Despite the great power and scope of modern computers, there remains yearning for intuitive, pedagogically appealing ways to understand electronic structures in atoms, molecules, and more complicated systems. Niels Bohr’s century-old model, in which electrons parade around atomic nuclei much like planets orbit the Sun, retains such appeal. In its historical context, the Bohr model managed to elucidate the hydrogen-atom spectrum and thereby gave great impetus to the birth of quantum mechanics.1–4 But it proved incompatible with quantum theory, which found that the ground state of the H atom was spherically symmetric and had zero orbital angular momentum, contrary to Bohr’s assumption of a planar, circular electron orbit with angular momentum $\hbar/2\pi$, specified by Planck’s constant. Even so, today the Bohr model has valid roles in describing highly excited Rydberg atoms,5 cavity quantum electrodynamics,6 and quasi-Rydberg states in graphene.7

From early on, Bohr’s model was considered to fall far short of his earnest aim to provide a physical basis for chemical bonding. Helge Kragh states, “Bohr’s original and most ambitious project of establishing a common theory for atoms and molecules—one that would be of equal significance to physics and chemistry—turned out to be a failure” (see the article by Kragh in PHYSICS TODAY, May 2013, page 36; quote, page 41). A few years ago, however, redemption arrived.8–10 Bohr’s model was found to emerge from the Schrödinger equation in the limit of infinitely many dimensions, where quantum mechanics morphs into classical mechanics.11 Here we revisit Bohr’s H-atom model to show how his postulates conform to quantum theory in its infinite-dimension limit. With that perspective, we take a fresh look at Bohr’s treatment of the H$_2$ molecule. Simple extensions of his molecular model, requiring just elementary algebra, turn out to give potential-energy curves, for both the H$_2$ ground electronic state and several excited states, that agree well with those obtained from highly accurate ab initio quantum mechanical computations done with supercomputers. Further examples...
illustrate that a rudimentary Bohr-like model also gives respectable results for electronic geometry of multielectron atoms. All told, at its centennial, his model deserves a recently bestowed accolade:12 “Bohr’n again.”

Bohr’s hydrogen atom

In his 1911 doctoral thesis dealing with the electron theory of metals, Bohr concluded that classical physics could not explain why electrons bound in atoms behaved differently from those carrying current. That led him to embark on a postdoctoral stint with J. J. Thomson, the discoverer of the electron, at Cambridge University in England. Naive and brash, Bohr was disillusioned when parts of his thesis critical of Thomson’s classical theory failed to arouse interest at Cambridge.

Bohr retreated to Manchester in March 1912 to work with Ernest Rutherford doing experiments that probed how much energy alpha particles lose as they traverse matter. That began an intense, mutually supportive, lifelong friendship.13 (Figure 1 shows them at a sporting event.) Rutherford had published his discovery of the atomic nucleus nearly a year before, but it was not yet taken seriously; Thomson’s “plum-pudding” atomic model, which presumed positive tidbits were sprinkled among rings of electrons, was still in vogue. By May Bohr had switched to theory, prompted by his recognition of why a previous treatment of alpha-particle energy loss was inadequate. His thesis had prepared him to spot the fault: Electrons had been treated as free rather than bound in atoms. Hence, almost inadvertently, Bohr came to focus on finding an electronic architecture that would be compatible with the nuclear atom model.

In July Bohr submitted to Rutherford a seven-page manuscript, referred to since as the Manchester or Rutherford Memorandum. Precursor to the three long papers—dubbed the trilogy—that Bohr published a year later, the memorandum emphasized two key problems with the nuclear model. In classical mechanics, the centrifugal force on an orbiting electron is balanced by the coulombic attraction to the nucleus. But the classical orbits became unstable when populated with more than one electron. Moreover, nothing in classical physics determines orbital radii or frequencies. Bohr proposed to introduce a hypothesis, as yet speculative but in-

Bohr’s model predictions for the orbits of electrons (red dots) in molecular hydrogen, superimposed on electron-density distributions (curves) obtained from quantum mechanical calculations. The distances along the molecular axis $z$ are given in atomic units, where 1 a.u. is equal to the Bohr radius $a_0$; blue dots represent nuclear positions. Results are shown for $H_2$ in the electronic ground state with internuclear distances (a) $R = 0.8$ and (b) $R = 1.4$, corresponding to configurations I and II, respectively, depicted in figure 3a. The Bohr-model calculations assume that the pair of electrons rotate synchronously with a constant distance of separation and a fixed dihedral angle of 180°. Although such orbits don’t exist in quantum mechanics, the locations of the Bohr orbits correspond roughly to the maxima in the electron probability distributions. (Adapted from ref. 8.)
volving Planck’s constant, from which he could determine specific allowed orbits. He frankly acknowledged that he considered it hopeless to try to justify such a hypothesis.

In part 1 of his trilogy, Bohr developed four versions of the hypothesis. His concluding and most familiar version invoked stationary circular orbits specified by quantized orbital angular momentum, \( L = n\hbar \), with \( n = 1, 2, 3, \ldots \). Introducing that quantum constraint into classical expressions, Bohr derived the radii \( r_n = (n^2/2Z)\alpha_0 \) and energies \( E_n = -(Z^2/2n^2)\alpha_0^2 \) of the allowed orbits for a one-electron atom. The quantity \( \alpha_0 = \hbar^2/m_e^2 \) was soon christened the Planck constant, \( m \) is the electron mass, \(-e\) the electron charge, and \( Z \) the atomic number.

Bohr’s simple formula for the energy levels \( E_n \) was a spectacular success. It gave quantitative agreement with the H-atom spectral series seen in laboratory experiments and in stellar observations, and it predicted other spectral lines that were soon verified. It also identified the Fe⁺ ion from stellar spectral lines that had been mistakenly attributed to atomic hydrogen.

**Superseded by quantum theory**

Although impressed with Bohr’s success, many contemporary scientists were offended by his blithe introduction of amenable postulates. Yet three of his key postulates were destined to become pervasive in quantum mechanics. Foremost was his concept of stationary states, although bereft of electron orbits. Another was his assertion that an electron in the lowest-energy stationary state, the ground state \((n = 1)\), does not emit radiation. That was contrary to classical electrodynamics, which would require an orbiting electron to continuously radiate energy and spiral into the nucleus.

Likewise fundamental was Bohr’s attribution of spectra to radiation emitted or absorbed in transitions between stationary states, with spectral-line frequencies determined by the energy difference between states. That, too, contradicted classical electrodynamics by disconnecting the frequencies appearing in spectra from those of mechanical motions of either of the communicating states. As a consequence, Bohr was led to his correspondence principle, which says that the close approach of stationary states at high energies renders classical and quantum frequencies nearly the same at large \( n \).

Bohr’s H-atom model enjoyed further success for about a dozen years. Especially impressive were extensions in 1916 by Arnold Sommerfeld. He included elliptical orbits and found the energy levels remained the same as those obtained by Bohr. He then added relativistic mechanics, which produced fine structure in agreement with observations. Also striking was the result of the celebrated 1922 experiment by Otto Stern and Walther Gerlach, underlain to test the Bohr model (see the article by Bretislav Friedrich and Dudley Herschbach, PHYSICS TODAY, December 2003, page 53). The experiment determined, to within 10% error, the magnetic moment of a silver atom. (That moment is due to the atom’s single valence electron.) The result

\[ E_n = (-\frac{Z^2}{2n^2}) \alpha_0^2 \]

in customary atomic units. (Distance is in units of the Bohr radius \( a_0 \) energy is in Hartree units \( \alpha_0^2 \) via the relationship \( r = \hbar \alpha_0^2/2m_e \), the equation can be recast in terms of \( \phi \), the radial probability amplitude:

\[ -\frac{1}{2} \frac{\partial^2}{\partial r^2} \phi + \left( -\kappa \frac{\Lambda(\Lambda + 1)}{r^2} - \frac{Z}{r} \right) \phi = E \phi. \]

Thereby the sole D-dependence appears in the centrifugal potential, where

\[ \Lambda = \ell + (D - 3)/2 \]

replaces the orbital angular momentum quantum number, and the principal quantum number becomes \( n + (D - 3)/2 \).

**Box 1. Relating Bohr to Schrödinger**

For a one-electron atom with nuclear charge \( Z \) and orbital angular momentum \( \ell \) in D-dimensional spherical coordinates, the radial Schrödinger equation is:

\[ -\frac{1}{2}\partial^2 \phi/\partial r^2 + \left( -\frac{\kappa}{r} - \frac{Z}{r} \right) \phi = E \phi. \]

in customary atomic units. (Distance is in units of the Bohr radius \( a_0 \) energy is in Hartree units \( \alpha_0^2 \) via the relationship \( r = \hbar \alpha_0^2/2m_e \), the equation can be recast in terms of \( \phi \), the radial probability amplitude:

\[ -\frac{1}{2} \frac{\partial^2}{\partial r^2} \phi + \left( -\kappa \frac{\Lambda(\Lambda + 1)}{r^2} - \frac{Z}{r} \right) \phi = E \phi. \]

The transcriptions for \( n \) and \( \ell \) enable all properties of D-dimensional hydrogenic atoms to be readily related to those for D = 3. Shown here, for instance, are the radial probability distributions \( |\psi|^2 \) for ground-state atoms with \( D \) between 2 and 100. Each curve is normalized with respect to its maximum, at \( r_{\text{max}} = (D - 1)/4Z \). The ground-state energy is \( E_0 = -2Z^2/(D - 1)^2 \).

Scaling the radial coordinate via \( r \rightarrow (D - 1)/2r \) and the energy by \( E \rightarrow (2/D - 1)^2E \) transforms the ground-state wave equation into

\[ \left(-\frac{2}{D - 1} \frac{\partial^2}{\partial r^2} + \frac{1}{2} (D - 3) \frac{1}{(D - 1)^2} - \frac{Z}{r} \right) \phi = E \phi. \]

In the limit \( D \rightarrow \infty \), the derivative term is quenched, and the wave equation reduces to

\[ E(r) = 1/(2r^2) - Z/r, \]

which is equivalent to the Bohr-model hydrogen-atom energy function. The minimum of \( E(r) \) determines the large-D limit for the scaled location and energy in the ground state: \( r = 1/Z \) and \( E = -2Z^2 \).

Thus far, only the radial wave equation has been considered. The angular part is separable, and for the ground state its wavefunction is spherically symmetrical. However, the D-dimensional volume element contains a factor \( \sin^D \theta \), so for \( D \rightarrow \infty \), the polar angle will be restricted to \( \theta = 90^\circ \). Hence, in the large-D limit, the electron distribution corresponds to the planar circular orbit of the Bohr model.

For other atoms or molecules, D-scaling proceeds in essentially the same way. Via the \( \psi \rightarrow \phi \) transformation, the Schrödinger equation is recast so that the explicit D-dependence appears solely in the centrifugal energy, always as a simple, quadratic factor.\(^{10,11}\)
which agreed with that predicted from classical electrodynamics for an electron rotating in a circular orbit with angular momentum $\hbar$, was hailed as compelling evidence for the Bohr model.

By 1926 the advent of quantum mechanics and the discovery of spin had discredited Bohr’s model. Although the predicted H-atom spectrum, including the fine structure, was not altered, the principal quantum number was redefined to be $n = l + k + 1$, where $l$ and $k$ are the number of angular and radial nodes in the wavefunction—are both zero for the ground state. The fine structure, was not altered, the principal quantum number was redefined to be $n = l + k + 1$, where $l$ and $k$ are the number of angular and radial nodes in the wavefunction—are both zero for the ground state. The Stern–Gerlach result had to be modified to creating actual Rydberg states with large $n$, the Bohr model applies nicely. Such an atom can be treated as hydrogenic, because the lone excited electron is far away from its home base, which has a net effective charge of $+1$ due to shielding of the nucleus by the nearby electrons. For large $n$, especially for states with few radial nodes, the Schrödinger equation indeed gives results that agree with the Bohr picture: The excited electron moves in a planetary orbit with radius proportional to $n^2$ and energy proportional to $n^2$.

**Dimensional scaling**

As applied to electronic structure, dimensional scaling is not at all exotic, although it is borrowed from quantum chromodynamics. (See the article by Edward Witten, PHYSICS TODAY, July 1980, page 38.) The procedure operates in a space in which all vectors have $D$ Cartesian coordinates. It involves generalizing the Schrödinger equation to $D$ spatial dimensions and rescaling coordinates and energy to absorb generic $D$-dependence. For the simple case of the H atom, the $D$-dependence is exactly known and the principal quantum number becomes $n + (D - 3)/2$. (See box 1.) Consequently, for large $D$, the scaling of the electron radius becomes proportional to $D^2$ and scaling of energy proportional to $D^2$. Thus going to large $D$ for fixed $n$ is equivalent to creating actual Rydberg states with large $n$ at fixed $D = 3$.

Taking $D$ to infinity with $n = 1$ converts the wave equation into the ground-state Bohr-model energy function. In particular, the centrifugal term representing Bohr’s orbiting electrons naturally appears in the infinite-$D$ limit, even for states with no orbital angular momentum. That seeming paradox (which might have delighted Bohr!) is accommodated by $D$-scaling. In the large-$D$ limit, the electrons are not orbiting but rather sitting still at fixed locations corresponding to the minimum of the energy function.

**Figure 3. The Bohr molecule.** (a) In his model of the hydrogen molecule, Niels Bohr proposed that both electrons (1 and 2) traced a shared orbit around the molecular axis $z$, as shown in configuration I. (Here $R$ is the distance between the two protons, A and B, and $\rho$ is the orbital radius.) But his formulation allows two other solutions: configuration II, in which $0 < |z_\text{2} - z_\text{1}| < R$, and electrons are on opposite sides of the molecular axis; and configuration III, in which $|z_\text{2} - z_\text{1}| > R$, and electrons are on the same side of the molecular axis. Configurations I and II represent the lowest triplet state $3\Sigma^+_g$; configuration III represents the lowest triplet state $3\Sigma^+_u$.

(b) Potential energy curves (plotted in atomic units) display the variation of electronic energy with internuclear distance $R$. Bohr did not calculate such curves, but results derived from his 1913 formulation are shown for the three configurations (black curves). For comparison, results are shown from highly accurate quantum mechanical calculations (blue points). The Bohr-model result for the $1\Sigma^+_g$ state has been improved (red curve) by including a perturbation term, as described in box 2. (Adapted from refs. 8 and 10.)

**Figure 4. Potential-energy curves** for ground states of the helium hydride molecule (HeH) and of $\text{He}_2^+$ calculated from Niels Bohr’s original 1913 formulation, compare well with accurate quantum mechanical calculations (data points). Energies and distances $R$ are plotted in atomic units. As Bohr anticipated, neither molecule is stable; rather, the constituent atoms repel each other at all internuclear distances $R$. The large-$R$ asymptotes have been adjusted to the correct dissociation limits. (Adapted from ref. 8.)
energy function. That does not violate Heisenberg’s uncertainty principle. When D-scaling factors are introduced into the coordinates, the inverse factors enter into the conjugate momenta. Hence the coordinate–momentum products remain unchanged. Moreover, Bohr’s bilithe assumption, considered outrageous in 1913, that an electron in the $n=1$ state does not emit radiation while accelerating about the proton, is justified in the large-D limit. Since the electron configuration in that limit corresponds to the minimum of the energy function, energy conservation forbids the electron to emit a photon.

At first blush, the infinite-D limit may seem absurdly distant from the “real world” at $D=3$. In typical dynamical problems, however, after taming any singularities by a suitable choice of scaling factors, the major dimension dependence of quantities of interest varies as 1/$D$. Hence the large-D limit, where 1/$D \to 0$, is closer to the real world (1/$D = 1/3$) than is the oft-used $D=1$ regime. Indeed, results obtained at large $D$ usually resemble those for $D=3$ and therefore provide a good first approximation. For the H atom, the $D$-dependence is known exactly, so incorporating it in the scaling factors enables the large-D limit to give the same results as $D=3$ for the scaled energy and most probable electron location.

Bohr’s hydrogen molecule

In part 3 of his trilogy, Bohr presented chiefly calculations for the hydrogen molecule in its ground state. As depicted in configuration I of figures 2a and 3a, he assumed that the two electrons (labeled 1 and 2) each orbit the molecular axis with angular momentum $h$ in a common circular path midway between the protons (A and B). His calculation procedure was equivalent to determining the electronic energy and geometry, for a fixed internuclear spacing $R$, by evaluating the minimum of the energy function,

$$E(R) = \frac{1}{2} \left( \frac{1}{\rho_{1}^2} + \frac{1}{\rho_{2}^2} \right) + V(r_{1A} r_{1B} r_{2A} r_{2B} r_{12} R),$$

in atomic units. Here $\rho_{1}$ and $\rho_{2}$ are the electron orbit radii, $r_{ij}$ is the distance between two particles $i$ and $j$, and $V$ is the Coulomb potential energy, which includes the attractive electron–nucleus interactions

$$(1/r_{1i} \ldots)$$

and the repulsive electron–electron $(1/r_{1j} \ldots)$ and nucleus–nucleus $(Z^2/R)$ interactions.

As with the H atom, Bohr’s $E(R)$ energy function for $H_2$ corresponds to the Schrödinger equation in the large-D limit. Again, that is a redeeming grace. Even before the advent of quantum mechanics, a fatal conceptual flaw in the Bohr $H_2$ model was recognized.14 Bohr had assumed the two electrons orbit synchronously around the molecular axis in the same direction. That would produce a large magnetic moment and cause the ground state of $H_2$ to be paramagnetic. In actuality, however, the ground state is weakly diamagnetic and has no electronic orbital angular momentum.

The conceptual quandary is banished at the large-D limit, where the electrons are motionless and therefore do not generate magnetic moments. From the $D$-scaling perspective, such orbits should be viewed not as tracing an electron trajectory but as the locus of the electron’s most probable location. Ironically, however, by virtue of the cylindrical symmetry about the molecular axis, those loci coincide with the Bohr orbits. Figure 2 compares, for two internuclear distances, the electron distributions of the Bohr orbits with those calculated using a good-quality wavefunction.

Bohr reported numerical results only for configuration I, at the internuclear distance that corresponds to the minimum of the $E(R)$ function. That minimum occurs for $R = 1.10a_0$ and $\rho_{1} = \rho_{2} = 0.95a_0$ and it yields a bond dissociation energy of 0.105$e^2/a_0$ or 2.86 eV, relative to the $H + H$ asymptote. (We updated his result using the modern value of $e^2/a_0$.) Accurate values for the equilibrium bond distance and bond energy are 1.40$a_0$ and 4.745 eV, respectively.15

A comparison more fair to Bohr is with the results 1.51$a_0$ and 3.14 eV, obtained from an approximate wavefunction in 1927 by Walter Heitler and Fritz London,16 ever since cited as the first a priori calculation of chemical bonding.

Minimizing Bohr’s energy function admits two other configurations, labeled II and III in figure 3a, in which the two electrons have separate orbits. Configurations I and II, in which the electrons remain inside the protons and on opposite sides of the molecular axis, constitute the singlet ground state.

Figure 5. The ground-state configurations of various multielectron atoms, calculated using a Bohr-like model. For both the $n=1$ and $n=2$ shells, the electron locations (red dots) found from that simplistic model agree closely with the maximum charge densities obtained from standard quantum-theory calculations. (Distances are given in atomic units.) A sole exception occurs for lithium’s lone valence-shell electron. The Bohr-like model also captures for beryllium, boron, and carbon, respectively, the linear, trigonal, and tetrahedral geometry characteristic of the $sp$, $sp^2$, and $sp^3$ hybridized orbitals in conventional treatments of chemical bonding. (Adapted from ref. 10.)
Box 2. Modest extensions

The accuracy with which the Bohr model describes small molecules can be enhanced via simple strategies:

**Perturbation approach.** For diatomic hydrogen, the Bohr model corresponds to the Schrödinger equation in the limit of infinitely many dimensions. The large-$D$ result can be improved by expanding the $D$-dependence of the Schrödinger equation in powers of $1/D$ and applying standard perturbation theory. An equivalent procedure is to expand the Bohr energy function in powers of the displacement from its minimum. The term quadratic in the displacement describes harmonic oscillations about the minimum and provides the first-order $1/D$ contribution. For $H_2$, the first-order calculation is given in detail in reference 8; for discussion of higher-order perturbation calculations for helium and $H_2^+$, see references 10 and 11.

**Switching-quantization approach.** The Bohr model assumes quantization of the electron angular momentum relative to the molecular axis. As seen in figure 3b, that yields quite accurate results for $H_2$ at internuclear distances up to nearly $R = 1$ (in units of the Bohr radius $a_0$). At larger $R$, where each electron feels mainly the nearest nuclear charge, better results can be obtained by quantizing momentum relative not to the molecular axis but to the nearest atomic nucleus. The centrifugal term in the Bohr energy function changes from $1/\rho_i^2 + 1/\rho_j^2$, where $\rho_i$ is the $i$th electron’s distance from the molecular axis, to $1/r_i^2 + 1/r_j^2$, where $r_i$ is the distance of the $i$th electron from its nearest nucleus.

The atomic quantization (AQ) has a local minimum for configuration II in figure 3 as long as $R > 2.77$; below that the electrons collapse into the opposite nuclei. Using molecular quantization (MQ) for $R < 1$ and AQ for $R > 2.77$ and connecting them by a third-order interpolating polynomial gives good agreement with quantum mechanical results over the full range of $R$.

**Constrained-Bohr approach.** The collapse of the AQ Bohr model at small $R$ occurs because the coulombic attraction of each electron to the closest nucleus is not prevented by centrifugal terms. A simple quantum constraint on the electron locations removes the instability and enables AQ to be used over the full range of $R$. The key is to include a quantum potential $QP(r, R)$ between each electron and its non-nearest nucleus. The Bohr picture treats the electron as a point particle on a spherical surface of radius $r$ centered about the nearest nucleus. A circular surface of that surface will give the correct quantum interaction energy with the non-nearest nucleus. Since $QP(r, R)$ is finite, the constraint ensures that an electron cannot collapse onto its opposite nucleus. The effective potential $QP(r, R)$ can be derived from any two-electron wavefunction. Calculations carried out using two prototypical wavefunctions, Heitler–London and Hund–Mulliken, gave $E(R)$ curves close to the quantum mechanical results shown in figure 3b; details are given in reference 9.

$1^3\Sigma_g^+$; configuration III, in which the electrons orbit outside the protons and on the same side of the molecular axis, corresponds to the triplet state, $3^3\Sigma_g^-$. Bohr recognized that configuration I would dissociate ultimately to $2^+ + 2e^-$, so he inferred, rather vaguely, that there must exist another configuration—configuration II—that dissociates to $H + H$. Configuration III, not recognized by Bohr, represents repulsively interacting $H$ atoms.

Figure 3b plots the dependence of the electronic energy on $R$ for the three configurations, as derived from Bohr’s $E(R)$ function. Such curves, in accord with the Born–Oppenheimer approximation, specify the potential energy for molecular vibrations. Also shown are the results (blue points) from extensive quantum variational calculations for the ground singlet state and the lowest triplet state. Bohr’s model fairly accurately predicts the energy of the ground singlet state both at small $R$, where configuration I has the lowest energy, and at large $R$, where configuration II has the lowest energy. (Configuration II is the lowest-energy configuration for $R > 1.20\alpha_0$; it merges with configuration I at small $R$.) The Bohr model accurately predicts the repulsive triplet state, configuration III, over the full range of $R$. But it does poorly at predicting the depth of the attractive well of the singlet state.

Simple enhancements of the Bohr model markedly improve results for the attractive well of the singlet state. (See box 2.) The most straightforward extension—the perturbation approach—is to expand the energy function about its minimum in powers of $1/D$. Adding the first-order $1/D$ perturbation term gives the red curve in figure 3b, for which the equilibrium bond length and dissociation energy are 1.38$a_0$ and 4.50 eV, close to the accurate results. Similar results were obtained by two other methods—the switching-quantization approach and the constrained-Bohr approach. Those extensions have also yielded fairly accurate potential curves for some excited states of $H_2$ and for ground states of lithium hydride, beryllium hydride, diatomic lithium, and other simple diatomic combinations.

Bohr offered qualitative arguments indicating that the ground states of a helium hydride molecule and of $He_2$ would be entirely repulsive. Figure 4 shows remarkably accurate potential curves we obtained using his original formulation.

**Multielectron atoms**

In part 2 of his trilogy, Bohr discussed He and larger atoms, simply postulating that each electron circles the nucleus with orbital angular momentum of $h$. For those atoms, unlike $H$, $H_2$, and Rydberg atoms and molecules, the model based on Bohr’s wishful postulate does not correspond to the Schrödinger equation in the large-$D$ limit. Curious nonetheless to see what it would give, we examined a simplistic energy function:

$$E = \frac{1}{2} \sum_{i=1}^{N} \left( \frac{n_i^2}{r_i^2} + V(r_i, r_{2i}, \ldots, r_N) \right),$$

where $r_i$ is the distance from electron $i$ to the nucleus. In analogy to Bohr’s hydrogenic function and to its large-$D$ limit, the multielectron energy function consists merely of centrifugal kinetic energy terms plus the coulombic potential energy. It is akin to a heuristic approximation employing $D$-scaled quantum numbers for excited electronic states of multielectron atoms. The quantum numbers $n_i$ for each of the $N$ electrons are assigned using the familiar prescription for sequential filling of the atomic shells: $n = 1, 2, 3, \ldots$, with $2n^2$ the maximum occupation of each shell. At a crude level of approximation, minimizing the energy function gives the fixed locations that the electrons attain at the large-$D$ limit in the $D$-scaled space, which for $D = 3$ represent the most probable configuration.

Figure 5 shows the electron configurations obtained for neutral atoms with $2 \leq Z \leq 6$. The results agree remarkably well with the radius of maximum
radial charge density in atomic shells and subshells, determined from $D = 3$ self-consistent field calculations using Roothaan-Hartree-Fock (RHF) wavefunctions. For the $n = 1$ shell, the radii are within 1% of the RHF most probable radii. For the $n = 2$ shell in Li, the model result ($3.85a_0$) is much larger than the RHF value ($3.09a_0$), but for beryllium, boron, and carbon the agreement between the Bohr and RHF results ($2.04a_0$, $1.53a_0$, and $1.21a_0$, respectively) is good.

Not surprisingly, the net ground-state energies given by the model compare poorly with RHF results. However, a striking aspect is that simply minimizing the energy function predicts that in the $n = 2$ shell the valence electrons for Be, B, and C are disposed in linear, trigonal, and tetrahedral geometry, respectively. Those geometries correspond to the $sp$, $sp^2$, and $sp^3$ modes of hybridization of the $s$ and $p$ orbitals invoked in myriad discussions of chemical bonding. Conventional wave-mechanics treatments of hybridization have to neglect differences in orbital energies to obtain those modes. In the simplistic Bohr-like scheme, they appear without any ado.

The Bohr model may acquire more progeny. The prototype examples described here and others presented elsewhere provide fairly accurate results that support qualitative insights for a variety of electronic states of atoms and molecules, including excited electronic states and quasi-stationary states. Both the computations required and the guiding concepts are elementary and exemplary of Bohr’s enterprising spirit and acceptance of paradox.

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References


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