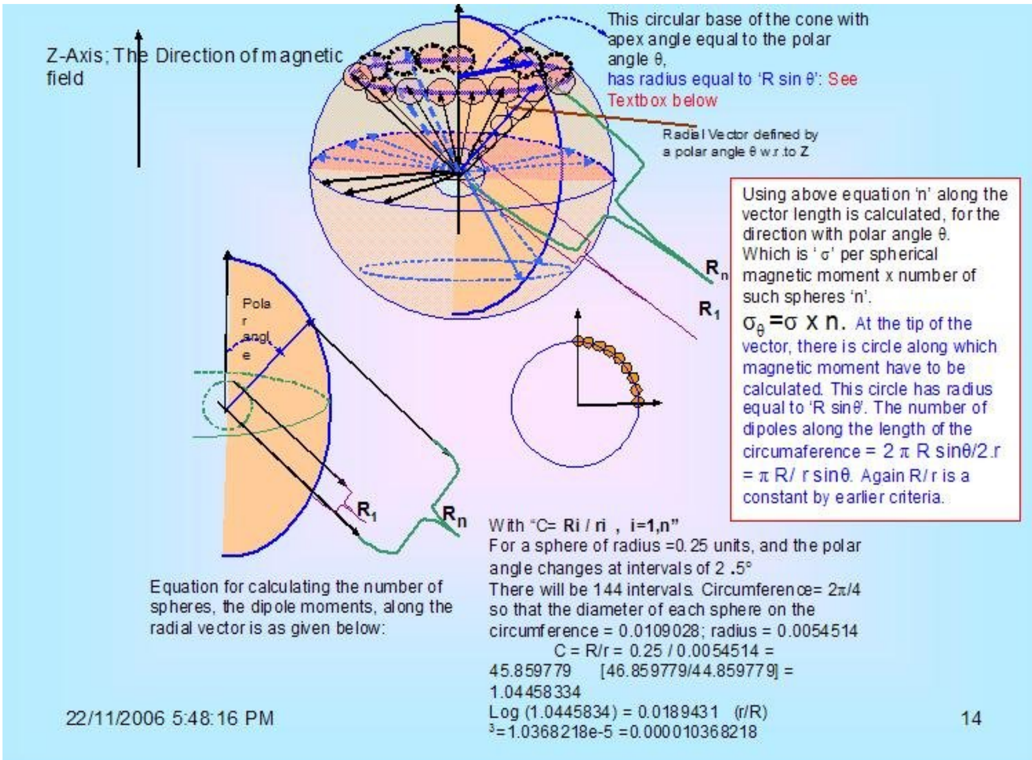
σ_i will be the same for all 'i' , i= 1,n and the value of 'n' can be obtained from the equation below

$$n = 1 + \frac{\log \frac{R_n}{R_1}}{\log \frac{C+1}{C-1}}$$

With **"C= R_i / r_i , i=1,n"**

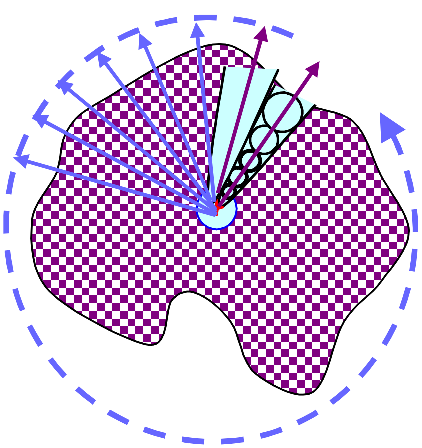
3. Summation procedure for Induced Field Contribution within the specimen from the bulk of the sample.

To slide #1



As can be evidenced by the approach in the previous two sheets, the method results in the contribution of the induced filed value at the centre of the IVE by the summation using the point dipole approximation. Thus there is no necessity to describe in terms of surface charges to simplify by an integration procedure.

More details for this calculation-method are made available in the next Sheet.



With the help of an optical Goniometer and a Travelling microscope, it should be possible to measure the sets of r,θ,φ values conveniently define the specimen shape with respect to a internal coordinate reference frame, even though an analytical equation may not be possible. Since it is only a question of finding appropriate 'n' (number of dipoles for given polar coordinates, the task of arbitrary shape can be within the realms of calculation by this summation procedure.

Along each of the radial vector direction of polar angle θ, spheres can be closely packed with the specified constraint. It is this constraint which brings in the simplicity that, every one of the spheres along a radial vector contributes the same induced filed at the specified point (site) within the material. Thus if the value for one sphere is known, and the number of closely packed spheres are calculated (as given by the equation stated earlier), then, the total contribution from that direction can be obtained by multiplying by the number 'n' of such spheres.

Let the contribution of (one) i-th sphere along the vector direction θ be = $\sigma^{i,\theta}_{\varphi}$

Then the contribution from 'n' spheres would be $= n \times \sigma^{i,\theta}_{\varphi} = \sigma^{\theta}_{\varphi}$

This is only along the line of a radial vector which is for a fixed φ. The φ dependent contributions for a given polar angle, θ can be obtained by recognizing the rotational symmetry around the magnetic field direction and this above value of σ^{θ} would be the same for all radial vectors on the surface of rotational cone with apex angle θ. If the circle described by the base of the cone is considered its radius would be, '$R \sin\theta$' where R is the radial distance to the surface of the sphere from the site. By calculating the circumference of the circle described by the base, (to be $2 \times \pi \times R \sin\theta$) and dividing the circumference length by the diameter of the Sphere in that base layer, which is $2 \times r$, the number of such closely packed spheres on the circumference can be known. This number $[(2 \times \pi \times R \sin\theta) / 2 \times r]$ would be the number of radial vectors with the same polar angle θ and all the radial vectors would contribute each the same as calculated for one of vector . Thus the final value for the given polar angle would be

$\sigma_\theta = [(2 \times \pi \times R \sin\theta) / 2 \times r] \times \sigma^{\theta}_{\varphi}$. This procedure is repeated for all values of θ discretely at known (specified before) interval and sum over the polar angles would give the total contribution from the entire specimen. R/r value would be the same as the value set as constraint.

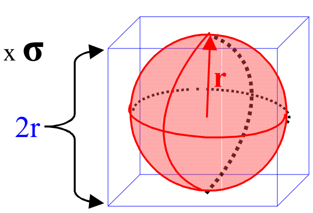
For one sphere = $\sigma^{i,\theta}_{\varphi}$ For 'n' spheres $= n \times \sigma^{i,\theta}_{\varphi} = \sigma^{\theta}_{\varphi}$

Summed for all azimuthal angle values for the given polar angle = σ_θ .

Summing Over all polar angles thus gives final total contribution from the specimen material corresponding to spherical filling = **σ.** Since the spheres at their respective points can be replaced by cubes with the side equal to the diameter of that sphere, there can be no further void to account for. This step increases the magnetic moment at each point by the ratio of the cube to sphere volume. i.e.,

$(8 \times r^3) / (4/3 \times \pi \times r^3)$ = **1.909859 .** Final value = **1.909859** x **σ**

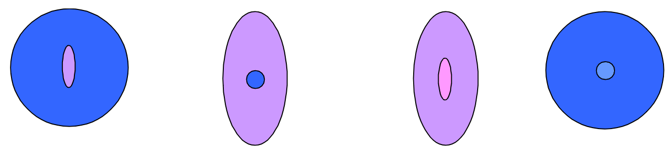
This induced field value obtained finally can be related to the demagnetized factor values of the Inner and Outer shapes to arrive at the standard values.



http://www.geocities.com/amudhan20012000/Confview.html
http://www.geocities.com/amudhan20012000/Confview_link.html

Advantages of the summation method described in the previous sheets: (An alternative method for demagnetization factor calculation)

1. First and Foremost, it was a very simple effort to reproduce the demagnetization factor values, which were obtained and tabulated in very early works on magnetic materials. Those Calculations which could yield such Tables of demagnetization factor values were rather complicated and required setting up elliptic integrals which had to be evaluated.
2. Secondly, the principle involved is simply the convenient point dipole approximation of the magnetic dipole. And, the method requires hypothetically dividing the sample to be consisting of closely spaced spheres and the radii of these magnetized spheres are made to hold a convenient fixed ratio with their respective distances from the specified site at which point the induced fields are calculated. This fixed ratio is chosen such that for all the spheres the point dipole approximation would be valid while calculating the magnetic dipole field distribution.
3. The demagnetization factors have been tabulated only for such shapes and shape factors for which the magnetization of the sample in the external magnetic field is uniform when the magnetic susceptibility of the material is the same homogeneously through out the sample. This restricts the tabulation to only to the shapes, which are ellipsoids of rotation. Where as, if the magnetization is not homogeneous through out the sample, then, there were no such methods possible for getting the induced field values at a point or the field distribution pattern over the entire specimen. The present method provides a greatly simplified approach to obtain such distributions.
4. It seems it is also a simple matter, because of the present method, to calculate the contributions at a given site only from a part of the sample and account for this portion as an independent part from the remaining part without having to physically cause any such demarcations. This also makes it possible to calculate the field contribution from one part of the sample, which is within itself a part with homogeneously, magnetized part and the remaining part being another homogeneously magnetized part with different magnetization values. Hence a single specimen which is inherently in two distinguishable parts can each be considered independently and their independent contribution can be added. For the point 1 mentioned above view http://www.geocities.com/inboxnehu_sa/nmrs2005_icmrbs.html



Inner ellipsoid a/b=0.25 demgf= **0.697**	Outer ellipsoid a/b=0.25 demagf= **0.708**	Ellipsoid Outer a/b=0.25 Inner a/b=0.25 demagf=0.333	Outer sphere Inner sphere a/b=1 demagf=0.333

From the standard tables demagnetization factor for a/b=0.2: =0.750484
for a/b=0.3: =0.661350

interpolation yields for 0.25: = **0.705** 417

It is only conventional in material physics consideration to have a spherical (Lorentz) cavity while calculating the demagnetization factors for regular outer shapes of the magnetized specimen. By the procedures used in this work,it is a matter of simple alteration in sequence in which certain equations defining the shpes and forms are considered which makes it possible,without any resulting complications in the calculation,to get values for Facotrs, based on the definition of demagnetization factors,as reported above by applying the shapes inside out . This seems to be very favourable for studying shapes, with added susceptibility reagents in membrane-media, by spin-echo NMR techniques.The details are deferred to future presentations.

To Slide #1

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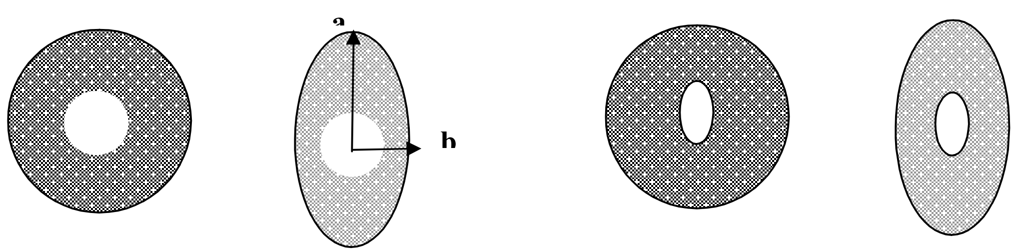


Outer a/b=1 **D**emagf=0.33	outer a/b=0.25 **D**emagf=0.708
inner a/b=1 **D**emagf=-0.33	inner a/b=1 **D**emagf=-0.33
0.33-0.33=0	*0.708-0.33=0.378*

conventional combinations of shapes

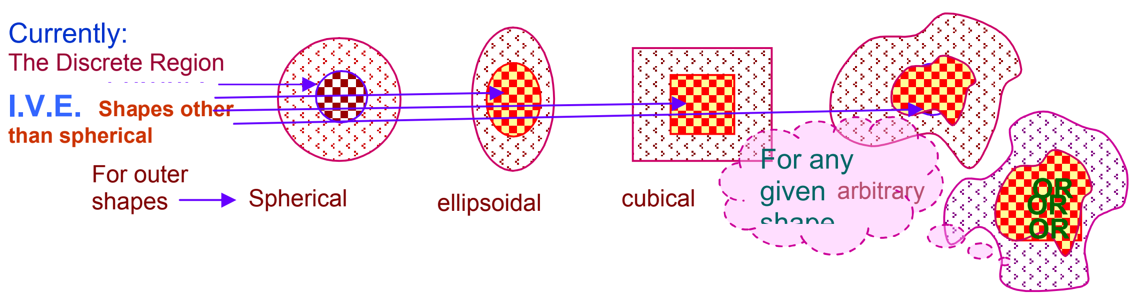
Current propositions of combinations

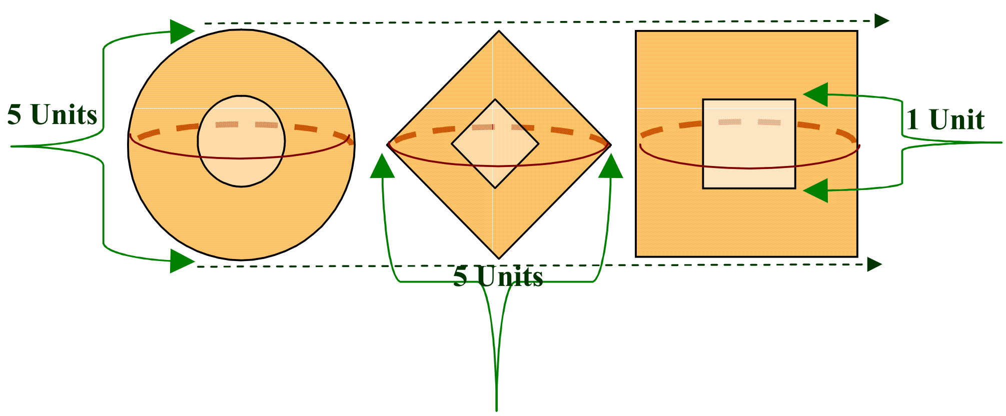
Outer a/b=1 **D**emagf=0.33	outer a/b=0.25 **D**emagf=0.708
inner a/b=0.25 **D**emagf=-0.708	inner a/b=0.25 **D**emagf=-0.708
0.33-0.708=-0.378	**0.708-0.708=0**

Download the display materials from http://nehuacin.tripod.com/id6.html

It becomes necessary to define an Inner Volume Element [I.V.E] in most of the contexts to distinguish the nearest neighbors (Discrete Region) of a specified site in solids, from the farther elements which can be clubbed in to be a continuum. The shape of the I.V.E. had always been preferentially (Lorentz) sphere. But, in the contexts to be addressed hence forth the I.V.E. need not be invariably a sphere. Even ellipsoidal I.V.E. or any general shape has to be considered and for the sake of continuity of terms used it may be referred to as *Lorentz Ellipsoids / Lorentz Volume Elements.* It has to be preferred to refer to hence forth as I.V.E. (Volume element inside the solid material: small compared to macroscopic sizes and large enough compared to molecular sizes and intermolecular distances).

The several combinations of Outer Macroscopic specimen shape and the Shape of Inner Volume Elements are displayed below. And for such combinations, at any point within the specimen, the calculation of induced field contribution seems to be merely a question of handling the analytical solid geometry and subsequent summation. Thus a single demagnetization is not possible but the induced field distribution can be calculated by a point by point calculation of the induced field and an algorithm is simple enough to evolve for a computation much faster using a program in a computer.



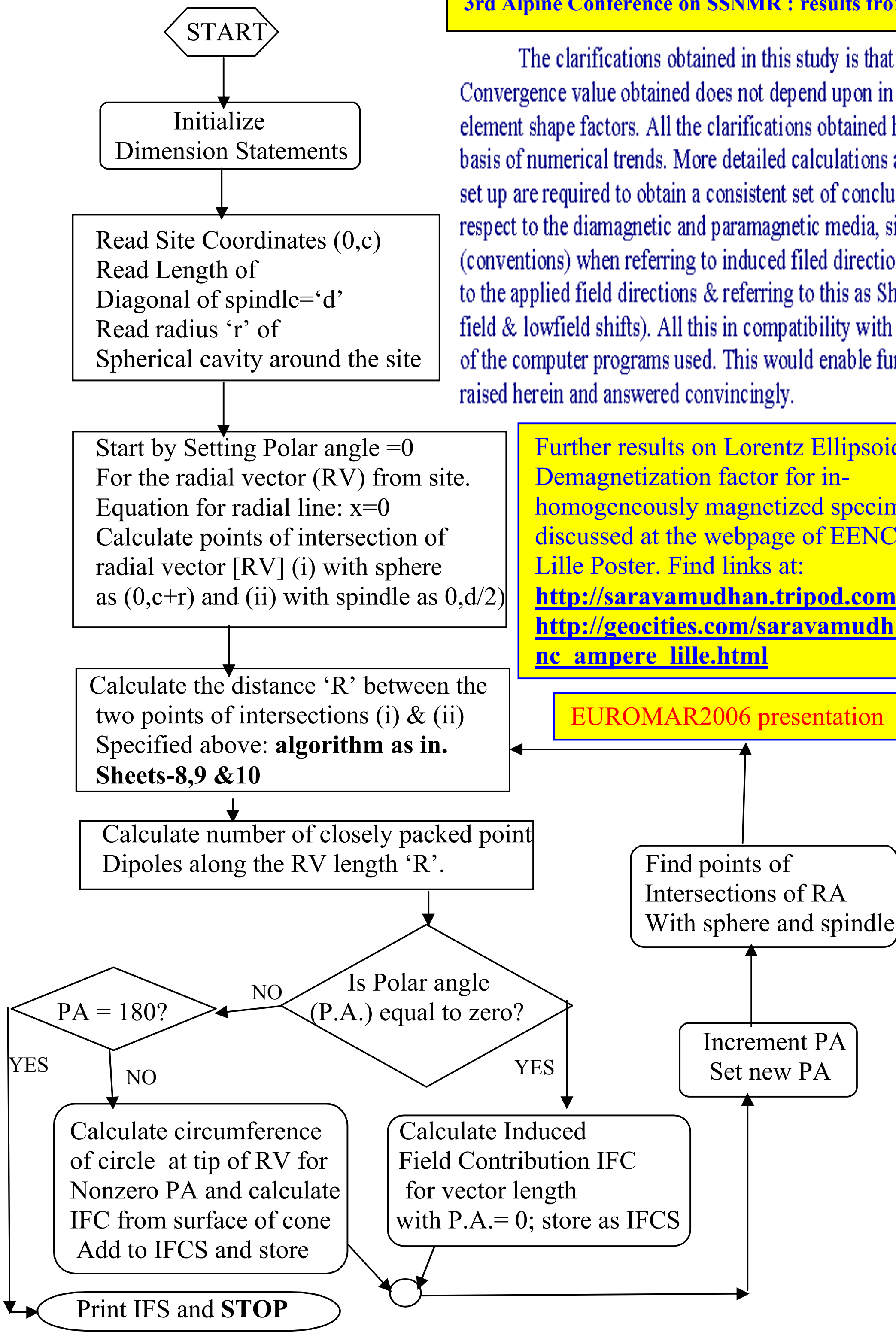


These are the specific shapes which were considered and a typical algorithm and a flow chart of a computer program used is illustrated in the next sheet

3rd Alpine Conference on SSNMR : results from Poster

The clarifications obtained in this study is that the Convergence value obtained does not depend upon in the inner element shape factors. All the clarifications obtained have been on the basis of numerical trends. More detailed calculations and trend –line set up are required to obtain a consistent set of conclusions with respect to the diamagnetic and paramagnetic media, sign of (conventions) when referring to induced filed directions with respect to the applied field directions & referring to this as Shieldings (high field & lowfield shifts). All this in compatibility with the Algorithms of the computer programs used. This would enable further questions raised herein and answered convincingly.

Further results on Lorentz Ellipsoids, and Demagnetization factor for in-homogeneously magnetized specimen, are discussed at the webpage of EENC-Ampere-Lille Poster. Find links at:
http://saravamudhan.tripod.com/id12.html
http://geocities.com/saravamudhan1944/eenc_ampere_lille.html



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At this URL: http://nehuacin.tripod.com/id3.html an insight is provided to the questions enlisted below which provides ample indications for the future directions in which these questions would lead to investigations and thus provide to NMR spectroscopic results to convincingly explain the electronic structures which can result in the trends of Shielding constants as observed in the variety of contexts with much less ambiguity than now what is prevailing.

1. *What is the root source for these Questions? **Sheet 2***
2. *What are the Contributions to Induced Fields at the site of the nucleus from the different parts of the specimen that makes up the Experimentally Measured Shielding Tensor?. **Sheet 3***
3. *Why is the Bulk Susceptibility Contribution zero for Spherical Samples? **Sheet 4***
4. *How is the Intermolecular Contribution calculated by the Discrete Summation Procedure? **Sheet 5***
5. *How to ensure that all the neighboring molecules of significance have been considered in the summation? How can the boundary of Lorentz Sphere [the semi micro volume element] be constructed? **Sheet 6***
6. *Can the Semi micro Volume element be Ellipsoidal instead of being Spherical; can there be Lorentz Ellipsoids? **Sheet 7***
7. *What is the Intermolecular contribution to the Shielding Tensor if the neighboring molecules are enclosed within a Ellipsoidal Volume Element instead of Spherical volume Element? **Sheet 8***
8. *Can the Experimentally measured Values of the Shielding Tensor for the spherical shape and the Ellipsoidal shape be related by an equation? **Sheet 9***
9. *What are the questions still remain at this stage to be answered? **Sheet 10***
10. *What are the considerations when the induced fields within the specimen can be inhomogeneous? **Sheet 11***
11. *Why the Discrete Summation procedure cannot be extended to the entire extent of the macroscopic specimen? **Sheet 12***
12. *Where are the sources for finding a description of the simpler summing method of calculating demagnetization factors? **Sheet 13***
13. *Can the simple method be useful for tackling the difficult calculations for the case of inhomogeneous magnetization? Have there been any specific shapes considered till date? **Sheet 14***
14. *Can there be zero Induced Fields inside a specimen of inhomogeneous magnetization, if the shape of inner volume element and the outer specimen shapes are same as argued out for ellipsoids? **Sheet 15***
15. *Can the Shielding tensor results be obtained with simple calculations in the case of an experimental determination in the in-homogeneously magnetized specimen even when provided that the shapes are describable by regular equations? **Sheet 16***

The numbers against the Sheet indicated in above list are the display sheet numbers at the POSTER site of the 4th Alpine Conference. This Abstarct and display sheet contents are downloadable from the URL *http://nehuacin.tripod.com/id3.html* , given also above. Abstract Title: *A Consideration of the Enduring Questions for the Possibility of Using Arbitrary Shapes of Specimen for HR PMR Studies in Single Crystalline Solid State*

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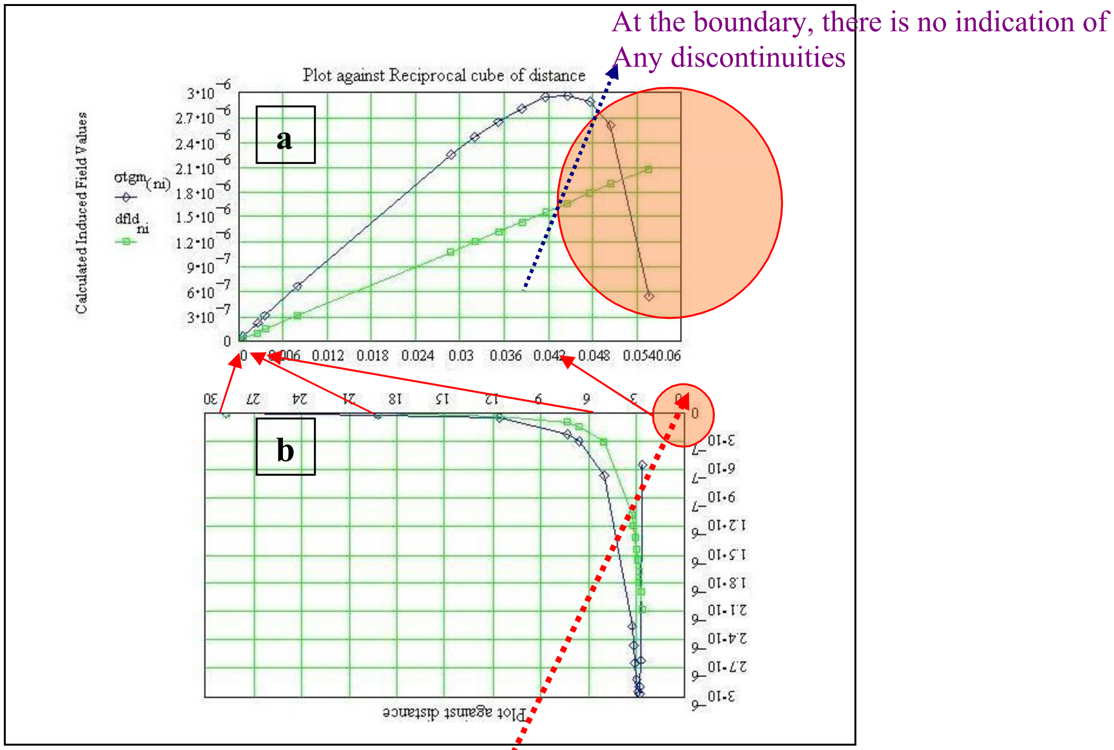
The consequences external to the material due the internal magnetization is the prime concern in finding the utilization priorities for that material.

Calculating Induced Magnetic Field outside the specimen: Improvement due this recent alternate method of summation procedure.

The induced field distribution in materials which inherently possess large internal magnetic fields, or in materials which get magnetized when placed in large external Magnetic Fields, is of importance to material scientists to adequately categorize the material for its possible uses. It addresses to the questions pertaining to the structure of the material in the given state of matter by inquiring into the details of the mechanisms by which the materials acquire the property of magnetism. To arrive at the required structural information ultimately, the beginning is made by studying the distribution of the magnetic field distributions within the material (essentially magnetization characteristics) so that the field distribution in the neighborhood of the magnetized (magnetic) material becomes tractable. **The consequences external to the material due the internal magnetization is the prime concern in finding the utilization priorities for that material.** In the materials known conventionally as the magnetic materials, the internal fields are of large magnitude. To know the magnetic field inducing mechanisms to a greater detail it may be advantageous to study the trends and patterns with a more sensitive situation of the smaller variations in the already small values of induced fields can be studied and the Nuclear Magnetic Resonance Technique turns out to be a technique, which seems suitable for such studies. When the magnetization is homogeneous through out the specimen, it is a simple matter to associate a demagnetization factor for that specimen with a given shape-determining factor. When the magnetized (magnetic) material is in-homogeneously magnetized, then a single demagnetization factor for the entire specimen would not be attributable but only point wise values. Then can an average demagnetization factor be of any avail and how can such average demagnetization factor be defined and calculated .It is a tedious task to evaluate the demagnetization factor for homogeneously magnetized, spherical (ellipsoidal) shapes. An alternative convenient mathematical procedure could be evolved which reproduces the already available tables of values with good accuracy. With this method the questions pertaining to induced field calculations and the inferences become more relevant because of the feasibility of approaches to find answers.

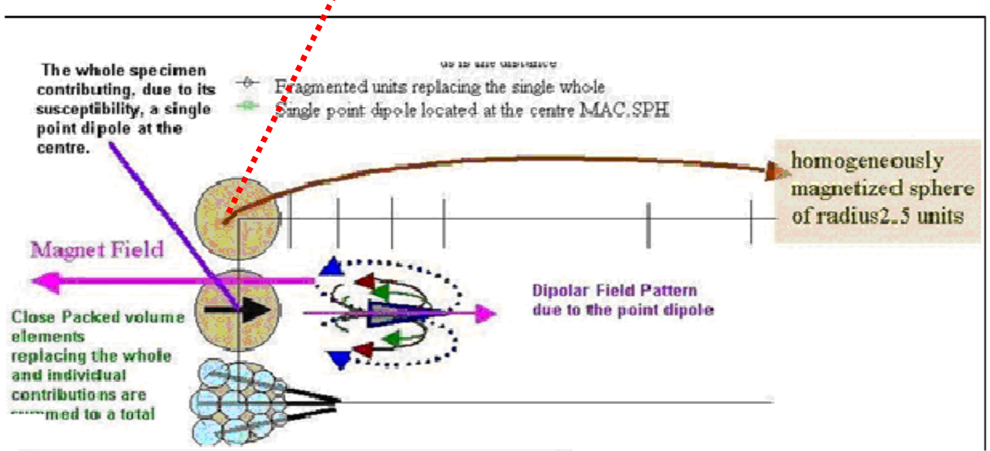
THE RESULTS FOR THE CALCULATION OF INDUCED FIELD OUTSIDE THE SPECIMEN ILLUSTRATED IN THE NEXT PAGE INDICATES THE SUPERIORITY OF THE ALTERNATE SUMMING METHOD IN WHICH THE MATERIAL COULD BE SUBDIVIDED INTO CLOSE PACKED VOLUME ELEMENTS WITH CONSTRAINT FOR POINT DIPOLE APPROXIMATION TO BE VALID AT THE SPECIFIED DISTANT LOCATION FOR ALL THE SUBDIVIDED VOLUME ELEMENTS/DIPOLES

http://saravamudhan.tripod.com/id6.html



Green Line in the graph is calculated when a single total dipole moment is at the centre of the specimen.
When the specimen is subdivided and the moments distributed according to the specified constraints, the resulting curve is the **Black line**. As indicated by the black line, the "**field within the homogeneous specimen is zero**".
Top: a. Induced field plotted as function of 1/R^3
Lower: b. The same plotted as a function of R

FIGURE-10



DISCUSSION OF THE CRITERIA FOR SUBDIVIDING

The contents of the Sheets-08,09,10 would make evident the following consequence of splitting dipoles into equal parts and/or unequal parts distributing them about the origin of the total moment. The simplest symmetrical criterion for distributing the equally subdivided moments would be to place them in symmetrical disposition around the original undivided dipole centre to get the electrical centre of gravity of the moments to be same before and after the division. By this criterion, the equally divided parts may be placed at equal intervals of distances around, which bring some parts away from the point where the induced field is calculated and equal numbers nearer to that site. Displacing the equal parts by same interval of distance away and near would ensure the electrical centre of gravity to be retained as the same, but the dipole which is away would contribute much less and the nearer part contribute much more (due to inverse cube dependence on distance). Moreover, the sum of the contributions would not be the same as that of undivided dipole. This brings in the arbitrariness and makes the division (splitting) of dipole questionable.
Thus, it is required to divide the dipoles as weighted parts (and not equal parts) in such a way that the electrical centre of gravity is retained. In addition, the requirements for the validity of point dipole approximation must be fulfilled for each divided part at its location to which it is distributed. Then the contribution of induced field from each divided part would be the same at a specified distant point. That is, *"the magnitude of divided dipoles is equal"* is not a necessary criterion. But, irrespective of its size and distance (for same θ and φ) each divided part contribute the same value of induced field so that simply multiplying by the number of parts into which the original dipole is subdivided, the total induced filed value is obtained. As much as the sample specimen has a homogeneity consideration for the susceptibility value through out the specimen, a kind of homogeneity in contribution (equal contribution) is held as constraint while subdividing, instead of the division into equal parts. Ensuring this kind of "homogeneity/uniformity" of induced filed contribution, makes the induced field value independent of the distance. The criterion of point-dipole approximation is built-in in the choice of the (R/r) factor with the "uniformity" of contribution. This seems to simulate factually the single "undivided" moment contribution when the dipole approximation is valid. *But, the fact is, in reality, "with the undivided dipole, the point dipole approximation is not valid".*

It is essentially the distance dependence, which is critical for the validity of the point dipole approximation. The angular dependence hence is to the same extent as it is in the case of undivided case of moments. Thus for a given set of (θ, φ) values, meaning along a given radial vector, the number of dipoles closely packed would depend upon the ratio of (C=R/r) chosen. Depending upon this value of 'C', the number of dipoles along each of the radial vector, '$n_{\theta,\varphi}$' would vary. For the spheres packed closely along the line the center of all spheres of varying radii lie on the radial vector. These spheres would have radii such that it would be possible to draw a cone containing these spheres, which would have an apex at the site where the induced filed contribution is required. The axis of the cone would be the radial vector. Which means that the material in the given set of such spheres are contained in the spherical specimen within a solid angle "Δω" (see Figure-7) where as the material of the entire specimen can be included only if the solid angle '4π' is covered. Hence for each set of (θ, φ), a '$\Delta\omega_{\theta,\varphi}$' and an '$n_{\theta,\varphi}$' are associated with every of one of the $n_{\theta,\varphi}$ spheres contributing the same induced field value.

Then for all conical sections (packed radially adjacent, and closely packed to cover the solid angle 4π) the (θ, φ) associated would determine the angular dependence and the number 'n' would determine the dipoles which all contribute the same induced field at the conical apex where the contribution is calculated. When spheres are closely packed, there would be voids in the closed packed structure. This would mean the materials in the volume of the voids (for the corresponding magnetic moments) have to be taken into account which is accomplished by describing a cube enclosing each of the spheres, the 'side-length' being the same as the radius of that corresponding sphere. This has been explained already earlier in the previous section.

CONCLUSION

It is known that a division of a magnetized material into smaller volume elements would not provide in general a unique possibility for assessing the induced field distribution calculated by applying the point dipole approximation to sum the contributions from the extent of the material. In spite of such established ambiguities, it has been shown that a criterion for subdividing the materials into smaller elements is possible; by which, a induced dipole moment can be associated corresponding to every subdivided elemental-volume and, then the point dipole approximation can be employed. Thus, a convenient alternate method could be evolved to calculate demagnetization factors. This procedure yields values, which are reasonably accurate and are the same as the values available from the standard table of demagnetization factors.

This alternate procedure, which is very convenient to calculate induced filed contributions, it has been found to enable the calculation of demagnetization factors for the combination of shapes of inner semi-micro volume element and the outer macroscopic specimen shape as in Figure-10. More over, with the confidence thus ensured for the criteria of subdividing magnetized materials, it has been found that this procedure enables the applicable ranges and chemical contexts for the use of point dipole approximation. As can be found from the descriptions above the induced field distributions can be calculated without invoking surface charges and hence, from the point of view of applications in chemistry, the appreciation of induced field distributions in chemistry gets better and more elegant with the point dipole approximation. Specifically, interpretation of spectral parameters in terms of molecular electronic structure seems to be rendered much less ambiguous with this magnetic dipole model.

The consideration in this presentation **holds out possibilties for further investigations** in the study of *"Line Shapes in Magnetic Resonance and the Average Static Magnetic Field at a Site: The Role of Discreteness and Continuum within the Material"* with particular reference to the remarks by W.C.Dickinson in Physical Review., **81**, 717 (1951). An effort along these indications has been initiated as per the documentation at the webpage for the MRSFall2006 at http://nehuacin.tripod.com/id4.html