servable difference in this respect between fission of thorium with helium ions and $U^{235}$ with slow neutrons would occur in the length of the chains between the primary products and the stable nuclei, those chains on the heavy side of the distribution curve being shortened. This has not been investigated.

The depth of the dip in the mass yield curve must be related to the excess excitation in the fissioning nucleus. The results with slow neutron fission of $U^{235}$, where the factor in yield between dip and peaks of the distribution curve is about 600, fast neutron fission of thorium where the factor [a6] is about 10, and fission of thorium with 37.5-Mev helium ions where the factor was found to be only about 2, indicate that there is a definite relation between the excitation of the nucleus and the occurrence of symmetrical fission. While the results at alpha-energies lower than 37.5 Mev do not give a complete picture of the distribution at these energies, enough is given to indicate that the dip is always much shallower than that found in slow neutron fission of $U^{235}$.

**ACKNOWLEDGMENTS**

The author wishes to express his thanks to Professor I. Perlman and Professor G. T. Seaborg for valuable suggestions and criticisms, to Dr. N. Ballou for aid in separating samarium and europium, and to Dr. J. G. Hamilton and the crew of the Crocker Laboratory cyclotron for making the bombardments.

This work was performed at the Radiation Laboratory, University of California, Berkeley, California under the auspices of the Atomic Energy Commission.

PHYSICAL REVIEW VOLUME 75, NUMBER 1 JANUARY 1, 1949

# A Note on the One-Electron States of Diatomic Molecules

Henry A. Erikson and E. L. Hill
*Department of Physics, University of Minnesota, Minneapolis, Minnesota*
(Received July 26, 1948)

The explicit formulation of an integral of the motion is given for a single electron moving in the field of two fixed nuclei, for both the classical and the quantum mechanical cases. The corresponding quantal operator together with the Schrödinger Hamiltonian and the operator for the component of the orbital angular momentum of the electron about the internuclear axis form a complete set of commuting observables of the problem. This supplies the dynamical interpretation of the separation parameter of the energy equation.

## I. INTRODUCTION

It is well known that the equations of motion of the electron moving in the field of two fixed nuclei are separable in elliptic coordinates in both classical and quantum mechanics. In the latter case the separability of the Schrödinger equation falls under Case VII of Eisenhart's classification.[1] The separated differential equations have been studied in detail for the special case of the hydrogen molecular ion ($H_2^+$) by Burrau,[2] Wilson,[3] Teller,[4] Hylleraas,[5] and others.

The purpose of the present note is to establish the form of a general integral for the problem. While the use of this integral is implicit in all of the work which has been done on the two-center problem, back to that of Euler,[6] its explicit formulation and dynamical significance have not been given previously, to our knowledge. The possession of the integral does not give one any information which cannot be derived from the separation of the variables in the Schrödinger equation, but it is of theoretical interest as an important example of the use of first integrals in quantum mechanics. Actual examples of this

[1] L. P. Eisenhart, Phys. Rev. **74**, 87 (1948).
[2] Ø. Burrau, K. Danske Viden. Selskab **7**, Nr. 14 (1927).
[3] A. H. Wilson, Proc. Roy. Soc. London **A118**, 617 (1928); **A118**, 635 (1928).
[4] E. Teller, Zeits. f. Physik **61**, 458 (1930).
[5] E. Hylleraas, Zeits. f. Physik **71**, 739 (1931).
[6] E. T. Whittaker, *Analytical Dynamics* (Cambridge University Press, Cambridge, 1927), third edition, p. 97.

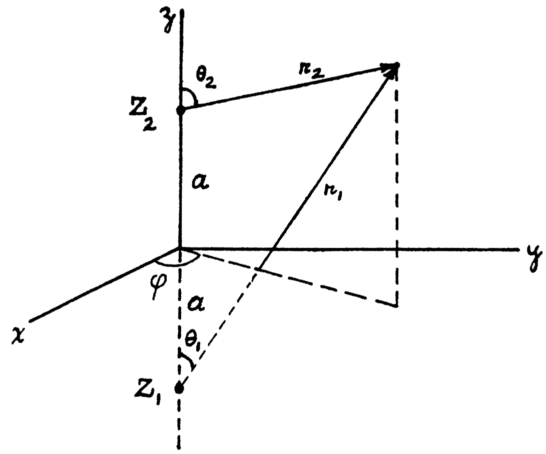


FIG. 1. Coordinate system for the two-center problem.

type are rather difficult to discover for the Schrödinger equation.[7]

## II. THE CLASSICAL INTEGRAL

The basic cartesian reference system $S$ is chosen as indicated in Fig. 1, the origin being at the midpoint between the nuclei. We let $\mathbf{L}'$ and $\mathbf{L}''$ be the orbital angular momentum vectors of the electron as referred to the two nuclei 1 and 2 respectively as origins. A short calculation from the Newtonian equations of motion of the electron shows that the following quantity is an integral of the motion[8]

$$\Omega_c \equiv \mathbf{L}'\cdot\mathbf{L}'' + 2me^2a(Z_1\cos\theta_1 - Z_2\cos\theta_2), \quad (1)$$

that is, we have $d\Omega_c/dt=0$ as a consequence of the equations of motion of the particle. The notation in Eq. (1) is as indicated in Fig. 1, with $m$ as the electronic mass. A curious feature of this expression is that it involves the angular momentum vectors of the electron computed about two different points. For vanishing internuclear distance this reduces to the square of the angular momentum about the origin of the system $S$.

## III. THE QUANTUM MECHANICAL INTEGRAL

We wish to formulate expression (1) as a self-adjoint linear operator $\Omega$ which will satisfy the identical commutation relation

$$[\mathcal{H}, \Omega] \equiv \mathcal{H}\Omega - \Omega\mathcal{H} = 0, \quad (2)$$

with the Schrödinger energy operator $\mathcal{H}$, the latter being

$$\mathcal{H} \equiv -\frac{\hbar^2}{2m}\nabla^2 - \frac{Z_1e^2}{r_1} - \frac{Z_2e^2}{r_2}. \quad (3)$$

This is the standard condition which, when satisfied, assures one that the wave functions of the stationary states of the system can be arranged to be simultaneous eigenfunctions of the two operators $\mathcal{H}$ and $\Omega$; i.e., the wave functions will satisfy the two simultaneous equations

$$\mathcal{H}\psi = E\psi, \quad \Omega\psi = \bar{\omega}\psi, \quad (4)$$

where $E$ and $\bar{\omega}$ are eigenvalues of the two operators.

Calculation shows that this can be accomplished by the usual simple procedure of taking the symmetrized form of Eq. (1)

$$\Omega \equiv \tfrac{1}{2}\hbar^{-2}(\mathbf{L}'\cdot\mathbf{L}'' + \mathbf{L}''\cdot\mathbf{L}') + \gamma(Z_1\cos\theta_1 - Z_2\cos\theta_2), \quad (5)$$

with

$$\gamma = 2me^2a/\hbar^2 = 2a/a_0, \quad (6)$$

where $a_0$ is the Bohr radius.

The angular momentum operators in (5) can be formulated in terms of the corresponding operators in the reference system $S$ by the relations

$$\begin{aligned} L_x' &= L_x + i\hbar a\partial_y, & L_x'' &= L_x - i\hbar a\partial_y, \\ L_y' &= L_y - i\hbar a\partial_x, & L_y'' &= L_y + i\hbar a\partial_x, \\ L_z' &= L_z, & L_z'' &= L_z. \end{aligned} \quad (7)$$

On insertion of these expressions into (5) we find that

$$\Omega \equiv \hbar^{-2}L^2 + a^2(\nabla^2 - \partial_z^2) + \gamma(Z_1\cos\theta_1 - Z_2\cos\theta_2). \quad (8)$$

The proof of the commutation relation (2) is a somewhat onerous task, but since it requires only elementary techniques it will not be given here. The work is perhaps performed most readily with the expressions (3) and (5) for the operators, but can also be carried out with the formulations in terms of elliptic coordinates given below.

We give for reference the forms of the operators in terms of elliptic coordinates $(\xi, \eta, \varphi)$ defined by the relations

$$r_1 = a(\xi+\eta), \quad r_2 = a(\xi-\eta). \quad (9)$$

[7] J. M. Jauch and E. L. Hill, Phys. Rev. **57**, 641 (1940).

[8] An attempt to find the remaining integrals of the problem in explicit form by the standard procedures of classical theory (reference 6, p. 323) fails by reason of the appearance of elliptic integrals.

The transformation of the energy operator follows readily from the usual formula for the laplacian operator in curvilinear coordinates, and yields the result

$$\mathcal{H}\equiv-\frac{\hbar^2}{2ma^2}\left\{\frac{1}{\xi^2-\eta^2}\frac{\partial}{\partial\xi}\left[(\xi^2-1)\frac{\partial}{\partial\xi}\right]+\frac{1}{\xi^2-\eta^2}\frac{\partial}{\partial\eta}\left[(1-\eta^2)\frac{\partial}{\partial\eta}\right]+\frac{1}{(\xi^2-1)(1-\eta^2)}\frac{\partial^2}{\partial\varphi^2}\right\}-\frac{e^2}{a}\frac{(Z_1+Z_2)\xi-(Z_1-Z_2)\eta}{\xi^2-\eta^2}. \quad (10)$$

The transformation of the operator $\Omega$ is more laborious, but again it requires only elementary techniques and will not be given here. The result is

$$\Omega\equiv\frac{1-\eta^2}{\xi^2-\eta^2}\frac{\partial}{\partial\xi}\left[(\xi^2-1)\frac{\partial}{\partial\xi}\right]-\frac{\xi^2-1}{\xi^2-\eta^2}\frac{\partial}{\partial\eta}\left[(1-\eta^2)\frac{\partial}{\partial\eta}\right]+\left[\frac{1}{\xi^2-1}-\frac{1}{1-\eta^2}\right]\frac{\partial^2}{\partial\varphi^2}+\gamma\frac{(Z_1+Z_2)\xi(1-\eta^2)+(Z_1-Z_2)\eta(\xi^2-1)}{\xi^2-\eta^2}. \quad (11)$$

The operators $\mathcal{H}$, $\Omega$, and $L_z\equiv-i\hbar\partial_\varphi$ which gives the component of orbital angular momentum of the electron about the internuclear axis, thus form a complete set of commuting observables defining the stationary states of the system.

The Schrödinger equation with the energy operator (10) permits separation of the variables with the wave function written in the form

$$\psi(\xi,\eta,\varphi)=F(\xi)G(\eta)\exp(i\Lambda\varphi), \quad (12)$$

with

$$\Lambda=0,\ \pm1,\ \pm2,\ \cdots.$$

Considered by itself, the operator $\Omega$ allows separation into individual equations for the functions $F(\xi)$ and $G(\eta)$ alone only for $\Sigma$-states ($\Lambda=0$). Nevertheless, we can employ it to give a dynamical interpretation of the separation parameter in the Schrödinger equation, by the introduction of the operator

$$\mathbf{A}=-\Omega-2ma^2\mathcal{H}/\hbar^2. \quad (13)$$

When the operator $\mathbf{A}$ is applied to a complete wave function of the form (12), which is a solution of the Schrödinger equation for an energy eigenvalue $E$, we find that

$$\mathbf{A}\psi=A\psi \quad (14)$$

where $A$ is the separation parameter of the Schrödinger equation.[9] The operator $\mathbf{A}$ of Eq. (13) thus gives us the interpretation of the separation parameter in terms of the dynamical operators of the problem.[10]

[9] H. A. Bethe, *Handbuch der Physik*, (Edwards Brothers, Ann Arbor, 1943) second edition, vol. 24, part 1, p. 530.

[10] The explicit formulation of the operator of Eq. (13) is made following a remark of the referee who suggested its use as part of the set of commuting observables instead of $\Omega$. While this is quite possible, it leads to no particular simplification since the separated form of the Schrödinger equation shows that the eigenvalues $E$ and $A$ both appear in each of the two separated equations.