Low-energy collisions of D^+ with D and He^{2+} with He

J. M. Wadehra
Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, Pennsylvania 15260
(Received 25 May 1979)

Quantum-mechanical calculations for differential cross sections and various transport cross sections describing the thermal-energy collisions of D^+ with D and He^{2+} with He are presented. Lowest-order Viehland-Mason theory is used to calculate mobility of D^+ in D. The zero-field mobility at 77, 303, and 10000 K is, in units of $cm^2 V^{-1} s^{-1}$, 10.5, 7.0, and 2.1, respectively.

I. INTRODUCTION

Recent efforts concerning the inertial confinement of plasma for fusion purposes using intense ion beams have been quite successful.[1] In this scheme tiny pellets of deuterium, used as fuel, are imploded by powerful ion beams. The data on the low-energy collisions of deuterons with deuterium have therefore become of great practical importance in the design of ion sources and ion beams. Considerable interest has also been shown in low-energy collisions of He^{2+} with He in recent experimental[2] as well as theoretical[3,4] studies. The purpose of this paper is to present theoretical results of transport cross sections of D^+ in D and He^{2+} in He and of mobility of D^+ in D. The mobility is calculated for various gas temperatures for electric field strength to number density ratio $\mathcal{E}/N$ between 0 and 250 Td where 1 Td $=10^{-17}$ V cm^2. Finally, the angular distribution for collisions of D^+ with D and He^{2+} with He is shown in the form of low-energy differential cross sections.

II. CROSS SECTIONS AND MOBILITY

The interaction of the atomic ion $D^+(^1S_0)$ or $He^{2+}(^1S_0)$ with ground-state atom $D(^2S_{1/2})$ or $He(^1S_0)$ is governed by two potential curves: $^2\Sigma_g^+$ and $^2\Sigma_u^+$ for D_2^+ and $^1\Sigma_g^+$ and $^1\Sigma_u^+$ for He_2^{2+}. If δ_l^g (δ_l^u) is the lth-order phase shift associated with the elastic scattering by gerade (ungerade) potential, then, taking appropriate account of the nuclear spin and statistics (the nuclear spin is $S=1$ for deuterium and $S=0$ for helium), the square of the absolute scattering amplitude for an integer spin can be written as[5]

$$|f(\theta)|^2=\frac{S+1}{2S+1}\left|\sum_{l\text{ even}} f_l^g(\theta)+\sum_{l\text{ odd}} f_l^u(\theta)\right|^2 +\frac{S}{2S+1}\left|\sum_{l\text{ even}} f_l^u(\theta)+\sum_{l\text{ odd}} f_l^g(\theta)\right|^2, \tag{1}$$

where

$$f_l^{g,u}(\theta)=(2ik)^{-1}(2l+1)[\exp(2i\delta_l^{g,u})-1]P_l(\cos\theta), \tag{2}$$

k being the wave number of relative motion.

Various transport cross sections involving weighted deflection angles are defined as

$$Q^{(l)}=\frac{2\pi}{C_l}\int_0^\pi (1-\cos^l\theta)I(\theta)\sin\theta\, d\theta, \tag{3}$$

where

$$C_l=1-\frac{1+(-1)^l}{2(l+1)}$$

and $I(\theta)$ is the differential cross section; $I(\theta)=|f(\theta)|^2$. The total cross section is

$$Q_{\text{tot}}=2\pi\int_0^\pi I(\theta)\sin\theta\, d\theta. \tag{4}$$

A general expression for all the transport cross sections in the form of sums over partial waves can be written down[5,6] in a straightforward but tedious manner.

The zeroth-order Viehland-Mason theory[7] for the calculation of the mobility starts by assuming that the relative motion of the ions and the atoms obeys the Maxwell-Boltzmann distribution with an effective temperature given by Wannier's law:

$$\tfrac{3}{2}k_B T_{\text{eff}}=\tfrac{3}{2}k_B T_{\text{gas}}+\tfrac{1}{2}mv_d^2, \tag{5}$$

where m is mass of the ion and k_B is Boltzmann's constant. The drift velocity v_d is related to the field strength $\mathcal{E}$ by the reduced mobility K_0, $v_d=K_0\mathcal{E}$, and K_0 is calculated from

$$K_0=\frac{3}{8}\frac{q}{N_0}\left(\frac{\pi}{mk_BT_{\text{eff}}}\right)^{1/2}\frac{1}{\Omega^{1,1}(T_{\text{eff}})}, \tag{6}$$

where q is the charge on the ion, N_0 is the standard atomic number density (2.69×10^{19} cm^{-3}), and $\Omega^{1,1}(T)$ is the collision integral

$$\Omega^{1,1}(T)=\frac{1}{2}\int_0^\infty x^2Q^{(1)}(x)\exp(-x)dx, \tag{7}$$

with $x=E/k_BT$.

III. CALCULATIONS AND RESULTS

A. D^+ with D

The lowest $^2\Sigma_g^+$ and $^2\Sigma_u^+$ potential curves of D_2^+ dissociating into $D(^2S_{1/2})$ and $D^+(^1S_0)$ for large separations are tabulated numerically by Peek,[8] up to internuclear separations of $30a_0$. For internuclear separations greater than $30a_0$ the two states become degenerate within the accuracy considered and both the potential curves are approximated by the asymptotic form

$$V(R) = -C_4/R^4 - C_6/R^6\,, \qquad (8)$$

where $C_4 = 2.25$ a.u. and $C_6 = 9.45$ a.u. The coefficient C_4 is one-half the dipole polarizability of hydrogen[9] and C_6 is obtained by fitting the asymptotic form (8) to the potential curves[8] of D_2^+ around $30a_0$.

The phase shifts δ_l^g and δ_l^u are computed by direct integration of the Schrödinger equation using the Numerov algorithm. The integration was done up to $R = 300a_0$ in steps of $0.01a_0$. The Born approximation to the phase shift for the asymptotic potential defined by Eq. (8) is

$$\delta_{l\,\mathrm{Born}} \approx \frac{\pi m k^2}{(2l+3)(2l+1)(2l-1)\hbar^2} \times \left(C_4 + \frac{3C_6k^2}{(2l+5)(2l-3)}\right). \qquad (9)$$

For each value of the relative energy E the Numerov phase shifts are calculated for all values of l up to those for which the Born approximation agrees within a specified accuracy. For example, for $E = 0.005$ and 5.0 eV (the lowest and the highest relative energy considered for D^+ in D), the Numerov phase shift agrees with the Born shift within 1% for $l = 31$ and 457, respectively. For higher partial waves the phase shifts are obtained by adding to the Born shifts a small term obtained by extrapolation of the Numerov shifts at smaller l. The bulk of the computer time is used in the calculation of the Numerov phase shifts, and the sum over partial waves in the evaluation of various cross sections takes only a fraction of the computer time. Typically, 1000 partial waves were summed to calculate the various cross sections.

B. He^{2+} with He

The states of He_2^{2+} relevant to present calculations are the lowest $^1\Sigma_u^+$ state and the first excited $^1\Sigma_g^+$ state, both separating into $He^{2+}(^1S_0)$ and $He(^1S_0)$ for large internuclear separations. The lowest $^1\Sigma_g^+$ state of He_2^{2+} dissociates into $He^+(^2S_{1/2}) + He^+(^2S_{1/2})$. *Ab initio* calculations of these potential curves, using the generalized valence bond method, have recently been reported.[3]

Again, for a given relative energy E, the Numerov phase shifts are matched to the Born phase shift [Eq. (9)] for higher partial waves by a small correction factor. In the present case, $C_4 = 2.766$ a.u. and $C_6 = 4.652$ a.u. The coefficients C_4 and C_6 are derived from the dipole and the quadrupole polarizabilities of helium which have been previously calculated.[10]

IV. DISCUSSION

Figure 1 shows the differential cross section for the scattering of D^+ by D at a relative energy of 5 eV. Calculated differential cross sections are useful in the design of beam experiments performed at thermal energies. The significant enhancement in the forward and backward directions is due to the usual glory effects.

The total cross section as well as the two lowest transport cross sections for motion of D^+ in D are shown as a function of relative energy in Fig. 2. The higher transport cross sections, which appear only in the correction terms and higher approximations in the kinetic theory,[7] are shown in Fig. 3. For center-of-mass energies higher than 5 eV the momentum-transfer cross section is dominated by charge transfer and has the logarithmic energy dependence

$$Q^{(1)} = (a - b\ln E)^2\,. \qquad (10)$$

When $Q^{(1)}$ is in a_0^2 and E is in eV, the constants are $a = 18.9$ and $b = 1.12$. The analytic form, Eq. (10), is used in the calculation of the mobility. The mo-

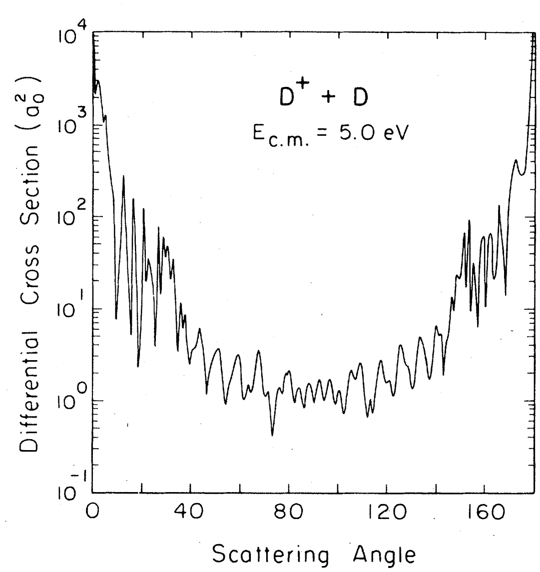

FIG. 1. Differential cross section for elastic collisions of D^+ with D for a center-of-mass energy of 5 eV.

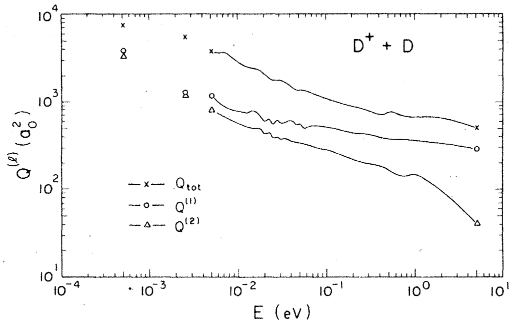

FIG. 2. Total Q_{tot} and transport cross sections $Q^{(1)}$ and $Q^{(2)}$ for collisions of D^+ with D.

bility of D^+ in D for gas temperatures of 77, 303, and 10 000 K is shown in Fig. 4, as a function of the ratio of the electric field strength to number density. The zero-field mobility of 10.5, 7.0, and 2.1 $cm^2 V^{-1} sec^{-1}$ at gas temperatures of 77, 303, and 10 000 K, respectively, agrees very well with the previous calculation.[11]

If the scattering amplitudes $f_l^{g,u}(\theta)$ are rapidly falling functions of θ, as is evident from Fig. 1, Eq. (1) for the differential cross section becomes almost independent of spin.[12] Assuming the energy dependence of the phase shift to be given by the Born approximation, Eq. (9), one obtains an *approximate* scaling law,

$$Q_{H^+-H}(E)/Q_{D^+-D}(\tfrac{1}{4}E) \approx 0.5 ,$$

where Q_{D^+-D} is a cross section (either differential or total or any transport) of D^+ in D and Q_{H^+-H} is the corresponding cross section for H^+ in H. Extensive calculations of various cross sections for H^+ in H have recently been reported.[13] For Q_{tot} the ratio $Q_{H^+-H}(E)/Q_{D^+-D}(\frac{1}{4}E)$ has the values 0.55, 0.44, and 0.57 for $E = 0.002$, 0.10, and 0.20 eV, respectively.

In order to interpret the results of a beam experiment on He^{2+} in He, we show in Fig. 5 the differential cross section at a center-of-mass energy of 0.5 eV; the dissociation energies of the relevant

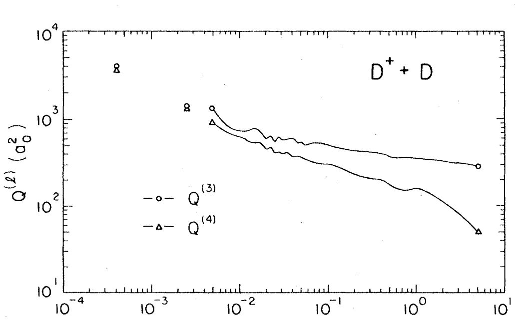

FIG. 3. Higher transport cross sections $Q^{(3)}$ and $Q^{(4)}$ for collisions of D^+ with D.

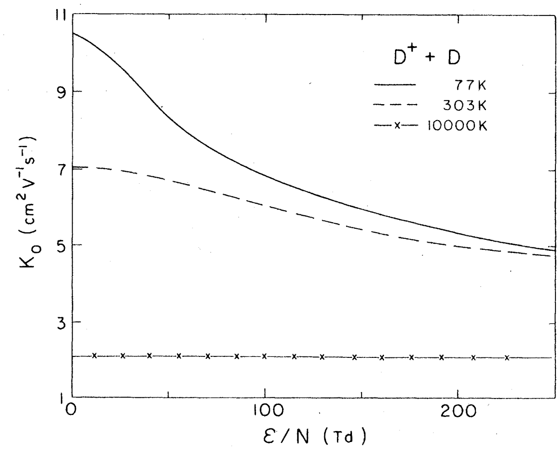

FIG. 4. Reduced mobility of D^+ in D as a function of electric field strength to number density ratio at three different gas temperatures.

${}^1\Sigma_u^+$ and ${}^1\Sigma_g^+$ states of He_2^{2+} are 0.44 eV and 0.33 eV, respectively. The slightly attractive long-range force between the He^{2+} ion and the He atom is due to the polarization induced in the atom. This long-range polarization potential also causes orbiting resonances, as is evident from the asymmetric nature of the differential cross section of He^{2+} in He in Fig. 5. Neither of the relevant ${}^1\Sigma_g^+$ and ${}^1\Sigma_u^+$ states of He^{2+} + He intersects the ${}^3\Sigma_g^+$ and $X\,{}^1\Sigma_g^+$ states of He^+ + He^+ at thermal energies, and therefore the process of single-charge transfer is possible only through a radiative transition.[3] The

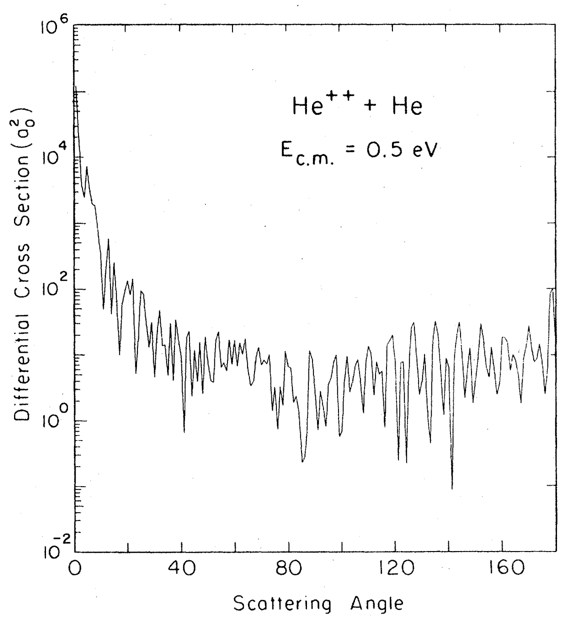

FIG. 5. Differential cross section for elastic collisions of He^{2+} with He for a center-of-mass energy of 0.5 eV.

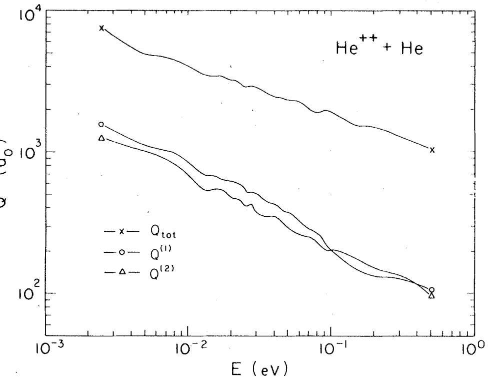

FIG. 6. Total Q_{tot} and transport cross sections $Q^{(1)}$ and $Q^{(2)}$ for collisions of He^{2+} with He.

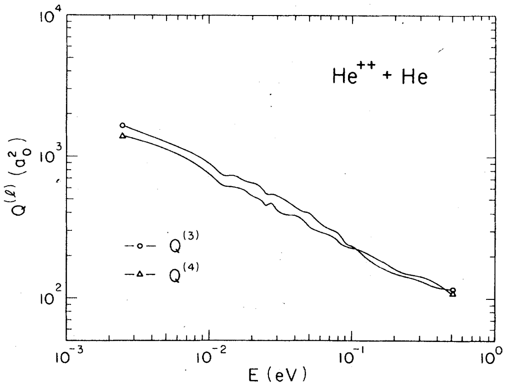

FIG. 7. Higher transport cross sections $Q^{(3)}$ and $Q^{(4)}$ for collisions of He^{2+} with He.

rate constant for radiative single-charge transfer in He^{2+} + He collisions is estimated theoretically[14] to be 4.24×10^{-14} $cm^3\,sec^{-1}$ at 300 K, which agrees quite well with the measured value of 4.8×10^{-14} $cm^3\,sec^{-1}$. The total and first two transport cross sections of He^{2+} in He are shown in Fig. 6 and higher transport cross sections are shown in Fig. 7. For E_{CM} higher than 0.5 eV the momentum-transfer cross section of He^{2+} in He is also fitted to the analytic form (10) with $a=8.79$ and $b=2.24$. This analytic form for $Q^{(1)}$ was used in the calculation of the mobility of He^{2+} in He in our previous work.[4]

Almost no experimental information is available for a direct comparison with our present theoretical results and an experimental effort concerning thermal-energy collisions of D^+ with D and He^{2+} with He would be worthwhile. Present experimental difficulties include the formation of pure beams of atoms in their ground state. There are considerable amounts of metastable and Rydberg atoms in most experiments involving either crossed or merged beams. Difficulties are also encountered in the formation of pure ion beams at thermal energies. Any impurities of H_2^+ in D^+ are difficult to remove by magnetic means since both D^+ and H_2^+ have the same charge-to-mass ratio. The difficulty associated with He^{2+} at thermal energies arises from its high ionization potential.

Various transport cross sections in Figs. 2 and 6 exhibit quantum structure due to orbiting resonances, glory and rainbow oscillations, and the *g-u* interference.[15] At low energies a contribution to the structure is also due to the discrete nature of the sum over partial waves. In the case of He^{2+} in He, the quantum structure associated with shape resonances has been analyzed to estimate resonant contributions to single-charge transfer between He^{2+} in He.[14] A detailed analysis of oscillations due to orbiting resonances in the total cross section of a closely related system (protons on ground-state hydrogen) has also been carried out.[16]

ACKNOWLEDGMENTS

Special thanks are due Professor J. N. Bardsley for helpful discussions concerning this subject material on various occasions and for constant encouragement. I also wish to thank Professor J. E. Bayfield for his kind advice. A liberal use of computer facilities of Group T4, Los Alamos Scientific Laboratory is gratefully acknowledged. This research was supported by the Advanced Research Projects Agency of the Department of Defense and was monitored by ONR under Contract No. N00014-76-C-0098.

[1]G. Yonas, J. W. Poukey, K. R. Prestwich, J. R. Freeman, A. J. Toepfer, and M. J. Clauser, Nucl. Fusion 14, 731 (1974); P. A. Miller, R. I. Butler, M. Cowan, J. R. Freeman, J. W. Poukey, T. P. Wright, and G. Yonas, Phys. Rev. Lett. 39, 92 (1977).
[2]R. Johnsen and M. A. Biondi, Phys. Rev. A 18, 989 (1978); 18, 996 (1978).
[3]J. S. Cohen and J. N. Bardsley, Phys. Rev. A 18, 1004 (1978).
[4]J. M. Wadehra, J. S. Cohen, and J. N. Bardsley, Phys. Rev. A 18, 1009 (1978).
[5]E. W. McDaniel and E. A. Mason, *The Mobility and*

Diffusion of Ions in Gases (Wiley, New York, 1973).
[6]H. T. Wood, J. Chem. Phys. 54, 977 (1971).
[7]L. A. Viehland and E. A. Mason, Ann. Phys. (N.Y.) 91, 499 (1975); 110, 287 (1978).
[8]J. M. Peek, J. Chem. Phys. 43, 3004 (1965).
[9]L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1968).
[10]J. Lahiri and A. Mukherji, J. Phys. Soc. Jpn. 21, 1178 (1966); Phys. Rev. 141, 428 (1966).
[11]A. Dalgarno, Philos. Trans. R. Soc. London A 250, 426 (1958).
[12]N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University, London, 1965), p. 646.
[13]G. Hunter and M. Kuriyan, Proc. R. Soc. London A 353, 575 (1977).
[14]J. N. Bardsley, J. S. Cohen, and J. M. Wadehra, Phys. Rev. A 19, 2129 (1979).
[15]R. J. Munn, E. A. Mason, and F. J. Smith, J. Chem. Phys. 41, 3978 (1964).
[16]A. V. Matveenko and L. I. Ponomarev, Sov. Phys.-JETP 41, 456 (1975).