Semiclassical Calculation of Elastic H^+-He Differential Scattering Cross Sections*

H. F. Helbig, D. B. Millis, and L. W. Todd
Department of Physics, Clarkson College of Technology, Potsdam, New York 13676
(Received 3 December 1969)

Elastic differential cross sections for proton-helium scattering are calculated in the semiclassical approximation for two assumed interaction potentials. Both potentials are of the form

$$V(r; A, B, C) = (2/r)e^{-r/A}[1 + r/A + \tfrac{1}{2}r^2(1/A^2 - U/B)] - U[1 + r/B + (r/C)^2 + 2Ur^4/\alpha]^{-1},$$

where U is the difference between the ground-state energies of He and Li^+ (4.373 11 hartree) and α is the polarizability of He (1.3835 bohr^3). The first potential $V_M \equiv V(r; 0.423, 0.483, 0.441)$ fits the He-H^+ ground-state energies which Michels has calculated. The second, $V_W \equiv V(r; 0.442, 0.505, 0.451)$, is similar to V_M except that its minimum is decreased by 10% to agree with the value obtained by Wolniewicz. The cross sections for these two potentials are shown for protons incident at energies T of 7, 19, 58, and 116 eV in the laboratory frame and for scattering angles, at each energy, out to the rainbow angle θ_R. θ_R is given in center-of-mass coordinates by the expression $\theta_R T \cong 0.1$ rad hartree. As the collision energy decreases, the cross sections develop oscillatory structure not present in the classical cross sections. This structure and the rainbow angle are sensitive to the choice of potential, which suggests that measurements of H^+-He cross sections may be used to test the suitability of, e.g., the Born-Oppenheimer potential for scattering phenomena. It is also suggested that many-body calculations of these cross sections would allow, by comparison with the present results, an evaluation of the potential scattering model.

INTRODUCTION

While the potential scattering model has proved effective for describing collisions between composite systems, a complete understanding of its utility must await comparison between its predictions and those of an *ab initio* many-body calculation. The proton–helium-atom collision has many advantages as the site for such a comparison. It involves four particles whose interactions are well understood and, through the Born-Oppenheimer[1] approximation, lends itself to a fairly straightforward potential scattering analysis. (The H^+-H system, in addition to its experimental difficulties, possesses a degenerate ground-state energy at large internuclear separations, thus requiring a two-state description at all collision energies. There is evidence[2] that a single state is adequate to describe the H^+-He collision at energies below 1 keV.)

Within the context of the potential scattering model itself, it is of interest to determine the relevance of the quasistatic Born-Oppenheimer potential energy to scattering situations. Low-energy proton-helium scattering affords a comparison between relatively simple measurements and clean-cut theoretical predictions involving a single (well-studied) Born-Oppenheimer energy curve.

Apart from its archetypal qualities, the proton-helium collision is interesting in its own right, a not surprising result for the interaction between the two most prevalent atoms in the universe. Michels[3] gives an excellent review of recent areas of concern.

Previous calculations of the differential scattering cross section for H^+-He date back to the work of Massey and Smith[4] who used classical scattering theory and the Hartree[5] field of the helium atom to represent the interaction. Their results differed from the measurements of Ramsauer and Kollath[6] in a way which was in qualitative agreement with their oversimplification of the interaction. Everhart, Stone, and Carbone[7] presented results of a classical calculation of the differential cross section for scattering from a screened Coulomb potential which might be applied to the H^+-He collision. Helbig and Everhart[2] gave the results of a classical calculation of the deflection function for H^+-He, from which high-energy differential scattering cross sections might be derived. Green and Johnson[8] obtained the differential cross section for scattering from the ground- and first-excited state potentials of He-H^+ which were computed by Michels[3] and Wolniewicz.[9] Their attention was limited, however, to the region of large angles and high energies, where quantum effects in the elastic cross section are unimportant.

In this paper it is shown that the interaction potential reveals its structure most clearly in the region where quantum effects begin to emerge. In particular, small changes in the assumed potential energy function are shown to produce sig-

nificant differences in the resulting cross sections.

It is hoped that the present results, besides providing workaday cross sections for this system, will stimulate further progress, both theoretical and experimental, toward tests of the potential scattering model and of the application of Born-Oppenheimer energies to scattering interactions.

Atomic units ($\hbar = a_0 = m_e = 1$) are used unless otherwise indicated.

CALCULATION

The calculation procedure described by Bernstein[10] was used.[11] In brief outline, the scattering amplitude $f(\theta)$ was obtained by replacing the Rayleigh-Faxen-Holtsmark[12] sum over partial waves of angular momentum l with an integral which was then evaluated by the method of stationary phase.[13]

Phase Shifts

The required phase shifts $\eta(l)$, where l is the angular momentum, were calculated in the JWKB approximation.[12] To check the accuracy of this approximation, a few of the η's were compared with exact[14] values. Approximately constant differences of about 0.1% were found. To find the effect of these inaccuracies in η, all of the cross sections were recomputed from phase shifts containing an artificial systematic[15] error of 5%, i. e., 50 times the error we estimate for the JWKB phases. A typical recomputed cross section (marked X) is shown at the bottom of Fig. 1 along with the corresponding cross section computed from JWKB phase shifts. From such results we conclude that the JWKB approximation introduces no more than a 1% inaccuracy in the present cross-section calculations.

Interaction Potentials

We found it convenient to use the analytic function

$$V(r; A, B, C) = (Z_1 Z_2 / r) e^{-r/A} P_1 - U/P_2 ,$$

where $$P_1 \equiv 1 + r/A + r^2 (\tfrac{1}{2} A^2 - U/BZ_1Z_2)$$

and $$P_2 \equiv 1 + r/B + (r/C)^2 + 2Ur^4/\alpha ,$$

to represent the potential energy of $He\text{-}H^+$. In this expression A, B, and C are adjustable parameters, U is the difference between the ground-state electronic eigenenergy of the united atom (Li^+, in the present case) and the separated atoms, and α is the polarizability of the target atom. The other symbols have their customary connotations. With $U = 4.37311$ hartree and $\alpha = 1.3835$ bohr^3, $V_M(r) \equiv V(r; 0.423, 0.483, 0.441)$[16] fits the Born-Oppenheimer energies calculated by Michels[3] within 0.001 hartree (except at 0.1 bohr, the inner limit of Michels's calculation). With the same values for U and α, $V_W(r) \equiv V(r; 0.442, 0.505, 0.451)$ is deepened so as to pass through the value -0.075 hartree at its minimum in accord with the accurate variational calculation of Wolniewicz.[9] Except for the increase in well depth from -0.067 to -0.075 hartree, V_W is quite similar to V_M.

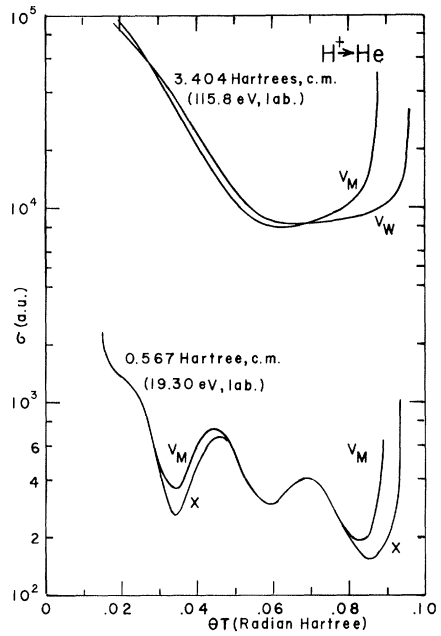

FIG. 1. Differential cross sections, marked with the potentials from which they are derived, are plotted versus the product θT of c.m. scattering angle and c.m. impact energy. The upper curves show that measurable differences may be distinguished between two reasonable choices of interaction potential. In the lower pair, the curve marked X shows the consequences of a systematic 5% error in the phase shifts which produced its companion.

While the necessary interpolations between Michels's values for the interaction energy could be obtained in other ways, a reasonable potential function has obvious utility for coordinating the single energy value of Wolniewicz with Michels's work on the general shape of the energy function. In addition, other variations of $V(r; A, B, C)$ may be made easily should experimental measurements indicate the need for yet a different potential. Finally, this form of the potential function may be useful for representing similar interactions, such as those between protons and other noble gases.[17]

RESULTS

Differential cross sections $\sigma(\theta)$ for center-of-mass (c.m.) collision energies of 3.404, 1.702, 0.567, and 0.213 hartree are shown in Fig. 2 for calculations based on semiclassical and classical

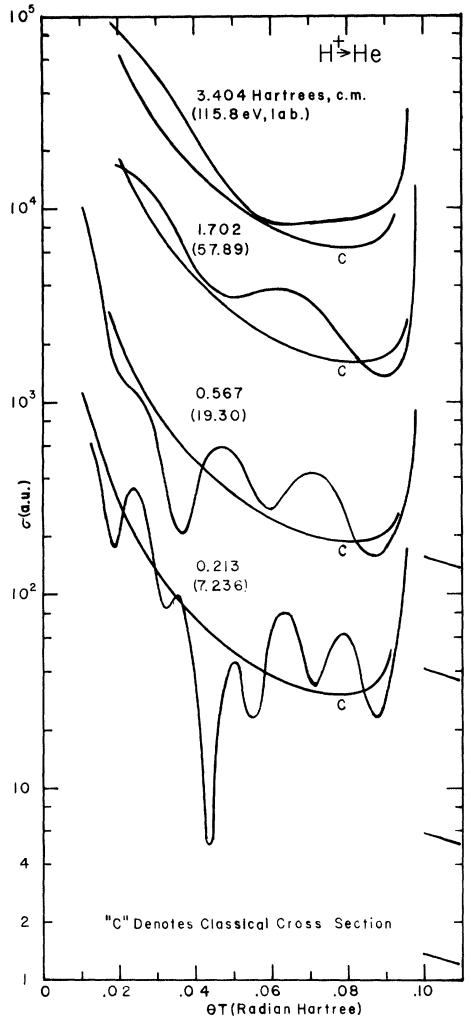

FIG. 2. Proton-helium differential cross sections, calculated from the potential V_W, are plotted versus θT for several incident energies. θ is the c.m. scattering angle; T the c.m. impact energy.

methods. The energies were chosen to be in the center of the efficient scattering region.[18] (In both Figs. 1 and 2, the cross sections are plotted versus the product θT of c.m. scattering angle and c.m. collision energy to counteract the compression of the scattering pattern into the forward direction at increasing energies.)

The development of nonclassical effects with decreasing energy (increasing proton wavelength) is evident in Fig. 2, which shows the cross sections determined from the potential V_W. The classical cross sections (marked C) are shown for comparison. The possibility for collision spectroscopy, so aptly named by Smith *et al.*[19] is clear.

The abrupt rise in each of the cross sections which occurs just outside $\theta T = 0.09$ rad hartree is an artifact of both the classical and semiclassical analyses. By utilizing a simple correction[20] in terms of the Airy function, it can be shown that some remnant of this rainbow effect would survive a full wave treatment of the collision. Indeed, when the Airy correction is applied at the rainbow angle θ_R (the position of the classical pole in σ), one finds that the cross sections have values lying between the tops of the semiclassical curves and their continuations at the right-hand edge of Fig. 2. The indication, then, is that the rainbow effect will be marked, in fact, by a relatively abrupt change in the slope of the cross section in the vicinity of θ_R. Unfortunately, the Airy correction is valid only very near θ_R for the present calculations and therefore cannot be used to delineate the transition between the left- and right-hand portions of the cross-section curves.[21,22]

The possibility of utilizing the rainbow effect to decide between the assumed interaction potentials is indicated at the top of Fig. 1. Here predicted cross sections for the scattering of 115.8-eV protons from helium atoms at rest in the laboratory frame are shown, based on each of the two potentials V_M and V_W. The outward shift of the rainbow angle for the deeper potential (V_W) is evident. Calculations with potentials of equal depth but different minimum *locations* show little change in the rainbow position, as has been pointed out by Mason[23] for an "exp-six" potential. Thus an experimental determination of θ_R should allow the potential-well depth to be found rather accurately. This is of particular interest in the case of He-H^+ for which no dissociation-energy measurements exist.[24]

In summary, it appears that the proton-helium collision is unusually well suited for testing at least two basic aspects of scattering theory. Since the potential scattering model proves to yield cross sections which are quite sensitive to the assumed potential function, its predictions can be compared with experimental measurements to determine the relevance of, e.g., the Born-Oppenheimer energy to scattering problems. The simplicity of the system makes it a likely candidate for many-body studies which will allow assessment of the potential scattering model itself.[25]

Note added in proof: Recently we have succeeded in computing the 0.567 hartree H^+-He differential scattering cross section by summation of the Rayleigh-Faxen-Holtsmark (RFH) equation. The result agrees with the present calculation inside the rainbow angle and shows considerable structure beyond the rainbow region before running parallel to the classical result at larger angles. Phase shifts out to $l = 4000$ (JB approximation after $l = 140$) were required for three-place convergence in σ. With the phase shifts in hand, it required

about 6 min to compute the stationary-phase cross section and about 66 min for the RFH sum.

ACKNOWLEDGMENTS

The authors wish to express their thanks to Professor A. W. Czanderna, Professor F. L. Moore, Professor D. J. Kaup, and Professor A. Rotsstein for helpful discussions, and to Warren E. Ferguson, Jr., for his assistance with some of the machine calculations used.

---

*Work supported by the National Science Foundation.

[1]M. Born and J. R. Oppenheimer, Ann. Physik 84, 457 (1927); see also J. C. Slater, *Quantum Theory of Matter*, 2nd ed. (McGraw-Hill, New York, 1968), Chap. 19.

[2]Intrusion of the lowest-lying excited states of $He-H^+$ would be marked by the inelastic process of electron transfer to the proton. Measurements indicate that the probability of this transfer is less than a few percent at low collision energies. See H. F. Helbig and E. Everhart, Phys. Rev. 136, A674 (1964).

[3]H. H. Michels, J. Chem. Phys. 44, 3834 (1966).

[4]H. S. W. Massey and R. A. Smith, Proc. Roy. Soc. (London) A142, 142 (1933).

[5]D. R. Hartree, Proc. Cambridge Phil. Soc. 24, 89 (1928); 24, 111 (1928); 24, 426 (1928).

[6]C. Ramsauer and R. Kollath, Ann. Physik 16, 570 (1933).

[7]E. Everhart, G. Stone, and R. J. Carbone, Phys. Rev. 99, 1287 (1955).

[8]T. A. Green and R. A. Johnson, Phys. Rev. 152, 9 (1966); this and many other calculations on the $He-H^+$ system have been concerned with the inelastic process of electron capture by the incident proton.

[9]L. Wolniewicz, J. Chem. Phys. 43, 1087 (1965).

[10]R. B. Bernstein, *Advances in Chemical Physics* (Wiley, New York, 1966), Vol. X, p. 75.

[11]Details of the numerical techniques appear in the Ph. D. dissertation of D. B. Millis, Clarkson College of Technology, Potsdam, N. Y. (unpublished).

[12]See, for example, N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions*, 3rd ed. Oxford U. P., London, 1965).

[13]See, for example, H. Jeffries and B. S. Jeffries, *Mathematical Physics*, 3rd ed. (Cambridge U. P., Cambridge, England, 1956)

[14]Fourth-order Runge-Kutta methods were used to solve for the zeros of the radial wave equation and of the corresponding spherical Bessel functions. Only a few of the exact phase shifts were calculated since each of them required about 30 min on the Clarkson College IBM 360 computer. Since the present calculations require the order of 100 phase shifts at each energy, working with exact values was impractical.

[15]While *systematic* inaccuracies in η distort the cross sections, *random* inaccuracies can obliterate them altogether. This is because the cross sections depend not only on η, but upon its first and second derivatives as well. The numerical procedures for obtaining (and interpolating between) these quantities thus require that η be a smooth function of l up to the third derivative. Random inaccuracies in η will destroy this required smoothness, resulting in erratic derivatives and unrecognizable cross sections.

[16]The parameters A, B, and C for $V_M(r)$ were determined by a systematic search of A-B-C space for the minimum of the sum of the squares of the fractional differences between $V(r; A, B, C) - 2/r$ and the electronic energies of $He-H^+$ which Michels gives at twelve internuclear separations. For $V_W(r)$, A, B, and C were determined from numerical studies of the behavior of $V(r; A, B, C)$ which are being extended for future publication.

[17]Recent work on the $Ar-H^+$ system indicates the need for a more realistic potential function than the traditional (and analytically elegant) forms provide. See F. A. Herrero, E. M. Nemeth, and T. L. Bailey, J. Chem. Phys. 50, 4591 (1969).

[18]This region is defined by the conditions that (i) the proton wavelength λ is small enough so that the scattering will be sensitive to the shape of the attractive-repulsive (AR) potential ($\lambda < \frac{1}{2}a$, where a is characteristic of the AR potential-well width); yet (ii) the proton momentum $2\pi/\lambda$ is small enough that the nominal classical deflection angle $\theta = \epsilon/2T$ is larger than a typical experimental resolution of 2×10^{-3}. Here ϵ is the well depth of the AR potential and T is the c.m. impact energy. These conditions lead to the inequalities $16\pi^2/2\mu a^2 < T < 250\epsilon$ (where μ is the system's reduced mass) which define the region of efficient collision energies. See N. F. Mott and H. S. W. Massey, Ref. 12, p. 111 for a discussion of condition (i) and the formula used for θ. It is interesting to note that the condition $\mu a^2\epsilon > 0.3$, which guarantees a range of efficient collision energies for scattering from an AR potential is very close to the condition that the potential will support a bound state.

[19]F. T. Smith, R. P. Marchi, W. Aberth, and D. C. Lorents, Phys. Rev. 161, 31 (1967).

[20]Ref. 10, p. 104.

[21]The right-hand portions of the cross-section curves shown in Fig. 2 connect smoothly with the results of Green and Johnson (Ref. 8) at larger angles and energies.

[22]Preliminary efforts to sum the Rayleigh-Faxen-Holtsmark equation directly reveal a slow rate of convergence at the present energies and the consequent need to generate a much larger set of phase shifts than for the semiclassical calculation. Nonetheless, it is clear that the classical rainbow spike is survived only by a rapid decrease in the cross section outside θ_R. Most interesting is the appearance, in the exact calculation, of pronounced structure outside θ_R. Further work on this problem is in progress.

[23]E. A. Mason, J. Chem. Phys. 26, 675 (1957).

[24]B. G. Anex, J. Chem. Phys. 38, 1652 (1963).

[25]It would be interesting to see what success classical analysis might have, treating the helium atom as a dynamic multipole. See M. Gryzinski, Phys. Rev. Letters 24, 47 (1970).