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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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Even when Spherically Shaped Single Crystalline Solid Specimens have been used for HR PMR measurements , for the subsequent interpretation of the Shielding Tensor parameters, it required a further calculation of intermolecular contributions to Shielding Tensor. These intermolecular contributions, when subtracted from the experimental shielding parameter values, could yield the truly and only molecular contributions which is of relevance for infering about the molecular electronic structure.

The question as to why a spherical shape was required, and, whether it would be possible to relax the stringency of this constraint has been the consideration of the presentations made (1) till now. Such deliberations led to the possibilities of calculating the induced field contributions inside a magnetized material by a simple summation procedure. It had also been shown that handling these types of calculations seem possible , for contributions only within the Lorentz ellipsiods, as well as, for the contributions from within the entire macroscopic specimen with shapes other than the regular ellipsoids of revolution (2).

At this juncture making progress with the question of arbitrary shapes as stated in the title of this abstract would require a consideration of the possibilities of the shape and location of the Lorentz semi micro volume element so that the intermolecular contributions can be disentangled from the total contribution unambiguously. This raises the issue of the microscopic averaging and the macroscopic averaging for arriving at the induced field at a point within the magnetized material. A discussion on the requirements seem due before actually proceeding with the calculations of this type and this context would at this juncture be highlighted and a strategy to be followed would be laid out in this presentation.

1. http://geocities.com/amudhan_nehu/graphpresent.html
2. http://geocities.com/saravamudhan1944/eenc_ampere_lille.html