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Quantum Spin Coherent Electron Correlation

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1. Introduction

A data-driven quantum chemical re-investigation and characterisation of the nature of the singlet-coupled e-pair interaction in weak interactions in physics and chemistry is discussed, in order to bring out its surprisingly broad implications for our understanding of some of the most fundamental aspects of nature.

1.1 Outline

The central conceptual difficulty in standard non-relativistic quantum chemistry, as for relativistic quantum mechanics, remains that in the absence of a satisfactory, physically intelligible representation of the phenomenon of spin, spin is represented in our models as a topological constraint on many-particle interactions. All of chemistry is dominated by the phenomenon of spin-pairing, derived from the Aufbau principle of filling electron shells in atoms. However determinantal expression of antisymmetry requirements effectively maintains separation of same spin electrons (exchange effects) while degrading the details of coupling between opposing spin electrons to electrostatics. This chapter investigates quantum mechanically the implications of a semiclassical model of spin proposed and formally defended some time ago (Burton 1988; including a formal modification of coupled pair theory), extending my previous published conjectures (Burton 2009). Its simple new idea touches a vast area of contemporary physics and chemistry.

1.2 Basic motivation

The stimulus for this research was a program focused on weak molecular interactions involving small neutral molecules whose interactions are well known to be very sensitive to electron correlation effects (Burton 1977, 1979, 1980; Burton, Gray & Senff 1982; Senff & Burton 1985, 1986, 1989). The particular focus of our investigations was interactions involving He and H_2 molecules involving well-localised e-pairs. Aside from their fundamental relevance to our prehistory in cool interstellar, molecular clouds, from a technical viewpoint these molecules were ideal to minimise the impact of artefacts arising from the various approximations involved in implementing the conventional correlation algorithms we employed at the time.

Interactions involving such well-separated e-pairs should represent ideal candidates for investigation with pair correlation algorithms (Sinanoglu 1961, Hurley 1976) designed to isolate intra-pair and interpair contributions to electron correlation corrections to many-electron wavefunctions, and their simple electronic structures were amenable to relatively

complete Hartree-Fock Self-Consistent-Field modelling. Being confident of control over artefacts from these sources, we carefully investigated basis set completion effects in the pair-correlation ansatz. The weak van der Waals interaction potentials in He...He, He...H_2 and H_2... H_2 were available experimentally by several routes, including direct scattering in crossed molecular beam experiments, and with these as reference we embarked on a program to test regions of the more polarisable inter-atomic interaction zones for basis set incompleteness.

What we found told us that even very large conventional, nuclear-centred, gaussian basis sets were subject to improved electron correlation energies when augmented by additional s,p probe sets aligned between nuclear centres. Our approach to their disposition was to locate these basis set additions off nuclear centres along the line of interaction, but to keep these located a fixed distance from the nearby atomic centre while intermolecular distance coordinates were varied to sample van der Waals interaction, to minimise basis set extension error (Boys & Bernardi, 1970), an artefact well-known in HF-SCF calculations but possible also in the computation of pair-correlation energies.

The results, admittedly involving small effects, but systematically accumulated over more than a decade, eventually led me to question why the low density region at the polarisable edge of interacting atoms & molecules should be so sensitive to details of basis set disposition. Surely, I had thought, electron correlation is dominated by the dynamics of inter-electron interactions in regions of higher rather than lower electron density[1]. The details of our calculations however were asking me to revisit this assumption: maybe electron correlation is better understood as an *edge effect* of e-pairs?

1.3 Reviewing the basic conventions of quantum chemistry

Multi-electron wavefunctions in quantum chemistry are conventionally characterised by aggregating individual electron spin-orbitals into an antisymmetrised, determinantal notation devised in 1929 by J.C. Slater. The spatial and spin parts of multi-electronic wavefunctions fail to factorise except in the special case of a single e-pair, so the burden of the determinantal expansion of electronic spin-orbitals having m_s= +½ and -½ spins is accepted to ensure that the exclusion principle devised by Wolfgang Pauli in 1925 (Pauli 1945) is satisfied for the electronic structure, even though most molecular electronic structures in chemistry are strongly paired. At least the antisymmetry required of sets of fermions, the wavefunction changing sign with respect to pairwise particle interchange, was guaranteed by the determinantal formalism.

Much of the chemistry of molecules formed of light atoms reflects their electronic structure being comprised of relatively localised e-pairs with close-coupled singlet pairing of spins, reminiscent of the simplified (and pre-quantum mechanical) models of locally-paired electron dot diagrams introduced by Gilbert N Lewis (1916) to explain the covalent bond. This has led to extensive theoretical investigation of pair correlation methods both formally (Sinanoglu 1961, Hurley 1976) and subsequently by a wide range of computational methods in quantum chemistry, including those used in our program of investigating weak van der Waals interactions.

The determinantal notation, which succeeds by construction to keep electrons of the same spin widely separated in the quantum chemistry models, ensures conformance to

[1] The weak assumption embedded in density functional approaches to correlation effects, rather than correlation being localised in *polarisable* regions .

antisymmetry and the exclusion principle but its cost is that it de-emphasises the natural tendency to e-pair formation in chemistry. If the close coupling between electrons of opposite spin is more relevant to the physics of the system under investigation, as theorists Sinanoglu and Hurley have chosen to emphasise by treating these structures as clusters of e-pairs, the pair-correlation formalism (rather than the more conventional configuration interaction or CI approach) may be advantageous. By emphasising correlations between e-pairs of opposing spin, and of pair-pair interactions between them, such an approach seemed ideal for investigating weak intermolecular forces, as was the case in our interactions involving He and H_2.

When one focuses upon weakly interacting systems with one or two closely localised electron pairs (e-pairs), and these are light neutral molecules such as He or H_2, the interaction energy between the localised pairs is *purely repulsive* when modelled at the uncorrelated level of the Hartree-Fock-Self-Consistent-Field model. HF-SCF approximates each electron (spin-)orbital self-consistently in the time-averaged, 'electrostatic' field of the other electrons. Correcting the approximate HF-SCF wavefunction requires adding electron correlation corrections to the zero-order 'independent electron' wavefunction, by introducing either explicit inter-electron distance parameters (e.g. Hylleraas 1930; Boys and Handy 1969, Gill et al. 2006) or by constructing configuration interaction (e.g. Shavitt 1977, 1981) expansions to implicitly (statistically) model more flexibly the details of electron-pair interaction. Either strategy, at the considerable expense of very extended and diffuse representation of the resulting correlation, and being hard to interpret, can realise excellent agreement between computed and empirical total electronic energy for molecules in their ground states. In particular for our neutral, light molecule systems, total energies can be expected which quite closely mimic the rather weak van der Waals *attraction* between these close-shell molecules as they approach one another. This is a critical achievement, required because otherwise it would be impossible to *liquefy* He(g) or H_2(g) albeit at temperatures close to zero Kelvin: He boiling point is -268.6 °C (4.55 K); H_2 boiling point (1.013 bar) is -252.8 °C (20.8K). Statistical mechanical models of these phase changes, and molecular beam scattering experiments, are completely consistent with *attractive* van der Waals interaction potentials for the respective molecular interactions. So one can conclude that it is impossible to model the (g) to (l) phase change in these liquids without taking electron correlation effects into account.

1.4 Challenging the conventional approach to representing spin

Our van der Waals interaction calculations, using well-matched electron correlation algorithms and more and more complete basis sets to avoid obvious basis set superposition artefacts, showed some small but unexpected effects which led us to reconsider the conventional wisdom of electron correlation theory. The topological separation of same-spin electrons enforced by the determinantal wavefunction formulation leads to very long multi-configuration expansions for the correlated wavefunction expressions which approach exact ground-state energies of these molecules[2]. The physical interpretation of these correlation effects are best shown from e-pair cluster expansions, which show the correlation corrections are dominated by the principal correlating natural orbitals[3] for each localised e-pair, which

[2] This is already true for *single* two-electron ground-state pairs, such as He (Hylleraas 1930; Pekeris 1958) or H_2 (Kolos et al. 1986), when e-pair correlation is explicitly modelled by r_{12} expansion.

[3] The significance of natural orbitals lies in the fact that CI expansions based on these orbitals have generally the fastest convergence.

introduce nodal surfaces to intersect the occupied orbitals of the e-pair either angularly or radially. This tends to create an impression that electron correlation effects are derived from regions of higher rather than lower electron density within the e-pair. This long held assumption was now the focus of my concern, because, as with direct conventional Configuration Interaction (CI) expansions, even the PNO-CI expansions of cluster pair theory tend to aggregate many small contributions whose physical nature is difficult to discern.

What our strange off-nuclear-centred basis set augmentations were telling us (in our investigation of the interaction of light non-polar molecules) was that significant regionally specific correlation contributions were arising from low-density, highly polarisable, outer reaches of atoms, well away from the respective nuclear centres which tightly constrain electrons by nuclear attraction.

I began in 1988 to investigate a semi-classical model of correlation in a two-electron, axially symmetric bound-state (Burton 1988), starting from first principles and the helicity equations, and to review Hurley's formal specification of e-pair correlation. In determinantal formulations customary in quantum chemistry, the spin wavefunctions have a purely topological significance consistent with the exclusion principle but what I was coming to realise instead was that spin should be explicitly and physically instantiated *directly* as peripheral wavelet disturbances in the superficial parts of electron orbitals themselves.

The idea of physically embodied but peripheral wave-matter spin, considered semiclassically as a *fractional* electron disturbance, could be a significant effect but remain rather well hidden by the general acceptance of spin being modelled as a determinantal topology. It had just the features to physically explain the Stern-Gerlach 1925 effect in a superior way to that proposed by Uhlenbeck & Goudsmit in 1925 & 1926, which supposed the ultimately untenable notion that the *whole* electron was subject to spin. In semiclassical terms, replacing the electronic charge to mass ratio e/m in expressions for the electron magnetic moment due to spin by the expression δe/δm proposed in Burton 1988, a ratio of identical magnitude for identical fractions of mass and charge, was entirely consistent with fundamental treatments of spin effects (Merzbacher 1970; Landau & Lifshitz 1977). This heretical idea, one certainly not excluded by the history of the concept (Tomonaga 1974/1997), warranted further investigation.

Much later in 2003-5 (Burton 2009), I realised that the dominant or principal correlating orbital for He could in fact be *identified with* the antisymmetrised singlet-coupled spin wavefunction of the spin-orbital coupling itself. Furthermore, in this special case, a single variational parameter corresponding to its radial mixing with the HF-SCF reference (introduced as a conjecture in Burton 1988) was all that remained to exactly determine the He $(1s)^2$ ground state singlet energy, once the angular interaction effects were *completely specified* by the symmetry of the antisymmetrised singlet coupling formula (Section 2.7; see Figure 1).

2. Electron correlation problem in quantum chemistry

During the decade around my hosting an *International Workshop in Atomic and Molecular Physics and Quantum Chemistry* at the University of Wollongong in June 1980 and whose proceedings I edited (Burton 1980), my small research group's activities centred on two ways of testing the validity of then current models of electron correlation in quantum chemistry. We were focused upon investigating models of the electron correlation energy contribution itself at various degrees of approximation for weak van der Waals molecular interactions (Senff & Burton 1985, 1986, 1989), in particular by appraising the impact of

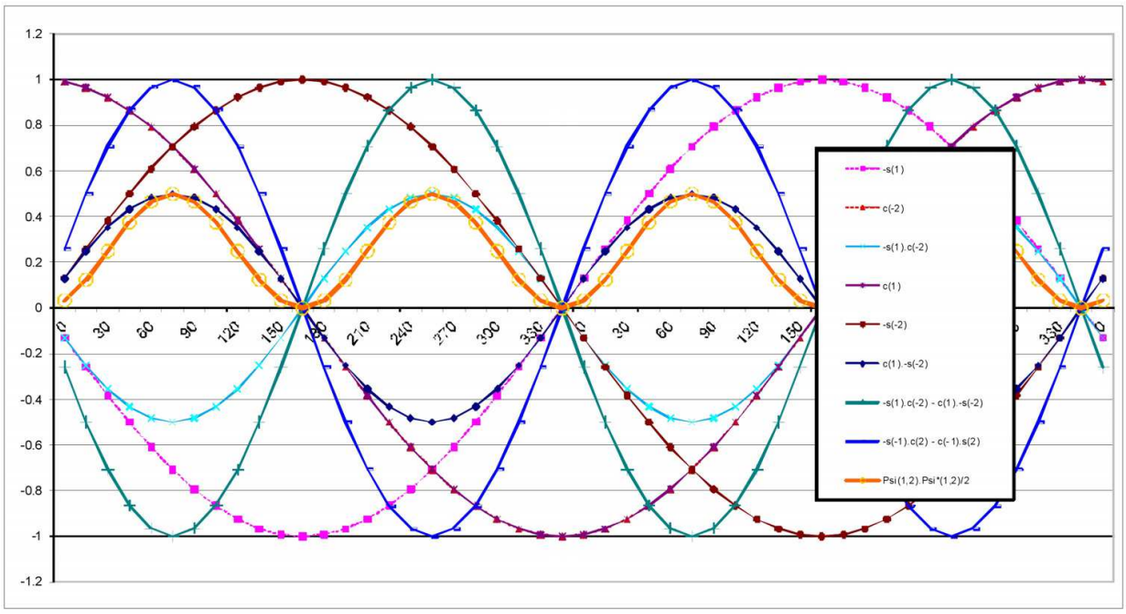

Fig. 1. Angular representation of m = +/- ½ spin wavefunctions for He $(1s)^2$ configuration, in antisymmetrised singlet form, with relative phase optimized to illustrate axially circumferential quadrupolar beats in the periphery of the pair function. The circumferential angular form for a given distance ρ off-axis is illustrated beginning with explicit sinusoidal (s) or cosine (c) forms for m_s = +/- ½ as shown in the legend.

innovative ways of assessing the basis set limitations implicit in those models by the choice of strategy to build more completeness (accessing yet more subtle correlation effects) into those, still approximate, models of the correlation contribution (Burton 1977, 1979, 1980; Burton, Gray & Senff 1982).

2.1 Issues in conventional computational approaches

Before Isaiah Shavitt's (1981) '*Graphical Unitary Group Approach*' led to making Full CI calculations practical to exhaust the correlation energy contributions of a given molecular basis set, methods tracing their heritage back to Oktay Sinanoglu (1961) and focused on pair correlation energies were formally analysed for completeness by Andrew Hurley (1976, *Electron Correlation in Small Molecules*) and made practical in for computational quantum chemistry in basis set representation by several groups led by Werner Kutzelnigg, Wilfried Meyer and Reinhart Ahlrichs *et al.* (1975a, 1975b) in Germany.

At that time, through focusing upon relatively localised intra-pair-correlation energies which were known to dominate the correlation energy contributions (corrections) to much simpler molecular Hartree-Fock, Self-Consistent Field estimates of molecular electronic energies, it was left to the relatively weak coupling between the correlation energy effects of *different* pairs to represent the uncertainty of various "coupled pair" methods of assessing total correlation energies within the constraints of a given basis set (Ahlrichs *et al.* 1975A, 1975b).

2.2 Interactions involving localised electron pairs

While the transformation to a localised formulation of occupied molecular orbitals in, say, the methane molecule, CH_4, generates four equivalent bonding orbitals, the canonical

orbitals in the SCF-MO representation begin symmetry adapted. We preferred to work in a localised orbital representation to assess pair correlation energies to concentrate the nominal impact of intra-pair correlation in a less diffuse, localised orbital representation, consistent with the supposed strength of the formal methods for treating electron correlation we chose to pursue.

In time we narrowed our focus to the simplest of molecules: He, Li^+, H_2, H_3^+ having a single (localised) electron pair, and concentrated on assessing the nature of the weak inter-pair correlation energy effects corresponding to the van der Waals interaction between these species, including weakest of interactions of neutral molecules He...He, He...H_2 in various angular alignments and H_2...H_2 in its various representative configurations.

Molecular beam scattering analyses of these neutral molecule interactions provided the external reference for our internal analysis of systematic errors from the approximations we were forced to make in our calculations because of our access to relatively modest computational resources.

The basis set superposition error (BSSE; Boys & Bernardi 1970) was of particular significance to our approach, since poor representation by way of local basis set limitation led to the correlation ansatz "borrowing" flexibility from nearby centres as they were brought nearer, generating artificially higher (less limited) correlation contributions for more compact molecular forms (close collision) than those more distantly interacting (van der Waals asymptote) molecular forms: this artefact acted apparently to deepen the attractive van der Waals well.

In order to independently appraise the quality of the representations of each counterpart molecule in these molecular interaction calculations, we adopted the pragmatic device, in addition to using large, well-tempered s,p,d,f basis sets on each nuclear centre, of scanning the sensitivity of calculated correlation energies with a free-floating s,p set to probe where in the molecule additional basis set flexibility might still be required.

We reported this approach at the *AMPQC* workshop in Burton, Gray & Senff (1980), and two of us (myself and Ulrich Senff) subsequently found in a careful series of calculations that in the close interface between weakly interacting neutral systems (in the region where the SCF-MO energies are in fact repulsive, and only correlation effects generate an attractive intermolecular potential energy to qualitatively match experiment) involving He...He, He...H_2 and H_2...H_2 that even quite large nuclear-centred basis sets appeared systematically inadequate to fully represent the intermolecular correlation energy of these weakly interacting systems.

Our focus on weak interactions between light, non-polar molecules such as He or H_2 allowed us to effectively eliminate the BSSE correction at the HF-SCF level, so the impact of free-floating s,p function specifically in the correlation energy correction could be assessed. What we found consistently (despite correcting for the BSSE itself) was for each atom centre, additional correlation energy arose with s,p sets being located at the 'edge' (say fixed at 50-100pm off-nucleus) of each atom, on the line of centres of their interaction. This remained true as we increased the well-tempered s,p,d,f bases on each centre.

This was a small but persistent effect, and it raised an important question in my mind: Why was the atomic or molecular *edge* of these interacting systems, each just a localised correlated pair of electrons, seemingly so vulnerable to additional degrees of local basis set freedom?

2.3 Back to first principles of spin and correlation

By 1988, my reflecting on this question turned active again, but from an entirely different angle. I went back to first principles in the structure of the helicity equations in Landau & Lifshitz (1977) for a free electron and contemplated what they would reduce to for the case of an electron constrained axially by being bound on the attractive nucleus of an atom.

I discovered (Burton 1988) that a semiclassical, fractional electron effect – like ion cyclotron resonance but considered as a fractional electron wavelet circulating circumferentially around a Schrödinger-like delocalised electronic matterwave – could support all the formal equations representing electron spin effects without change if instead of the electronic charge e and the electronic mass m occurring everywhere as the electronic charge to mass ratio (e/m) I notionally attributed spin effects in these equations to there being a localised disturbance involving a *small fraction* of the electronic matter wave ($\delta e/\delta m$) localised in the axially distant and relatively polarisable periphery (well away and self-shielded from the attraction of the nuclear centre) of each electron distribution.

I also discovered that Andrew Hurley's (1976) careful formal analysis of electron pair coupling had a single minor defect: he had assumed that (single-valued) L^2 orbital representations of basis sets for correlation calculations in molecules could in principle exhaust electron correlation effects in a full-CI formulation. This led him to wrongly conclude that conventional correlation corrections in quantum chemistry should be attributed solely to reduced electron repulsion. As I confirmed directly with my earlier mentor, this conflicted with the need in correcting the energy of an HF-SCF model of an e-pair (e.g. He, or H_2) to satisfy the Virial Theorem *both* at the level of the HF-SCF model representation (already Virial Theorem compliant at limit basis set), *and* at the level of the additionally correlated representation of the electronic ground-state of that same molecule. If the HF-SCF representation of He satisfies the Virial Theorem, and the true (correlated) ground state of He does also, then changes in *both* the one-electron terms <T> (to elevate one electron kinetic energy terms) and the two-electron terms <V> (to diminish electron interaction energies) of the correlation-corrected total energy expressions relative to the HF-SCF model must be required from the correlation corrections. Assigning the correlation correction solely to a reduction of electron repulsion without a corresponding change to increase one-electron kinetic energy (increased wave-function curvature), as Hurley had concluded, must be wrong.

The implication of this was that no single-centred L^2 basis of reasonable size could expect to rapidly converge correlation energies, even in Full-CI models of that correlation, and that the weakly interacting systems we had been studying, embellished with off-nucleus 'probe' s, p sets, were reflecting *additional physical requirements* for basis set freedom in each atom's periphery.

2.4 Identifying the singlet-coupled spin wavefunction with the principal pair correlating natural orbital of each localised e-pair

There is a special case, that of singlet-coupled $m_s = +½$ and $-½$ spins in a two-electron atomic wavefunction, where one can explicitly write the angular behaviour of the spin coupling. Taking the specific case of ground state singlet of atomic He, the e-pair wavefunction can be written:

$$\text{He } (1s)^2 = 1s(1).1s(2)\ \{a(1).b(2)-b(1).a(2)\}/\text{Sqrt2} \qquad (1)$$

where $a(1)$ and $b(1)$ represent spin wavefunctions, each a two-valued angular function periodic in 4π corresponding to $m_s = +½$ and $-½$ spins, respectively.

Burton (2009) shows a diagram of each angular contribution of the singlet-coupled two electron wavefunction, and interprets these contributions and their resulting interaction as peripheral surface disturbances oriented about the Z=0 axis of the helicity equation, through the He nuclear position, in this case (Figure 1). Counter-propagating fractional electronic surface disturbances corresponding to m_s= +½ and -½ spin periodicity (over 4π) were shown there to interact in the physical space domain of their *relative angle* (over 2π, i.e. single-valued in physical space) to yield a resultant quadrupolar form of oscillating angular coupling, transverse to the helicity axis, centred on Z=0.

Conventionally, the separation of spatial and spin variables in forming Slater determinantal representations of anti-symmetrised many-electron wave-functions leads spin to be represented and considered as a topological variable not directly interactive with the underlying spatial orbital of each spin-orbital, exactly as is being portrayed in Eq. 1. What Burton (1988, 2009) discovered instead is that a stable (circumferential) quadrupolar miss-match between the two otherwise spherical orbital forms for each electron arises in singlet coupling: the singlet coupling leads to a *physical resonance* in the counter-propagating angular forms of the two independent electrons in close-matched singlet coupling, where the respective interacting disturbances are built-in to the spin-orbital representation in a multiplicative manner. This resonance corresponds *simultaneously* to an increase in curvature of the underlying one-electron wavefunctions due to the circumferential disturbance, and a systematic circumferential mismatch between the two independent electrons. The former has the effect of increasing <T> for the two electron wave-function (relative to HF-SCF with no spin representation) while the latter has the effect of decreasing the electron interaction energy <V> due to the *systematic persistence* of the resonantly stable circumferential mismatch in the angular behaviour of the two electrons. Hurley's analysis determined the form of the correlation change in its impact on (changes in) <V> but missed the necessary complement to it on (changes in) <T> because he restricted his consideration (in complete consistency with universal practice at the time) to L^2 orbital excitations as the correlating orbitals.

Burton's semiclassical interpretation of electron correlation suggests that one should deny any formal physical separability of spin effects from the underlying spatial wavefunction of each spin-orbital, rather to include them directly as surface modifications to those spatial forms.

2.5 Quantum spin coherence using an integrated spin-orbital representation for e-pair

In the models of physical interaction involving two well-separated electron pairs that Ulrich Senff and I considered, very large L^2 orbital basis sets (including off-centred functions) were required to begin to converge the correlation energies of systems even as simple as He...H_2 or H_2 ...H_2 , despite the fact that the HF-SCF wave-functions could be well-represented by modest DZ+P nuclear centred basis sets. The startling conclusion we are forced to reach, against eighty years of history in LCAO-MO models of quantum chemistry, is that it is a mistake to topologically separate spin from its physical impact on underlying spin-orbital representations of interacting electrons when these are closely singlet coupled. The implication of this in singlet coupling is that the multiplicative spin-coupled wavefunction form of each pair *is precisely* the form of the principal correlating natural orbital of the HF-SCF version of that pair.

Going back to the helicity equations for this model of He, we find that just a single (ρ/a_H) parameter (see below) scales the off-axis form of the multiplicative disturbance due to spin

(Burton 1988, pp. 12-14), and as this varies, the relative *angular* curvature of each independent electron's wavefunction varies but so also does the phasic amplitude mismatch with the co-bound second electron. The optimum value of this parameter serves to restore the required Virial Theorem balance between $\langle V \rangle_{Exact}$ and $\langle T \rangle_{Exact}$ for the correlated ground state as correlation increases to alter these, in a balanced way but in the opposite sense, from reference HF-SCF values of $\langle V \rangle_{SCF}$ and $\langle T \rangle_{SCF}$.

Of course, such a simplified one-parameter optimisation per pair of electron correlation in molecules comprised of relatively localised singlet coupled e-pairs (most of chemistry in fact, and virtually all of protein-dominated biology) would lend itself to very efficiently computed semi-empirical models of explicitly correlated many-electron wave-functions, with the major benefit of needing only HF-SCF level basis set representations, and all other virtual excitations in the CI being dispensed with in favour of a single correlating natural orbital representation for each localised orbital pair.

2.6 Coherent e-pair correlation function

Burton (1988) recounts the outcome of the Bernardi & Boys (1973) analysis of the pair correlation function employed in Boys & Handy (1969a, 1969b) exemplars of accurate direct correlation in Ne and LiH using their trans-correlated wavefunction formalism. Roby (1971, 1972) had already shown that the transcorrelated wavefunction and the cluster expansion wavefunctions for the Independent Pair Approximation (IPA) and the Coupled Pair Approximation (CPA) are related for spatially well separated pairs[4] by equivalence between the strong orthogonality constraint of pair theories and the canonical contraction conditions of the trans-correlated approach to the correlated wavefunction, when (see Note):

$$\mu_{ij}(1,2) = [f(1,2)-1]\ |\Psi_i(1).\Psi_j(2)| \tag{2}$$

Hurley commented on this supposed universal form to pair correlation f(1,2):

> 'One would expect that an accurate description would require quite unrelated functions f(1,2) for the various pairs and that any restriction of the pair functions would seriously affect the correlation energy' (Hurley 1976; p.254)[5].

It is precisely this surprising result from the detailed analysis of an effective direct correlated method, coupled with its generalisation from Burton (1988; see Equations 12 through to 23) to include non-single-valued Pair Natural Orbitals for the principal correlation effect circumferential to the axial that we conjoin to propose modelling e-pair correlation *universally*, at least for the case of axially symmetric pairs in $|L,S\rangle$ representation. The general expression (Burton 1988, Eq.31) for the correlation function is given by Eq. 3:

$$f(1,2) = R_f(\rho_1,\varphi_1,\tau_1)\, R_f(\rho_2,\varphi_2,\tau_2)\, \mathbf{S}(\rho_1,\varphi_1,\tau_1;\, \rho_2,\varphi_2,\tau_2) \tag{3}$$

Burton (2009) advanced this semiclassical analysis suggested by Burton (1988) to *identify* the angular analysis required of the optimised semiclassical correlation interaction **S** in [3] with

[4] Consistent with the van der Waals interactions involving He and H_2 that we were pursuing.

[5] This proposal has seemingly not been directly pursued, although numerical approaches along this line have been cast in terms of an 'inter-particle' distance operator (Boys & Handy 1969; Bernardi & Boys 1973), or seek to model particle position *and* momentum in joint distributions (see Gill, Crittenden et al. 2006).

the fully quantum mechanical, antisymmetrised singlet-coupling of the two-electron singlet spin function from Eq.1.

The crucial point of the argument at this stage is that the function **S** in Eq.3, which is designed to establish and maintain coherence in the opposing sense of Ripple propagation for each electron of the pair, can, at least for stationary state wavefunctions, be **presumed** to have achieved this goal (Burton 1988, p.22). In our chosen context of the He $(1s)^2$ ground state, to respect the known topology of spin in antisymmetrised e-pairs, means that the angular degrees of freedom for the m_s = +/- ½ spin components in the e-pair interaction must be constrained. The angular form of the peripheral correlation interaction of the pair is fully determined by the *assumption* of singlet coupling. The resulting angular behaviour around the orienting axis of the 1s(1).1s(2) orbital product for ground state He is given in Figure 1.

2.7 Angular characterisation of a singlet-coupled antisymmetrised e-pair

Burton (2009) devised an angular characterisation of the m_s = +/- ½ spin e-pair interaction. Figure 1 shows the build-up of the resulting angular probability distribution for the circumferential singlet-coupled spin wavefunction Φ(1,2) and the corresponding angular density function Φ(1,2).Φ*(1,2) (shown in orange, showing peripheral quadrupolar form over 2π), where

$$\Phi(1,2) = \{ \sigma(1; \rho, \phi, a'_H)\, \sigma(2; \rho, -\phi, a'_H) - \sigma(2; \rho, \phi, a'_H)\, \sigma(1; \rho, -\phi, a'_H) \} / \text{sqrt } 2 \qquad (4)$$

and

$$\Phi^*(1,2) = \{ \sigma(1; \rho, -\phi, a'_H)\, \sigma(2; \rho, \phi, a'_H) - \sigma(2; \rho, -\phi, a'_H)\, \sigma(1; \rho, \phi, a'_H) \} / \text{sqrt } 2 \qquad (5)$$

The incorporation of the singlet-coupled spin wavefunction's angular dependence from Fig.1 leaves (for the ground-state e-pairs of He or H_2 we are considering) just a single axial function R_f dependent upon $\rho_1=\rho_2$ being left to optimise. The radial mixing parameter determines the effective fraction of the e-pair in the periphery being subject to the physically (electromagnetically) coupled disturbance between the fractional matter-wave counter-propagations. Therefore, to variationally maximise the pair correlation energy for the pair corresponds to a variational optimisation of the mixing parameter depending upon ρ. As this function increases off-axis starting from ρ=0 the radial behaviour of R_f for each electron begins with unit value (Burton 1988, see Equations 8, 9 and 10), and follows a scale parameter ρ^2/a_H^2 which increasingly intersects the polarisable periphery of the e-pair off-axis as the mutually induced *and self-consistent* effective magnetic field H linking the circulation of the counter-propagating spins increases. Burton 1988 notes that the a_H parameter has the dimensions of distance and for a laboratory scale field of **H** = 1 Tesla has the value of 36.2617 nm. The variation of this single parameter to reach the exact correlation of the pair is therefore a simple variational optimisation.

Three decades after Hurley's mooted universal form of pair-correlation function (Eq. 2), in our realization of a direct matter-wave representation of the pair function (called the Quantum Spin Coherence model), we have an interesting new context in which to re-examine the systematics of electron correlation, including the amazing consistency of $(1s)^2$ pair correlation energies as diverse in size as in H^- and U^{90+} (around 1.1ev[1]: see Gill, Crittenden et al. 2006), a long recognised fact of quantum chemistry, that on its own is suggestive of more regularity in the dynamics of electron pair correlation than had yet been appreciated.

$$\tilde{\varepsilon}_{ij} = \left(1+\langle\hat{\mu}_{ij}|\hat{\mu}_{ij}\rangle\right)^{-1} \left\{ \left\langle |\psi_i\psi_j| \left| \frac{1}{r_{12}} \right| \hat{\mu}_{ij} \right\rangle + \left\langle \hat{\mu}_{ij} \left| \frac{1}{r_{12}} \right| |\psi_i\psi_j| \right\rangle + \left\langle \hat{\mu}_{ij} | H_{ij} + E^o_{ij} - E_o | \hat{\mu}_{ij} \right\rangle \right\} \quad (12)$$

where E^o_{ij} is the energy of the core of the other (N-2) electrons,

and $H_{ij}(1,2) = F_{ij}(1) + F_{ij}(2) + \frac{1}{r_{12}}$, where $F_{ij} = F - R_i - R_j$ and F is the Fock operator.

Noting that the form of the correlated wavefunction used in the Appendix is unnormalized and $\langle\Psi|\Psi\rangle = 1 + \langle X|X\rangle$. Assuming a normalized correlation function, $\tilde{\mu}_{ij}(1,2)$, such that

$$\hat{\mu}_{ij}(1,2) = \lambda_{ij}\tilde{\mu}_{ij}(1,2) \quad (13)$$

we have

$$\tilde{\varepsilon}_{ij} = \left(1+\lambda_{ij}^2\right)^{-1} \left\{ \lambda_{ij}\left\langle |\psi_i\psi_j| \left| \frac{1}{r_{12}} \right| \tilde{\mu}_{ij} \right\rangle + \lambda_{ij}\left\langle \tilde{\mu}_{ij} \left| \frac{1}{r_{12}} \right| |\psi_i\psi_j| \right\rangle + \lambda_{ij}^2 \left\langle \tilde{\mu}_{ij} | H_{ij} + E^o_{ij} - E_o | \tilde{\mu}_{ij} \right\rangle \right. \quad (14)$$

Note from Burton 1988

2.8 Peripheral field dynamics of surface beats arising from coherent e-pair correlation: Quantum spin coherence

The multiplicative semi-classical pair-correlation function f(1,2) from Eq. 3 is to be identified in its angular behaviour **S** about an axis defining of spin orientation with the multiplicative fully quantum mechanical, constrained antisymmetric topology of singlet coupling given by Φ(1,2) from Eq. 4. Optimisation of the multiplicative interaction of the radial profile of pair correlation function's angular behaviour with the underlying orbital radial profiles is then a single parameter optimisation. This parameter is derived by Burton (1988; Equations 8-10) as ρ^2/a_H^2 where the off-axis distance scale parameter a_H reflects the both effective semiclassical magnetic moment of the partial electron disturbances linked in coherent counter-propagation in the singlet coupling and the counter-propagation frequencies of that coupling. Since the coupling is magnetic in character, higher effective self-consistent fields in the coupling draw the effective radius of the circumferential counter-propagation inwards to intersect a larger fraction of the electrons of the pair being subject to correlation mismatch.

This entirely explicit and variationally-determined form of peripheral correlation interaction within an e-pair is what we denote Quantum Spin Coherence.

Its primary signature in the introduction of circumferential beats transverse to the spin axis, in the form of a dynamic quadrupolar interaction arising from the spatio-temporal mismatch between the coherently correlated electrons of the pair. This beat phenomenon corresponds in turn to a conservative standing wave whose impact is to effect an oscillating, transverse, quadrupolar magnetic field oriented along the spin axis of the pair (see Figure 1). Arising from singlet coupling for which no magnetic field residue would be expected in first order, this higher order side effect of pair correlation is an unprecedented form of diamagnetic field. Derived from very small fractions of electronic charge subject to interactive coupling in the correlation, the corresponding diamagnetic field is expected to represent one of the weaker fields of atomic physics.

The QSC model has one more surprise: the *ground state* of the pair correlation is what is being determined by the above identification with the conventional singlet coupling topology. Higher harmonics of this correlation stabilisation of the e-pair are possible.

2.9 The possibility of a spectral manifold of higher order harmonics of the singlet-coupled spin wavefunction for each e-pair

Burton (2009) saw several implications of the basic QSC model. In particular, as a physically large bound electron pair, He looks capable of subtending an extensive spectrum of singlet-coupled higher spin harmonics, for which evidence may in due course be found.

In the helicity equation model, a uniform magnetic field is assumed to apply to the electronic wavefunction. We can however imagine the two electron version of He represented in this manner beginning with zero spin coupling, in identical spherical orbital forms for each electron 1s(1) and 1s(2). A minor fluctuation on the surface of one electronic wave-function will have an immediate polarising impact on the independent second electron, to generate a counteracting fluctuation (Maxwell's equations) in the space-time form of the second electron's wave-function. Two counter-propagating disturbances will resolve into a set of interaction harmonics in the circumferentially bounded system, of which the fundamental has the form already given by Eq. 1[6].

The *higher harmonics* of this ground state singlet spin interaction have to my knowledge never before been contemplated. These will correspond semiclassically to smaller fractional-electron and more angularly intersected two-electron mismatch resonances, converging to the HF-SCF (zero spin) limit, as the effective fractional electron subject to mismatch diminishes asymptotically through the higher manifold states of this harmonic spectrum.

The spectral manifold of standing wave or harmonic representations of pair correlation, is bounded by the exact ground state (conventional or fundamental mode of singlet coupling) of the pair and the completely uncorrelated (HF-SCF) representation, where the effective correlation stabilisation from minuscular coherent correlation mismatch in the higher harmonics converges to zero. These figures are illustrated in Table 1A. where HF-SCF and exact ground state estimates for He $(1s)^2$ are shown.

The He ground state correlation energy of 1.1439eV or 9227cm^{-1} is located as the fundamental spin-coupling mode of the QSC stabilisation w.r.t. the uncorrelated HF-SCF representation of the electron pair (the latter being a purely electrostatic model of the e-pair). On the assumption that higher harmonics intersects less of the bulk of the e-pair distribution, and so represent both engagement of smaller fractional electronic charge and greater radial distance off-axis of the effective correlation, Table 1B. indicates via a semiclassical, first-order series how one might anticipate the spectrum of this manifold.

3. History of spin & spinors

Schrödinger (1931) associated the 'Zitterbewegung' (or *jitter*, an intricate internal structure of the electron) of the Dirac formulation with spin. According to Barut & Zanghi (1984) more than fifty years later: 'historically spin was introduced as a classically indescribable two valuedness,' but 'spin is the angular momentum of the Zitterbewegung.' For the

[6] The orientation of the circumferential counter-propagation and the resulting non-spherical quadrupolar beats (Fig. 1) about the axis of an appropriate atomic |L, S> coupling scheme, implies the need for a compensating sphericalisation of the two-electron wavefunction by a J = 0 rotational wavefunction.

A. Helium e-pair energies for $(1s)^2$ / mE_h

vdW well			-0.063
ε_C		-42.04	*0.150%*
E_{exact}	-2903.74	*1.448%*	*0.0022%*
$E_{HF\text{-}SCF}$	-2861.70		

ε_C	42.04 mE_h	e_{vdW}	0.06 mE_h
	1.1439 eV		0.0017 eV
	9227 cm^{-1}		14 cm^{-1}

B. Helium e-pair spin-harmonics for $(1s)^2$ / cm^{-1}

n	Nominal	ΔE (1hv) excitations	Level spacing	QSC harmonics N		e-pair correlation	ΔE (2hv) excitations
1	-1.000	-				S=0 resonances	
2	-0.250	**-9226.7**		2	-0.250	**-9226.7**	**-9.227**
3	-0.111	-4100.7	*5.126*			4100.7	
4	-0.063	**-2306.7**	***6.920***	4	-0.063	**2306.7**	**-2.307** ***6.920***
5	-0.040	-1476.3	*7.750*			1476.3	
6	-0.028	**-1025.2**	***8.201***	6	-0.028	**1025.2**	**-1.025** ***8.201***
7	-0.020	-753.2	*8.473*			753.2	
8	-0.016	**-576.7**	***8.650***	8	-0.016	**576.7**	**-577** ***8.650***
9	-0.012	-455.6	*8.771*			455.6	
10	-0.010	**-369.1**	***8.858***	10	-0.010	**369.1**	**-369** ***8.858***
11	-0.008	-305.0	*8.922*			305.0	
		{…}		…	…	**…**	**…** **…**
	{SCF}	0.0	*9227*	0	{SCF}	0.0	{limit} ***{9227}***

Table 1. **A**. Electron correlation energy of He $(1s)^2$ electronic singlet configuration. **B.** QSC model of spin-coupled harmonics projected to lie between the uncorrelated SCF limit and the fully quantum-spin-coherent correlation of He $(1s)^2$. The lowest bound state of the spin-harmonic manifold (see Fig. 1) can be identified with the optimally correlated pair (N=2), providing a pair-correlation 'stabilisation energy' ε_c of the constructive interference between ground state singlet coupled spin functions. The distance in energy below the uncorrelated HF-SCF orbital energy of other successively less correlated spin-harmonic states lie in a manifold which converges to the asymptotic state that lacks symmetry breaking i.e. the HF-SCF orbital pair. In the case of circular boundary conditions, the manifold of excited states is determined—to first order—as $E_N = -\varepsilon_c/N^2$; N even.

zitterbewgung itself one has, following Huang (1952): 'the expectation value of the position (of a localized electron, includes) a time dependent part involving interference terms …between positive and negative energy states of the electron and represents the Zitterbewegung.' See also Barut & Bracken (1981) and Barut (1988).

3.1 Ongoing confusion about spin & spinors

Going back to the foundations of relativistic quantum mechanics (RQM), Dirac's (1928a, 1928b) original operator formulation, following Pauli's matrix algebra lead, produced *ab initio* both antimatter and a technical representation of spin, later named by Ehrenfest, as a *spinor*. In Tomonaga's (1974/1977) account, p.128-130, the two component wave functions so produced (a *large* part corresponding to the hydrogen-like orbitals, and a *small* part, rather ill-defined, representing the spin) correspond to spinors whose physical interpretation still remains unclear even today: spinors form a "mysterious tribe." According to M. Atiyah in Goddard (1998) celebrating Dirac: "unlike differential forms, which are related to areas and volumes, spinors have no such simple interpretation. They appear out of some slick algebra, but the geometrical meaning is obscure" (p. 113-4 in Goddard 1998).

Kutzelnigg (1984) attempted to apply orbital basis-set-expansion methods to Dirac's equations of motion, only to produce non-physical, non-bounded variational states, together

with states low in the continuum[7] which appear equally unphysical, in part due to the matrix representation of the Dirac equation in a finite basis not having the correct non-relativistic limit (Schrödinger limit) for $c \rightarrow \infty$.

Mathematically, spinors correspond to *double-valued representations* of the rotation group representative of particles of half-integral spin (i.e. fermions), and are neither vectors nor tensors. This lack of clarity on the physical or geometrical structure of - not just electrons but all fermions - in respect of spin (see again Atiyah in Goddard (1998) and Tomonaga (1974/1977)) follows Schrödinger (1927) himself, reflecting upon what is "missing" in his original hydrogen atom model:

> "in the language of the theory of electron orbits, the *angular momentum* of the electron round its axis, which gives it a *magnetic moment*. …[there is] no doubt that, by the paradoxical yet happy conception of the spinning electron, the orbital theory will be able to master disquieting difficulties which latterly have begun to accumulate [in modeling atomic spectra, including the Paschen-Back effect of line splittings in strong magnetic fields]... We shall be obliged to attempt to take over the idea of Uhlenbeck and Goudsmit (1926) into wave mechanics. I believe that the latter is very fertile soil for this idea, since in it the electron is not considered as a point charge, but is continuously flowing through space, and so the unpleasing conception of a "rotating point charge" is avoided. In the present paper, however, *the taking over of this idea is not yet attempted.*" [emphasis at end added; Schrödinger 1927, p.64.]

The continuing lack of a clear physical- or geometrical-model of spin[8] has remained like a cloud over particle physics, and has allowed (R)QM to suffer interminable stress as to its interpretation, no less that that enforced by the 'Copenhagen' interpretation being extended from single particle wavefunctions to those for multiple particles. Spin is surely modern physics' biggest single conceptual barrier: we know how it works; we just do not yet fully appreciate its physics.

3.2 Realisation of hidden variable theory with spin as a partial matter-wave

In the spirit of de Broglie & Einstein, Schrödinger (1926), Bohm & Bub (1966) and Bell (1987), our partial matter-wave formulation of spin leads directly to a one-parameter variational model of coherent correlation within each close-coupled e-pair. This model applies the mathematics of a freely propagating electron in a magnetic field to a quantum model of electron pairs. The QM helicity equations given by Landau & Lifschitz (1977) for a free electron in a homogenous field are taken as the template for the *radial* behaviour of the free electron.[9] For the *angular* behaviour, when applied to a non-propagating electron bound to a fixed nucleus, the model is developed with the aid of two assumptions.

The *first*, at last implementing Schrodinger's suggestion of modeling spin via the electron matter-wave itself, contemplates some to-be-determined 'volume' *fraction* of the electron matter-wave being subject to coherent circumferential disturbance. This fraction δ should correspond semiclassically to comparable fractions $\delta\mathbf{e/e}$ of the electronic charge and

[7] Where the 'uncoupled' or non-coherent spin representations of our Quantum Spin Coherence model would reside.

[8] As opposed to familiar mathematical-, topological-, Pauli matrix-, symmetry representation- or empirical angular momentum vector-representations of spin.

[9] This would generate an effective semi-classical orbiting frequency of 88.04GHz for a laboratory scale field of 1 Tesla, corresponding to a cyclotronic orbital radius of 36.26 nm.

fractions δ**m/m** of the electronic mass, so that the *ratio* between these, δ**e/**δ**m** maintains the same *whole* charge to *whole* mass ratio **e/m** which (following the Uhlenbeck & Goudsmit hypothesis) enters the helicity equations on the presumption that the *whole* electron is spinning. This fraction δ**e/e** = δ**m/m** is determined variationally by the shape of the radial function off-axis, which is determined to deviate from the multiplicative value of unity, only in the peripheral and polarisable outermost regions of the nuclear-centred electron.

The *second*, based upon two counter-propagating electrons, involves determining the *relative phase* of the lowest stationary state coupling between a m_s = + ½ and a m_s = - ½ oriented spin circulations, whose amplitudes are periodic over 4π, but whose relative angle values circulate for the pair in the real physical range of 2π.

The formal equation for the intra-pair correlation interaction is provided for the QSC model by Eq. 31, p.22 of Burton (1988), where the dynamic correlation is taken (following Hurley's prompting) to conform to a universal form, given here as Eq. 3 for ease of reference.

Consideration of the continuity boundary conditions over 2π around the periphery, and variation of the relative phase of the coupling, leads by way of *constructive interference* between the spins to an *l*=2, quadrupolar beat phenomenon in the circumferential periphery of the electron pair, orthogonal to the spin axis. The result of the *angular form* of the pair correlation formula for the least energy coupling in axially symmetric situations is essentially available by inspection, as the Figure 1 reveals.

In the absence of the QSC insight, a rather more elaborate computational strategy, via the appropriate RQM equations provided in their quaternion formulation of 'scale relativity' by Celeriere & Nottale (2003, 2005)[10], might be extended to fully accommodate the spin-spin interaction of QSC so long deleted (in advance) as lacking physical "significance" in Dirac's equation for the spin-spin-interaction of two electrons (Breit, 1932):

> 'The modification required consists in the removal of terms in e^4 in the result of eliminating the "small" components of the wavefunction. These terms do not involve *h* so that their physical significance is doubtful even for this reason alone."(Breit 1932, p.617) … "The coupling of motions of particles due to their interactions with transverse waves is small compared to that due to electrostatic forces."(p.621)

It remains true that in QSC these effects are small compared to coulomb interactions, but hardly insignificant: thus RQM calculations adopting the Breit Hamiltonian also ignore correlation effects See Whittaker (2007).

4. Interaction fields between QSC-correlated He atoms: Gravity?

Spectral theory suggests that the He spin-manifold is capable of propagating its field of influence relatively far. Burton (2009) suggested that cool astrophysically distributed He gas can mediate a cooperatively aligned physical interaction through the interstellar "aether" of He which orients the quadrupolar resonant form of individual singlet coupled He atoms, so forming a background electromagnetic field in which all 'matter' is bathed. Gravity thus could

[10] While the Celerier & Nottale's 'scale relativity' quaternion framework is not set up in a manner in which the current spinor model has obvious application, or vice versa, the framework admits of *deriving* the Schrödinger and Dirac equations as special cases, and also admits *non-differentiable* functions (such as our two-valued spin functions). I anticipate that the QSC model will represent a highly pre-diagonalised form of basis representation of equations accessible via Celerier & Nottale's equations of motion.

be a side-effect of basic chemistry in cool distributed gas clouds, and so be fundamentally quantum mechanical in origin: if so, it is also *emergent* in the history of the Universe.

4.1 The strange weakness of the gravitational background

It remains of outstanding current interest, many years after Einstein's (1916) formulation of the space-time topology of General Relativity, how gravity can be integrated with quantum mechanics (QM, now eighty five years old: Landau & Lifshitz 1977; Merzbacher 1970, 1992) in general and with the standard model at the *atomic* (QED) and *sub-nuclear* (QCD) levels of particle physics (Fritzsch 1992), also both decades old. The nature of the gravitational field, of relative scale forty orders of magnitude weaker than the coulombic force and – apparently - universally *attractive* between macroscopic bodies, continues to challenge particle theorists, whose 'strings' and 'branes' with 10-dimensional support seek to capture its elusive essence, so far without success. The apparently universal background force field of gravity, empirically identified by Newton more than three centuries ago and re-described as a topology in coupled space-time by Einstein almost a century ago, has remained *unexplained*[11] beyond attributing the action-at-a-distance force of unknown fundamental origin to the interaction of classical 'masses'. What is actually *causing* Einstein's curvature of space-time?

The modern focus of investigations on gravity itself include: (i) galactic modeling, which raises a question of deviation from perfect inverse-square behavior of the gravitational force field, or else the existence of some form of so-far unobserved (or identified) 'dark matter' throughout the universe[12]; (ii) the search for, observation of, and characterization of properties of massive interstellar gravitational 'black holes' which assume that gravity does not change in form at small distances; and (iii) the search for direct observational evidence of 'gravitational waves'.

So far, gravitational waves (GW) have eluded direct detection, although their existence has been inferred from measurement of the orbital decay of the binary neutron stars PSR 1913 + 16 (Taylor & Weinberg 1989). Two huge experimental consortia aimed at directly observing astronomical gravitational waves are currently underway, both focused on observing such *dynamic perturbations* to the gravitational background: LIGO[13] is just attaining its design sensitivity and discrimination to detect gravitational pulsation from binary pulsars such as PSR 1913 +16; and LISA[14], which spectrally complements LIGO, being readied for 2013 flight and aimed at detecting gravitational waves from galactic binaries and super-massive black hole binaries.

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[11] As David Hume in 1739 already recognized in *A Treatise of Human Nature*, of Newton's *Principia Mathematica*, that he advanced a description rather than an explanation of gravity. Einstein's topological reformulation of gravity into an observer independent tensor formulation of curved space-time does not escape the same charge.

[12] See Da Rocha & Nottale (2003) and Nottale (2004), who instead propose another explanation.

[13] Laser Interferometer Gravitational Observatory (Gustafson, Shoemaker et al.1999; Allen, Anderson et al. 2001); multiple earthbound laser interferometer pairs of up to 4 kilometre pathlength, positioned thousands of kilometers apart, with high signal-to-noise efficiency in the 10Hz-10kHz region. See Laser Interferometer Gravitational Wave Observatory, LIGO-T0100017-00-Z, www.ligo.caltech.edu, (23 Feb 2001); see http://www.ligo-wa.caltech.edu/ligo_overview/ligo_overview.html and http://www.ligo.caltech.edu/advLIGO/.

[14] Laser Interferometer Space Antenna (Tinto & Dhurandhar 2005); a giant triangulation of three identical spacecraft $5x10^6$ km apart, to observe and detect cosmic low frequency GWs not visible from earth, in the spectral region 10^{-4}Hz to 1Hz.

LIGO (version II) and the spaceborne LISA is designed capable of resolving changes of 1 part in 10^8 of an interference fringe relative to feedback-controlled dark-fringe resonance in the carrier 180W Nd:YAG 1064nm laser beams, so is capable of resolving differential GW impact on (30kg sapphire) test-masses situated remotely in each arm of the interferometer down to 10^{-19} m, i.e. a rather small part of a single atom's 10^{-15} m nuclear radius. They supposedly may also detect a 'continuous wave' background signal that comprised the Newtonian Background 'gravity gradient' of gravity. This could appear as a 'stochastic' source, a seemingly random waveform generated by a large number of weak, independent sources of gravitational radiation. One possible source of such a signal could be emissions from the early universe – the unthermalised gravitational equivalent of the cosmic microwave background radiation (CMBR). Searches in stochastic backgrounds are conducted by cross-correlating the outputs of two or more interferometers.

The *particle physics* complement of gravity, Higgs bosons exchanging information between masses, remain as yet unidentified[15], so we lack insight into the frequency domain of the Higgs field[16], although the *symmetry* of the interaction, by way of an especially intriguing (to this work) 'transverse quadrupolar' field, has been determined. No physical candidate for such dynamics has yet emerged from string theory and other models directed at incorporation of gravity into a unified four-fundamental-force 'theory-of-everything'.

One major issue is the relative strength of gravity in relation to the electromagnetic, weak-nuclear and strong-nuclear forces, given by the dimensionless scaling constants: $a_g \sim 3 \times 10^{-41}$; $a_e \sim 1/137$; $a_w \sim 1/30$, $a_s \sim 1/3$. So, while macroscopic inverse-square/curved space-time understanding of gravity is clear enough from its success in planetary and galactic modeling, in the context of fundamental QM and particle physics models, its attractive nature yet its extraordinary weakness remains deeply mysterious to science: one could say, as mysterious as consciousness itself[17].

4.2 From explicit spinor correlation in atomic He to Meso-Scale interstellar gravitation?

Rewriting Basic Physics of Spin: A geometrically specific spinor model in physical, matter-wave terms is devised. A *coherent analytical* model of electron-pair correlation is introduced, invoking the phenomenon of Quantum Spin Coherence (QSC) as a Virial-theorem-compliant – and computationally scalable -- correlation strategy in quantum chemistry. Superficial e-pair spin-coupling *beats* are identified as a *constructive interference* in coherent counterposed spin coupling as a consequence of the model. A spin-harmonic manifold of possible spin-coupled stationary states for (axially) symmetric e-pair is predicted. Novel electromagnetic force-fields, including a 'transverse, quadrupolar' pulsating magnetic field

[15] CERN's $2.3B Large Hadron Collider (LHC) has two 'general purpose' detectors, *Atlas* and the *Compact Muon Solenoid*, both of whose teams are aiming to identify the elusive Higgs boson. The Higgs boson, 'known as the "God particle" because of its importance to the Standard Model' [BBC commentary], provides an account in particle physics of why all other particles have mass.

[16] The Higgs mechanism is considered to fill all of space with a relatively uniform field, whose energy is regarded as the best candidate for the 'dark energy' of the Universe. 'Dark energy' is thought to make up the greater part (~70%) of the Universe, and be the 'cause' of the accelerating expansion of the Universe, following findings in 1998 by two teams studying supernovae.

[17] Burton, P.G. (2011). Human Cognition: higher brain function and the science of human consciousness. ISBN 9781456307400. See www.createspace.com/3494821

attending coherent e-pair correlation, are adduced, the latter being a form of diamagnetism, *dynamic diamagnetism*, which is a direct implication of the QSC model. This is a novel, attractive and resonant, form of diamagnetism limited to conspecific peer e-pair interactions.

The Special Role of He: Atomic helium is a major element in interstellar regions, and present in cool molecular clouds which are astrophysically significant in the formation of new stars. The QSC phenomenon of coherent correlation is particularly significant in the isolated e-pair case of ground state He $(1s)^2$ because, even though the correlation in the K-shell of all atoms has a similar magnitude (Section 2.8), the small positive charge on the He nucleus means that the electron distribution of this e-pair is especially large, and therefore able to subtend a more extended spectral manifold of harmonics of the fundamental singlet-coupled ground state configuration than from any other atom. This large size and high peripheral polarisability in the He case in turn means that the penetration distance of field interaction involving resonant information exchange between distant conspecific peer atoms is also unusually great.

He...He interaction: Isolated He atoms are completely isotropic (Footnote 6). However, once He atoms begin to weakly interact, their natural internal correlated structure, which in QSC is axially oriented, becomes 'exposed' by the interaction. The propagation of the correlation field of each e-pair acts to co-orient and so slightly stabilise the relative interaction. Specifically, the anisotropic interaction of the transverse quadrupolar beat phenomenon tends to co-orient interacting He atoms. Nearby He...He interaction is capable of collisional stabilisation to create a very weakly bound state of He_2 (Luo, McBane et al. 1993) which may amplify orientational alignment in the general He...He interaction field, but the model being proposed does not rely upon this potential amplification of the basic phenomenon. Quantum-spin-coherently sourced, dynamic diamagnetic interactions between e-pair peers are then active even in extremely dilute interstellar He at the direct & local (micro-), proximally co-operative (meso-) and regional source-aggregated (macro-) level of consolidation to form a cooperative and coherently implicative force field.

What is Mass?--from Spin Coherent Cooperativity to Gravity: Macro-level dynamic diamagnetic cooperativity sourced *chemically*, between e-pairs in He atoms, acts as a symmetry-compliant source--in fact the *fundamental explanatory source*--of the dynamics of the primary gravitational interaction. Implications for current searches for gravitational waves are considerable and implications of the quantum-spin-coherence model in particle physics, including the removal of 'mass' as an *intrinsic* property of matter, are to be noted.

5. Implications of the QSC model of spin & spin-pairing

The adoption and use of coherent partial matterwave electron representation of the spin component of spin-orbitals in chemistry would have many implications. It provides a new conceptual basis to:

1. Satisfy every equation in Landau & Lifschitz or Merzbacher texts on Quantum Mechanics on spin, by substituting fractional $\delta e/\delta m$ wherever e/m appears in the formula for the electron-magnetic moment.
2. Variationally optimise electron pair correlation as a coherent matter-wave phenomenon between opposing spins paired in each orbital (i.e. as a purely local, single parameter optimization), with results which, in contrast to most correlation algorithms, are

consistent with the requirements of the Virial theorem, yet scale reasonably with molecular size because of the intrinsically local nature of their impact.

3. Understand the electron magnetic moment at the first semiclassical level as a fractional electron, peripheral circulation effect $\delta e/\delta m = e/m$, and at a deeper quantum level, interpret the idea of any fundamental particle having as an empirical attribute something called mass being derived from the strength (low mass) or weakness (high mass) of that particle's interaction from the universal background field mediated astrophysically by distributed yet implicate He atoms.
4. Understand gravity (described but not explained by Einstein, 1916) as an intrinsically coherent, quantum-mechanical indirect interaction between apparent 'masses', whose effect is transmitted onto the local particle from implicate aggregation of field effects due entirely to (intrinsically stable, coherent correlations within) the electronic part of the wave function of remote He-bound spin- pair couplets. In this formulation, mass becomes a secondary and empirical result of engagement of any (electromagnetic) particle with a primary *dynamic diamagnetic* magnetic field interaction between distant but implicate electron peer pairs. The empirical appearance of mass is then understood as the result of implicate cooperation in a background micro-field alignment at the meso-scale, where each micro-field is essentially derived from QSC coupling in correlated e-pairs, and where at large or asymptotic distances the pulsating magnetic field lines are essentially collinear. In this formulation, there is little/no role/contribution of the (electronically shielded) *nuclear* 'hadrons' in aggregating such inertial drag on a particle, at least from nuclear-shielded neutral atoms: the effect is essentially *electronic* in its nature and being derived from atom-based interactions, *chemical* in origin.
5. Tidy up the unification of the four forces of physics, to bring gravity into a formulation of R(QM). This is goal Einstein couldn't see a way to reach, and which is not in principle possible to achieve, without his first having taken QM seriously enough in this context (see also item 12.) to understand that gravity could be *caused* by close-coupling in pair interactions. In this way, gravity is positioned as an *outcome* of quantum entanglement[18].
6. Convert to heresy the 'Copenhagen' dogma on non-deterministic QM interpretation, substituting a realized form of matter-wave spin following the heritage of Einstein, de Broglie, Schrödinger, Bohm & Bell, and in line with the present conjecture, describe exactly & precisely those few previously 'hidden' spin 'variables' that have been overlooked as a result of the repressively 'dogmatic' Copenhagen view (and along with it the persistent semiclassical, non- determined, determinantal interpretation) of QM.
7. Advance an account of the physical origin of the three colour forces in QCD (Fritzsch, 1992) as deriving from three complementary spatial orientations of spin interactions.
8. Develop new models the nature of the meson in the strong force, the neutrino in the weak force, and understand that the proton must not be immune from decay.
9. Predict the rest mass of the electron-antineutrino (0.575ev), as being displaced or decoupled from its coherent origin as a spin-only, low mass and low charge (virtual) partner in a coherently coupled fermionic correlation of an e-pair.
10. Understand that matter and antimatter is exactly in balance in our universe – that hadrons account for all the original positronic antimatter becoming captured in metastable QSC variant spin couplings with electron counterparts.

[18] In QSC, entanglement as *topology* becomes matter-wave *interaction*.

11. Recognise *dynamic* diamagnetism as a new fundamental force of nature, to account for the origin of an apparent, empirically attractive gravitational force, by being responsible ultimately for both internal 'mass' of any particle/ body/'matter'/planet/star/galaxy (i.e. drag w.r.t. the implicate background field) and, by directed difference, apparent gravitational forces between those bodies.
12. Quantum spin-coherence emerges, via the representational power of the 'ripple' model of spin, as a natural, principal and *determinable* solution of the 'small' parts of the quaternionic form of the relativistic quantum equations of motion, as provided by Celerier & Nottale (2003, 2005).

Predictions are also made concerning (a) the existence of, and (b) unique observational fingerprint of, hitherto unsuspected excited harmonics spin-states of electronic singlet coupling. These QSC spin harmonic states, occurring as previously unrecognized structure within the ground state electronic wave-function of an electron pair, are not yet observed. The special case of He $(1s)^2$, because of its size subtending an exceptionally large manifold of such harmonics, as illustrated in Table 1, and because of its ubiquity, becomes of outstanding astrophysical interest.

6. Directions for future research

The Quantum Spin Coherence model of the phenomenon of electron correlation entails a novel conception of realised electron spin and a new physical and geometric interpretation of the spinors of relativistic quantum mechanics. A simple and direct physical interpretation of the most fundamental Stern-Gerlach experiment arises, originated by the chaotic Zitterbewegung of an originally non-magnetised electron interacting with the inhomogeneous magnetic field to generate its magnetic moment. The fundamental philosophy of modern quantum theory is revised by this model, which defends a realization of the 'hidden-variables' matter-wave interpretation of quantum mechanics. The model is also defensible by consistency with two modern *ab initio* formulations of the applicable quaternion equations of relativistic quantum mechanics.

Three independently disprovable aspects of this reconception of spin and correlation are immediately apparent. Firstly, the ability to model individual filled-shell electron correlation by an essentially exact analytic model with a single variational dimension is available, whereby the *universality* of the pair correlation function f(1,2) suggested here can be assessed. The simplest test of the model itself is whether its prediction of the achievement of the exact energy of He $(1s)^2$ by this strategy is met. Secondly, a previously unrecognized quantisation and energy-state manifold in ground-state e-pair coherent spin coupling is predicated, including a manifold of states as I have predicted semiclassically for He. Direct spectroscopic transitions will fail to reveal this previously unsuspected intra-atomic manifold because of forbidden singlet-singlet selection rules, however more condensed states including liquid He (and especially He_2) may reveal previously unexpected atomic manifold structure in phonon bands in response to shock. Thirdly, the model predicts previously unsuspected coherent magnetic complement of a newly coherent QSC formulation of the weak dispersion interaction between e-pairs, despite their spin-singlet coupling which should (conventionally)close out the possibility of any residual magnetic interaction. Previously, dispersion interaction had been posed as being a rather chaotic interaction between instantaneous dipolar field arising in each structure. Along with a coherent, line-of-sight dipolar *electrical* interaction between remote e-pairs (corresponding to a revised understanding of the van der Waals interaction), a new kind of dynamic magnetic field provides a secondary, transverse, quadrupolar form of e-pair

interaction. This purely quantum phenomenon is called dynamic diamagnetism, and it is fundamentally *attractive* in nature, especially between otherwise identical coupled pairs, in contrast to all previously known forms of diamagnetism which give rise to repulsive forces of interaction, including the Meissner effect in superconductivity. Finally, the model predicts that both complementary fields of any e-pair interaction are fundamentally orientationally anisotropic. [The single exception lies in a hypothetical situation of an e-pair in perfect isolation, where the overriding J=0 rotational homogenization applies.]

In the QSC framework, gravity, apparently the simplest and certainly the first recognized of the four modern forces of nature, is derived as a force of purely quantum-mechanical origin. This result provides the first account of integration of all four forces in nature being quantum mechanical in origin. Einstein's approach (Davies 1995; Feynman 1998; White & Gribbin 2005) to developing a rapprochement between gravity and quantum theory, as though these were fundamentally independent of one another, thus could not have succeeded. Although the incorporation of relativistic concepts into quantum mechanics is *necessary* to explain gravity (through the phenomenon of electron spin and the implications of its singlet coupling) it has, until now, not been *sufficient* to explain gravity. It remains to the future therefore to consider appropriate formulation of the 'equations of matter-wave motion' in which the QSC model provides its insights without requiring the assumption of the empirical phenomenon of particle mass. However, it is extremely unlikely that the LHC design will ever see the ultra-weak signature of bound e-pair interactions.

In the QSC formulation of gravity, gravitational forces cannot be present at the origination of the Universe. Gravitational waves, as a composition of a stabilising gravitational background field and a multiplicity of dynamic perturbations from non-equilibrium meso-scale gravitational activity, are the current target of gravitational wave observatories, based upon laser interferometry. For the LIGO experiment, observations may well detect meso-scale perturbations relative to the background, but not the background itself, there being no gravitational complement of the CMBR in the QSC framework. The additional degrees of freedom in the forthcoming LISA experiment should be capable, subject to certain conditions, of observing the proposed intrinsic anisotropy of QSC gravitational forces at meso-scale.

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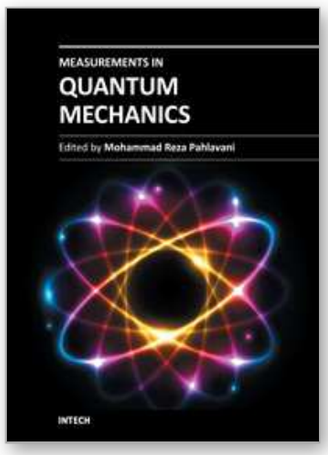

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