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**A DYNAMIC ENSEMBLE MODEL
FOR
INTENSITY PARAMETERS IN CHIROELECTRONIC SPECTROSCOPY**

by

Katarzyna M.E. Miedzinska

A thesis submitted to the
Faculty of Graduate Studies and Research
in partial fulfillment of
the requirements for the degree of
Doctor of Philosophy
Department of Chemistry

Carleton University
Ottawa, Ontario
September, 1992

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INTENSITY PARAMETERS IN CHIROELECTRONIC SPECTROSCOPY**

submitted by Katarzyna M.E. Miedzinska, M.Sc.
in partial fulfillment of the requirements for
the degree of Master of Science

Thesis Supervisor

Chair, Department of Chemistry

Carleton University

September, 1992

ABSTRACT

Polarized spectroscopy requires a model containing clear selection rules for both the sign and the intensity of spectra. The covering operator requires at least four dimensions in order to contain all the experimental observables. Dirac generated a Schroedinger equation from a four-dimensional Lagrangian that contained two conjugate Hamiltonians and was compatible with relativistic mechanics. A frame of reference convenient for chiral spectroscopy was designed and an atomic structure with a geometric relevance was constructed. Dirac's equation was used to construct the ideal geometry that contains all the experimental observables. This ideal geometry is the Moebius locus. The minimal set of eight Moebius Loci consists of four conjugate pairs of loci. Each pair is a natural coordinate axis of the event space. The minimal parent object of this set of Moebius Loci is a four-dimensional non-orientable Klein surface. The infinite group was established from the operations describing the Klein surface and an infinite number of Moebius rotations. Magnetic and electric representations for both the object and the probe were developed from the group and a three-dimensional Young Volume was established in order to allow product multiplication of the representations. Thus selection rules have been made available for polarized spectroscopy and a method for pulling out intensity parameter information has been acquired.

ACKNOWLEDGEMENTS

I would like to extend my appreciation to the Department of Chemistry and Faculty of Graduate Studies of Carleton University, without whose unfailing support this work would not have been completed. Their understanding of difficult and extenuating circumstances and willingness to accomodate my requirements was above and beyond their mandate.

I would also like to extend my thanks to my supervisor, Dr. Bryan R. Hollebone, for talking me into trying to work under these circumstances and for convincing me that anything was possible. I appreciate his patience and willingness to wait while I worked things out for myself. I would also like to thank Pam Wolff for acting as liason with the department on more occasions than I care to remember.

I appreciated the input from Dr. John Donini of Energy, Mines and Resources, Coal Research Laboratories (CRL), who often took on the role of sounding board. I would like to thank Eric Hollebone, also of CRL, for his painstaking efforts in creating the computer generated figures of the required functions. The remaining figures are courtesy of Glenn R. Lisle of GRL Desktop Design, whose facility with CorelDraw was greatly appreciated.

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I. INTRODUCTION

I.1. Spectroscopy and Polarized Light

The sharp, ordered lines of the emission spectrum of atomic hydrogen stimulated the development of quantum mechanics. The success of quantum mechanics in predicting the energies of these lines has made it an accepted model for describing the structure of atoms. However, the information from spectroscopy is much richer than simply energies of states. The probing light can be prepared with a known orientation phase and sense of rotation giving a known handedness or "*chirality*" to the beam. ¹ If the chiralities are equal, linearly polarized light results, if they are unequal, a circularly polarized beam is established. At the same time, the sample can be immersed in either or both electric and magnetic fields. ² In the simplest case the electric field at the sample may originate internally due to asymmetric electronic structure of an enantiomer. ¹ This leads to Stark or Zeeman spectra with unpolarized light and to Electric or Magnetic Circular Dichroism (ECD or MCD) spectra with circularly polarized light. ^{3,4,5,6} These techniques can be applied to

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¹ R. Faber, Differential Geometry and Relativity Theory, Pure and Applied Mathematics Series, Marcel Dekker, Inc. New York, 1983.

² E.U. Condon and G.H. Shortley, Theory of Atomic Spectra, Cambridge University Press, Cambridge, 1935.

³ a P.J. Stephens, *Inorg. Chem.*, **4**, 1690, 1965.

b P.J. Stephens, *J. Chem. Phys.*, **43**, 4444, 1965.

⁴ P.J. Stephens, *J. Chem. Phys.*, **52**, 3489, 1970.

⁵ P.J. Stephens, *Ann. Rev. Phys. Chem.*, **25**, 201, 1974.

⁶ P.J. Stephens, *Adv. in Chem. Phys.*, **35**, 197, 1974.

both absorption and emission methods. The dichroism spectra are recorded as differences in intensities between left and right circularly polarized light, generated alternately in one beam. ⁷

If observed carefully, the experiment yields information about the available degrees of freedom and limitations to that freedom for both light and matter. By allowing the experiment, and therefore Nature to guide the model, stringent requirements may be placed on the model development. It is possible to describe these phenomena in abstract algebra, as *ad hoc* extensions of traditional quantum mechanics. ^{2,7,8} However, there is a keenly felt need for an alternative geometric form which could express the observed polarizations, intensities and halfwidths directly in terms of the chiral topology of the electronic structure of atoms and molecules. ⁸ The two approaches can be compared to two methods of exploring an unknown landscape. The algebraic method is differential, in which the territory is discovered stepwise. The topological method establishes the basic global map first and is able to guide local exploration in terms of its most prominent features.

The traditional MCD description allows a left-handed photon to probe only a left-handed structure. However recent experimental evidence clearly shows that this is not so. ⁹ A series of transition metal model compounds was designed in order to investigate the possibility of the existence of magnetic hypersensitivity.

---

⁷ S.B. Piepho and P.N. Schatz, Group Theory in spectroscopy, John Wiley & Sons, New York, 1983.

⁸ U. Fano and G. Racah, Irreducible Tensor Sets, Academic Press, New York, 1965.

⁹ P. Wolff, MSc Thesis, Carleton University, 1990.

The series, $M-O-CO-C-X$ was designed with three concerns in mind; the effect of the molecular medium with respect to the inertial, magnetic and electric properties.

The ligand exchanged in the series was located far enough away from the small compact f orbitals of the metal atom that the only inertial effect of the electron mass felt by the metal atom was that of the first oxygen atom. The ligands chosen were of similar diamagnetism in order to maintain a constant magnetic inductance of the molecular background. The changes at the ligand were less than 1% of the magnetic properties of the unpaired electron on the metal. Therefore only the electron density in the p orbitals of the bound oxygen was affected by exchanging the outer X ligand.

The experimental results indicated a linear relationship (FIGURE I-1) between the electronegativity and the differential absorbance. At the highest ligand electronegativity the p orbitals of the bound oxygen are contracted, resulting in a minimal overlap between the metal and entire ligand. This small overlap has the least effect on the internal orbitals. By exchanging the ligand to one of lower electronegativity the overlap was allowed to increase and interfere with the metal f orbitals. The MCD intensity decreased and eventually changed sign. It is clear therefore that a left-handed photon is indeed capable of probing both left- and right-handed structures.

The purpose of this thesis is to examine the available experimental evidence and devise a description of the interaction between matter and polarized light which allows such probing to take place.

FIGURE I-1a Plot of χ_L vs MCD for 3 Nd(III) complexes

FIGURE I-1b Plot of χ_L vs MCD for 3 Sm(III) complexes

I.2. Polarized Spectroscopy

The development of polarized spectroscopy as a viable experimental and research tool spanned over a century and a half and involved many of the best-known figures of the day. Biot, Fresnel, Faraday, Maxwell, Cotton, Werner, Rosenfeld all contributed to the development of the technique. The phenomenon of polarized light was first observed in 1808 by Malus, who passed a single beam of light through a quartz crystal and observed the exit of not one but two beams. The major developments were:

1808	E.L. Malus ¹⁰	Polarization of light
1811	D.F. Arago ¹¹	Optical activity proportional to wavelength
1815	J.D. Biot ¹²	Optical activity of some organic molecule
1819	A. Fresnel ¹³	Transverse wave model for light
1846	M. Faraday ¹⁴	Magnetic optical activity

---

¹⁰ E.L. Malus, Mem. Soc. d'Arceuil 2, 143, 1808.

¹¹ D.F. Arago. Mem. Inst. 12, 93, 1811.

¹² J.B. Biot, Ann. Chim. Phys. 4, 90, 1815.

¹³ A. Fresnel, Ann. Chim. 10, 288, 1819.

¹⁴ M. Faraday, Phil. Mag. 28, 294, 1846.

1847	W. Haedinger ¹⁵	Discovery of circular dichroism (CD)
1865	J.C.Maxwell ¹⁶	Electromagnetic nature of light
1874	J. van't Hoff ¹⁷	Explanation for chiral carbon
1893	P. Drude ¹⁸	Optical rotary dispersion (ORD)
1895	A. Cotton ¹⁹	CD in solution
1911	A. Werner ²⁰	Optically active inorganic complexes
1928	L. Rosenfeld ²¹	Quantum model of optical activity
1955	H. Rudolph ²²	First commercial ORD spectrometer
1960	M. Grosjean ²³ M. Legrand	First commercial CD spectrometer

---

¹⁵ W. Haedinger, Ann. Phys. 70, 531,1847.

¹⁶ J.C. Maxwell, Phil. Trans. Roy, Soc. London 155, 459, 1865.

¹⁷ J. van't Hoff, Arch. Neederland Sci. Exact. Nat. 9, 445,1874.

¹⁸ P. Drude, Ann. Physik, 50, 595, 1893.

¹⁹ A. Cotton, Compt. Rend. 120, 989, 1895.

²⁰ A. Werner, Chem. Ber. 44, 1887, 1911.

²¹ L. Rosenfeld, Z. Physik 52, 161, 1928.

²² H. Rudolph, J. Opt. Soc. Am. 45, 50, 1955.

²³ M. Grosjean and M. Legrand, Compt. Rend. 251, 2150, 1960.

The development of Circular Dichroism (CD) and Optical Rotary Dispersion (ORD) spectrometers took place in a manner often seen in the research world, in which the technology for the observations outreaches the theoretical understanding of the phenomenon involved. The science of spectroscopy received considerable enlightenment with the development of quantum physics in the first quarter of the twentieth century. As this same century draws to a close, the environment is once again that of the first quarter, where the technological world has supplied science with the tools of Magnetic Circular Dichroism (MCD) and Magnetic Vibrational Circular Dichroism (MVCD), with the possibility of Electro-Magnetic Circular Dichroism (EMCD) and Electro-Magnetic Vibrational Circular Dichroism (EMVCD) already evident, and no comprehensive theoretical basis for assessment of experimental results.

The need for a comprehensive model for chiroelectronic spectroscopy is indicated by the potential of the spectroscopic techniques involved. Polarized spectra of all forms of matter are rich in tensorial information in all wavelength ranges. If the orientations of the sample and of the external fields are deliberately controlled, then irradiation with plane or circularly polarized light can yield unique, directional patterns of absorption or emission. ^{7,24,25,26}

-
- ²⁴ G. Herzberg, Molecular Spectra and Molecular Structure,
 I Spectra of Diatomic Molecules;
 II Infrared and Raman Spectra of Polyatomic Molecules;
 III Electronic Spectra and Electronic Structure of Polyatomic Molecules, D. Van Nostrand Company, New York, 1967.
- ²⁵ A.B.P. Lever, Inorganic Electronic Spectroscopy, 2nd ed., Elsevier Science Publishers, Amsterdam, 1986.
- ²⁶ D. Shaw, Fourier Transform NMR Spectroscopy, 2nd ed., Elsevier Science Publishers, Amsterdam, 1986.

These patterns are related to the structure of the sample material at the site of the interaction with radiation. ^{7,27} MCD in particular is an outstanding research and commercial tool due to its high resolution, high precision, ease and expense (or lack of) of sample preparation, and user-friendliness due to a high degree of automation. Although the application of MCD for identification and quantification purposes is clear and already implemented ⁷ it is not being utilized to nearly the degree it should be for structural and reaction mechanism studies. This is primarily due to the aforementioned lack of a theoretical basis for the interpretation of results. There is an inability to assign tensorial observables or to uniquely assign half-integer systems. This was recognized by Heisenberg in 1926, but not pursued, although Bethe did try to reinsert tensorial information in 1929. ²⁸

---

²⁷ S.F. Mason, Molecular Optical Activity and the Chiral Discrimination, Cambridge University Press, Cambridge, 1982.

²⁸ F. A. Cotton, Chemical Applications of Group Theory, Interscience Publishers, New York, 1963.

I.3.   Magnetic Circular Dichroism Spectroscopy

I.3.i   The MCD Experiment

The experiment consists of random light being directed through a polarizer such as a nicol prism, producing a plain polarized ray at a 45° angle to the horizontal. The light is propagated along the axis which is chosen to be the main axis of quantization, the z -axis (FIGURE I-2). This light is bending both left- and right-handedly and so is degenerate along the y -axis. The experiment has therefore decreed a degeneracy in one axis, that is in one of the dimensions. This is the first indication that there is a requirement for an extra dimension in the space that the experiment is taking place in.

The modulator creates a time-dependent double ray which is right-handed half the time and left-handed the other half of the time. The ray is then passed through the sample, which is distorted by the external magnetic field so that any rotational translation becomes a helical translation. The helical light wave does work upon an electron along a helix of the same hand. The result is a changing intensity at the photomultiplier tube, which cannot distinguish between the right- and left-handed light until it is coupled to the modulator by means of a lock-in amplifier which then recovers the signal. The analyzer, a second prism, then measures the amount by which the sample has rotated the plane of the light beam by being rotated itself until a null reading is obtained. The angle by which the analyzer is rotated is the conjugate of the angle by which the sample rotated the beam. ¹¹

FIGURE I-2 The MCD Experiment

Modern MCD experiments measure the difference in absorption of right and left circularly polarized (CP) light.^{5,6} The electric and magnetic field $\mathbf{E}$ and $\mathbf{H}$ of circularly polarized light of angular frequency $\omega = 2\pi\nu$ is supposed to propagate through the medium in the $+z$ direction through the absorbing medium are of the form :

$$E_{\pm}(z,t) = E_0^0 \exp \{ i\omega (t - \Delta \hat{n}z/c) \} (i \pm j) \quad (\text{I.3-1})$$

$$H_{\pm}(z,t) = (\Delta \hat{n}/\hat{\mu}) E_0^0 \exp \{ i\omega (t - \Delta \hat{n}z/c) \} (\mp \hat{u} + j) \quad (\text{I.3-2})$$

where $+$ and $-$ specify right and left circular polarizations, respectively, $\hat{n} = n - ik$ is the complex refractive index, $\hat{\mu}$ is the complex magnetic permeability in the xy plane (which must be isotropic), and both $\hat{n}$ and $\hat{\mu}$ are functions of the external magnetic field. The intensity $I(z)$ of the light at z is the energy passing per unit time through unit area normal to the z axis and is given by the time average of the Poynting vector $(c/4\pi)(\mathbf{E} \times \mathbf{H})$.

For a transition $A \rightarrow J$, assuming J to be unpopulated at ambient temperature, the spectrum can be characterized by:

$$\Delta I(z) = (c/4\pi) (\Delta \hat{n}/\hat{\mu})_r E_0^{02} \exp \{ -2\omega \Delta k z/c \} \quad (\text{I.3-3})$$

$$I_{\pm}(z) = (c/4\pi) (\hat{n}_{\pm}/\hat{\mu})_r E_0^{02} \exp \{ -2\omega \Delta k z/c \} \quad (\text{I.3-4})$$

where $(\hat{n}_{\pm}/\hat{\mu})_r$ is the real part of $(\hat{n}_{\pm}/\hat{\mu})$. k is referred to as the absorption coefficient of the medium in the z direction and the circular dichroism Δk in this direction is the difference in absorption coefficients ($k_- - k_+$) given by:

$$\Delta k = -4/3\gamma N_a^0 \left\{ \frac{\mathcal{A}(A \rightarrow J)}{h} f' + \left[\mathcal{A}(A \rightarrow J) + \frac{\mathcal{B}(A \rightarrow J)}{k_t} \right] f^0 \right\} \quad (1.3-5)$$

where

$$\gamma = \pi^2 a^2 / \hbar n.$$

and the sign of the circular dichroism is chosen to conform to the convention used for natural CD.

To transform this phenomenological form into a theoretical model, $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{C}$ are interpreted as arising from the differential rotation of charge around the imposed magnetic field during the transition. This generates a preferred transient magnetic moment aligning with or against the field, resulting in a positive or negative differential signal respectively.

The resulting signal has three forms of differential absorbance of right- and left-handed light with respect to energy (**FIGURE I-3**). These signals are represented by the three MCD terms which are assigned the following meanings in describing the spectrum.

INTERPRETATION

es

gs

FIGURE I-3 The MCD Terms

They are given by: ⁶

$$\mathcal{A}(I \rightarrow J) = -\frac{g}{4d_A} \sum_{a^0, j^0, j^0'} [\langle a^0 | m_- | j^0 \rangle \langle j^0' | m_+ | a^0 \rangle - \langle a^0 | m_+ | j^0 \rangle \langle j^0' | m_- | a^0 \rangle \\ * [\langle j^0 | \mu_z | j^0' \rangle - \langle a^0 | \mu_z | a^0 \rangle] \delta_j^0 \delta_{j'}^0 \quad (1.3-6)$$

$$\mathcal{A}(I \rightarrow J) = -\frac{g}{2d_A} \sum_{a^0, j^0} \text{Re} \left\{ \sum_{k^0 \neq J} [\langle a^0 | m_- | j^0 \rangle \langle k^0 | m_+ | a^0 \rangle - \langle a^0 | m_+ | j^0 \rangle \langle k^0 | m_- | a^0 \rangle] * \langle j^0 | \mu_z | k^0 \rangle / \omega_{kJ}^0 \hbar \right. \\ \left. + \sum_{k^0 \neq A} [\langle a^0 | m_- | j^0 \rangle \langle j^0 | m_+ | k^0 \rangle - \langle a^0 | m_+ | j^0 \rangle \langle j^0 | m_- | k^0 \rangle] * \langle k^0 | \mu_z | a^0 \rangle / \omega_{kA}^0 \hbar \right\} \quad (1.3-7)$$

$$= -\frac{g}{4d_A} \sum_{a^0, j^0} [\langle a^0 | m_- | j^0 \rangle \langle j^0 | m_+ | a^0 \rangle - \langle a^0 | m_+ | j^0 \rangle \langle j^0 | m_- | a^0 \rangle] \\ * \langle a^0 | \mu_z | a^0 \rangle \quad (1.3-8)$$

The $\mathcal{A}$ terms are the result of transitions from a ground state which may be degenerate or non-degenerate to a degenerate excited state. The degenerate state is split by the magnetic field and the right-handed light is preferentially absorbed by the more stable level, the left-handed by the less stable level. This results in a difference spectrum that goes negative to the low energy side of the original transition centre and positive to the high energy side, crossing the axis at the band centre. The intensity of the $\mathcal{A}$ term is, to a first approximation, inversely proportional to the zero-field linewidth of the transition.

The $\mathcal{B}$ term is present for all transitions regardless of degeneracy, and is inversely proportional to the zero-field state separations $(\Delta E^0)^{-1}$. It has the same appearance as a $\mathcal{V}$ term, but can be distinguished based on the temperature dependence of the $\mathcal{V}$ term as the $\mathcal{B}$ term is independent of temperature. $\mathcal{B}$ terms are usually weak in comparison to $\mathcal{A}$ terms, with either a negative or positive sign.

$\mathcal{V}$ terms arise from transitions out of degenerate states which split in the magnetic field, although at low temperatures the number of molecules in the stabilized state is larger than that in the destabilized state. Therefore the absorption of the band is greater from the stabilized state and dominates the spectrum up to 100° C. A normal $\mathcal{V}$ term is a single strong negative or positive curve with a temperature sensitive molar ellipticity and is diagnostic of a degenerate ground state in a molecule.

In fact, there are not three terms but six, two of each type with signs reversed, as has been seen experimentally.⁹ The equations describing each of these terms must be tensorial in nature. They are traditionally solved by scalar techniques such as perturbation theory which cause them to lose all of their phase information.⁷ The standard phases are arbitrarily re-inserted to match the experimentally observed phases. The drawback to this empirical approach is that it does not allow the prediction of phases for new compounds.

MCD spectroscopy yields the same information as absorption spectroscopy in terms of the position (energy) of an absorption band. In many cases, however, the differential intensities offer considerably more information, because they carry the magnetic moment in addition to the square of the electric moment. In the first case,

it is often possible to detect bands in the MCD that were too weak to be detected by absorption spectroscopy; this occurs when the absorption is small, but the magnetic difference between the absorption of left and right circularly polarized light is relatively large. When two transitions overlap in the absorption, MCD has the possibility of resolving them, as they may have opposite magnetic properties and hence MCD sign.

Since the magnetic field splits the Zeeman levels of degenerate states, MCD can contribute new information that is not available at all from the absorption spectrum. Since $\mathcal{A}$ and $\mathcal{B}$ terms depend on the excited and ground state degeneracies respectively, bands can be positively assigned based on their degeneracies. In organic molecules in particular, this is useful for distinguishing singlet to singlet transition from singlet to triplet transitions.

I.3.ii   MCD and Perturbation Theory

The MCD phenomena is one of a transition between an initial and a final state. Traditional treatment considers only the states and not the actual process of the transition. The transitions are considered to be virtually instantaneous and the Franck-Condon principle is applied. Perturbation theory yields a set of mixing coefficients for the states which determine the sign of the phenomenon observed. The process is entirely empirical. No geometrical consideration or quantum mechanical requirements are involved. The right-hand rule is applied as an arbitrary choice of sign.

However the experimental evidence indicates an irreconcilable difference between the implications of MCD and absorbance spectra of transition metal compounds. The model compound series described earlier was subjected ⁹ to an absorption as well as an MCD analysis. Whereas the changing sign of the MCD spectra would indicate a need for the application of perturbation theory, the absorption spectra show no change (FIGURE I-4). This would indicate that remixing of initial and final states does not in fact occur. As both requirements cannot coexist, a new model must be developed which will account for this discrepancy.

The states involved in the absorption band have not changed, therefore the observed change of chirality in the MCD band must arise from a change in the type of transition taking place. ΔJ does not change in character, indicating the validity of the quantum numbers as the ligand is altered. The constant energy indicates the photon does not change. The operator must be different in some way. The changeable characteristics of the operator lie in the three components of the phase.

I.3.iii   MCD and Phase

In the MCD experiment, the phase must be understood to be a relative rather than an absolute phenomenon. The instrument locks the phase positions to the external force fields. The phase factor is a general term which must encompass all the experimentally observable properties of the atom that are also apparent in the photon probe, the χ , s and c .

FIGURE I-4 Absorption Spectra of Model Compound Series

It is possible to describe the phase conditions in terms of coherence and complementarity between the atom and probe as opposed to mixing coefficients. The experimental evidence indicates a change in chirality. This type of change may possibly arise out of a 2π coherence shift which is observable in the time constant. The model will have to have the potential to be able to discriminate such shifts. In order to do so all the information for the geometry must be in the operator, particularly with respect to time constants.

I.3.iv   MCD and the Transition Process

MCD is the phenomenon of a transient magnetic moment. Therefore if there is a change in the space within which an event takes place by electronic, magnetic or inertial means, the resulting transition takes place in a different way. The experiment described above is an observation of the transition moment from the ground state to the excited state. Such a transition has been considered instantaneous under the Franck-Condon principle. This assumption would allow no change in the structure of the system. However a change has been observed. Furthermore the Born-Oppenheimer principle states that only the electron moves, thus there is no transfer of momentum to the nucleus.

Experimental evidence shows otherwise. The experiment described above results only in excitation. It takes time ⁹ and requires a movement of electron vectors in space to accomplish this. Therefore both space and time are non-zero vectors. Therefore both the Franck-Condon and Born-Oppenheimer principles are not valid as inertia is involved. An electromagnetoinertial vector is being moved around the

space, requiring time to move through all the backgrounds of the molecule. The electric background observes the dielectric constant, the magnetic structure observes the diamagnetic constant, and by the masses one observed the inertial constants. If a characteristic is changed (for example by changing a ligand) and the molecule is probed again the process of moving through the background will take a longer or shorter time as the electromagnetoinertial vector is effectively moving through a different space. The change is seen as a change in sign and/or intensity. Thus in MCD one observes a change in phase factors as the same phenomenon occurs in different but related compounds such as those in the model series described. Thus the same ground and excited states with the same accurate quantum number descriptions in a series of compounds will undergo a different transition process and thus yield identical absorption spectra but different MCD spectra.

Each state is considered to have a + or - phase factor.⁷ Therefore changes in magnetic behaviour in MCD spectra from one compound to the next are seen to indicate a different state. Perturbation theory is applied and the new state is mixed with the old one. However it is known from the experimental evidence that the state is not changed, only the transition process. Therefore attention must be centred on the chemical processes involved.

Recent femtosecond photochemistry²⁹ indicates vibrational states of molecules were populated in less than 20 femtoseconds during an electronic excitation. Therefore molecules are being heated when being hit with UV and visible light.

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²⁹ S.T. Repinec, R.J. Sension, A.Z. Szarka, R.M. Hochstrasser, J. Phys. Chem., 95, 10380, 1991.

The molecule in question is stilbene:

The double bond is heated to 1000 C in 20 phemptoseconds. Photochemistry observed the rotation from a *cis* to a *trans* conformation. The entire process was decided upon within the first phemptosecond and required only a picosecond to take place, as observed by infrared spectroscopy. Therefore the impact to begin the rotation took place within the first 20 phemptoseconds, and the cooling off and rotation took thousands of phemptoseconds.

As it has until recently been not possible to observe only 20 phemptoseconds, transitions were considered to be instantaneous. The process actually observed in photochemistry was the cooling. Therefore theories were being developed on the wrong phenomenon, as selection rules are really only valid for the process of impact and the resulting choice of rotation.

It has been proven experimentally that the Franck—Condon principle, Born—Oppenheimer principle and perturbation theory are invalid for MCD due to time, inertia and transition process considerations. However the principles of physics involved in quantum mechanics still must be strictly obeyed in any model being developed. It is the intention of this thesis to do so.

II. THE MCD MODEL

II.1 Introduction

II.1.i Model Development

The MCD phenomenon is in reality a transient magnetic moment. As such it is the property of the transition process itself as opposed to being a property of the particular states involved. It is possible therefore to derive a model which observes the transition process and the electromagnetic nature of both the atom and photon. The atom behaves in a manner observable by the MCD experiment. It is necessary to develop a language which yields a description of this behaviour.

Given the output as experimental data, one needs only to treat the situation as a reverse engineering problem and design a device which yields the same output. Designing an instrument to correlate spectral data to the parameters is an observational as opposed to a derivational approach. There are precedents in the field of spectroscopy for the derivation of empirical fitting parameters from the regularity of spectral data. The Rydberg power rule, the Block equations for NMR and Van Vleck's crystal field theory, where no quantum mechanical analysis was used, are viable examples. Such an approach will be applied to the MCD problem in this thesis by relating polarized spectra to scalar parameters.

In order to design such a device a phenomenological approach may be taken. Inspiration will be forthcoming from the state of the art physics available and from the experimental observables of nature. The standard physical conditions of isolated systems must be included in order for the device to behave as an atom would.

Conservation of energy and momentum must be observed. The full degrees of freedom available and constraints on those degrees of freedom must be included. The principles of relativity and uncertainty must be included in order to conclude the correlation process. This approach will allow a transformation of the spectral data to a set of parameters from which selection rules may be derived.

II.1.ii   MCD Expressions

This thesis is an investigation of the forms of equations as opposed to their content. This is not an investigation of correlations between MCD and quantum mechanics as the phenomena of MCD have not been investigated to a degree which allows correlation with quantum mechanical definitions or relationships.

The phenomenological approach will devise a set of equations that behave in the same manner as the observable facts and phenomena. This will be accomplished by uniting geometry to physics in order to achieve a set of rules. In the past scalars have been used for convenience ³⁰ as the problem has been deemed too difficult. The standard approach has been to employ a series of nested parameters with no connections to motion or coherence.

By reproducing visible polarization processes seen in the instrument, a transform may be created which is useful in creating a set of arbitrary evaluation parameters from spectra. The form of the transform equations will be based on a set of abstract

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³⁰ J.B. Marion, Classical Dynamics of Particles and Systems, Academic Press, New York, 1965.

parameters that will be given names for convenience but have no physical meaning. For example the use of the terms *current* and *flux* will be used to describe objects which behave in a manner identical to that of conventional current and flux. Although it may well be an entirely different phenomenon, if it looks like and is observed to behave like the conventional term, it will be labelled as such.

The model is really about how to set up non-orientable axes as the simplest description of the observable phenomena in order to use that description to predict spectral data. There is a total separation of form and content. Content will emerge from the future use of the MCD model in much the same manner as crystal field parameters (DQ, DS, DT) have developed by common use, although their exact meaning is still unknown.

Heisenberg's Action is describable with a four-dimensional Lagrangian because position/momentum spaces are initially coupled in some way until uncertainty destroys it. The Lagrangian is a description of the intensity of the transition as $(T - V)$ by describing the remnant of ideal geometry after uncertainty has had its effect. The Lagrangian still exists after uncertainty because it describes the energy content.

The Hamiltonian is a description of the energy of the transition of the state. It identifies the location of the phenomenon in the spectra as wavelength. It describes the energy $(T + V)$ of the states involved. By allowing the possibility of a fully coupled energy state, where all the kinetic energy is coupled to all the potential

energy, a chiral, non-orientable Hilbert space is created in which a state vector can operate. The state vector travels along a work pathway defined by a geometrical function. This pathway is describable by the geometric function $\tanh$ because this $\tanh$ is capable of exploring the entire Hilbert space. This is a necessary requirement of the coordinate axis, to explore from zero to infinity, and $\tanh$ is the simplest geometric function which can perform this task.

II.2. MCD and Geometry

II.2.i Chirality, Sense of Rotation, and Coherence

For over a century chirality has been regarded as a property of molecules arising either from the arrangement of atoms or the superposition of a magnetic field. It was essentially regarded as a perturbation of isotropic systems, irrelevant to the basic structure of atoms. However the observation of parity breakdown in β emission and the recent discovery of the parity selection role of the Z^0 Boson ³¹ has revealed that chirality is a fundamental property of matter at the subatomic level. Its influence is detectable as an observable residual left-handed circular dichroism of heavy atoms and the probable spontaneous preference for crystallization of their salts in a left-handed habit. The same influence has been evoked to explain the evolution of all life forms in a left-handed morphology.

The object of this thesis is to develop the tensorial form ⁸ and illustrate the unambiguous geometric assignment of polarized spectra which is made possible with this topological approach. This unambiguous assignment is not possible in the traditional, algebraic form because it is based on both philosophical and practical simplifications. Philosophically, the original authors seemed to accept and employ an oversimplified, Kantian definition that atomic or molecular systems exist in isolation, with the implication expressed by Max Born ³² that atomic structure required no definition of static or dynamic geometric phases. ³³ The absence of any

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³¹ R. Walgate, *Nature* **303**, 473, 1983.

³² M. Born, *Zeit. fur Physik* **38**, 803, 1926.

³³ E.W. Hobson, The Domain of Natural Science, Cambridge University Press, Cambridge, 1923.

such phases allowed the reduction of the description of the physical system to that of a scalar, spherically symmetric structure in three-dimensional positional space and permitted the analysis of structure and spectra by spherical harmonics. These functions and all of the derived forms of coupling to which they lead, have actually been oversimplified to the point that they cannot describe any of the observable, non-orientable aspects of atomic structure or events.

To overcome this, some authors have introduced arbitrary, algebraic phase factors to assign polarized phenomena.⁷ However, since they have not been derived from the geometry of the system, they do not solve the basic inadequacy of the traditional model. There is no currently available point group capable of resolving left-handed rotation from right-handed rotation except by definition. The solution requires instead, a return to the original expressions of classical mechanics and a redevelopment of a relativistic form while keeping the explicit, complete geometry.

The absence of a phase criterion is unimportant in the derivation of energies or probability densities of states and in the estimation of electronic transition intensities in atoms and molecules because for these scalar properties, phase always appears in squared form. However the description of any polarization or coherence properties requires an explicit phase definition of the relative phase of the phenomenon. The phase for these purposes has usually been chosen to optimize convenience of manipulation of the description being used, leading to a variety of options in the literature.

In general, the experimental requirement for inclusion of arbitrary factors in a theory is usually an indication that the postulates are incomplete and that the assumptions used to define the physical model may be too restrictive. The ability of the Z^0 Boson to influence the chirality of the bound electrons of atoms is a mechanism which cannot be denied experimentally but has instead been confirmed by the residual left-handedness of Fermions in atoms, and should remain in the physical model.

The consequences of explicit inclusion of reflection or inversion as physical mechanisms are observable. The phase in the differential equation, the operations and phases of vector coupling and the number and behaviour of symmetry elements and representations in point groups are all affected. Refining the physical model appears to reduce the arbitrariness of manipulations in the different formats and increases the symmetry of functions, matrix or vector relationships. As well, it removes the ambiguity of double point groups and allows a direct unitary mapping of basis functions onto unambiguous components of these representations for the first time.

II.2.ii   Geometry and Spectroscopy

The spectra of atoms or molecules are usually measured as wave length resolutions of resonant interactions of radiation with matter. This observation of a scalar intensity ² does not display either the spatial or temporal complexity of the process. This complexity can be resolved by measuring intensities, at each wave length, as function of both the geometry and duration of the interaction by the appropriate experimental apparatus.

In these experiments, the various types of spectroscopy are based on the fact that there are many aspects of both geometry and duration that can be controlled. The radiation may be linearly or circularly polarized. It can be used to probe material samples in specific alignments and under imposed electric or magnetic fields. At the same time, the radiation can be generated in pulses as short as 10^{-15} seconds and the electromagnetic fields applied to the sample can be oscillated, at any frequency, in either position or intensity. These oscillating fields are equivalent to irradiation of the sample with a second beam at a different frequency, direction and polarization from the first.

These various forms of positional and temporal spectroscopy are known by the wide variety of names described above but each of them is a method for investigating some aspect of the extensive degeneracy and complexity of resonant processes in matter. The complexity of equipment needed to make these measurements is greater than for unaligned absorption spectroscopy but the wealth of structural information available is making these techniques more common.

In all these techniques the resonant intensity is measured as a function of the spatial or temporal phase angle between the initial conditions and the conditions of radiation after interaction with the sample. The amount of information available in any single technique depends on the number of positional and temporal parameters which are well defined in the experiment. In traditional absorption or emission spectroscopy there is no such parameter. In linear dichroism spectroscopy the linear polarization of radiation defines a plane transverse to the direction of the ray which has two possible extremes. In circular dichroism spectroscopy, two counter-acting senses of rotation transverse to the ray are coupled to the initial linear polarization

phases. In magnetic or electric circular dichroism spectroscopy, the static magnetic or electric dipole aligned along the ray couples with the linear and circular phases to define opposing hands of helical polarization about the ray. In pulsed electric or magnetic circular dichroism spectroscopy, the temporal phase, defined by the reaction of matter to the interaction with a photon, couples with the three positional phase conditions defined by the matter.

The resulting interaction space must allow for all individual combinations of binary phase choices. The total of allowed physical situations, for a single energy photon, therefore becomes $2^4 = 16$. With modern spectroscopic technologies, all these phases can be resolved for any interaction between radiation and matter. The preference of a specific substance in magneto-electric fields for radiation of predetermined polarization, sense of rotation, hand and temporal delay can be measured at all energies. Each interaction therefore carries a unique geometry since each event occurs at a different energy and represents a specific way that the matter can exchange energy with the radiation field.

This geometry is describable by a set of coordinates that are not positional so much as procedural in that they imply movement along a potentially non-linear workpath or object. The minimal basis set of independent objects defining the structure carries in it four such workpaths, which may be labelled as the "*dimensions*". Since transitions represent changes of state of matter, the geometry and energy of the radiation required for each event are probing the difference in

electro-magneto-inertial structure between states. The observable four-dimensionality (as defined above) of these differences in structure implies that with limits of uncertainty, the states themselves must exist in characteristic symmetry in these four objects (or pathways) and their conjugates.

These geometries result from all the possible degrees of freedom available to the electrons of an atom or molecule, within the limits imposed by the binding forces necessary to maintain a stable state. Therefore, the minimum necessary features of these geometries can be deduced from applying these limits to the properties of free electrons. At the same time, the geometries of electronic stable states must be consistent with all spectroscopic geometric information because the purpose of discovering these geometries is to use them to predict the dependence of transition intensities on spatial and temporal probe conditions.

There are two philosophically opposite approaches to deriving a complete description of geometries of stable states and transitions. One is the reductionist approach in which the properties of individual fundamental particles are subjected to the laws of mechanics. This presents two associated difficulties; the solutions are approximate for more than two particles and tractable solutions in complicated systems are usually defined by omitting the geometry. In the absence of geometry, the structure of polarized transitions are assigned with a series of arbitrary phase factors. While these provide the facility to catalogue the polarizations of transitions, the absence of a formal relationship with state structures precludes their ability to predict behaviour.

The alternative approach employs the physics of ensembles. Any set of particles is in motion above absolute zero and tends towards complete disorder. However, binding forces prevent the attainment of complete disorder and lasting conformations of the structure are established. External influences which are capable of performing work in specific directions can rearrange these cooperative structures to new conformations. This process takes place when the external influence couples with the system in a shared event space. Within this space, work can only be performed on the system if the structures within the forces and the system correlate for a finite amount of time. Thus, transitions can only occur if the geometry of the influence is coherent with some part of the geometry of the system.

There is no uniquely necessary geometry which can be assigned to bound systems. However, the measurability of polarization, sense of rotation, hand and period of reaction of transitions defines a minimum set of properties which the system geometry must possess. By initially limiting the description to atomic systems the binding force geometry becomes radial.

In ensemble models the individual particles have no separate identity. Their positional and temporal properties, including electron spin, are coupled in all possible ways, yielding resultant overall geometries and stabilities. The fact that all particles remain bound means that these geometries are periodic in space and time simultaneously so that a state vector can be defined which oscillates through all available dimensions of a non-orientable Hilbert space. Likewise, all the components of the higher properties including momentum, energy and action must

oscillate, without any net loss or gain. The limits of oscillation amplitudes are classically zero to infinity for each state property. In reality finite binding forces and uncertainty limit allowable displacements, and relativity limits allowable velocities to finite values, removing the classical singularities from the full position-momentum space.

From these spectroscopic requirements and mechanical limits together, the simplest sufficient geometry for the oscillations of the state vector is the four-dimensional hyper-Klein surface.^{34,35} This surface is a nesting of a fundamental Klein surface and an infinite set of overtone surfaces about one origin. The fundamental surface can be projected down to either a three-dimensional positional space or a three-dimensional inertial space. In each case, the fourth dimension becomes a singularity of the other dimensional type at the origin. A further projection to two dimensions is useful in revealing the basic structure. In the plane, the component of the state vector executes its changing momentum around a heart shaped path described by a hyperbolic tangent function while the velocity follows the coupled hyperbolic cotangent. This full period spans 4π radians. Coupled to this is an oscillation of the vertical component on a sine function while the velocity follows the cosine. The full path in three dimensions is therefore a Mobius locus.³⁶ Since the total length of the state vector must be constant, but its components vary in length, a conjugate locus, coupled to the initial one is generated simultaneously with all inverted properties.

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³⁴ P.J. Giblin, Graphs, Surfaces and Homology, Chapman and Hall, London, 1977.

³⁵ J. Hayden and E.C. Zeeman, Math. Proc. Can. Phil. Soc. **89**, 193, 1981.

³⁶ D. Hilbert and S. Cohn-Vossen, Geometry and the Imagination, Chelsea Publishing Company, New York, 1952.

II.2.iiiSpace and Physical Phenomena

Traditional spectroscopy is defined by intensity (a relative condition), band width (in units of Joules) and energy or position (also in units of Joules) as obtained by ordinary absorption. However these modern polarization and differential polarization techniques yield other types of information and in the process introduce the concept of "*space*" to quantum mechanics. In the simplest case, a polarimeter splits a field and yields two intensities of light. A two-dimensional spatial coordinate (degrees) is required to describe the polarization. Space is therefore measurable in an experiment in the sense that intensities vary with position. Both CD and MCD were in fact originally plotted as degrees of rotation, that is a form of molar rotation, or extinction coefficient.

It is necessary therefore to begin developing a model for polarized spectroscopy by putting space explicitly into the description of an atom which is capable of interacting with the rotation of a beam of circularly polarized light. There can be two reasons for the rotation, assymetry in either the electric or magnetic fields imposed on an atom. As these fields act perpendicularly to each other, two independent axes of rotation exist, so some form of space cannot be denied. Rotation about two axes implies the existance of a third axis. Adding this axis and coupling the rotation of the electric vector and the rotation of the magnetic vector requires a non-orientable geometry. In fact, non-orientable motion of electromagnetic vectors of static and transient states is a fundamental property of space.

The passage of polarized light through matter yields three observable properties (FIGURE II-1), each implying its own dimensional requirements. The first is seen in one dimension ³⁷ in which the electromagnetic state vector points along (in phase, 0π) or against (completely out of phase, π radians) an axis which can be considered a coherence (c) to either an external or internal field. In the MCD experiment this could be observed as a coherence to the molecular electric or internal Stark field.

The second observable phenomenon is seen in two dimensions. ^{6,7} Here the highest function is a quadratic, which allows for the greatest amount of curvature and is observed as a sense of rotation (s) of the state vector about the independent orthogonal Zeeman axes. ^{38,39}

The third observable ^{27,40} is the three dimensional handedness, or chirality (χ). ^{1,2,41} The three dimensional solution is a cubic about three orthogonal axes, yielding a helix as the shape of the state vector motion with the most curvature.

The three bifurcated aspects of state vector behaviour are therefore coherence, sense of motion and chirality (of the helix), are all simultaneous properties of any axis.

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³⁷ E. Fredericq and C. Houssier, Electric Dichroism and Electric Birefringence, Clarendon Press, Oxford, 1973.

³⁸ B.R. Judd, Angular Momentum Theory for Diatomic Molecules, Academic Press, New York, 1975.

³⁹ J.C. Kemp, J. Opt. Soc. Am. 59,950, 1969.

⁴⁰ L. Velluz, M. Legrand and M. Grosjean, Optical Circular Dichroism, Academic Press, New York 1965.

⁴¹ W. Kauzmann, Quantum Chemistry, Academic Press, New York, 1959.

One dimension   Coherence

Two dimensions   Sense of Motion

Three dimensions   Chirality

FIGURE II-1   Observable Phenomena of Polarized Spectroscopy

The three levels of duality imply the necessity of $2^3 = 8$ orthogonal but confluent coordinate axes for a complete definition of the supporting space.

These are not axes in the usual sense, only in the sense that they can be used to parametrize the space. They are non-orientable and may be closed to form a Moebius locus ³⁵ in order to define the atomic space, or open to define the photon space. The experiment observes an adiabatic rearrangement of vectors within the combined event space defined by overlap of the photon structure with the atom structure.

Within the conventional definitions available for MCD ^{5,6} it is evident that there is no explicit definition of coherence, sense of motion or chirality in either the general ground state $|a\rangle$ or the excited state $|j\rangle$ of a transition. Furthermore, in the traditional description of transitions the electric part is squared, so that the x and y directions have become equivalent. This means that the helical nature of the interaction has been lost along with any ability to predict the observed sign. At the very least, a definition of the degeneracy in the spaces supporting the function $|a\rangle$ and $|j\rangle$ is required, whether in x or y is immaterial.

The advent of polarized spectroscopy data makes it necessary to interpret at least the major characteristics of the observables i.e. sign, and preferably the intensity as well. Spatially defined selection rules are obviously involved in transitions, and it is necessary to establish the nomenclature that will give specify them in unambiguous language in order to provide the algorithm to calculate the sign and the intensity.

Thus a need has been established for a transition operator which has to be at least four-dimensional in order to contain the experimental observables. The spaces required to support unambiguous descriptions of observable particles and events consists of pairs of real confluent orthogonal three dimensional spaces for both position and momentum. These pairs of spaces which are related by an apparent reflection symmetry on each of three axes, represent the phase reversal of particles, so that overall the spaces are related by inversion. Spaces with all these attributes will be defined as bilateral. Pairs of bilateral spaces can be defined in any dimensionality and are characterized by the inversion operation which represents vestigial C_2 rotations through spaces of the next higher dimension.

In keeping with traditional, single spin spaces, bilateral spaces require definitions of metrics before being employed for descriptions of dynamics. Well behaved metrics permit definitions of continuous functions and their derivatives between unambiguous boundaries. Two types of metrics are needed for the two types of spaces of interest, a positional metric in some measure of length and a dynamic or Eckart metric in the unit of momentum. These are traditionally related by non-singular Fourier transforms in which derivatives are always taken in the positive sense of either translation or rotation. In this development, such arbitrary assumptions cannot be maintained because they eliminate sets of experimentally observable phenomena.

The definition of a metric in any space implies that the Fourier transform gives concurrent definitions of allowed operations, which in turn permits the construction of functions in the space. Thus velocity functions can be constructed in a position space or vice versa. In bilateral space pairs there is the further requirement to define

operations which relate the metrics and hence the functions of the two orthogonal spaces. The explicit form of this bilateral operator set relies ultimately on the objective of describing the chirality of matter in its combined position-momentum manifestation, that is, the space of the Action of the system.

Chirality is a function of simultaneous and coherent translation and rotation and in either handed component space. This locus is not explicit in traditional "*helicity bases*" because translation is not formally coupled to rotation and the phases, senses and chirality are all indeterminate.

In anticipation of defining steady chiral states of atoms and molecules, open ended helical coordinates are inappropriate. Rather, reciprocal helical loci are required so that closed momenta or bounded distributions can be described. This can be accomplished with a set of Mobius coordinates in each of the confluent orthogonal spaces with a handedness defined for the positive senses of coherent translation and rotation.

II.3. MCD and Ensembles

II.3.i Description of Spectroscopic Phenomena

Modern spectroscopy needs an unambiguous language to describe observable tensorial phenomena. The traditional approach, anticipated by Maxwell and culminating in Dirac, is implicitly capable in its most general form of providing this language for several reasons. It contains a sufficient number of dimensions. The necessary tensorial structure can be specified on these generalized dimensions. The basic theory fully accomodates relativistic behaviour and uncertainty within its derivation. Therefore it is possible to adapt the Dirac–Maxwell description to polarized phenomena.

Phenomena are transformations of whole atoms or chromophores of molecules, that is, they are processes imposed on states of cooperative behaviour of particles. States can be represented by vectors of cooperative electromagnetoinertial behaviour in Action space, the space of the Lagrangian. Stable states can be represented by Action (the repetitive development of one form of energy, while the total energy is held constant) on maximally disordered geometry allowed by the atomic or molecular potential. This ideal geometry set up by the Action of the state vector can be used to define fundamental coordinate axes to reveal the full geometry of position–momentum space and the full degeneracy of the state.

Since this description applies to all states of any ensemble of bound, cooperatively acting particles, revised postulates for this quantum mechanics of ensemble are desirable as spectroscopy measures ensemble behaviour and not individual atomic behaviour. In fact, the experimentally verifiable laws of thermodynamics both at equilibrium and far-from-equilibrium are sufficient postulates for this purpose.

II.3.ii   Early Observations of Ensemble Behaviour

There have been several interesting observations of atomic behaviour in this century. In 1912 Harry Mosely observed absorption of X-rays by the nucleus in Rutherford's lab. ⁴² In a letter to his sister Margery on February 2 of 1913, Mosely described his conclusions in the following terms;

"The X-ray spreads out in a spherical form from a source as a wave through the aether can, when it meets an atom, collect up all its energy from all around and concentrate it on the atom. It is as if when a circular wave on water met an obstacle, the waves were all suddenly to travel round the circle and disappear all round and concentrate its energy on attacking the obstacle. Mechanically of course this is absurd, but mechanics have in this direction been for some time a broken reed. There is some most mysterious property of energy involved which the Germans have for some years been groping after but which we see no immediate hope of comprehending."

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⁴² D. Wilson, Rutherford A Simple Genius, MIT Press, Cambridge, 1983.

This observed behaviour provides a starting point for the model developed in this thesis. By combining Mosely's observations with Rutherfords interpretation, Bohr's Correspondence Principle and the geometric consequences hinted at in the work of both Heisenberg and Schroedinger, a tensorial model may be derived which fully describes the observable polarizations and intensities measured in modern spectrophotometry.

Although it was shown by Bourcault in 1790 that light through a translucent medium slows down, it has recently been seen that it slows down by 90%. ⁴³ This suggests that the interaction involves light in a non-resonating form which tests every molecule and then moves on. Indeed, the long testing period suggests that the assessment of each atom involves an extended tensorial test of coherence of the electromagnetic vectors of the light wave with those of the ground state of the atom or molecule, establishing the relative phase of the MCD phenomenon. Scattering and resonance are then only different in the range that full coherence is achieved for resonant absorption or stimulated emission but is not achieved in scattering. This also suggests that the real part of the index of refraction is a measure of the degree of incoherence at the scattering event

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⁴³ R.W. Schoenlein, L.A. Peteanu, R.A. Mathies, C.V. Shank, Science, **254**, 412, 1991.

II.3.iii   Laws and Postulates: Existence of States

The existence of a state is determined by two competing influences, all the available degrees of freedom and the limitations on those degrees of freedom. These two influences result in a new system of particles in a stationary state of repetitive motion. In order to include in the description all the tensorial observables of the state it is necessary to include the full degrees of freedom and to allow full coupling at all times and amongst all particles simultaneously. Such an ensemble system will behave adiabatically and thus the particles within the ensemble will follow the laws of thermodynamics. The dynamics of the individual particles is limited by relativistic and uncertainty constraints.

II.3.iv   Laws of Thermodynamics

The first two laws of thermodynamics establish the full degrees of freedom for the bound system. The first law establishes the principle of conservation and the requirement of the system for a conservative event space within which all events occur and within which mass and energy intersect with any or all allowed tensorial properties. The pathway of bound electrons must have momentum in all three dimensions at once, and the natural coordinates must remain fully coupled. The second law is a statement of order in that order decreases as time evolves in an open system. In a bound system, order decreases to the greatest minimum possible. This law determines the existence of a least complex path and establishes the need for non-orientability.

The implications for adiabatic systems indicate that coupled cooperative motions of bound electrons must fall on closed pathways which simultaneously exploit all available dimensions. In one dimension there exists a coherence choice for positive or negative motion away from the origin. In two dimensions there is the additional choice of sense of motion either clockwise or counterclockwise. In three dimensions there is the additional choice of handedness.

The least complex non-orientable pathway available which can fulfill these requirements is a Moebius locus. The Moebius locus represents the ideal geometry for the fundamental stationary state. In adiabatic systems all allowable positions and velocities must fall on non-orientable Moebius loci about the origin. Positioning all eight available Moebius Loci upon a common origin induces the parent object, the Klein surface, which is the event space. Each Moebius locus requires a 4π rotation, resulting in a four-dimensional Klein surface which can be mapped onto unitarily by the Lagrangian operator. At the limit for the bound system, the correspondence limit, there are an infinite number of nodes with an infinite amplitude and the assembly behaves like a solid classical object.

The final two laws define limitations upon the full degrees of freedom. The third law specifies zero point behaviour of the system. Minimum disorder at $T=0K$ requires the dynamic behaviour to act along a path of minimum complexity. Coupled motion must occur even at lowest real temperatures. As the temperature decreases, entropy also decreases, so coupled motion becomes more ordered. Least complex behaviour consistent with the first and second laws requires that individual bound electrons move along the simplest Moebius locus, thus defining the ground state. This requires a 4π revolution between repetition points. Prigogine's fourth law of

maximum entropy ⁴⁴ defines the allowed excited states. It is a statement about closed systems far from equilibrium. The addition of energy into such a system increases order. The number of structural features (nodes) can be specified as harmonics of the basic locus. Hence at $T > 0K$, the path is of greater than minimum complexity and contains overtones. As more energy is added (temperature increases) the number of nodes increases. Eventually the pathway appears to form a solid object. This provides the Correspondence Limit when sufficient energy is added to a bound system. Prigogine's fourth law allows the substitution of complete disorder for Rutherford's original use of aether.

Whereas creation operators occur in the nucleus, annihilation operators appear progressively after leaving the nucleus. Therefore creation operators are associated with condensed matter where there is structure. Conversely annihilation operators are associated with space where there is no ordering structure. Therefore annihilation is the progressive addition of uncertainty and space is just complete disorder, as seen in Prigogine's fourth law of thermodynamics.

Whereas the standard approach is to create order in a vacuum or aether, the model of this thesis will put order in the condensed matter rather than in the space. The well known relationship $E = mc^2$ is an expression of energy as an evaporated form of matter and mass as the condensed form with the possibility of conversion from one form to the other. The energy that is seen by the observer is entirely kinetic. To put order back into the system some potential energy must be involved. However the

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⁴⁴ I. Prigogine and I. Stengers, Order Out of Chaos, Bantam Books, New York, 1984.

standard definition of free space had no potential and so could not have order. The fourth law states that in order to see order there has to be a confinement of matter with a potential which is a characteristic of condensed matter, and even a photon is condensed matter in a certain sense.

II.3.v   Relativistic Mechanics

Applying relativistic mechanics to a system at constant energy allows conclusions to be made with regards to the behaviour of the electron as it nears the nucleus. As the electron pathway radius tends to infinity, the potential energy reaches a maximum, and kinetic energy a minimum. Conversely, as the radius tends to zero, the kinetic energy reaches a maximum and potential reaches a minimum. Thus the total energy E remains constant for the state. As the electron approaches the nucleus it must shrink in all dimensions and it is no longer observable as it enters the nuclear radius. The nucleus itself is a unique point where the electron velocity is so great as to make it approach Boson mass and its presence is manifested as a degeneracy in chirality. The electron couples to the Z^0 Boson which reestablishes the pathway by redefining chirality, sense and coherence. Therefore definitions can be made for normality and orthogonality and gauges can be defined uniquely in such a way that if all relevant dimensions of the particle are kept, a smooth function of position and momentum can be written.

Application of the uncertainty principle when position and velocity paths are fully characterized allows an analysis of the uncertainty limits and the definition of an uncertainty pathway that can be described as a wave function of coupled uncertainty of position and velocity. Heisenberg's uncertainty principle, due to its non-zero nature, may be represented to demonstrate its true vectorial nature as cross products of three-dimensional vectors. In any open or closed three-dimensional non-orientable coordinates, the differentials of position and momentum vary continuously along the coordinates and reverse behaviour with reversal of the sense of motion of the state vector on the coordinate. Thus Heisenberg's statement becomes:

$$\Delta \vec{p} \times \Delta \vec{x} - \Delta \vec{x} \times \Delta \vec{p} \neq 0$$

Reversing the multiplication implies a reversal of direction of the vectors, which cannot be accomplished in one hand. Therefore the two hands must coexist and require four dimensions to do so. Furthermore the nonzero nature of the relationship implies an infinite barrier and therefore a phase factor. This behaviour is recognized in the Carrington reversal of sense in EPR.⁴⁵ By choosing a coordinate system of natural coordinate pathways and defining the event space, one defines the quantum mechanics of the classical limit. By adding the uncertainty behaviour one allows the definition of fully coupled four-dimensional action, perceived after integration on the natural coordinate as three-dimensional energy.

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⁴⁵ A. Carrington, D.H. Levy and T.A. Miller, Adv. Chem. Phys. 18, 149, 1970.

There are only two points where the uncertainty vector properties are certain and therefore observable. These two points are the origin, and the 2π rotation point (the maximum radius, or limit), although classical observation is never achieved. At the nucleus, as the velocity of the electron tends to the speed of light, the observer cannot observe the radius. It is here that there can be an exchange of geometric integrity with the nucleus and if not achieved, emission may be initiated. At the limit, the observer loses track of the direction of the velocity vector on the pathway. Before reaching the Stark field, the velocity vector wobbles and is susceptible to external perturbation and the likelihood of a transition process. The uncertainty accompanying the ideal pathway can be described therefore only as a wave function of the coupled uncertainty of position and velocity. Pathways and the ideal periodic behaviour of the observables chirality, sense and coherence can be written as natural coordinates while wave functions of states and can be used in the Schroedinger format to calculate the remaining certainty of the observables. They can also be identified by group theoretical labels which do not yet exist but will be developed in this thesis. Thus there is now an available description for stationary states which to date have only been assumed to exist.

II.4. MCD and Topology

II.4.i Bound Quantal Action

In traditional mechanics, the Bohr Complementarity suggests an incompatibility between objects and processes.⁴⁶ Their dimensional equivalence can be recognized through realizing that time is necessary to define both concepts but that it is recursive in objects compared to being open ended in processes. In other words, the steady states of repetitive motion of field vectors which represent objects (or more precisely, stable states of systems) have the same dimensionality as the transitions of unbound vectors representing processes, but the coordinate axes of objects are periodic and hence *quantized*, while the vectors on the open axes of processes are *chaotic*.

From this, it becomes clear that the distinction between "*objects*" or "*processes*" is an apparent rather than an absolute situation and depends simply on the space/time scale of observation and conceptualization. At any particular scale of magnification, the entire repetitive behaviour of one set of field vectors may be visible as a single object, while only part of another set can be seen and thus will be interpreted as a singular change or process. Thus, the apparent structure and behaviour of every space is characterized by the choice of scale.

In considering this, there could be any number of degrees of freedom, depending on the relevant number of objects and their allowed processes. The fundamental decision is the discrimination between the system and the surroundings. Following

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⁴⁶ a N. Bohr, Nature 121:78, 580 (1928);

b N. Bohr, Naturwiss 16, 245 (1928).

the D'Alembertian Principle of Zero Work, ⁴⁷ an operational decision is imposed which defines an arbitrary origin for a local system. The structure and behaviour of objects in the local system are described relative to this origin and any fields identified with the surroundings are normalized to performing Zero Work on the system. In any such local system the scale must be decided, then the relevant objects and processes may be defined and the *effective* number of degrees of freedom calculated as the product of all objects in discrete processes. This effective number of degrees of freedom defines the number of independent coordinate axes needed to establish the mechanical space. This is the space of $\vec{x} \times \vec{v}$, which are perpendicular to each other so that the resulting space is handed and results in a third vector pointing out into the space. The most convenient description of the behaviour can then be based on a choice of "*natural coordinates*", defined as a set of coordinate axes which incorporate all the unchanging physical information. The unit of measurement on each of these coordinates, called the unit vector, is chosen to represent the minimum behavioural change of importance in the description.

The shape of the natural coordinates can be determined by applying Prigogine's concept that structure of a system appears as the consequence of imposing limits on degrees of freedom. ⁴⁴ In mechanical space order is a function of the Action on the pathway, not of position alone and therefore order decreases as the complexity of Action. At the limit of minimal kinetic energy content in the system, the minimal structure of repetitive motion of objects is the most disordered pathway allowed

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⁴⁷ S.W. Grossberg, Advanced Mechanics, J. Wiley & Sons, New York, 1968.

within the bounds of the local space. In topological terms, these shapes are the most non-orientable paths which can be taken by the objects through the space allowed by the confining forces. Depending on their geometry, the fields restrict and couple processes of completely free motion into either less random processes if they provide partial confinement or into new objects if the motion is restricted completely into repetitive paths. In this sense, objects are coherent, repetitive processes executed by smaller objects on a recognizable topology. Since coherence can only be achieved with integral periodicity of a process, the imposition of limits *quantizes* both the energies and topologies of stable objects allowed within the mechanical space. It is stipulated that these objects conserve energy and obey the first law of thermodynamics. Successive couplings progressively reduce the number of independent dimensions until the mechanical space is confined to a single point object or "*singularity*" acting as the pseudoscalar of the space.

II.4.ii   Ideal Mechanical Geometry

The assembly of bound objects obeys the second law of thermodynamics and displays the most disordered process geometries allowed by the imposed limits. In this mechanical space, this criterion produces non-orientable pathways. Orientable paths, such as spherical harmonics are demonstrably more ordered because they can be constructed as paired sets of non-orientable paths. ³⁴ There can be two types of behaviour of bound objects on these pathways; coherent and incoherent processes. The coherent processes of the Hilbert space are described by the excursions of a "*state vector*", representing the coupled motion of bound objects around any of the

allowed, closed, pathways. At any instant, the system can only be in one of these "states". In this sense, the coherent, coupled processes become the effective objects of the space. The state of the system can be altered by interaction with external quanta of Action.

As predicted by the third law of thermodynamics, when all possible quanta of kinetic energy are expelled and the lowest effective "temperature" is reached, the remaining object is the most ordered and hence the least convoluted, non-orientable path of action. This path displays the simplest topology which can carry all the essential information about the structure of the mechanical space. Together with any equivalent but orthogonal paths, whose number is determined as 2^n where n is the number of degrees of freedom, it is uniquely suited to be identified as a "natural coordinate", carrying all the ideal geometry of the space.

Observable, local mechanical systems incorporate three dimensions each of position and momentum, defining a joint space of 2^6 degrees of freedom since each coordinate is two-valued about its origin. The union of the origins and the locking together of coordinate axes of these two contributing spaces to eliminate all relative translation and rotation creates a four-dimensional mechanical space with 2^4 degrees of freedom. Applying Occam's Razor, the simplest geometric figure which can represent a repetitive coordinate of this space is the Klein surface.³⁴ In three dimensions this decomposes to pairs of handed orthogonal loci. In general this curvature is demonstrated by a helix. Closing a helix creates a Moebius locus (FIGURE II-2) which retains the handedness or "chirality", χ and carries as well, a sense of rotation about the principal axis, s and a phase of coherence with fields perpendicular to the principal axis, c . Hence, there are 2^3 such loci. The last degree

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FIGURE II-2 Möbius Locus

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of freedom allows for a sign on the pseudoscalar, which creates sets of conjugate, inverted pairs of loci which act as the four natural coordinate axes of the four-dimensional mechanical space.

At any instant, on a given coordinate locus, the vector cross product of the position and velocity vectors which are defined at all points on the Moebius locus can be specified. The result of this product is the state vector, perpendicular to both components, creating with them a sub-space of one hand. The conjugate vector on the coupled, inverse locus must define the corresponding sub-space of opposite hand. These conjugate vectors of opposing chirality can be compared by calculation of their vector difference;

$$\vec{r} \times \vec{v} - \vec{v} \times \vec{r} = \vec{r} \times \vec{v} + \vec{v} \times \vec{r} = 2\vec{k} \quad (\text{II.4-1})$$

which yields a non-vanishing "*commutator*" $\vec{k}$ projecting onto the principal axis of rotation. Thus the vectorial difference cancels all the in-plane properties between conjugate state vectors but leaves addition of the vertical projections of them at all points on the coupled loci.

Projection of these natural coordinates onto standard three-dimensional positional axes is necessary to describe the ways in which experimental conditions interact with the mechanical structure. This can be stated in simple trigonometric terms. Two projections of the locus are required; one onto the horizontal plane and one onto the vertical axis of rotation of three-dimensional positional space.

FIGURE II-3 is the two dimensional projection in the x,y plane of the Moebius locus, looking down the z axis, including the "*cone of uncertainty*". The projection onto the plane resembles an Archimedean spiral, except that the curve is closed by reversal of its rate of spiraling, called its "*pitch*", every π radians. When uncertainty is superimposed, a cornucopian figure of density results. The radius of the curve is directly described by a hyperbolic tangent function of the horizontal angle ϕ . Therefore, any point on the mechanical coordinate is specified by the angle α whose hyperbolic tangent is any desired value, a .

This point on the new ideal geometry coordinate can be expressed in terms of the inverse hyperbolic tan function which yields a path covering the entire space;

$$\vec{r} = \vec{\rho} \times \alpha = \vec{\rho} \times \tanh^{-1}(a) \quad (\text{II.4-2})$$

in which, $\vec{\rho}$ is a tensorial scaling factor of position on the coordinate α which depends on the mechanical properties of the space, and $\tanh^{-1}$ are slopes taken for one sense of rotation.

Since the system is assumed to be adiabatic, having equal total energy at all positions of the state vector, the corresponding velocity coordinate is the directed derivative of the position on the locus with respect to time. It is always orthogonal to the position vector and since energy is conserved on this locus, it varies inversely in magnitude to position. This behaviour can also be expressed in inverse hyperbolic form;

FIGURE II-3 Two Dimensional Projection of Three Dimensional Moebius Locus (including "cone of uncertainty")

$$\vec{v} = \vec{\sigma} \times \frac{d\vec{\alpha}}{dt} = \vec{\sigma} \times \coth^{-1}(a) = \vec{\sigma} \times \frac{\vec{I}}{\alpha} \quad (\text{II.4-3})$$

in which $\vec{\sigma}$ is a tensorial scaling of angular velocity to the space.

The projection on the vertical axis of rotation can be stated in parallel fashion. The behaviour is sinusoidally coupled to the projection in the plane. This "*imaginary*" axial projection of the locus is calculated from the "*real*" behaviour in the plane by the outer product of the position and velocity vectors at any point on the locus and the points of inflection occur at the same values of ϕ . In inverse angle terms;

$$m\vec{\mu} = (\vec{\rho} \times \vec{\sigma}) \times \sinh^{-1}(a) \quad (\text{II.4-4})$$

in which the scaling of the vertical projection $\vec{\mu}$ is specified by the tensorial product $\vec{\rho} \times \vec{\sigma}$ and $\sinh^{-1}(a)$ represents the coupling of $\tanh^{-1}(a)$ to $\coth^{-1}(a)$.

On each path, the total energy is constant but oscillates from completely potential at the infinite point to kinetic at the origin. As the state vector is performing its excursion from 0 to 2π it is concurrently performing its conjugate excursion from 2π to 4π on the conjugate locus which is defined by the Moebius of the original locus. This guarantees that the total length of the state vector plus its conjugate is constant, representing the conservation of total energy in the coupled state.

At the origin of the "*process*" space objects approach light speed and behave relativistically. ¹ Then the vector must shrink in all three dimensions of coherence, sense and chirality together and enter an extra dimension in the "*origin*" to conserve energy. This point on the locus will be defined as a *node* in the natural coordinate. In atoms this passage of the state vector through the origin corresponds to the entry of the Fermionic electron into an unexpanded dimension created by nuclear forces, especially the Z^0 Boson incorporated in the proton. The weak force associated with this Boson is known to reorient Fermions, including electrons, to left handedness in any single pass. The effects are visible in the polarized spectra of heavy atoms. If only the scalar aspects of energy were conserved, the vector could re-enter three-dimensional space with binary choices of orientation phase, sense of rotation and chirality, on any one of the $2^3 = 8$ orthogonal paths. However, the conservation of momentum demanded in a state forces the state vector to follow the unique conjugate path for the completion of the excursion from 2π to 4π . Taken in these inverted, conjugate pairs, the eight Moebius loci are then the four "*natural coordinates*" of the four-dimensional mechanical space because they describe all the equivalent paths of least Action in the space.

Since these conjugate natural coordinates do not commute, their vertical projections into three dimensions must vectorially subtract to a non-vanishing, tensorial moment on the principal axis of rotation. From (II.4-1) and (II.4-4);

$$\begin{aligned}
 \vec{K} &= [(\vec{\rho} \times \vec{\sigma})^* - (\vec{\sigma} \times \vec{\rho})] \times \sin^{-1}(a) \\
 &= [\vec{t}^* - \vec{t}] \\
 &= \vec{K}
 \end{aligned}
 \tag{II.4-5}$$

in which $\vec{l}^*$ and $\vec{l}$ are the projections of the state vector on the principal axis form both the conjugate and chosen loci repectively, and $\vec{A}$ is the net commutation "*moment of scaled Action*".

Motion of vectors on fewer or less convoluted paths could not support the full structure of the four mechanical dimensions. In particular, traditional, *orientable* paths divide space into inside vs outside and only support one subspace in any one excursion.

II.2.iii   Wave Functions on Mechanical Coordinates

Thus far, this development gives a model of an ideal geometry of bound Fermion states, expressed as the natural coordinates of mechanical space. In observable systems, uncertainty limits the precision for the simultaneous observation of position and momentum. This limit was first expressed by Heisenberg as a constant calculated from the squared product of individual uncertainties in position, $\Delta\vec{x}$ and momentum, $\Delta\vec{p}$. The result was a squared property with dimensions $[ml^2t^{-1}]^2$, in which the dimensions $[ml^2t^{-1}]$ are equivalent to Action, $\vec{A}$ as defined by Hamilton. Heisenberg recognized that this minimum limiting Action, $\Delta\vec{A}$ had the dimensions and size of Planck's constant. The squared property defined the apparently scalar product;

$$[\Delta\vec{x} \cdot \Delta\vec{p}]^2 = \Delta A^2 = \hbar^2 \quad (\text{II.4-6})$$

However, Heisenberg indicated that taking the square root of this property to define

the *uncertainty of a state* implied a non-scalar geometry in the result.^{48,49,50,51} This was unavoidable because the time vector occurs to an odd power in the dimensions of Action, hence Action must be a vector. In fact, $\hbar^2$ must be a pseudoscalar formed by the product of inverted vectors

$$\overleftarrow{\hbar} \times \overrightarrow{\hbar} = \overline{\hbar}^2 \quad (\text{II.4-7})$$

By definition, $\overrightarrow{\hbar}$ itself can only be a vector if it is formed by cross multiplication of its two constituent vectors. This implies the recognition of Δx and Δp as *vectorial* or *directed* differentials. The ideal, classical positions and momenta are defined in orthogonal directions on the natural coordinate Moebius loci. The respective uncertainties themselves are likewise both anisotropic and orthogonal to each other at any point on the locus. Indeed, this orthogonality could not exist if the differentials were scalar because they would then be indistinguishable. Each directed component of uncertainty has two influences on its associated property; change of the magnitude in the direction of the property and change of direction at right angles to it. The first defines uncertainty concerning the scaling of the magnitudes of the space, the second about the geometric integrity of the path taken by the state vector. These deviational tendencies can be expressed as functions coupled to the position α of the state vector on the natural coordinate, so that in mechanical space terminology;

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⁴⁸ W. Heisenberg, Z. Physik **40**, 501, 1926.

⁴⁹ W. Heisenberg, Z. Physik **43**, 172, 1927.

⁵⁰ W. Heisenberg, Z. Physik **44**, 326, 1927.

⁵¹ W. Heisenberg, Nature **121**, 580, 1928.

$$\Delta \vec{r} = \Delta \vec{\rho} \times \vec{\alpha} \quad (\text{II.4-8})$$

$$\Delta \vec{v} = \Delta \vec{\sigma} \times \frac{\vec{v}}{\alpha} \quad (\text{II.4-9})$$

in which $\Delta \vec{\rho}$ and $\Delta \vec{\sigma}$ are the uncertainty scaling tensors in position and velocity respectively. Since they are tensors and must be combined as an outer product to completely fulfill the degrees of freedom in mechanical space, they provide the same geometric reason for the non-vanishing commutator in the reversal of the order of uncertainties as was found for defining the commutator of conjugate Moebius natural coordinate loci;

$$[\Delta \vec{r} \times \Delta \vec{v} - \Delta \vec{v} \times \Delta \vec{r}] = \Delta \vec{A} = \vec{h} \quad (\text{II.4-10})$$

In parallel with the commutation of the ideal geometry of the natural coordinates, the chiralities of the two conjugate uncertainty vector products are opposite, giving moments in opposite directions on the principal axis at all values α on the natural coordinate. Vectorial subtraction of one moment of the uncertainty from the other again gives a nonvanishing result. Geometrically, this new "*commutator*" is a position-momentum directed volume of minimum uncertainty of the mechanical space, at each locus point. It represents the "*Minimum Action*" needed to allow the state vector to reverse chirality at any point during its excursion on the natural coordinate defining a specific state. Since Action is work integrated over time, this Minimum Action, and hence the reversal of chirality, may be achieved in the finite time represented by the length of the position uncertainty along the path.

This model leads to a geometric definition of the wave function of a state. It can be stated as a ratio of the locus uncertainty to the ideal locus geometry for any position α of the state vector on the natural coordinate. The ideal geometry is implied by the ideal scaled Action, A_c . The uncertainty at any position on the locus is the extent of loss of this geometry through mechanisms dependant on the strong nuclear force. The wave function, representing the remaining fraction of certain, observable, classical Action at each point on the excursion of the state vector, can therefore be defined as the product of the scaled inverse of uncertainty of Action with the ideal scaled Action;

$$\psi_c = \left[\frac{\hbar}{\Delta A} A_c \right] \quad (\text{II.4-11})$$

Since this wave function is still dependant on the orientation of the coherence phase c , it implies its own conjugate through the Moebius inversion;

$$\psi_c^* = \left[-\frac{\hbar}{\Delta A} A_c^{-1} \right] \quad (\text{II.4-12})$$

Normalization is stated as the integrated scalar product of these two tensors ψ^* and ψ over respective ranges of the independant variable a which is implied in the tensor A_c so that;

$$\int \psi_c^* \times \psi_c da = A^2 \quad (\text{II.4-13})$$

in which A^2 is the net, Classical Lagrangian Energy, L , for the state ψ in the scaled space of the system.

In this normalized form, the inverse uncertainty of action specified by ψ_c defines the traditional "*quantum mechanical amplitude*" in terms of the explicit but progressively decaying three-dimensional geometry of non-orientable, mechanical space. Only the remaining classical Action component can contribute to the observable scaled Action. Thus, the accumulated uncertainty of Action is the agent which *reduces* the intensity of observable properties below the prediction for the normalized wave function without certainty.

II.5. MCD: Dimensions and Units

II.5.i Normalization

The definition of wave functions as the dependance of uncertainty on Action is equivalent to a reduction in the symmetry of the state from ideal geometry to a "real", but more poorly defined dynamic structure. The relationship between a geometric or topological approach and standard quantum mechanical practices is demonstrated by the Fourier transform between frequency and wavelength scales. The pathway in wavelength terms is seen as geometry, while in the frequency scale is seen as a periodicity. Uncertainty is a blurring of these pathways, in wavelength terms seen as a tube instead of a line, in frequency seen as an uncertainty in periodicity. At an equal energy a late arrival would be due to a longer pathway travelled, an early arrival would be due to a shorter than ideal pathway travelled. A shorter than ideal pathway is characterized by states with shorter paths, i.e. those of higher energy with a greater number of nodes. The equivalent description in terms of quantum mechanics invokes the Addition Rule, where selected states are added in certain amounts to obtain a new geometry. Any state not displaying ideal geometry can be described by the quantum mechanical Addition Rule as it distorts the ideal geometry by addition, thus causing a reduction of symmetry. Normalization is a compensation for this partial loss of classical identity. Since the wave function is defined by the product of the ideal and uncertainty tensors, the integration of the function with its conjugate performs two roles. The integration of the ideal function $\vec{\rho}_{\chi sc}$ represents the generation of a circular photon as the state vector executes its locus. The stability of the state as a whole depends on the destructive cancellation of this photon by the photon of the conjugate excursion. Thus, the normalization of the ideal part of the functions establishes the Moebius

Inversion multiplication of the function to its conjugate to establish this exact cancellation.

In contrast, the normalization of the uncertain part of the functions establishes the extent of *loss* of structural integrity of the state from the integration of the direct product of the uncertainties accumulated during the coupled excursions of the state vector and its conjugate. There is no geometric conjugacy of the uncertainties that permits mutual cancellation of the accumulated effects, since, by definition, they describe the randomization of the dynamic geometry. In sum, each normalized state exists in its own unique mechanical space.

The probability that the orientation and magnitudes of the properties of the state can be detected decreases from the total certainty of a hypothetical classical space towards zero since the uncertainty accumulates as the state vector executes the locus. Thus, the magnitudes characterizing any state are determined by the time τ taken to complete the excursion. Since this period cannot be exact, the magnitude of the property will display a maximum value at a particular value of its defining parameter and decay to zero above or below this value, as it becomes less probable. This characteristic of uncertain systems is called the "*width*" of the property.

Thus the normalization procedure has defined the unique shape and size of each state in terms of its ideal scaled Action, A_c . Traditionally, the probability integral is arbitrarily equated to unity so that all the calculated probability is contained within conventional three-dimensional space. In effect, all states are defined on one origin and given the same positional degree of magnification. In this calibration or gauge, the states are discriminated only in terms of scalar energies.

In non-orientable Moebius loci, this single adjustment to one guage is not possible, since eight orthogonal combinations of chirality, sense and coherence coexist on one origin in the same volume. These eight spaces are energetically degenerate in isolation but must all be used for calibration because they can be resolved by external fields into discrete observable states. In this sense, these spaces are "pro-observables" and must reside in the parental structure before symmetry descent imposed by external perturbations.

Normalization is performed on the fundamental eight-fold tensor to accomodate all geometries. On one origin, it adjusts the magnitudes of internal dimensions so that the radius of the state vector, which is coupled to the horizontal angle, can vary from zero to infinity of the scaled Action space as the angle α varies from zero of an arbitrary coherence direction to 2π radians. The meaning of terms "zero" and "infinity" in observable position or velocity spaces relies upon the magnitude of the electro-magneto-mechanical potential. This separate question can be explored by evaluating limiting behaviour of state vectors in an arbitrary potential.

II.5.ii   Energy Geometry and Conservation

The stability of bound states is usually evaluated in an operational form of Hamilton's expression of energy in which the energy dimensions are specified in the operator. The definition of natural coordinates in the dimensions of scaled Action indicates that the operator need only carry the dimensionless relative change in scaled Action. This format can be derived from classical mechanics. The chiral form of quantum mechanics requires the full four-dimensional Lagrangian rather than the

Hamiltonian which is restricted to a single choice of chirality and sense of rotation.⁵² It is usually expanded as the sum of the spherical kinetic and potential contributions;³⁰

$$L = T - V \quad (\text{II.5-1})$$

In contrast with $H = T + V$ where it is implied that the electron is exposed to a constant potential and, to conserve energy, the kinetic energy must also be constant. This is possible in an orbital of orientable geometry such as a sphere or a spherical harmonic. It is not possible for an electron in a non-orientable orbital. In such topology, the chiral energy is conserved but its composition varies periodically between entirely potential at the largest radius at the top of the potential well (which represents the Correspondence Limit where the Lagrangian vanishes and the atom dissociate);^{53,54} to entirely kinetic at the origin as the coupled conjugate state vectors sweep in opposite senses from 0 to 2π radians on their inverse Moebius loci which make up the natural coordinate axis. To illustrate this non-orientable energy, the kinetic and potential terms of the Lagrangian can be expanded in dimensional forms of velocity and position respectively.

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⁵² P.A.M. Dirac, Lectures on Quantum Mechanics, Belfer Graduate School of Science, Yeshiva University, 1964.

⁵³ J.H. Van Vleck, Quantum Principles and Line Spectra, National Research Council Bulletin #54, Washington, 1926.

⁵⁴ E.U. Condon and H. Odabasi, Atomic Structure, Cambridge University Press, Cambridge, 1980.

$$m l^2 t^{-2} = m \left[\frac{\vec{l}^*}{t} \right] \times \left[\frac{\vec{l}}{t} \right] + m \frac{(\vec{l}^*) \times (\vec{l})}{2} \quad (\text{II.5-2})$$

$$= \left[m^{1/2} \left(\frac{\vec{l}}{t} \right) \right] \times \left[m^{1/2} \left(\frac{\vec{l}}{t} \right) \right] + \left[m^{1/2} \left(\frac{\vec{l}}{t} \right) \right] \times \left[m^{1/2} \left(\frac{\vec{l}}{t} \right) \right]$$

in which; $\vec{l}$ is the displacement in "*momentum space*", parallel to the locus, $\vec{l}^*$ is the displacement from the origin to the locus in "*position space*", and $m^{1/2}$ is the root mass. Each of the four terms is the root inertia per unit time, $I^{1/2}/t$ as on a changing pathway the Inertia changes at all times and the changes are being observed. The sum is the total energy, $L = T + V$ which is a pseudoscalar in which the locus twists are being canceled out, thus cancelling out the geometry of Energy. The observable behaviour therefore arises from the root mass, which needs to be defined in geometric terms.

$$\frac{l}{t} = f \left[\frac{\sinh^{-1} \phi}{\cosh^{-1} \phi} \right] = f [\tanh^{-1} \phi] \left\{ \frac{l}{t} \right\}^* = f \left[\frac{\cosh^{-1} \phi}{\sinh^{-1} \phi} \right] = f [\coth^{-1} \phi]$$

Then, by substitution for these velocity and displacement dimensions on natural coordinates;

$$L = \left[m^{1/2} \left(\frac{\vec{\sigma}}{\alpha} \right) \right] \times \left[m^{1/2} (\vec{\sigma} \cdot \alpha) \right] + \left[m^{1/2} (\vec{\rho} \cdot \alpha) \right] \times \left[m^{1/2} \left(\frac{\vec{\rho}}{\alpha} \right) \right] / t^2 \quad (\text{II.5-3})$$

Two further steps are required; identification of the apparent topology of the time dimension to be substituted into the potential term and the mapping of the velocity and position of the conjugate functions into the space of the original functions so that the conservation of energy can be demonstrated. The first requirement can be solved by extracting the time topology from the velocity definition.

$$\vec{v} = \frac{\vec{l}}{\vec{\sigma}} = \frac{\vec{\sigma}}{\vec{\sigma}} = \vec{\sigma} \quad \tanh^{-1}a = \vec{\sigma} \frac{\sinh^{-1}a}{\cosh^{-1}a} \quad (\text{II.5-4})$$

This full definition of the velocity must, by Einstein's analysis, be tracked by the mass. The simplest interpretation of these definitions when considering only the ideal geometry is the set of identities;

$$m^{1/2} = f(\sinh^{-1}a) \quad \vec{l} = f(\sinh^{-1}a) \quad \vec{t} = f(\cosh^{-1}a) \quad (\text{II.5-5})$$

and

$$m^{1/2*} = f(\cosh^{-1}a) \quad \vec{l}^* = f(\sinh^{-1}a) \quad \vec{t}^* = f(\cosh^{-1}a)$$

Therefore equation (II.5-5) is seen to indicate that the l and t relationships cancel out to a normalized velocity space, while the mass space normalized onto itself. Furthermore, the derivative of the root mass with respect to path position ($d/dx \sinh^{-1}a$ or $d/dx \cosh^{-1}a$) yields $1/(a^2 + 1)^{1/2} da/da$ where $a = (-v/c)$ which is the Einstein definition of inertial mass. Therefore the path scales all the observable phenomena.

These cross products are observable phenomena because it appears that in heavy metal alloys the positive metallic lattice slows down the motion of the electrons to such an extent that they scatter off each other. This novel scattering produces a "*dynamic*" contribution to the electrical potential. It is the principle origin of the enormous mass of the heavy metal electrons. ⁵⁵

The geometric relationships are seen to be physically correct as can be illustrated by examining behaviour at the inflection points. **FIGURE II-4** is not entirely mathematically accurate as the axes have been distorted deliberately in order to present a point of view which allows the imagination to project the behaviour of the state vectors within the object.

$$a = 0 \qquad \tau = 1 \qquad \vec{t} = 0$$

the velocity starting from the origin of the locus is infinite so that for a coincident displacement of one unit $\vec{\sigma}$, the time elapsed is a characteristic minimum interval.

$$a = 1 \qquad \tau = \alpha \qquad \vec{t} = \alpha$$

the coincident displacement length approaches infinity slightly faster than the time period within the magnitude of the vectorial scaling factor $\vec{\sigma}$. However, as the ratio approaches unity the curve stops expanding, the displacement from origin reaches its maximum and then starts to decrease.

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⁵⁵ S. Law, "Electrons Switch On to Heavy Metal", New Scientist, 126, 57-60 (1990).

FIGURE II-4 State Vector Behaviour on a Moebius Locus

This derivation is valid for time in both the $\vec{T}$ and $\vec{t}$ spaces so that;

$$\vec{t} = \vec{\tau} \cosh^{-1} a \quad (\text{II.5-6})$$

will define mechanical Moebius time in terms of a period $\vec{\tau}$ which is vectorial because it refers to the direction along the locus in which the time is measured.

The second requirement is solved by applying the Moebius Inversion to the geometry of the original functions. This operator inverts all properties, including, chirality, sense of rotation, coherence phase and the length of the position vector. In the real horizontal plane, the one dimensional projected position vector is only affected by the inversion of the coherence phase ;

$$\vec{r}^* = -\vec{\rho} \frac{1}{\alpha} \quad (\text{II.5-7})$$

The inversion of the coherence phase and the sense of rotation impose a two-fold inversion on the velocity so that;

$$\vec{v}^* = \left[\vec{\sigma} \left(\frac{1}{\alpha} \right)^{-1} \right]^{-1} = -\vec{\sigma} (\alpha)^{-1} = -\vec{\sigma} \left(\frac{1}{\alpha} \right) \quad (\text{II.5-8})$$

Substitution of these conjugate properties, seen now in the locus of the original space, the final Lagrangian becomes;

$$\begin{aligned} L &= \left[-m \vec{\sigma}^2 \left(\frac{1}{\alpha} \right)^2 \right] - \left[m \vec{\rho}^2 \left(-\frac{1}{\alpha} \right) \cdot (\alpha) / \vec{\tau}^2 (\cosh^{-1} a)^2 \right] \\ &= \left[-m \vec{\sigma}^2 (\tanh^2 \phi) \right] - \left[-m \vec{\rho}^2 \vec{\tau}^{-2} (\text{sech}^2 \phi) \right] \end{aligned} \quad (\text{II.5-9})$$

Since the dimensions of both the kinetic and potential energy terms are unaffected by these geometric restatements, the Lagrangian in this form becomes a normalized identity describing a constant energy of the system because, by definition;

$$-\tanh^2 \phi + \operatorname{sech}^2 \phi = 1 \quad (\text{II.5-10})$$

II.5.iii   Ideal Natural Energy Coordinates

A comparison of the formal Lagrangian (II.5-1) with its dimensional expansion in (II.5-2) suggests that L could be regarded as a difference of "energy squares". Traditionally, L and hence T and V are described in one position space so that kinetic energy is defined as a scalar product of velocities and potential as a scalar product of positions defined in that chosen space. However, the four-dimensional $\mathcal{L}$ actually represents the inner direct products of velocity and position vectors from their respective, conjugate three-dimensional spaces. Thus, the factorization as a difference of squares in the four-dimensional mechanical space, explicitly restates the energy as an inner product of conjugate sums of root kinetic energy, t and root potential energy, v ;

$$\begin{aligned} L &= (T - V) \\ &= (t + v)^* (t - v) \end{aligned} \quad (\text{II.5-11})$$

The star (*) symbol represents an operation algebraically similar to conjugation whose geometric meaning will be developed later. The simplest dimensions of the sum or difference of t and v can be derived as the conjugate square roots of energy;

$$m l^2 t^{-2} = \left[m^{1/2} \begin{pmatrix} \vec{1} \\ t \end{pmatrix} \right]^* \times \left[m^{1/2} \begin{pmatrix} \vec{1} \\ t \end{pmatrix} \right] = "1" \quad (\text{II.5-12})$$

which can be recognized as conjugate velocities scaled to $m^{1/2}$ normalized to the energy of the state. Therefore any standard trigonometric relationship that reflects normalization can be validly applied. However, the minimum unit vector of quantum mechanical space is derived from Planck's constant in dimensions of Action, ml^2t^{-1} . To employ this vectorial unit, the dimensionality must be restated as Action scaled to the moment of inertia of the mechanical space. One of the consequences of dealing with a non-orientable surface is a constancy in total energy. However the distribution of that energy can change, as can the distribution of the energy on the conjugate partner.

Multiplying both numerator and denominator of (II.5-12) by the moment of inertia $I = ml^2 = (m^{1/2}l)(m^{1/2}l)$ yields the relationship

$$= \left[\frac{m l^2 t^{-1}}{m^{1/2} l} \right]^* \times \left[\frac{m l^2 t^{-1}}{m^{1/2} l} \right]$$

which is now in the form of Action scaled to the root moment of inertia. This is a scaling factor for the entire space, that is the basic constant of the entire space.

The purpose is to put the functions from equation (II.5-5) back in order to allow an explicit factorization in the form of kinetic and potential energies on *non-orientable natural coordinates*. Any standard real trigonometric normalization relationship can be used, the least complex available being the hyperbolic function based on $(\tanh^2 x - \text{sech}^2 x = 1)$.

The real hyperbolic functions are required to avoid turning axes inside out, an operation which will be demonstrated in (II.5-29). Turning the axes inside out is an inversion operation which is required as an operation of its own in order to observe Moebius rotations with group theory. Simplifying equation (II.5-10) by removing the common term yields

$$= \left[\frac{\cosh}{\sinh} + \frac{1}{\sinh} \right] \times \left[\frac{\cosh}{\sinh} - \frac{1}{\sinh} \right] = \left[\frac{1}{\sinh} \times (\cosh + 1) \right] \times \left[\frac{1}{\sinh} \times (\cosh - 1) \right]$$

Recognizing that $(\cosh + 1) = [(t + v)/m^{1/2}]^*$ and $(\cosh - 1) = [(t + v)/m^{1/2}]$ since $1/\sinh = m^{1/2}$, the energy relationship is seen as:

$$= \overrightarrow{(t + v)}^* \times \overleftarrow{(t - v)} \quad (\text{II.5-13})$$

where $\left[\frac{\cosh}{\sinh} + \frac{1}{\sinh} \right] = (t + v)^*$ and $\left[\frac{\cosh}{\sinh} - \frac{1}{\sinh} \right] = (t - v)$

thus generating a root energy wave function which enables the probe to "sit" on the potential and watch the kinetic energy, the traditional technique used as kinetic behaviour has been unknown and now can be specified. Having created an axis that permits tracking Action it is possible to track the change in kinetic energy for the first time.

This sum and difference were identified as the *conjugate* states of scaled Action in the initial description of states on natural coordinates. As in the case for energy, the total Action remains constant, although it is redistributed between the conjugate pathways as one partner gains action to a maximum at the nucleus and the other loses action at the infinite node. The root kinetic and potential energies of (II.5-12) can be redefined as the kinetic and potential scaled Action of the Lagrangian.

The factoring of this explicitly conjugate pair of scaled Action states can be projected into a three-dimensional 3D mechanical space to allow descriptions of observable properties of the system. In this tensorial subspace, the reconstruction of the difference of squares shows that the usual algebraic difference of squares of scalar multiplication is not obtained. Instead, the *cross terms* of the momenta with position survive;

$$\begin{aligned}
 \overrightarrow{(t + v)}^* \times \overleftarrow{(t - v)} &= \vec{t}^* \times \vec{t} - \vec{t}^* \times \vec{v} + \vec{v}^* \times \vec{t} - \vec{v}^* \times \vec{v} \\
 &= \left[\left(\frac{\vec{\sigma}}{\alpha} \times \vec{\sigma} \alpha \right) - \left(\frac{\vec{\sigma}}{\alpha} \times \frac{\vec{\sigma}}{\alpha} \right) + (\vec{\sigma} \alpha \times \vec{\sigma} \alpha) - (\vec{\sigma} \alpha \times \frac{\vec{\sigma}}{\alpha}) \right] \\
 &= \left[(1) - \left(\frac{\vec{\sigma}}{\alpha} \times \frac{\vec{\sigma}}{\alpha} \right) + (\vec{\sigma} \alpha \times \vec{\sigma} \alpha) - (1) \right] \\
 &= \left[-\vec{t}^* \times \vec{v} + \vec{v}^* \times \vec{t} \right] \quad (\text{II.5-14})
 \end{aligned}$$

This factorization shows that the state energy can be defined as a difference between a negative, attractive and a positive, repulsive scaled Action. Each is defined in turn as a vector product of conjugate kinetic, $\vec{t}$ and potential, $\vec{v}$ root scaled Action, which

indicates that both potential and kinetic Action occur in these two forms. The attraction and repulsion forms of potential are familiar and are represented by $\vec{v}$ and $\vec{v}^*$. Kinetic Action is usually understood only as a repulsive influence since its addition to a system is thought to reduce order. However, in a fully chiral space, the kinetic coupling of a bound particle can occur either constructively or destructively. Constructive coupling of conjugate Kinetic scaled Action represented by $\vec{t}$, permits an additive coherence of state vectors, producing a net transient projection on the principal axis. This allows radiation of energy and destabilization of the mechanical space of the state. Destructive coupling, $\vec{t}^*$ causes the mutual cancellation of coherence phase at all positions of the state vector, preventing radiation and stabilizing the state.

Since only the coherence phases of the scaled Action functions are correlated in three dimensions by this conjugate coupling, the difference $\overleftarrow{(t - v)}$ and the conjugate sum $\overrightarrow{(t + v)}^*$ must represent in turn, further differences of squares to describe the coupling of chirality and sense of rotation within the scaled Action states. On formal factoring, the tensorial difference becomes;

$$\begin{aligned}
 \overleftarrow{(t - v)} &= (\varphi \vec{t} \iota)^* (\varphi \vec{v} \iota) \\
 &= (\vec{\varphi}^* \times \vec{t}) - (\vec{\varphi}^* \times \vec{v}) + (\vec{t}^* \times \vec{\varphi}) - (\vec{v}^* \times \vec{\varphi}) \\
 &= [(-\vec{\varphi}^* \times \vec{t}) + (\vec{t}^* \times \vec{\varphi})]
 \end{aligned}
 \tag{II.5-15}$$

following the previous vectorial procedure.

The factoring of the conjugate sum $(\vec{t} + \vec{v})^*$ follows the same rules;

$$\begin{aligned}
 (\vec{t} + \vec{v})^* &= [(\vec{\varphi} - \vec{v})(\vec{\varphi} + \vec{v})]^* \\
 &= [(\vec{\varphi}^* \times \vec{v}) - (\vec{v}^* \times \vec{\varphi})]^* \\
 &= [(\vec{\varphi} \times \vec{v}^*) - (\vec{v} \times \vec{\varphi}^*)]
 \end{aligned}
 \tag{II.5-16}$$

This defines a second set of parameters $\vec{\varphi}$ and $\vec{v}$, the kinetic and potential forms of root scaled Action of a state. Each state is normalized to the parameters of the supporting space, which are collected in $\vec{\sigma}$, or equivalently, in the product $\rho \vec{x} \tau^{-1}$. Thus the normalized energy of the state can be written directly as;

$$\begin{aligned}
 L &= [(\vec{\varphi} - \vec{v})(\vec{\varphi} + \vec{v})]^* [(\vec{\varphi} + \vec{v})(\vec{\varphi} - \vec{v})] \\
 &= [\vec{\varphi}^* \vec{v} - \vec{v}^* \vec{\varphi}]^* [-\vec{\varphi}^* \vec{v} + \vec{v}^* \vec{\varphi}] \\
 &= [\vec{\varphi} \vec{v}^* - \vec{v} \vec{\varphi}^*] [-\vec{\varphi}^* \vec{v} + \vec{v}^* \vec{\varphi}] \\
 &= [-\vec{\varphi} \vec{v}^* \vec{\varphi} \vec{v}^* + \vec{\varphi}^* \vec{v} \vec{v}^* \vec{\varphi} + \vec{v}^* \vec{\varphi} \vec{\varphi} \vec{v}^* - \vec{v} \vec{\varphi}^* \vec{v}^* \vec{\varphi}] \\
 &= [-\vec{v} \vec{\varphi}^* \vec{\varphi}^* \vec{v} + \vec{v}^* \vec{\varphi} \vec{\varphi} \vec{v}^*] \\
 &= [(-\vec{v}^* \times \vec{v}) + (\vec{v} \times \vec{v}^*)]
 \end{aligned}
 \tag{II.5-17}$$

since only the non-orientable cross products do not commute and the surviving terms represent respectively the stabilizing and destabilizing combinations of kinetic and potential energy. In essence, this is a topological expression of the concept of "exchange energies" of bound electrons.

II.5.iv   Normalization in the Electromagnetoinertial Gauge

The model of atomic structure has been developed in the four-dimensional mechanical space to provide unambiguous definitions of all tensorial properties. In particular, this space avoids the singularities of either of the constituent velocity or position spaces. The smooth inversion of the Action state vector through the fourth dimension at the origin of these natural coordinates, replaces the apparent singularity of an undefined phase reversal which arises in a traditional description of orbitals in a purely position or velocity space description. Similarly, the smooth recursion of the vector from an increasing to a decreasing radius due to uncertainty resolves the apparent singularity of an infinitely long vector as it passes through the horizontal plane. The recursion occurs because the vectors of position and velocity reach extreme values. While position tends to infinity, velocity is at right angles, point across the position node to the next segment of the path. As long as the velocity vector is not so uncertain as to also point to a position of infinity, the state vector can cross to the next segment. As long as the energy of the state is finite, this outer limit of the mechanical space actually corresponds to a vector of finite length in position space. As the stability of the state approaches zero, the projection of this vector in position space increases until it becomes infinite as the electron becomes a free particle. This behaviour is completely consistent with the De Broglie Wave-Particle Duality of atomic structure.

However, the properties of atoms are usually observed in experiments done in position space. Since the size and shape of the mechanical space projected into position space depends inversely on the energy content, a description of the state structure in positional space requires a calibration of the mechanical space which

depends on this inverse relationship. In this sense, the internally "*guage invariant*" mechanical spaces for each state are "*guage dependant*" in the larger experimental positional space. The same circumstances apply to a description of the state in an experimental velocity or "*momentum*" space, such as used in electron energy loss spectroscopies.

The guage invariance of the experimental space is achieved by placing all the guage information into the coordinates. Thus, the energy of the state is expressed in terms of a scaling factor of the mechanical coordinate to observable properties of the supporting spaces. This provides an expectation value of the state energy in terms of fundamental physical constants. The form of each of the velocity and position supporting spaces is defined by the topology of the significant forces in each subspace.

In atomic systems, both electric and magnetic forces act between charged, spinning, massy particles. For any orbiting electron or coupled set of electrons characterized by a net orbiting vector, the electric and magnetic forces are orthogonal. The electrical forces set up an orthogonal three-dimensional mechanical position subspace, whereas the magnetic forces set up a three-dimensional mechanical velocity subspace. In many-electron atoms these forces do not act through vacuum but through the background of all rotating charged particles. Thus, the relevant sizes and shapes of the mechanical subspaces are scaled to C , the *electric capacitance* of the state and L , the *magnetic inductance* of the state. In this format, the mechanical properties are still specified as attributes of vectors on the coordinates of the subspaces instead of as properties in the definition of the coordinates themselves. A simpler and more general form can be derived by attributing inertial,

magnetic, and electric permeabilities to the space and defining an electromagnetoinertial Action metric on the natural geometric coordinates. The obvious unit for the metric of their combined mechanical space will be the smallest observable unit of Action, as defined by Planck's constant, $\hbar$. The redefined functions can be constructed by first using the definitions of inductance and capacitance;

$$C = \epsilon \vec{r} \text{ and } L = \mu \vec{r} \quad (\text{II.5-18})$$

in which μ is the *magnetic* and ϵ is the *electric permeability* of the atomic space and r is the instantaneous position of the state vector. In parallel, an equivalent definition of the moment of inertia I becomes necessary to describe the full obedience of the system to the laws of conservation of energy and momentum;

$$I = \gamma \vec{r} \quad (\text{II.5-19})$$

in which γ is an "*inertial permeability*". Now the instantaneous position of the state vector $\vec{r}$ on the locus is always associated with the completely general, tensorial spatial properties, ϵ , μ and γ .

II.5.v   Electromagnetoinertial State Coordinates

The electromagnetoinertial normalization means that expressions for both the kinetic and potential contributions to the total Lagrangian are readily derived and substituted for the traditional mechanical form; ⁴⁵

$$\begin{aligned}
 L &= T - V \\
 &= \frac{1}{2} \left[L \frac{d^2 q}{dt^2} - \frac{q^2}{C} \right] \\
 &= \frac{1}{2} \left[L i^2 - \frac{i^2 t^2}{C} \right]
 \end{aligned} \tag{II.5-20}$$

By differentiating with respect to time to define the steady state associated with this energy;

$$\frac{dL}{dt} = \left[Li \frac{di}{dt} + \frac{i^2 t}{C} \right] = 0 \tag{II.5-21}$$

On simplification by dividing by i^2 , this becomes a first order expression in a dimensionless current and in time;

$$\frac{di}{i} = \frac{-1}{LC} t dt \tag{II.5-22}$$

In this form, the Lagrangian operator cannot display Hermitian properties but the differential equation is solved by Hermite expressions of the form;

$$i = \exp \left[\frac{-\bar{t}^* \times \bar{t}}{2 LC} \right] \tag{II.5-23}$$

in which this dimensionless "current" i can be recognized as a pair of oppositely polarized motions of charge, each following one of the conjugate pair of loci in the direction indicated by the time vector of the space, $\bar{t}$ or $\bar{t}^*$. In this current model, the Lagrangian description of steady states places the first of two levels of Hermitian requirements in the wave functions, revealing that states can be modelled as Mobius pairs of completely counteracting currents in orthogonal but conjugate spaces.

These spatial gauge correlations between the generalized mechanical space and the more specific electromagnetioinertial space can be incorporated into the full description of steady states by a dimensional analysis which explicitly recognizes that ϵ , μ and γ are not in general unity, especially in real atoms. ⁴⁵ Introduction of these additional scaling components, (II.5-18) and (II.5-19), requires energy in (II.5-17) to be written;

$$L = \frac{(m^2 \mu \epsilon \text{ l }^6 \text{ t}^{-4})(\text{t}^2)}{I L C}$$

This general form can be projected into three dimensions onto the magnetic axis as follows;

$$\begin{aligned} L &= \left[\left(\frac{m^{1/2} \mu^{1/2} \text{ l }^{3/2} \text{ t}^{-1}}{I^{1/2} L^{1/2}} \right) (\vec{t}) \times \left(\frac{m^{1/2} \epsilon^{1/2} \text{ l }^{1/3} \text{ t}^{-2}}{C^{1/2}} \right) (\vec{t}^* \times \vec{t}) \right]^2 \\ &= \left[\left(\frac{\vec{J}}{I^{1/2} L^{1/2}} \right) (\vec{t}) \times \left(\frac{\vec{I}}{C^{1/2}} \right) (\vec{t}^* \times \vec{t}) \right]^2 \end{aligned} \quad (\text{II.5-24})$$

in which $\vec{J}$ is the *magnetic flux* of a one-dimensional time subspace and $\vec{I}$ is the rotating *electric current* of the accompanying, orthogonal two-dimensional time subspace. On comparing this development with (II.5-17), two identities can be established between the formal vectors and those derived by dimensional analysis;

$$\vec{\varphi} = \left[\frac{\vec{J}}{I^{1/2} L^{1/2}} \right] (\vec{t});$$

$$\iota = \left[\frac{\vec{i}}{C^{1/2}} \right] (\vec{t}^* \times \vec{t}) = \left[\frac{(\vec{i} \times \vec{t})^*}{C^{1/2}} \right] (\vec{t}) \quad (\text{II.5-25})$$

The formal *flux* $\vec{\varphi}$ is the conventional flux $\vec{J}$ scaled to the root moment of inertia and the inductance of the mechanical space, multiplied by the time vector of the periodic rotation between nodes. Thus, $\vec{\varphi}$ plays the role of root kinetic Action in a three-dimensional velocity subspace of the state by representing the flow of magnetic lines of force along the principal axis. This conventional magnetic flux $\vec{J}$ is mechanically equivalent to the magnetic pole or quantity of magnetism and could be called the "*magnetic charge*" projected onto the principal three-dimensional axis. This *flux* $\vec{\varphi}$ is stabilizing or its conjugate $\vec{\varphi}^*$ is destabilizing depending on the sign of the time vector. This is known as the Zeeman splitting.

Similarly, the formal *current* $\vec{\iota}$ is the *electric current* $\vec{i}$, scaled to the capacitance of the mechanical space, multiplied by the direct product of the conjugate time vectors. This conventional current is mechanically equivalent to the magnetomotive force and the magnetic potential of the two-dimensional time subspace. Thus, $\vec{\iota}$ plays the role of the root potential Action in the three-dimensional position subspace, representing the strength of the magnetic field in the horizontal plane. The formal current $\vec{\iota}$ is stabilizing or its conjugate $\vec{\iota}^*$ is destabilizing depending on the sign of the remaining time vector.

In the *magnetic flux* subspace, the time vector defines the direction of motion of the flux with respect to any external magnetic field along the principal axis of the three-dimensional mechanical space. In the *electric current* subspace, the two-dimensional time axes define the orientation and curvature of the electric field in the horizontal plane with respect to the horizontal component of any external electric field. This geometric expression is formally equivalent to the curl of the Maxwell equations. At the origin, the time component will be directed with or against the horizontal electric external field. This defines the coherence phase of the state. However, since the natural coordinates are Moebius loci, the emerging vector must also define a boost of this curl about the principal axis, requiring the existence of an additional operator in the Maxwell equations to describe the handed "*pitch*" of the state vector. Taken together, all possible vector products of motion in the two subspaces define the coupling possibilities of these three properties, creating all eight projected magnetic subspaces of the four-dimensional mechanical space.

A completely equivalent projection of the eight electric subspaces is factored to project onto the electrical axis of a three-dimensional mechanical space instead of the magnetic axis of (II.5.2-25). Thus;

$$\begin{aligned}
 L &= \frac{(m^2 \mu \epsilon l^6 t^{-4})(t^2)}{I L C} \\
 &= \left[\left(\frac{m^{1/2} \epsilon^{1/2} l^{3/2} t^{-1}}{C^{1/2}} \right) (\vec{t}) \times \left(\frac{m^{1/2} \mu^{1/2} l^{3/2} t^{-2}}{I^{1/2} L^{1/2}} \right) (\vec{t}^* \times \vec{t}) \right]^2
 \end{aligned}$$

2

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or

$$L = \left[\left(-\frac{\vec{f}}{C^{1/2}} \right) (\vec{t}) \times \left(-\frac{\vec{t}}{I^{1/2} L^{1/2}} \right) (\vec{t}^* \times \vec{t}) \right] \quad (\text{II.5-26})$$

in which; f is the *electrical flux* of the mechanical space and $\vec{t}$ is the *magnetic current* of the space. Again by comparison with (II.5-17);

$$\begin{aligned} \vec{\phi} &= \left[\frac{\vec{f}}{C^{1/2}} \right] (\vec{t}); \\ \vec{t} &= \left[\frac{\vec{t}}{I^{1/2} L^{1/2}} \right] (\vec{t}^* \times \vec{t}) \end{aligned} \quad (\text{II.5-27})$$

In this alternative but equivalent definition, the *electrical flux* now lies along the principal time coordinate and plays the role of the root kinetic Action. This *flux* is mechanically equivalent to an "electric pole" and can likewise be defined as the electric charge projected onto the principal axis of the alternative three-dimensional mechanical subspace. The formal *flux* is stabilizing or destabilizing depending on the alignment of the electric pole with an external electric field. This is known as the Stark splitting.

The two-dimensional *magnetic current* is mechanically equivalent to the electromotive force and consequently, the electric potential of this three-dimensional mechanical subspace. Since it depends again on two time coordinates, the coherence phase to any horizontal, external magnetic field and the curvature in the sense of rotation around the principal axis are both defined. Again the eight possible mechanical subspaces in three dimensions are defined.

These alternative projections each yield an "axial" subspace characterized by a "vertical" principal axis perpendicular to a "horizontal" plane. In (II.5-3), projections of the four-dimensional natural coordinates into the horizontal plane of a three-dimensional *position* subspace were established for general, orthogonal position and velocity vector components. The general two-dimensional position vector in this plane depends on both the coherence phase, for its initial orientation and the sense of rotation, or more appropriately, the sense of expansion, for its complete description. The orthogonal velocity vector in this plane is couple to this locus with only the single decision of the sense of rotation with or against the sense of expansion. Thus for the magnetic projection, (II.5-28),

$$\begin{aligned}\vec{\varphi} &= \left[\frac{\vec{J}}{I^{1/2} L^{1/2}} \right]^* (\vec{t}) = (\vec{\sigma})^{1/2} = (\vec{\sigma} \times \tanh^{-1} \mathbf{a})^{1/2} \\ \vec{t} &= \left[\frac{\vec{I}}{C^{1/2}} \right] (\vec{t}^* \times \vec{t}) = (\vec{\rho} \alpha)^{1/2} = (\vec{\rho} \times \operatorname{sech}^{-1} \mathbf{a})^{1/2}\end{aligned}\quad (\text{II.5-28})$$

leading to the identities;

$$\begin{aligned}\left(\frac{\vec{J}}{\alpha}\right)^{1/2} &= (\vec{\sigma} \operatorname{sech}^{-1} \mathbf{a})^{1/2} = \vec{J}^* \times \vec{t} \\ (\vec{\sigma})^{1/2} &= \frac{\vec{I}}{I^{1/2} L^{1/2}} \\ (\vec{\alpha})^{1/2} &= (\tanh^{-1} \mathbf{a})^{1/2} = \vec{I} \times \vec{t}^* \times \vec{t}\end{aligned}$$

and

$$(\vec{\rho})^{1/2} = \frac{\vec{l}}{C^{1/2}} \quad (\text{II.5-29})$$

The electric projection can be expressed equivalently as;

$$\begin{aligned} \vec{\phi} &= \left[\frac{\vec{l}}{C^{1/2}} \right]^* (\vec{l}) = \left(\frac{\vec{\sigma}}{\alpha} \right)^{1/2} = (\vec{\sigma} \times \tanh^{-1} \mathbf{a})^{1/2} \\ \vec{l} &= \left[\frac{\vec{l}}{I^{1/2} L^{1/2}} \right]^* (\vec{l}) = (\vec{\rho} \alpha)^{1/2} \\ &= (\vec{\rho} \times \text{sech}^{-1} \mathbf{a})^{1/2} \end{aligned} \quad (\text{II.5-30})$$

leading to the identities;

$$\begin{aligned} \left(\frac{\vec{l}}{\alpha} \right)^{1/2} &= (\vec{\sigma} \times \tanh^{-1} \mathbf{a})^{1/2} = \vec{l}^* \times \vec{l} \\ (\vec{\sigma})^{1/2} &= \frac{\vec{l}}{C^{1/2}} \\ (\vec{\alpha})^{1/2} &= (\tanh^{-1} \mathbf{a})^{1/2} = \vec{l} \times \vec{l}^* \times \vec{l} \\ (\vec{\rho})^{1/2} &= \frac{\vec{l}}{I^{1/2} L^{1/2}} \end{aligned} \quad (\text{II.5-31})$$

Alternatively, all projections could be taken into a three-dimensional velocity space, reversing the roles, so that;

$$\vec{\sigma} \alpha = \vec{sech}^{-1}a \quad \text{and} \quad \vec{\rho} \alpha = \vec{tanh}^{-1}a \quad (\text{II.5-32})$$

and all expressions are adjusted accordingly.

In either case, the vector product of one-dimensional *current* with two-dimensional *flux* ($r_3 \times r_3$ with a common origin and coherently placed axis) leads to a *four-dimensional property* defined as the *scaled Action*. Since this dimension lies outside the dimensions of both the position or velocity subspaces, it is *imaginary* to both. As described in (II.4-4), this cross product exists in a coordinate with a composite scale of $\vec{\rho}^* \times \vec{\sigma}$, on the *imaginary projection* of the real, hyperbolic coordinates. Since circular angle functions are imaginary with respect to hyperbolic angle functions, the appropriate description of these projects can be stated as;

$$m\vec{\mu} = (\vec{\rho}^* \times \vec{\sigma}) \sin^{-1}a; \quad e\vec{\epsilon} = (\vec{\sigma}^* \times \vec{\rho}) \cos^{-1}a \quad (\text{II.5-33})$$

representing the magnetic and electric components of the projected Action from the alternative subspaces.

Since these projections originate from orthogonal subspaces and are out of phase on the Action coordinate, the net projection on the Action coordinate is the result of the combined values of these two properties. Thus, a "*magnetic quantum number*", m , defined from the magnetic subspace carries an electric degeneracy and the

equivalently necessary electric quantum number e must carry the magnetic degeneracy. Therefore both $\vec{\mu}$ and $\vec{e}$ must be specified before the description of any state is complete and before any assignment of spectroscopic transitions is realized. This explicit expression of current and flux defines the metrics on the electromagnetoinertial axes of the full mechanical space. It is clear from (II.5-29) and (II.5-31) that these metrics are not constant displacements. Along the locus illustrated in **FIGURE II-4**, a metric of constant current $\vec{J}$ corresponds to a *continuously changing* unit length of path in the hyperbolic space. An equivalent variation occurs in the metric of flux on the perpendicular axis in its circular space. Thus the curvature of this non-orientable space applies to the metrics on the natural coordinates and to all their derived properties. In particular this non-linearity defines the accumulation of uncertainty for processes on these coordinates and applies to the final normalization of the whole relativistic and partially uncertain structure.

The normalization of the mechanical space to the field properties $\vec{\epsilon}$, $\vec{\mu}$ and $\vec{\gamma}$ has established a four-dimensional, classical mechanical space in which all the information needed to describe the stability and full, non-orientable, dynamic geometry is built into the four natural coordinate axes of the space. The full scaled Action, A of a state is defined by the excursion of the state vector along the four-dimensional coordinate in the time t necessary between adjacent nodes. Stability and geometry are the two observable three-dimensional consequences of the complete Action of four-dimensional space.

Since the transform from traditional position/velocity to flux/current language is unitary then at every point along the classical natural coordinates of scaled Action, a finite amount of uncertainty in the relationship of *flux* to *current* is necessarily present. Since this uncertainty both reduces the stability and degrades the dynamic structure randomly, a conjugate uncertainty which nullifies the effect of the original influence cannot be defined. Thus, the uncertainty acts as a linearly additive function along the natural coordinates. It defines the "*amplitude*" of the complete wave function as the proportion of the classical properties of the state vector which remain certain at the end of an excursion on the locus. As expressed in (II.4-11) and (II.4-12), the "certainty wave functions" ψ_c are the products of the uncertainty functions measured on the unit vectors on the natural coordinates, A_c in time t ;

$$\psi_c = \left[\left(\frac{dA}{dt} \right) (A_c t) \right] \quad \text{and} \quad \psi_c^* = \left[\left(\frac{dA}{dt} \right) (A_c^* t) \right] \quad (\text{II.5-34})$$

The general normalization stated in (II.4-13) can now be made specific for scaled Action certainty wave functions in the four-dimensional mechanical space or for any property projected into a three-dimensional observational, mechanical subspace. The natural coordinates A_c are already normalized to the mechanical properties of the system but the uncertainty (dA_c/dt) must be normalized over time. The topology of time in these states defines periods τ , for the time necessary for the state vector to complete an excursion between nodes of the locus. Thus, the certainty is found normalized on a *path integration* of the instantaneous uncertainty over the period τ . The infinitesimal of the path integration, dA , specifies the projection of the classical properties of the full four-dimensional coordinate onto the principal, Action coordinate from each point on the coordinate.

Path integration on the natural coordinate α for one excursion therefore predicts the degraded value of the projected classical properties of the coordinate. However, these expectation values can only be observed in a projected, three-dimensional subspace in which they retain all the tensorial properties of the projected principal axis, including preferred chirality and sense of rotation. Physically, this would mean the state must radiate during the excursion. This can only be prevented by coupling to the conjugate excursion, so that a double integration is required across the pair of coupled coordinates $\psi_c^* \psi_c$, to yield the expectation energy, L from the net reciprocal Action of the coordinate pair. Moreover, this double integration applies to both constructive and destructive forms of coupling;

$$L = - \int \int \left[\frac{h}{\Delta A} A_t^* \right] \times \left[\frac{h}{\Delta A} A_v \right] d\alpha + \int \int \left[\frac{h}{\Delta A} A_v^* \right] \times \left[\frac{h}{\Delta A} A_t \right] d\alpha \quad (\text{II.5-35})$$

This normalization differs from the conventional Schroedinger form in three distinct ways. The first is the adaptation of the coordinates to the full symmetry of the underlying mechanics together with their scaling to both the magnitudes of the underlying electromagnetic fields and the inertia of the coupled electrons. This means that the normalization itself defines the Ideal net expectation energy of the state for its projection into the chosen, observational subspace.

Secondly, as is required in (II.5-35), the normalization applies equally to the stabilized, destructively coupled and the destabilized, constructively coupled scaled Action contributions to L . For a properly normalized state this normalization should explicitly confirm that the net expectation, in any observation space, must arise entirely from the destructively coupled term. Any contribution from the constructively coupled term means that the state is in transition. This can be illustrated by the normalization of the axially projected part of the total Action which defines either the magnetic or electric quantum vector, aligned to an external field. The appropriate projection from (II.5-35), ignoring uncertainty which will only reduce the strength (g), yields the pair of normalization contributions;

$$\begin{aligned}
 n &= \left[-\int \int \alpha^* \alpha d\alpha + \int \int \frac{1^*}{\alpha} \frac{1}{\alpha} d\alpha \right] \\
 &= \left[-\int_0^{2\pi} \int_0^{2\pi} \sin^2 \phi/2 d\phi + \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{1}{\sin^2 \phi/2} d\phi \right] (g\beta) \\
 &= \left[-(\phi/4 \mid_0^{2\pi}) + (-\cot \phi/2 \mid_{-\pi}^{\pi}) \right] (g\beta) \\
 &= [-(\pi/2) + (0)](g\beta)
 \end{aligned} \tag{II.5-36}$$

in which the Moebius inversion of mechanical axes requires integration appropriate to the unique conjugate excursion of the state vector. Taken between limits defined by these coordinates, the definite integrals confirm that the stabilized contribution is finite, while the destabilized contribution vanishes. The coordinates α carry the varying metric which defines the topology so that the result can be stated as multiples of Planck's constant of Action normalized to the Lagrangian energy, $h/2$;

$$\begin{aligned} n &= (m \text{ or } e) = [\pi/2] (h/2)(\text{unit vector}) \\ &= (m \text{ or } e) = [1/2] (\hbar)(\text{unit vector}) \end{aligned} \quad (\text{II.5-37})$$

This relationship shows that the fundamental, half-integer quantum number system emerges as a consequence of the Moebius topology executed by Fermions in chiral, three-dimensional observational spaces. Thus, the association of half-integer algebra with state topology, hinted at by Heisenberg and Schroedinger, becomes explicit in non-orientable geometry.

The third aspect of the normalization is the explicit treatment of uncertainty as the accumulated decay of structure during the excursion of the state vector. From (II.4-9) and (II.4-10), the uncertainty can be viewed as a vector product of deviations in the position and velocity space scaling factors, $\Delta\rho$ and $\Delta\sigma$. In such a model, uncertainty arises from *imperfections* in the through-space fields which couple the position and velocity subspaces. The deviations of the vectors from classical behaviour are merely symptoms of these field limitations. The origin of these imperfections is clearly a time dependant influence from dimensions beyond those used in constructing the four-dimensional mechanical space from the weak

nuclear and electromagnetic forces. A possible origin will be discussed in the context of the topology of energy and time.

The topology of the volume of uncertainty $U(\alpha)$, on the four-dimensional surface depend on the position of the state vector. At the origin, $\vec{r}$ is small and $\Delta\vec{r}$ is relatively large, conversely, $\vec{v}$ is near light speed and $\Delta\vec{v}$ is insignificant. In contrast, when the state vector reaches its extreme displacement, the opposite uncertainty volume shape is achieved but the volume itself remains constant. Thus, as shown in (II.4-11), the uncertainty is a simple, linear function of α . This can be explicitly introduced into the non-vanishing term of (II.5-35);

$$\begin{aligned}
 L &= - \int \int \alpha^* \times \alpha d\alpha \\
 &= - \int_0^{2\pi} \int_0^{2\pi} \left[\frac{\hbar}{\Delta A_t} A_t \right]^* \times \left[\frac{\hbar}{\Delta A_v} A_v \right] d\phi \\
 &= -\hbar^2 \int_0^{2\pi} \left[\frac{1}{\Delta A_t^* \Delta A_v} \right] d\phi \cdot \int_0^{2\pi} \int_0^{2\pi} A_t^* \times A_v d\phi \quad (\text{II.5-38})
 \end{aligned}$$

The factorization indicates that the integrated, hence accumulated uncertainty reduces the ideal, classical energy, hence stability, of the state. This phenomenon must accompany all the properties of the state as they are projected for observation into any other subspace such as magnetic or electric fields.

These steps of normalization are needed each time the structure of a mechanical space is projected from four dimensions into a three-dimensional subspace for observation of a property. While the basic vectors fully occupy the four-dimensional space, ranging across the full extent of the natural coordinates, the projected images can occupy very assymmetric and limited values when adapted to the chosen axes of the subspaces. Hence, atoms can appear to be "distorted" or "very small" in observational position spaces, depending on the ratio of the mechanical space energy tensor to that of the subspace.

The topologies of time and displacement in both velocity and position subspaces have been defined in (II.5-5). Since bound particle behaviour can be relativistic, a topology of apparent mass is also required before all aspects of these projections can be described. This can be derived from the dimensions of scaled Action wave functions;

$$\vec{\psi} = m^{1/2}(\vec{r} \cdot \vec{a}) = (m_e^{1/2} \coth^{-1} a) \times (\sigma \tanh^{-1} a) \quad (\text{II.5-39})$$

in which the mass topology counterbalances the velocity to conserve both energy and momentum in the stable state. This dependence on the relative velocity angle ($\coth^{-1} a$) explicitly displays the required relativistic role of mass since the directed derivative can be expanded as;

$$\frac{d}{da} \left[\coth^{-1} \frac{v}{c} \right] = \left[\frac{1}{1 - (v/c)^2} \right] \frac{d(v/c)}{da} \quad (\text{II.5-40})$$

Now the limiting values of energy wave function properties can be estimated in terms of fundamental constants upon projection into three-dimensional position space. The following inequalities can be defined to estimate the magnitudes of the projected potential position and kinetic, velocity vectors at their two limits of observable behaviour, near the atomic nucleus and at the extreme point of excursion away from the nucleus;

$$\begin{aligned}
 \vec{r}_N &\geq \Delta r = \vec{\rho} \coth \alpha_N \\
 \vec{v}_N &\leq c = \vec{\sigma} \tanh \alpha_N \\
 \vec{r}_M &\leq \alpha = \vec{\rho} \coth \alpha_M \\
 \vec{v}_M &\geq \Delta v = \vec{\sigma} \tanh \alpha_M
 \end{aligned}
 \tag{II.5-41}$$

in which α_N and α_M are respectively, the magnitudes of the angles of the state vector projected into the horizontal plane of the three-dimensional positional space as it "disappears" into the nucleus and as it nears its maximum displacement. Since these angles are both defined by differences between classical and uncertain positions, their behaviour at reciprocal positions is coupled as;

$$\begin{aligned}
 \tanh \alpha_M &= \coth \alpha_N \\
 \coth \alpha_M &= \tanh \alpha_N
 \end{aligned}
 \tag{II.5-42}$$

These relationships allow $\vec{r}_M$ and $\vec{v}_M$ to be defined in terms of fundamental constants and $\vec{r}_N$ which is defined by the local gravo-magneto-electric field strengths.

$$\begin{aligned}\vec{r}_M &= \vec{\rho} \coth \alpha_M = \vec{\rho} \tanh \alpha_N = \frac{\vec{c}}{\vec{\sigma}} \\ \vec{v}_M &= \vec{\sigma} \tanh \alpha_M = \vec{\sigma} \coth \alpha_N = \frac{\vec{\sigma} \vec{r}_N}{\rho}\end{aligned}\quad (\text{II.5-43})$$

However, the scaling parameters $\vec{\sigma}$ and $\vec{\rho}$ must first be defined in terms of the uncertainty of the projected state vector;

$$\begin{aligned}\Delta r \times \Delta p &= \Delta r \times (\Delta m \times \Delta v) = \vec{r}_N^* \times \vec{v}_M = \hbar \\ &= \vec{\rho} \coth \alpha_N^* \times (m \coth \alpha_M \times \vec{\sigma} \tanh \alpha_M) \\ &= \vec{\rho} \coth \alpha_N^* \times (m \tanh \alpha_N \times \vec{\sigma} \coth \alpha_N) \\ &= \vec{\rho}^* \times m \times \vec{\sigma} \coth \alpha_N\end{aligned}\quad (\text{II.5-44})$$

since

$$\tanh \alpha_N \times \coth \alpha_N = 1 \quad (\text{II.5-45})$$

Thus, since;

$$\Delta v = \vec{v}_M = \frac{\hbar}{\vec{r}_N \Delta m} = \frac{\hbar}{\vec{r}_N m \tanh \alpha_N}$$

then;

$$\vec{\sigma} = \frac{\hbar}{\vec{r}_N m} \quad (\text{II.5-46})$$

Similarly, by substitution;

$$\vec{\rho} = \frac{\vec{r}_N}{\coth \alpha_N}$$

but since

$$\tanh \alpha_N = \frac{\vec{c}}{\sigma} = \frac{c \vec{r}_N m}{h}$$

then;

$$\coth \alpha_N = \frac{h}{c \vec{r}_N m}$$

and

$$\vec{\rho} = \frac{\vec{c} \vec{r}_N^2 m}{h} \quad (\text{II.5-47})$$

Finally, by substitution for $\vec{\rho}$ and $\vec{\sigma}$;

$$\vec{v}_M = \vec{\sigma} \coth \alpha_N = \frac{h}{\vec{r}_N m} \times \frac{h}{c \vec{r}_N m} = \frac{h^2}{c \vec{r}_N^2 m^2}$$

$$\vec{r}_M = \vec{\rho} \tanh \alpha_N = \frac{\vec{c} \vec{r}_N^2 m}{h} \times \frac{c \vec{r}_N m}{h} = \frac{c^2 \vec{r}_N^3 m^2}{h^2} \quad (\text{II.5-48})$$

Since c , m and h are all known quantities, one assumption about r_N will define the values r_M and v_M , the radius and velocity of the state vector at its outer limits in position space. A reasonable approximation would be the Bohr radius since there is no stable orbital with a smaller mean radius in the hydrogen atom. Then on substitution;

$$v_M \simeq 10^8 \text{ cm/sec} \quad \text{and} \quad r_M \simeq 10^{-6} \text{ cm.} \quad (\text{II.5-49})$$

and these estimates suggest that the vector is moving at 1% of the speed of light at a distance 100 times larger than the Bohr radius when it reaches its extreme displacement on the Moebius locus. If r_N is chosen one order of magnitude smaller, v_M approaches c even at its slowest point, putting a clear lower limit on r_N .

This "*nuclear radius*" is 10^6 larger than the radius observed by nuclear particle scattering experiments and has no direct relation to it. Instead, this r_N represents the radius at which the vector of the incoming electron, or the net vector of coupled electrons, achieves light speed, c on its excursion around the Moebius coordinate locus. In this sense, r_N defines an "*event horizon*" below which the electric vector is invisible because no information about its behaviour can be transmitted faster than its own motion. At this radius the electronic vector has essentially entered the fourth dimension which three-dimensional observers cannot directly "see into". This also implies that no geometric structure of electric vectors lying within this "*nuclear radius*" can be detected by any observer, *including any other atom*. In this sense, these electrons or their coupled motion are irrelevant to the visible features and can be regarded, in chemical language, as "core electrons". The electrons which have

excursions beyond this radius carry observable structure and hence can interact with other such electrons in constructive or destructive correlations as chemical, "valance" electrons.

This atomic model is similar in form to a "Saturnine" model of the atom first proposed by Nagaoka in Rutherford's laboratory in 1904.⁴² Like the relation of Saturn to its moons, the nucleus appears to fill the space inside the innermost observable orbit. This effectively defines the repulsive part of the potential in a system of two mutually attractive particles, the proton and the electron.

V.2.viii   Topology of Energy and Time

Traditionally, it is assumed that the shape of the mechanical space of atoms is defined by the potential of the central field. The derivation of scaled Action wave functions shows that the dynamic structure of kinetic energy and the static structure of potential energy *contribute equally* to the complete, non-orientable topology. The static topology derived in (II.5-9) to satisfy the conservation of energy requirement had been proposed earlier on an empirical basis as the stabilizing part of the full Poeschl-Teller potential for anharmonic oscillators including atoms. Using this model, the traditional form of the Hamiltonian can be written;

$$H = - \frac{\hbar^2}{2m} \frac{d^2}{dx^2} - (\lambda + 1) k^2 \operatorname{sech}^2(kx) \quad (\text{II.5-50})$$

and the corresponding Schroedinger equation has solutions;

$$|\lambda m_\lambda\rangle = (-1)^m \lambda \left[\left[\frac{2\lambda+1}{2} \right] \left[\frac{\lambda-m_\lambda}{\lambda+m_\lambda} \right] \right]^{1/2} \left[P_{m_\lambda}^\lambda(-\tanh(kx)) \right] \quad (\text{II.5-51})$$

By comparison of this traditional description of the energy of the state to that arising from the full energy conservation requirement in (II.5-9), the associated Legendre functions solutions on $\tanh(kx)$ are identical to the description of the topology of the kinetic energy. In other words, the traditional solutions of the Schroedinger form of quantum mechanics are the coordinate transformations needed to describe the kinetic energy contribution in the same coordinates as those specified for the potential. Since the kinetic contribution is usually specified in spherical symmetry, these Poschl-Teller hyperbolic solutions essentially represent the distortion of the orientable kinetic space needed to create the non-orientable stabilizing, destructively interfering couple to the potential.

Since they are merely coordinate transforms of the kinetic contribution, these traditional wave functions do not provide any explicit definition of Uncertainty because it is left implicit in the squared term $\hbar^2$ in the definition of the kinetic contribution in the Hamiltonian. Therefore, in contradiction to conventional assumptions, these "wave functions" are actually classical, non-orientable geometry transforms and *carry no information* beyond the digital selection rules about the magnitudes or intensities of any physical phenomena. Instead of using this differential treatment of kinetic and potential while leaving the uncertainty completely obscured, the coordinate of kinetic energy can be described explicitly as

one of the two orthogonal Action components on the classical, natural coordinate, A_c . This completely separates the description of the ideal geometry, which establishes the selection rules, from the uncertainty which describes the intensity by the linear functions of (II.5-34).

Applying this discrimination between ideal geometry and accompanying uncertainty, the conjugate coupling and summation of kinetic and potential contributions on the ideal natural coordinates cancels all chirality, sense of rotation or coherence phase in the description of energy. This stable energy topology can be constructed, following Lagrange, by uniting a three-dimensional position space with a three-dimensional velocity space through the coupling of the origins and the coordinate axes of the two spaces. This coupling removes two of the initial six degrees of freedom and yields a four-dimensional energy topology, free of any singularities. The projection of atomic structure from this ideal four-dimensional topology into three-dimensional mechanical space requires breaking the achiral surface into two coupled, orthogonal chiral three-dimensional spaces. This structure would remain apparently achiral after projection however, because all states would be composed of equivalent Moebius loci of opposite chirality.

For Fermions which interact with protons this strict achirality is not observed. Instead, neutrinos from hydrogen fusion are dominantly left handed, likewise β decay is preferentially left handed, as is atomic structure itself, observed in the circular dichroism spectra of heavy atoms, the morphology of their salts and the configuration of biochemicals. This preferential left chirality means that neither a model of atomic structure based on ideal bichiral nor on an exclusively left chiral proto-electron interaction in four-dimensional space is adequate. Instead, the

simplest necessary model requires the presence of a time-dependant perturbation of the geometry of the left handed locus, randomizing it towards the bichiral limit of a pair of coupled, oppositely chiral loci. In effect, this perturbation, traditionally identified as Uncertainty, is equivalent to a finite uncoupling of the coordinate axes of the position and velocity spaces, leaving only the origins superimposed. Thus uncertainty must be regarded as a symptom of a fifth dimensional, high frequency force field capable of disorienting the state vector during its chronon of excursion.

Nuclear models suggest that "baryons", including protons can exert both the left orienting and the randomizing forces on electronic state vectors. Protons are constructed of three quarks bound together by the strong nuclear force. Two conjugate quarks of the proton are known to act like a meson with a relationship of counter-chiral spaces. The third, acting like a hadron, carries an uncompensated, left polarized tensor of the weak nuclear force. The electronic state vectors must pass through this proton structure as they enter the origin of their space. Depending on the topology of these ingoing vectors, they should emerge ballistically, carrying restructured χ , s and c properties dictated by this weak force.

At the same time however, these electronic vectors are exposed to the strong nuclear force in the proton which couples the two heavy quarks. Since the strong force is so much more intense than the electromagnetic or weak forces, it is capable of short range binding of quarks carrying high kinetic energy, which is expressed as high frequency counter-rotation. Since quarks are asymmetric partially charged particles, this motion creates an oscillating strong force field at a frequency far higher and out of phase with the frequency of oscillation of the state vector through its nuclear nodes. Thus in this model, the strong force oscillation acts simply as a

randomizing perturbation on the chiral atomic structure. In essence, this rate of randomization is constant for all matter at the atomic structure level of organization because protons are present as the fundamental building particle in all atoms. The period of this oscillation establishes the minimum time during which the energy of the state vector can evolve to a new quantity and hence defines the minimum quantum of Action, $\hbar$, of atomic systems.

The final structural consequence of the mechanical space model, including the roles of weak and strong nuclear forces, is the resolution of the wave-particle duality paradox. It is essentially a physical example of the Bohr complementarity which is resolved in general by a change in scale of observation. In the model, the conservation of energy (II.5-9) shows that the particle-like behaviour near the origin and the complementary wave-like behaviour at the outer extreme of the Moebius excursion are coupled aspects of overall motion. The only difference in moving between these limits is the continual change of scale of the four-dimensional time base and the coupled relativistic topology of the mass.

The attribution of topologies to both energy and time provides a firm foundation for interpreting the energy-time alternative formulation of the uncertainty definition. In the traditional position-momentum form, the uncertainty condition is the minimum Action for inversion of chirality, defined as the finite difference between the reversed vector products of directed derivatives of position and momentum at any point on the locus. The equivalent energy-time form was difficult to interpret since directed derivatives of apparently scalar energy or of unidirectional time seemed inconceivable. In this model, the deviation in energy is measured by the extent of incoherence of the counter-rotating state vectors and the deviation of time

is defined by the incoherence of the state vector phase with the proton quark phase. This relationship is implicit in the estimation of the projected size and shape of atoms in three—dimensions and can be employed to define the initiation and progress of scattering or absorption of photons in transitions between atomic states.

III. REPRESENTATIONS FOR THE MCD MODEL

III.1. Ideal Symmetries

III.1.i Symmetry Operations of Coupled Systems

In any description of a system, the structure of the language is determined by the complexity of the structure of the system. Symmetry descriptions of systems are unique in that the goal in constructing the language is to achieve an unambiguously complete description without any redundancy. This is done by defining classes of symmetry operations which together describe all the available indistinguishable reorientations of the system with respect to an external coordinate reference.

The relevant structure of the electromagnetoinertial systems of interest here is defined by the dynamic repetitive Action permitted within the confining forces of the system. Assuming that the strong force is only relevant to uncertainty, the ideal structure is maintained by the weak and electromagnetic fields of the atomic nucleus. A corollary to Bell's inequality ⁵⁶ predicts that under these circumstances, there is a formal requirement for coupling of position and velocity. In these systems, the coupling of origins and axes of translation and rotation is equivalent to coupling electric dipoles with translational symmetry to magnetic quadrupoles with rotational symmetry. Since electric and magnetic fields are at right angles to each other, the effect of coupling them is to create coherent patterns of precession and nutation of the coupled vector as it explores the remaining dimensions of allowed motion. These patterns are recognizable as the Moebius loci of the full, four-dimensional Klein surface.

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⁵⁶ Gribbon, J, "The Man Who Proved Einstein was Wrong", New Scientist
43-45, 24 November 1990.

Sets of symmetry operators which map these loci of ideal geometry onto themselves and the equivalent orthogonal loci of the degenerate set can be defined in the full four-dimensional electromagnetoinertial space of the Klein surface.

Within this space the constant metric on the Moebius loci is the minimal Action. As described above, this has the appearance of a differential of variable length when projected onto the three-dimensional position space. Based on this constant aspect of the locus or its predictable projected variation in three dimensions, a Casimir symmetry operator can be defined. Thus, just as infinitesimal point groups are well defined for orientable spherical geometry in three dimensions, an infinitesimal point group can be defined for the four-dimensional Klein surface.

The Casimir operator is the fully symmetric representation of the structure from which it is derived.⁵⁷ The Casimir theory allows a transformation from differential operators to a family of finite axes as a power series in hypergeometric algebra. This family set contains all of the lesser symmetry operators. In the power series format it can be expanded to make explicit all the details of the structure. In algebraic terms, this means that the infinitesimal form may be restated as an infinite sum of finite symmetry axes. In three-dimensional orientable spherical geometry the Casimir operator⁵⁴ becomes a sum of circular rotations labelled C_n for all finite orders n . In the case of the Klein geometry, the Casimir operator becomes an infinite sum of non-orientable recursions, the simplest being a Moebius locus. For this reason, these closed path motions will be defined as "*Moebius Rotation Axes*",

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⁵⁷ B.R. Judd, Operator Techniques in Atomic Spectroscopy, McGraw-Hill Book Company, New York, 1963.

labelled $\hat{M}_n$. On projection to three-dimensional position space, these closed path motions appear as rotations of 0 to 4π radians around the Mobius locus and its conjugate.

This projection can be illustrated by cutting the projected Klein surface along its one surviving symmetry plane in three dimensions.³⁴ This cut (**FIGURE III-1**) reveals that the surface comprises a pair of oppositely handed basic Moebius loci about the principal axis which is perpendicular to the symmetry plane. From the complete four-dimensional hyper-Klein surface, higher order cuts will produce the infinite set of nested hyper-Moebius closed path motions. These will project into three dimensions as Mobius operators performing multiple twists of the object being operated upon.

FIGURE III-2 (a) through (f) is a computer generated sequence of figures of $(\tanh^{-1} \times \sinh^{-1})$ for the $J = 1/2$ state as the Klein surface is generated from the initial Moebius strip.⁵⁸

III.1.ii   Projected Chiral Operators

Projection of the Klein surface into three dimensions destroys most of its symmetry.³⁴ As shown in **FIGURE III-1**, only one Moebius axis (seen as S_2) and a symmetry plane perpendicular to it survive the procedure. Axes orthogonal to the principal axis survive only as sets of reflections, shown in **TABLE III-1**.

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⁵⁸ Courtesy of Eric Hollebome, Energy, Mines and Resources, CANMET, Coal Research Laboratories, FPL, Devon, Alberta.

TABLE III-1 Fundamental Operator Reflections

$\hat{E}$	$\hat{\sigma}_h$	$\hat{\sigma}_v^{xz}$	$\hat{\sigma}_v^{yz}$
$\hat{\sigma}_v^{xz} \hat{\sigma}_v^{yz} (= \hat{C}_2^z)$	$\hat{\sigma}_h \hat{\sigma}_v^{xz} (= \hat{C}_2^x)$	$\hat{\sigma}_h \hat{\sigma}_v^{yz} (= \hat{C}_2^y)$	$\hat{\sigma}_h \hat{\sigma}_v^{xz} \hat{\sigma}_v^{yz} (= \hat{S}_2)$

This finite set of operations defines a closed permutation group of order eight. Each of these operations has the potential to act independently upon any of the three components of the Moebius loci; the chirality, sense of motion and coherence. The generic matrix allows for all eight possible motions from any original horizontal address to any possible new vertical address.

The effects of the fundamental symmetry operators may be seen in their respective matrices which represent the changes to any of the loci (TABLE III-2). In the case of those operations that require successive reflections the order of application of these operations is immaterial as the results are identical. It is worth noting that the $\hat{\sigma}_v^{xz} \hat{\sigma}_v^{yz}$ operation is the dynamic equivalent of a $\hat{C}_2^z$ rotation in a point group. Similarly the $\hat{\sigma}_h \hat{\sigma}_v^{xz}$ operation is equivalent to a $\hat{C}_2^x$ rotation and the $\hat{\sigma}_h \hat{\sigma}_v^{yz}$ operation is equivalent to a $\hat{C}_2^y$ rotation. The combined operation of $\hat{\sigma}_h \hat{\sigma}_v^{xz} \hat{\sigma}_v^{yz}$ is the dynamic equivalent of an $\hat{S}_2$ operation.

These eight operations define a closed permutation group of order eight, which is the Identity ($\hat{I}$) class of operators for the fundamental natural coordinate system, as demonstrated in the group multiplication table (TABLE III-3).

FIGURE III-1 Klein Surface

FIGURE III-2 (a) Computer Generated Klein Surface
for the $J = 1/2$ State

FIGURE III-2 (b)

FIGURE III-2 (c)

FIGURE III-2 (d)

FIGURE III-2 (e)

FIGURE III-2 (f)

TABLE III-2 Fundamental Chiral Operators

$$\hat{\mathbf{E}} = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +1 \end{bmatrix}$$

$$\hat{\sigma}_h = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$\hat{\sigma}_v^{xz} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & +1 \end{bmatrix}$$

$$\hat{\sigma}_v^{yz} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$\hat{C}_2^z = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$C_2^x = \begin{bmatrix} +1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & +1 \end{bmatrix}$$

$$\hat{C}_2^y = \begin{bmatrix} +1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$\hat{S}_2 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

TABLE III-3 Group Multiplication Table for Identity Class I

I	E	σ_h	σ_v^{xz}	σ_v^{yz}	C_2^z	C_2^x	C_2^y	S_2
E	E	σ_h	σ_v^{xz}	σ_v^{yz}	C_2^z	C_2^x	C_2^y	S_2
σ_h	σ_h	E	C_2^x	C_2^y	S_2	σ_v^{xz}	σ_v^{yz}	C_2^z
σ_v^{xz}	σ_v^{xz}	C_2^x	E	C_2^z	σ_v^{yz}	σ_h	S_2	C_2^y
σ_v^{yz}	σ_v^{yz}	C_2^y	C_2^z	E	σ_v^{xz}	S_2	σ_h	C_2^x
C_2^z	C_2^z	S_2	σ_v^{yz}	σ_v^{xz}	E	C_2^y	C_2^x	σ_h
C_2^x	C_2^x	σ_v^{xz}	σ_h	S_2	C_2^y	E	C_2^z	σ_v^{yz}
C_2^y	C_2^y	σ_v^{yz}	S_2	σ_h	C_2^x	C_2^z	E	σ_v^{xz}
S_2	S_2	C_2^z	C_2^y	C_2^x	σ_h	σ_v^{yz}	σ_v^{xz}	E

III.1.iii Projected Chiral Representations

The Grand Orthogonality Theorem ^{24,28} (GOT) defines the number of ordered sets or permutations of projected independent loci which can be discriminated by these projected operators. ⁵⁷ In this case it is equal to the number of operators. Each of the eight resulting permutations "represents" an allowed reordering of the set. Physically, each such "*representation*" identifies one of the eight possible self-conjugate sets of loci which can be reached by the use of the operators.

$$\begin{aligned}
&= \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +1 \end{bmatrix} + \begin{bmatrix} -1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +1 \end{bmatrix} + \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & +1 \end{bmatrix} + \\
&\hspace{15em} \text{(III.1-2)} \\
&+ \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \begin{bmatrix} +1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & +1 \end{bmatrix} + \\
&+ \begin{bmatrix} +1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} + \begin{bmatrix} -1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -1 \end{bmatrix}
\end{aligned}$$

The positive sign represents the conventional right-handed, counter-clockwise, in coherence choices. The negative sign represents the other binary choice.

These matrices may be reduced to a simpler dimensional (χsc) notation, in which case the above summation would appear as;

$$\begin{aligned}
&(+1,+1,+1) + (-1,+1,+1) + (-1,-1,+1) + (-1,-1,-1) + (+1,+1,-1) + (+1,-1,+1) \\
&\quad + (+1,-1,-1) + (-1,+1,-1) \\
&= (+++) + (-++) + (--+) + (---) + (++-) + (+-+) + (+--) + (-+-) \quad \text{(III.1-3)}
\end{aligned}$$

The eight Moebius loci have been defined (III.1-3), however the definitions extend only to the first window, the $0-2\pi$ rotation of the total 4π rotation of the locus. The natural coordinates are a set of four conjugate pairs of Moebius loci, each pair representing a complete $0-4\pi$ rotation. The conjugate is the $2\pi-4\pi$ portion of the

original locus after having undergone a horizontal reflection. The notation for a natural coordinate is therefore written as:

$$\kappa = (\chi sc)_{0-2\pi}(-\chi sc)_{2\pi-4\pi}^* \quad (\text{III.1-4})$$

which can be reduced to the simpler form

$$\kappa = (\chi sc)(-\chi sc)^* \quad (\text{III.1-5})$$

where the conjugate notation κ^* implies the $2\pi-4\pi$ rotation, or second window. The conjugate wave function κ^* can therefore be defined as

$$\kappa^* = (-\chi sc)(\chi sc)^* \quad (\text{III.1-6})$$

Therefore the eight Moebius loci can be defined as a set of four natural coordinates, an accompanying set of four conjugate natural coordinates, as shown in **TABLE III-4**.

TABLE III-4 Natural Coordinates and Wavefunctions

$\kappa = (-++)^{*}$	$= p$	$\kappa^* = (+++)^{*}$	$= p^*$
$\kappa = (--+)^{*}$	$= q$	$\kappa^* = (+-+)^{*}$	$= q^*$
$\kappa = (---)^{*}$	$= r$	$\kappa^* = (+--)^{*}$	$= r^*$
$\kappa = (-+-)^{*}$	$= s$	$\kappa^* = (++-)^{*}$	$= s^*$

Thus, the set of natural coordinates can be reduced in notation to the set of (p,q,r,s) . These four, binary natural coordinates form a direct topological realization of the four spinor coordinates of the Dirac equation.⁵⁹ (Refer to Historical Appendix, pg 182) Both the topological and the algebraic Dirac expressions of state energies are derived from the Lagrangian definitions, hence this one-to-one mapping of all properties of the solutions, including specification of the coordinates is inevitable. While the spinor coordinates define the minimum necessary properties of any set of coordinates in four dimensions, the natural coordinates provide an unambiguous geometric specification of predictable, observable properties of states because the contributing particles, forces and the thermodynamic consequences of their interactions have all been recognized in constructing these coordinates.

The explicit specification of χ , s and c which leads to the coordinates of **TABLE III-4**, provides explicit definitions to the abstract Dirac phase factors of the spinor coordinates. In performing this mapping, no special order of p , q , r or s can be specified from physical principles. However, since the Dirac factors are arbitrary the nomenclature can be made consistent with traditional practice. As conventions, in the Dirac phase choices, right handedness, counter-clock-wise rotation and positive minor axis coherence are taken as "*real*" geometric attributes and algebraically assigned as positive phase factors. Only one of the four natural coordinates is fully defined by these three "*real*" attributes. Any of the three other possible orientations are considered as "*imaginary*" and assigned phases depending

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⁵⁹ A. Sudberry, Quantum Mechanics and the Particles of Nature: an Outline for Mathematicians, Cambridge University Press, Cambridge, 1986.

on $[(-1)^{1/2}]^n$. The present derivation of the natural coordinates shows that this convention is too restrictive in its viewpoint. All four coordinates are *equally real* in the sense that they are all of equal importance in completely defining the atomic structure.

Dirac's notation of symmetry was deliberately developed to avoid the complexities of Wigner's notation. However, because of the distinction between real and imaginary coordinates in the Dirac format, specific but assymetric real and imaaginary sign conventions were assigned to kets, operators and bras which had to be followed in unique sequences as triangular rules.^{2,24,41} In the most compact Wigner form, the basis functions display the same asymmetry and it is also implicit in the Condon and Shortley choice of convention.^{2,54} This asymmetry applies to both the processes of conjugation and normalization. The restatement of the form of those coordinates in **TABLE III-4**, renders all coordinates equally "real" in their own spaces, defined by dimensions χ , s and c . This eliminates the need for phase factors based on $(\sqrt{-1})^n$ but the requirement for an ordered process for combining coordinates remains since the spaces do not commute.

III.2. Fundamental Operators and Representations

III.2.i Natural Coordinates and Conjugacy Operators

The fundamental chiral operators can be represented as two sets of four natural coordinate operators that allow any one natural coordinate to become any one other natural coordinate. These four operators have the same (χ_{sc}) components as the $0-2\pi$ window of the pathway of the unconjugated natural coordinate (TABLE III-5).

TABLE III-5 Wave Function (Natural Coordinate) Operators $\hat{I} = \hat{i} + \hat{i}^*$

$$\hat{i} = \hat{p} + \hat{q} + \hat{r} + \hat{s} = (+++)(-++)^* + (---)(--+)^* + (+--)(---)^* + (++-)(--+)^*$$

$$\hat{i}^* = \hat{p}^* + \hat{q}^* + \hat{r}^* + \hat{s}^* = (-++)(+++)^* + (---)(++-)^* + (---)(+--)^* + (---)(+-+)^*$$

These four operators can be mapped onto the fixed matrix set from the Dirac equation,⁵⁹ where $[\hat{p}, \hat{p}^*]$ is γ^0 and $[(\hat{q}, \hat{q}^*)(\hat{r}, \hat{r}^*)(\hat{s}, \hat{s}^*)]$ are the three γ^i . The importance of the operator $\hat{p}$ lies in its ability as the horizontal reflection plane $\hat{\sigma}_h$ to convert both the $0-2\pi$ window of the pathway into its conjugate and thus create the entire natural coordinate, and to convert the natural coordinate itself into its own conjugate.

$$\begin{array}{ccc}
 (\chi sc)(-\chi sc)^* & \longleftrightarrow & (-\chi sc)(\chi sc)^* \\
 \left| \begin{array}{c} \uparrow \quad \uparrow \quad \uparrow \\ (\hat{\sigma}_h \ 0-2\pi) \end{array} \right. & & \left| \begin{array}{c} \uparrow \quad \uparrow \quad \uparrow \\ \hat{\sigma}_h(0-2\pi) \end{array} \right. \\
 \hline & \hat{\sigma}_h(2\pi-4\pi) & \hline
 \end{array} \quad (VI)$$

The closed nature of the set is demonstrated in TABLE III-6. The operations on the conjugate wave functions result in a diagonal matrix that demonstrates the fixed matrix behaviour of the Dirac equation, as seen in TABLE III-7.

III.1.ii Chiral Topology and Point Group Description

To identify the simplest appropriate symmetry point group for these natural coordinates and operations, the salient features of the topology must be characterized. Individually, the non-orientable coordinates followed by the state vector are Moebius loci. Together, they describe a Klein topology which contains all the geometry of the bound system. ³⁴ It exists as an infinite set of defect surfaces in three-dimensional position spaces, each carrying a discontinuity. By topological rearrangement, this defect can be reduced to a point at the origin of the three-dimensional space, where all paths of motion must meet. Here, motion can pass smoothly from "*inside*" to "*outside*" the surface, altering any property of chirality, sense or coherence on any single Moebius locus. The discontinuity is resolved in four dimensions in which the Moebius loci merge into Klein surfaces. This provides the extra dimension for smooth rotation between Moebius attributes on each surface since chirality is unresolved in four dimensions. This basic

TABLE III-6 Wave Function Multiplication Table

	pp^*	qq^*	rr^*	ss^*
pp^*	$\hat{p}$	$\hat{q}$	$\hat{r}$	$\hat{s}$
qq^*	$\hat{q}$	$\hat{p}$	$\hat{s}$	$\hat{r}$
rr^*	$\hat{r}$	$\hat{s}$	$\hat{p}$	$\hat{q}$
ss^*	$\hat{s}$	$\hat{r}$	$\hat{q}$	$\hat{p}$

TABLE III-7 Conjugate Wave Function Multiplication Table

	pp^*	qq^*	rr^*	ss^*
$p^* p$	$\hat{p}^*$	$\hat{q}^*$	$\hat{r}^*$	$\hat{s}^*$
$q^* q$	$\hat{q}^*$	$\hat{p}^*$	$\hat{s}^*$	$\hat{r}^*$
$r^* r$	$\hat{r}^*$	$\hat{s}^*$	$\hat{p}^*$	$\hat{q}^*$
$s^* s$	$\hat{s}^*$	$\hat{r}^*$	$\hat{q}^*$	$\hat{p}^*$

requirement of appealing to four dimensions for the nondefect structure indicates that the simplest point group will be the one describing the geometry of nested Klein surfaces of increasing convolutions which can be defined as the hyper-Klein surface.

This basic four-dimensional structural information is absent in conventional descriptions of atomic structure. Even in the explicit four spinors described in Dirac's notation, as in Schroedinger's and in conventional group theoretical notation, there is a loss of geometric discrimination as the cross products do not carry complete information on the physics of the system. These problems are explicitly apparent in the description of fermion behaviour. In these conventional descriptions, arbitrary phases must be employed but in addition, a further ambiguity is introduced for odd numbers of Fermions which is most readily recognized in the group theory format as a duplication of representations in the reduction of direct products. Whenever finite double groups are constructed using the Bethe operator $R^{24,60,61}$ direct products of the half integer representations can contain a given irreducible representation more than once. This implies that the description is incomplete because it fails to account for the observable orthonormality of the states of the system being investigated. The description therefore fails in predicting the eigenvalues of these pairs of representations and requires the addition of non-group-theoretic mixing parameters to permit assignment.¹² The existence of these parameters depends on the quantum

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⁶⁰ J.S. Griffith, The Theory of Transition Metal Ions, Cambridge University Press, Cambridge, 1961.

⁶¹ J.S. Griffith, The Irreducible Tensor Method for Molecular Symmetry Groups, Prentice-Hall, Englewood Cliffs, New Jersey, 1962.

mechanical addition rule to construct a description of observables from the inadequate set of representations of conventional groups.

It is possible however to expand the group theory in such a way as to describe observables unambiguously. This model will replace the nondeterministic spinor coordinates which provide an indeterminate physical picture with a physical definable locus. This model provides a tensorial space of eight coupled Moebius vectors and allows for the construction of a full infinite group of all overtone structures of natural coordinates on operators. This Moebius point group is shown in **TABLE III-8**, constructed from the actions of operators of **TABLE III-2** on the natural coordinates of **TABLE III-4**.

III.2.iii   Infinite Moebius Symmetry Operators

The set of eight symmetry operators which define the point group for the fundamental set of eight Moebius loci represent the residual finite symmetry after projection of these loci from the four-dimensional Klein space. However the full Klein space includes an infinite set of higher order Mobius loci which project into three-dimensional space as pathways with multiple twists. Since the original eight operators can be amplified to describe these projected Moebius overtones, this simple set can be identified as the basic Moebius Identity Operator class in three dimensions.

In its fully expanded form this Identity Operator is inconvenient. It can be made much more compact and formally useful through linear combinations of the reflection operations which together generate changes in the basic dimensions of chirality, sense and coherence.

With respect to the principal axis S_z aligned on the z -axis shown in **FIGURE II-4**, different sets of planes can reverse each of these three dimensions. The simplest dimension, coherence, can be reversed by reflection in σ_v^{yz} to convert $+c$ to $-c$. The two-dimensional property of sense of rotation, starting from $+\chi$, is reversed by reflecting the Action on the pathway through the horizontal plane σ_h^{xy} . Since this is not an orientable space, a simple σ_v^{xz} reflection cannot accomplish this sense reversal. The three-dimensional property of chirality is reversed by a combination of horizontal and vertical reflections which may be regarded as a dihedral reflection σ_d . These are illustrated in **FIGURE III-3**.

This correlation allows matrix **III.1-1** to be generated in terms of the eight operations of the Identity group. Expansion of this matrix to define the higher order Moebius operators needed to describe the overtone natural coordinates is very simple. About the principal axis both the basic and overtone natural coordinates can only display one choice of both chirality and sense of rotation. While the basic coordinate carries the minimum chiral pitch which results in 4π rotation, the overtones have higher pitch values which carry the overtone coordinates back to the origin in submultiples of 4π radians. This symmetry is described by more frequent vertical reflections at appropriate angles to the basic σ_v^{yz} . The position of these additional planes can be denoted by $\cos\phi$ for ϕ in the xy plane.

FIGURE III-3 Reflections which Correspond to Chiral Dimension Reversal

$$\sigma_d \sigma_h \sigma_v \implies \chi s c$$

Thus the generalized Moebius operator becomes:

$$\begin{array}{c} \chi \\ s \\ c \end{array} \begin{bmatrix} \pm 1 & 0 & 0 \\ 0 & \pm 1 & 0 \\ 0 & 0 & \cos \phi \end{bmatrix} \quad (\text{III.2-2})$$

The first overtone to the fundamental locus would involve an additional twist for a total of two. As a result of this twist, the pathway returns to the origin at $\phi = \pi$ as well as a 2π . This overtone can be represented by the matrix pair;

$$\begin{bmatrix} \pm 1 & 0 & 0 \\ 0 & \pm 1 & 0 \\ 0 & 0 & \pm 1.000 \end{bmatrix} \quad \begin{bmatrix} \pm 1 & 0 & 0 \\ 0 & \pm 1 & 0 \\ 0 & 0 & \pm 1.000 \end{bmatrix} \quad (\text{III.2-3})$$

where the *cosine* ϕ represents the location of the return to the origin. Thus each matrix represents to location of the "node" of the locus. To have any meaning the two matrices must always be taken as pairs.

Similarly a fundamental locus with two additional twists can be represented by a trio of matrices.

$$\begin{bmatrix} \pm 1 & 0 & 0 \\ 0 & \pm 1 & 0 \\ 0 & 0 & \pm 1.000 \end{bmatrix} \begin{bmatrix} \pm 1 & 0 & 0 \\ 0 & \pm 1 & 0 \\ 0 & 0 & \pm 0.500 \end{bmatrix} \begin{bmatrix} \pm 1 & 0 & 0 \\ 0 & \pm 1 & 0 \\ 0 & 0 & \pm 0.500 \end{bmatrix}$$

An analysis of the fundamental chiral operators reveals that rotations of dynamic pathways are in fact pairs of reflection planes. A true rotation $\hat{C}_n$ is in reality $\hat{\sigma}_v^{\pi/n} \hat{\sigma}_v^{2\pi/n}$. The Moebius rotations are seen therefore as pairs of appropriate reflection planes (TABLE III-9). In keeping with the compact notation (χsc), the Moebius rotation operators may be expressed as shown in TABLE III-10.

III.2.iv   Infinite Moebius Representations

Having established the behaviour of the compact form of Moebius symmetry operators, the Moebius representations can be explicitly defined. A description in terms of dimensions χ , s and c is available directly from the operator matrices. However these properties are not those measured by direct spectroscopic experiment. Thus, it is more useful for spectroscopic interpretation to transform the dimensional description of representations to a description in terms of the electromagnetic properties of atomic states carrying such dimensions.

TABLE III-9 Moebius Rotations

$$M_r = \sigma_r / \sigma_r^* = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \cos 2\theta \end{bmatrix}$$

$$M_1 = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +1.000 \end{bmatrix}$$

$$M_2 = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -1.000 \end{bmatrix}$$

$$M_3 = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.800 \end{bmatrix}$$

$$M_4 = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +0.000 \end{bmatrix}$$

$$M_5 = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.309 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.809 \end{bmatrix}$$

$$M_6 = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +0.500 \end{bmatrix}$$

$$M_7 = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.623 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.223 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.907 \end{bmatrix}$$

$$M_8 = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +0.707 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.707 \end{bmatrix}$$

$$M_9 = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +0.765 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +0.174 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.940 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.655 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.939 \end{bmatrix}$$

$$M_{10} = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.809 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.309 \end{bmatrix}$$

$$M_{11} = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +0.841 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +0.415 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.142 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.355 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +0.747 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.871 \end{bmatrix}$$

$$M_{12} = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.806 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.806 \end{bmatrix}$$

$$M_{13} = \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.883 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & +0.568 \end{bmatrix} \quad \begin{bmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -0.171 \end{bmatrix}$$

TABLE III-10 Compact Notation for Moebius Rotations

$\hat{M}_1$	=	$(\pm 1, \pm 1, +1.000)$		
$\hat{M}_2$	=	$(\pm 1, \pm 1, -1.000)$		
$\hat{M}_3$	=	$(\pm 1, \pm 1, -0.500)$		
$\hat{M}_4$	=	$(\pm 1, \pm 1, -0.000)$		
$\hat{M}_5$	=	$(\pm 1, \pm 1, +0.309)$	$(\pm 1, \pm 1, -0.809)$	
$\hat{M}_6$	=	$(\pm 1, \pm 1, +0.500)$		
$\hat{M}_7$	=	$(\pm 1, \pm 1, +0.623)$	$(\pm 1, \pm 1, -0.223)$	$(\pm 1, \pm 1, -0.907)$
$\hat{M}_8$	=	$(\pm 1, \pm 1, +0.707)$	$(\pm 1, \pm 1, -0.707)$	
$\hat{M}_9$	=	$(\pm 1, \pm 1, +0.766)$	$(\pm 1, \pm 1, +0.174)$	$(\pm 1, \pm 1, -0.940)$ $(\pm 1, \pm 1, -0.655)$
		$(\pm 1, \pm 1, -0.959)$		
$\hat{M}_{10}$	=	$(\pm 1, \pm 1, +0.809)$	$(\pm 1, \pm 1, -0.309)$	
$\hat{M}_{11}$	=	$(\pm 1, \pm 1, +0.841)$	$(\pm 1, \pm 1, +0.415)$	$(\pm 1, \pm 1, -0.142)$ $(\pm 1, \pm 1, -0.355)$
		$(\pm 1, \pm 1, -0.749)$	$(\pm 1, \pm 1, -0.971)$	
$\hat{M}_{12}$	=	$(\pm 1, \pm 1, +0.866)$	$(\pm 1, \pm 1, -0.866)$	
$\hat{M}_{13}$	=	$(\pm 1, \pm 1, +0.885)$	$(\pm 1, \pm 1, +0.565)$	$(\pm 1, \pm 1, +0.121)$

In a spectroscopic event, a photon interacts with the atom or molecule to inject energy into a stable state and increase the kinetic energy to the point of establishing a well defined excited state. In chiral space this implies that a helical photon, prepared in one hand enters the atomic space and is able to perform work on the state vector to alter it from following a fundamental locus to an overtone locus. This is physically possible only if the coherence, sense of motion and chirality of the photon and atomic state are identical since the vectors of electric and magnetic fields of the photon can only perform work along the locus of the atomic vectors. Atoms which fail to present their internal structure coherently to the vectors of the photon cannot interact and are irrelevant to the spectroscopic experiment.

With these assumptions, the dimensions χ , s and c can be given electromagnetic interpretations for those atoms which are visible by absorption or emission spectroscopy.

For low energy excitations or de-excitations wave lengths are many orders of magnitude larger than the average radius of the atom or molecule. Only when the state vector approaches the limit of complete potential does it become long enough, in position space, to couple with the electronic vector of a photon passing up or down the z -axis of the atom (FIGURE II-4). At this point, the coherence c between the state and photon electrical vectors is defined. A Stark electric field imposed on the system in this same direction would stabilize or destabilize the atomic state depending on the relative polarization of the field. The amount of stabilization depends on the imposed electric field strength. Thus, for a degenerate orthogonal pair of loci oriented with opposite polarities along the z -axis, a static electric field will raise the Stark degeneracy and the transient electric vector of the

photon will cohere with one but not the other. Both phenomena reveal the projection of the electrical component of the state vector on the x -axis. Thus, a quantum number can be defined for this projected electrical component and for convenience will be labelled e_j . In terms of the fundamental dimensions, e_j corresponds to coherence c and defines the number of electrical quanta projected to the positive or negative ends of c .

In this same geometry, the magnetic projection of the state vector lies in the principal z -axis because it results from the rotating electrical current i from equation II.5-28. This associates the magnetic quantum number m_j with the sense of rotation s .

Since both e_j and m_j are bidirectional they together account for 2^2 dimensions of electromagnetic space. There remains a degeneracy in chirality which is resolved in circular polarization spectroscopy techniques by deliberate alignment of the sample coupled with circular preparation of the photon. The preferential chirality detected by these techniques would in principle generate a vector component requiring a quantum number to evaluate the length of projection. However, the dependance of chirality on the nuclear Z^0 Boson indicates that this vector is associated with the unexploded fourth dimension. Therefore the basic dimension of chirality χ cannot be replaced by a detectable quantum number similar to e_j and m_j . However the degeneracy of the set of chiral states can be defined by the tensor specification of $J_{(k)}$ where k is the degeneracy number.

The representations of the infinite Moebius group, specified by these quantum identifiers $J_{(k)} m_j e_j$ are listed in TABLE III-11 up to $k = 5$ ($n = 10$).

TABLE III-11 Representations and Fundamental Quantum Numbers

$J_{n/2}(m_j, e_j)$	n	$\Gamma_n(\gamma_n^m \dots \gamma_n^m) \gamma^e$
$J_{1/2} m_{\pm 1/2} e_j$	1	$(\Gamma_1 \gamma_1^m \gamma^e)(\Gamma_{-1} \gamma_1^m \gamma^e)$
$J_1 m_{\pm 1} e_j$	2	$(\Gamma_2 \gamma_2^m \gamma^e)(\Gamma_2 \gamma_0^m \gamma^e)(\Gamma_2 \gamma_{-0}^m \gamma^e)(\Gamma_2 \gamma_{-2}^m \gamma^e)$
$J_{3/2} m_{\pm 3/2} e_j$	3	$(\Gamma_3 \gamma_3^m \gamma^e)(\Gamma_3 \gamma_1^m \gamma^e)(\Gamma_3 \gamma_{-1}^m \gamma^e)(\Gamma_3 \gamma_{-3}^m \gamma^e)$
$J_2 m_{\pm 2} e_j$	4	$(\Gamma_4 \gamma_4^m \gamma^e)(\Gamma_4 \gamma_2^m \gamma^e)(\Gamma_4 \gamma_0^m \gamma^e)(\Gamma_4 \gamma_{-0}^m \gamma^e)(\Gamma_4 \gamma_{-2}^m \gamma^e)(\Gamma_4 \gamma_{-4}^m \gamma^e)$
$J_{5/2} m_{\pm 5/2} e_j$	5	$(\Gamma_5 \gamma_5^m \gamma^e)(\Gamma_5 \gamma_3^m \gamma^e)(\Gamma_5 \gamma_1^m \gamma^e)(\Gamma_5 \gamma_{-1}^m \gamma^e)(\Gamma_5 \gamma_{-3}^m \gamma^e)(\Gamma_5 \gamma_{-5}^m \gamma^e)$
$J_3 m_{\pm 3} e_j$	6	$(\Gamma_6 \gamma_6^m \gamma^e)(\Gamma_6 \gamma_4^m \gamma^e)(\Gamma_6 \gamma_2^m \gamma^e)(\Gamma_6 \gamma_0^m \gamma^e)(\Gamma_6 \gamma_{-0}^m \gamma^e)(\Gamma_6 \gamma_{-2}^m \gamma^e)$ $(\Gamma_4 \gamma_{-4}^m \gamma^e)(\Gamma_4 \gamma_{-4}^m \gamma^e)$
$J_{7/2} m_{\pm 7/2} e_j$	7	$(\Gamma_7 \gamma_7^m \gamma^e)(\Gamma_7 \gamma_5^m \gamma^e)(\Gamma_7 \gamma_3^m \gamma^e)(\Gamma_7 \gamma_1^m \gamma^e)(\Gamma_7 \gamma_{-1}^m \gamma^e)(\Gamma_7 \gamma_{-3}^m \gamma^e)$ $(\Gamma_7 \gamma_{-5}^m \gamma^e)(\Gamma_7 \gamma_{-7}^m \gamma^e)$
$J_4 m_{\pm 4} e_j$	8	$(\Gamma_8 \gamma_8^m \gamma^e)(\Gamma_8 \gamma_6^m \gamma^e)(\Gamma_8 \gamma_4^m \gamma^e)(\Gamma_8 \gamma_2^m \gamma^e)(\Gamma_8 \gamma_0^m \gamma^e)(\Gamma_8 \gamma_{-0}^m \gamma^e)$ $(\Gamma_8 \gamma_{-2}^m \gamma^e)(\Gamma_8 \gamma_{-4}^m \gamma^e)(\Gamma_8 \gamma_{-6}^m \gamma^e)(\Gamma_8 \gamma_{-8}^m \gamma^e)$
$J_{9/2} m_{\pm 9/2} e_j$	9	$(\Gamma_9 \gamma_9^m \gamma^e)(\Gamma_9 \gamma_7^m \gamma^e)(\Gamma_9 \gamma_5^m \gamma^e)(\Gamma_9 \gamma_3^m \gamma^e)(\Gamma_9 \gamma_1^m \gamma^e)(\Gamma_9 \gamma_{-1}^m \gamma^e)$ $(\Gamma_9 \gamma_{-3}^m \gamma^e)(\Gamma_9 \gamma_{-5}^m \gamma^e)(\Gamma_9 \gamma_{-7}^m \gamma^e)(\Gamma_9 \gamma_{-9}^m \gamma^e)$
$J_5 m_{\pm 5} e_j$	10	$(\Gamma_{10} \gamma_{10}^m \gamma^e)(\Gamma_{10} \gamma_8^m \gamma^e)(\Gamma_{10} \gamma_6^m \gamma^e)(\Gamma_{10} \gamma_4^m \gamma^e)(\Gamma_{10} \gamma_2^m \gamma^e)(\Gamma_{10} \gamma_0^m \gamma^e)$ $(\Gamma_{10} \gamma_{-0}^m \gamma^e)(\Gamma_{10} \gamma_{-2}^m \gamma^e)(\Gamma_{10} \gamma_{-4}^m \gamma^e)(\Gamma_{10} \gamma_{-6}^m \gamma^e)(\Gamma_{10} \gamma_{-8}^m \gamma^e)$ $(\Gamma_{10} \gamma_{-10}^m \gamma^e)$

A graphical form of these representations can be based on an expansion of the Young Tableaux format. Standard Young Tableaux are two-dimensional objects containing at most three pieces of information: the identity by row, by column and by content of each box. Five pieces of information are now required to be included in the Young Tableaux; the state J , the magnetic moment m_j , the electric moment e_j , and the projection of of unit moment vectors m_j and e_j , including the concept of magnitude which defines the relative dimensions of each three-dimensional unit. Thus a three-dimensional Young Volume must be developed for both the fundamental state and all the more complex states with their overtones. The essential feature required in this three-dimensional version is explicit specification of the conjugation conditions for the three identifiers J , m_j and e_j . A typical Young Tableaux for a typical component m_j and e_j of tensor $J_{(k)}$ is shown in FIGURE III-4.

The length of the unit vector in the $J_{(k)}$ dimension is defined by the cross products:

$$J_{(k)} = m_j \times e_j \quad \text{III.2-4}$$

so that this unit vector varies with the degeneracy k . Likewise, the cell volume may be defined as the cross product;

$$V_{(k)} = J_k \times m_j \times e_j \quad \text{III.2-5}$$

so that the volume itself varies with k .

FIGURE III-4 3D Young Volume

In this formalism, the three-dimensional Tableaux represent the projected properties of the four-dimensional Lagrangian for each J_k , m_j and e_j and the vector associated with the fourth axis of Lagrangian space projects as the volume of the cell. Thus volume is the density of states available on that missing axis and acts as a normalization condition for the three-dimensional state.

Both J_k and $V_{(k)}$ are defined by vector cross products and both are directional entities. The tensor specification of J defines its chirality since it relies on choices of sense in m_j and coherence in e_j in the cross product of these vectors. Similarly the volume specification of V is directed because it relies upon all the eight choices of chirality, sense and coherence. Traditionally, the directed nature of the construction of two-dimensional Young Tableaux has been expressed by limiting the allowed shapes of the Tableaux.⁵³ By extending these limitations to the three-dimensional Tableaux, a set of eight orthogonal allowed shapes is generated, occupying the octants of a Cartesian coordinate vector space. This allows the definition of geometric cross product rules defining the stages of conjugation in evaluation of selection rules.

However the analysis is not yet complete because the degeneracies have not yet been explored. The magnetic degeneracy arises due to the inability to distinguish between the particular arrangements of magnetic moments within a 2π rotation as the coherence phase is not identified. Individual nodes and pathways are not seen, but the effective magnetic moments are summed up and the overall moment is observed. The total number of possible arrangements for each positive or negative m_j value is $n!/m!(n-m)!$, where n is the total number of nodes, and m is the total number of moments projected in the chosen direction of either North or South. As each

projection, whether North (N) or South (S), can be created by any one of four possible pathways or Moebius loci, the total degeneracy for any one m_j per wavefunction ψ or ψ^* is further expanded:

$$\text{half-integer } m_j \quad \left[\frac{n!}{m!(n-m)!} \right] 4^{[(n+1)/2]} \quad (\text{III.2-6})$$

$$\text{full integer } m_j \quad \left[\frac{n!}{m!(n-m)!} \right] 2 \times [4^{(n/2)}] \quad (\text{III.2-7})$$

The resulting magnetic degeneracies for J and m_j states are seen in TABLES III-12 and III-13.

III.2.v   Representations of Overtones

The representations of overtones are generated by operating on the fundamental set of chiral loci with the Moebius symmetry operators of successively higher order. There is an infinite set of classes of these finite operators, each of which is constructed by multiplying the fundamental class by successively more frequent inversion during rotation of the state vector about the principal axis. This infinite set generates an infinite set of irreducible representations, each of successively higher order, in parallel with the development of traditional, infinite point groups. Since this group is a unique extension of the finite fundamental chiral group, it is an infinite permutation group (TABLE III-14)

TABLE III-12 Number of Arrangements for Each $\pm m_j$ State

J, m_j	± 0	$\pm 1/2$	± 1	$\pm 3/2$	± 2	$\pm 5/2$	± 3	$\pm 7/2$	± 4	$\pm 9/2$	± 5	$\pm 11/2$	± 6	$\pm 13/2$
$1/2$		1												
1	1		1											
$3/2$		3		1										
2	3		4		1									
$5/2$		10		5		1								
3	10		15		6		1							
$7/2$		35		21		7		1						
4	35		56		28		8		1					
$9/2$		126		84		36		9		1				
5	126		210		120		45		10		1			
$11/2$		462		330		165		55		11		1		
6	462		792		495		220		66		12		1	
$13/2$		1716		1287		715		286		78		13		1

TABLE III-13 Total Magnetic Degeneracies

J, m_j	± 0	$\pm 1/2$	± 1	$\pm 3/2$	± 2	$\pm 5/2$	± 3	$\pm 7/2$	± 4	$\pm 9/2$	± 5	$\pm 11/2$	± 6	$\pm 13/2$
$1/2$		4												
1	8		8											
$3/2$		48		16										
2	96		128		32									
$5/2$		640		320		64								
3	1280		1920		768		128							
$7/2$		8960		5376		1792		256						
4	17920		28672		14336		4096		512					
$9/2$		129024		86016		36864		9216		1024				
5	258048		430080		245760		92160		20480		2048			
$11/2$		1892352		1351680		675840		225280		45056		4096		
6	3784704		6488064		4055040		1802240		540672		98304		8192	
$13/2$		28114944		21086208		11714560		4685824		1277952		212992		1638

TABLE III-14 Magnetic Representations

Γ_n	$\gamma(\pm m_j)$	$J_n/2$	I	M_1	M_2	M_3	M_4	M_5	M_6	M_7	M_8	M_9	M_{10}	M_{11}	M_{12}	M_{13}
Γ_1	$1/2$	$1/2$	1	1	0	0	0	0	0	0	0	0	0	0	0	0
Γ_2	1, 0	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0
Γ_3	$3/2, 1/2$	$3/2$	1	1	0	1	0	0	1	0	0	0	0	0	0	0
Γ_4	2, 1, 0	2	1	1	1	0	1	0	0	0	1	0	0	0	0	0
Γ_5	$5/2, 3/2, 1/2$	$5/2$	1	1	0	0	0	1	0	0	0	0	1	0	0	0
Γ_6	3, 2, 1, 0	6	1	1	0	1	0	0	1	0	0	0	0	0	1	0

IV. MCD AND TRANSITIONS

IV.1 Topology of Transitions

To promote a state of a system to a less stable, more complex state in the same system an event involving union with input energy must occur. In the event space the system and the excitation must have identical shapes in order to interact. In the process of excitation the quantum of energy is totally absorbed because it alters the original locus to have exactly one more twist per revolution.

Any perturbation of an atomic state must have an external cause. However there are two environments that an external probe can act upon. One is a totally degenerate state, the other a state that has been split by a static external magnetic field. In the latter case every m_j or e_j is labelled discretely, however the observable moment truly yields only orientation information, not energy information. Therefore each individual m_j or e_j must have a slightly different J value if it is truly non-degenerate. These states can be labeled by means of the quantum mechanical addition rule by addition of shapes and energy of excited states. Therefore m_j or e_j yields purely orientation information only if all the m_j or e_j states are fully degenerate. An equivalent approach is to perturb the system in order to split m_j or e_j , having lowered the symmetry by the external field in the process.

The group theoretical description of transitions can be used because the photon has an origin superimposed upon that of the atom within the event space. This allows the geometric features of the photon to be described in terms of the language of the atom. The group theory and direct products see the point of view of the recipient, not the incoming probe. The photon is an *electric dipole* and *magnetic quadrupole*.

Although it is a transverse wave in and of itself, its electric dipole vector is spinning around along the direction of travel. In the case of absorption, it is necessary to know what that electric vector looks like to the receiving atom. In the case of emission, statistical distributions of the separation of energies are observed as the analysis is incomplete due to a missing dimension.

The transitions are indicated in **FIGURE IV-1**, which illustrates the difficulty in differentiating which of two possible transitions has created the MCD term. The two possible wave functions involved are distinguished by their coherence and require the application of an external field to differentiate them.

The operators and the resulting transitions can also be defined in Maxwellian terms. Previous difficulties in mapping Maxwell's equations onto the Dirac four-dimensional formalism has been due to a missing dimension in Maxwell's field equations. Whereas Dirac's γ^0 and γ^i have four components, Maxwell provided only a three-dimensional analysis with gradient, curl and divergence. However, by boosting the origin on the field one can obtain a pitch on the curl. (Refer to Historical Appendix, page 168) The behaviour of this pitch determines the operator behaviour.

The operator is the first derivative $d(\text{pitch})/d\phi = \rho$. If $\rho = 0$ then $\hat{I} = \hat{i} + \hat{i}^*$ are identity operators and there is no interaction — the photon has zero energy. If $\rho \neq 0$ and the pitch of the photon and wave function are superimposed, absorption can take place, as outlined in **TABLE IV-1**. If $\rho \neq 0$ and there is no match between the pitch of the photon and the pitch of the wave function then there is scattering. In

ABSORPTION

$$|(-\hat{++})|q\rangle = |(-\hat{++})|(-\cdot\cdot+)(+\cdot+)^*>$$

$\Delta J > 0 \quad \Delta m_j > 0$
Operator accelerates
0-2 π window pathway.

$$|(+\hat{++})|q\rangle = |(+\hat{++})|(-\cdot\cdot+)(+\cdot+)^*>$$

$\Delta J > 0 \quad \Delta m_j < 0$
Operator descelerates
2 π -4 π window pathway.

$$|(-\hat{--})|r\rangle = |(-\hat{--})|(-\cdot\cdot\cdot)(+\cdot\cdot)^*>$$

$\Delta J > 0 \quad \Delta m_j > 0$
Operator accelerates
0-2 π window pathway.

$$|(+\hat{--})|r\rangle = |(+\hat{--})|(-\cdot\cdot\cdot)(+\cdot\cdot)^*>$$

$\Delta J > 0 \quad \Delta m_j < 0$
Operator descelerates
2 π -4 π window pathway.

$m_j > 0$	+1	R.H.
$m_j = 0$		Forbidden
$m_j < 0$	-1	L.H.

FIGURE IV-1 MCD Transitions

the 2π – 4π window of time the sign of the derivative reverses, the photon unwraps itself from the atom causing scattering. The angle of scattering can be calculated as the mismatch in wrapping and unwrapping of the photon about the atom yields the angle of the outgoing photon and the real part of the refractive index is seen as a function of the wavelength of the photon.

If $d(\text{pitch})/d\phi$ reverses sign then emission occurs as the pitch has been decreased as a result of the photon unwrapping itself from the atom. As a result the wave functions are seen to be π out of phase.

TABLE IV–1 Photon–Wave Function Interactions – Absorption

	q	r
$\hat{p}$	$\Delta J > 0 \Delta m_j < 0$	
$\hat{q}^*$	$\Delta J > 0 \Delta m_j > 0$	
$\hat{r}$		$\Delta J > 0 \Delta m_j > 0$
$\hat{s}$		$\Delta J > 0 \Delta m_j < 0$

IV.2 Electromagnetic Description of Transitions

As an electromagnetoinertial gauge and state coordinates have been described (II.5), the total energy of any state of the system may be described in both mechanical and electromagnetic terms. The energy contained in the system oscillates from the magnetic to the electric. At its farthest limit the energy is mechanically all potential, and electromagnetically all capacitive (electric). Near the nucleus the energy is all kinetic in mechanical terms and all inductive (magnetic) in electromagnetic terms. Referring to section II.5.v and equation (II.5-20), the transformation from potential ($\frac{1}{2} kx^2$) to capacitive ($\frac{1}{2} q^2/C$) energy and kinetic ($\frac{1}{2} mv^2$) to inductive ($\frac{1}{2} Li^2$) energy is clear. Assuming a zero resistance for the vector current for the atomic states in order to maintain a constant energy content of the state, the equation (II.5-22) expresses the conventional description of oscillating current in an LC circuit. The solution ⁵⁹ is the "conserved current" which carries no dimension or units and takes the form of the vector (II.5-23). Each occurrence of this vector must be separated into its two Moebius inverted, conjugate paths of motion for the electronic vectors L and C which define the state.

When the operator, such as the photon probe, acts on the state, it can accelerate only one of these vectors along its path as it is by definition orthonormal to the conjugate vector. It increases the value of the inductive term L of the current which has the same original orientation as the photon. As it cannot affect the conjugate current, the two current vectors are dephased. As the two currents were initially fully coupled, the unaccelerated current will attempt to equilibrate with the

accelerated current. If this equilibration is successful, a transition is said to have occurred and a new state will emerge. If not, the photon is released and no transition will have taken place. The transition is dependent on the ratio of the inertia, inductance and capacitance of the initial and final states.

IV.3 Fundamental Direct Product Selection Rules

TABLE III-6 has illustrated the point group operator table for the $J=1/2$ state and is applicable to the photon-atom interaction as the photon can be represented by this operator set. There are four possible representations for the photon $(\hat{p}, \hat{q}, \hat{r}, \hat{s})$ which can act on any one of the four possible left-handed wave functions $\psi(p, q, r, s)$.

All the formalisms apply to these representations of operators and the Young Tableaux can be used to display the structure of the representations and their direct product algebra with atomic states. Thus, the unique and unambiguous description is extended to the analysis of structures and spectra of many-body atoms.

Therefore for transitions a cross product description of an event is a cross product of a state with a probe acting upon that state, being described in terms of the shape and energy of yet another state. Distribution of the incoming energy over all available m_j states is a real time process in a real direction with an accompanying real vector change. Translation of the photon probe along its own path is converted to rotation by a coupling of the photon to the state of the atom. The resulting absorption requires the time of one full wavelength. This process requires a movement of nodes within the space as the configuration of the ground state is altered. The ground state is by Hund's Rule the most degenerate state and as the nodes are displaced by the incoming energy the atomic structure is recoiling from the impulse of the photon, as expected according to Newton's first law of motion. The atom needs to recoil by converting the translational energy into rotational energy within the atom itself. This is a totally inelastic process as all the energy disappears inside the atom. It is this process that is described by the direct product.

This analysis illustrates that a complete polarization instrument should involve the intersection of both external magnetic and electric fields probed by circularly polarized light. Since such an instrument has not yet been developed, coherence information and therefore electric information cannot currently be extracted from experimental data. Therefore the three-dimensional Young Volume representation of operators and states collapses to a two-dimensional Young Tableaux for current practices. The coherence information is lost in this process. A two-dimensional Young Tableaux is used only because of limitation to the instrumentation, not because of limitations to the theory or indeed to practice, as the instrument can be built. As a result of the necessary conversion from three dimensions to two dimensions, in the Young Tableaux only magnetic information is revealed.

IV.4 Intensities of Allowed Transitions

In any description of a system, the language used to define the energy content is chosen as a consequence of recognizing the numbers and interactions of the particles and forces. The system based on the interactions of the strong, weak and electromagnetic forces on one proton-electron pair would formally require 2^4 dimensions. Up to three interactions could arise, coupling protoelectron motion into reduced numbers of independent dimensions. Experimental experience suggests that there is weak-electromagnetic coupling, usually denoted as the "*spin-orbit*" interaction which depends approximately on the fourth power of the number of protons.⁴⁹ The weak-electromagnetic coupling reduces the number of independent dimensions to 2^3 , and the influence of the missing dimensions is reduced to a binary degree of freedom on the value of the "*coupling constant*". As a result, there are two types of atoms, those with "*positive*" and those with "*negative*" coupling constants.

In contrast, the strong force appears only to randomize this weak-electromagnetic structure, no significant coupling to these other forces can be defined. The extent of randomization is found by integration of the state vector pathway. The path integration of natural coordinates identifies the properties of a stable state if it couples the vector coordinate dynamically to its conjugate. The ideal component of this "*normalization*" depends on the coincidence of the ideal portion of the coordinates. The extent of normalization depends on the degree of non-classical decay in the ideally allowed cases. The longer the time taken by the state vector in executing its locus, the greater the accumulation of uncertainty, as described in

equations II.5-38. In a transition, the intensity is determined by the overlap of uncertainties of the ground and excited state via the change in Action imposed by the probe.

Intensities of circularly polarized transitions involve combining the effects of ideal spin-orbit coupling from the weak-electromagnetic interaction with the randomizing influence of the strong field interaction. The magnitude of ideal spin-orbit coupling would be infinite and of a particular sign if there were no randomization of geometry in the extended dimensions of three-dimensional space. In this ideal limit, the spectroscopic intensity would be the change in magnetic flux, added by the probe, which directly measured the change in electromagnetic dimensions of the atom. This would be definable in fundamental physical units of current and flux with appropriate vectorial structure in the event space.

The degree of loss of intensity can be estimated from the overlap of uncertainties from the participating states in the transition using the path integral to define a joint uncertainty along the excitation locus. Thus, while the path integral for a state establishes the cone of uncertainty, illustrated in **FIGURE II-3**, the path integral for a transition defines a more asymmetric object with a changing pitch. The volume of this uncertainty space defines the degradation of the ideal intensity. This model of atomic structure would make possible, for the first time, the separate definition and calculation of these two contributions to intensities. An initial set of experiments showing the variation of intensity and sign of MCD magnetic hypersensitive transitions shows that the effects of the two contributions may be discriminated in real systems. ⁹ Thus, the formal discrimination can be tested in new applications designed to permit recognition of ideal and real intensity contributions.

V. CONCLUSIONS

There are two situations which are guaranteed to intrigue any scientist and therefore drive one on to new dimensions. When one knows that the information one seeks, or behaviour one expects to see is just out of reach due to a lack of technology to perceive it, one is challenged to design the experiment or technology required. Another challenge arises from being inundated with data which one knows contains information when there is no current viewpoint or interpretive model capable of extracting that information. Here the challenge is to conduct a thought experiment, to bend ones mind in new directions and observe the data from a new perspective in order to place the available information in a slightly different context and recognize a different pattern of behaviour. The ultimate challenge is to describe that behaviour in a manner which will allow a prediction of that behaviour under various conditions.

There are two facts which lead one to believe that some highly selective form of selection rules must exist. The relatively high refractive index of coloured molecules indicates that virtually every photon collides with an atom. However it has been calculated that only one in every 10^{12} molecule has actually captured a photon. Therefore there must be a very small window of tolerance which allows an interaction between photon and atom. Initial estimates of this window lie in the range of .005 degrees. There is therefore a high degree of selectivity that must be met within any model to be presented.

As polarized spectroscopy is essentially a chiral spectroscopy, it was necessary to invent a frame of reference that is the most convenient for chiral spectroscopy. This frame of reference was derived from the observable phenomena of polarized spectroscopy, specifically MCD. The coherence, sense of motion and chirality behaviour led to the construction of an atomic structure with a geometric relevance. It was initially startling to find that the specific structure, the Klein surface, and its perceivable behaviour had been observed previously in early experiments by Harry Mosely, and that Erwin Schroedinger had deduced a similar structure for electron pathways nearly six decades earlier.

It was interesting to discover that other routes of deductive reasoning had led others to the need for a four-dimensional analysis and the use of the Lagrangian as an operator. Whichever route was taken, all led to the same conclusion, that the ideal geometry must allow for two orthogonal three-dimensional pathways of least action (the Moebius loci), which when induced to their parent object are seen to arise from a Klein surface. The discovery of the Moebius loci as the natural coordinate axes allowed the development of a mechanics built about an event space which contained all the atomic behaviour within its bounds, as opposed to a mechanics built about a space which had to be continually renormalized to accommodate extraneous behaviour. In short, the space does the work, not the matter, thus allowing an interaction between light and matter to be described within that same space.

Having recognized the ensemble nature of matter within such a space, the atomic behaviour within the space was deduced from an interpretation of the laws and postulates governing ensemble behaviour. The four laws of thermodynamics and the relativity principle allowed a description of all possible behaviour within the ideal

geometry. The application of the uncertainty principle led to a clearer understanding of the dual nature of matter, and to a greater understanding of the observables of that nature. In short, the observable to any probe is not the ideal behaviour as induced by the nucleus, but the loss of this behaviour as the atom feels the effects of the external environment. This impurity is in fact the saving grace of matter, for it is that same loss of ideality that allows matter to interact with external perturbations and thus support life as we know it.

Having described the operators which represent the coordinate axes, the group was expanded to accomodate an infinite atomic structure. There have been several algebraic methods used in the past to define and describe such groups of operators. The choice to employ group theory was made in order to provide as compact, concise and unambiguous description as could be imagined at the time. There was no current group theoretical description available which was capable of describing the geometry and dynamic behaviour of the event space, and so the eight-fold Moebius group evolved of its own volition as a minimal descriptive requirement. The process was aided considerably by the permutative nature of the operators and their innate acquiescence to the Casimir operator conditions.

The group theoretical construction allowed a simple, concise description of atomic states, including those of a half-integer nature. The algebra for the product multiplication of the group representations is again concise and compact as both wave functions and conjugate wave functions can be easily portrayed on several levels. It is worth noting that the multiple levels of conjugacy are easily and clearly demonstrated as separate individual conjugate mechanisms of different aspects of the atomic behaviour, and no longer an indecipherable conglomerate behaviour

which consistently led one to the need for complex numbers in describing that same atomic behaviour.

It is now possible to describe the underlying atomic characteristics and selection rules which define the limits of the interaction of light and matter. Whether or not an atom will interact with a photon, and whether that interaction will be absorption, emission or scattering is now definable and almost predictable. The descriptive mathematics are in place. However it is not complete because the work has come full circle and there is now a requirement for information that is not currently available.

It has become clear that yet another quantum number, an electric moment e_j is required in order to fully describe any atomic behaviour. The source of this electric moment is known and has been described. It is yet another source of ambiguity which must be resolved. In order to do so one must conduct an experiment in which an external electric field is added orthogonal to the external magnetic field already available in polarized spectroscopy. Thus a new era of technology is required and further work will continue once Electro-Magnetic Circular Dichroism (EMCD) has been established. Any true resolution of polarized spectra is dependent upon the understanding of the behaviour of this electric moment. Having gained the observable information required from such spectroscopy, the mechanism for interpreting the data has already been established in the form of the Young Tableaux. One needs only to fill in the required information on the final axis.

It is anticipated that such an instrument could be built in the near future. It is projected that building such a spectrometer would take a year or two at most, and that the definable information could be extracted within another one to three years.

An investigation of the intensities of EMCD spectra should yield capacitance and inductance data for the states, leading to information regarding the bond strengths. An examination of $\mathcal{E}$ terms should lead to a characterization of excited states for capacitance.

In the interim it will be possible to begin to develop the intensity parameters required. The methodology will parallel that of developing the crystal field fitting parameters of DQ, DS and DT. The dipole, quadrupole and octupole operators must be defined in terms of the descriptions available from this study. These operators will represent the electric, magnetic and inertial influences of the atomic or molecular background upon the state. It will be necessary to describe all possible subspaces in terms of that parent space.

The standard technique in spherical harmonics is to use mixing coefficients of the major axes in order to estimate internal field gradients that allow one to see a change in motion from the parental sphere to the (cubic, tetrahedral etc.) distorted subspace. This same technique may be applied to the Klein surface. As an example, in the model series described at the start of this study, a change of ligand was seen to bring on a change of intensity as a result of a change in chirality. It is necessary to examine the possible phenomena that would cause the atomic dielectric, diamagnetic and di-inertial constants to twist to such an extent that handedness changes. Fields that affect motion are obviously being inverted due to the change in

ligand. There is a new path of least resistance being created, and this path must be described by a different linear combination of the dipole, quadrupole and octupole for every ligand changed in the compound.

Having described a pattern of behaviour that describes all possible changes, the correlation to spectra may begin. Again, carefully designed model compound series may be used. As there are three observable parameters, spectra containing a minimum of three bands of the same ΔJ value are required as the bands used must represent identical behaviour. It is proposed that the resulting intensity parameters be labeled as DH, DI, and DJ.

The dipole may be described by the group Γ_1 , the quadrupole by Γ_2 and the octupole by Γ_6 . The relative intensity is describable by the relationship:

$$\text{Relative Intensity} = \text{Klein surface} + (\text{DH})[\Gamma_1] + (\text{DI})[\Gamma_2] + (\text{DJ})[\Gamma_6]$$

The work involved in pulling out this intensity information has been proposed and accepted as a post-doctoral project.

HISTORICAL APPENDIX

Introduction

Description and Structure

In order to be certain that a description of atomic and molecular structure which does satisfy all the needs of the most highly resolved measurements is achieved, it is useful to examine the process by which descriptions, and their accompanying mathematical models, are derived. This examination of the process will permit the recognition and separation of limits imposed by natural conditions and limits employed to make models mathematically tractable. The former must all be present in explicit form and the latter need to be minimized while the consequences are made clear. The artificial limits to structure or behaviour serve to reduce the number of defined entities in a model and hence apparently simplify manipulation. In fact, the undefined entities are not eliminated from actual observations so their effects still govern observed magnitudes. In attempting to describe these magnitudes with any such artificially truncated model, the contributions of the undefined entities become indefinably combined with the declared parameters. As is the case with analysis of polarized spectra, attempts are often made to reintroduce the information.^{2,8,27,37,41} In most cases however, this is done without reference to the underlying physical structure in the experiment. As a result many alternative, ideosyncratic models are proposed to "*calibrate*", or renormalize, the data, none of which provide any physical insight into the process being observed. To assess the state of any particular area of interest in science and to determine whether its current models are appropriate to the tasks involved, an overview of the development of models in general is very useful.

Traditional Model Development

The role of tradition in science is manifested in three major areas; the selection of problems to be studied, the method of the scientific process itself, and the concepts required in formulating the question to be studied.⁶² Problems can be studied only by first formulating the question to be answered. To formulate a question, there first needs to be a concept with which to grasp the phenomenon of interest. Concepts arise from the present level of understanding, which arises in turn from past history. These concepts suggest a possible direction of study.

This direction may foster progress or it may stifle new insight by continuing to feed a collection of prejudices. However the concepts themselves are unavoidable as they are the basis of the same current understanding that led to the asking of the question. Therefore it is important to recognize the traditions for exactly what they are and to assess their relevance in the current study.

One of the great stimulants of scientific discovery is society and its needs. Pythagoras discovered the relevance of mathematical relations in natural phenomena and triggered a long period of development in mathematics, astronomy and natural philosophy precisely because of the needs identified during a time of great philosophical debate which stimulated intellectual development within the society of his time. No further fundamental understanding of nature was achieved until the discoveries of Copernicus, Galileo and Kepler, whose interests in

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⁶² W. Heisenberg, Encounters with Einstein, Princeton University Press, Princeton, 1983.

astronomy and mathematics were stimulated by navigational and land surveying requirements of this time of great westward exploration. Their interest in the practical aspects of science led to further studies as well as the invention of mechanical devices such as optical instruments.

At the same time however, the practical application of science performs a valid function as a check on the validity of the results and as a justification for the initial effort. This tradition was being followed still when atomic physicists searched for practical applications of atomic physics to check if they had correctly understood nature. However the methods followed by modern physicists differ from those of their predecessors. The change was evoked by Galileo, who abandoned the traditions of his time and the descriptive approach of Aristotle to replace it by the philosophy of a structural science of Plato. Thus, causality replaced empiricism and science was directed away from simple observation to discovery of rules of behaviour.

Concepts and Constructs

Whereas Aristotle sought solutions by intuition, Galileo and Copernicus created a so-called "empirical" science by idealizing experience in order to discover mathematical structures in phenomena and thus gain a simplicity as a basis for a new understanding. Such a "scientific reasoning" was an important achievement in the history of human thought and is considered to be the real beginning of physics.⁶³

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⁶³ A. Einstein and L. Infeld, The Evolution of Physics from Early Concepts to Relativity and Quanta, Simon and Schuster, 1938.

Instead of simply describing what is visible, this new method aimed to design experiments and produce phenomena not normally seen, and to calculate these phenomena on the basis of mathematical theory. This effectively compares the newly observed phenomena with mathematical constructs known as natural laws.

This radical change of approach required a level of confidence that Galileo and Kepler found in their theological beliefs. They felt that physics is a reflection on the divine Ideas of Creation (hence physics was named natural philosophy), and consequently, causality must be the fundamental principle of science. The philosopher Kant ⁶⁴ pointed out that causality is not an empirical law but is a pre-condition for this kind of science, which has been elaborated upon ever since.

One of the assumptions made consistently with this attitude in science is that new phenomena are not really produced, but that they are natural occurrences that have been effectively isolated, independent of the probe designed to study them. If it were true that science is empirical and that the concepts and mathematical constructs involved are drawn from empirical data, then any new field of endeavor would contain only such quantities that can be observed directly, and natural laws would be formulated only on the basis of these observed quantities.

Einstein felt that the transition from observation to definitions of phenomena must make use of theory and theoretical concepts and that the empirical process of observation cannot be separated from the mathematical construct and its concepts. Thus observations and experiments provide examples of the concept and its

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⁶⁴ a E. Kant, Critique of Pure Reason, 1781;

b E. Kant, Prolegomena to Any Future Metaphysics, 1783;
 Liberal Arts Press Ltd., Bobbs-Merrill Company, Inc., 1950.

mathematical predictions. An important characteristic of modern physics is that the conclusions drawn from initial information are not only qualitative but also quantitative, a process which requires the language of mathematics. Mathematics as a tool of reasoning is necessary to draw conclusions which may be compared with experiment. The price for abandoning the language of mathematics is a loss in precision. The discovery of the uncertainty relationships by Heisenberg is an example of this process as uncertainty is required to represent the loss of precision. Einstein and his colleagues continued to hold strong personal feelings regarding the relationship between God and nature, although in developing quantum theory they were forced to let go of the nearly four hundred year old traditional reliance on strict causality.

A natural extension of the empirical tradition is the derivation of statistical distributions from repeated observations, which has become a standard method in particle physics. Although Goethe tried to return to a descriptive science which is interested only in the visible natural phenomena, modern science is still essentially that of a causal nature.

New Science : Mechanics to Quantum Mechanics

Thus, the purpose of any modern physical theory is to explain as wide a range of phenomena as possible in terms of a minimal set of defined properties and relations. It is justified in so far as it does make events predicatable. The results of scientific research often force a change in the philosophical view of problems that extend far beyond the restricted domain of science itself. Scientific concepts often begin with those used in ordinary language but they are transformed and lose the ambiguity

associated with them in ordinary language, gaining in rigourousness so they may be applied to scientific thought. Pioneer work consists of finding new and unexpected paths of development. Such paths usually arise out of a dissatisfaction with the predictive power of the initial model. The model then undergoes an analysis of its weaknesses in order to identify missing concepts. It is here that the theory of "*freedom vs. limits*" is often brought into play. By exploring the extent of freedom available and discerning the reduction of this freedom due to constraining influences, two new concepts can be introduced into the model. The nature of the constraining influences and the types of remaining freedom of movement can be identified by a name represented by any nouns from common language, but because the concepts are unique, the nouns become very specific. The initial and fundamental steps are always of a revolutionary character.⁶³ Scientific imagination finds old concepts too confining and replaces them by new ones. The continued development along any line already initiated is more in the nature of evolution until the next turning point is reached when a still newer field must be conquered.

The underlying principle of Natural Philosophy⁶⁵ is this systematic reduction of apparent complexity to a simple set of fundamental ideas and relations. This was achieved in classical mechanics and supported by the success of its application to astronomy, the kinetic theory of matter, etc. The original concepts of the new science arose from astronomy as the positions and velocities of bodies. Newton added the concepts of mass, force and momentum as well as kinetic and potential energy to complete the conceptual basis of mechanics and in the process introduced the use of vectors to physics. Newtonian mechanics was so successful that whenever

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⁶³ T.S. Kuhn, The Structure of Scientific Revolutions, University of Chicago Press, 1970.

new observed phenomena required or suggested new concepts, attempts were made to reduce them to or place them in parallel with the old ones of mechanics. When electricity and magnetism were being explored in the eighteenth century, the concept of force was introduced in a mechanical sense. By the nineteenth century it became clear that electromagnetic phenomena could not be so easily reduced. Faraday introduced the concept of the electromagnetic field in 1849, and Maxwell completed the theory in 1861. Inverting the traditional view, fields were now seen to be as "*real*" in a space–time space as in a position–velocity (mechanical) space. Our entire knowledge of the acting forces can be summarized in the construction of the field. Fields provided a more compact way of describing acting forces, poles, currents and velocities than was possible in classical mechanics concepts and they allowed a simple description of electric and magnetic phenomena in accordance with the law of conservation of energy.

Fields Mechanics

The quantitative mathematical description of the laws of the field appears in Maxwell's equations without redundancy. The equations represent the functionally two–dimensional STRUCTURE of the instantaneous field by means of the radial gradient, the angular divergence and spiral curl. All three terms are functionally two–dimensional because Maxwell thought of what is now described as the photon as a transverse wave.

An instantaneous field surface has two variable independent position parameters and is thus functionally two–dimensional. Each pair on this surface possesses the property of a position in time as well as electric and a magnetic field gradient (with

magnitude and direction) vectors. Each gradient is defined by three parameters (magnitude and direction). Therefore in order to describe two independent electric and magnetic transverse waves, six parameters are required. Thus each point would have associated with it eight descriptors, the position (θ, ϕ) , the electric gradient $(|e|, \theta_e, \phi_e)$, the magnetic gradient $(|m|, \theta_m, \phi_m)$. Given certain known relationships, the number of independent parameters may drop.

The gradient represents the contours of the field and has no angular dependence. In spherical coordinates the divergence is the rate of change of the field as the angle is changed. The curl is the spirality of the field. These can all be represented in circular polar coordinates. If one were to boost the origin up the z-axis to obtain three dimensions, there results a pitch on the curl and for three dimensions there would be four terms in total, the gradient, divergence, curl and pitch. Maxwell's equations differ in form and character from equations of classical mechanics by idealizing the experiment and describing the closed pathway in a generalized set of dimensions. Then everything concerning size is quite irrelevant and vanishes from our considerations. The classical mechanical definitions of positions and velocities are replaced by the electromagnetic, which is regarded as something real, which once created exists, acts and changes according to Maxwell's laws. Maxwell's equations describe the structure and development of the electromagnetic field. All space is the scene of these laws and in contrast to mechanical laws in which only points of matter or charge are present. In causal classical mechanics, if the position and velocity of a particle in one single instant, and the acting forces are known, the whole future path of the particle can be foreseen. This is replaced in Maxwell's

theory by knowledge of the field at one instant from which one can deduce how the whole field will change in space and time. Maxwell's equations allow one to follow the history of the field just as mechanical equations enable one to follow the history of material particles.

There is still another essential difference between classical mechanical laws and Maxwell's field laws. Field theories are global and as such express behaviour on continuously varying tensorial gradients. In contrast, the classical mechanical model describes behaviour in terms of parameters evaluated at specific, discrete points. In any mechanics system a frame of reference is required to illustrate the mechanical properties of interest. The frame, which may be constructed of any particular mechanical property is called a coordinate system. Transformation laws allow movement between coordinate systems which provides an alternative view in terms of a different mechanical property. In classical mechanics the laws of transformations were formulated for coordinates and velocity and the laws of mechanics were invariant with respect to classical transformations.

In field mechanics the simultaneous description of position and velocity in one coordinate system led to the development of Minkowsky spaces. Here however position and time were not kept separate on distinct axes. Space and time were no longer seen to be independent of each other as Newton believed, but related by a Lorentz transformation. Maxwell's equations or field laws are invariant with respect to a Lorentz transformation. Every coordinate system has its own internal clock. However, as seen from Einstein's work, time is not globally invariant and the next step away from classical mechanics, the theory of relativity is introduced. The state of a system in quantum mechanics was now seen to be characterized by a vector in a

many-dimensional space, which implied statements concerning the statistical behaviour of the system under given observational conditions. This was the first indication within field mechanics of the need for a four-dimensional space of mixed and generalized position and velocity properties. This mixture will be seen to be Action, and is an indication the the requirement of field mechanics for an Action space, or Lagrangian.

The concept of the field was throughout its development related to the existence of a background aether, apparently required as a completely elastic medium for electromagnetic theory in order to set up a fixed classical background which could oscillate without causing loss of energy during transmission of a wave. The development of special relativity ⁶⁶ freed electromagnetic theory from a need for aether. The background need not be seen as the support of the system since the uncertainty in the classical motion of the vector can be substituted for the aether. In fact, the model developed in this study will exploit this condition by setting up the classical ideal non-orientable motion that progressively (integratably) loses certainty, that is the path integral will add up continuously until the cycle is reinitiated by passage of the state vector through the origin. This can be alternately described by placing the uncertainty in the pathway instead of the space, which becomes undefinable vector positions.

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⁶⁶ ^a A. Einstein, Ann. Phys. 17, 891, 1905;

^b A. Einstein, Ann. Phys. 17, 905, 1905;

^c A. Einstein, Ann. Phys. 18, 639, 1905.

Dirac felt that Maxwell's equations were not complete ⁵² and might need to be modified in order to be made into a non-linear electrodynamics. In this study the suggested expansion of Maxwell's field equations to four terms will represent the photon in photon-matter interactions. As will be shown, the atom represented by Dirac's four-dimensional expressions can then directly participate in a photon-atom interaction, which can be represented by a coherent overlap of Maxwellian and Diracian four-dimensional spaces into an event space created by superimposing respectively a four-dimensional open photon space upon a four-dimensional closed atomic space. The major advance will be in using the two sets of expressions to express the full extent of geometric coherence necessary by using group theory.

Traditions of Quantum Physics

Concepts and Constructs

Three main schools of thought were pursued in the early development of the concepts of quantum physics. The Munich school characterized by Sommerfeld was phenomenological in nature – it attempted to unite new observational findings in intelligible fashion, present their connection by means of mathematical formulae which appeared plausible from the standpoint of current physics. The Göttingen school was represented by Born and Franck who tried to represent natural processes by means of a carefully worked out mathematical formalism which satisfied the demand for rigour. The Copenhagen school of Nils Bohr was a conceptual/philosophical approach which attempted to clarify the concepts by means of which events in nature are ultimately to be described.

Standing away from the personalities, each of these approaches represents a necessary step in formulation of a working model. The phenomenology is needed to define the required degrees of freedom within recognizable constraints. Once found, the concepts of constraints and remaining degrees of freedom must be defined. Once defined, the concepts must be given dimensions and units to achieve predictive capabilities within a physically and mathematically rigorous framework. Such concepts of constraints and permitted behaviours are required whenever one enters a new field.⁶² These new concepts often appear initially as unclear and undeveloped and are either modified later or abandoned for other new ideas. In either case one ends up with clear and well-defined views. The theories of quantum physics were developed over a relatively short span of only five years. The preparatory work took place from 1922 to 1924, the decisive concepts were published in 1925 and the

exploitation of the ideas began in earnest in 1926 and 1927. However even the preparatory work did not arise directly from classical and field mechanics, for several concepts introduced during the first two decades of the twentieth century were necessary intermediate steps. Quantum physics contains three essential concepts; the concept of a state of matter (which was clearly understood only after quantum and wave mechanics were developed): the more sophisticated concept of a discrete stationary state; the concept of the elementary particle whose behaviour creates the state.

The concept of a discrete stationary state as an unexplained axiom was introduced by Bohr in 1913 and was intended to show a connection between three main phenomena; the stability of the atom even upon perturbation, spectral laws and Rutherford's experiments and atomic model. It is worth noting that even the concept of stability of the atom arose out of previous work, the discovery of X-rays (1895), radioactivity (1896) and the existence of negative electrons of small mass (1897). To begin combining these three phenomena a discrete stationary state was required as an initial state. In order to connect the stability of the atom with Rutherford's model it was necessary to believe that the behaviour of the state was describable by mechanics. The only connection to the spectral laws was obtained by accepting Einstein's light quanta, a concept arising from Planck's introduction of quanta in 1900 that Einstein expanded in 1913. Bohr achieved his interpretation of atomic spectra by assessing the older ideas, eliminating those aspects which appeared irrelevant and then adding whatever new ideas were deemed necessary. In particular he felt it necessary, against Rutherford's objections, to propose what was then a radical new concept, that any attempt to visualize or to explain the behaviour of the electron during a transition of an atom from one stationary state to

another must be renounced. Sommerfeld extended the Bohr theory to elliptical as well as circular orbits and in 1915 invented the radial quantum number n , the azimuthal quantum number l and the inner quantum number j to represent the quantization of an unknown kind of angular momentum responsible for the doublet lines.⁶⁷ Schroedinger pointed out⁶⁸ that these circular/elliptical orbits cannot occur for non-hydrogen atoms and concluded that the supposedly elliptical orbit of outer electrons must occasionally penetrate the shielding shell. An approximate calculation was made based on a model in which the electron passes smoothly from the larger outer elliptical orbit to a smaller inner one as it penetrates the shielding shell. The advent of quantum mechanics and Bohr's renouncement caused the demise of all models based on classical electron orbits, but the concept of penetration remained valid.

In 1916 Einstein introduced the general theory of relativity and of gravity and Rubens confirmed Planck's quantum theory by measurements of thermal radiation. 1918 was an important landmark as Einstein introduced initial and final states and transition probabilities; Bohr introduced the Correspondence Principle; Born and Jordan introduced matrix manipulation; and Dirac and Heisenberg independently introduced the first steps to the Uncertainty Principle which allowed a simple mathematical scheme for quantum mechanics. In 1923^{69,70,71} de Broglie introduced

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⁶⁷ A. Sommerfeld, Atomic Structure and Spectral Lines, Braunschweig:Friedr. Vieweg & Sohn, 1919.

⁶⁸ E. Schroedinger, Z. Phys. 4, 347-354, 1921.

⁶⁹ ^a L. de Broglie, Compt. Rend. 177, 507, 1923;

^b L. de Broglie, Compt. Rend. 177, 548, 1923;

^c L. de Broglie, Compt. Rend. 177, 630, 1923.

⁷⁰ ^a L. de Broglie, Compt. Rend. 179, 39, 1924;

^b L. de Broglie, Phil. Mag. 47, 446, 1924.

⁷¹ L. de Broglie, Ann. Phys (10) 3, 22, 1925.

the concept of matter waves which was to be one of the mainstays of quantum mechanical thought. In May of 1925 ⁷² Heisenberg's Uncertainty Principle was fully unveiled in its squared form in order to ensure a scalar result. Born and Jordan ^{73,74} (and later Heisenberg) ^{75,76} described commutation with matrix calculations and Dirac developed an equivalent mathematical scheme with no matrix components. Born and Jordan⁴⁷ introduced the principle axis of transformation and Heisenberg introduced a physical content and an absence of pathways. Uhlenbeck and Goudsmit discovered that a previously known double-value in the states of an atom could be interpreted in terms of the electron having a spin-angular momentum of $1/2 \hbar$. Soon after Heisenberg identified unexpectedly large spin-spin interaction energies in atoms with many-electron quantum dynamical systems. In 1926 Schroedinger wave mechanics were derived from de Broglies' theorems. ^{77,78,79} Although they looked different from the Bohr model, they obtained the same results and were shown to be mathematically equivalent to the quantum mechanics of Born and Heisenberg, and like Heisenberg's work also contained no pathways. At this time the assumption was made that a scalar result would be obtained if the positive real square root was taken in the Schroedinger format, ^{77,78,79} an arbitrary convention that soon became the rule. Dirac and Jordan then introduced transformation theory. In 1927

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⁷² W. Heisenberg, *Z. Physik* **34**, 858, 1925.

⁷³ M. Born and P. Jordan, *Z. Physik* **34**, 858, 1925.

⁷⁴ M. Born and N. Wiener, *J. Math. Phys.* **5**, 84, 1926.

⁷⁵ W. Heisenberg, *Z. Physik* **33**, 879, 1925.

⁷⁶ M. Born, W. Heisenberg, P. Jordan, *Z. Physik* **35**, 557, 1926.

⁷⁷ E. Schroedinger, *Ann. Phys.* **79**, 361, 1926.

⁷⁸ ^a E. Schroedinger, *Ann. Physik* **79**, 489, 1926;

^b E. Schroedinger, *Ann. Physik* **80**, 437, 1926.

⁷⁹ E. Schroedinger, *Ann. Phys.* **81**, 109, 1926.

Heisenberg ^{50,80} refined his uncertainty principle and introduced electronic spin and Dirac quantized the electromagnetic field. Pauli developed Pauli matrices for the spin--angular momentum vector of the electron as the appropriate means for dealing with systems having angular momentum equal to an odd multiple of $1/2 \hbar$. Weyl and Wigner independently initiated work showing the usefulness of group theory in studying quantum mechanical systems. In 1928 Dirac introduced the relativistic theory of electron and Bohr extended Heisenberg's ideas and formulated the Complementarity Principle. ^{46,81,82,83} In 1929 Slater developed a simplified application of the spin and exclusion principle to the calculation of energy levels of atoms having several electrons outside of closed shells. Bethe initiated ligand field theory, and Dirac discovered the positron and creation and annihilation operators.

This rapid series of developments left the world of physics reeling. At the time, most of theoretical physics was described in terms of the classical mechanical philosophy and the majority of new concepts made these old views obsolete. The concepts of space and time were altered by the theory of relativity, quantum theory and uncertainty affected causality, atomistics affected views of substance and matter, and complementarity was an entirely new way of thinking. Between them, Schroedinger and Heisenberg devalued the philosophy of materialism that had been held since Newton, changed the concepts of boundaries and isolation, contradicted strict determinism and predictability and raised questions on the role of the mind in nature, returning the human observer to a central position in natural philosophy.

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⁸⁰ W. Heisenberg, The Physical Principles of Quantum Theory, University of Chicago Press, 1930.

⁸¹ N. Bohr, Naturwiss. 17, 483, 1929.

⁸² N. Bohr, Naturwiss. 18, 73, 1930.

⁸³ N. Bohr, J. Chem. Soc. (London) 349, 1932.

Einstein originally felt that a physical theory should contain only quantities that can be directly observed, to provide a guarantee of connections between the mathematical formulae and the phenomena. This led to a mathematical formalism which really seemed to fit the atomistic phenomena and gave Born, Jordan and Dirac a starting point which they elaborated to a closed system of quantum mechanics. However Einstein eventually abandoned this belief when he realized that although an electron path could not be observed inside the atom it MUST exist. ³² In 1926 Einstein insisted that there must be an electron path in the interior of the atom and Heisenberg began to look for geometric meaning within the uncertainty principle which he never stopped searching for. It is obvious therefore that the concepts of the time contained the geometry, whereas the working models had none. The matter was not rigorously pursued as the relevance was not obvious at the time since polarized spectroscopy was in its infancy. To include geometry it would have been necessary to use topology as no other form of relevant and effective mathematics existed. Furthermore Born felt that there was no need for phases and even if there were, there was no effective way of manipulating them at the time. ³² Any phase choice was considered acceptable as long as it was used consistently. ³⁸ The entire matter of geometry was dropped and has only recently begun to interest spectroscopists as the opportunities to perform polarized experiments become more common.

Wave Mechanics

Bohr wanted to develop a liason between quantum theory and classical electrodynamics. He set forth the correspondence principle where at the limit of large quantum numbers the frequency, intensities and other properties of radiating systems as calculated by quantum theory must pass over into those calculated classically.

Schroedinger's first concept was that the wave function represented a real disturbance, a "*matter wave*" in space or even a novel kind of aether analogous to electromagnetic waves of Maxwell's theory, but he abandoned these matter waves because he saw no way to make them interact with electromagnetic waves in processes of emission and absorption. He saw matter as qualitatively and quantitatively different from electromagnetic functions and turned to an electromagnetic interpretation where the relationship $\psi\psi^*$ was a measure of the density of electric charge.

This initial matter wave concept essentially identifies the defining property of the bound electron wave as inertia, I . The replacement of this by the electric charge redefined the dominant property of the electron wave as its capacitance, C . Later, the magnetic property was recognized so that the inductance L of the electron wave was also employed to interpret Zeeman effects. In this form his wave mechanics did offer a renewal of confidence in the kind of causal determinate laws found in Maxwellian electrodynamics and Einsteinian gravitation. In his first paper ⁷⁷ he replaced quantum conditions by a variation problem and made no reference to the wave properties of particles, quantization of energy or Planck's constant, although

he does mention that K has the dimensions of Action which, as Heisenberg has shown required four dimensions. This implicit requirement for a four-dimensional function is represented by his use of the Euler-Lagrange (II.2-1) equation for the variational problem, and will be referred to in this study.

$$\left[\frac{\delta\psi}{\delta x}\right]^2 + \left[\frac{\delta\psi}{\delta y}\right]^2 + \left[\frac{\delta\psi}{\delta z}\right]^2 + \frac{2m}{K^2}\left[E + \frac{e^2}{r}\right]\psi = 0$$

$$\Delta\psi + \frac{2m}{K^2}\left[E + \frac{e^2}{r}\right]\psi = 0 \quad (\text{APP-1})$$

Schroedinger knew that one limitation of his wave mechanics was that it was not consistent with relativity theory and was not invariant under a Lorentz transformation, but he wanted to use his math formalism as a pathway back to classical physics based on a continuum undisturbed by sudden transitions, where quantization was only a misleading approximation and he hoped relativistic theory would complete his theorem. Initially, the introduction of relativistic behaviour forced Schroedinger to use half-integer rather than whole integer Legendre functions to fit the complete potential. However, this was abandoned in his first paper because it seemed to have no physical significance and was replaced by linear combinations to give whole integer functions. In private notes however he seems to have speculated that the relativistic behaviour of vectors is essential for the passage of the vector through the nucleus and this implies a need for the half-integer.⁸⁴

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⁸⁴ W. Moore, Schroedinger, Life and Thought, Cambridge University Press, Cambridge, 1989. See private notes page.

Lorentz said⁸⁵ that he preferred wave mechanics over other formalisms when using only the Cartesian coordinates, but when using greater degrees of freedom the waves and vibrations of momentum space could not be interpreted physically, and so matrix mechanics must be used. Schroedinger's reply was that with respect to the interpretation of waves in q -space, $\psi\psi^*$ was charge density. He felt that as ψ was surely fundamentally a real function, there should not be a need for complex numbers and did not at the time realize that complex numbers are carriers of the unobservable phase information of the wave functions,⁸⁶ a concept included in this thesis. The essential difficulty arose from attempting to place an entire function within a space that could not contain it. A function will be real only within its own real space.

In his fourth paper,⁷⁹ Schroedinger was concerned about the appearance of the $\sqrt{-1}$ that occurred in his theory, but he avoided any trouble by using only the real part of the complex number and using i as a convenient device for calculations. Heisenberg had originally introduced the $\sqrt{-1}$ in his commutation relation but with no concrete interpretation, although he did comment on an implied geometric meaning.⁷² In this paper Schroedinger uses the wave function simply as the product of the amplification factor and an imaginary phase factor. Dirac commented⁸⁶ that quantum mechanics had not been invented earlier because the phase quantity was well hidden in nature, but he felt that although its discovery was a cornerstone, its physical significance was still obscure.

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⁸⁵ H. Lorentz, correspondence with E. Schroedinger, 1926, seen in Karl Przibbaum (ed.) *Briefe zur Wellenmechanik*, Wien:Springer, 1963.

⁸⁶ P.A.M. Dirac, *Fields and Quanta*, 3, 139-164, 1972.

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Schroedinger discussed the physical significance of the wave function ψ , which he called a field scalar.⁸⁴ The complex conjugate ψ^* was seen as a weight function in the configuration space of the system, but could not be given a direct interpretation in three-dimensional space because the function was in configuration space and not in real space. Schroedinger himself was still uncomfortable with the complex wave function but stated that if it was fundamentally unavoidable and not a mere convenience for calculation, it would mean that actually two wave functions exist "which only together give conclusions about the state of the system".⁸⁴

Dirac Formalism

Dirac recognized Nagaoka's "Saturnian atom" radius⁴² as the radius at which Maxwell's equations resulted in a nonlinearity. Therefore he began dealing with general fields by placing the classical theory into an operator form.⁵² However to do so he began with an action integral A denoted by $A = \int \mathcal{L} dt$ where $\mathcal{L}$ is the Lagrangian, and then passed on to the Hamiltonian by specializing $\mathcal{L}$ to three dimensions. In doing so he recognized the requirements for a theory to be relativistic via an invariant action integral. To pass over from the Lagrangian to the Hamiltonian via the Lagrangian equations of motion, the momentum variables were introduced.

However his initial use of the Lagrangian indicates his acceptance of the requirement for four dimensions, although he arrived at this conclusion as a theoretical mechanic and without the benefit of the experimental evidence from polarized spectroscopy. By his analysis, all mechanics involve position and motion

(momentum). Therefore a function is required over the entire space that couples motion and position. Thus one always needs twice the number of dimensions, one set of three dimensions for motion, one set of three for position, for a total of six. However six are too many, for in order to maintain a mutual origin, one dimension must be removed. In order to disallow translation and to keep the velocity space from rotating, the axes had to be kept together, and another dimension was removed, leaving four. The resulting four-dimensional Lagrangian falls into two conjugate three-dimensional Hamiltonians⁵³ that represent two orientable three-dimensional hands with a common origin, $\mathcal{L} = \mathcal{H}^* \mathcal{H}$.

His insistence on using Hamiltonians arose from his belief that the Balmer series could not be solved on a Lagrangian.⁴² In essence however, Dirac did not use a Hamiltonian but a Lagrangian with Hamiltonian axes. For this reason some of his physics found itself outside the Hamiltonian space and required an imaginary axis. Each appearance of an imaginary axis represents the existence of some physics in the conjugate Hamiltonian $\mathcal{H}^*$, not the Hamiltonian $\mathcal{H}$, and therefore really in the Lagrangian, $\mathcal{L}$. As long as both $\mathcal{H}$ and $\mathcal{H}^*$ are both subsets of $\mathcal{L}$, the Lagrangian could be used instead of the Hamiltonian.

The only real purpose in forcing the use of a Hamiltonian is to keep the description down to three dimensions by getting rid of one dimension by means of specifying a path of least action (or least elapsed time). This however leads to a set of four paths of least action, so that any attempt to use the Hamiltonian yields an imaginary axis as the fourth set cannot be avoided.

Dirac generated a Schroedinger equation with a set of spinors as solutions. The Dirac equation ⁵⁹ can be isolated into the Schroedinger part, which as a standard first order differential equation that can be solved by the wave function of ψ .

$$i\gamma^\mu \delta_\mu \psi = m\psi \quad (\text{APP-2})$$

where m = rest mass of particles whose state is described by ψ
 ψ = four component wave function known as the Dirac spinor, dependent on frame of reference
 δ_μ = $\delta/\delta x^\mu$ where $x^\mu = (t, \vec{r})$ is the space-time position 4-vector
 γ^μ = a set of four 4x4 fixed matrices that are independent of the frame of reference and satisfy the condition

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2g^{\mu\nu}$$

where $g^{\mu\nu}$ = diagonal (1,-1,-1,-1) is the metric tensor of special relativity and the fixed matrices are:

$$\gamma^0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad \gamma^i = \begin{bmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{bmatrix}$$

where all the entries including σ_i are 2x2 Pauli matrices.

Dirac specified this more rigidly with a set of four binary 4×4 fixed matrices which are independent of the local frames specifying the wave function. This binary four-space is the basis of the formalism as it defines the dimensions and effectively yields an eight-fold space. Whereas the Lagrangian, as was well known at the time, included all the necessary geometry for this space, the Hamiltonian did not.³² However the Hamiltonian was used because it was felt at the time that an atom could be defined by a single path of least resistance⁴⁷ since the geometric implications of sense of rotation and orientation phase were thought to be irrelevant from Born's analysis. The actual result of the passage to the Hamiltonian is a loss of seven-eighths of the geometry in three-dimensional space and hence the failure to recognize the full eight-fold degeneracy of the state.

By definition, both the operator and wave function must also be binary 4-spaces. The product is in fact the Lagrangian, which Dirac separated into the operator and the basic coordinate format, that is, four bifurcated independent directions which do NOT have to be linear and are free to be curved.

Foundations of Explicitly Geometric Quantum Mechanics

The Lagrangian mechanics are four-dimensional. Dirac has produced a Schroedinger format of the Lagrangian mechanics upon which to build a theory which is totally compatible with relativistic mechanics. In his formalism the relativistic mechanics are required to the theory, and are not simply added on, but included from the beginning as they are compatible with Dirac's Lagrangian format.

Therefore the Dirac formalism may be used to construct the simplest analytical geometry in a combined position momentum space and non-orientable coordinates convenient to chiral spectroscopy. On these coordinates uncertainty wave functions will be used to document the loss of ideal geometry and a path integral. However it is important to note that the intensities of the observable phenomena will depend upon the proportion of ideal geometry remaining after the path uncertainty integral. If uncertainty eliminates the ideal geometry, then there are no observable phenomena for the spectroscopist since the ideal geometry is the only real observable. Therefore clear and unambiguous predictions of observables can be made only on the remaining ideal geometry, not on the uncertainty. Dirac has not limited his formalism to either a stable or transient state, leaving open the possibility of studying both photons and atoms. As this study will begin with atoms, it will begin by defining steady states on closed coordinate axes which will display all of the four-dimensional properties so that each coordinate will select one of the bifurcation choices from the Dirac set.

As there are one scalar and three non-scalar portions, the bifurcation will be done on the three non-scalars, yielding $2 \times 2 \times 2$ such coordinates, which are the eight spaces of the natural coordinates. Therefore eight spaces will be constructed with three bifurcated properties on closed coordinates.

SYMBOL INDEX

I	moment of inertia
C	electric capacitance
L	magnetic inductance
m	rest mass
ψ	wave function
A	Lagrange's Action integral
$\mathcal{H}$	Hamiltonian
$\mathcal{L}$	Lagrangian
I	intensity
$\mathcal{A}$	MCD A term
$\mathcal{B}$	MCD B term
$\mathcal{C}$	MCD C term
A	ground state
J	excited state
a	ground state
j	excited state
c	coherence
s	sense of motion
χ	chirality
p	momentum
x	position
v	velocity
r	radius
k	non-vanishing commutator
ρ	tensorial scaling factor of position
a	coordinate of position
ϕ	vertical angle off vertical axis to plane
A	moment of scaled Action
A	Hamiltons Action
L	classical Lagrangian energy
T	kinetic energy
V	potential energy
i	electric current
i	magnetic current or root potential Action
f	magnetic flux or charge
φ	flux
f	electric flux
ψ_c	certainty wave function

END

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FIN