CHEMICAL SCIENCES

Fragmenting the Total Moment of a Magnetized Specimen; the Scalar and Vector Potentials in Magnetism Revisited

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Some of the recent considerations on calculation of induced field distribution within a magnetized specimen required fragmenting the total moment conveniently for the point dipole approximation to be rendered more valid than what was hitherto possible. Then the definitions of the **H** field and the **B** field, which require invoking a Vector Potential, seem to becoming less tangible and in particular, to prescribe a procedure for use in chemical contexts requires sorting out this newly arising vagueness about these physical quantities. An effort would be made to clarify the kind of approaches and stand points to this particular procedure of dividing magnetic moments.

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Suggested reading:
http://www.ugc-inno-nehu.com/isc2009nehu.html
Dividing a Magnetic Moment and Distributing the Parts, can it ensure a Better Validity of the Point Dipole Approximation?
And also in the Proceedings of the 96th ISC, held at NEHU Shillong

http://www.ugc-inno-nehu.com/cmdays2011_gu.html
When A Magnetic Moment Is Subdivided, Do The Fragmented Moments Interact Among Themselves?

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The two kind of Electric charges, + and **–, can** occur as isolated charges.

Magnetic charges, the magnetic North And south poles occur as dipoles only; as poles equal in magnitude and opposite in nature (sign for the pole) with a well defined distance of separation; which means, magnetic poles always occur with a well defined magnetic dipole moment.

Electric dipoles are also encountered most often. Then the question of what keeps the charges (which can be isolated charges) separated, and, without neutralizing each other, is a question though not always simple enough to answer. The contexts of Chemical sciences can be content, if it is borne in mind, that a non conducting dielectric medium holds the charges separated and these electric dipoles arise as induced dipoles in a medium due to the presence of an External electric field.

In the context of the subject of chemistry, mostly what is important in atoms and molecules is the positively charged nucleus of Atoms with electrons in the outer orbits to compensate for the positive charge of the nucleus. With fixed atomic nuclear framework in molecules, it is the electron charges or the electron charge clouds which is all pervasive and the presence of due number of electron on an atom making that atom neutral in the molecule. When fractional electrons -by charge cloud descriptions- are moved from one atom to the next, then, a fractional positive charge is created due to the movement of fractional electron charge (resulting in uncompensated fractional nuclear charge). Then, a fractional negative charge is created on the neighboring atom since the positive nuclear charge of that atom is more than compensated by the inflow of electron charge. Thus, a positive charge only means a electron charge moving away from an atomic centre rather than a movement of positive charge. This can be in turn said to be a delocalization of electron charge cloud.

The static electric charges (the source charges) result in Forces on test charges at a distant point the coulombs law governing the magnitude of such forces is most often used in chemical science and hence c an be considered familiar as far as the descriptions in the present circumstances. The equations relating the amount of charges, forces, electric fields and the electric potential at a distant point due to the source charges, are all well described with static charges and conceptually it is not too difficult in chemical sciences to visualize as and when necessity arises.

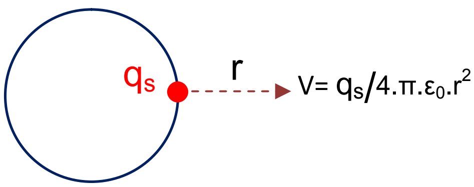
It is necessary to consider flowing (moving unlike static) charges to account for the magnetic fields. It is quite common to consider bar magnets or horseshoe shaped magnets to realize a magnetic intensity i.e the magnetic field in vacuum (no materials present where the magnetic field is supposedly measured). In this case, no flowing charges are required to explain the existence of North Pole and South Pole of certain strength. Magnetic lines of forces can be visualized for bar magnet. When the magnetic field (the magnetic intensity) is such that it is between magnetic North and South Pole faces, then there is the possibility of realizing uniform magnetic fields within certain volume/area or even along a line. But between the magnetic pole faces if a material is placed (which does not have inherently any magnetic moments within itself) then the presence of the magnetic intensity would cause or induce a magnetic moment and the magnetic field at such points (where the material is also present) would be additively the magnetic intensity with the induced magnetic moment. The topic of this contribution, fragmented moments, refers to such contexts of magnetic fields within magnetized specimen. Such induced magnetic moments within materials are usually explained using the charges in the material acquiring motional characteristics due to forces exerted by magnetic intensity. Which means, magnetic dipole moments arise due flowing charges: or, in other words, due to the currents set up inside the material due to the external magnetic field intensity.

The electro static quantities which arise due to the presence static charges and there can be equations relating one such quantity to the other. That is static charges (source charges) exert forces on test charges placed in the neighborhood; and account for the presence of electric fields, generate electric potentials at a distant point where a test charge can be placed. Then how would these electro static quantities, manifest when the charges are moving, namely, when flowing currents are present. Electrostatic force and field are vector quantities; where as the electrostatic potential is a scalar quantity. All these quantities are defined at a point relative to the static source charge. When the source is moving how this point does stand specified and is it possible to define time independent measurable quantities analogus quantities for the case of moving charges? Is magnetic moment (or a magnetic field) arising due to such currents a time independent measurable quantity - an electro dynamic property? When do the scientists preoccupied with chemical problems have to be concerned about these details for the electro-static and magneto-static quantities – concepts in physics?

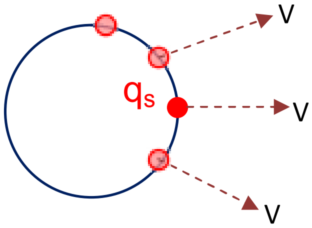
Then is it a converse that moving magnetic dipoles, that is, time dependent changes in magnetic flux, can generate electrical voltage – namely the phenomenon of electromagnetic induction?

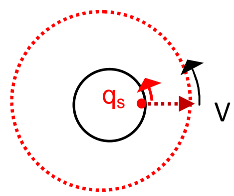
When all these queries, which arise in chemical sciences, have to be answered compactly, it becomes necessary to transcend to the subject matter of physics. The popular Maxwell equations in electrodynamics are a familiar topic in physics. These equations require the foundations in mathematical physics to retain the compactness for handling this phenomenon and thus make it a remote subject to chemistry.

Those who can revise their school physics would be able to get the grip again on the potential energy of a test charge placed in the neighborhood of a source charge. Tthe derivation of the expression for potential energy requires this to be the work done on the test charge (negative of the potential it gains to do work). This is as far as the significance of electrostatic potential at point, which enables the calculation of the electrostatic field at the point as the derivative (gradient) for the variation of the potential at that point. However, the necessity and significance of the magnetic vector potential is not immediately evident though similarity of magnetic field derivable at a point from the vector potential is stated along with the definitions. There have been several efforts in the available tutorials to explain the physical significance, which probably helps the students at university-level physics courses. Appealing to the students of chemistry is still not popular. Hence an effort is made to explain this concept in more elementary steps and simpler terms. This was found wanting in order that the demagnetization effects and the nuclear shielding (*Nuclear Magnetic Resonance chemical shift values are measures of nuclear shielding; this shielding is an electronic property of the nuclei in presence of an external magnetic field*) can be appreciated better for the interpretations in chemical contexts. This can also add a substantial clarity in the subject of physics as to the microscopic and macroscopic aspects of the magnetic fields within the magnetized specimen. The descriptions may be found supplementary to the chapters on Magneto statics as in the books on Electrodynamics / Electricity and Magnetism *(by 1. Gupta, Kumar & Singh and 2. B.B.Laud).* The book with title “Concepts in physics” by H.C. Verma does not contain descriptions on Magnetic Vector Potential. In this book, the chapter on ‘Magnetic Field’ brings about clearly the relation between electric field and magnetic field; the chapter on ‘Magnetic Field Due to Electric Current’ the emphasis is on magnetic field as resulting from moving charges (flowing currents); Magnetic Scalar potential due to a dipole is described in the chapter on Permanent Magnets. However, the differences between magnetic field, magnetic (dipole) moment, induced fields and moments, the diamagnetic induced moments as the cause of “magnetization” and the permanent dipole moments of particles with intrinsic spins and their reorientation as the of “magnetization” phenomena are all described in one place but appear scattered, even when the chapters are well organized in a book. That the Magnetic Scalar potential is useful mainly when there are no flowing currents is well emphasized in the book by B.B. Laud in the chapter on magneto statics on page 129 in the beginning of the section introducing Vector Potential. It is essential that in these books while describing clearly the classification of the currents in material media, the various physical quantities related to magnetism must find a detailed delineation of where which property and which physical quantity becomes significant why the others have not so much of a significance with a comparison of the situation in electrostatics. This contribution is to find how to fill the gaps as found wanting in the currently prescribed standard text books in view of the fact the dividing the magnetic moment seems conveniently possible for the additive characteristics of the consequences. For this examining in detail as to what is the status of the interaction among moments when a total moment is divided and treating the resulting fragments as independent non-interacting moments.



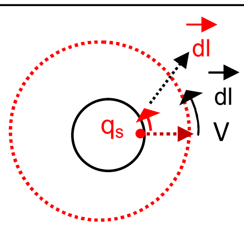
Consider a source charge q_s, can be an electron, placed at the circumference of a circle. The potential energy (a scalar) of unit test charge is ‘V’ at a distant point ‘r’ from the charge. Or simply stated, the potential at that point is V due to the charge q_s.





If the static charge is placed at other points along the circumference, then the point where the same potential ‘V’ can be experienced by a test charge will also be displaced as shown in the figure.

If the charge moves with uniform speed along the circumference, then the point at distance ‘r’ where the potential of magnitude ‘V’ exists also should be moving with the same speed all the time keeping the distance r from the source charge. Thus when such a current flows, there is a circle described by the locus of points where the potential ‘V’ exists due to the moving charge causing the current. This potential, which is a scalar quantity, has to be associated with a direction for its displacement, which is along the tangent to the circle at the point where ‘V’ is the potential.

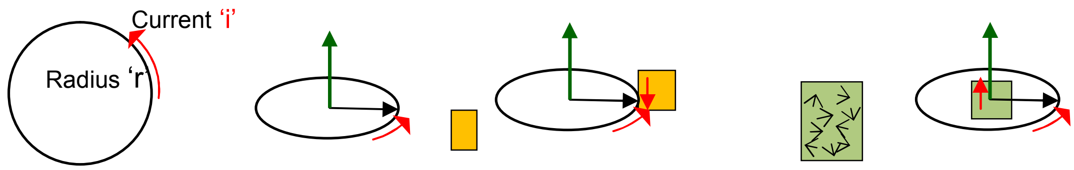


For the charge q_s flowing along the circumference, the current can be the q_s . $[2\pi r_c / T]$ with r_c and T time period of uniform rotation. This is simply the definition of current that it is the rate of charge flow. The term within brackets is the velocity. And the $2\pi r_c$ is the circumference of circle. And, for any closed loop the length is $\oint dl$ which is a $\vec{\text{vector}}$ tangential to circle at the point where the charge is instantaneously present. This assigns the direction for the velocity with $[2\pi r_c / T]$ as the magnitude.

This depicts the scene where the potential (at a point) ‘V’ is rotating with the velocity correspondingly with the circumference of the larger circle divided by T for the magnitude and a $\vec{dl}$ vector on that circle defines a direction. Thus the scalar quantity in electrostatics has acquired a directional property and hence may now be Vector potential. Thus vector potential would correspond to the static scalar potential when the test point is always viewed with reference to the instantaneous location of the moving source charge. http://hyperphysics.phy-astr.gsu.edu/hbase/magnetic/magvec.html

When the various currents that can be present in a material medium are considered, the following nomenclature probably would stand a better appeal for simple minded approaches.

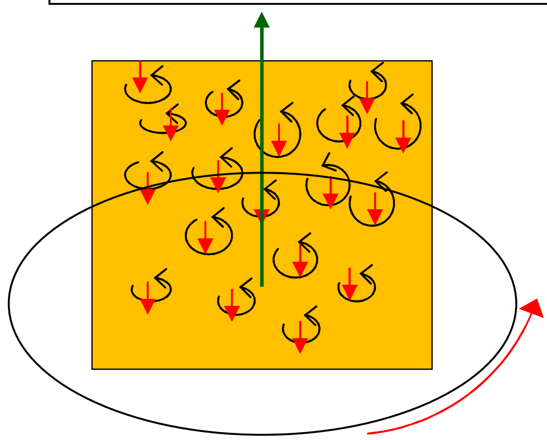
If a current 'I' flows through a circular path with a certain radius,



Diamagnetic substance gets induced with a dipole moment opposite to the field direction

Substances with randomly oriented permanent tiny moments undergo an alignment of these moments and acquire magnetization parallel to the magnetic fields

In the case of diamagnetic substances tiny atomic currents are set up when external field is applied and these tiny atomic currents induced magnetic moments.



The atomic currents can be due circulation of charge clouds or partial charges clouds and these are magnetization currents. It has also been pointed out (for example by C.P.Slichter) that even though the magnetic fields due to inherent circulation of electrons in orbits can be producing magnetic fields larger than the laboratory fields, such fields are not encountered in materials because of the phenomenon of orbital quenching.

True current is due to transport of charges (electrons) along the circular path. And the magnetic Vector potential for the Magnetic Intensity due to the true current must correspond to the circulating charges.

The Magnetic Induction Field or the Magnetic Field is due to the total current. And hence the Magnetic Vector potential must correspond to the total current flowing.

There is other class of currents mentioned in the text books, but in the present context of fragmented moments, these two types are most appropriate.

For Magnetic induction **B**, $\nabla \times \mathbf{B} = \mu_0 \mathbf{J}_{\mathbf{Total}}$

J stands for current density. Similarly $\nabla \times \mathbf{M} = \mu_0 \mathbf{J}_{\mathbf{atomic}}$

and, for Magnetic Intensity $\nabla \times \mathbf{H} = \mu_0 \mathbf{J}_{\mathbf{True}}$

Conventions and symbols in accordance with contents of pages 173-174 of *"Electrodynamics" by S.L.Gupta, V.Kumar, and S.P.Singh, Pragati Prakashan Publishers.*

Discussion at cmdays2011 was to emphasize the fact:

The Magnetization is merely the appropriate sum of the atomic moments induced in the specimen. The magnetization M does not include the interaction between the atomic microscopic moments. The total magnetization of the macroscopic specimen is conveniently fragmented for reasons of simplicity to calculate out the demagnetization factors. When the interaction between the microscopic atomic moments is considered the result is a specimen shape dependent geometric factor is obtained as premultiplying factor to M. And, this premultiplying factor precisely happens to be the required Demagnetization factor. Thus it is the non interacting moments which are contributing to Magnetization and fragmenting them conveniently does not bring in complications of any kind.

As quoted from the presentation file for cmdays2011:

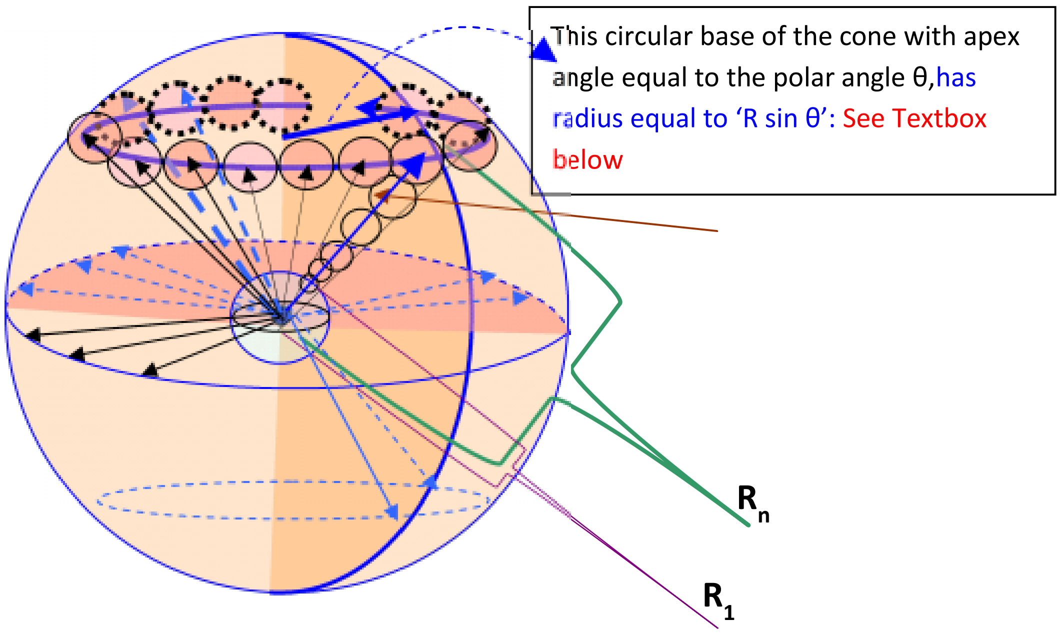
It is to be pointed out at this juncture, the total induced field values at a point within the spheroidal specimen results only in a shape (and not the size) dependent pre-multiplying factor to the value of the induced moment (generated by the interaction with external field). It would be true that the individual elemental moments interact among each other but what matters is the effective total interaction. It is only in a spectroscopic analysis as for the Proton Magnetic Resonance Spectroscopy, it is possible to demarcate the intra molecular versus the intermolecular around a particular site and distinguish the strengths and significance of the long-range & short-range interaction scales. And, disentangle the microscopic and macroscopic consequences and observe the effects distinctly as if these are two different physical quantities even though it is all induced fields.

In the Appendix-1 (next page) the picture depicts the way the fragmenting and close packing is achieved for calculating demagnetization factors. In view of the explanations, in the early pages, to differentiate various types of currents, and the expressions for quantities, M, H and B in terms of appropriate type of current, it should be obvious for purposes of chemical sciences that viewing the fragmentation patterns for the demagnetization factor calculations is entirely in concurrence with the terms and physical quantities used in Electrodynamics (electricity and magnetism). An appreciation of this fact would encourage the adaptation of the summation technique in several other chemical and biological contexts confidently.

Refrences:

1. *The Theory Of Magnetism Made Simple,* by Daniel Mattis, World Scientific, London, 2006, ISBN 981-238-579-8 (pbk)
2. *Electrodynamics,* by S.L.Gupta, V.Kumar, and S.P.singh, Pragati Prakashan, Meerut (U.P.), Eighth edition, 2005 ISBN 81-7556-868-2
3. *Concepts of physics,* by H.C.Verma, Vol.2, Bharati Bhavan, New Delhi, 2008, ISBN 10:81-7709-232-4, ISBN 13: 978-81-7709-232-5
4. *Principles of Magnetic Resonance,* by Charles P.Slichter, Harper & Row, New York, 963, Library Congress catalogue Number 63-11293. Particularly pages 65 &66 with Section 4.2 on Experimental Facts About Chemical Shifts, Section 4.3 on Quenching of Orbital Motion.
5. *http://www.ugc-inno-nehu.com/cmdays2011/*
6. *http://www.ugc-inno-nehu.com/cmdays2011_gu.html*

APPENDIX-1



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.