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Search for Simplicity: Quantum mechanics of atoms

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Search for Simplicity: Quantum mechanics of the hydrogen atom

In the last essay we introduced the minimum kinetic energy $K_{\min} \sim \hbar^2/(2mR^2)$ of an electron of mass m confined to a volume of linear dimension R. We observed that it will try to expand (Schrödinger pressure) if it is not kept from doing so by a confining force. With these concepts we can directly determine the energy and size of the hydrogen atom. The electron wavicle surrounds the nucleus in a spherical cloud with an average radius R. The lowest state is the result of two forces in equilibrium: the electrostatic attraction e^2/R^2 of the nucleus and the tendency of the cloud to expand. This tendency can also be expressed in terms of a force, the "Schrödinger force." Whenever an energy depends on a coordinate x, there is a force to change x; it is the negative derivative of the energy with respect to x. Thus the Schrödinger force is the negative derivative of the minimum kinetic energy with respect to R. Setting these two opposing forces equal gives

$$\frac{e^2}{R^2} = -\frac{dK_{\min}}{dR} \sim \frac{\hbar^2}{mR^3}. \quad (1)$$

That relation determines R, which happens to come out equal to the "Bohr radius":

$$R \sim \hbar^2/(me^2) \equiv a_B = 0.53 \times 10^{-8} \text{ cm}. \quad (2)$$

The energy E of the electron in this state is

$$E \sim -\frac{e^2}{R} + \frac{\hbar^2}{2mR^2}. \quad (3)$$

Inserting (2) gives

$$E \sim -me^4/2\hbar^2 = -\tfrac{1}{2}e^2/a_B = -13.6 \text{ eV}. \quad (4)$$

The energy $|E|$ is called Ry(rydberg); it is the amount necessary to liberate the electron. It is remarkable that we get the exact result for the ionization energy of hydrogen by using our approximate estimates.

The relation (1) happens to be the condition for the energy (3) to be a minimum. Therefore the results (2) and (4) can also be interpreted as resulting from finding the lowest possible value of the energy as one would expect for the lowest quantum state.

The excited states of hydrogen can be found by a similar procedure. Higher quantum states have n nodes in their wave functions. Then the characteristic wavelength $\bar{\lambda}$ is R/n, giving rise to a higher kinetic energy $K_n \sim n^2\hbar^2/(2mR^2)$. The corresponding stronger expanding force

$$-\frac{dK_n}{dR} = \frac{n^2\hbar^2}{mR^3}$$

is balanced by the Coulomb attraction e^2/R^2 and gives rise to larger radii $R_n = n^2\hbar^2/(me^2)$. Inserting this into the energies $E_n = -e^2/R + K_n$ yields the well-known Balmer formula $E_n = -(me^4/2\hbar^2)(1/n^2)$. Note that the energy is smaller than mc^2 by a factor $(e^2/\hbar c)^2$ which shows that the use of a nonrelativistic expression for kinetic energy is justified.

What about atoms with more than one electron? We will treat helium and atoms with many electrons in greater detail later on. For the moment we use a very crude picture: such atoms contain a core consisting of the nucleus and most of the electrons. It carries a charge ne where n is the small number of the remaining outer electrons. Thus, qualitatively, the situation is not unlike an atom with a few electrons. We then expect again dimensions of the order a_B and an energy of the order of a Ry to liberate one of these outer electrons.

These results are perhaps the greatest triumph of quantum mechanics. The existence of atoms was known for a century and conjectured for many more, but their size and internal energies were only deduced from experiments such as the ones mentioned in the previous essay. Quantum mechanics showed that they are of the order of a_B and of Ry, respectively, both of which are simple combinations of the three fundamental constants, m, e, and $\hbar$.

It is instructive to apply the same method to nuclear systems. The force between the nucleons is more complicated than the Coulomb force; it is repulsive for small distances and drops exponentially for larger ones. We may very roughly approximate the potential of the attractive part by $-g^2/r$. Figure 1 shows that $g^2 \sim 10e^2$ (taken from Ref. 1). It is about ten times stronger than the attraction between two opposite charges e. The repulsion at the center is important—it keeps the nucleons apart—but does not influence the energy very much because it acts only at distances which will turn out to be much smaller than the separations between nucleons. Replacing the electron mass by the nucleon mass $M \sim 2000\,m$ and e^2 by g^2, we obtain for the nuclear Bohr radius a_N and the nuclear rydberg Ry_N

$$a_N \sim a_B/20\,000 = 2.7 \times 10^{-13} \text{ cm},$$

$$\text{Ry}_N \sim 200\,000 \text{ Ry} = 2.7 \text{ MeV}.$$

These are indeed typical distances and energies in nuclear physics, but they are very rough estimates, not only because of the complicated form and of the symmetry dependence of the nuclear force but also because of the intricacies of the many-body problem in ordinary nuclei. For the deuteron, however, our method should give reasonably good results if we replace M by the effective mass $M/2$. This would double a_N and halve Ry_N, not too far from the actual values 4.3×10^{-13} cm and 2.2 MeV.

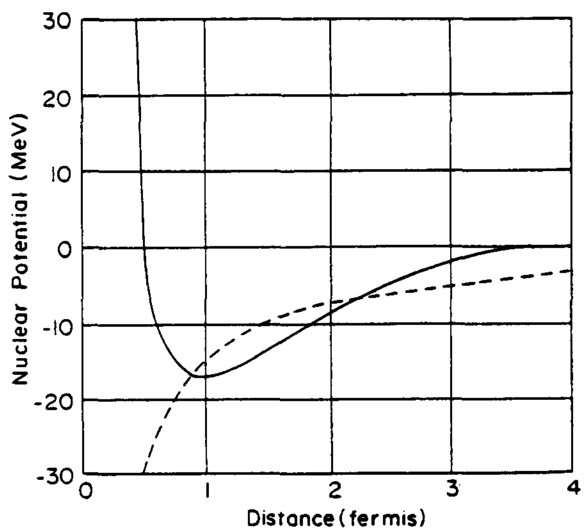

Fig. 1. Sketch of the potential of the nuclear force as a function of internucleon separation as measured in fermis, 10^{-13} cm. (This curve is not quantitative, because it ignores the dependence on spin and symmetry.) For comparison, the dashed curve gives the attraction of two opposite, but equal, charges 3.2 e. [Reprinted from Ref. 1.]

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We now answer the question of last month as to why the Pauli principle is equivalent to the assumption that each of N equal particles in a volume V is confined to a "private" volume V/N. There are two explanations. Here is the first. A quantum state of a free particle with a well-defined momentum is stationary; its momentum stays constant and its position is spread over the whole volume V. This is not the only kind of state. We can construct nonstationary states where the momentum and the position are spread over finite intervals Δx and Δp which obey Heisenberg's relation $\Delta x \Delta p = \hbar$. N equal particles must be distributed over N different quantum states. Let us choose states that are blobs of a spatial extension Δx and which have all the same momentum distribution. To prevent any overlap the size Δx must be smaller or equal to $d = (V/N)^{1/3}$. We choose the maximum $\Delta x \sim d$ in order to minimize the momentum spread Δp. This leads us directly to the "private room" of dimension d, and to an average momentum $\sim \hbar/d$.

For the second approach we remember that the Pauli principle is equivalent to the antisymmetry of the wave function Ψ. The latter changes sign if the coordinates of two equal particles are exchanged. From this follows immediately that the wave function vanishes if two equal particles have the same coordinates; they cannot be at the same place. (This is the last remnant of the classical concept of impenetrable particles.) Let us look at the dependence of ψ on the distance r of two electrons (Fig. 2). It is zero for $r = 0$ and reaches its typical values $\pm |\bar{\psi}|$ roughly like $\psi \sim \bar{\psi} \sin kr$ between $r = -\pi/2k$ and $+\pi/2k$. This is a wave function corresponding to a relative momentum $p_r = \hbar k$. The probability $|\psi|^2$ is low as long as $|r| < k^{-1}$. Thus the electrons stay apart at a distance of the order of $d \sim \hbar / p_r$. The average momentum p of the electrons is of the same order as the relative momentum p_r and we get again the relation $p = \hbar/d$ between the momentum and the size d of the "private room."

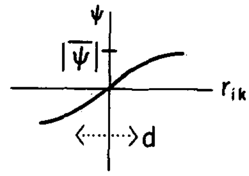

Fig. 2. Dependence of the wave function on the relative distance of two equal particles.

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[1]K. Gottfried and V. Weisskopf, *Concepts of Particle Physics* (Oxford University Press, New York, 1984).

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