

PHYSICAL REVIEW LETTERS

VOLUME 19

16 OCTOBER 1967

NUMBER 16

EXPANSION APPROACH TO LOW-ENERGY ELECTRON-HYDROGEN-ATOM SCATTERING

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(Received 30 August 1967)

A new expansion method for calculating scattering phase shifts has been described previously by one of us and applied to *s*-wave scattering by an attractive Yukawa potential.¹ We report here the first numerical results obtained from this method for electron-atom scattering. We consider the low-energy collision of electrons with atomic hydrogen in its ground state. The stationary-state wave function is written as

$$\Psi = a_1\psi_1 + a_2\psi_2 + \Phi, \quad (1)$$

where ψ_1 and ψ_2 are asymptotic forms, and Φ is a compound-state wave function represented by a configuration-interaction (CI) expansion built solely from Slater-type orbitals (STO). The role of Φ is to describe short-range interactions and it therefore includes components corresponding to states of H^- . Forms ψ_1 and ψ_2 are built from properly antisymmetrized and spin-projected functions which can be written for a general target atom as

$$\psi_i = A_{N+1} \Theta_{S+\frac{1}{2}, N+1} (A_N \Theta_{S, N} \Xi_N \theta_N) \varphi_i \alpha, \quad (2)$$

where A_N represents an N -electron antisymmetrizer and $\Theta_{S, N}$ is an N -electron spin projector for total spin quantum number S . $\Xi_N \theta_N$ is an N -electron function for the isolated target atom. The free-wave spatial orbitals φ_i are taken, following Armstead,² for waves of

angular quantum number l and energy $\frac{1}{2}k^2$, as

$$\varphi_1 = j_l(kr); \quad \varphi_2 = j_{l+1}(kr) + [(l+1)/kr]j_{l+2}(kr). \quad (3)$$

The coefficients a_1 and a_2 in Eq. (1) are determined by a procedure¹ which causes Ψ to converge toward a solution of the Schrödinger equation for scattering energies determined by the choice of Φ . With the forms chosen for ψ_i , the phase shift is $\eta = -\tan^{-1}(a_2/a_1)$. Actual computations require matrix elements involving the functions represented by Eq. (2) and the basis functions for Φ . The necessary integrals can be evaluated with relative ease, but the matrix element formation is a rather complicated algebraic problem which will be described later.

We have studied singlet and triplet *s*- and *p*-wave scattering of electrons from the $1s$ state of hydrogen in the static exchange approximation. Exact solutions of the differential equations for this approximation have been given by John³ and Omidvar.⁴ The compound-state wave function Φ is built from Slater-type orbitals of *s* and *p* symmetry. The STO form as taken as $r^{n-1} \exp(-\zeta r + im\varphi) P_l^{lm}(\theta)$. As an example of how this compound-state function is constructed for *S* states, Φ is taken as a configuration interaction expansion built from *s*-type STO's of differing principal quantum number. For the results shown in Fig.

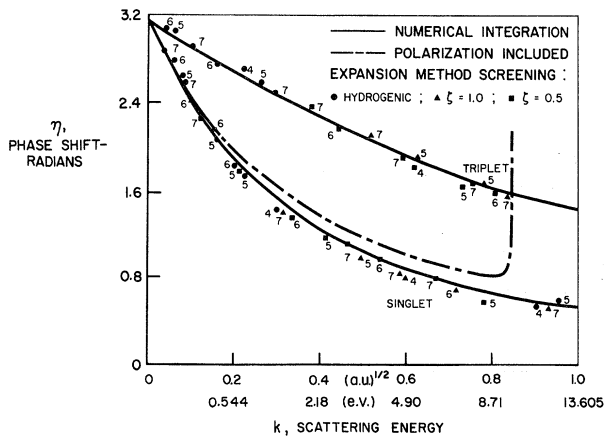


FIG. 1. *S*-wave phase shifts for electron-hydrogen-atom scattering. Numbers adjacent to points indicate the expansion lengths. Scattering energy defined by $k^2 = 2E$, with E in a.u.

1, this expansion consisted of configurations of the type $(1s ns)$ with $n=1, 2, \dots, 7$ and with screening constants, ζ , chosen to reach different regions of the scattering energy. For *p*-wave scattering, the expansion consisted of configurations of the type $(1s np)$. These configurations are appropriate to the static exchange approximation. For the singlet-state *s*-wave function, one bound level exists, and the basis of Φ permitted its description. The results are given in Fig. 1 for *s*-wave and in Fig. 2 for *p*-wave scattering. The calculated phase shifts are somewhat more sensitive to the basis of Φ for the case of *p*-wave scattering but

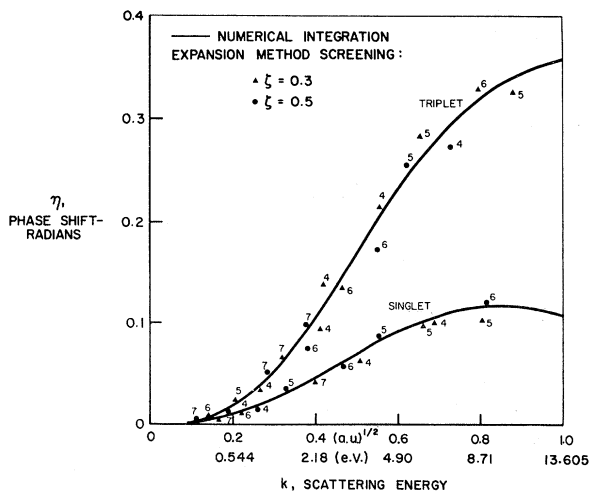


FIG. 2. *p*-wave phase shifts for electron-hydrogen-atom scattering.

exhibit proper convergence with increased expansion length. This expansion method requires that the scattering energies be chosen as the eigenvalues of the secular equation which corresponds to the CI expansion for Φ . This requirement is not restrictive, however, since small changes in the screening values cause a shift in the eigenvalues, thus allowing one to reach almost any scattering energy.

Additional calculations, which include distortion and polarization effects, are now in progress. Preliminary results for singlet *s*-wave scattering are shown in Fig. 1. These results indicate a first resonance at $k = 0.838$ in excellent agreement with previous studies.^{5,6} These calculations include in Φ , in addition to configurations of the type $(1s ns)$, correlation functions such as $(ns n's)$, $(np n'p)$, $(nd n'd)$, etc., properly projected and antisymmetrized to insure over-all 1S symmetry. Some calculations for triplet *s*-wave scattering have also been performed. These initial studies show a scattering resonance at $k \approx 0.86-0.87$.

The results reported here, which give a good definition of the scattering from zero energy to the first excitation level, were produced at the total expense of 9 min of over-all computer time (UNIVAC 1108). More significantly, the described procedure is applicable to scattering from much heavier target atoms where direct numerical integration or other variational approaches are prohibitive owing to the immense effort and time involved. We have programmed this procedure to handle elastic scattering from atoms containing as many as 36 electrons and will report results on alkali and atmospheric gas atoms in the near future.

We acknowledge the assistance of Miss Roslie Scolsky in the development of the computer programs.

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