New quantum numbers in collision theory. IV. Separation of the first Born contributions

Chun Woo Lee and U. Fano
James Franck Institute, University of Chicago, Chicago, Illinois 60637
(Received 18 February 1987)

The major contribution to forward scattering amplitudes for inelastic electron collisions, from the first Born approximation, is separated out from the remainder in the expressions of differential cross sections and of target orientation, for purposes of analysis. Simple results of this analysis are presented for $e+\mathrm{He}$ collisions, as a preliminary to a more detailed analysis of the same data in a separate paper.

The first Born approximation affords an adequate representation of the contribution of long-range Coulomb interactions to the inelastic scattering of charged particles, a contribution that accounts for most of the total cross section. The Born scattering amplitude S_B depends mainly on the momentum $\mathbf{q}=\mathbf{p}_a-\mathbf{p}_b$ transferred from projectile to target in the collision; it is represented simply by $S_B \propto F(q)/q^2$, where the "form factor" $F(q)$ is the Fourier transform of the charge density associated with the transition between target states induced by the collision. The large value of the differential cross section for 0° scattering stems from the small value of the corresponding value of $q_{\min}=\Delta E/v_a$, where ΔE indicates the energy imparted to the target and $v_a=p_a/m$ the impact velocity.[1]

On the other hand S_B alone would yield *no contribution* to the target's orientation, which hinges on the interference of scattering amplitude terms 90° out of phase on account of its odd parity under time reversal. Contributions of S_B to orientation occur nevertheless from its interference with the residual scattering amplitude

$$S_R=S_{\text{exact}}-S_B \ . \tag{1}$$

Systematic sorting out of the contributions of S_B and S_R thus emerges as a *promising tool of analysis* in collision theory, a point that may not have been stressed in the past. Note, as a preliminary to this analysis, that S_R is conveniently evaluated by partial-wave analysis, being a far smoother function of the scattering angle θ than S_B is; S_B itself is nevertheless readily expanded into its partial-wave contributions.

The previous papers of this series[2] have represented the invariant scattering matrix element S_{exact} in the form $(L_B l_B \mid S(j_t) \mid L_A l_a)$. Here (l_a,l_b) indicate orbital quantum numbers in the partial-wave analysis of the projectile wave functions with momenta $\mathbf{p}_a$ and $\mathbf{p}_b$, before and after an inelastic collision, respectively; (L_A,L_B) indicate the

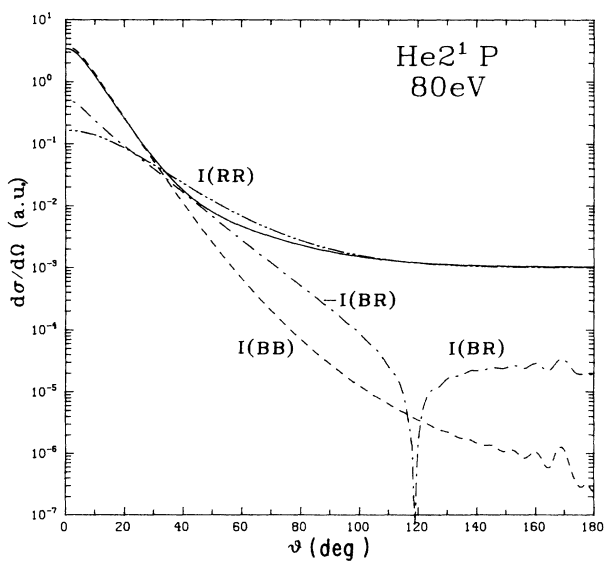

FIG. 1. Contributions of the first Born $I(BB)$, residue $I(RR)$, and cross term $I(BR)$ to the differential cross section in atomic units a_0^2 vs θ: for process (3) at 80 eV. ——, total; — — —, $I(BB)$; —·— $I(BR)$; —··—, $I(RR)$.

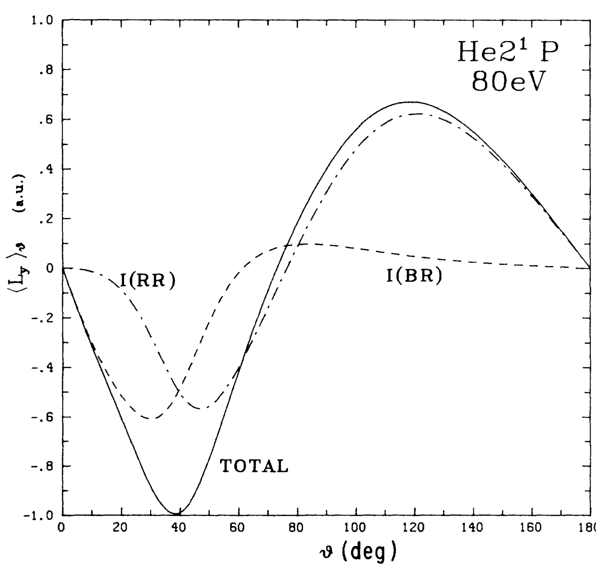

FIG. 2. Contributions of the cross term $I(BR)$ and residue $I(RR)$ to the orientation $\langle L_y\rangle_\theta$. ——, total, — — —, $I(BR)$, —·—, $I(RR)$.

corresponding angular momenta of the target; and $\mathbf{j}_t = \mathbf{l}_a - \mathbf{l}_b^* = \mathbf{L}_B - \mathbf{L}_A^*$ represents the angular momentum transferred in the collision (Ref. 2, paper III). The differential cross section for target excitation with projectile deflection θ and the expectation value $\langle L_y \rangle_\theta$ of the target's final angular momentum in the direction y parallel to $\mathbf{p}_b \times \mathbf{p}_a$ are bilinear functions of S_{exact} and of its Hermitian conjugate $S_{\text{exact}}^\dagger$.

Reference 2 has replaced the pair of orbital momenta labels (l_a, l_b) of S_{exact} and the corresponding pair (l_a', l_b') of $S_{\text{exact}}^\dagger$ by a set of linear combinations $\{\sigma,\tau,\zeta,\eta\}$, which have even or odd parity under the permutation P of (l_a, l_b) with (l_a', l_b') and under the permutation Q of (l_a, l_a') with (l_b, l_b'). Paper III has also shown how collision cross sections and other observables are represented by linear combinations of matrix elements of the direct product $S_{\text{exact}}^\dagger \times S_{\text{exact}}$ labeled by the new quantum numbers. (The coefficients of these matrix elements are standard algebraic functions of $\{\sigma,\tau,\zeta,\eta\}$, even or odd under the permutation P and Q.) The first Born and residual contributions to observables are then sorted out by representing each matrix element in the form

$$\begin{aligned}(S_{\text{exact}}^\dagger \times S_{\text{exact}})_{\sigma\tau\eta\zeta} &= [(S_B^\dagger \times S_B) + (S_B^\dagger \times S_R) + (S_R^\dagger \times S_B) + (S_R^\dagger \times S_R)]_{\sigma\tau\zeta\eta} \\ &= [I(BB) + I(BR) + I(RR)]_{\sigma\tau\zeta\eta} ,\end{aligned} \tag{2}$$

where $I(BB)$ stands for $S_B^\dagger \times S_B$, $I(BR)$ for the pair of cross terms, and $I(RR)$ for $S_R^\dagger \times S_R$. Note that the contributions of $I(BB)$ and $I(RR)$ to cross sections are nonnegative but that of $I(BR)$ is not.

We illustrate the general result (2) using the scattering matrix S_R obtained for the collision process

$$e + \text{He}(1s^2\,{}^1S) \rightarrow e + \text{He}(1s2p\,{}^1P^\circ) \tag{3}$$

by a distorted-wave Born approximation to be described in a following paper. Figure 1 presents the separate contributions to the differential cross section from the terms labeled $I(BB)$, $I(BR)$, and $I(RR)$ in (2). Figure 2 presents the corresponding contributions to the orientation $\langle L_y \rangle_\theta$, where $I(BB)$ vanishes (as noted above) because the $I(BB)$ terms are invariant under the permutations P and Q but their coefficients are odd under Q in the case of orientation according to paper III, Eq. (29).

Figure 1 shows a predominance of the contributions $I(BB)$ at small θ which is very striking in view of the logarithmic scale of ordinates. The contribution $I(RR)$ predominates instead at $\theta > 40°$, where $I(BB)$ is very small. The cross term $I(BR)$ is less important and is negative at $\theta < 120°$. The oscillations of $I(BR)$ and of $I(BB)$ at $\gtrsim 150°$ are artifacts of calculation amplified by the poor convergence of partial-wave expansions in spherical harmonics whose sign *oscillates* at large angles. This artifact, which has plagued many collision calculations,[3] could presumably be removed by an appropriate rearrangement of the harmonic expansion.

Figure 2 provides an interesting analysis of the orientation into two components only: The cross term $I(BR)$ contributes most at $\theta \lesssim 20°$, thus reflecting the large values of S_B where S_R nearly vanishes as $\theta \rightarrow 0°$. Conversely $I(BR)$ nearly vanishes at $\theta \gtrsim 50°$ where $I(RR)$ predominates.

This work has been supported by the U.S. Department of Energy, Division of Basic Chemical Sciences. One of us (C.W.L.) wants to thank Y. S. Lee for providing the ATMSCF computer code. This work was submitted in partial fulfillment of the requirements for a Ph.D. degree from the Department of Chemistry at the University of Chicago.

[1]See, e.g., Chap. 3 of U. Fano and A. R. P. Rau, *Atomic Collisions and Spectra* (Academic, New York, 1986).

[2]C. W. Lee and U. Fano, Phys. Rev. A **33**, 921 (1986), paper I; C. W. Lee, Phys. Rev. A **34**, 959 (1986), paper II; C. W. Lee and U. Fano, preceding paper, Phys. Rev. A **36**, 66 (1987); C. W. Lee (unpublished).

[3]This artifact has required many more partial waves than necessary, e.g., in Madison and Shelton's calculation, Phys. Rev. A 7, 499 (1973).