one of calcite, using the value for N_0 as derived in the foregoing.

Note added in proof:—The new value for λ_g/λ_c recently calculated by DuMond and Cohen[18] is 1.002063. Substituting this value for 1.00202 in Eq. (4), $N_0=6.02489\times10^{23}$ (physical scale) is obtained, which is even in a better agreement with 6.02472×10^{23}, the newest $N_{\text{universal}}$ of the two authors,[18] than those of Table I. But if one uses the newest N_0, the respective λ_g/λ_c also must be used.

[18] J. W. M. DuMond and E. Cohen, Revs. Modern Phys. **25**, 691, 706 (1953).

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The Binary Rearrangement Collision*

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The theory of the general binary collision is discussed, and it is demonstrated that the rearrangement scattered amplitude can be derived from the integral equation which is convenient for determining the direct (no rearrangement of particles) scattered amplitudes. As a consequence, it is shown that no ambiguity in matrix element for the rearrangement amplitude in Born approximation exists.

THE binary rearrangement collision is a process in which a system A in state n collides with a system B in the state m, and systems C in state s and D in state t emerge. We shall consider events in which no photons are involved and that no particles appear or disappear. In previous treatments[1,2] of the general two-body collision different unperturbed Hamiltonians are employed for developing the stationary state integral equations. If no rearrangement of particles occurs in the collision, the relevant unperturbed Hamiltonian is that describing the relative motion of the two noninteracting systems A and B. If a rearrangement of particles occurs so that systems C and D appear, then it is convenient to select as unperturbed Hamiltonian that pertaining to the relative motion of C and D as noninteracting systems. However, with the latter procedure it is not clear from the derived integral equation in what way the boundary conditions are met since the incident wave, which is an eigenfunction of the alternative unperturbed Hamiltonian referring to systems A and B, is manifestly not present. Indeed, it is not apparent that the corresponding integral equations resulting from the separate imposition of the outgoing boundary condition describe the same wave function. Clearly, a single integral equation satisfying the boundary conditions should provide the amplitudes pertinent to any event, rearrangement or otherwise. It is the purpose of this note to demonstrate that this is indeed the case, and incidentally to remove the serious ambiguity in matrix element arising in the Born approximation for rearrangement amplitudes. This ambiguity stems from the fact that either of the interaction energy operators between systems A and B, or C and D, yield the same matrix element[2] when exact wave functions for the unperturbed systems are presumed. However, such wave functions do not exist except in the very special three-body collision of electrons with hydrogen atoms, so that, in general, a difference in matrix element necessarily arises. For rearrangement (exchange) scattering of electrons from atoms this ambiguity has been referred to as "prior-post discrepancy,"[3,4] and has been clarified by an analysis[5] which will now be extended to the general binary collision.

We wish to solve the wave equation

$$(H-E)\Psi=0, \tag{1}$$

where the Hamiltonian can be written in either of two ways,

$$H=H_{AB}+V_{AB}=H_{CD}+V_{CD}. \tag{2}$$

Since the entire calculation is performed in the center-of-mass system, the unperturbed Hamiltonians for the initial and final systems may be written as

$$H_{AB}=H_A(\mathbf{r}_a)+H_A(\mathbf{r}_b)-\frac{\hbar^2}{2\mu_{AB}}\nabla_{\mathbf{r}_{ab}}^2,$$

$$H_{CD}=H_C(\mathbf{r}_c)+H_D(\mathbf{r}_d)-\frac{\hbar^2}{2\mu_{CD}}\nabla_{\mathbf{r}_{cd}}^2.$$

Here $\mathbf{r}_a$, $\mathbf{r}_b$, $\mathbf{r}_c$, and $\mathbf{r}_d$ are the internal coordinates of the respective systems, while $\mathbf{r}_{ab}$ and $\mathbf{r}_{cd}$ denote the vectors that connect the centers of mass of the systems A, B and C, D respectively. For the internal motion we

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[1] N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Oxford University Press, New York, 1949), second edition.

[2] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), p. 230.

[3] Bates, Fundaminsky, and Massey, Trans. Roy. Soc. (London) **243**, 93 (1950).

[4] Corinaldesi, Trainor, and Wu, Nuovo cimento **9**, 436 (1952).

[5] S. Altshuler, Phys. Rev. **91**, 1167 (1953).

introduce the sets of eigenfunctions and eigenvalues $u_n{}^A(\mathbf{r}_a)$, $u_n{}^B(\mathbf{r}_b)$, $u_n{}^C(\mathbf{r}_c)$, $u_n{}^D(\mathbf{r}_d)$ and $\epsilon_n{}^A$, $\epsilon_n{}^B$, $\epsilon_n{}^C$, $\epsilon_n{}^D$, corresponding to the internal energy operators $H_A(\mathbf{r}_a)$, $H_B(\mathbf{r}_b)$, $H_C(\mathbf{r}_c)$ and $H_D(\mathbf{r}_d)$.

In order to deduce the appropriate integral equation for the problem, we introduce the outgoing Green's function which is defined by

$$(E-H_{AB}(\mathbf{r}_{ab},\mathbf{r}_a,\mathbf{r}_b))(\mathbf{r}_{ab},\mathbf{r}_a,\mathbf{r}_b|G_{AB}|\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b')=\delta(\mathbf{r}_{ab}-\mathbf{r}_{ab}')\delta(\mathbf{r}_a-\mathbf{r}_a')\delta(\mathbf{r}_b-\mathbf{r}_b'), \quad (3)$$

where

$$(\mathbf{r}_{ab},\mathbf{r}_a,\mathbf{r}_b|G_{AB}|\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b')=\frac{-\mu_{AB}}{2\pi\hbar^2}\sum_{\alpha,\beta}\frac{\exp[ik_{\alpha\beta}|\mathbf{r}_{ab}-\mathbf{r}_{ab}'|]u_\alpha{}^A(\mathbf{r}_a)u_\beta{}^B(\mathbf{r}_b)u_\alpha{}^{A*}(\mathbf{r}_a')u_\beta{}^{B*}(\mathbf{r}_b')}{|\mathbf{r}_{ab}-\mathbf{r}_{ab}'|}. \quad (4)$$

Here the sums include integration over continuum states, $k_{rs}{}^2\equiv(2\mu_{AB}/\hbar^2)(E-\epsilon_r{}^A-\epsilon_s{}^B)$, and μ_{AB} denotes the reduced mass associated with the motion of systems A and B. We are now prepared to write the integral equation for the motion in the usual form of an incident plus scattered wave,

$$\Psi(\mathbf{r}_{ab},\mathbf{r}_a,\mathbf{r}_b)=\exp[i\mathbf{k}_{nm}\cdot\mathbf{r}_{ab}]u_n{}^A(\mathbf{r}_a)u_m{}^B(\mathbf{r}_b)+\Phi(\mathbf{r}_{ab},\mathbf{r}_a,\mathbf{r}_b), \quad (5)$$

where

$$\Phi(\mathbf{r}_{ab},\mathbf{r}_a,\mathbf{r}_b)=\int\int\int(\mathbf{r}_{ab},\mathbf{r}_a,\mathbf{r}_b|G_{AB}|\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b')\times V_{AB}(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b')\Psi(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b')d\tau_{ab}'d\tau_a'd\tau_b' \quad (6)$$

and

$$\operatorname*{Lim}_{r_{ab}\to\infty}\Phi=\sum_{\alpha,\beta}\frac{\exp[ik_{\alpha\beta}r_{ab}]}{r_{ab}}F_{\alpha\beta}u_\alpha{}^A(\mathbf{r}_a)u_\beta{}^B(\mathbf{r}_b).$$

It is the scattered part of the total wave function which provides the amplitudes for any prescribed process. Consequently, we proceed to deduce the amplitude for finding system D in state t while system C is in the state s. To do so, we shall demonstrate that

$$\operatorname*{Lim}_{r_{cd}\to\infty}\Phi=\sum_{\alpha,\beta}\frac{\exp[iK_{\alpha\beta}r_{cd}]}{r_{cd}}G_{\alpha\beta}u_\alpha{}^C(\mathbf{r}_c)u_\beta{}^D(\mathbf{r}_d), \quad (7)$$

which then identifies the required rearrangement amplitude as G_{st}. The F_{ij} are the direct scattered amplitudes (no rearrangement of particles).

We begin with the observation that the Jacobian of the transformation between the two sets of coordinates $\mathbf{r}_{ab}$, $\mathbf{r}_a$, $\mathbf{r}_b$ and $\mathbf{r}_{cd}$, $\mathbf{r}_c$, $\mathbf{r}_d$ is unity. The proof is elementary and will be omitted. Therefore, the element of integration can be represented either as $d\tau_{ab}d\tau_a d\tau_b$ or $d\tau_{cd}d\tau_c d\tau_d$ and is abbreviated in what follows as $d\tau$. Furthermore,

$$\delta(\mathbf{r}_{ab}-\mathbf{r}_{ab}')\delta(\mathbf{r}_a-\mathbf{r}_a')\delta(\mathbf{r}_b-\mathbf{r}_b')=\delta(\mathbf{r}_{cd}-\mathbf{r}_{cd}')\delta(\mathbf{r}_c-\mathbf{r}_c')\delta(\mathbf{r}_d-\mathbf{r}_d').$$

With this result, we now define the Green's function for the operator $(E-H_{CD})$,

$$(E-H_{CD}(\mathbf{r}_{cd},\mathbf{r}_c,\mathbf{r}_d))(\mathbf{r}_{cd},\mathbf{r}_c,\mathbf{r}_d|G_{CD}|\mathbf{r}_{cd}',\mathbf{r}_c',\mathbf{r}_d')=\delta(\mathbf{r}_{cd}-\mathbf{r}_{cd}')\delta(\mathbf{r}_c-\mathbf{r}_c')\delta(\mathbf{r}_d-\mathbf{r}_d'), \quad (8)$$

or

$$(E-H_{CD}(\mathbf{r}_{cd}',\mathbf{r}_c',\mathbf{r}_d'))(\mathbf{r}_{cd},\mathbf{r}_c,\mathbf{r}_d|G_{CD}|\mathbf{r}_{cd}',\mathbf{r}_c',\mathbf{r}_d')=\delta(\mathbf{r}_{cd}-\mathbf{r}_{cd}')\delta(\mathbf{r}_c-\mathbf{r}_c')\delta(\mathbf{r}_d-\mathbf{r}_d'), \quad (9)$$

because of the symmetry character of the Green's function for Hermitian operators. This alternative Green's function is explicitly given by

$$(\mathbf{r}_{cd},\mathbf{r}_c,\mathbf{r}_d|G_{CD}|\mathbf{r}_{cd}',\mathbf{r}_c',\mathbf{r}_d')=\frac{-\mu_{CD}}{2\pi\hbar^2}\sum_{\gamma,\mu}\frac{\exp[iK_{\gamma\mu}|\mathbf{r}_{cd}-\mathbf{r}_{cd}'|]u_\gamma{}^C(\mathbf{r}_c)u_\mu{}^D(\mathbf{r}_d)u_\gamma{}^{C*}(\mathbf{r}_c')u_\mu{}^{D*}(\mathbf{r}_d')}{|\mathbf{r}_{cd}-\mathbf{r}_{cd}'|}, \quad (10)$$

with $K_{\gamma\mu}{}^2\equiv(2\mu_{CD}/\hbar^2)(E-\epsilon_\gamma{}^C-\epsilon_\mu{}^D)$. Proceeding with the analysis, we rewrite (6) as follows:

$$\begin{aligned}\Phi(\mathbf{r}_{ab},\mathbf{r}_a,\mathbf{r}_b)&=\int\int\int\int\int\int\delta(\mathbf{r}_{ab}-\mathbf{r}_{ab}')\delta(\mathbf{r}_a-\mathbf{r}_a')\\&\times\delta(\mathbf{r}_b-\mathbf{r}_b')(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b'|G_{AB}|\mathbf{r}_{ab}'',\mathbf{r}_a'',\mathbf{r}_b'')\\&\times V_{AB}(\mathbf{r}_{ab}'',\mathbf{r}_a'',\mathbf{r}_b'')\Psi(\mathbf{r}_{ab}'',\mathbf{r}_a'',\mathbf{r}_b'')d\tau'd\tau''\\&=\int\int\int\int\int\int\delta(\mathbf{r}_{cd}-\mathbf{r}_{cd}')\delta(\mathbf{r}_c-\mathbf{r}_c')\\&\times\delta(\mathbf{r}_d-\mathbf{r}_d')(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b'|G_{AB}|\mathbf{r}_{ab}'',\mathbf{r}_a'',\mathbf{r}_b'')\\&\times V_{AB}(\mathbf{r}_{ab}'',\mathbf{r}_a'',\mathbf{r}_b'')\Psi(\mathbf{r}_{ab}'',\mathbf{r}_a'',\mathbf{r}_b'')d\tau'd\tau'' \quad (11)\end{aligned}$$

after transformation to the set of coordinates $(\mathbf{r}_{cd},\mathbf{r}_c,\mathbf{r}_d)$. That is, the sets $(\mathbf{r}_{ab},\mathbf{r}_a,\mathbf{r}_b)$ and $(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b')$ are now regarded as functions of $(\mathbf{r}_{cd},\mathbf{r}_c,\mathbf{r}_d)$ and $(\mathbf{r}_{cd}',\mathbf{r}_c',\mathbf{r}_d')$, respectively. Upon substituting (9) into (11) and utilizing the Hermitian[5–7] property of H_{CD}, we are led to

$$\begin{aligned}\Phi=\int\int\int\int\int\int\int\int(\mathbf{r}_{cd},\mathbf{r}_c,\mathbf{r}_d|G_{CD}|\mathbf{r}_{cd}',\mathbf{r}_c',\mathbf{r}_d')\\\times[(E-H_{CD}(\mathbf{r}_{cd}',\mathbf{r}_c',\mathbf{r}_d'))\\\times(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b'|G_{AB}|\mathbf{r}_{ab}'',\mathbf{r}_a'',\mathbf{r}_b'')]\\\times V_{AB}(\mathbf{r}_{ab}'',\mathbf{r}_a'',\mathbf{r}_b'')\Psi(\mathbf{r}_{ab}'',\mathbf{r}_a'',\mathbf{r}_b'')d\tau d\tau''. \quad (12)\end{aligned}$$

[6] The Hermitian behavior of H_{CD} with respect to G_{AB} and G_{CD} is established by applying Green's theorem and proving that the resulting surface integrals vanish. The proof is analogous to that carried out in detail in reference 5 for the special case of electron exchange impact with hydrogen atoms. A less elaborate, albeit formal, approach is to treat the modified problem in the usual way through the use of a large but finite space for the scattering process with periodic boundary conditions (reference 7).

[7] Reference 2, p. 102.

By making use of the identity given in (2), (12) may be rewritten as

$$\Phi=\int\int\int\int\int\int(\mathbf{r}_{cd},\mathbf{r}_c,\mathbf{r}_d|G_{CD}|\mathbf{r}_{cd}',\mathbf{r}_c',\mathbf{r}_d')\times[\{E-H_{AB}(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b')+V_{CD}(\mathbf{r}_{cd}',\mathbf{r}_c',\mathbf{r}_d')-V_{AB}(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b')\}\times(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b'|G_{AB}|\mathbf{r}_{ab}'',\mathbf{r}_a'',\mathbf{r}_b'')]\times V_{AB}(\mathbf{r}_{ab}'',\mathbf{r}_a'',\mathbf{r}_b'')\Psi(\mathbf{r}_{ab}'',\mathbf{r}_a'',\mathbf{r}_b'')d\tau'd\tau''; \quad (13)$$

and, finally, upon employing (3) and (6) the scattered part of the wave function becomes

$$\Phi=\int\int\int(\mathbf{r}_{cd},\mathbf{r}_c,\mathbf{r}_d|G_{CD}|\mathbf{r}_{cd}',\mathbf{r}_c',\mathbf{r}_d')\times V_{AB}(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b')\Psi(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b')d\tau'+\int\int\int(\mathbf{r}_{cd},\mathbf{r}_c,\mathbf{r}_d|G_{CD}|\mathbf{r}_{cd}',\mathbf{r}_c',\mathbf{r}_d')\times\{V_{CD}(\mathbf{r}_{cd}',\mathbf{r}_c',\mathbf{r}_d')-V_{AB}(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b')\}\times\Phi(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b')d\tau'. \quad (14)$$

In the Born approximation the scattered part of the wave function in (5) is set equal to zero under the integral, with the result that

$$\Phi_{(\mathrm{Born})}=\int\int\int(\mathbf{r}_{cd},\mathbf{r}_c,\mathbf{r}_d|G_{CD}|\mathbf{r}_{cd}',\mathbf{r}_c',\mathbf{r}_d')\times V_{AB}(\mathbf{r}_{ab}',\mathbf{r}_a',\mathbf{r}_b')\exp[i\mathbf{k}_{nm}\cdot\mathbf{r}_{ab}']\times u_n{}^A(\mathbf{r}_a')u_m{}^B(\mathbf{r}_b')d\tau'. \quad (15)$$

Consequently,

$$\lim_{r_{cd}\to\infty}\Phi_{(\mathrm{Born})}=\frac{-\mu_{CD}}{2\pi\hbar^2}\sum_{\alpha,\beta}\frac{\exp[iK_{\alpha\beta}r_{cd}]}{r_{cd}}u_\alpha{}^C(\mathbf{r}_c)u_\beta{}^D(\mathbf{r}_d)\times\int\int\int\exp[-i\mathbf{K}_{\alpha\beta}\cdot\mathbf{r}_{cd}]u_\alpha{}^{C*}(\mathbf{r}_c)u_\beta{}^{D*}(\mathbf{r}_d)\times V_{AB}(\mathbf{r}_{ab},\mathbf{r}_a,\mathbf{r}_b)\exp[i\mathbf{k}_{nm}\cdot\mathbf{r}_{ab}]\times u_n{}^A(\mathbf{r}_a)u_m{}^B(\mathbf{r}_b)d\tau, \quad (16)$$

and the Born rearrangement amplitude for finding systems C in state s and D in the state t after A in state n collides with B in state m is given by

$$G_{st}{}^{(\mathrm{Born})}=\frac{-\mu_{CD}}{2\pi\hbar^2}\int\int\int\exp[-i\mathbf{K}_{st}\cdot\mathbf{r}_{cd}]\times u_s{}^{C*}(\mathbf{r}_c)u_t{}^{D*}(\mathbf{r}_\alpha)V_{AB}(\mathbf{r}_{ab},\mathbf{r}_a,\mathbf{r}_b)\times\exp[i\mathbf{k}_{nm}\cdot\mathbf{r}_{ab}]u_n{}^A(\mathbf{r}_a)u_m{}^B(\mathbf{r}_b)d\tau. \quad (17)$$

In a similar manner (14) will provide the exact functional for the rearrangement amplitude.

In conclusion, it is evident from (17) that V_{AB}, and not V_{CD}, is the correct interaction energy so that, in principle, no ambiguity in matrix element exists. It should be pointed out that we have treated all the particles as if they were distinguishable. This produces no loss in generality, since linear combinations of the exchange degenerate wave functions can be conveniently formed in the end so that the proper symmetry in each group of identical particles is assured.