Angular Momentum in Chemistry

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Dedicated to Prof. Helgard G. Raubenheimer on the occassion of his 65th birthday

Noting that current chemical theory is based almost exclusively on electronic energy and spin variables the equal importance of orbital angular momentum is explored in this paper. From its classical definition the angular momentum of electrons in an atom is shown to obey Laplace's equation, which automatically leads to discrete values in terms of spherical harmonics. This analysis assumes a continuous distribution of electronic charge, which resembles a fluid at equilibrium. It serves to elucidate the success and failure of Bohr's conjecture and the origin of wave-particle duality. Applied to atoms, minimization of orbital angular momentum leads to Hund's rules. The orientation of angular momenta in lower-symmetry molecular environments follows from the well-known Jahn-Teller theorem.

Key words: Bohr Conjecture, Laplace's Equation

Introduction

Study of the physical world is made possible by the recognition of several fundamental symmetries. According to Noether's theorem each symmetry leads to the recognition of a *conservation law* [1]. In dynamical systems conservation of mass, energy, momentum and angular momentum derive from the assumed *homogeneity* and *isotropy* of space-time. Together with the conservation of electronic charge, which arises from the internal symmetry of the electromagnetic field, all of these conservation laws are of basic importance in the theoretical understanding of chemistry.

The conservation laws of mass and energy are the cornerstones of the theories of chemical composition and thermodynamics. The kinetic theory of gases relies on the conservation of linear momentum and the conservation of electronic charge underpins all models of chemical transformation. In contrast, the conservation of angular momentum is largely ignored, except by reference to electron spin, which is only one quantum-mechanical aspect of the total angular momentum of an electron. This omission leaves an unbridgeable gap in the theory of molecular structure and conformation, which has been a source of endless frustration for almost a century. The reason for this state of affairs can be traced to the uncritical embrace of an unreasonable model of directed chemical bonding that gained universal recognition in chemistry.

Angular Momentum

Angular momentum in classical mechanics is a vector quantity that describes rotational motion and must be of obvious importance for the understanding of electronic motion in atoms and molecules. The angular momentum vector that quantifies circular rotation of a particle about an axis is defined as the moment of the linear momentum, $\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$, *i. e.* the vector product of the linear momentum and the radius vector from the point of rotation. It is directed along the axis of rotation, perpendicular to the plane of rotation, and is positive in the direction that drives a right-handed screw (Fig. 1).

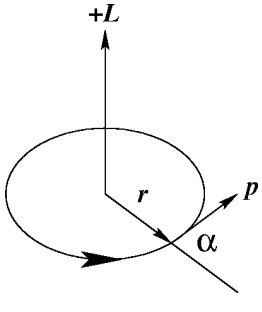

Fig. 1. Definition of the angular momentum vector.

The classical angular momentum vector decomposes into cartesian components. From the definition of

$$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p} = \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = \boldsymbol{rp} \sin\alpha \qquad (1)$$

simple vector algebra [2] defines the components of $\boldsymbol{L}$ as

$$L_x = yp_z - zp_y, \qquad (2)$$

$$L_y = zp_x - xp_z, \qquad (3)$$

$$L_z = xp_y - yp_x \qquad (4)$$

and

$$\boldsymbol{L}\cdot\boldsymbol{L} = L^2 = L_x^2 + L_y^2 + L_z^2. \qquad (5)$$

The moment of the force, or *torque* associated with temporal change of angular momentum, $\boldsymbol{N} = \partial L/\partial t$, is also defined as a vector product, $\boldsymbol{N} = \boldsymbol{r} \times (\mathrm{d}\boldsymbol{p}/\mathrm{d}t)$, in the same way as the angular momentum.

On analyzing the angular momenta of electrons in an atom another important factor comes into play. With the total positive charge concentrated at the point-like nucleus the electron density is considered to be in a central Coulomb field with rotation about a fixed point rather than an axis. In the absence of external torque, *e. g.* a magnetic field, the electronic charge on an atom constitutes a stable mechanical system. With all forces and torques in balance the angular momentum L therefore satisfies an equation like that of Laplace. Allowed rotational modes appear as the solutions to the angular-dependent part of the equation, the precise details of which depend on the assumed nature of the extranuclear electrons.

The Bohr conjecture

The most advanced model, that of quantum field theory, defines the electron as a zero-dimensional point particle. Its properties of mass, charge and spin are considered to be of mathematical significance only. Efforts to form a physical picture of the electrons are considered meaningless. Nevertheless, the first successful account of atomic structure was based on such a particle model and Bohr's conjecture that the angular momentum of an orbiting electron is quantized in units of $\hbar$.

The mystery of Bohr's conjecture and the calculation of Rydberg's constant, based on this conjecture, has never been resolved satisfactorily. The mystery consists therein that the quantum number (n), which quantifies the angular momentum

$$mvr = n\hbar \qquad (6)$$

is combined with the Coulomb potential $V = e\phi = -e^2/4\pi\varepsilon_0 r$ to yield the total energy

$$E = -\frac{Ry}{n^2} \qquad (7)$$

of the hydrogen ground-state electron in rydberg units. In reality however, the ground state requires values of $n = 0$ and $n = 1$ in eq. (6) and (7) respectively. The confusion arises from the fact that the quantum number of eq. (6) is the azimuthal quantum number m_l, whereas n of eq. (7) is the principal quantum number, and both of these are integers. The wrong assumption is that (6) refers to the hydrogen ground state. In fact, it simply defines the smallest unit of non-zero orbital angular momentum, $\hbar = mvr/m_l$, as equivalent to the angular momentum of a point particle of mass m and linear velocity v, in a circular orbit of radius r, about a fixed point. The energy of such a hypothetical point particle on a stable orbit defines the corresponding *rydberg* unit of energy,

$$Ry = \frac{me^4}{8\varepsilon_0^2 h^2} = \frac{me^4}{2(4\pi\varepsilon_0)^2\hbar^2}.$$

The Bohr model introduced the enduring concept of stationary quantum states and first defined fundamental concepts such as the bohr magneton, $\mu_B = e\hbar/2mc$ and the fine-structure constant, $\alpha = v_1/c = e^2/\hbar c \simeq 1/137$, still in common use. However, inability to extend the description to more complex atoms made it unacceptable as a chemical model. The unphysical definition of the stationary state in terms of an accelerated electron that fails to radiate, remained the major objection against the model.

Although this major problem could not be resolved Sommerfeld [3] extended the Bohr treatment to give reasonable accounts of atomic structure in general, the formation of chemical bonds and the periodic table of the elements. This was achieved by the introduction of elliptic orbits in line with Kepler's laws of planetary motion and widening of Bohr's conjecture by the formulation of quantum rules for periodic systems in

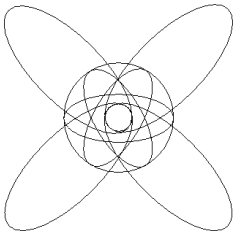

Fig. 2. Sommerfeld model of the neon atom in terms of four elliptic and four circular orbits, both types in tetrahedral array.

terms of action integrals such as $\oint p_k \mathrm{d}q_k = n_k h$, $k = 1,2,..,n$ = integer, where q and p are generalized coordinates and their canonically conjugate momenta. Use of these rules enabled the assignment of electronic, vibrational and rotational molecular spectra and predicts Bragg's law for the interpretation of diffraction phenomena.

Success of the Sommerfeld model was due to the introduction of two additional quantum numbers, required to describe elliptic orbits. The scheme is illustrated by the electronic structure that it proposed for the neon atom. Ten electrons, as shown in Fig. 2, are distributed over two shells, or energy levels, on sets of two and eight orbits respectively. The inner shell accommodates two electrons[1] while the second shell consists of four elliptic and four circular orbits, arranged in space, such that the total electronic angular momentum is quenched.

Quenching is achieved by directing the angular momentum vectors of the electrons on elliptic orbits towards the corners of a regular tetrahedron. Angular momentum vectors of the electrons on circular orbits are in turn directed to tetrahedral sites which complete the cube that also contains the corners of the first tetrahedron. For the carbon atom only the four equivalent elliptic orbits in tetrahedral array are occupied. By analogy with the Lewis-Langmuir model of electron-pair bonds, this predicted arrangement was argued with great effect, to account for the structure of aliphatic compounds. This proposition has turned out to be the most persistent legacy of the Sommerfeld model, although the sound principle of quenched angular momentum on which it was based, has been abandoned in modern theories of chemical bonding. The idea of defining tetrahedral orbitals by hybridization is an obvious attempt to emulate the attractive Sommerfeld construct, albeit at the expense of the fundamental principle of angular momentum conservation.

The need to introduce half-integer quantum numbers can now be seen to have arisen from inappropriate use of Bohr's conjecture, assuming non-zero angular momentum for electrons in *s*-states. This dilemma signalled the ultimate failure of Sommerfeld's model.

The unsuccessful Bohr-Sommerfeld model was based on the assumption that an orbiting particle provided the only possible source of electronic orbital angular momentum in an atom. A valid alternative is defined by a hydrodynamic model that pictures the electron as an ideal compressible fluid that surrounds the nucleus. At equilibrium, in a stationary state, the fluid appears incompressible, in accord with one of the pioneering interpretations [4] of the Schrödinger function, which has never been fully appreciated. In this model angular momentum derives from the hydrodynamic circulation, or vorticity, of the fluid, which is subject to the central Coulombic attraction [5] and becomes observable in an applied magnetic field. The components of vorticity, at equilibrium, are defined in terms of the components of flux, u, v, w as:

$$\xi = \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z}, \quad \eta = \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}, \quad \zeta = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}. \quad (8)$$

For an electron of mass m_e the relationship between vorticity and angular momentum follows from (2) as $\int \xi \cdot \mathrm{d}r(x,y,z) = L_x/m_e$, *etc.*

The continuity equation

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

through (8), implies the Helmholtz relation

$$\frac{\partial \xi}{\partial x} + \frac{\partial \eta}{\partial y} + \frac{\partial \zeta}{\partial z} = 0$$

and hence[2] a circulation potential ρ, which corresponds to an angular momentum that satisfies Laplace's equation.

Laplace's equation

Laplace's equation, in cartesian coordinates, reads

$$\nabla^2 V = \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = 0. \quad (9)$$

[1] The helium problem remained unsolved in the Sommerfeld scheme as quenching of the angular momentum of two electrons, both with quantum number $n = 1$ and together on the same circular orbit ($L_z = \pm\hbar$), requires them to orbit in opposite sense on a collision course. A tentative solution pictures the electrons as moving in phase on elliptic orbits with $L_z = \pm\hbar/2$, as shown in the diagram. This model, however crude, anticipated the description of two *s*-electrons with paired spins.

[2] Note that $\partial\rho/\partial x = \xi$, *etc.*

It describes the situation in which the potential has the least mean gradient. For instance, the condition $d^2y/dx^2 = 0$ requires only that the curve described by the moving point shall have zero curvature, *i. e.* $y = mx + c$, a straight line. The equation may be solved by separation of the variables under the assumption that the potential may be written as a product function

$$V = X(x) \cdot Y(y) \cdot Z(z) \tag{10}$$

in which X, Y and Z are functions of only one independent variable. On substitution of (10) into (9) and division by V, the equation becomes

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2} = 0. \tag{11}$$

Whereas the value of each term in (11) is independent of the other two, each of them must be equal to a constant, to give three equations of the type

$$\frac{d^2V}{dx^2} = KX.$$

Writing K as a squared quantity, $K = k_i^2$, each equation has a simple solution[3], such that

$$V(k_1, k_2, k_3) = e^{k_1x + k_2y + k_3z}, \tag{12}$$

$$k_1^2 + k_2^2 + k_3^2 = 0. \tag{13}$$

These solutions describe both the distribution of charge density as well as the orbital angular momentum states of electronic charge on the atom. Without loss of generality it is sufficient to consider only the one-electron case of hydrogen-like atoms. In this instance it makes no sense to consider the electron as a point particle, but rather as unit charge, symmetrically distributed over the available space that surrounds the nucleus [1, 7]. Eq. (13) shows that the three separation constants cannot all be real numbers, except for three equal constants of zero, which imply $L = 0$, the state of spherical symmetry, quantum-mechanically known as an *s*-state. The case of two zero constants will later be shown not to be allowed quantum-mechanically, and classically it corresponds to the Bohr model of the H ground-state electron on a circular orbit with $L_z = \hbar$.

Of particular interest is the case where one of the constants (k_3 say) is equal to zero. To satisfy (13) the remaining two must be complex quantities, giving solutions

$$X = c_1 e^{\pm kx}, \quad Y = c_2 e^{\pm iky}.$$

Solutions of (9) follow as

$$V_k = c_1 e^{\pm k(x \pm iy)}, \tag{14}$$

$$V_z = c_2 z + c_3. \tag{15}$$

These equations describe the components of angular momentum on an arbitrary scale that depends on the value of k. Non-zero $\pm k$ implies electronic rotation, in either direction, on a plane perpendicular to $\boldsymbol{L}$. The total angular momentum vector is directed at an arbitrary angle, θ, with respect to Z and it may be considered as precessing about Z as shown in Fig. 3. The z-component, L_z, has a fixed value, but the components L_x and L_y are variable and depend on the azimuthal angle φ.

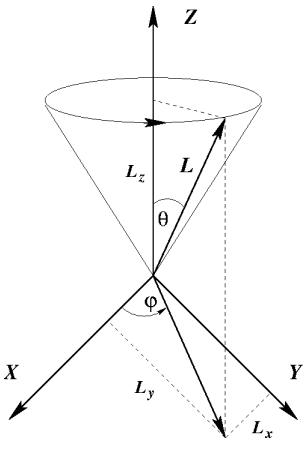

Fig. 3. Cartesian components of angular momentum $\boldsymbol{L}$.

On writing the Laplacian in spherical polar coordinates it consists of a radial part and an angular part, Λ^2, such that

$$\nabla^2 = \frac{1}{r^2}\left\{\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \Lambda^2\right\}, \tag{16}$$

$$\Lambda^2 = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2}\frac{\partial^2}{\partial\varphi^2}. \tag{17}$$

The angular momentum evidently depends on Λ^2 only. Separation of the variables is achieved by writing the potential as the product function $V = R(r) \cdot \Theta(\theta) \cdot \Phi(\varphi)$, first multiplied by $r^2 \sin^2\theta$ and divided by V to isolate the azimuthal function, with separation constant m^2.

[3] The roots of the auxiliary equation $D^2 - k^2 = 0$ are $\pm k$. Hence $X = c\exp(\pm kx)$.

Hence

$$\frac{\sin^2\theta}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right)+\frac{\sin\theta}{\Theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)=m^2, \quad (18)$$

$$\frac{\mathrm{d}^2\Phi}{\mathrm{d}\varphi^2}=-m^2\Phi, \quad \Phi=ce^{\pm im\varphi}. \quad (19)$$

Single-valued solutions for (19) require that $\Phi(\varphi) = \Phi(\varphi+2\pi)$ which implies integer m. Eq. (18) is next divided by $\sin^2\theta$, to give

$$\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right)=c, \quad (20)$$

$$\frac{1}{\Theta}\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)-\frac{m^2}{\sin^2\theta}+c=0. \quad (21)$$

Eq. (21) is recognized as Legendre's associated equation, in which the separation constant $c = l(l+1)$ ensures well-behaved solutions for integer l [2]. Written in the form

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2}+l(l+1)Y=0. \quad (22)$$

Eq. (22) is the general differential equation of spherical surface harmonics of integral order and finite over the unit sphere. At the surface of a sphere of constant radius $r = a$, $\mathrm{d}V/\mathrm{d}r = 0$, the first term of the Laplacian (16) vanishes and the remainder reduces to (22).

Any solution V_l of Laplace's equation of degree l is called a solid spherical harmonic, and has the form $V_l = r^l Y_l^m(\theta,\varphi)$. After separation of variables there are $2l+1$ independent functions $Y_l^m(\theta,\varphi) = \Theta(\theta)\cdot\Phi(\varphi) = Ne^{im\varphi}P_l^m(\cos\theta)$ for each value of l. For $r = 1$, $V_l = Y_l^m$ so that Y_l^m is the value of the solid harmonic at points on the surface of the unit sphere defined by the coordinates θ and φ, and hence Y_l^m is called a *surface harmonic* of degree l. Surface harmonics are orthogonal on the surface of the unit sphere. The associated Legendre polynomials $P_l^m(\cos\theta)$ have $l-m$ roots (zeros). Each of them defines a nodal cone that intersects a constant sphere in a circle, which defines a constant latitude. These nodes are in the surface of the sphere and not at $r = 0$, as commonly assumed in the definition of atomic orbitals. Surface harmonics are undefined at $r = 0$.

A moment's reflection on the geometry outlined in Fig. 3 suggests that the total angular momentum L^2 is described by Y_l^m and the projection L_z by (19). This surprising result shows that classical theory predicts the angular momentum of an electron on an atom as restricted to discrete values depending on the integers l and m. Only the units are lacking and the success of the Bohr model of the atom consisted in correctly guessing the unit of angular momentum quantization as $\hbar$. The guess implies that $L^2 = -\hbar^2\Lambda^2$ and transforms eq. (17) into the eigenvalue equation

$$L^2Y_l^m(\theta,\varphi)=l(l+1)\hbar^2Y_l^m(\theta,\varphi) \quad (23)$$

which defines the allowed values of $L^2 = l(l+1)\hbar^2$. Likewise

$$L_zY_l^m=m\hbar Y_l^m \quad (24)$$

defines the eigenvalues of the Z-component of angular momentum.

The fact that these values agree exactly with the quantum-mechanical results is hardly surprisingly seeing that Schrödinger's amplitude equation

$$\nabla^2\psi=-\frac{2m}{\hbar^2}(E-V)\psi \quad (25)$$

is the appropriate modification of Laplace's equation that leads to the correct quantization of the kinetic energy $(T = E-V)$ and angular momentum.

Hydrodynamic Model

It remains to be demonstrated that the hydrodynamic model correctly predicts the same numerical results as the Bohr model. In order to produce a stable atom it is necessary, as before, to assume that an electrostatic force of attraction be balanced by some other force, presumably of quantum-mechanical origin[4]. Whatever the nature of this force, it should be of the same magnitude as a classical centrifugal force. Assuming the negative charge to be effectively concentrated at a radial distance r from the nucleus, the force balance requires that

$$\frac{e^2}{4\pi\varepsilon_0 r^2}=\frac{m_e v_\varphi^2}{r}=\frac{p^2}{m_e r} \quad (26)$$

i. e. (dropping subscripts)

$$\frac{1}{r}=\frac{me^2}{4\pi\varepsilon_0(pr)^2}.$$

[4] Identified in Bohmian mechanics as the quantum potential.

This r should not be interpreted to define a circular orbit. Conservation of energy requires

$$E = T + V = \frac{1}{2}mv^2 + V = \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{2r} - \frac{1}{r}\right) = -\frac{me^4}{2(4\pi\varepsilon_0)^2(pr)^2} = -Ry\left(\frac{1}{n^2}\right). \quad (27)$$

The last equality is inferred from the spectroscopic Rydberg formula,

$$\Delta E = Ry\left(\frac{1}{n_1} - \frac{1}{n_2}\right),$$

for integer n_i. Noting that Planck's constant $h = 2\pi\hbar$ has units of angular momentum (Js), an obvious way of introducing the quantum-mechanical interaction and establish the Rydberg formula is by substituting, with Bohr, $pr = n\hbar$ in (27), to give

$$E = -\frac{me^4}{2(4\pi\varepsilon_0)^2 n^2\hbar^2} = -\frac{me^4}{8\varepsilon_0 n^2 h^2} = -Ry\left(\frac{1}{n^2}\right) \quad (28)$$

with the correct value of Rydberg's constant. It is important to understand that the final expression (28) for total energy does not imply non-zero angular momentum of the ground state.

The dynamic model for hydrogen, assumed here, is equivalent to the hydrodynamics of a liquid globe with free surface, around a gravitational nucleus, used in the analysis of tidal waves [5]. During free motion of the system surface elements of fluid undergo simple harmonic oscillation along a normal coordinate. These surface oscillations represent the infinite sum over all surface harmonics of integral order. They combine to form progressive waves that travel over the surface with no change in form. The motion of surface elements keep in step, passing simultaneously through their equilibrium positions. Any free motion may be simulated by superposition of the surface modes with a proper choice of amplitude and phase. One of the simplest solutions represents a system of standing waves, which in the case of an electron, leads directly to the condition $2\pi r = n\lambda$, $n = 0, 1, \ldots$ that, combined with De Broglie's relation $\lambda = h/p$, produces the Bohr conjecture, $pr = nh/2\pi$.

Oscillations at the surface of a sphere are properly described by the spherical surface harmonics, $Y_l^m(\theta,\phi)$, *i. e.* those harmonics that satisfy Laplace's equation on the surface of a sphere. The surface harmonic $Y_1^0 = \sqrt{3/4\pi}\cos\theta$ is shown on the left in Fig. 4.

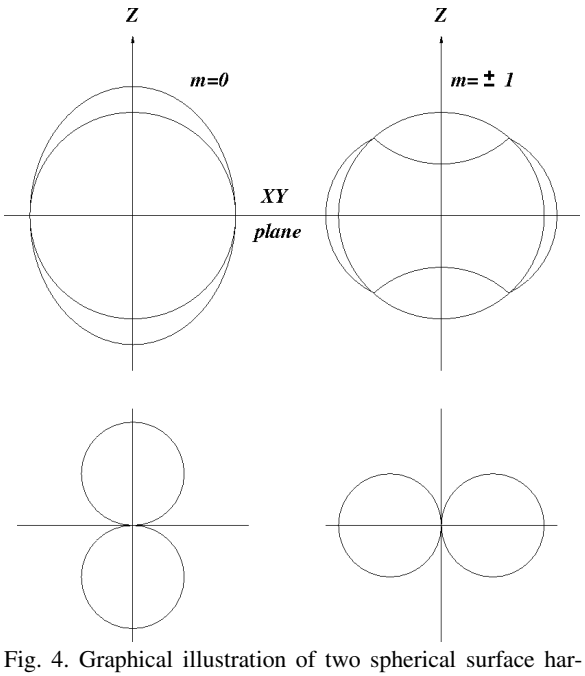

Fig. 4. Graphical illustration of two spherical surface harmonics on the unit sphere. The lower part of the diagram shows the mapping centred on a point at $r = 0$. In all cases 3D images require rotation about Z.

It has a node along the equator. $Y_1^{\pm 1}$ is on the right. In hydrodynamics surface oscillations are linked to a velocity potential due to a point source at the origin [5].

Electronic structure

Resolution of the Bohr paradox depends on the assumed nature of an electron. It is intuitively clear that any such picture should be more detailed than the zero-dimensional point-particle of elementary-particle physics, or the alternative notion of pure wave motion. It seems self-evident that the definition of an entity, which occurs in a void as either particle or wave, requires that it has substance. The alternative is that it exists in a substantial medium. In this case the ultimate description of matter, when analyzed beyond the elementary-particle level, must correspond to a distortion of, or an inhomogeneity, in the vacuum, assumed to be a continuous fluid, or aether. An object such as an electron is therefore considered made up of the same homogeneous stuff as the aether and owing its unique features to characteristic wave patterns that occur in its interior or at its interface with the vacuum.

A completely free electron, considered as a highly compressible fluid, will presumably be of infinite extent and its most prominent property will be the wave

motion. A closely confined electron resembles a mechanical particle with less obvious wave properties. In all intermediate situations both wave-like and particle-like properties may be observed.

Bohm interpretation

A consistent quantum theory of matter and motion, based on Madelung's hydrodynamic analogy, adapted by Bohm [6], has been developed. By substituting a wave function in polar form, $\Psi = R\exp(iS/\hbar)$, Schrödinger's equation is decomposed into

$$\frac{\partial R^2}{\partial t} + \nabla \cdot \left(\frac{R^2 \nabla S}{m} \right) = 0, \tag{29}$$

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} - \frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} + V = 0. \tag{30}$$

Madelung interpreted R^2 as the density $\rho(\boldsymbol{x})$ of a continuous fluid, which has the stream velocity $\boldsymbol{v} = \nabla S/m$. Eq. (29) becomes a continuity equation, $\partial\rho/\partial t + \mathrm{div}(\rho\boldsymbol{v}) = 0$, and (30) determines changes of the velocity potential S in terms of the classical potential V and a quantum potential

$$V_q = -\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R} = -\frac{\hbar^2}{4m}\left[\frac{\nabla^2\rho}{\rho} - \frac{1}{2}\left(\frac{\nabla\rho}{\rho} \right)^2 \right],$$

arising in the effects of internal stress in the fluid.

In his interpretation Bohm emphasized that in the classical limit ($V_q \to 0$) eq. (30) reduces to the classical Hamilton-Jacobi equation. It is further argued that, by analogy, eq. (30) defines an ensemble of possible trajectories of a particulate electron, for which a definite trajectory is predictable if an initial position can be specified. This interpretation gives equal weight to particle and wave aspects. The electron moves like a mechanical particle guided by a wave, but the association between particle and wave remains artificial. The main advantage is recognizing the role of the quantum potential to emphasize the holistic nature of quantum systems. The Bohm interpretation adds nothing to quantum formalism and all conclusions, although less obvious, still hold in terms of conventional theory.

Madelung interpretation

All models, from Bohr to Bohm and beyond, have a problem with the assumed particle nature of electrons. Madelung's proposal, in its original form, has, for the same reason, never been taken seriously. Despite the claim that the hydrodynamic model is in all respects equivalent to that of Schrödinger, Madelung [4] admits that a continuous distribution of electronic charge density presented an intractable problem with respect to the interaction between charge elements. Like the molecules that make up macroscopic fluids he seems to be looking for sub-electronic particles to make up the electron. This is an unnecessary assumption. For an electron without parts quantum units of charge, mass and spin indivisibly belong to the total electron [7], without internal self-interaction. Non-classical behaviour exists in the flexibility of the electron.

Any fermion could be seen as a topological chiral knot in the fabric of space-time. It changes shape in interaction with its environment and disperses in the form of a boson on contact with an enantiomer. The centre of mass follows the trajectory which Bohm assigns to a particle. Bohm's pilot wave is no more than harmonic undulation in the interior of the electron, which undergoes perpetual rotation in spherical mode. As suggested by Madelung electrons that come into contact do not fuse together like bosons. They may appear to interpenetrate, but change their shape to avoid one another; they never coincide and maintain individual integrity.

A proton, because of its different wave structure is more massive and less flexible than an electron. When these particles meet the electron wraps itself around the proton under the electrostatic attraction directed towards the proton. This interaction modifies the electronic wave structure and effective size of what is now described as an atom. In interstellar space where it exists as a *rydberg atom* it has dimensions orders of magnitude larger than, for instance, in a terrestrial hydrogen plasma. At the effective surface the wave pattern follows the surface harmonics, consistent with the angular momentum and excitation of the electron. Orbital angular momentum is observed in a magnetic field $\boldsymbol{B}$ where the electron is subject to a vector potential $\boldsymbol{A}$ in addition to the scalar potential $e\phi$, such that eq. (30) becomes [10]

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\nabla S - \frac{e}{c}\boldsymbol{A} \right)^2 + e\phi - \frac{\hbar^2\nabla^2 R}{R} = 0.$$

In hydrodynamic analogy the flow velocity, as in

$$m\boldsymbol{v} = \nabla S - \frac{e}{c}\boldsymbol{A}$$

is no longer irrotational; $\mathrm{curl}\,\boldsymbol{v} = -(e/mc)\boldsymbol{B}$. Because

of the wave pattern orbital angular momentum and energy of the electron assume only those discrete values allowed by the integers associated with the wave pattern. This behaviour of the electron is conveniently described by Schrödinger's equation.

Quantum model

The quantum-mechanical description of angular momentum follows from substitution of the operator equivalent of classical momentum, *e.g.* $p_x \rightarrow -\hbar i\partial/\partial x$ into eqs. (1)–(4). As the order of multiplication is important in vector products, the operator components

$$\hat{L}_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

etc., do not commute amongst themselves. The commutators, such as $(L_x, L_y) = (L_xL_y - L_yL_x)$, are nonzero and have the values $(L_x, L_y) = i\hbar L_z$, $(L_y, L_z) = i\hbar L_x$, $(L_z, L_x) = i\hbar L_y$. It means that more than one component can never be measured simultaneously. The commutation properties of orbital angular momenta is a nonclassical effect arising from the Lévy-Leblond (LL) quantum condition [11], $L_z = \hbar m$, which is also the basis of the Bohr conjecture. This condition is as fundamental as the Planck-Einstein and De Broglie conditions, $E = \hbar\omega$, $p = \hbar k$, which respectively specify quantized energy and linear momentum.

The quantum operators lead directly [2] to the eigenvalue eqs. (23) and (24) for a central field. If L_z, the eigenvalue in a central field, is known, L_x and L_y remain unidentified within the limitation

$$L_x^2 + L_y^2 = L^2 - m^2\hbar^2 = \left[l(l+1) - m^2\right]\hbar^2$$

The maximum allowed value of $m = l$ shows that, always, $L_z < L$. It is therefore impossible to have $L_x + L_y = 0$, a situation identified before as the Bohr model.

The eigenfunctions of L^2 and L_z are the spherical harmonics $Y_l^m(\theta, \varphi)$. The first few of these, in normalized form, are

$l = 0$, *s*-state:

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}, \tag{31}$$

$l = 0$, *p*-state:

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\cdot\frac{z}{r}, \tag{32}$$

$$Y_1^{\pm 1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\varphi} = \mp\sqrt{\frac{3}{8\pi}}\cdot\frac{x \pm iy}{r} \tag{33}$$

like (14) and (15) for $k = 0, \pm 1$.

The chemical implications of the LL condition are as dramatic as those of the P-E and DB conditions. It shows that only one of the real eigenfunctions L_x, L_y and L_z is defined at any instance. The common practice of using linear combinations of so-called "real orbitals" to describe "directed chemical bonds" is therefore forbidden by fundamantal quantum theory. Structural chemists will have to look for an alternative principle that defines molecular shape. The quenching of orbital angular momentum, as pointed out by Sommerfeld [3], is such an alternative.

Atomic Structure

All quantum-mechanical atomic models are based on solution of Schrödinger's equation for an electron in the field of a stationary proton, *viz.* eq. (25) with $V = -e^2/4\pi\varepsilon_0 r$. The eigenvalues of total energy, L^2 and L_z, respectively, are ordered in terms of the quantum numbers $n = 1, \ldots; l = 0, 1, \ldots, (n-1); m_l = -l, \ldots, +l$. Bound states are those with $E < 0$. The single electron on the H atom is assumed to be at the lowest ground-state energy level, $n = 1$, $l = m_l = 0$. The experimental finding that this state was doubly degenerate meant that at least one more eigenfunction was needed to describe the behaviour of the electron.

Electron spin

The so-called spin variable that accounts for the observed degeneracy enters [8] the Schrödinger theory through the factor $i\hbar$ in the time-dependent equation

$$\left(i\hbar\frac{\partial}{\partial t} - H\right)\Psi = 0 \quad (\Psi = \psi e^{-iEt/\hbar}). \tag{34}$$

On substituting from (23) it follows that

$$\left(\frac{\hbar^2\nabla^2}{2m} - V\right)\Psi = -i\hbar\frac{\partial\Psi}{\partial t}$$

or in terms of a squared Schrödinger operator for a free particle $(V = 0)$,

$$S^2\Psi = \left(\frac{\hbar^2\nabla^2}{2m} + i\hbar\frac{\partial}{\partial t}\right)^2\Psi = 0.$$

The complex square root of S^2 does not exist and a linear form such as

$$S = \left(2mi\hbar\frac{\partial}{\partial t}\right)A - (i\hbar\nabla) + C$$

becomes meaningful only if A and C are defined as square matrices. The immediate effect of such formulation [2] is that the wave function need to be defined as a row vector, called a spinor,

$$\Psi = \begin{pmatrix}\psi_+\\ \psi_-\end{pmatrix},$$

which represents different (spin) angular-momentum states. Spin, like orbital angular momentum, is also described by two quantum numbers, but unlike l and m_l these are half-integer numbers. Total spin has eigenvalues of $s(s+1)\hbar^2$, $S = \sqrt{3/4}\hbar$, and multiplicity $2s+1 = 2$, for $s = 1/2$, as found experimentally. Spin components, *e.g.* $S_x = m_s\hbar \quad (m_s = \pm 1/2)$ obey the same commutation rules as the components of L.

The first theoretical account of electron spin was provided by the relativistic wave equation of Dirac. Consequently, it is often stated that spin, or intrinsic angular momentum, is a quantum and/or relativistic property. This conclusion is not warranted. A more convincing physical model is based on the hydrodynamic model outlined above.

It remains to be explained how an inhomogeneity in the aether, said to constitute an electron, manages to move about freely without getting entangled with the environment. One possible mechanism is through spherical rotation of the region that defines the electron. The effect of axial rotation is to wind up the connecting medium until it shears and develops a surface of discontinuity. During spherical rotation the interconnecting medium relaxes after every 4π cycle and does not shear. The rotating electron neither transmits nor receives rotational energy, but is surrounded locally by a medium that undergoes cyclical wave motion. This undulating region constitutes the spin. The fact that the symmetry group of spherical rotation also satisfies the spinor version of both Dirac's equation [9] and Schrödinger's equation [1] provides final support for the proposed hydrodynamic formulation of electron spin.

The appearance of electron spin indicates that the conservation of atomic angular momenta must involve both orbital and spin angular momenta and the conserved quantity their vector sum $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$.

Energy levels

The spin quantum number $s = 1/2$ for all one-electron states, while the magnetic spin quantum number has the possible values $m_s = \pm 1/2$, defining states of equal energy. The doubly degenerate ground state of the hydrogen atom therefore has the configuration denoted by $1s$ and characterized by the quantum numbers $n = 1$, $l = 0$, $m_l = 0$, $m_s = \pm 1/2$. The first and second excited states are the doubly degenerate $2s$ state, $(n = 2, l = 0, m_l = 0, m_s = \pm 1/2)$ and the six-fold degenerate $2p$ state, $(n = 2, l = 1, m_l = 0, \pm 1, m_s = \pm 1/2)$, a total of 8 electronic states with $n = 2$. Likewise, for $n = 3, 4$, *etc.* there are 18, 32 *etc.* possible states.

The reasonable expectation that the ground state of all more-electron atoms should also be the $1s$-state is not confirmed by spectroscopic analysis. It is found instead that no more than two electrons of any atom can share the $1s$ level. Likewise, a maximum of 6, 10 or 14 electrons can share the degenerate p, d or f levels of a given atom. Detailed analyses have shown that this distribution is a manifestation of a more general fundamental rule known as the exclusion principle, which applies to all sub-atomic entities with non-integral spin, known as *fermions*. It requires the total wave function, with space and spin parts, to be anti-symmetric with respect to particle exchange.

To understand the electronic configuration of an atom it is sufficient to note the equivalent formulation of the exclusion principle, that no more than two electrons on the same atom can have the same set of four quantum numbers n, l, m_l, m_s. In principle the electronic energy for each set of allowed quantum numbers can therefore be calculated from Schrödinger's radial equation:

$$\frac{\mathrm{d}^2\psi(r)}{\mathrm{d}r^2} + \frac{2m}{\hbar^2}\left[E_n - V(r) - \frac{l(l+1)}{2mr^2}\right]\psi(r) = 0.$$

For an atom of atomic number Z, the term $V(r)$ represents the potential energy of the electron in the field of the nucleus and the $Z-1$ other electrons. The calculation of $V(r)$ is not a trivial operation and the interpretation of electronic energy and angular momentum no longer follows the hydrogen pattern, which only applies in an approximately central potential field. In the hydrodynamic model however, electrons at deep energy levels should be constrained in their motion and

m_l / σ	−2	−1	0	1	2
1			↑		
2	↑		(↑↓)		↑
3	↑		↑		↑
4	↑	↑		↑	↑
5	↑	↑	↑	↑	↑
4	↑	↑	↑↓	↑	↑
3	↑	↑↓	↑	↑↓	↑
2	↑	↑↓		↑↓	↑
1	↑↓	↑↓	↑	↑↓	↑↓
0	↑↓	↑↓	↑↓	↑↓	↑↓

Fig. 5. Spin orientation in d-multiplets with up to 10 electrons in spherical atoms that obey the exclusion principle. The pair in brackets represent the unlikely alternative singlet state. The spin count is defined as $\sigma = 2\sum m_s$.

those at the highest (valence) level would still find themselves in a central potential field of an atomic core, which is equivalent to having an effective positive charge at the nuclear position. The energy and angular momentum of only the valence shell are therefore adequately described in terms of hydrogenic quantum numbers.

Based on the previous conclusion it is possible to rationalize the electronic structure of the first 20 elements and the general ordering of all elements of the periodic table.

Spin ordering

A conspicuous feature of the electronic configuration of atoms, not determined by energy calculations based on n and l only, namely the relative spin orientation of valence-shell multiplets, is correctly specified by Hund's empirical rules: "The first $(2l+1)/2$ electrons on a given energy sub level have the same spin orientation. Addition of more electrons causes stepwise pairing of spins". The same predictions are seen to follow from the assumption that all atoms are spherically symmetrical and therefore have zero resultant angular momenta. This condition is satisfied if one of an odd number of electrons that constitute a multiplet has $m_l = 0$ and all others occur as pairs with $\pm m_l \neq 0$. Given n, l and m_l, the spin orientation m_s (up or down) is controlled by the exclusion principle, as demonstrated for the two-electron system in the d-multiplet $l = 2$) shown in Fig. 5. In this case there are two possibilities consistent with zero orbital angular momentum, for an even number of electrons, a singlet state with paired spins at $m_l = 0$ and a triplet state with $m_l = \pm 2$ (say). Only the triplet state has antisymmetric space functions, which imply that the probability density tends to zero as the electrons approach a common position. The Coulomb repulsion is therefore lower for the triplet state than for the singlet state, which has a wave function symmetric in space coordinates.

The predicted spin ordering for all multiplets of a degenerate d-state, shown in Fig. 5, is consistent with Hund's rules.

Molecular Structure

It is known from chemical practice that atoms join up to form electrically neutral molecules consisting of positively charged nuclei dispersed in an electronic fluid. Like the surface of a free electron or atom, the outer surface of a molecule will also tend to define a minimum gradient that satisfies Laplace's equation, albeit in an environment of lower symmetry. Although the solutions are no longer the spherical harmonics of a central field, they still characterize a minimum angular momentum, commensurate with the highest symmetry allowed by intramolecular interaction.

To anticipate the geometrical distribution of atomic nuclei in a molecular interior it is necessary to consider the realignment of spherical harmonic angular-momentum vectors in the field of multiple nuclei. A closely related problem was considered by Jahn and Teller [12] (JT) who formulated a theorem that clarifies several issues around the prediction of molecular shapes.

Jahn-Teller theorem

JT investigated the effect of electronic orbital degeneracy on the symmetrical nuclear configurations of polyatomic molecules. Any molecule has a continuous set of configurations consistent with a given symmetry. Among these one equilibrium configuration of minimum energy is stable with respect to all totally symmetrical displacements, *i. e.* those which do not disturb the symmetry. However, this configuration is not necessarily stable against all other types of nuclear displacement, not if the electronic energy for neighbouring conformations depends linearly upon any of the nuclear displacements. By analyzing the motion of a single electron in the respective fields of three colinear nuclei and of four nuclei in square-planar array, it is demonstrated that linear and non-linear molecules respond in fundamentally different ways to nuclear displacement.

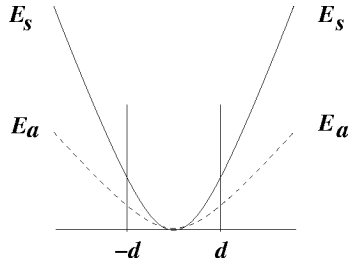

Fig. 6. Energy change on symmetrical and antisymmetrical distortion of trinuclear arrangement with angular momentum degeneracy.

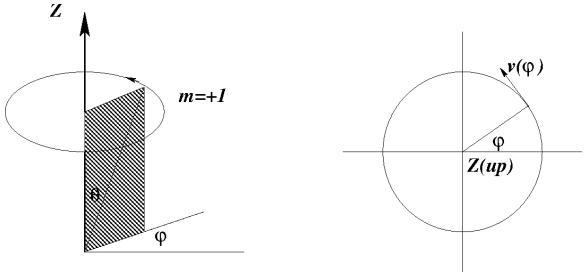

Fig. 7. Illustration to demonstrate the rotation of an orbital angular momentum vector.

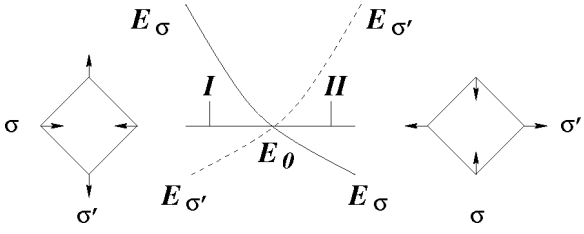

Fig. 8. Energy changes on in-plane symmetry breaking in a square-planar arrangement with electronic orbital degeneracy.

The states of the electron are classified as σ, π or δ for orbital angular momentum projections of 0, ±1, ±2 (in units of $\hbar$) along the polar axis, which is not in an arbitrary direction, but is fixed by symmetry. The σ states are non-degenerate, while the π, δ, *etc.* states are each two-fold degenerate, corresponding to either clockwise or anti-clockwise rotation of the electron about the polar axis. For the trinuclear molecule an unsymmetrical displacement can, without loss of generality, be considered as displacement of the central nucleus by a distance d perpendicular to the nuclear axis. This displacement destroys the axial symmetry and removes the degeneracy. Each degenerate state splits into two states, one symmetrical with respect to reflection in the plane of the nuclei and the other antisymmetrical with respect to the same plane. These states have different energies E_s and E_a. As the nuclear displacement is varied these states and their energies change continuously, but their symmetry remains. Displacements of d and $-d$ result in the same state and energy, as shown in Fig. 6. The energies E_s and E_a are even functions of d, and all that is required for stability with respect to nuclear displacement is that the function be positive in both cases. This condition is assured by the orbital angular momentum, which is therefore responsible for stabilizing the linear arrangement. The effect of displacement is to change the alignment of the angular momentum vector $L_z = m\hbar$ associated with the eigenfunction $e^{\pm im\varphi}$, shown in Fig. 7. To change the direction of L_z requires work against kinetic energy and consequently the angular momentum acts like a gyroscope to realign the vectors.

As a counter example the motion of a single electron in the field of a square-planar arrangement of four identical nuclei is considered. In the previous example the total wave function was generated by rotation of the angular-momentum eigenfunction in any half-plane (shaded in Fig. 7) about the polar axis, *i. e.* multiplication by $e^{im\varphi}$. In the square-planar arrangement four half-planes rotate together about the four-fold symmetry axis, with $-\pi/2 \leq \varphi \leq \pi/2$ for $m = \pm1$. The displacements shown in Fig. 8 may be regarded as positive and negative values of the same nuclear displacement. This nuclear displacement reduces the four-fold symmetry to two-fold. The degenerate state splits into two states Φ_σ and $\Phi_{\sigma'}$, the first with angular momentum projected perpendicular to the symmetry plane σ and the second perpendicular to σ'. Because the configurations *I* and *II* are equivalent the energies E_σ and $E_{\sigma'}$ are related, such that

$$E_\sigma(I) = E_{\sigma'}(II)$$

and *vice versa*. As seen from Fig. 8 the energy levels cross at the energy E_0 of the undisplaced configuration. There is no symmetry reason which precludes a linear dependence of the energy levels upon the nuclear displacement in the neighbourhood of E_0, and the square-planar configuration can in general not be a stable equilibrium configuration.

The results obtained from the two illustrative examples were generalized by examination of the pathways of allowed symmetry breaking for all relevant symmetry point groups, excluding those of complete axial symmetry. It was found that all non-linear nuclear configurations with an orbitally degenerate one-electron

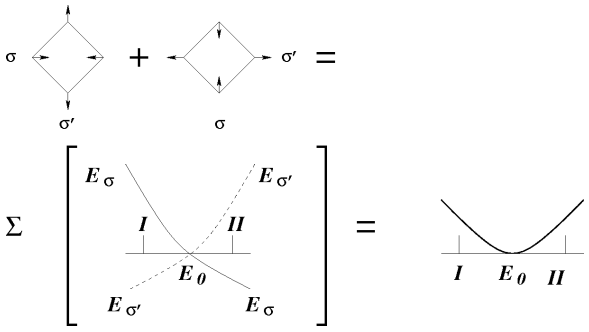

Fig. 9. Diagram to demonstrate the stability of an electronically non-degenerate square-planar system against distortion.

state are unstable against some normal displacement, not the totally symmetrical.

Non-degenerate states

One aspect of Jahn and Teller's theorem which is repeatedly emphasized in the chemical literature is the distortion of symmetrical molecules with one-electron orbital degeneracy. These cases are the exceptions to a general rule which is rarely emphasized nor applied to problems of molecular conformation. The rule applies wherever the pair of degenerate levels $(\pm m_l)$ accommodate two electrons, with total electronic energy $E_\sigma + E_{\sigma'}$ as shown in Fig. 9. The total conformational energy in this case has a minimum at E_0 which stabilizes the symmetrical arrangement of nuclei. The reason for this stabilization is hinted at, but not explicitly stated by JT. It relates to the electronic orbital angular momentum.

Orbital angular momentum arises from the rotation of electronic charge about axes that depend on the environment, represented by either an applied magnetic field or the polarization by ligand nuclei that surround the reference atom. The total angular momentum, which is the vector sum of the individual contributions, reduces to zero if the component charge rotations occur in opposite sense with respect to a single axis of rotation. The angular momentum is said to be quenched and the corresponding minimum kinetic energy of rotation stabilizes this symmetrical situation.

In a free atom the electrons move in the symmetrical central Coulomb field of the nucleus and the angular momenta of electrons at a degenerate pair $(\pm m_l)$ of energy levels is quenched identically. For an atom in a molecule the spherical symmetry is broken and the angular momentum vectors are redirected as demanded by the symmetry of the molecular environment. The

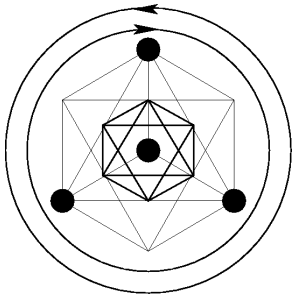

Fig. 10. Diagram to demonstrate the quenching of orbital angular momentum in the methane molecule. Magnetic moments cancel in projection along each possible H-C polarization direction, because of *p*-electron charges rotating in opposite sense, as shown.

principle of minimum orbital angular momemtum still implies that the favoured conformation will be of a symmetry that quenches the orbital angular momentum.

The symmetry groups considered by JT are all of the type that quenches the orbital angular momenta of electrons derived from free-atom energy levels that constitute degenerate pairs $(\pm m_l)$ in a spherically symmetrical environment. The only molecules excluded from the set are those without any symmetry, *i. e.* the *chiral* molecules. An important consideration is that chiral molecules have residual orbital angular momentum in projection along a polar direction, *e.g.* an applied magnetic field. The JT distortions consist of spontaneous breaking of molecular symmetry by a normal displacement that introduces an interaction, which lowers the energy of the system, without affecting the polar projection of the angular momentum[5]. JT distortion therefore does not cause optical activity.

Molecular shape

The central JT theme describes the relationship between the symmetry and stability of non-linear molecules, analyzed as a function of orbital degeneracy. This, somewhat misleading terminology, refers specifically to degenerate states available for one single electron. The enormous volume of more recent work devoted to the study of JT effects [13] focusses exclusively on vibronic interactions at symmetry-related degenerate intersections on potential energy surfaces. The more common and more important prediction of symmetrical structures stabilized by non-degenerate angular momentum states is largely forgotten.

The first step in the formation of a molecule is to consider a given atom as surrounded by a number of non-interacting secondary atoms, or ligands, which is

[5] As for free atoms the unpaired electron has an effective magnetic quantum number $m_s = 0$.

also the assumption of crystal field theory. The energy and angular momentum of the primary atom are conserved, but differently distributed, depending on the symmetry of the secondary shell of atoms. These quantities are still the eigenvalues of an atomic Schrödinger equation, in a central field modified by interaction with the secondary shell. To first approximation it is correct to assume that the orbital angular momentum is conserved in magnitude, but not in orientation. The JT approach is to modify the central-field description of energy and angular momentum eigenvalues in terms of the representations of each symmetry group concerned. It is almost axiomatic to assume that the arrangement of identical ligands around a central atom should be of the highest possible symmetry; like assuming a spherical shape for free atoms. According to JT the resulting molecular structure automatically ensures quenching of the orbital angular momentum. Introduction of unlike ligands lowers the symmetry, which remains sufficient to quench the angular momentum, until no two ligands are alike. This property has been demonstrated [14] to produce a tetrahedral structure for methane. It relies on the presence of two p-electrons on the free carbon atom, with $m_s = \pm 1$.

The significant new result is that the p-electron density should rotate in sets of parallel planes, perpendicular to the lines connecting H and C nuclei. For fixed nuclei these planes intersect in points that define regular octahedra, shown in Fig. 10 for two different spacings with respect to the central carbon nucleus. The smaller octahedron is defined by midpoints of the lines connecting the hydrogen nuclei. The larger one contains the hydrogen positions, on the black dots. Uncertainty associated with the circulation radius is sensitive to the chemical nature and electronegativity of the ligands.

Qualitatively however, the prediction is well in line with the various criteria for the definition of atomic shape based on charge-density distribution [15] and reflects the statement of the author:

> In reality, chemical bonding is a molecular property, not a property of atomic pairs.

Many larger molecules resemble an assembly of unsaturated fragments consisting of the symmetrical cellular units of the methane type, after removal of one or more ligands, *e.g.* CH_3, CH_2, *etc.* When such fragments combine to form saturated molecules their relative orientation in the final product must ensure that the orbital angular momentum stays quenched.

[1] J. C. A. Boeyens, *New Theories for Chemistry*, Elsevier, Amsterdam, **2005**.

[2] J. C. A. Boeyens, *The Theories of Chemistry*, Elsevier, Amsterdam, **2003**.

[3] A. Sommerfeld, *Atombau und Spektrallinien*, 4th ed., Vieweg, Braunschweig, **1924**.

[4] E. Madelung, *Quantentheorie in hydrodynamischer Form, Z. Physik*, **1926**, *40*, 322 – 326.

[5] H. Lamb, *Hydrodynamics*, 6th ed., Cambridge, University Press London, **1957**.

[6] D. Bohm, *A Suggested Interpretation of Quantum Theory in terms of "Hidden" Variables, Phys. Rev.* **1952**, *85*, 166 – 193.

[7] J. C. A. Boeyens, *Structure of the electron, Trans. Roy. Soc. S. Afr.* **1999**, *54*, 323 – 358.

[8] C. J. H. Schutte, *The Theory of Molecular Spectroscopy. Volume I*, North-Holland, Amsterdam, **1976**.

[9] E. P. Batty-Pratt and T. J. Racey, *Geometric Model for Fundamental Particles, Int. J. Theor. Phys.* **1980**, *19*, 437 – 475.

[10] T. Takabayashi, *On the Formulation of Quantum Mechanics associated with Classical Pictures, Prog. Theor. Phys.* **1952**, *8*, 143 – 182.

[11] J.-M. Lévy-Leblond, *Quantum heuristics of angular momentum, Am. J. Phys.*, **1976**, *44*, 719 – 722.

[12] H. A. Jahn and E. Teller, *Stability of Polyatomic Molecules in Degenerate Electronic States, Proc. Roy. Soc. (Lond.)* Series A, **1937**, *161*, 220 – 235.

[13] I. B. Bersuker, *Modern Aspects of the Jahn-Teller Effect Theory and Applications to Molecular Problems, Chem. Rev.* **2001**, *101*, 1067 – 1114.

[14] J. C. A. Boeyens, *Quantum Potential Chemistry, S. Afr. J. Chem.* **1999**, *53*, 49 – 72.

[15] P. G. Mezey, *Shape in Chemistry*, VCH, New, York **1993**.