

Quantum Defect Method for Linear Molecules and $e\text{-H}_2^+$ Scattering*

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The quantum defect method is extended to permit calculation of short-range phase shifts for electron scattering states in the field of a linear molecule-ion. The method is applied to the low-energy ($k < 0.2$ a.u.) scattering of electrons by H_2^+ ; the differential scattering cross section is calculated and compared with that derived by Temkin and Vasavada.

I. INTRODUCTION

The close relationship between highly excited bound states of an atomic electron and the low-energy scattering states of an electron around the corresponding ion is the basis of the quantum defect method (QDM) for treating electron scattering by atomic ions.^{1,2} The quantum defect and the short-range, non-Coulombic part of the phase shift both express the effect of the short-range potential due to bound electrons in the scatterer.

The success of the QDM for atoms has prompted us to extend it to obtain short-range phase shifts for electron scattering by molecule-ions, and by diatomic and linear polyatomic molecule-ions in particular. The ultimate motivation for this method is part of a program to treat inelastic electron-molecule scattering processes in a quantitative way. The development of a molecular QDM represents one step, in which one makes use of accurate spectroscopic information to obtain the phase shifts. These then may serve as long-range boundary values for other methods, e.g., a pseudopotential calculation,³ which provides the continuum function of interest in and near the region of the molecular core electrons.

We shall summarize the quantum defect method here, repeating only enough of the details to define the notation and sketch the physical ideas. Then we shall describe the calculations as applied to the $e\text{-H}_2^+$ problem and compare our semiempirical elastic differential scattering cross section with the *a priori* cross section calculated recently by Temkin and Vasavada.⁴

II. QUANTUM DEFECT METHOD AND EXTENSION TO MOLECULES

A. Extension of the One-Electron QDM to Molecules

An electron far from but in the potential field of an atomic or molecular ion is essentially an electron in a

Coulomb field, so that the forms of the wavefunctions of such an electron are Coulomb functions when the distance r , between electron and atom or center of the molecule, is large. The energy of a bound state of such a system is conveniently expressed as

$$E_n = -K_n^{-2}, \quad (1)$$

in atomic units, where

$$K_n = n - \mu(E_n), \quad (2)$$

n is the integer index analogous to the principal quantum number for a pure Coulomb state and $\mu(E_n)$ is called the quantum defect. For atoms, the relation between the quantum defect $\mu(E)$ for excited bound states ($E < 0$) and the short-range contribution $\delta(E)$ to the phase shift for low-lying continuum states ($E > 0$) was obtained by an analytic continuation procedure described in detail by Seaton^{1,2} and in part, by Ham.⁵ If the energy in the continuum is given as $E = \gamma^{-2}$, then continuation of $\mu(E)$ into the continuum gives

$$\tan \delta(E) = \tan[\pi \mu(E)] [(1 - \exp(-2\pi\gamma))^{-1}], \quad (3)$$

with γ positive. Hence, for low-energy scattering with $\gamma > 1$, the phase shift is essentially

$$\delta(E) \cong \pi \mu(E). \quad (4)$$

The extension of the quantum defect method to linear molecules may be carried out in either of two ways. Flannery and Öpik⁶ suggest that the core potential be represented by two point charges whose separation is treated as a parameter. They then separate the wave equation for the Rydberg electron in prolate spheroidal coordinates. In this way, the asymptotic-continuum scattering states are expressed as sums of regular and irregular solutions of the Coulombic Schrödinger equation in terms of the variable $(r_A + r_B)/2R$. This method has not yet really been carried out, insofar as Flannery and Öpik were able to justify setting the quantum defect equal to zero for the states of interest for their treatment of the photoionization of H_2 .

Rather than introduce a parameter, we have chosen to express our asymptotic one-electron scattering functions as eigenstates of orbital angular momentum. This procedure, when applied in a semiempirical quantum defect

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¹ M. J. Seaton, Monthly Notices Roy. Astron. Soc. **118**, 504 (1958).

² M. J. Seaton, Proc. Phys. Soc. (London) **88**, 809, 815 (1966); O. Bely, *ibid.* **88**, 833 (1966); D. L. Moores, *ibid.* **88**, 843 (1966).

³ B. Schneider, M. Weinberg, J. Tully, and R. S. Berry, "A Pseudopotential Method for Low-Energy Electron Scattering" (to be published).

⁴ A. Temkin and K. V. Vasavada, Phys. Rev. **160**, 109 (1967).

⁵ F. S. Ham, *Solid State Physics* (Academic Press Inc., New York, 1955), Vol. 1.

⁶ M. R. Flannery and U. Öpik, Proc. Phys. Soc. (London) **86**, 491 (1965).

method, is tantamount to a very specific physical assumption. We use spectroscopic term values to obtain quantum defects into the continuum, to obtain phase shifts. We can justifiably assume that our one-electron Rydberg and scattering functions are eigenfunctions of l_z (Z the axis being the internuclear axis) from the symmetry of the problem. Our association of the quantum defects with eigenfunctions of l^2 is a different matter altogether; for a molecule, we cannot be sure on any general symmetry ground that the spectroscopically allowed Rydberg states or the continuum states beyond them are also eigenstates of l^2 . In an atom, the allowed states are eigenstates of l^2 , if correlation is neglected. In a molecule, they need not be. Nevertheless both the analysis given by Mulliken⁷ and model calculations indicate that the amount of "l spoiling" is quite small, at least for H₂ or H₂⁺ near its equilibrium position. We therefore have carried out our calculations with continuum functions that are eigenfunctions of l^2 , and assumed that these correspond closely to the extensions of the spectroscopic Rydberg states into the continuum.

The method formally follows very closely the approach used by Seaton. The one-electron Schrödinger equation in Born-Oppenheimer approximation, (in terms of the distances r and r_α from Rydberg electron to origin, and to nucleus α) is

$$\left[-(\hbar^2/2m)\nabla^2 - \sum_{\text{nuclei } \alpha} (Z_\alpha e^2/r_\alpha) + \sum_{\text{core electrons } j} e^2 V_j\right] \Psi_{nlm}(\mathbf{r}) = \epsilon \Psi_{nlm}(\mathbf{r}), \quad (5)$$

where the effective potential V_j is analogous to that derived by Feshbach.⁸ This becomes a Coulomb equation for large r :

$$\left[-(\hbar^2/2m)\nabla^2 - (e^2/r)\right] \Psi_{nlm}(\mathbf{r}) = \epsilon \Psi_{nlm}(\mathbf{r}). \quad (6)$$

Replacing the true potential with the effective V_j 's in (5) reduces the problem to one with axial symmetry. This reduces the equation to

$$\left[-(\hbar^2/2m)\nabla^2 + V'(r, \theta) - (e^2/r) + (M^2/r^2 \sin^2\theta)\right] \times \Psi + (1/K^2)\Psi = 0 \quad (7)$$

with $\epsilon = -K^2$ and

$$V'(r, \theta) = - \sum_{\alpha} (Z_\alpha e^2/r^2) + \left(\sum_j (e^2/r_j)\right) + (e^2/r); \quad (8)$$

$V'(r, \theta)$ thus goes to zero much faster than r^{-1} as r increases without limit.

Strictly, the asymptotic function is

$$\Psi_m(\mathbf{r}, \theta) = \sum_l a_l Y_l^m(\theta) \times [y_1(K, l; r) - \beta_{lm}(\epsilon) y_4(K, l; r)], \quad (9)$$

with $\psi_m(0, \theta) = 0$. Note that the sum over l is taken only over even l (for gerade Ψ 's) or over odd l (for ungerade Ψ 's). The assumption that Ψ is an eigenfunction of l^2 gives the form

$$\Psi_{lm}(\mathbf{r}, \theta) = Y_l^m(\theta) \times [y_1(K, l; r) - \beta_{lm}(\epsilon) y_4(K, l; r)]. \quad (10)$$

The functions y_1 and y_4 are Coulomb functions:

$$y_1(K, \lambda; \rho) = [K^{\lambda+1}/\Gamma(2\lambda+2)] M_{K, \lambda+1/2}(2\rho/K) \quad (11)$$

and

$$y_4(K, \lambda; \rho) = [A(K, \lambda) \cot\pi(2\lambda+1) - G(K, \lambda)] \times y_1(K, \lambda; \rho) - y_1(K, -\lambda-1; \rho)/\sin\pi(2\lambda+1). \quad (12)$$

The subsidiary functions

$$A(K, \lambda) = \Gamma(K+\lambda+1)/K^{2(\lambda+1)}\Gamma(K-\lambda), \quad (13)$$

$$G(K, \lambda) = [A(K, \lambda)/2\pi][\psi(K+\lambda+1) + \psi(K-\lambda) - 2 \ln K], \quad (14)$$

$$\psi(x) = d \ln \Gamma(x)/dx, \quad (15)$$

$$M_{k, \mu}(Z) = [\Gamma(2\mu+1)/\Gamma(\mu-k+\frac{1}{2})] \times \exp(-i\pi K) W_{-k, \mu}(-Z) + \Gamma(2\mu+1)/\Gamma(\mu+k+\frac{1}{2}) \times \exp[i\pi(\mu-k+\frac{1}{2})] W_{k, \mu}(Z), \quad (16)$$

and

$$W_{k, \mu}(Z) = \frac{Z^k \exp(-Z/2)}{\Gamma(\mu-k+\frac{1}{2})} \times \int_0^\infty \mu^{-k-1/2} (1+t/Z)^{\mu+k-1/2} \exp(-t) dt. \quad (17)$$

For the one-dimensional problem, ψ , y_1 , and y_4 are entire analytic functions of ϵ ; therefore $\beta(\epsilon)$ is also an analytic function of ϵ and can be continued into the continuum, the region of positive ϵ . We assume without proof that the same holds true for the case where β depends on m as well as on l . In this case we obtain the same formed expression for β as one finds for the atomic problem,

$$\beta_{lm}(\epsilon) = \{A(K, l) \cot[\pi\mu(l, m; \epsilon)] - \text{Re}G(K, l)\}^{-1}. \quad (18)$$

We have explicitly indicated the dependence of the quantum defect on l and m . The phase shift is also related to the quantum defect by the same formal expression as in the atomic case:

$$\tan\delta(l, m; \epsilon) = \tan\pi\mu(l, m; \epsilon)/[1 - \exp(-2\pi\gamma)]. \quad (19)$$

The actual procedure by which one obtains the phase shift from known quantum defects may take any of several forms. Seaton² has recently shown that the

⁷ R. S. Mulliken, J. Am. Chem. Soc. **86**, 3183 (1964).

⁸ H. Feshbach, Ann. Phys. (N.Y.) **19**, 287 (1962).

function

$$Y_l(\epsilon) = \left\{ \sum_{j=0}^p \alpha_j \epsilon^j / 1 + \sum_{j=1}^q \beta_j \epsilon^j \right\} \\ = \tan \pi \mu_l(\epsilon) / \prod_{r=0}^l (1 + \epsilon^r), \quad (20)$$

with $q > p$, is a particularly useful form for fitting experimental bound state energies ϵ with the constants α_j, β_j to obtain continuum phase shifts by extrapolation. However for our calculations, for which relatively few Rydberg state energies are available in any one manifold, we used the simpler procedure of Ham,⁵ in which one lets n be defined by the relation

$$\cot \pi n = A(K, l) \cot \pi \mu \quad (21)$$

and expands n about $E=0$:

$$n = \sum_j a_j \epsilon^j. \quad (22)$$

The coefficients a_j are found by fitting a truncated series to the available experimental energies.

B. The Effect of Nuclear Motion

The one-electron approach just described deserves closer examination because of the effects of vibrational and rotational motion in molecules. If one works entirely within the framework of the Born–Oppenheimer approximation, one computes theoretical Rydberg term values as functions of R , the internuclear distance; from the one-electron procedure, one then obtains phase shifts for scattered waves as functions of R as well as of ϵ, l , and m . One can obtain R -dependent differential and total elastic scattering cross sections from these phase shifts; to compare these cross sections with experimental values, one should average the cross sections over the distribution function for internuclear distances,

$$P(R) = \sum_{\alpha} |\Psi_{\alpha}(R)|^2 e^{-E_{\alpha} l / kT} / \sum_{\alpha} e^{-E_{\alpha} l / kT}, \quad (23)$$

where E_{α} is the vibrational energy of the α th vibrational state of the molecule–ion scatterer. Computing the scattering cross sections in this way is the free-state analog of using the Born–Oppenheimer approximation for bound-state calculations. This is a reasonable first approximation even for scattering of very low-energy electrons because the attractive Coulomb field makes the duration of essentially all electron collisions with positive ions short compared with the nuclear vibration period. Even in the case of electron–neutral-molecule collisions, the attractive polarization potential has this effect.

One need not use theoretical electronic energies for the Rydberg states, and in many ways it is desirable to use the QDM as a semiempirical procedure. In this case, one extracts from spectroscopic energy levels the values of D_0 , the energy of the ground vibrational level of the

electronic state in question, and one or more level spacings; for these, one infers D_e , the energy of the static system at equilibrium, and the effective potential in the general neighborhood of the minimum. The value of D_e so obtained is not generally quite the same as the theoretical value for the nuclear-plus-electronic energy in the Born–Oppenheimer approximation because the actual “vibrational” levels include small effects due to finite nuclear velocities. These can be expressed in terms of perturbations due to the nuclear kinetic energy operators, $-\frac{1}{2}(\hbar^2/2M)\partial^2/\partial R^2$ and the nuclear rotational-energy operator $L^2/2MR^2$ (M is the reduced mass),^{9,10} which couple the Born–Oppenheimer vibronic states. One can use model calculations to estimate the magnitude of these perturbations and make approximate allowance for them to obtain approximate Born–Oppenheimer scattering phases. Alternatively, when the perturbations are fairly regular, one can use the empirical effective potential curves directly, and thereby implicitly take into account the small effects of nuclear vibration on the electronic bound-state energies and therefore on the scattering phases. We shall pursue the latter course here, and discuss the effect of nuclear vibration on Rydberg-state energies elsewhere.¹¹ In general these effects are small but occasionally one can expect to find large perturbations roughly analogous to the phenomenon of Fermi resonance of vibrational levels in different normal modes, which occurs in polyatomic molecules.

C. Open-Shell Cores and Spin States

If the core or ion–molecule scatterer does not have a closed-shell structure, more than one Rydberg (or scattering) state arises from a specification of core state and the principal quantum number (or asymptotic energy) and angular momentum quantum numbers of the outer electron. One has the familiar singlet–triplet splitting in the Rydberg states of H_2 , for example. Mulliken has pointed out⁷ that the interpretation of experimental quantum defects in such systems is ambiguous: the singlet and triplet energies would be split by twice the Rydberg-core exchange interaction, $2K$, even if the Rydberg orbitals of the singlet and triplet were identical. So long as the core has spherical, closed-shell symmetry, the same quantum defect simultaneously describes two quantities unambiguously, the energy of a state and the position of the outermost maximum for the corresponding bound-state wavefunction. If the core does not have this symmetry, and in particular if it has an open shell, then the quantum defect can be defined to describe one but not both of these quantities without ambiguity. Thus we can define

⁹ W. Kolos and L. Wolniewicz, *J. Chem. Phys.* **41**, 3663 (1964).

¹⁰ See, for example, R. S. Berry, *J. Chem. Phys.* **45**, 1228 (1966) and J. N. Bardsley, *Chem. Phys. Letters* **1**, 229 (1967).

¹¹ R. S. Berry and S. E. Nielsen, *J. Chem. Phys.* **49**, 116 (1968), preceding paper.

two limiting situations of approximation for which one can use the quantum defect to correlate energies and phase shifts or shapes of wavefunctions. At one limit, one can suppose that all the singlet-triplet splitting is due to exchange interactions and that the singlet and triplet asymptotic one-electron functions (for high n and large r) have the same shape. In this limit, one should determine the quantum defect from the average energy of corresponding singlets and triplets. This first limit was the one used by Mulliken⁷ and recently by Berry and Nielsen.¹¹ The other limit corresponds to the assumption that the singlet-triplet splitting can be ascribed principally to differences in the phases of the asymptotic one-electron Rydberg orbitals, and that one can neglect those parts of the exchange and correlation which cannot be included in an effective one-electron Hamiltonian. In this case one should compute separate quantum defects for singlet and triplet manifolds. One has such a situation when one writes different Hartree-Fock equations or different pseudopotentials for singlets and triplets. At this time it is not clear which extreme is closer to the truth. We have followed the latter approach in this work; a recent pseudopotential treatment also used this, with considerable success.¹²

III. PHASE SHIFTS AND ELASTIC SCATTERING IN e -H₂⁺

The principal use for the quantum defect method, as we pointed out previously, is probably as a tool to help

TABLE I. Quantum defects for H₂.^a

n	l	m	Singlet	Triplet
3	0	0	-0.0729	0.0652
4	0	0	(-0.0200)	...
3	1	0	0.2084 ^b	0.5124
4	1	0	0.2374 ^c	0.4689
3	1	1	-0.0431 ^b	0.0730
4	1	1	0.0117 ^c	0.0795
5	1	1	0.0331 ^d	0.0924
3	2	0	0.0624	0.0644
4	2	0	(0.1087)	0.0502
5	2	0	...	0.0125
3	2	1	0.0304	0.0372
4	2	1	-0.0116	0.0222
3	2	2	-0.0107	0.0146
4	2	2	(-0.0200)	0.0428

^a All values besides those in Footnotes b-d were taken from the summary compiled by F. A. Matsen and J. C. Browne in *Molecular Orbitals in Chemistry, Physics and Biology*, P. O. Löwdin and B. Pullman, Eds. (Academic Press Inc., New York, 1964), p. 539.

^b T. Namioka, *J. Chem. Phys.* **41**, 2141 (1964).

^c A. Monfils, *Bull. Acad. Sci. Roy. Belg.* **47**, 599, 816 (1961).

^d A. Monfils, *J. Mol. Spectry.* **15**, 265 (1965).

¹² A. U. Hazi and S. A. Rice, *J. Chem. Phys.* **47**, 1125 (1967).

in the calculation of inelastic processes. However its most immediate application is to the calculation of differential elastic scattering cross sections. We present here such a calculation for e -H₂⁺ scattering.

The problem requires three steps. First, one must compute the short-range phase shifts $\delta(l, m; \epsilon)$ with the reference axis for m taken as the internuclear axis. Second, one obtains the contribution to the scattered intensity, in a molecule-fixed frame, due to the short-range and Coulomb contributions, f_s and f_c , to the scattering amplitude, and transforms this to the intensity in a laboratory frame. Finally, one must compute the intensity $I(\theta) d\theta$ due to all the molecules by summing the contributions from the entire distribution of molecular orientations. The first step was described by Sec. II, above. The second is based on the separation described by Mott and Massey¹³ for the Coulomb and short-range scattering amplitudes; the Coulomb contribution can be determined directly in laboratory coordinates, but the short-range part requires transformation.

If θ' and φ' are the polar angles in the molecule-fixed frame, and θ and φ are the corresponding angles in the laboratory frame; then

$$Y_{lm}(\theta, \varphi) = \sum_k D_{mk}^l Y_{lk}(\theta', \varphi')$$

and

$$D_{mk}^l(\alpha, \beta, \gamma) = \sum_j (-1)^j \times \frac{[(l+k)!(l-k)!(l+m)!(l-m)!]^{1/2}}{(l-m-j)!(l+k-j)!j!(j+m-k)!} \times e^{(-ima)} \cos^{2l+k-m-2j}(\frac{1}{2}\beta) \sin^{2j+m-k}(\frac{1}{2}\beta) e^{(-ika)}.$$

Here, α , β , and γ are the Euler angles describing the rotation of the coordinate system relating one reference frame into the other.

The third step, the averaging over molecule orientation, has been described for randomly oriented molecules by Temkin and Vasavada⁴ and checked by ourselves. The cross section, repeated here for convenience, consists of a pure Coulomb term, a short-range term, and an interference term. If Ω' is the unit of solid angle in the laboratory frame ($\sin\theta' d\theta' d\varphi'$), then

$$\sigma(\Omega') = I_c + I_s + I_i, \quad (24)$$

where

$$I_c = [4k^2 \sin^4(\theta'/2)]^{-1}, \quad (25)$$

$$I_s = k^{-2} \sum_{l, l', m, m', L} \{ [(2L+1)(2l'+1)/(2L+1)] \times (ll'00 | L0)^2 \times (ll'mm' | Lm+m')^2 \cos(\varphi_{lm} - \varphi_{l'm'}) \times \sin\varphi_{lm} \sin\varphi_{l'm'} P_L(\cos\theta') \}, \quad (26)$$

¹³ N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Oxford University Press, Oxford, England, 1965), 3rd ed.

TABLE II. Short-range phase shifts for $e\text{-H}_2^+$ scattering. (Parenthetical values are extrapolated values for $k^2=0$; number of states indicates the number of bound states used for extrapolating the quantum defect into the continuum.)

k^2	Q.D.	T and V^a	Q.D.	T and V^a
	Singlet S wave (2 states)		Triplet S wave (1 state)	
0.01	0.057(0.032)	-0.430	0.205(0.205)	0.117
0.1	0.284	-0.440	0.205	0.094
0.2	0.536	-0.449	0.205	0.071
	Singlet $P_{m=0}$ (2 states)		Triplet $P_{m=0}$ (2 states)	
0.01	0.841(0.856)	0.493	0.938(1.312)	1.377
0.1	0.699	0.489	0.694	1.308
0.2	0.544	0.489	0.144	1.246
	Singlet $P_{m=1}$ (3 states)		Triplet $P_{m=1}$ (2 states)	
0.01	0.174(0.191)	-0.308	0.272(0.276)	0.220
0.1	-0.102	-0.304	0.236	0.224
0.2	-0.643	-0.298	0.199	0.186

^a See Ref. 4.

and

$$I_{\nu} = [k^3 \sin^2(\theta'/2)]^{-1} \sum_{l,m} \times \{ \sin \delta_{lm} \cos [k^{-1} \ln \sin^2(\theta'/2) + 2(\sigma_0 - \sigma_l) - \delta_{lm}] \times (2 - \delta_{m0}) P_l(\cos \theta') \}, \quad (27)$$

where

$$\sigma_l = \arg \Gamma(l+1 - ik^{-1}), \quad (28)$$

the Coulomb phase, and

$$\varphi_{lm} = 2\sigma_l + \eta_{lm}. \quad (29)$$

The index L must satisfy

$$l + l' + L = \text{even integer}; \quad (30)$$

$l, l', m,$ and m' are the usual angular-momentum quantum numbers, and $(l' m m' | L M)$ is a Clebsch-Gordan coefficient.

The computed phase shifts were based on the spectroscopically determined quantum defects given in Table I. Computations were performed on the IBM 7094 of the

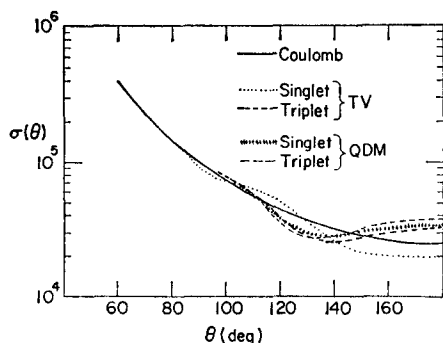


FIG. 1. Differential scattering cross section for electrons on H_2^+ for $k=0.1$ a.u. (0.136 eV).

Computation Center, University of Chicago, with two programs, one for determining phase shifts and one for determining the elastic scattering cross sections. Some typical phase shifts are given in Table II, where they are compared with the values found by Temkin and Vasavada by an *a priori* calculation based on polarized single-center orbitals. Figure 1 shows differential scattering cross sections for singlet and triplet states as determined by QDM calculations and by Temkin and Vasavada.⁴ Figure 2 exhibits the ratios of differential cross sections for $e\text{-H}_2^+$ scattering to the pure Coulomb contribution. It is very clear from the figures that the principal effects of the molecular core on elastic scattering occur at large scattering angles and that the effects are not large compared with the integrated cross section

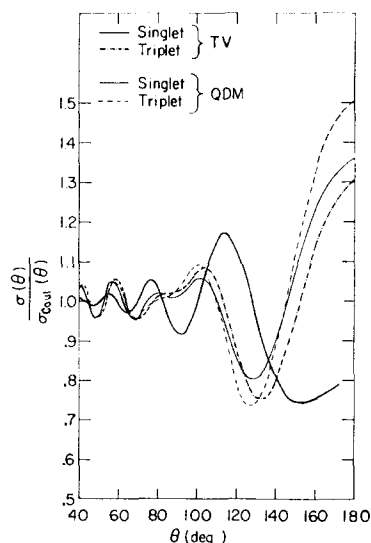


FIG. 2. Ratio of the $e\text{-H}_2^+$ differential elastic scattering cross section to pure Coulomb scattering, for $k=0.1$ a.u.

for scattering through angles greater than a few degrees. On the other hand the oscillations in the large angle scattering might offer a useful probe for studying ion-molecules.

The agreement between QDM and polarized single-center orbitals is quite good for the triplet cross section, but the results are quite different for the singlet. We would be inclined to prefer the QDM results because of their semiempirical nature if we could be completely confident of the experimental-input data. However, the identification of some of the Rydberg term values are not altogether certain, and we definitely do not have as many terms in any series [except perhaps the $^1P(m=1)$] as we would like, to obtain reliable phase shifts. At the moment, we can only say that the QDM and polarized orbital results are at variance and that we require either more spectroscopic data or some large-angle scattering experiments, or both, in order to resolve the differences.