

Dividing a Magnetic Moment and Distributing the Parts, can it ensure a Better Validity of the Point Dipole Approximation?

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When a homogeneously magnetized material is sub-divided into close-packed volume elements, then, each volume element gives rise to a dipole moment in presence of external field. Summing of the contribution of the induced fields due to these divisional moments calculated at a point within the sample, reproduces the already known values of demagnetization factors. Dividing a given total dipole moment into parts and distributing them to calculate the summed contribution of induced field at a distant point need not always result in the same value. The above alternate method of equivalent distribution of divided parts would be described with certain simple exercises as illustration.

Suggested Reference Materials:-

<http://saravamudhan.tripod.com/>

<http://nehuacin.tripod.com/>

http://www.geocities.com/inboxnehu_sa/conference_events_2005.html

http://www.geocities.com/inboxnehu_sa/conference_events_2006.html

http://in.geocities.com/saravamudhan2002/events_2007.html

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INTRODUCTION:

The table of demagnetization factors, which are available, consists of values calculated by a procedure of mathematical Integration, starting from defining “*infinitesimally small*” charge circulations giving rise to *dipole moments* placed at the centre of circulation. Thus such infinitesimal charge circulation is placed over the entire extent of the specimen and integration carried out of the induced field at a given point in the specimen due to all such infinitesimal dipole moments. If it is recalled here that a procedure of integration is effectively a summing over all the infinitesimal quantities, then the question arises as to whether within a certain tolerance, the infinite number of dipole moments envisaged can possibly find an equivalent distribution of finite number dipole moments arising from the entire material. Then the calculation of the contribution to the induced field due to all these finite number of dipoles would require finite number of calculations for summing, and the limit of infinite number of calculations and additions would not be encountered. The approach then would be to merge the cells in the mesh of infinite number of cells to reduce the count appropriately to finite number of cells in the mesh, which describes the material specimen without leaving any material away from counting for the contribution. Alternately, to get such a set of finite number of dipoles, first, the single dipole due to the bulk susceptibility of the entire specimen-volume is to be considered as having been placed at an appropriate electrical centre of gravity within the specimen. Then devise appropriate criteria for a subdivision for this single total dipole moment to distribute the resulting finite number of dipoles to appropriate locations within the specimen. Either merging the cells or subdividing the total, requires a rearrangement, correspondingly, either to get the equivalent origin for a set of distributed locations or for a given single location to get a set of distributed origins to be equivalent to the singular location. With respect to the induced field at a given point from all these dipoles using the point dipole approximation, placing effectively a single dipole at an origin need not result in the same value as the distributed situation for the dipoles that constitute the totality of dipoles. If it does, then it would be as if the point dipole approximation is valid for the effective single dipole as much as for the distributed dipoles, in which case there should not be any requirement for the “*subdividing*” procedure. In the following, this aspect of the necessity for subdividing the specimen into smaller volume elements would be illustrated for the compliance with the point dipole approximation to calculate induced field contribution at a given point.

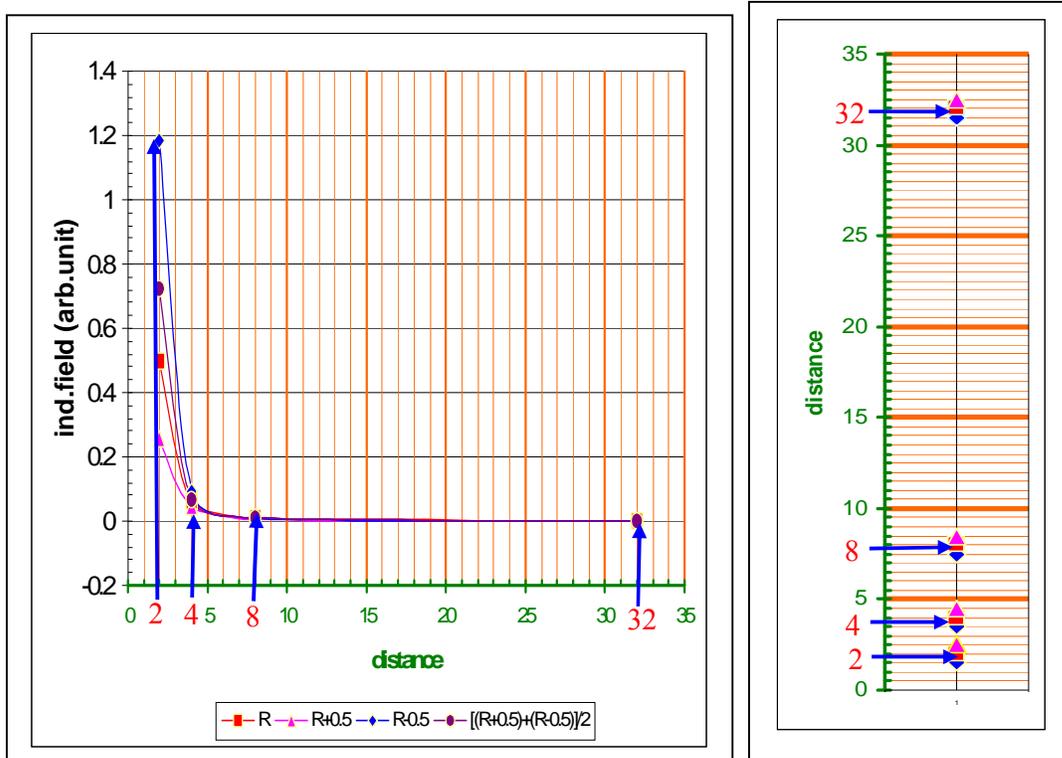
A DESCRIPTION OF SUBDIVIDED VOLUME ELEMENTS

In Figure 1, the illustration depicts the trends of induced field values for a dipole moment of a given magnitude, split into two equal parts and placed at symmetrically distant points on both sides of the original location. The data is on the Table-1 for this graphical illustration. An elaboration of the materials discussed in this section can be found at Appendix-A

Table-1:

	For moment value '-2 units' Induced field values at			
'R' values	R	R-0.5	R+0.5	[(R-0.5)+(R+0.5)]/2
2	-0.5	-0.256	-1.18519	-0.720595
4	-0.0625	-0.0439	-0.09329	-0.068595
8	-0.00781	-0.00651	-0.00948	-0.007995
32	0.00012207	0.000116523	-0.000127976	-0.00012225

Figure-1



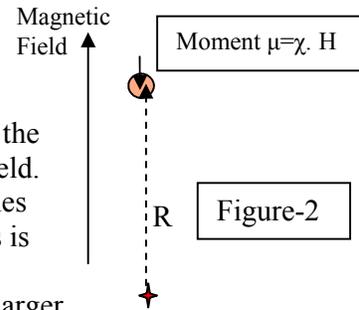
An equation of the type

$$\sigma_i = \sum \chi_i / R^3_i [1 - (3 \cdot R \cdot R_i / R^5_i)] \text{ -----Equation -1}$$

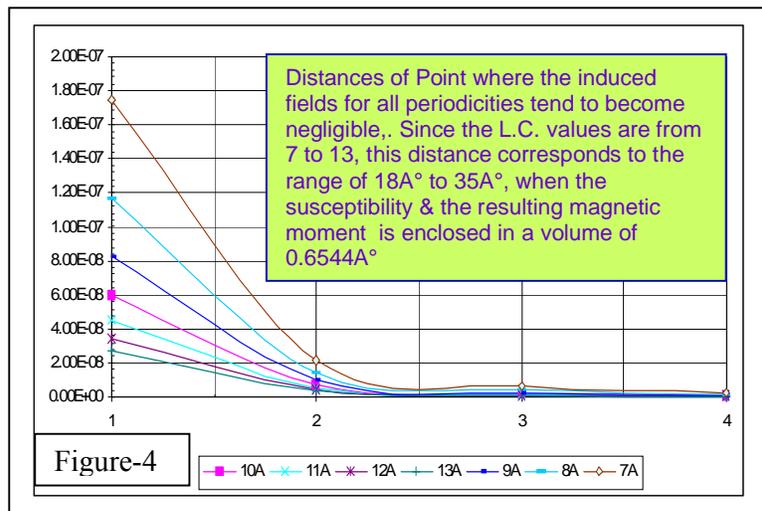
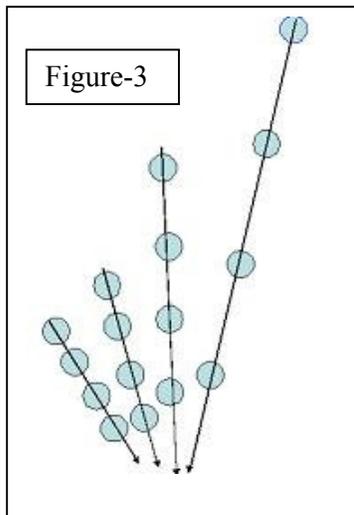
Can be used for the calculation of the induced field (a shielding tensor ' $\underline{\sigma}$ ' multiplied by the applied field value gives the induced field in the tensor forms.) For an 'isotropic susceptibility', characterizing the system can give the induced field component value along the field direction by the much simpler formula (derivable from the above by a simplification), as follows:

$$\{\chi \cdot (1-3 \cdot \cos^2 \theta)\} / (R)^3 \text{ -----Equation 2}$$

For the above calculation $\chi = -2$ was used and $\theta = 0^\circ$ where the θ is the angle between the distance vector and the direction of magnetic field. When the R-value increases, the splitting distance of 1 unit becomes relatively smaller and the consequence on the induced field values is obvious from the graphical results. It can be noted that the above equation for the point dipole approximation is more valid at such larger distances.



For a different perspective on this situation, the following illustration is included without much description. In this case, the volume 'v' of the spherical volume element considered here for the calculation is $1.17E-24$ c.c. The radius 'r' of this volume element is 0.00000006544 cm $0.6544E-08$ cm which is 0.6544 \AA using this radius value and the equation for the volume of sphere $(4/3) \cdot \pi \cdot r^3$ the value of 'v' has been calculated. The value of the susceptibility of the spherical volume used is $6E-29$ cgs units. The calculated values are at Lattice periodicities (one-dimensional) of 10 \AA ; 11 \AA ; 12 \AA and 13 \AA ; 9 \AA ; 8 \AA ; 7 \AA , (Figure-3). These are plotted graphically in Figure-4.

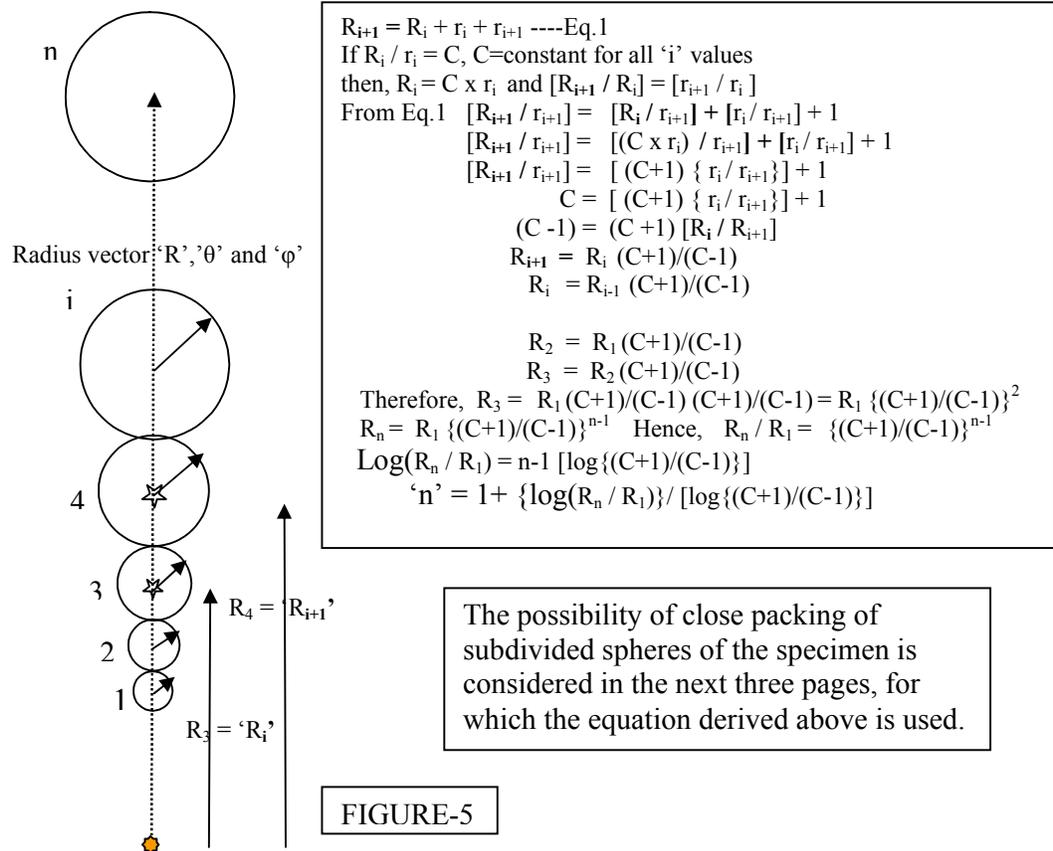


With the above remarks on the consequences of “splitting dipoles” and calculating contribution to the induced field at a distant point, the Calculation of the Demagnetization factor is described in the following section.

CALCULATING DEMAGNETIZATION FACTOR:

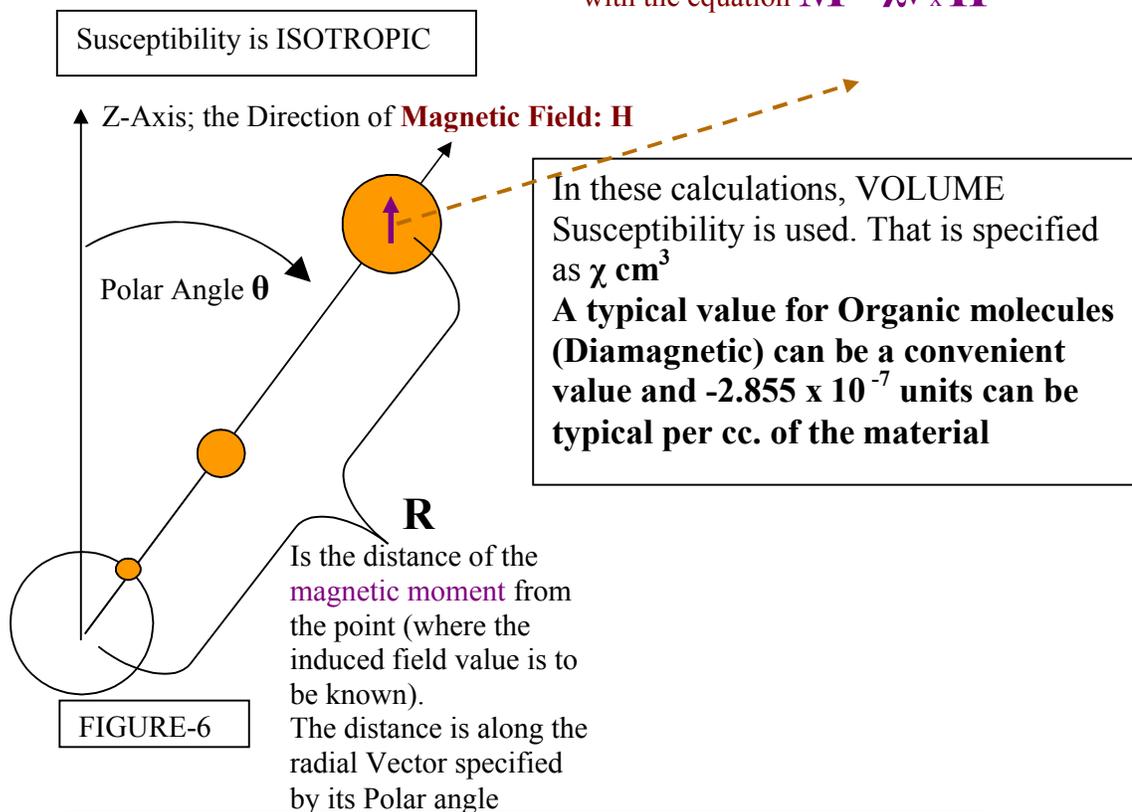
In the context of a demagnetization factor, it is necessary to remark that a single demagnetization factor value is obtainable for the whole specimen when (i) the specimen is a homogeneous substance with uniform volume susceptibility through out the sample and (ii) the shape of the specimen is an ellipsoid of revolution, a sphere being a typical special case. Splitting the magnetic moment would correspond to subdividing the specimen into smaller volume elements, each describable in terms of an associated moment in presence of the field.

If the totality of the specimen material is accounted for by the corresponding summation of the volume elements, the single dipole moment of the entire specimen material would have been equivalently subdivided, and the dipole moments of the individual elements would be placed at the appropriate central location within the respective volume elements. The susceptibility of the volume elements would be proportional to the volume and which in turn determines the magnitude of the moment. Thus from the equation 2 the following criteria can be inferred: the subdivided volume elements will all be at different distances from the point where the induced field is calculated. If the subdivision were such that the volume elements are equal in size, then the entire specimen would be subdivided into specified number of equal volume elements. This would result in the obvious inappropriate splitting as illustrated in the previous section. On the other hand noting that the divided susceptibility values would be proportional to the volume, if the shape of the volume elements is spherical, then the susceptibility would be a product of $(4\pi r^3/3) \cdot \chi_v$ with r being the radius of the spherical, divided element and χ_v being the volume susceptibility of the homogeneous specimen. Then, it is noteworthy that the r^3 factor in the numerator is as much cube dependence as the R^3 factor in the denominator. Note that the 'r' and 'R' are not related by any specified ratio. Therefore, same 'r' value occurs for the varying 'R' values in the case of equally subdivided elemental case. If the ('r' / 'R') value can be held constant, then all subdivided elements along a radial vector with the same θ value can all contribute the same value irrespective of the variation of 'R'. In such a case, with these criteria of r/R constant, would it be possible to subdivide the entire volume into smaller elements in such a way that the elements are all closely packed to account for the undivided material within that shape? If such a coincidence occurs, then possibly there can be a way out of the complication due to splitting dipoles. Then how many dipoles 'n' can be closed packed along a vector R, θ and ϕ ?



Commensurate with the Susceptibility the magnetic moment \mathbf{M} would be in accordance

with the equation $\mathbf{M} = \chi_v \times \mathbf{H}$



r is the radius of the **spherical magnetized material** specifically demarcated.
 $(4/3) \pi r^3$ will be the spherical volume of the material at a distance R contributing at the point of origin in the illustration on the left

The equation for induced field based on a dipolar model would then be

$$\sigma = -2.855 \times 10^{-7} \times [(4/3) \pi r^3] \chi_v \times (1 - 3 \cos^2 \theta) / R^3$$

From the above equation it is obvious that along this radial vector with the specified polar angle if spherical volume elements of the material are placed such that they all have the 'radius- r ' to 'distance- R ' ratio the same, then every one of such sphere would contribute the same induced field at the specified point.

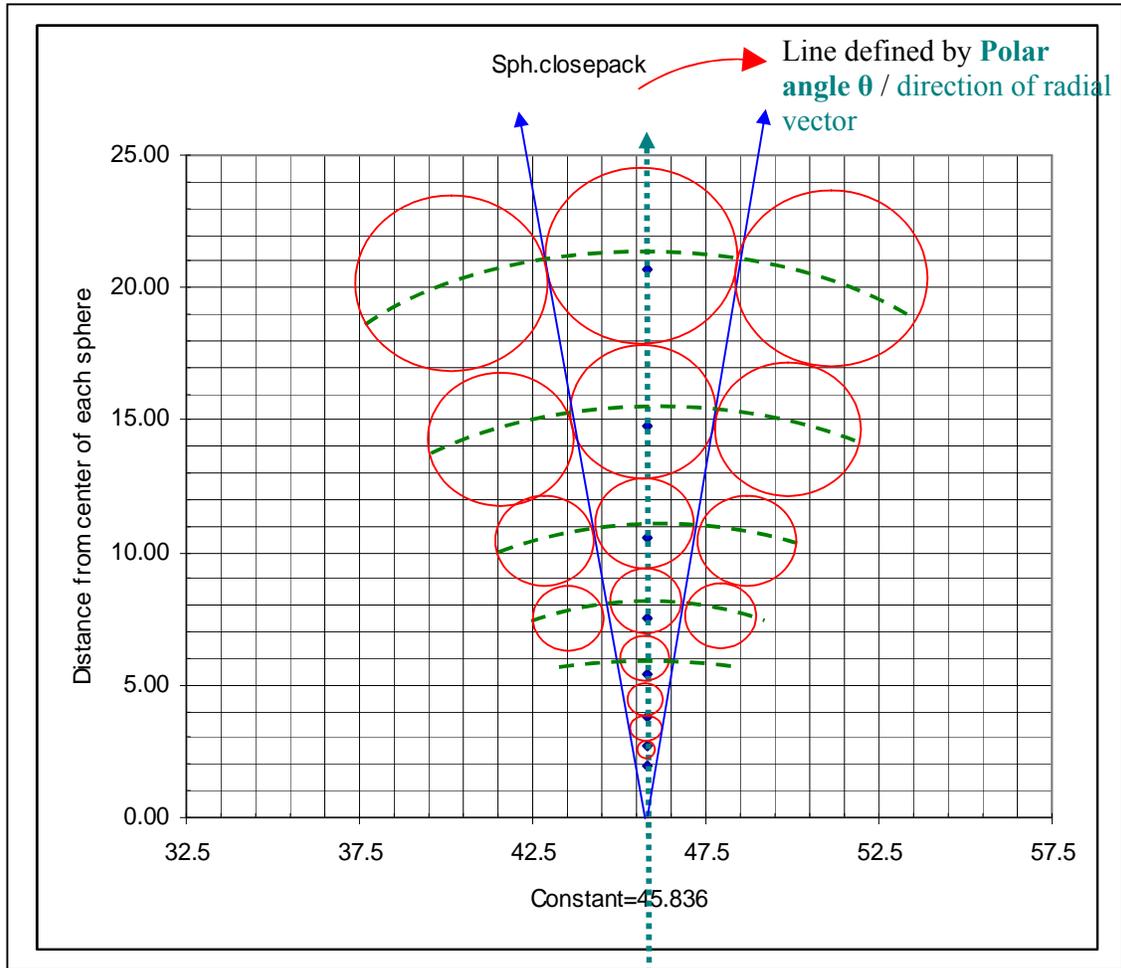
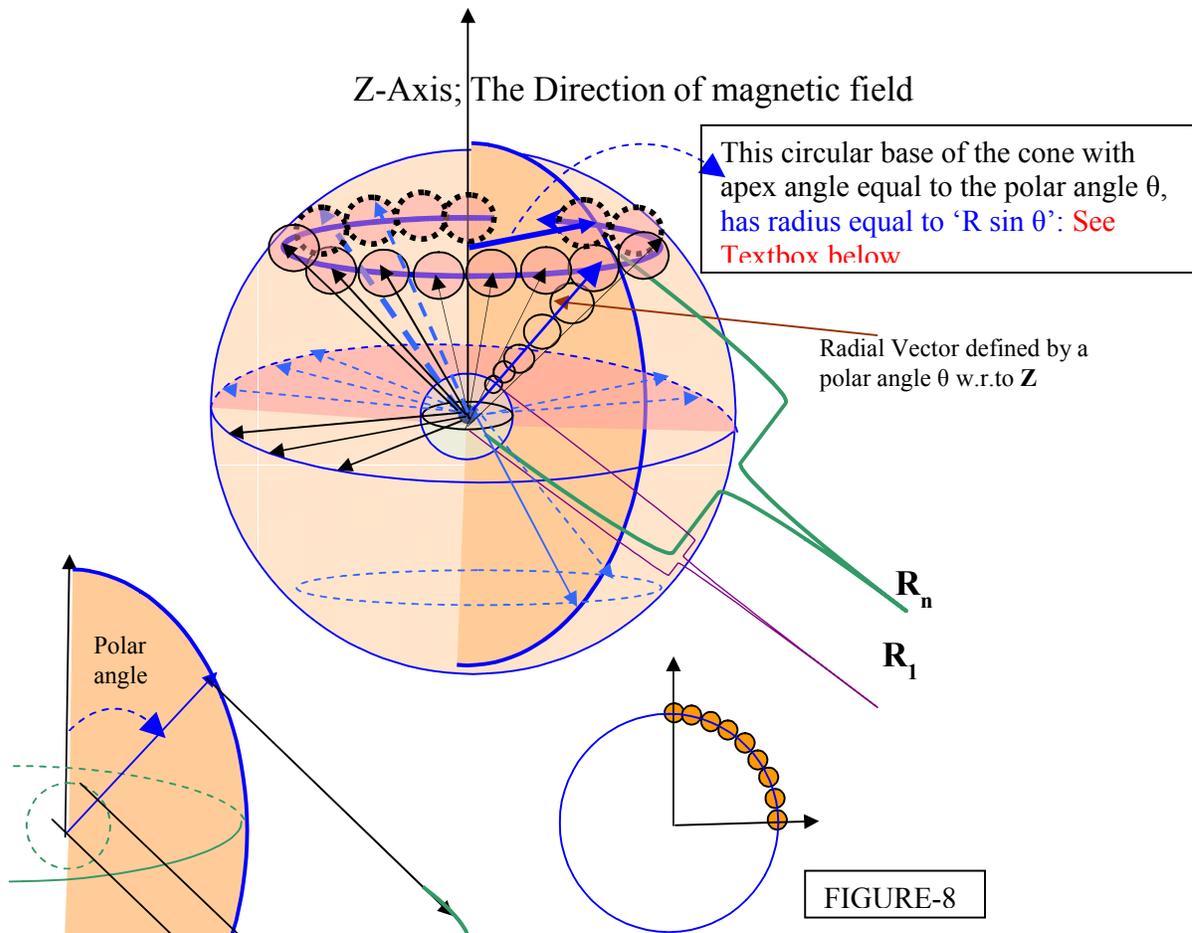


FIGURE-7

Quantitative ILLUSTRATION of Close packing with the constraint $r_i/R_i = \text{Constant}$

A Rotation by 360° results in a cone in conformity with the filling above and the cone is filled with the spheres closely packed. This is cone is a section of the full sphere and the sphere can be well envisaged with the closely filled spheres. The specimen then is left with the voids due to the regions not filled by the spheres. Hence, the material, in the actual specimen, corresponding to the amount filling the void must be taken into account and its contribution to induced field at the point.



Equation for calculating the number of spheres, the dipole moments, along the radial vector is as given 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”

For a sphere of radius =0.25 units, and the polar angle changes at intervals of 2 .5°

There will be 144 intervals. Circumference= 2π/4 so that the diameter of each sphere on the circumference = 0.0109028; radius = 0.0054514

$$C = R/r = 0.25 / 0.0054514 = 45.859779$$

$$[46.859779/44.859779] = 1.04458334$$

$$\text{Log}(1.0445834) = 0.0189431 \quad (r/R)^3 = 1.0368218e-5 = 0.000010368218$$

Using above equation ‘n’ along the vector length is calculated, for the direction with polar angle θ. Which is ‘σ’ per spherical magnetic moment x number of such spheres ‘n’.

$\sigma_\theta = \sigma \times n$. At the tip of the vector, there is circle along which magnetic moment have to be calculated. This circle has radius equal to ‘R sinθ’. The number of dipoles along the length of the circumference = $2 \pi R \sin\theta / 2.r = \pi R / r \sin\theta$. Again, (R/ r) is a constant by earlier criteria.

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 field 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 $= \sigma_{\varphi}^{i,\theta}$

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

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 $\sigma_{\varphi}^{\theta}$ 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 $[(2\pi R \sin\theta)/2r]$ 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

$\sigma_{\theta} = [(2\pi R \sin\theta)/2r] \times \sigma_{\varphi}^{\theta}$. 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 $= \sigma_{\varphi}^{i,\theta}$ For 'n' spheres $= n \times \sigma_{\varphi}^{i,\theta} = \sigma_{\varphi}^{\theta}$

Summed for all azimuthal angle values for the given polar angle $= \sigma_{\theta}$.

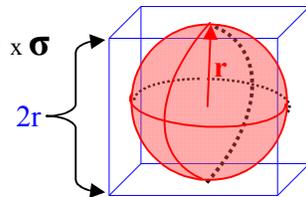
Summing Over all polar angles thus gives final total contribution from the specimen material corresponding to spherical filling $= \sigma$. Since the spheres at their respective points can be replaced by cubes with the side equal to the diameter of that sphere, there can be no further void to account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

$$(8 \times r^3) / (4/3 \times \pi \times r^3) = 1.909859. \text{ Final value } \sigma_T = 1.909859 \times \sigma$$

$$\sigma_T = [N_{INNER} - N_{OUTER}] \times (4\pi \times \chi_v) \text{ with } N_{INNER} = 0.3333 \text{ (stands for value for spherical cavity)}$$

From the above relation

N_{OUTER} can be calculated for the calculated σ_T



DEMAGNETIZATION FACTORS			
$a/b = m$		CALCULATED	STANDARD
0 / 3.0	= 0.0	1.000000	1.000000
0.3 / 3.0	0.1	0.854914	0.850804
0.6 / 3.0	0.2	0.744581	0.750484
1.2 / 3.0	0.4	0.582239	0.588154
1.8 / 3.0	0.6	0.469904	0.475826
2.4 / 3.0	0.8	0.388514	0.394440
3.0 / 3.0	1.0	0.328862	0.333333
4.2 / 3.0	1.4	0.244325	0.248803
5.4 / 3.0	1.8	0.189575	0.194056
6.6 / 3.0	2.2	0.151841	0.156326
7.8 / 3.0	2.6	0.124602	0.129090
9.0 / 3.0	3.0	0.104220	0.108709
10.5 / 3.0	3.5	0.085159	0.089651
12.0 / 3.0	4.0	0.070912	0.075407

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.

FIGURE-9A

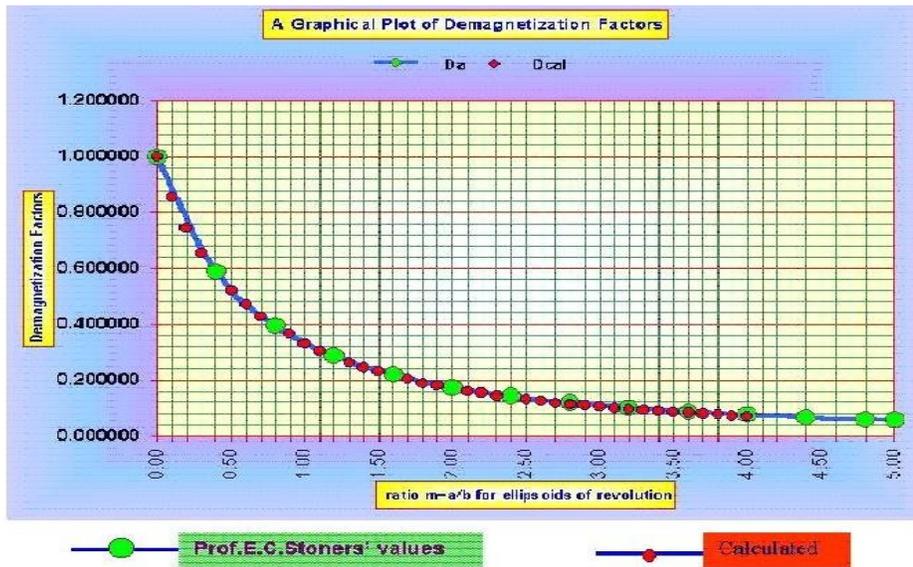


FIGURE-9B

The figures 9A & 9B, and the considerations related to the induced field distributions, calculations by point dipole approximation have been the subject matter in the contributions at several of the conferences and symposia, which are well documented, in the following websites, and the links specified in those WebPages:

- <http://saravamudhan.tripod.com/>
- <http://nehuacin.tripod.com/>
- http://www.geocities.com/inboxnehu_sa/conference_events_2005.html
- http://www.geocities.com/inboxnehu_sa/conference_events_2006.html
- http://in.geocities.com/saravamudhan2002/events_2007.html

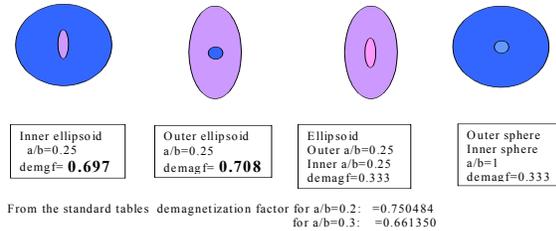


FIGURE-10

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 shapes and forms are considered which makes it possible, without any resulting complications in the calculation, to get values for factors, 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.

DISCUSSION OF THE CRITERIA FOR SUBDIVIDING

The contents of the figures 1, 3, and 4, and the materials included in Appendix-A would make evident the following consequence of splitting dipoles into equal parts and distributing them about the origin of the total moment. The simplest symmetrical criterion for distributing the 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 field 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 field 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 field 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 " $\Delta\omega$ " (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.

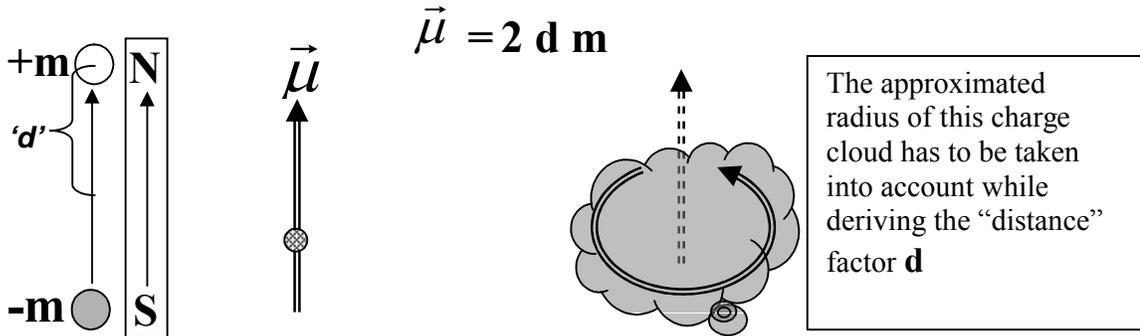
CONCLUSION

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 field 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.

APPENDIX: A - page1

Charge circulation, Magnetic Moment and the point dipole approximation

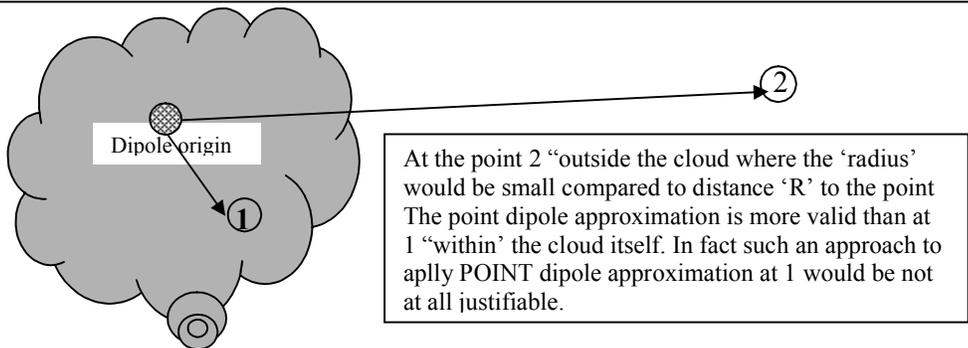


In case of either the electrical or the magnetic dipole moments a simple arrow can serve the purpose to indicate the presence of a “Dipole” as located at a given point ●



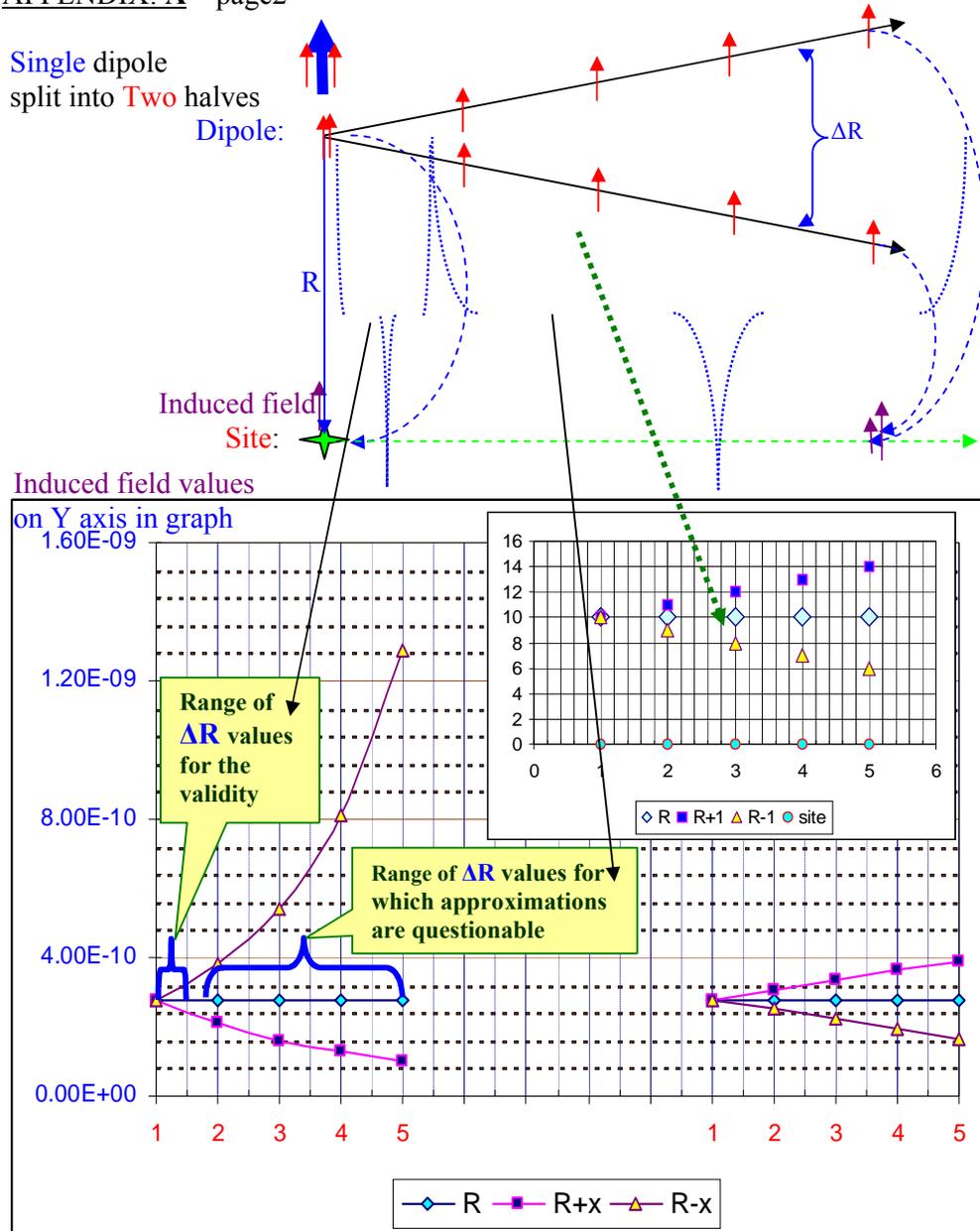
While considering the Field due to the dipole moment at ‘R’ it is possible to consider the two poles separately and find the contribution from each pole and sum up to get the total.

Instead of each time considering the poles of dipoles separately, it is possible to get an equation for this total at R by a single equation using the dipole moment. This implies that the distance d has to be considered while calculating the field at a distance **R**. It turns out that if **d ≅ R** then, the calculations result in unrealistic values. For validity, the value of **R >> d**. This means **R ≥ 10 • d**. This is referred to as the POINT-DIPOLE approximation. It is a consideration as to at what values of the distance **R** the given dipole can be arising from a single point and not from the consideration of the length **d** characteristic for the value of the moment **|μ|**.



At the point 2 “outside the cloud where the ‘radius’ would be small compared to distance ‘R’ to the point The point dipole approximation is more valid than at 1 “within’ the cloud itself. In fact such an approach to apply POINT dipole approximation at 1 would be not at all justifiable.

APPENDIX: A – page2

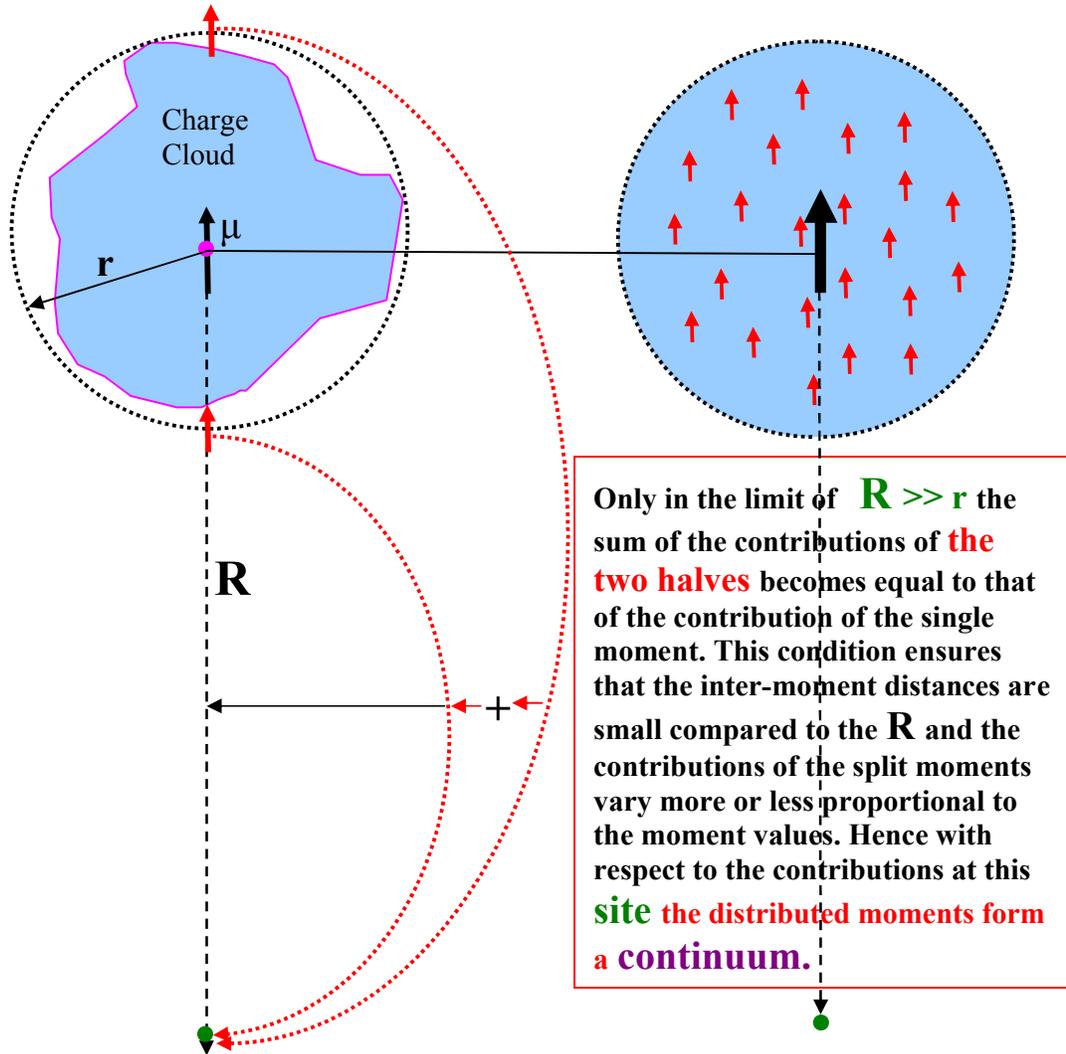


The INSET in the graph above is schematically enlarged in the drawing above which indicates how the single dipole is split and placed to have the same average distance as the un-split single dipole. Will the sum of contribution of the split halves be the same as the single un-split dipole? As seen in the left side of the graph, the contribution of the half placed below the average distance increases more rapidly with distance than the decrease of the contribution due to the half placed symmetrically above the average single dipole point. However, even when two split halves are considered, the effective magnitude of the vectorially added halves is the same as the un-split single dipole.

Materials given above in this SHEET should be added details to the considerations in SHEET-10 of the poster presented at the 6th NSC of the CRSI held in IIT/Kanpur during Feb. 2004: http://www.geocities.com/saravamudhan1944/crsi_6nsc_iitk.html

APPENDIX: A – page3

As pointed out earlier the induced field contribution at a distance R from the dipole varies as $1/R^3$. Therefore, the strength of the moment μ would be in the numerator, while the denominator would have the factor R^3 . The charge cloud which gives rise to this dipole moment is confined to a region which can be included completely within a sphere of minimum radius 'r', then the pictorially this situation can be envisaged as follows.



This is the detailed perspective of the contents of previous pages, and explains why for demagnetization factors, considering discrete distribution of magnetic moments would not be possible. That would be a question of calculating contributions from points within the cloud-region, at a point within the same region. The type of condition as above cannot be realized.