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 inhomogeneously magnetized specimen even when provided that the shapes are describable by regular eqautions*? ***Sheet 16***

Appendix: on ***Sheet 17 ; Sheet 18 ; Sheet 19 & Sheet 20***

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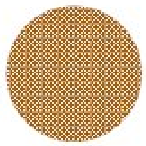
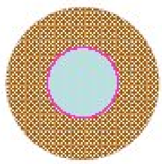
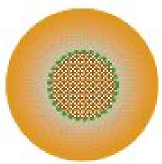
1 *What is the root source for these Questions?*



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.



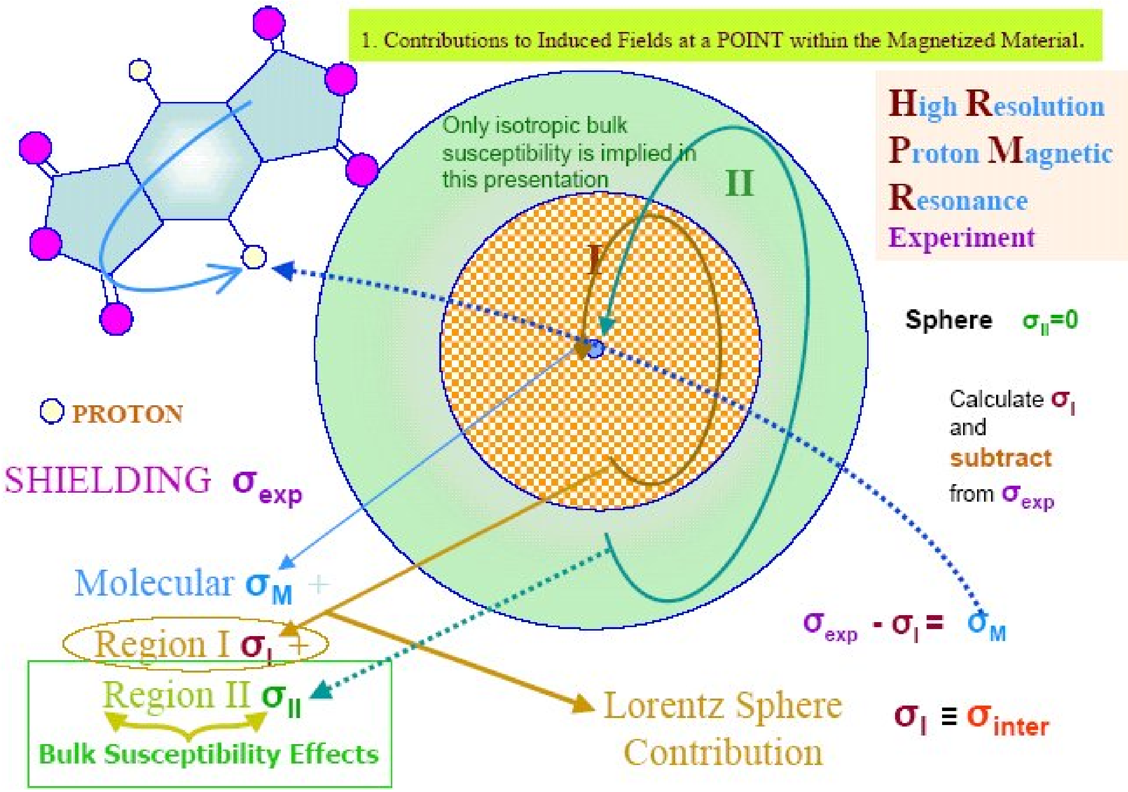
2. The above criterion requires that a semi micro **spherical volume element is carved out** around the site within the specimen and around the specified site this carved out region is a cavity which is called the **Lorentz Cavity**. Provided the Lorentz cavity is spherical and the outer specimen shape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

As stated above the HR PMR studies which are intended for determining Shielding tensor of protons are found to be beset by a difficulty; namely, every organic molecular system which is to be studied by HR PMR in single crystals had to be first of all made into spherically shaped specimens. Not all the crystals grown have the characteristics to realize the spherically shaped specimen. This is so because making sphere out of the naturally grown morphology of the crystals required a sort of grinding that the crystals would not withstand and so the specimen might break into pieces even before nearing the spherical shape. Thus the applicability of the Multiple Pulse Line narrowing technique was limited only by the properly shaped specimen while from the point of view of NMR instrumentation the progress was proving to be a highly promising. If there must be any necessity to study the improvement on the instrumentation part, it was necessary to find out whether there would really be so many numbers of samples to study. Instead of changing over, even from the point of view of basic research, the preoccupation was to find ways to circumvent the impediment and in simple terms the problem was to find out is there any way by which the intra molecular information on shielding can be retrieved from the experimentally determined Shielding tensor values from specimen of arbitrary shape.
Thus the basic approach had to be to sort out all the possible contributions to induced fields at a proton site in a single crystalline solid; and, find out how to disentangle them from the experimentally observed value. The beginning is made as in the next sheet #3.

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?.*

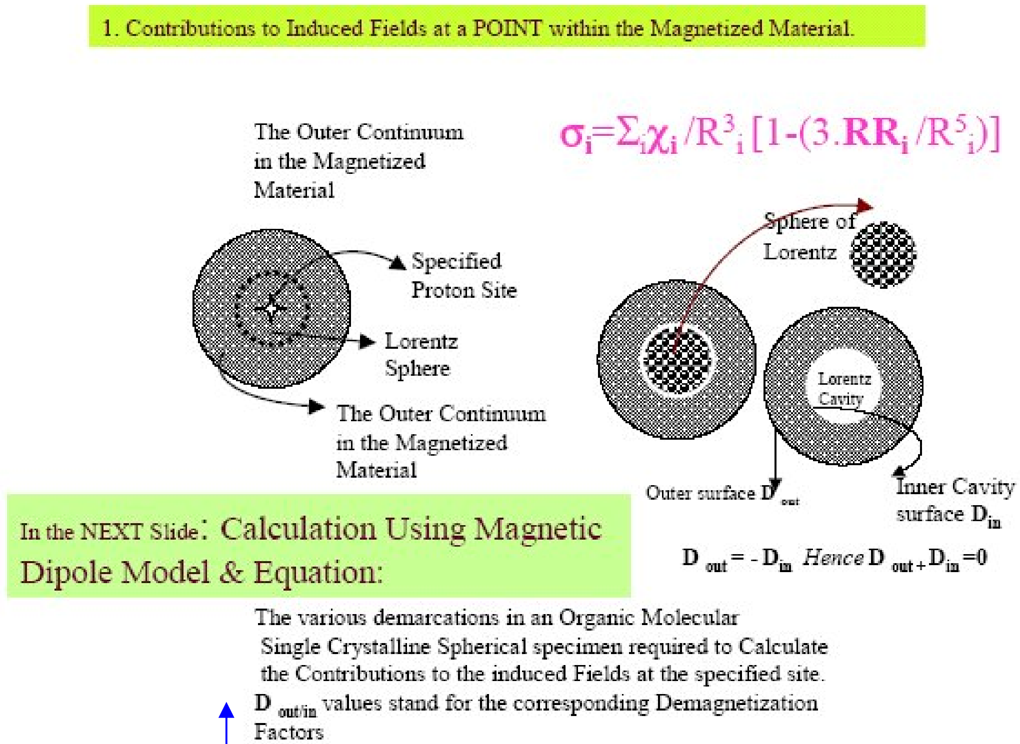


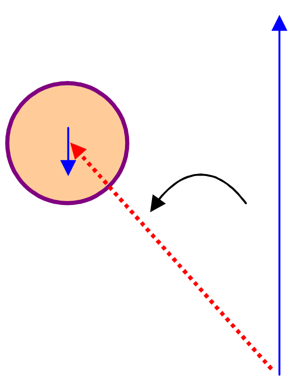
The above figure depicts the considerations discussed in the following reference:

Pyromellitic Acid Dianhydride; Crystal Structure and Anisotropic Proton Magnetic Shielding: S.Aravamudhan, U.Haeberlen, H.Irngartinger and C.Krieger, Molecular Physics, 38, 241 (1979).

The spherical sample is divided into two regions (1) the Lorentz sphere contributions from which are calculated by discrete sum of values from individual neighboring molecules σ_{inter}. (2) The continuum bulk region from where the induced field at proton is dependent on the shape dependent bulk susecptibility factor σ_{II}
In the following sheets more of this aspect would be displayed and discussed. First of all the equation used for the discrete summation of inter molecular contribution would be explained in the next sheet after explaining the reason for bulk susceptibility contribution being zero for spherically shaped specimen.

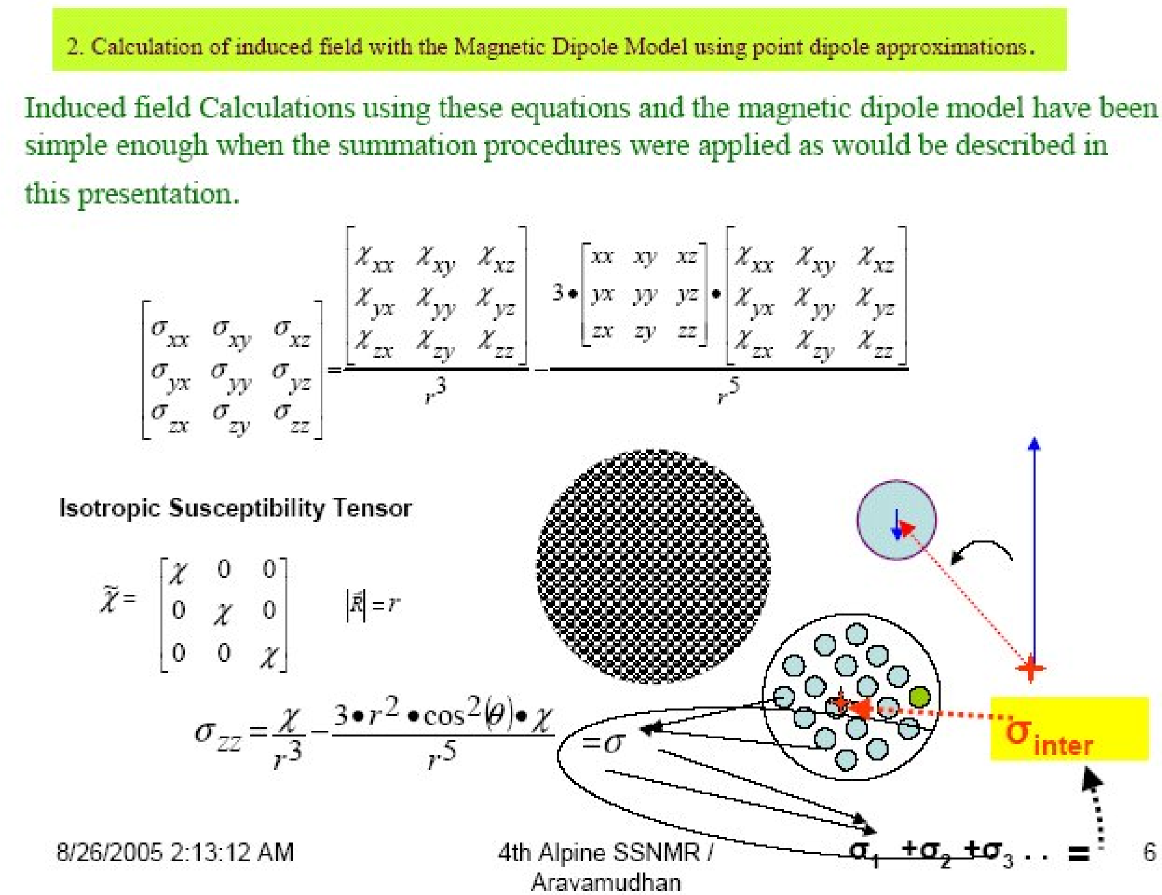
3. Why is the Bulk Susceptibility Contribution zero for Spherical Samples ?





The equation given above is based on the magnetic dipole model. The susceptibility gives rise to a induced dipole moment which is located at the center of gravity of that region. This dipole moment induces a field at neighboring locations which is calculated by the above equation.

4. How is the Intermolecular Contribution calculated by the Discrete Summation Procedure?



$$\sigma_{\mathbf{i}}=\Sigma_{i}\chi_{\mathbf{i}} /R^{3}_{i} [1-(3.\mathbf{RR_i} /R^{5}_{i})]$$

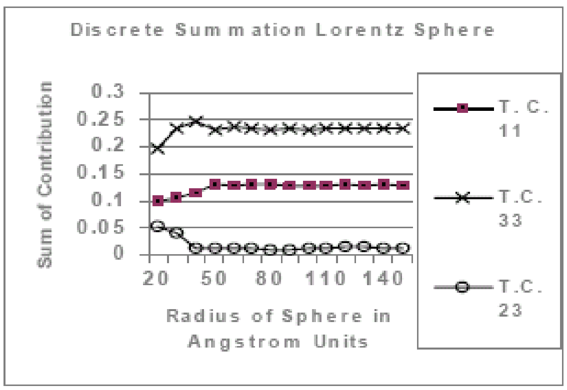
This equation in the tensor form is written in the expanded matrix form above to know the simplicity of the actual calculation.

Each blue sphere below indicates a dipole moment and the values for each one is substituted into the equation the resulting value added to result the final sum.

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?

How to ensure that all the dipoles have been considered whose contributions are signifiicant for the discrete summation ?

That is, all the dipoles within the Lorentz sphere have been taken into consideration completely so that what is outside the sphere is only the continuum regime.

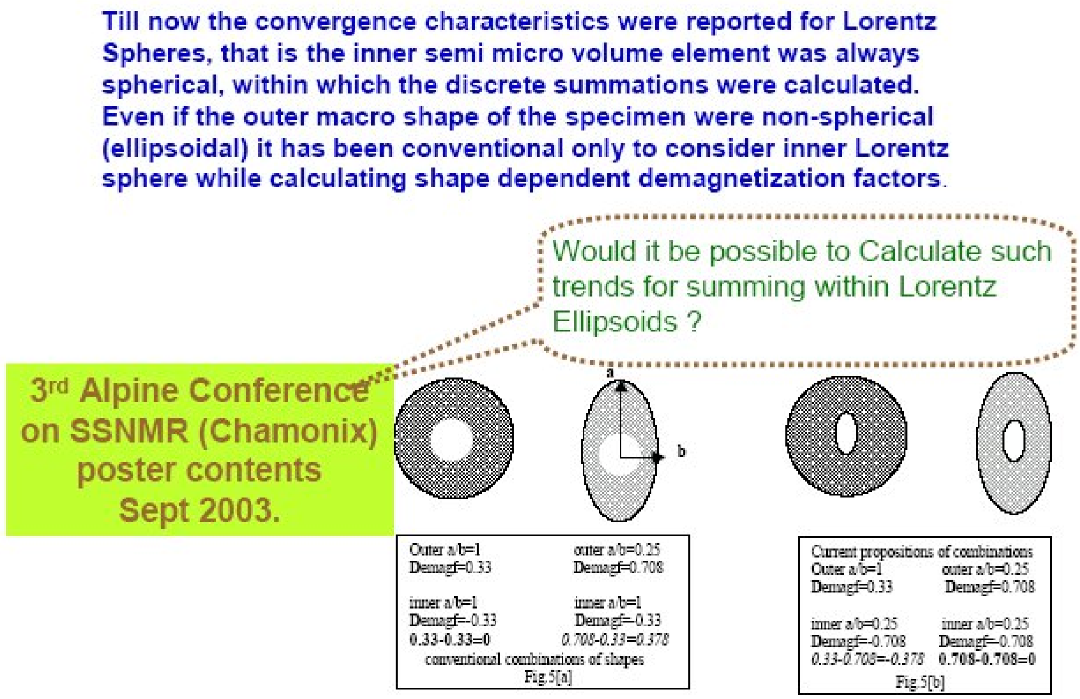


The summed up contributions from within Lorentz sphere as a function of the radius of the sphere. The sum reaches a Limiting Value at around 50A°. These are values reported in a M.Sc., Project (1990) submitted to N.E.H.University. T.C. stands for (shielding) Tensor Component

Thus as more and more dipoles are considered for the discrete summation, The sum total value reaches a limit and converges. Beyond this, increasing the radius of the Lorentz sphere does not add to the sum significantly

This is a convergence characteristic which gets more importance in the discussion at the succeeding sheets. Hence at this stage it is important to know the convergence criterion as above. This enables the precise demarcation of the Lorentz sphere from the remaining bulk.

6. *Can the Semi micro Volume element be Ellipsoidal instead of being Spherical; can there be Lorentz Ellipsoids?*



Here is the next step from the arguments in Sheet #4. For spherical samples the criteria was both inner and outer shape were same ad hence, inner element being a cavity has negative sign. Thus the two factors add up to zero.

Similarly inner and outer shapes were made ellipsoids and on the basis of similar argument the shape dependent bulk susceptibility contribution for this case can be also zero. The further consequence of this is depicted in the next sheet [Sheet#8] to look for the possible demarcation of ellipsoidal volume element by setting up convergence criteria for discrete sum.

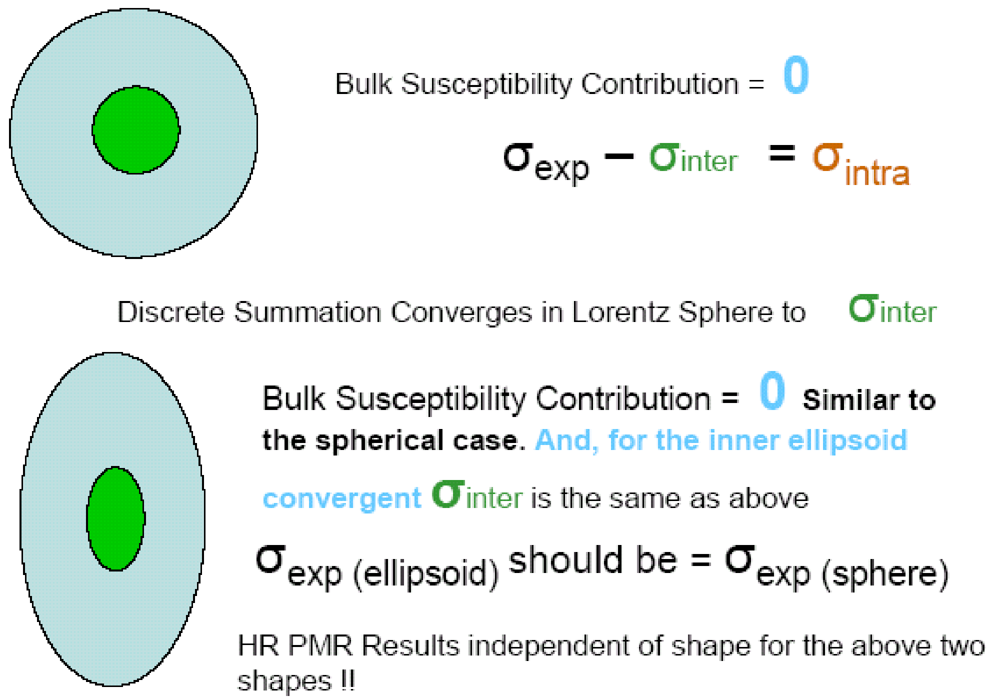
7. *What is the Intermolecular contribution to the Shielding Tensor if the neighboring molecules are enclosed within a Ellipsoidal Volume Element instead of Spherical volume Element?*

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.

That for Ellipsoidal volume element as well as the spherical volume element the summed up inter molecular contribution is the same warrants a careful consideration

8. *Can the Experimentally measured Values of the Shielding Tensor for the spherical shape and the Ellipsoidal shape be related by an equation?*



9. *What are the questions still remain at this stage to be answered?*

The questions which arise at this stage

1. How and Why the inner ellipsoidal element has the same convergent value as for a spherical inner element?

2. If the result is the same for a ellipsoidal sample and a spherical sample, can this lead to the further possibility for any other regular macroscopic shape, the HR PMR results can become shape independent ?

This requires the considerations on:

The Criteria for Uniform Magnetization depending on the shape regularities. If the resulting magnetization is Inhomogeneous, how to set a criterian for zero induced field at a point within on the basis of the Outer specimen shape and the comparative inner cavity shape?

10. *What are the considerations when the induced fields within the specimen can be inhomogeneous?*

The reason for considering the Spherical Specimen preferably or at the most the ellipsoidal shape in the case of magnetized sample is that only for these regular spheroids, the magnetization of (the induced fields inside) the specimen are uniform. This homogeneous magnetization of the material, when the sample has uniformly the same Susceptibility value, makes it possible to evaluate the Induced field at any point within the specimen which would be the same anywhere else within the specimen. For shapes other than the two mentioned, the resulting magnetization of the specimen would not be homogeneous even if the material has uniformly the same susceptibity through out the specimen.

Calculating induced fields within the specimen requires evaluation of complicated integrals, even for the regular spheroid shapes (**sphere and ellipsoid**) of specimen

http://nehuacin.tripod.com/id3.html

11. Why the Discrete Summation procedure cannot be extended to the entire extent of the macroscopic specimen?

Thus if one has to proceed further to inquire into the field distributions inside regular shapes for which the magnetization is not homogeneous, then there must be simpler procedure for calculating induced fields within the specimen, at any given point within the specimen since the field varies from point to point, there would be no possibility to calculate at one representative point and use this value for all the points in the sample.

A rapid and simple calculation procedure could be evolved and as a testing ground, it was found to reproduce the demagnetization factor values with good accuracy which compared well with the tabulated values available in the literature.

In fact, the effort towards this step wise inquiry began with the realization of the simple summation procedure for calculating demagnetization factor values.

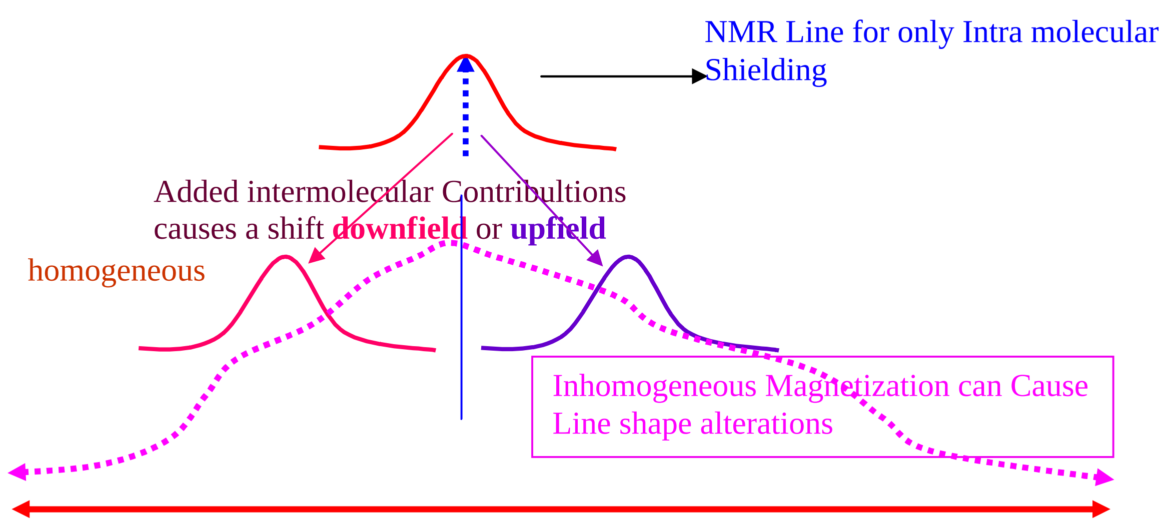
Results presented at the 2nd Alpine Conference on SSNMR, Sept. 2001

12. Where are the sources for finding a description of the simpler summing method of calculating demagnetization factors?

The following Web pages built by this author documents all the relevant presentations to provide details appropriately.

1. http://geocities.com/saravamudhan1944/eenc_ampere_lille.html
2. http://geocities.com/inboxnehu_sa/conference_events_2005.html
3. http://saravamudhan.tripod.com/id12.html

Further considerations would require a recapitulation from following diagram to differentiate the situations in homogeneous and inhomogeneous induced fields. Even regular shapes, if it is not ellipsoidal would have only inhomogeneously induced fields within.



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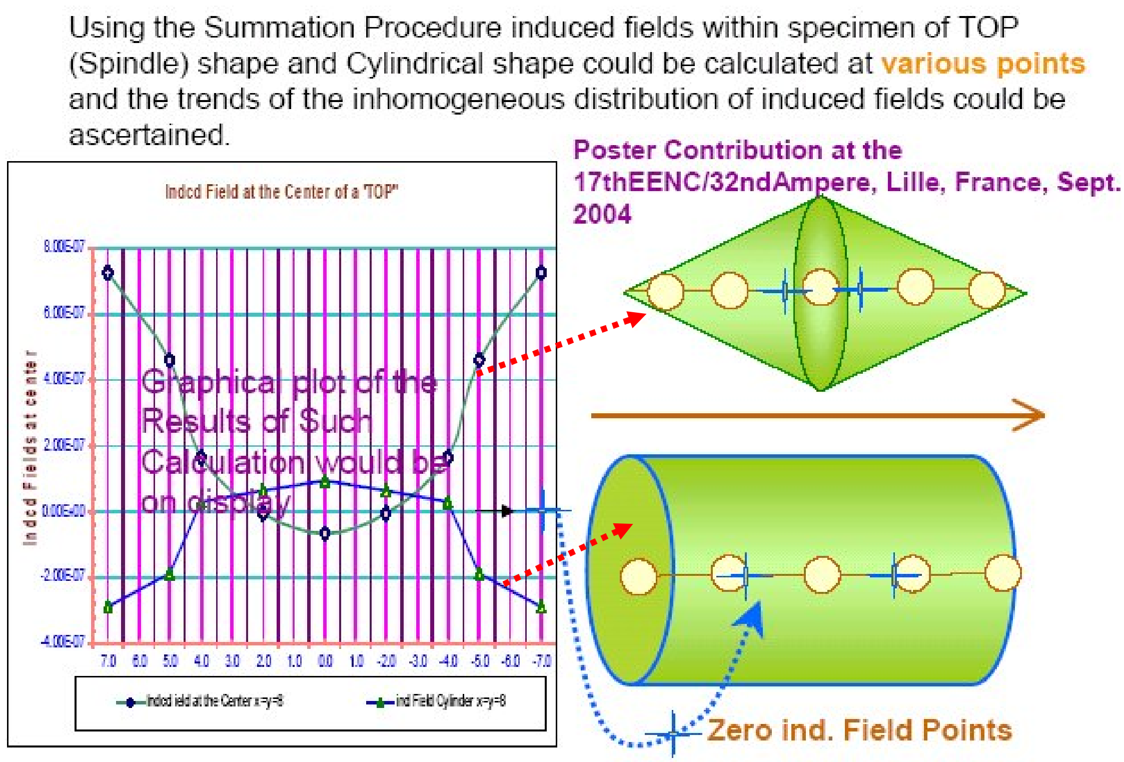
13. Can the simple method be useful for tackling the difficult calculations for the case of inhomogeneous magnetization? Have there been any specific shapes considered till date?



For a spherical sample a similar calculation at different points results zero value at all the points. The different trends above clearly distinguish cylindrical shape from the spindle shape.

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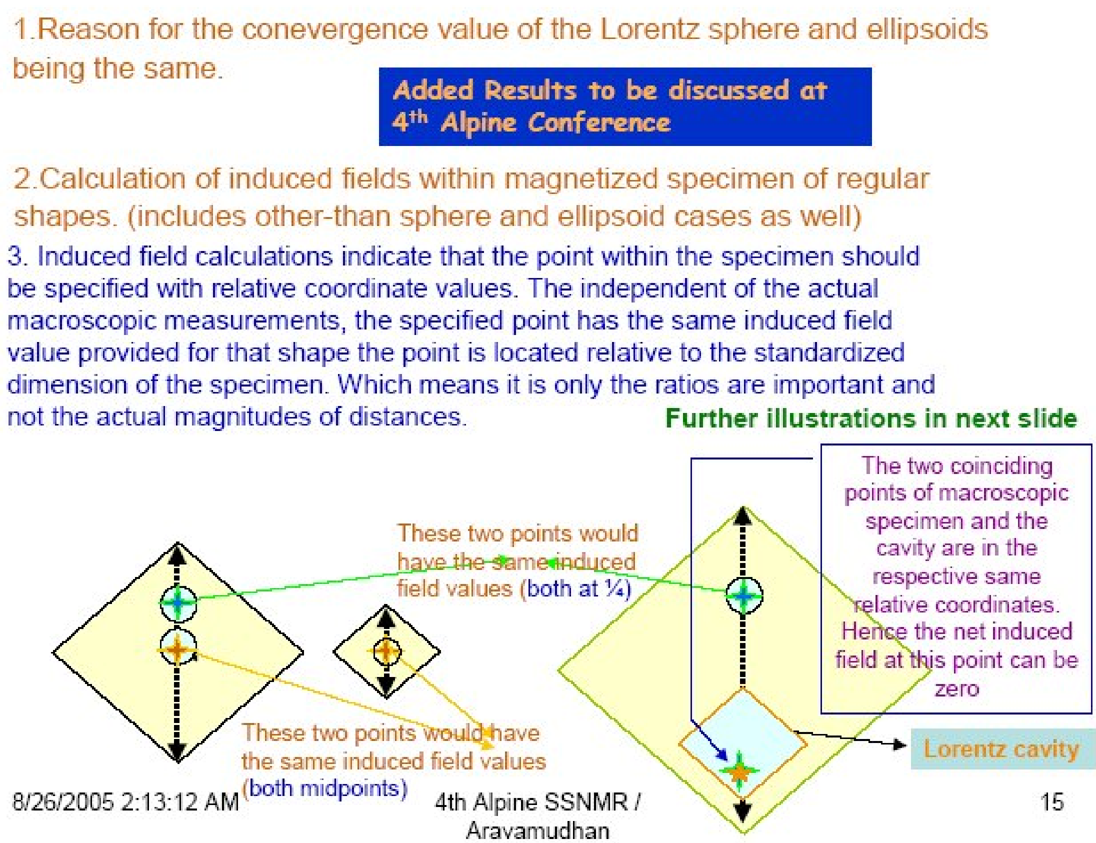
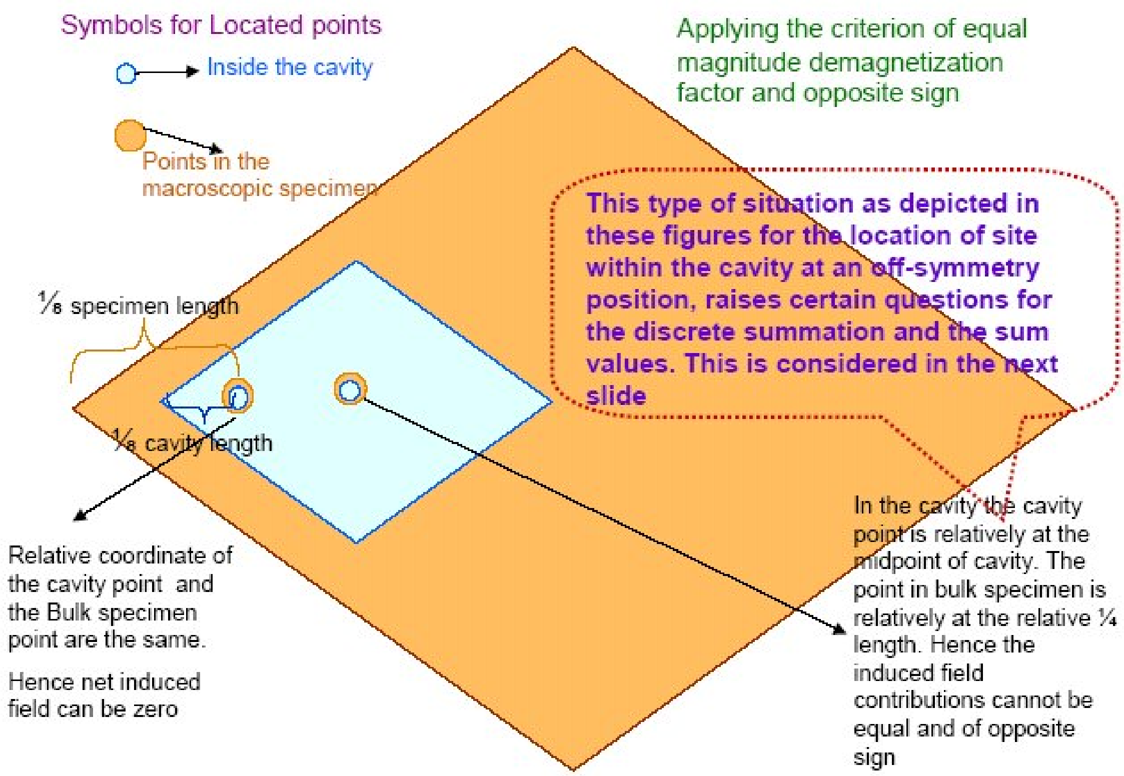
14. Can there be zero Induced Fields inside a specimen of inhomogeneous magnetization, if the shape of inner volume element and the outer specimen shapes are same as argued out for ellipsoids?

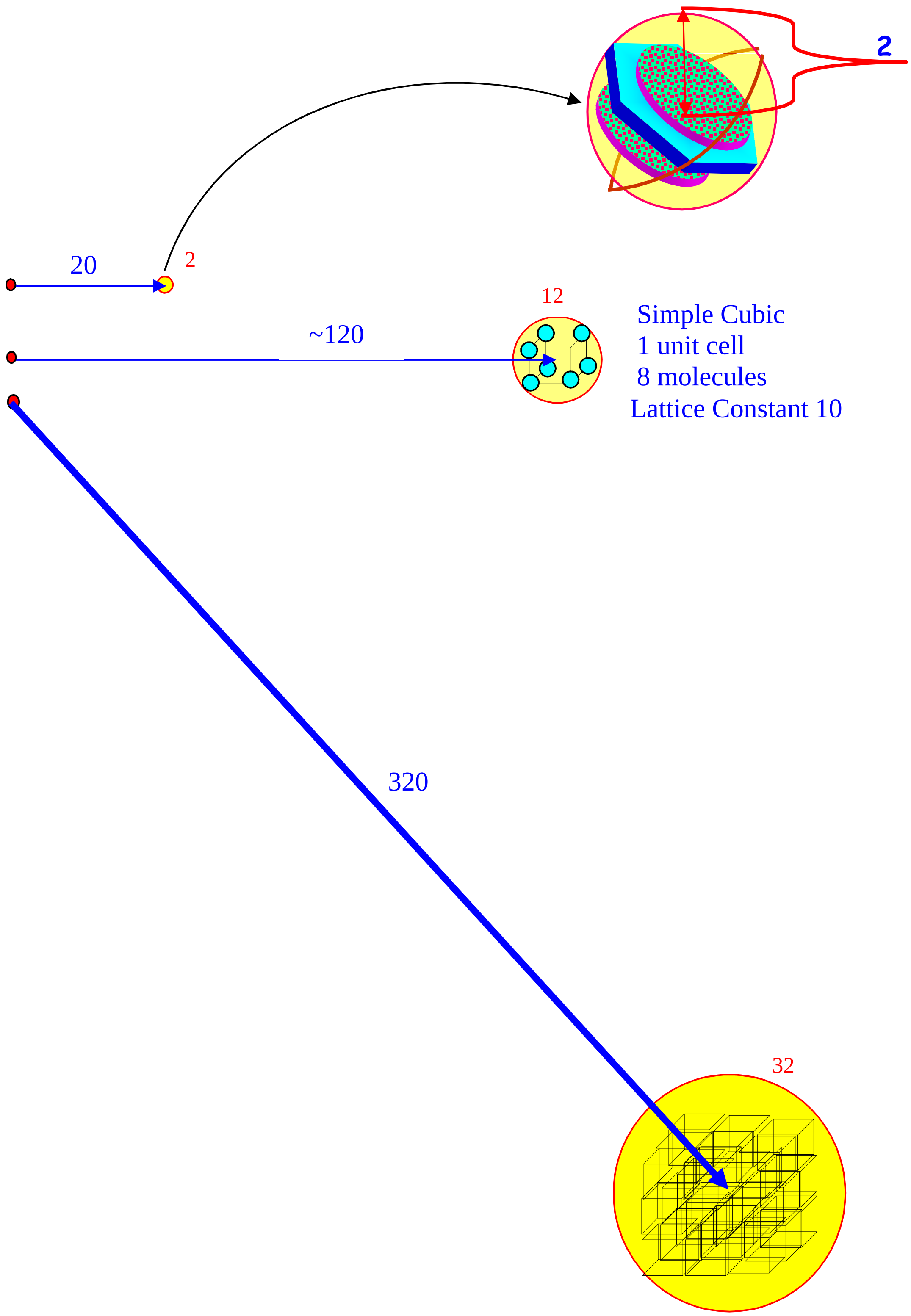


The item 1 mentioned above requires greater attention and hence this aspect is discussed separately in the appendix pages at the end. These have much more basic considerations of how to define discrete region quantitatively related to the continuum region. It is only with these basics discussed that question gets answered convincingly.

15. *Can the Shielding tensor results be obtained with simple calculations in the case of an experimental determination in the inhomogeneously magnetized specimen even when provided that the shapes are describable by regular eqautions*?



This above aspect can be discussed at length to consider the interesting consequences of the fact that the bulk susceptibility contribution to induced fields within the material depends only on the shape and size is not a factor. Only requirement would be that the relative coordinates of the points have to be the same [if the size is different] for induced field value to be the same.



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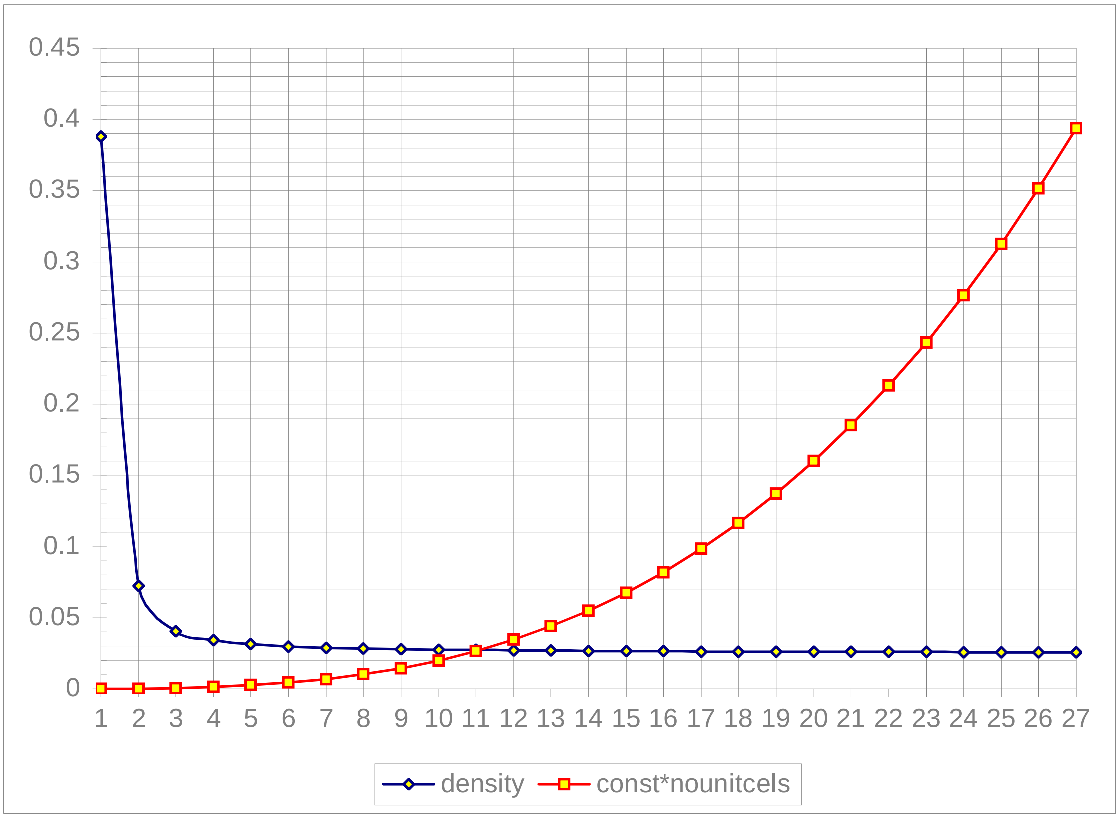
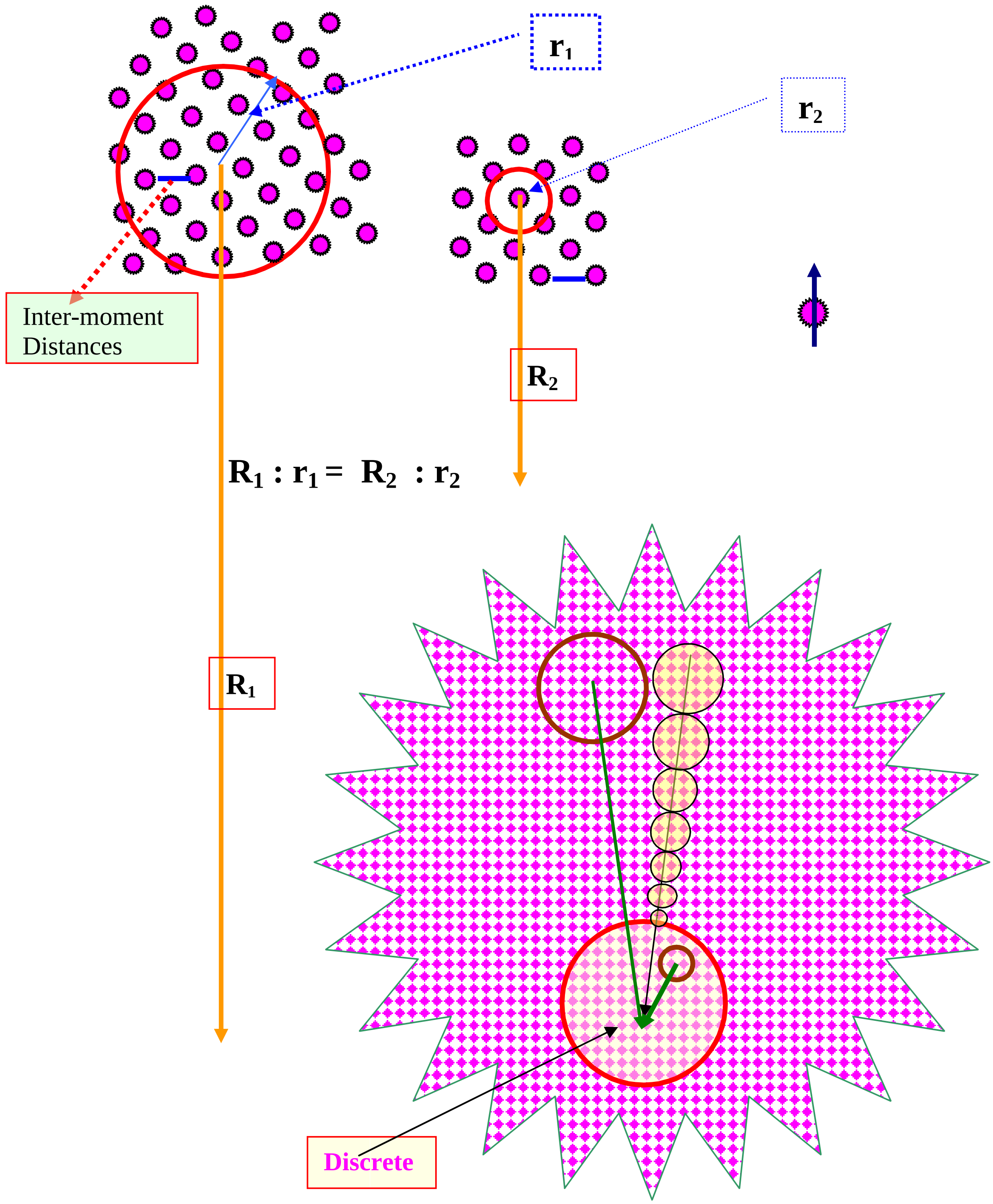


no untcel	d=wt/vol	no untcel	d=wt/vol
1	0.38794	10648	0.025923
8	0.072385	12167	0.025872
27	0.040429	13824	0.025826
64	0.034058	15625	0.025783
125	0.03137	17576	0.025744
216	0.029892	19683	0.025708
343	0.028958		
512	0.028315		
729	0.027845		
1000	0.027486		
1331	0.027204		
1728	0.026976		
2197	0.026787		
2744	0.02663		
3375	0.026495		
4096	0.026379		
4913	0.026279		
5832	0.02619		
6859	0.026112		
8000	0.026042		
9261	0.02598		



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For the reasons as explicable from the trends depicted in these appendices [the three sheets before] the contribution to the induced fields from the discrete summation predominates in magnitude to the sum of contribution from all the molecules which can be described as being in the continuum region. Since a sphere can be found within which the sum can converge, even if there are few molecules outside this region with anon spherical distribution, there net contribution is insignificant (can be negligible) compared to the intermolecular contributions. Hence even for a ellipsoidal Lorentz volume element, the total contribution is significantly from the sphere describable inside and the materials outside have already become insignificant numerically for the induced contributions.

As the distance increases, the induced field contributions decrease as the distance factor occurs in the denominator with exponent 3. The number of molecules available at a radial distance increases with distance. But the rate at which the number of molecules increase is less than the rate at which the contribution of each molecule decreases at larger distances hence the total effect becomes merely a question of geometry and less significant than the intermolecular contribution.