small back torque on the current itself mentioned above we have, as usual, $i\Phi/2\pi$.

Second distribution of the current

Going now to the other extreme, let the magnetized matter have the form of very flat narrow cylindrical rings placed coaxial with the bar, and let the current flow alternately radially and longitudinally through similar cylindrical slots between the rings, as suggested schematically in Fig. 1b; let us suppose that the current otherwise ignores the molecular structure and distributes itself with exact symmetry about the axis. (The current must also be prevented from slipping sidewise by a suitable constraint.)

In this case the torque arises from the field of the magnet acting upon the current. For in this case H_i is strictly symmetrical and the argument just given shows correctly that the torque on the magnetic material vanishes; all of the lines of B are cut by the current and the usual calculation gives for the torque exerted on the current alone $\int r i B \, dr = i\Phi/2\pi$ where $\Phi = \int B 2\pi r dr$.

The real case

Now so far as one can tell by inspection a magnet might actually be constructed according to either of the two models just described. If the conducting electrons were to move with entire disregard of the atoms, passing freely through them, then the mean force on the electrons would be determined by the mean value of the true magnetic intensity or B, and we should have an equivalent of our second distribution. It seems improbable, however, that the electrons do so move; they should tend to follow the spaces between the atoms (or to do something equivalent to this in quantum mechanics), and the result will then depend upon local conditions. If the interatomic space through which an electron slips resembles more nearly a longitudinal crack, we have an approach to the case of our first example (mean torque on magnet); if a transverse crack, an approach to the second (mean torque on the electron). It seems thus to the writer most probable that the torque in actual cases arises partly in one way and partly in the other, the amount arising from each cause being at present unknown.

If this be granted, then we cannot say that the force on a current is definitely either $j \times B$ or $j \times H$. We can only assert that either of these expressions, if paired off with the proper assumption as to forces on the magnetic material, will give correctly the total force-action upon a rigid body (or an incompressible liquid).

<div align="right">E. H. KENNARD</div>

Cornell University,
  March 20, 1933.

Improved Calculation of Ground State of H₂

The work of Hylleraas[1] on He shows that a great improvement in the treatment of a two-electron problem can be obtained by using wave functions in which the electronic separation enters explicitly. We have extended this method to the H_2 molecule, and wish to communicate our preliminary results.

The dissociation heat as measured experimentally is 4.46 ± 0.04 volts according to Richardson and Davidson,[2] 4.44 volts as given by Mulliken.[3] Adding the zero-point energy, 0.27 volt, gives -4.73 ± 0.04 as the energy of H_2 at the equilibrium nuclear separation, 1.4 Bohr radii (0.74A), referred to zero for separate atoms. Our computed values for three nuclear distances, R, are as follows, compared with the values read from a Morse curve constructed from spectroscopic data and passing through the minimum just described:

R	1.3	1.4	1.5
E(calc.)	−4.63	−4.69	−4.59
E(Morse)	−4.67	−4.73	−4.68

These results were obtained with a wave function in the form of a series:

$$\psi = \Sigma_{mnjkp} C_{mnjkp} e^{-\delta(\lambda_1+\lambda_2)} [\lambda_1{}^m \lambda_2{}^n \mu_1{}^j \mu_2{}^k \rho^p + \lambda_1{}^n \lambda_2{}^m \mu_1{}^k \mu_2{}^j \rho^p].$$

Here λ_1, μ_1 and λ_2, μ_2 are the ordinary elliptical coordinates of the two electrons respectively, and ρ is the ratio of their separation to $R/2$. The summation extends in principle over all not negative values of the indices such that $j+k$ is even, but we find such rapid convergence that no index need be carried higher than 2. The screening constant δ and the coefficients C are parameters to be varied in the usual way, in order to minimize the energy, and have different values for each R. So far, however, we have computed only with $\delta = 0.75$. The terms used, and their coefficients for $R = 1.4$, are as follows:

m	n	j	k	p	C	m	n	j	k	p	C
0	0	0	0	0	1	1	0	1	1	0	+0.0841
0	0	0	2	0	+0.5160	2	0	0	0	0	+0.0300
0	0	1	1	0	−0.2134	0	0	0	0	1	+0.1550
1	0	0	0	0	−0.3852	0	0	1	1	1	−0.0306
1	0	0	2	0	−0.0333	0	0	0	0	2	−0.0115
1	0	2	0	0	−0.0635						

A few other terms were tried and rejected, as they led to negligible decrease in the energy. In fact, the convergence is so rapid upon introducing the terms in succession, that we can state with some confidence that the inclusion of five or six more would bring the energy to within 0.01 volt of the convergence limit, and that this limit is -4.73 ± 0.02 volts, in complete agreement with experiment.

---

[1] E. A. Hylleraas, Zeits. f. Physik 65, 209 (1930).

[2] O. W. Richardson and P. M. Davidson, Proc. Roy. Soc. A123, 466 (1929).

[3] R. S. Mulliken, Rev. Mod. Phys. 4, 78 (1932).

Analysis of the problem indicates that the chosen value of δ is very nearly the optimum for $R=1.3$ and 1.4, but that for larger R a correspondingly larger δ would give slightly better results. We are now investigating this.

It may be of interest to give the best energy, -4.2 volts, obtainable from a combination of terms not including the electronic separation explicitly. This is the same value found by Hylleraas, by a long computation which he does not describe.

HUBERT M. JAMES
ALBERT SPRAGUE COOLIDGE
Harvard University,
Cambridge, Massachusetts,
March 17, 1933.

Influence of Inner Shells on Atomic Interactions

In applying wave mechanics to the study of the interaction of atoms more complex than He it has been customary to omit the inner shells from consideration. That the apparent success of computations of this sort does not justify this omission may be seen from a study of the normal state of Li_2.

The first attack on this problem was made by Delbrück.[1] In this work the inner electrons were included, but so many approximations were made in the numerical calculation that the results were seriously affected, as can be seen by comparing them with those of the writer, in obtaining which no such approximations were made. Bartlett and Furry[2] seem to misinterpret the work of Delbrück as showing the inner shells to be negligible and omit them entirely in a work which was otherwise more careful than Delbrück's, obtaining a result within 5 percent of the experimental value for the energy of dissociation. This close agreement must be viewed with some suspicion, however, for the corresponding computation in the case of hydrogen, that of Heitler and London, completed by Sigiura, gives a result in error by 34 percent.

There are three fundamental approximations made in work such as that of Bartlett and Furry: (1) an approximation in simplifying the operator used; (2) the omission of the inner shells; (3) the use of atomic wave functions to describe the outer electrons (the Heitler-London method). Such work does not seem to warrant a conclusion as to the importance of the inner shells in the interaction. The writer has, therefore, carried through without computational approximation a similar calculation including the inner shells and using the complete rigorous Hamiltonian operator. The wave functions for the outer electrons were the same as those used by Bartlett and Furry. The results of this computation are:

Internuclear distance (A)	2.78	2.98	3.18
Energy of interaction (volts)	-0.259	-0.294	-0.309

A Morse curve fitted to these points has its minimum very close to 3.18A, and the dissociation energy is thus computed as about 30 percent of the experimental value. By making the approximation of using an "interaction operator," as Bartlett and Furry do, the agreement with experiment was somewhat improved (dissociation energy 0.328 volt, equilibrium distance 3.07A). A comparison of these results with those of Bartlett and Furry indicates that the inner shells in Li_2 are responsible for a repulsion between the atoms which is decidedly important in comparison with the total energy of binding.

An attempt to better the results by adding functions of ionic type failed to give a perceptible improvement. By changing the shielding constant for the outer electrons the computed interaction energy can be increased by about 10 percent. It seems, however, that no rigorous computation designed along these lines can yield for the dissociation energy of Li_2 a value greater than 40 percent of that observed.

In view of these results it seems to be necessary to assume that the approximate agreement of the results of computations on the alkali metal molecules with experiment is due to a cancelling of errors, the neglect of the repulsion of the inner shells being counteracted by an underestimate of the attractive forces due to the outer shell. The interesting results of Rosen and Ikehara[3] must then be considered as of doubtful significance until some reason for expecting a systematic cancellation of these two types of error can be discovered.

The writer has for some time been of the opinion recently expressed by Furry,[4] that the best way to treat diatomic molecules is by using one-center functions for the electrons of inner shells, two-center functions for the others. A treatment of Li_2 by this method, using for the outer electrons the functions applied to the treatment of H_2 by Dr. A. S. Coolidge and the writer,[5] is now well under way. A more complete statement and analysis of the results of the research on which this note is a preliminary report, as well as a description of the methods used, will be published later in connection with a report on the more promising method mentioned above.

HUBERT M. JAMES
Harvard University,
Cambridge, Massachusetts,
March 17, 1933.

[1] M. Delbrück, Ann. d. Physik 5, 36 (1930).
[2] J. H. Bartlett, Jr. and W. H. Furry, Phys. Rev. 38, 1615 (1931).
[3] N. Rosen and S. Ikehara, Phys. Rev. 43, 5 (1933).
[4] W. H. Furry, Phys. Rev. 43, 361 (1933).
[5] Preceding letter.