Paramagnetism, Antiferromagnetism, And Magnetic Susceptibility Trends In The 3d Transition Metals

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ABSTRACT:

This paper explores the manner in which electron hybrid orbital geometry may facilitate important electron interactions within metal atoms — interactions that may account for the trend in magnetic susceptibility strength across the transition metals in the periodic table. These *pd*-hybridized orbital structures are considered in detail, along with the field and spin interactions that may collectively contribute to the strength of an atom's magnetic signature, relative to an external magnetic field. Specifically, various spin-related interactions, called spin bonding, are discussed, with respect to their influence over the magnetic field energy of a system of unpaired electrons, and thus, over properties such as paramagnetism, diamagnetism, and antiferromagnetism.

1. INTRODUCTION

1.1. Magnetic Susceptibility (χ_m)

The magnetic susceptibility (χ_m) of a substance is a measure of the degree to which it is drawn to or repelled from an external magnetic field. It is widely accepted that the degree to which an atom or molecule has paired versus unpaired electrons will determine its magnetic properties. Specifically, magnetic susceptibility is widely described as a proportionality constant between the magnetization, M, of a material — the density of its electron dipole moments — and the strength of the applied external magnetic field, H, in the relation $M = \chi_m H$.

Paramagnetism occurs when a substance is attracted to a magnetic field because it contains one or more unpaired electrons. In the presence of an external magnetic field, an unpaired electron's own magnetic moment will cause it to align with the external field. This causes cancellation of magnetic field to occur between the electron and the field, lowering energy through destructive interference [3]. The substance will therefore experience an attraction into the magnetic field because, according to the laws of thermodynamics, lower energy wave states are intrinsically favorable; they will be assumed when they are available. This is proposed as the physical reason for paramagnetic attraction.

Paramagnetic substances have a positive χ_m value. Most metals are paramagnetic, including the first five transition metals, scandium (Sc), titanium (Ti), vanadium (V), chromium (Cr, above 38°C)[1], and manganese (Mn).

When the external magnetic field is removed, the electrons on adjacent atoms in a paramagnetic substance lose their macroscopic magnetic coherence and return to a random distribution of alignments.

Diamagnetism occurs when a substance repels away from a magnetic field because it contains paired electrons. These paired electrons — superimposed, antiparallel, and with opposite spin — are in a state of perfect field cancellation with one another [3,4]. The presence of an external magnetic field disrupts the coherence of their *di-electron* state, raising their energy through constructive interference. As stated above, wave structures will naturally resonate away from higher energy states and towards lower energy states if they are able to do so. This is proposed as the physical reason for diamagnetic repulsion.

Diamagnetic substances have a negative χ_m value. Most covalently-bonded molecules are diamagnetic, and copper (Cu) and zinc (Zn) are examples of diamagnetic metals (*see §4*).

1.2: Questions Arising From Observed Magnetic Susceptibility Values:

At first glance, we might expect that the strength of the magnetic susceptibility of the transition metals should go up in accordance with the number of unpaired electrons in the atom. The more unpaired electrons there are, the stronger the magnetic response should be, but it is *not*. Nor is it simply a matter of *even* versus *odd* numbers of unpaired electrons.

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[1] Below 38°C — at room temperature — chromium is naturally antiferromagnetic. (*See §5*).

As such, certain questions immediately arise when the magnetic susceptibility trend is considered a little more closely. (*See graph in fig. 1, below*.)
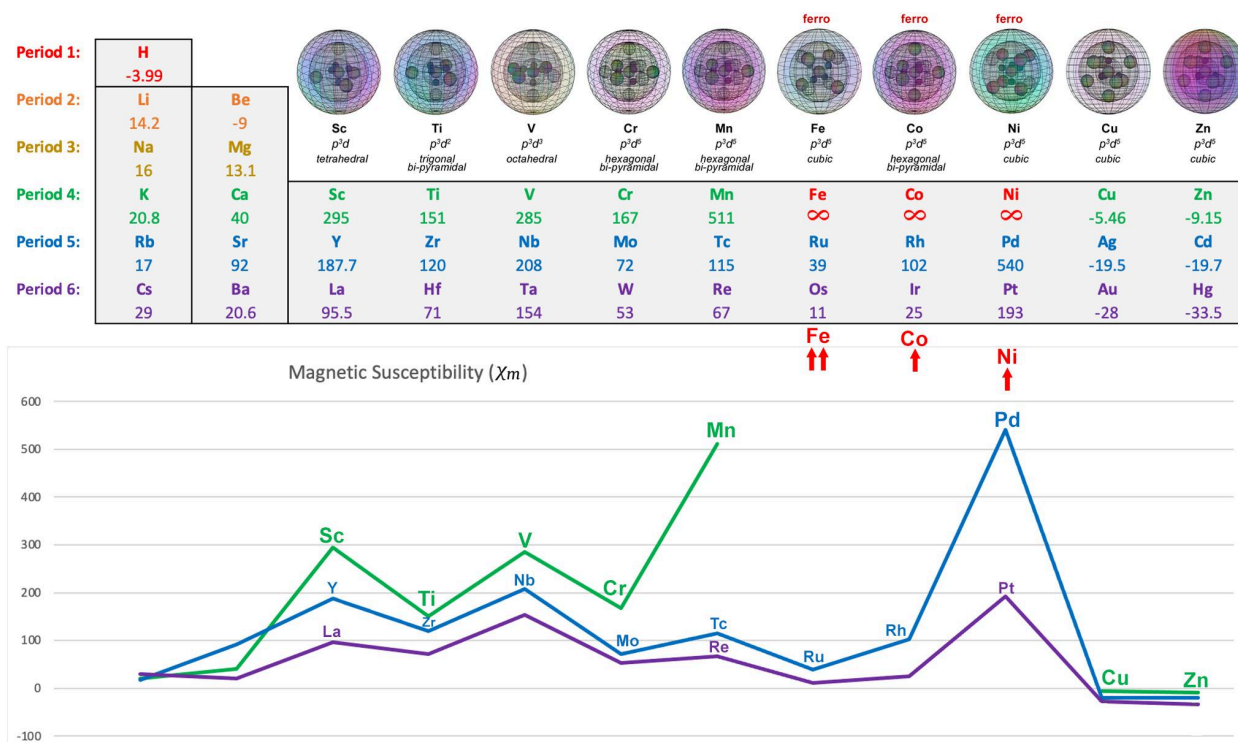
		Sc p^3d tetrahedral	Ti p^3d^2 trigonal bi-pyramidal	V p^3d^3 octahedral	Cr p^3d^4 hexagonal bi-pyramidal	Mn p^3d^5 hexagonal bi-pyramidal	Fe (ferro) p^3d^6 cubic	Co (ferro) p^3d^6 hexagonal bi-pyramidal	Ni (ferro) p^3d^6 cubic	Cu p^3d^6 cubic	Zn p^3d^6 cubic
Period 1: H −3.99											
Period 2: Li 14.2	Be −9										
Period 3: Na 16	Mg 13.1										
Period 4: K 20.8	Ca 40	Sc 295	Ti 151	V 285	Cr 167	Mn 511	Fe ∞	Co ∞	Ni ∞	Cu −5.46	Zn −9.15
Period 5: Rb 17	Sr 92	Y 187.7	Zr 120	Nb 208	Mo 72	Tc 115	Ru 39	Rh 102	Pd 540	Ag −19.5	Cd −19.7
Period 6: Cs 29	Ba 20.6	La 95.5	Hf 71	Ta 154	W 53	Re 67	Os 11	Ir 25	Pt 193	Au −28	Hg −33.5

Magnetic Susceptibility (χ_m)

Fig. 1: Magnetic susceptibility values for the s- and d-block elements [8]

If these magnetic effects were simply a matter of the *number* of unpaired electrons, scandium should have one of the smallest values with its single unpaired electron. Chromium (Cr) should have a larger value, with 6 unpaired electrons, than manganese (Mn) has with five. Or, since chromium's 6th electron is really the delocalizing $4s^1$ valence electron, the 5 core unpaired electrons should offer a similar value to that of manganese. But instead, chromium has a much smaller value.

When comparing the first three metals in the $3d$ row, scandium, titanium, and vanadium, we see they have 1, 2, and 3 unpaired electrons respectively. This implies that their relative magnetic susceptibility strengths should reflect this and present in the order: V > Ti > Sc. Instead, their relative strengths are Sc > V > Ti. The atom with the fewest unpaired electrons has the highest χ_m value while the atom with the most unpaired electrons has the middle χ_m value. Vanadium should have a much higher value, with 3 unpaired electrons, than scandium has with 1 unpaired electron, but Vanadium's value is slightly *lower*. This requires explanation.

In addition, despite the lower values in the $4d$ row, compared to the $3d$ row, palladium (Pd) has a larger value than both chromium and manganese, and with *fewer* unpaired electrons, in fact, with *no* unpaired electrons in the traditional view [8]. Further, if atoms with an odd number of electrons should have higher values than those with an even number of electrons, then

it becomes difficult to account for the high values of palladium and platinum in their respective rows.

Apart from the ferromagnetic gap in the 3d row, the basic trend in magnetic susceptibility seems roughly consistent between the 3rd, 4th, and 5th rows of the d-block metals. This indicates that their (ground state) electron structures are more than likely analogous, and thus, so are the interactions that determine their magnetic properties.

According to currently accepted theory, that is not the case, however, as electron configurations are believed to be different down the group in certain cases, for example nickel ([Ar]$4s^23d^8$) versus palladium ([Kr]$5s^04d^{10}$) versus platinum ([Xe]$6s^15d^9$). If each of these elements does indeed have a different number of unpaired electrons, it becomes difficult to explain why their magnetic properties (particularly Pd and Pt) show a similar group trend. On the other hand, identifying exact electron configurations for the d-block elements does pose various challenges [13] that are beyond the scope of this paper.

It is also important to note that the approach that will be taken here, by way of exploring the above questions, is made possible by and is built upon recent advances in sub-quantum mechanics [1,2]. It is proposed that it may shed light on the specific trend in magnetic susceptibility strength across the d-block, as well as the mechanisms underlying various forms of magnetism.

1.3. *pd*-Hybridization

In prior work [5] it was proposed that when *p*- and *d*-electrons occupy the same shell, their interactions invite us to consider them as a hybridized unit rather than as independent, superimposed harmonic structures. This is simply because electrons in the same shell cannot ignore the influence of each other's field, charge, and spin.

This *pd*-hybridization yields 4-, 5-, 6-, and 8-directional electron domain geometries, from p^3d (tetrahedral) through p^3d^5 (hexagonal bipyramidal or cubic) symmetry. These are shown in figure 2 (*below*) [6], and the details of each will be clarified in §2.
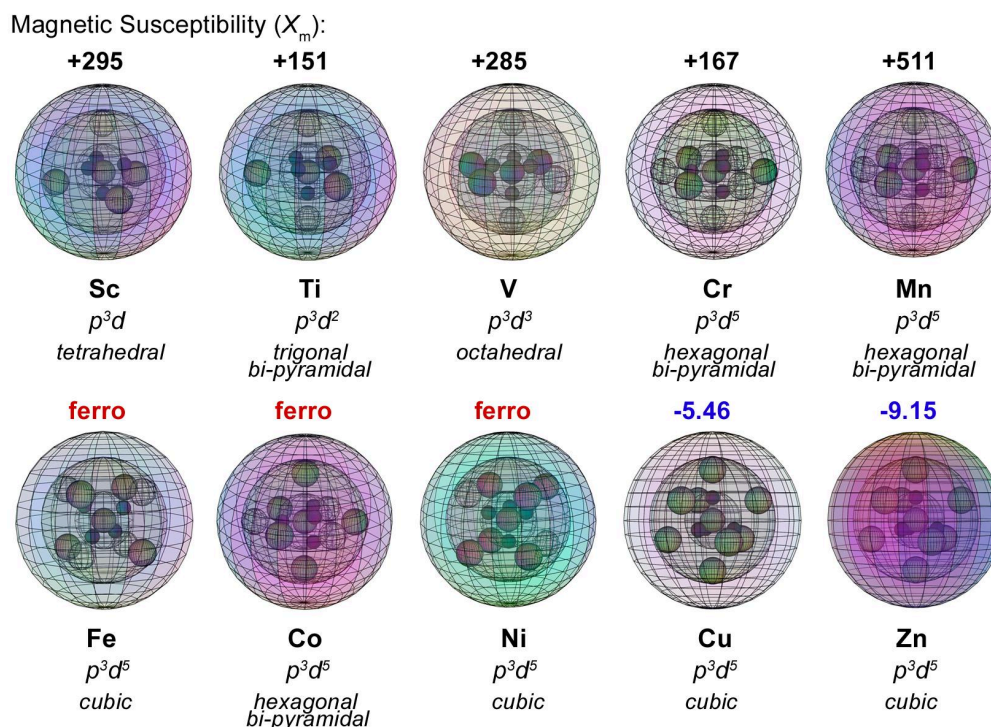
Magnetic Susceptibility (X_m):

+295	**+151**	**+285**	**+167**	**+511**
Sc	**Ti**	**V**	**Cr**	**Mn**
p^3d	p^3d^2	p^3d^3	p^3d^5	p^3d^5
tetrahedral	*trigonal bi-pyramidal*	*octahedral*	*hexagonal bi-pyramidal*	*hexagonal bi-pyramidal*
ferro	**ferro**	**ferro**	**-5.46**	**-9.15**
Fe	**Co**	**Ni**	**Cu**	**Zn**
p^3d^5	p^3d^5	p^3d^5	p^3d^5	p^3d^5
cubic	*hexagonal bi-pyramidal*	*cubic*	*cubic*	*cubic*

Fig. 2: pd-hybridization, including 3rd-shell electron domain geometries and χ_m values, for the 3d transition metals. (Note: Cu and Zn have the same cubic geometry as Fe & Ni. They are simply depicted at a different angle.)

Note carefully that the small dark-colored spheres inside the images above represent *di-electron* orbitals and the small lightly-colored spheres represent unpaired electron orbitals. These spheres represent only the *directions* of maximum electron density, *not* the actual shapes of the hybrid orbitals. (A more 'space-filling' representation of orbital shape can be seen in figure 3, below, in the case of scandium's proposed structure.)

In this paper, these *pd*-hybridized electron geometries will be applied to the questions mentioned in §1.2 above. It is suggested that they provide an essential foundation upon which to investigate the relevant electron interactions between core unpaired electrons and *di-electrons* in transition metal crystals.

1.4. The *Di-electron* 'Fundamental'

In 3rd-shell *pd*-hybridisation, the 3*s*-orbital electrons are not needed in order to achieve stable symmetry. It is proposed that they therefore remain in their spherical *s*-orbital *di-electron* state, *within* which (or perhaps *upon* which) the other 3rd shell hybrid electron orbitals resonate, like harmonics upon a fundamental. This is depicted in the image below.
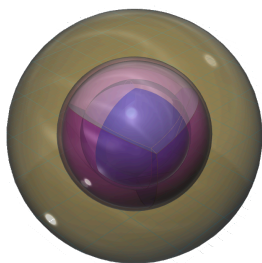
Fig. 3: Scandium's electron shells, showing the $3s^2$-di-electron sheath around the core shell, in addition to the outer $4s^2$ valence shell.

It may even be the presence of this spherical $3s^2$ resonance that allows for the possibility of unpaired core electrons to exist at all. As such, the significance of these unpaired core electrons cannot be overstated; it is *they* that determine an element's magnetic properties.

As we can see from the elemental χ_m values (*in figures 1 and 2 above*), it seems clear that the protected unpaired core electrons of the transition metals manifest a far stronger paramagnetic response than the valence electron(s) of an alkali or alkali earth metal, which have core *di-electrons* (or full shells) within them. In fact, as we will see in the case of chromium (and perhaps copper also), the presence of a single spherical valence electron appears to pose a disruptive magnetic influence to the inner atomic resonance.

We might also compare the alkali metals to the much more paramagnetic transition metals and conjecture that a single electron (or even a *di-electron*) in a spherical or delocalized distribution (such as in potassium or calcium) represents a far more diffuse electron density — and therefore a smaller magnetic signature — than an electron confined to a hybrid orbital lobe that takes up less than a quarter of a shell (as in the case of scandium), or perhaps even more so, a sixth or an eighth of a shell, as proposed for some of the other $3d$ metals.

2. *pd*-HYBRIDIZED ELECTRON GEOMETRIES

Before we look at the trend in magnetic susceptibility across the $3d$ row of the periodic table, let us first describe the proposed electron domain geometries within which the relevant electron interactions will occur.

2.1. Scandium (Sc)

Scandium is the first element to feature electrons in a *d*–orbital. Since *d*-electrons are resonating in the same space as *p*-electrons within their parent *s*-shell, we propose that these orbitals are able to hybridize together in search of lowest energy and highest stability. If that is the case, scandium would feature a 3rd shell containing 3 *di-electrons* and 1 unpaired electron in p^3d-hybridized tetrahedral symmetry (*see image below*). It is also proposed that the 3rd shell tetrahedral symmetry will align antiparallel (and antiprismatic) to the 2nd shell tetrahedral electron arrangement within, in order to minimize *di-electron* repulsion between shells.

Sc: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^1$

Fig. 4: pd-hybridization of scandium (Sc)

(Note again that the small spheres in the image above simply indicate the *directions* of maximum electron density.) The 3rd shell hybrid orbitals themselves will assume a spherical tetrahedral structure that divides the shell into four equal volumes. Each shell segment will be filled with electron density. It will be highest at the center of the face of each orbital (as in the traditional sp^3 lobe shapes) and will decrease toward the nodal regions between orbitals — as wave structures usually do — where electron density will be lowest (though not zero). (*This is depicted in figure 3 above*.)

It is also assumed, based upon known principles in chemistry, that the stronger repulsion and larger charge density of the three *di-electrons* will constrict the unpaired electron orbital, causing it to become somewhat extended radially outward. (This is similar to the constriction and radial extension, proposed in earlier work, for hybrid orbitals of fluorine and iron [5].)

Note also that, even though it is often useful to talk about these orbitals as separate, they are all — the entire atom is — part of a single, coherent, harmonic, resonant, phase-locked, spherically-symmetrical quantum wave state [3]. Orbitals and their 'boundaries' can therefore be seen as nodes and antinodes in this harmonic wave structure.

2.2. Titanium (Ti)

Titanium is the second element to feature electrons in the *d*–orbital. Building upon the *pd*-hybridization we introduced in regard to scandium (Sc), it is proposed that titanium has a 3rd shell containing 3 *di-electrons* and 2 unpaired electrons in $p^3 d^2$-hybridized, trigonal bipyramidal symmetry. The three *p*-orbital *di-electrons* will occupy the equatorial positions for maximum distance, since *di-electrons* repel more strongly than single electrons, forcing the 2 unpaired electrons into the two axial positions.

In such a configuration, the 4 tetrahedral 2nd shell *di-electrons* will align themselves with one *di-electron* opposite one of the single axial electrons in the 3rd shell, allowing the remaining 2nd and 3rd shell *di-electrons* to orient their directions roughly between one another, in order to minimize repulsion between shells.
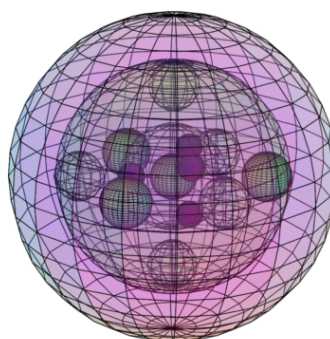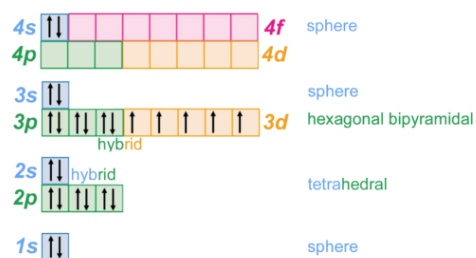
Ti: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^2$

Fig. 5: pd-hybridization of titanium (Ti)

As mentioned above, the stronger repulsion and larger charge density of the three *di-electrons* will constrict the unpaired electron orbitals, causing them to become somewhat extended radially outward in the axial directions.

2.3. Vanadium (V)

Vanadium is the third element to feature electrons in the *d*–orbital. It is proposed that vanadium has a 3rd shell containing 3 *di-electrons* and 3 unpaired electrons in a p^3d^3-hybridized, octahedral symmetry (*see image below*). The 3 *di-electron* and the 3 unpaired electron sets are each planar arrangements, and they lie orthogonal (90^0) to one another in making up the octahedral electron geometry.

In such a configuration, the 4 tetrahedral *di-electrons* in the 2nd shell will align themselves with two *di-electrons* roughly opposite two of the unpaired electrons in the 3rd shell, allowing the other *di-electrons* to orient their directions roughly between one another, in order to minimize repulsion between shells.

V: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^3$

Fig. 6: pd-hybridization of vanadium (V)

It is also proposed that the stronger repulsion and larger charge density of the three *di-electrons* will constrict the three unpaired electron orbitals, bringing these three degenerate electrons into closer proximity. In this case, this might serve to increase the coherence of the parallel spin bonding between them (*see §3.1 below*).

2.4. Chromium (Cr)

Chromium is the fourth element to feature electrons in the *d*–orbital. It is proposed that chromium has a 3rd shell containing 3 *di-electrons* and 5 unpaired electrons in p^3d^5-hybridized, hexagonal bipyramidal symmetry. The three *p*-orbital *di-electrons* occupy three symmetrically distant equatorial positions to minimize repulsion. The 5 unpaired electrons occupy the remaining equatorial and axial positions. (*See image below*.) In this case, one of the 4th shell valence electrons is required to join the 3rd shell hybrid resonance structure in order to maintain 8-directional symmetry (and avoid the asymmetry of 7 directions).

In such a configuration, the 4 tetrahedral 2nd shell *di-electrons* will align themselves with one *di-electron* opposite one of the single electrons in the 3rd shell, allowing all other *di-electrons* to orient their directions roughly between one another in order to minimize repulsion between shells.

Fig. 7: pd-hybridization of chromium (Cr)

The diagram below only shows chromium's eight 3rd shell p^3d^5-hybrid orbitals. *(The darker color represents di-electrons, the lighter color represents unpaired electrons. The sharp edges should not be taken too literally!)*

Fig. 8: One possible alternate view of only the 3rd shell pd-hybridized orbitals of chromium (Cr) in a hexagonal bipyramidal geometry

As mentioned above, the stronger repulsion and larger charge density of the three *di-electrons* will constrict the unpaired electron orbitals, causing them to become somewhat extended radially outward in their axial and equatorial directions.

2.5. Manganese (Mn)

Manganese is the fifth element with electrons in the *d*–orbital. It is proposed that manganese, like chromium (Cr), has a 3rd shell containing 3 *di-electrons* and 5 unpaired electrons in p^3d^5-hybridized, hexagonal bipyramidal symmetry. The three *p*-orbital *di-electrons* occupy three symmetrically distant equatorial positions to minimize repulsion. The 5 unpaired electrons occupy the remaining equatorial and axial positions. An electron from the 4s-orbital is therefore not needed (as it is in the case of chromium) in order to achieve 8-directional symmetry.

In such a configuration, the 4 tetrahedral 2nd shell *di-electrons* will align themselves with one *di-electron* opposite one of the single electrons in the 3rd shell, allowing all other *di-electrons* to orient their directions roughly between one another in order to minimize repulsion between shells.

Fig. 9: pd-hybridization of manganese (Mn)

(The diagram in figure 8 above (*for chromium*) could equally well depict manganese's eight 3rd shell p^3d^5-hybrid orbitals.)

As in the case of chromium, the stronger repulsion and larger charge density of the three *di-electrons* will constrict the unpaired electron orbitals, causing them to become somewhat extended radially outward in their axial and equatorial directions.

2.6. Iron (Fe), Cobalt (Co), and Nickel (Ni)

The two atomic criteria that give rise to ferromagnetism, along with a proposed electron structure for the iron atom, were introduced in prior work [5].
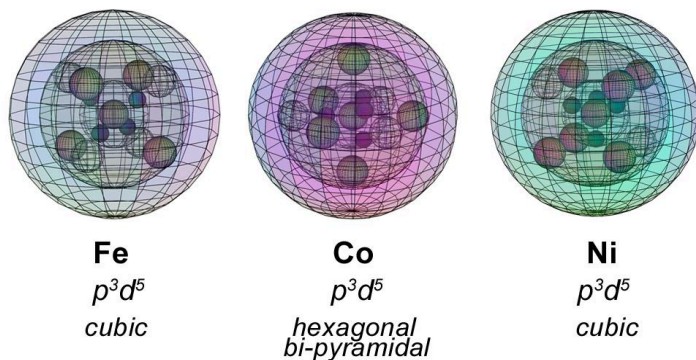
Fig. 10: pd-hybridization of iron (Fe), cobalt (Co), and nickel (Ni)

These three ferromagnetic transition metals will be covered in greater detail in future work on the topic of ferromagnetism. Additional detail can be found on the Quicycle website. [6,10]

2.7. Copper (Cu)

Copper is the ninth element with electrons in the *d*–orbital. It is proposed that copper features p^3d^5-hybridization. This enables a symmetrical, eight-directional cubic geometry containing 8 *di-electrons (see image below)*.

This *pd*-hybridization is achieved in the same way as in chromium, where one electron from the 4s-orbital joins the *pd*-hybridization in order to achieve 8-directional symmetry and lowest energy. (In the view below, this cube configuration is tilted to reveal that it is also a double-tetrahedral arrangement — two tetrahedra aligned antiparallel and antiprismatic.)

The 3rd shell cubic *di-electrons* will arrange their double tetrahedra in such a way that minimizes repulsion with the 2nd shell *di-electrons* beneath (*as depicted in the images below*).
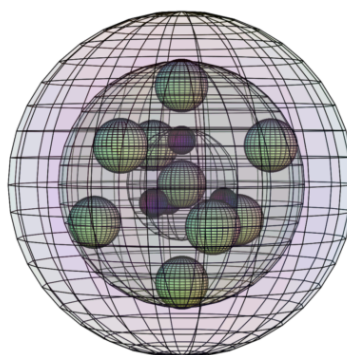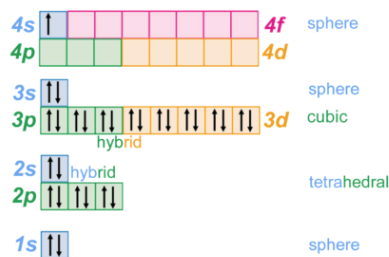
Fig. 11: pd-hybridization of copper (Cu)

Observational evidence may support such a proposed cubic structure for copper's 3rd shell. The images (*in figure 12 below*) of copper's Fermi surface were obtained using a process known as 2D-ACAR [9].

Fig. 12: Fermi surface of copper obtained with 2D-ACAR spectroscopy

2.8. Zinc (Zn)

Zinc is the tenth element with electrons in the *d*–orbital. Like copper, it is proposed that zinc features p^3d^5-hybridization. This enables a symmetrical, eight-directional cubic geometry containing 8 *di-electrons (see image below)*. This *pd*-hybridization is also achieved without the need of an electron from the 4*s*-orbital — as occurs in the case of copper.

The 3rd shell cubic *di-electrons* will arrange their double tetrahedra in such a way that minimizes repulsion with the 2nd shell *di-electrons* beneath (*as depicted in the images below*).

Fig. 13: pd-hybridization of zinc (Zn)

2.9. Metal Ion Electron Structure

When iron atoms bond with other metal atoms in a solid, they form a crystal structure in which their valence electrons become 'delocalized' — shared into a matrix of electron density within which the now-positive atomic cores remain suspended. They are held in their relative positions by a balance between attraction into the electron gas around them and repulsion from the adjacent positive atomic cores. This is the electrostatic nature of metallic bonding. Its electron delocalization is also the reason that metals are such good conductors of both heat and electrical potential.

When iron interacts ionically, it usually makes the Fe^{2+} or the Fe^{3+} ion (though there are other possibilities). The Fe^{2+} ion forms when the atom loses its 4s^2 valence electrons. The Fe^{3+} ion forms when the Fe^{2+} ion loses another electron. It is here proposed that the 3rd electron will be lost from one of the 3rd shell *di-electrons*, since this is the only way to retain 8-directional

symmetry. The Fe^{3+} ion will therefore achieve the same (hexagonal bipyramidal) electron configuration as proposed for chromium (Cr) and manganese (Mn), though without any (of the ionized) 4*s*-electron density.
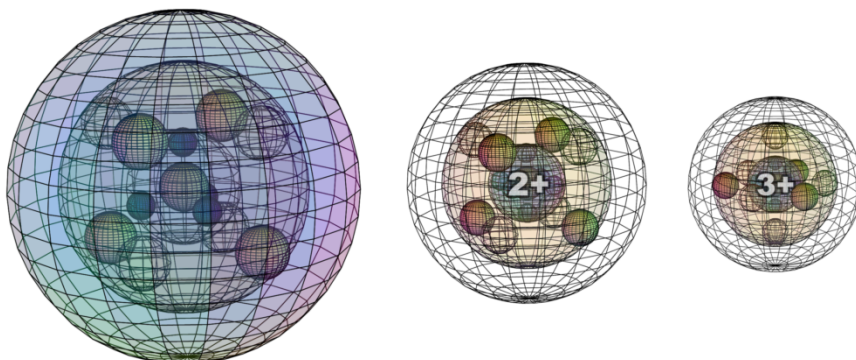
Fig. 14: Neutral Fe atom (left), Fe^{2+} ion (center), and Fe^{3+} ion (right).[2]

In ionic crystals — without delocalized electron density — iron ions no longer conduct electricity. They will, however, still be magnetically active because they still hold unpaired electrons. While metallic iron is ferromagnetic, iron ions will be strongly paramagnetic.

In the case of copper, the valence shell contains a single ($4s^1$) electron. When forming a metallic crystal, the $4s^1$ electron delocalizes to form the metallic bond, and when forming the Cu^+ ion, it is removed. In both cases, the core electron geometry remains the same.

It is proposed that, just as in the case of iron, a *second* ionization would shift copper's electron geometry by ionizing one of the hybrid *di-electrons*. This would retain 8-directional symmetry, but with one of the hybrid orbitals now containing an unpaired electron. The Cu^{2+} ion would therefore be expected to be strongly paramagnetic — due to its single and in this case *highly* constricted unpaired electron orbital — while the Cu^+ ion would still be diamagnetic. This is indeed the case. By way of example, copper (I) chloride (CuCl) has $\chi_m = -40$ while copper (II) chloride ($CuCl_2$) has $\chi_m = +1,080$. [11]

3. PARAMAGNETIC STRENGTH TREND

We might presume that the stronger the observed paramagnetism, the more 'unpaired electron character' is present. Surprisingly, though, the values do *not* go according to the number of unpaired electrons present, as the diagram below illustrates. There must therefore be other contributing factors, which we will investigate.

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[2] Increasing charge decreases atomic radius due to greater inward attraction (Z_{eff}).

by magnetic susceptibility:	+511		+295		+285		+167		+151
	Mn	>	Sc	>	V	>	Cr	>	Ti

by number of unpaired electrons:	6	>	5	>	3	>	2	>	1
	Cr		Mn		V		Ti		Sc
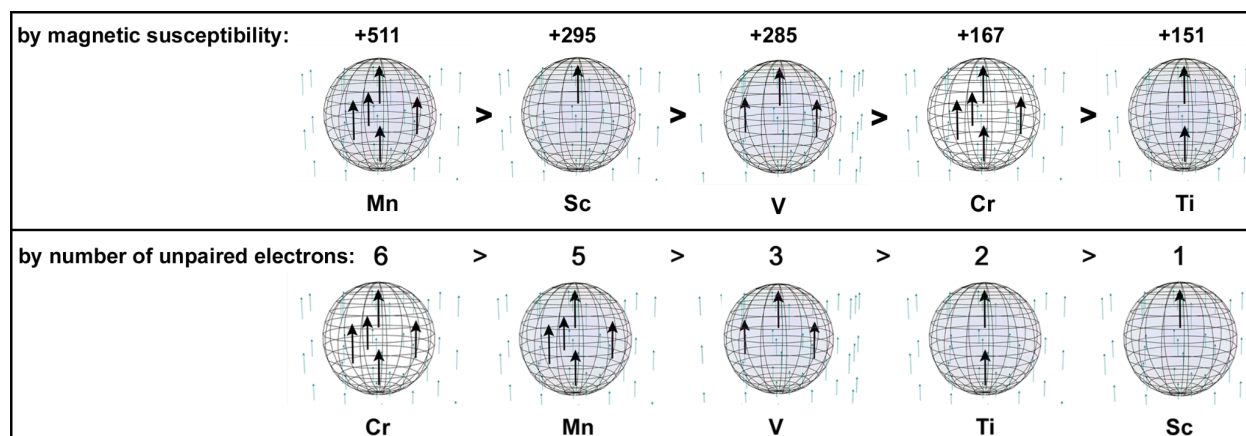
Fig. 15: Magnetic susceptibility strength trend in the metals of the 3d-block (excluding the ferromagnetic elements), compared to the number and geometry of unpaired electrons (arrows).

3.1: Spin Bonding:

The concept of spin bonding was introduced in earlier work [3] by way of explaining the spin-mediated 'inclusion' mechanism behind electron pair (*di-electron*) formation, named total *di-electron* inclusion (TDI). That case involves electrons of opposite spin, which should then also align magnetically antiparallel. This concept is expanded [3,4] to propose the spin-mediated mechanism behind Pauli's exclusion 'principle,' as well as introducing the concept of parallel spin bonding (*summarized below*) in order to account for the lower energy state described in Hund's 2nd Rule. In this paper, we propose an additional type of spin bonding — linear spin bonding (LSB).

The proposed *pd*-hybridized geometries, with their stabilized unpaired core electrons, allow for the possibility that unpaired electrons in the same shell — on opposite sides of the atomic core — can align both linearly and parallel. If they can do so, it cannot but have magnetic field (and perhaps also spin) consequences.

In earlier work [5], an additional form of spin bonding — ferromagnetic spin bonding (FSB) — was suggested as a mechanism for causing ferromagnetism in iron, cobalt and nickel. FSB will be investigated in more detail in future work.

3.1.1. Parallel Spin Bonding (PSB):

When unpaired, degenerate electrons share the same atomic shell, their lowest energy state is achieved when they possess the same spin, i.e. when spin is maximized. This is known as Hund's Second Rule. In earlier work [4], it was proposed that this will also involve a parallel magnetic alignment for these electrons[3].

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[3] Note: In the case of electrons, magnetically antiparallel does not mean the same as opposite spins. The former is a magnetic alignment distinction; the latter is a spin component phase relationship.

PSB was proposed as an explanation for the physical mechanism underlying this phenomenon. We might imagine that the internal photonic rotations within each particle are perfectly in phase with one another, and that the three electron wave states can therefore merge into a single, coherent flow state — a fermionic *tri-electron* state.
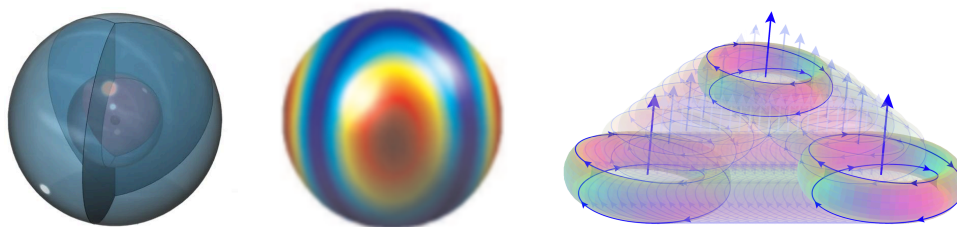
Fig. 16: Three different visualizations of boron's three 2nd shell sp^2-hybrid orbitals, parallel spin bonding into a single coherent harmonic spin state.

The effect of such a merging of wave structures, into a single stationary wave state, is that overall spin is reduced because quantum spin is a measure of overall spin, **J**. It is proposed that spin energy would thus be lowered, even as all of the spin components [4] within each electron remain present. It is proposed that this optimization of spin volume therefore amounts to a more attractive energy state, and this is the reason that adjacent *same-spin* electrons can attain a lower energy state than adjacent opposite-spin electrons. (Recall that the internal photons that constitute electrons[4], as propagating electromagnetic waves, are able to move through one another.)

3.1.2. Linear Spin Bonding (LSB):

When two unpaired, degenerate electrons share the same atomic shell and are able to align linearly and parallel to each other (as is proposed in the case of titanium), their parallel magnetic alignment and same spins allow for the reduction of energy through wave coherence and magnetic field cancellation [3].

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[4] According to the rotating photon model of condensed matter particles [1,2].
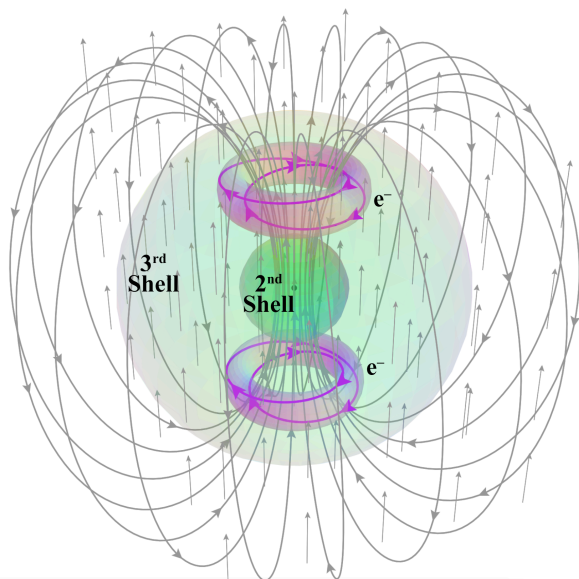
Fig. 17: Schematic of magnetic field connection between the two unpaired electrons in titanium's 3rd shell, linear spin bonding in an external magnetic field (gray vector field arrows).

The diagram above makes it easier to imagine the merging of quantum spin states into a single state, since we can imagine the literal merging and coincidence of magnetic flux lines from the two electrons, in a perfectly in-phase, columnar, rotational relationship.

This interaction topology is therefore not just a spin coherence but also one that involves a significant reduction in magnetic field energy (through destructive interference). As we will see below, it appears that such a linear spin bonding may lower the magnetic signature of each electron (with respect to an external magnetic field) more than does parallel spin bonding.

3.1.3. Diamagnetic Disruption & Total Di-Electron Inclusion (TDI):

It was described, in §1.1 above, that diamagnetic systems, such as *di-electrons*, repel away from external magnetic fields in order to preserve the electrons' perfect magnetic field cancellation with one another.

3.2: Effective Magnetic Electron (EME) Count:

In order to evaluate whether the *pd*-hybrid geometries, along with spin bonding, give rise to the observed χ_m trend, we will use scandium as our yardstick. It has 1 unpaired core electron, and there are therefore no mitigating electron interactions with other same-shell unpaired electrons. Scandium has a magnetic susceptibility value [8] of $\chi_m = +295$.

In order to assess how the presence of other electrons in the same core shell might affect their combined ability to interact with an external field, we propose a concept named the effective magnetic electron (EME) count. This number will reflect how much of the electrons' combined magnetic signature remains once internal spin-bonding and field cancellation have occurred between the unpaired core electrons.

Since the unpaired core electrons are fixed in their relative orbital positions, this brings their spins and fields into specific geometric interactions. It is proposed that these will either increase energy through constructive interference or decrease energy through destructive interference [3]. The net result of these internal interactions will determine how much of the electrons' magnetic signatures will be able to manifest beyond the boundary of the atom, and that will determine the atom's overall reaction to an external magnetic field.

According to this model, the EME value for an element is the result of two primary factors: (1) the number of unpaired electrons, and (2) the amount that this number is reduced by internal electron interactions, based upon their relative geometric positions.

Let us therefore consider scandium to have an EME = $1.0e^-$, at least as a first approximation, since it has one unpaired core electron orbital. (If we consider the unpaired electron in scandium to be constricted, as a result of the 3 *di-electrons* with which it shares the same shell, that would serve to increase its magnetic susceptibility.) We might then think of the other elements' χ_m values as representing an EME value that is proportional to scandium's χ_m value. We might then evaluate to what extent these EME values appear to match the *pd*-hybrid geometries, and whether their suggested electron interactions affect the values in the manner expected.

Recall that *di-electrons* are diamagnetic. We must therefore also understand χ_m values as the combination of both the paramagnetic and diamagnetic contributions within the atom; we must factor into our assessment the number of *di-electrons* sharing the 3rd shell with the core unpaired electrons. In the case of the first five *d*-block elements, they all have three 3rd shell *di-electrons*, making the comparison using their χ_m values appropriate, certainly to a first approximation.

3.3: Trend Analysis For The 3*d*-Row:

Let us now combine these ideas in order to match each geometry with its relative paramagnetic strength. (We will ignore the ferromagnetic iron, cobalt, and nickel, and the diamagnetic copper and zinc in the following discussion.)

Fig. 18: Magnetic susceptibility values for the Transition Metals [8]

	Sc	**Ti**	**V**	**Cr**	**Mn**
χ_m value	+295	+151	+285	+167	+511
Relative EME (e^-)	1.0	0.51	0.97	0.57	1.73
EME (per unpaired e^-)	1.0	~0.25	~0.32	~0.11	~0.35

Table. 1: Magnetic susceptibility values for the first five transition metals [8], along with their EME values, relative to scandium, and the EME per electron for each.

3.3.1. Scandium (Sc):

As proposed above, scandium has one unpaired electron in one position of a tetrahedral electron structure. The image below is intended to represent the orientation of this 3rd shell unpaired electron in an external (or adjacent atom's) magnetic field (whose north pole is pointing upwards). (*The purple arrow inside the atom represents the unpaired electron, and the black dots represent the relative positions of the 3 di-electrons in that shell.*)
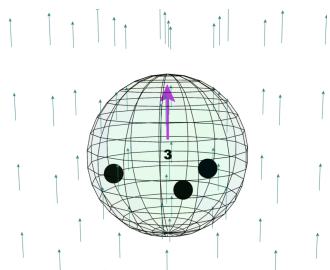
Fig. 19: The proposed paramagnetic alignment of scandium's single unpaired electron in an external magnetic field

This structure represents a rather simple case of one electron that is susceptible to an external magnetic field, and whose effects are not mitigated or affected by other unpaired electrons within the core electron topology. We might therefore consider scandium's one unpaired electron to have an EME ≈ $1e^-$, yielding a strong magnetic susceptibility of $\chi_m = +295$.

3.3.2. Titanium (Ti):

As described above, it is proposed that titanium has two unpaired electrons arranged linearly and axially in its trigonal bipyramidal electron structure. The images below are intended to represent the orientation of these 2 electrons in an external magnetic field (whose north pole is pointing upwards). (*The purple arrows inside the atom represent the unpaired electrons; the black dots represent the relative positions of the 3 di-electrons in that shell.*)
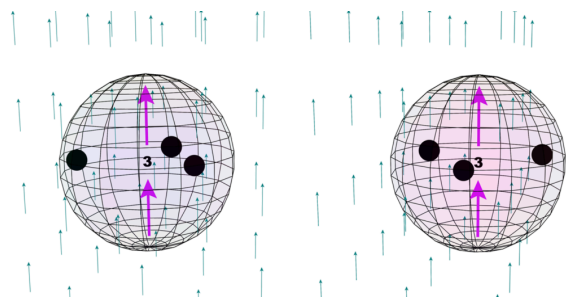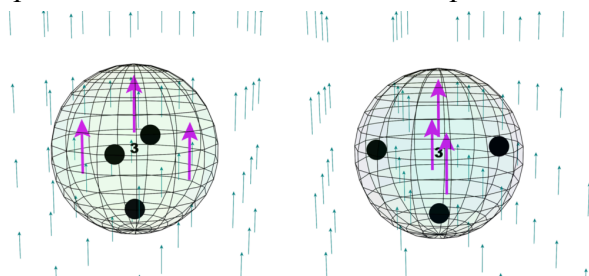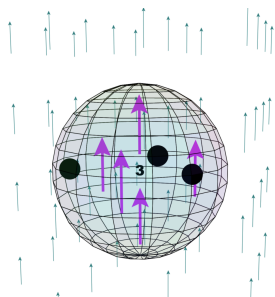
Fig. 20: The proposed paramagnetic alignment of titanium's two unpaired electrons in an external magnetic field

While titanium has two unpaired electrons — twice as many as scandium — it has a much lower magnetic susceptibility value of only χ_m = +151, about *half* of scandium's value (of χ_m = +295). It is proposed that this is due to the magnetic field cancellation that occurs between two unpaired core electrons when their geometry brings them into a linear spin bonding (LSB) relationship (*as described in §3.1.2. above*).

It is proposed that LSB significantly reduces the EME signature of these two coupled electrons with respect to an external magnetic field, and thus, will manifest as a weaker magnetic susceptibility for the atom.

If we consider scandium's single unpaired electron to have an EME ≈ $1e^-$ (wit*h* χ_m = +295), then titanium's 2 linear spin bonding electrons (wit*h* χ_m = +151) would have a relative EME ≈ $0.51e^-$. That equates to about $0.25e^-$ of electron signature, per electron, contributing to the magnetic response of the atom.

3.3.3. Vanadium (V):

As described above, it is proposed that vanadium has three unpaired electrons arranged in a planar arrangement within an octahedral electron structure. Due to orbital constriction by the 3 *di-electron* orbitals in the same shell, the 3 unpaired electron orbitals should be constricted into a slightly narrower wedge-like section of the spherical system, collectively occupying less than half of the shell volume.

The images below are intended to represent the orientation of these 3 electrons in an external magnetic field (whose north pole is pointing upwards). (*The purple arrows represent the unpaired electrons; the black dots represent the di-electrons.*)

Fig. 21: The proposed paramagnetic alignment of vanadium's three unpaired electrons in an external magnetic field

While vanadium has three unpaired electrons — three times as many as scandium — it has a slightly lower magnetic susceptibility value of $\chi_m = +285$, though still higher than titanium ($\chi_m = +151$). It is proposed here that this is due to the amount of field cancellation and spin optimization resulting from parallel spin bonding between these three unpaired electrons.

When unpaired electrons align linearly and parallel, as in the case of titanium (Ti), it was proposed that field cancellation occurs rather effectively between them, which significantly reduces their magnetic signature.

In the case of vanadium, there are *three* electrons spin-bonding together, but this time they are parallel spin bonding *adjacent* to one another. We might expect that this would increase the coherence of the spin bonding, and therefore decrease the EME. On the other hand, the unpaired electrons are also being constricted by the repulsion of 3 *di-electron* orbitals in the same shell, which should serve to increase their EME.

As such, it makes sense that each of vanadium's electrons might contribute a diminished EME, though not quite as diminished as in the case of titanium, and this appears to match the data. If we consider scandium's single unpaired electron to have an EME $\approx 1e^-$ ($\chi_m = +295$), and titanium's 2 linear spin bonding electrons to have an EME $\approx 0.51e^-$ ($\chi_m = +151$), then vanadium's 3 spin bonding electrons would have an EME $\approx 0.97e^-$. That equates to about $0.32e^-$ of electron signature contributed per electron for vanadium, which is both lower than scandium's $1e^-$ and a little larger than titanium's $0.25e^-$.

3.3.4. Manganese (Mn):

Manganese will be evaluated here before chromium (*see below*). While they are proposed to have the same core electron geometry, chromium is considered to be the variation on this electron structure due to its deficient valence shell.

Manganese's five unpaired electrons are arranged in a hexagonal bipyramidal structure. The images below are intended to represent the orientation of these 5 electrons in an external magnetic field.

Fig. 22: The proposed paramagnetic alignment of manganese's five unpaired electrons in an external magnetic field

Since this electron domain geometry contains five unpaired electrons, it makes sense that manganese should have the highest magnetic susceptibility ($\chi_m = +511$) of the (paramagnetic) $3d$ transition metals. It is proposed that this is due to the combination of spin bonding and field

cancellation that occurs between its five unpaired electrons, given their proximity, degeneracy, and slight orbital constriction.

If we consider scandium's single unpaired electron to have an EME ≈ $1e^-$ (χ_m = +295), and titanium's 2 linear spin bonding electrons to have an EME ≈ $0.51e^-$ (χ_m = +151), along with vanadium's 3 parallel spin bonding electrons to have an EME ≈ $0.97e^-$ (χ_m = +285), then manganese's 5 linear and parallel spin bonding electrons appear to have an EME ≈ $1.73e^-$ (with χ_m = +511). That equates to about $0.35e^-$ of electron signature contributed per electron for manganese.

This per-electron value of $0.35e^-$ is very similar to vanadium's $0.32e^-$, and when we compare the two geometries, there is an interesting similarity. The three hybrid unpaired-electron orbitals in vanadium are at 90° to one another, and in a planar arrangement through the atom. In the orbital structure of manganese (and chromium), this same planar, 90° relationship exists — except that there are three iterations of it (if we consider three axial sections). In all three cases, there are also 3 *di-electrons* in the shell, similarly constricting the unpaired electron orbitals. Each of these iterations should manifest a similar amount of electron energy reduction due to spin bonding, given the geometric similarity.

We might therefore expect their 'per electron' numbers to be comparable, and this might also shed light on what chromium's numbers might have been without the disruptive influence of its single valence electron (*see below*). Overall, manganese's χ_m value is larger than vanadium's because it has two more electrons (of roughly the same EME) contributing to its magnetic signature.

3.3.5. Chromium (Cr):

As mentioned above, chromium is antiferromagnetic at room temperature, but loses this in favor of paramagnetism at the relatively low Curie Temperature of 38°C. We will consider its antiferromagnetism below (*in §5*); in this section, we will consider its paramagnetism.

It is proposed that chromium has the same electron geometry as manganese, except that its (delocalized) valence shell only contains one electron. The images below are intended to represent the orientation of these electrons in an external magnetic field.
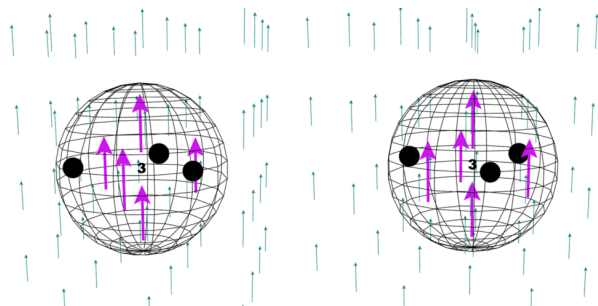

Fig. 23: The proposed paramagnetic alignment of chromium's five unpaired electrons in an external magnetic field

If we exclude the $4s^1$ electron, chromium has five times as many unpaired core electrons as scandium (with $\chi_m = +295$), yet chromium has a *lower* magnetic susceptibility of $\chi_m = +167$. This is also lower than manganese ($\chi_m = +511$), which also has five unpaired core electrons but with *both* of its $4s^2$ electrons.

As in the case of vanadium, the EME of both chromium and manganese's five 3rd shell unpaired electrons will be reduced due to spin bonding and field cancellation within its equatorial and axial symmetries. In the case of chromium, however, it is proposed that the presence of an electron deficient $4s^1$ orbital — or indeed, of the electron-deficient electron gas — may disrupt the electron coherence within, even if only with respect to the external field. If so, this would weaken the coherence of these electrons' response to an external field, which would result in a *weaker* χ_m value. Ini this case, it appears to diminish the EME of the 5 core electrons to a signature that is weaker, overall, than scandium's with its single unpaired electron.

If we consider scandium's single unpaired electron to have an EME $\approx 1e^-$ ($\chi_m = +295$), and titanium's 2 linear spin bonding electrons to have an EME $\approx 0.51e^-$ ($\chi_m = +151$), along with vanadium's 3 parallel spin bonding electrons to have an EME $\approx 0.97e^-$ ($\chi_m = +285$), and manganese's 5 linear and parallel spin bonding electrons to have an EME $\approx 1.73e^-$ ($\chi_m = +511$), then chromium's 5 linear and parallel spin bonding electrons appear to have an EME $\approx 0.57e^-$ (with $\chi_m = +167$). That equates to only $0.11e^-$ of electron signature contributed per electron. As stated, we propose that this is due to the $4s^1$ electron disruption.

4. DIAMAGNETISM

4.1. Copper (Cu):

Copper's 3rd shell is full, with a symmetrical arrangement of 8 field-repelling *di-electrons*. While it does have one unpaired $4s^1$ electron in its valence shell, it is presumed that the diamagnetism of its *di-electrons* overpowers any paramagnetism due to the $4s^1$ electron, giving copper a magnetic susceptibility of $\chi_m = -5.46$.

As mentioned above (*see §2.9*), according to the present model, when copper becomes a Cu^{2+} ion, its hybrid electron geometry should contain a single unpaired electron orbital that is being constricted and extended by 7 *di-electrons*, and it will therefore be strongly paramagnetic.

4.2. Zinc (Zn):

Zinc's 3rd shell is full, with a symmetrical arrangement of 8 field-repelling *di-electrons*, and, unlike copper, its 4th shell has a $4s^2$ *di-electron*. This gives zinc a lower magnetic susceptibility value than copper, with $\chi_m = -9.15$.

This may imply that the presence of copper's $4s^1$ electron may be disrupting the diamagnetism of its inner symmetrical arrangement of 8 field-repelling di-electrons, decreasing their diamagnetism slightly with respect to an external magnetic field. This is similar to the

disruption of magnetic coherence proposed in the case of chromium's paramagnetism (*see §3.3.5 above*).

5. ANTIFERROMAGNETISM IN CHROMIUM

As mentioned above, chromium is the only metal that is naturally antiferromagnetic at room temperature, though it loses this antiferromagnetism in favor of paramagnetism at a rather low Curie Temperature of 38ºC.

This means that there is something about chromium's electron structure that, when it is in crystalline metallic form at room temperature, its lowest energy state occurs when the electrons on adjacent atoms in the crystal are oriented with a magnetically antiparallel arrangement.

Note that, in the case of electrons, magnetically antiparallel does not mean the same as opposite spin. The former is a magnetic alignment distinction; the latter is a spin component phase relationship [4]. (Electrons of opposite spin can be either magnetically parallel or antiparallel.)

The precise mechanism behind chromium's antiferromagnetic state remains a matter under investigation, though it is believed to relate to the Fermi surface geometry within the crystal (rather than the crystal periodicity itself) [12].

If we were to speculate, based upon the present 'sub-quantum mechanics' model, it seems plausible that the driving force causing the electrons on adjacent atoms to align their magnetic moments antiparallel *and* their spins opposite might be the pairing up of the $4s^1$ electrons, from adjacent atoms, in the electron gas. This might then cause the degenerate, unpaired *pd*-hybrid electrons to orient their spins to match the spin of their valence electron, in order to resonate mutually at the lowest energy. (Their coherence might explain why and how they both affect the Fermi surface in a crystal.)

If this conjecture is correct, it would account for why none of the other $3d$ transition metals are naturally antiferromagnetic. Each of the other $3d$ metal atoms contributes 2 valence electrons to the electron gas. They therefore do not require a valence electron of opposite spin from an adjacent atom in order to find the stability of an electron coupling (or, at least, a spin-zero average), and this form of coupling is therefore not present to anti-align the core unpaired electron orbitals of adjacent atoms. (Copper is an exception, since it also donates a valence electron into its core. However, it contains no unpaired core electrons and a full 3rd shell containing 8 *di-electrons*, which is why it is diamagnetic.)

According to this conjecture, it would seem that chromium's antiferromagnetism does *not* arise from a crystal-wide spin bonding resonance, as is proposed in the case of ferromagnetism. This antiferromagnetism would therefore not be a form of ferromagnetism. (It is proposed that chromium's unpaired electron orbitals do not experience sufficient orbital extension to be ferromagnetic, due to constriction from only 3 same-shell *di-electrons*.) Consequently, the crystal structure of chromium — which is body-centered cubic (BCC) — should have no meaningful

bearing on the *mechanism* behind its antiferromagnetism (as it would have in the case of a ferromagnetic crystal).

It is therefore proposed that the antiferromagnetism of chromium arises from an electron coupling resonance within the (valence) electron gas that binds the crystal. (This region is where the above-mentioned Fermi surface, as well as the valence and conduction bands are located.) Thus, even though the unpaired core electrons are not significantly extended, it is proposed that they do not *need* to be in order to resonate in degeneracy — to *couple* — with their own valence electron. (*Perhaps we might even think of it as a kind of 'local paramagnetism.'*)

Since the coupling valence electron from each adjacent nearest-neighbor atom will have opposite spin, the (magnetic) core electrons of these adjacent atoms will therefore have opposite spins.

When the temperature increases enough to reach the Curie Temperature, however, there is enough thermalization present to disrupt this weak electron gas coupling resonance, to the point where an external magnetic field will overwhelm it in favor of a crystal-wide paramagnetic alignment with the now-dominant external field. If this field is removed, the crystal will remain paramagnetic — with random magnetic alignments of its core electrons — until it cools below its Curie Temperature, at which time the electron gas coupling resonance can gain enough 'traction' over thermalization to re-enable antiferromagnetism.

6. CONCLUSION & FUTURE WORK

In this paper we have proposed electron geometries for the $3d$ transition metals, as well as suggesting how electrons in *pd*-hybridized orbital geometries might interact to decrease their collective magnetic signature with respect to an external magnetic field. These spin bonding interactions and electron geometries are then invoked in order to account for the relative trend in magnetic susceptibility strength across the $3d$ row of the periodic table.

Diamagnetism and antiferromagnetism are also considered, and it is proposed that the latter results from a crystalline electron-gas coupling rather than being a form of ferromagnetism.

Possible applications involve the design of new crystalline materials that leverage the internal electron geometries of not only metal atoms but also paramagnetic metal ions. Within a crystal, these are fixed within specific geometries, and separated by diamagnetic anions of various sizes. In specific arrangements, materials with subtly varying magnetic properties can be engineered.

Future work will investigate the consequences of *pd*-hybridized electron structures in more detail. These will include:

- discussing the differences in paramagnetic strength that arise in the $4d$ and $5d$ rows, and how this may relate to the energy density of electron states in orbitals with different volumes
- accounting for palladium (Pd) as an apparent exception to the d-block paramagnetism trend
- the mechanism of ferromagnetism

- accounting for the *opposite* direction of the strength trends between ferromagnetism and paramagnetism, when comparing the 3*d* to the 4*d* and 5*d* rows
- accounting for why only iron, cobalt, and nickel are ferromagnetic in the *d*-block
- accounting for the opposite trend in melting points versus Curie Temperatures for iron and cobalt
- accounting for the easy and hard directions of magnetization in iron, cobalt, and nickel
- introducing *pdf*-hybridization and possible ground-state electron geometries for neodymium (Nd) and gadolinium (Gd).

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