Atomic ionization by electron impact: A hyperspherical approach

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An *ab initio* calculation, following a hyperspherical partial-wave method [J. N. Das, Aust. J. Phys. **47**, 743 (1994)], satisfactorily represents the recent experimental triple differential cross-section results of Röder *et al.* [Phys. Rev. A **53**, 225 (1996)] for electron hydrogen atom ionization collisions at low energies. The qualitative agreement with their theoretical results is also good. Moreover, our results are in absolute units and in some instances our results are in better agreement with the experiments compared to their theoretical results. Here it is also exhibited that the hyperspherical partial wave method is a promising formalism for studying atomic ionization problems. [S1050-2947(97)03706-2]

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I. INTRODUCTION

Electron-impact ionization of hydrogen atoms is an ideal Coulomb three-body problem. For low energies it is now a challenging theoretical problem. A considerable number of experimental results for triple differential cross sections (TDCSs) for low energies are now available [1–3]. However, present-day theories are far behind in explaining all these results. One may recall here that for intermediate and high energies the agreement between theory and experiment is now satisfactory (for a review see [4–7]). A simple first Born or second Born approximation or some of their variants [8–10], such as the distorted-wave Born approximation [11], Brauner-Briggs-Klar (BBK) theory [12], close-coupling theory [13], or multiple-scattering theory [14,15], satisfactorily describe the main features of the experimental results. The situation is completely different for low energies (see [16]); no existing theory is completely satisfactory. The major theoretical attempts in the past, in the low-energy domain, had been in modifying a distorted-wave calculation based on some physical (*ad hoc*) arguments, not always logically consistent. Thus the introduction of some effective charge of the distorting potential for the final outgoing electrons [17,18], the introduction of some dynamical screening factor [19], or the introduction of a Gamow factor [3,20] and an *ad hoc* polarization potential are some of the examples. Consequently, such theories have only limited success. The distorted-wave calculation of Röder *et al.* [3], which uses a Gamow factor for the post-collision interaction (PCI) and an *ad hoc* polarization potential, nicely reproduces the trends of the experimental results for certain kinematic condition but loses one of the essential properties of a predictive theory, as the results are expressed in *arbitrary units*. For low energies there are now two relatively rigorous theories. One of these is the convergent close-coupling (CCC) theory [21] and the other is the hyperspherical close-coupling theory [22]. These theories beautifully represent the total ionization cross sections for low energies. The CCC calculation also gives good differential cross-section results for energies of 54.4 eV. However, below this energy TDCS results are not known for these theories.

In the present work we consider the hyperspherical partial-wave method recently suggested by one of the present authors [23,24]. Here we confine our attention to the constant Θ_{12} geometry for low energies. This geometry has been considered by several authors [13,17,18] and very recently a large set of experimental and theoretical results, following modified distorted-wave Born approximations (DWBAs), have been presented by Röder *et al.* [3] for this geometry. The experimental results show important structures and their theoretical confirmation faces many difficulties. Their final results are not even in absolute units. Another reason for our consideration of the above geometry is that important simplifications may be made in the hyperspherical calculations.

It will be interesting at this point to draw a comparison between the hyperspherical method and some other methods generally used for TDCS calculations. The *Ansätze* on which different approaches are based are the *exact* expressions for the relevant T-matrix element given by (see [25])

$$T_{fi}=\langle \Phi_f | V_f | \Psi_i^{(+)} \rangle \tag{1a}$$

$$=\langle \Psi_f^{(-)} | V_i | \Phi_i \rangle. \tag{1b}$$

These expressions are obtained on the assumption that $\Psi_i^{(+)}$ and $\Psi_f^{(-)}$ are *exact* scattering-state wave functions and Φ_i and Φ_f are unperturbed but *asymptotically correct* wave functions in the initial and in the final channels and V_i and V_f are the corresponding perturbations. In a distorted-wave calculation one usually chooses form (1a) for the T-matrix element and takes for Φ_f a product of two Coulomb waves. This Φ_f does not represent *correctly* the final three-particle scattering state in the asymptotic domain (see [12]). As such, the basic equation, such as Eq. 1(a) of Ref. [3] (or the starting equation there with a product of plane waves), is unlikely to be *generally* valid. Additional factors such as a Gamow factor in [3] makes it far from a rigorous theory. Thus, with other different distorted-wave calculations the calculations of Röder *et al.* are subject to criticism.

The CCC method (21) for calculations of TDCSs also uses the form (1a) for the T-matrix element, uses for Φ_f a product of a plane wave and a Coulomb wave for the two outgoing electrons, and uses for Ψ_i^+ a close-coupling calculated scattering state. Since such a Φ_f does not satisfy the correct asymptotic condition, the CCC method is also subject to criticism. Moreover, the CCC calculation has some patho-

TABLE I. TDCS results for electron-impact ionization of hydrogen atoms of equal energy sharing a coplanar Θ_{12} constant geometry. E_i is the incident electron energy, Θ_{12} is the angular separation of the outgoing electrons, and θ_1 is the scattering angle of one of the outgoing electrons. Cross sections are in atomic units and correspond to cases where partial waves with $n \leq 6$, $l \leq l_{mx}$, $l_1 \leq l_{1mx}$, and $l_2 \leq l_{2mx}$ are included in Eq. (6a) (l_{mx} is the maximum value of l). Results display a convergence pattern.

		$E_i=30$ eV, $\Theta_{12}=100°$				$E_i=30$ eV, $\Theta_{12}=150°$			$E_i=20$ eV, $\Theta_{12}=150°$		
l_{mx}	$l_{1mx}=l_{2mx}$	$\theta_1=0°$	$\theta_1=120°$	$\theta_1=150°$	$\theta_1=240°$	$\theta_1=0°$	$\theta_1=50°$	$\theta_1=240°$	$\theta_1=0°$	$\theta_1=50°$	$\theta_1=240°$
0	0	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
1	1	0.20	0.29	0.31	0.03	0.46	0.11	0.06	1.64	0.33	0.15
2	2	0.51	0.57	0.35	0.02	0.92	0.16	0.01	2.50	0.67	0.19
3	3	0.61	0.63	0.28	0.04	1.97	0.03	0.02	5.03	0.23	0.13
4	4	0.82	0.77	0.20	0.02	2.57	0.05	0.01	5.90	0.26	0.05
5	5	1.02	0.81	0.21	0.01	2.82	0.03	0.01	5.98	0.24	0.04
6	6	1.11	0.88	0.19	0.01	2.85	0.02	0.01	5.49	0.24	0.06
7	7	1.13	0.93	0.20	0.01	2.76	0.02	0.01	5.18	0.28	0.05
8	8	1.08	0.99	0.17	0.01	2.56	0.02	0.01	4.85	0.28	0.05
9	9	1.04	1.05	0.17	0.01	2.45	0.02	0.01	4.79	0.28	0.05

logical difficulties such as the nonexistence of certain integrals for some of the angular momenta for the partial waves (see the second paragraph after Eq. (2) of Ref. [21] and also the last paragraph on p. 344 of Ref. [13]). It should be noted here that the CCC calculation for the total ionization cross section, which gives excellent results, follows a different route [26].

The BBK theory, on the other hand, uses the form (1b) for the T-matrix element. In the BBK theory the basic equation is correct and also the BBK $\Psi_f^{(-)}$ is asymptotically correct. So the approach is very satisfactory. The calculated results are also generally good for intermediate and high energies. However, the results are not good for low energies (see [16]). The BBK wave function $\Psi_f^{(-)}$ is so inaccurate for finite distances. It is also likely to be difficult to improve this wave function sufficiently in this approach.

The hyperspherical partial-wave method proposed by Das [23] and used in this calculation also starts from Eq. (1b) for the T-matrix element. There is no problem in choosing an asymptotically correct Φ_i. Here a plane wave suffices since it has the correct asymptotic behavior. Das attempted to determine $\Psi_f^{(-)}$ accurately from a hyperspherical partial-wave decomposition as outlined below (see [23] for details) and the approach is free from pathological difficulties. If a full calculation is made by solving the relevant coupled set of equations including a sufficiently large number of partial waves, arbitrarily accurate results are expected, at least in principle, in this approach. Now we describe the main points in this approach.

II. THEORY AND CALCULATIONS

In the electron-impact ionization of the hydrogen atom let the two outgoing electrons have coordinates $\vec{r}_1$ and $\vec{r}_2$ and momenta $\vec{p}_1$ and $\vec{p}_2$, respectively. The hyperspherical coordinates $(R,\alpha,\hat{r}_1,\hat{r}_2)$ are then defined by

$$R=\sqrt{r_1^2+r_2^2}, \quad \alpha=\tan^{-1}(r_2/r_1)$$

and we set

$$P=\sqrt{p_1^2+p_2^2}, \quad \alpha_0=\tan^{-1}(p_2/p_1).$$

The final three-particle scattering wave function is then expanded in terms of the orthonormal hyperspherical angular wave functions given by

$$\varphi_\lambda(\alpha,\hat{r}_1,\hat{r}_2)=p^n_{l_1l_2}(\alpha)Y^{lm}_{l_1l_2}(\hat{r}_1,\hat{r}_2). \tag{2}$$

Here $p^n_{l_1l_2}$ is the Jacobi polynomial and $Y^{lm}_{l_1l_2}$ is the coupled angular-momentum wave function. The expansion takes the form

$$\Psi_f^{(-)}(R,\alpha,\hat{r}_1,\hat{r}_2)=\sqrt{2/\pi}\sum_\lambda\left(\frac{F_\lambda(\rho)}{\rho^{5/2}}\right)\varphi_\lambda(\alpha,\hat{r}_1,\hat{r}_2). \tag{3}$$

For F_λ's one has the coupled set of equations

$$\left[\frac{d^2}{d\rho^2}+1-\frac{\nu_\lambda(\nu_\lambda+1)}{\rho^2}\right]F_\lambda(\rho)+2\sum_{\lambda'}\frac{\alpha_{\lambda\lambda'}}{\rho}F_{\lambda'}(\rho)=0, \tag{4}$$

where $\rho=PR$, $\lambda=2n+l_1+l_2$, $\nu_\lambda=\lambda+\frac{3}{2}$, and

$$\alpha_{\lambda\lambda'}=\left\langle\varphi_\lambda\left|\frac{1}{\cos\alpha}+\frac{1}{\sin\alpha}-\frac{1}{|\cos\alpha\hat{r}_1-\sin\alpha\hat{r}_2|}\right|\varphi_{\lambda'}\right\rangle\Big/P. \tag{5}$$

The symbol λ is used to denote the eigenvalue $2n+l_1+l_2$ or the multiplet (n,l_1,l_2,l,m) depending on the context.

The off-diagonal matrix elements $\alpha_{\lambda\lambda'}$ $(\lambda\neq\lambda')$ are generally much smaller than the diagonal elements (see [27]). Actually, the matrix elements of electron-nucleus interactions and the monopole part of the electron-electron interaction are diagonal in (l_1,l_2) and are approximately diagonal in n. Physically also, because of the screening effect, which is centrally symmetric, most of the three-body interactions are included in the diagonal elements. Moreover, the electron-electron interaction responsible for the off-diagonal elements is practically small when the electrons emerge at a large relative angle. So except for very low energies (when screening is only partial) and when the two electrons do not

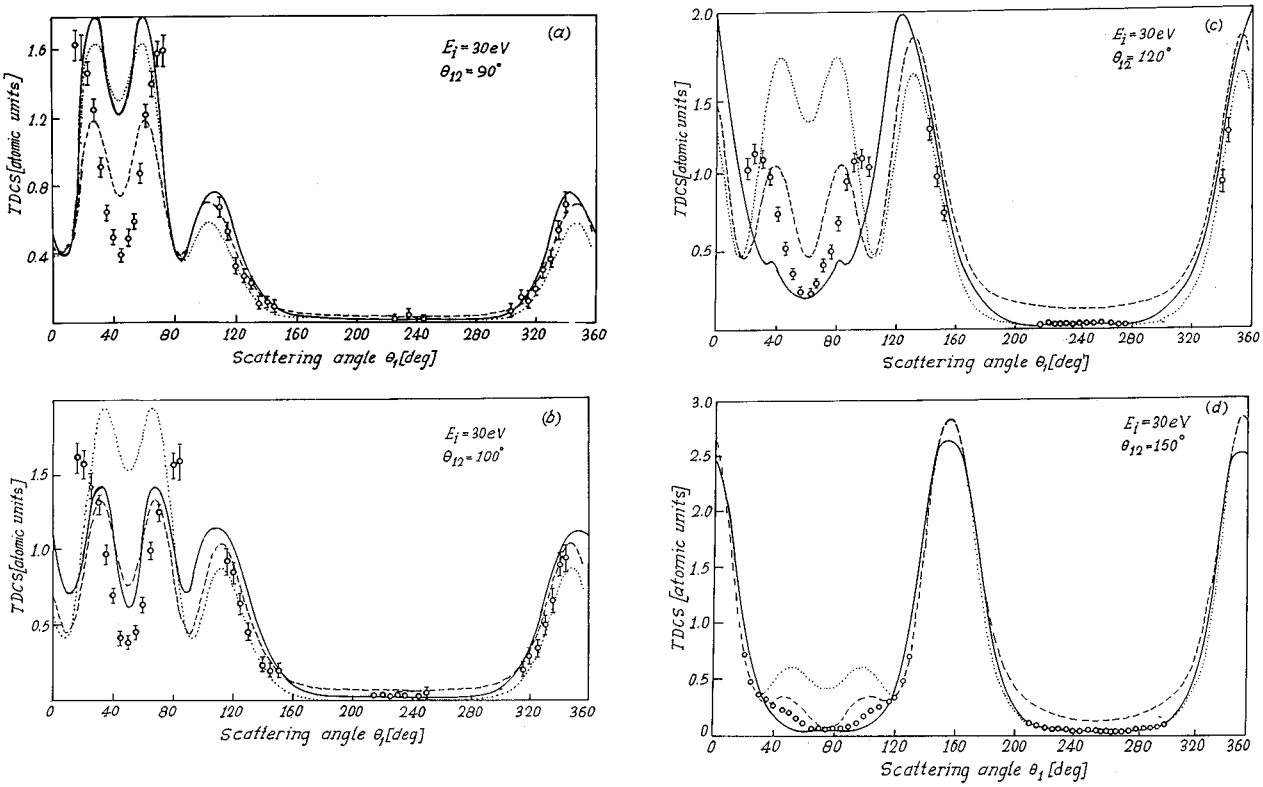

FIG. 1. TDCS in coplanar, equal energy sharing, Θ_{12} constant geometry for $E_i = 30$ eV. Theory: solid line, present results in atomic units; dashed curve, DWBA with (*ad hoc*) PCI and polarization effect included [3], normalized for each energy; dotted curve, DWBA with (*ad hoc*) PCI effect included [3], normalized for each energy. Experiment: circles with or without error bars, Röder *et al.* [3], normalized for each energy.

emerge at a small relative angle, the effect of the off-diagonal elements will be negligible. This is also clear from the results of the present calculation. When the off-diagonal elements are neglected in Eq. (4) the resulting equation becomes a Coulomb equation, different partial waves having different charges. The approximate state $\Psi_{0f}^{(-)}$ with converging boundary conditions is then given by

$$\Psi_{0f}^{(-)}(R,\alpha,\hat{r}_1,\hat{r}_2) = \sqrt{2/\pi}\sum_{\lambda} i^{\lambda} e^{-i\eta_\lambda}\varphi_\lambda^*(\alpha_0,\hat{p}_1,\hat{p}_2) \times \varphi_\lambda(\alpha,\hat{r}_1,\hat{r}_2)[F_\lambda^{(0)}(\rho)/\rho^{5/2}], \tag{6a}$$

where

$$F_\lambda^{(0)}(\rho) = \frac{e^{\pi\alpha_\lambda/2}|\Gamma(\nu_\lambda+1+i\alpha_\lambda)|}{\Gamma(2\nu_\lambda+2)} 2^{\nu_\lambda}\rho^{\nu_\lambda+1}e^{-i\rho} \times {}_1F_1(i\alpha_\lambda+\nu_\lambda+1,2\nu_\lambda+2,2i\rho) \tag{6b}$$

$$\sim \sin(\rho-\nu_\lambda\pi/2+\alpha_\lambda \ln 2\rho+\eta_\lambda), \quad \rho\to\infty \tag{6c}$$

and

$$\alpha_\lambda = \alpha_{\lambda\lambda'}, \eta_\lambda = \arg\,\Gamma(\nu_\lambda+1-i\alpha_\lambda). \tag{6d}$$

It may be noted here that $\Psi_{0f}^{(-)}$ does not satisfy the exact boundary condition at infinity. But with a sufficiently large number of partial waves it will be a good approximation to $\Psi_f^{(-)}$ for the kinematic conditions considered here and will satisfy approximately the asymptotic condition.

The symmetrized state corresponding to $\Psi_{0f}^{(-)}$ is

$$\Psi_{0s}^{(-)}(R,\alpha,\hat{r}_1,\hat{r}_2) = \frac{1}{\sqrt{2}}\{\Psi_{0f}^{(-)}(R,\alpha,\hat{r}_1,\hat{r}_2)+(-1)^S \times \Psi_{0f}^{(-)}(R,\pi/2-\alpha,\hat{r}_2,\hat{r}_1)\}. \tag{7}$$

$S=0$ corresponds to the singlet and $S=1$ corresponds to the triplet state. The corresponding scattering amplitude is then [15]

$$f = -(2\pi)^2\langle\Psi_{0s}^{(-)}|V_i|\Phi_i\rangle \tag{8}$$

and the triple differential cross section is

$$\frac{d\sigma}{d\Omega_1 d\Omega_2 dE_1} = \frac{p_1 p_2}{p_i}\left(\tfrac{1}{4}|f^{(0)}|^2+\tfrac{3}{4}|f^{(1)}|^2\right). \tag{9}$$

III. RESULTS

Table I displays the convergence pattern of the scattering cross section of the present calculation with the increase of the values of the parameters l_{mx}, l_{1mx}, and l_{2mx} for a few set of values of scattering angle θ_1 and angular separation Θ_{12} for energies of 30 and 20 eV. For θ_1 large, say, larger than Θ_{12}, convergence is practically obtained with a small number of partial waves. In such regions scattering is practically *S*-wave-, *P*-wave-, or *D*-wave-like. For Θ_1 close to the peaks, if any exist, a larger number of partial waves contribute, and often with l_{mx} as large as 9, convergence is not

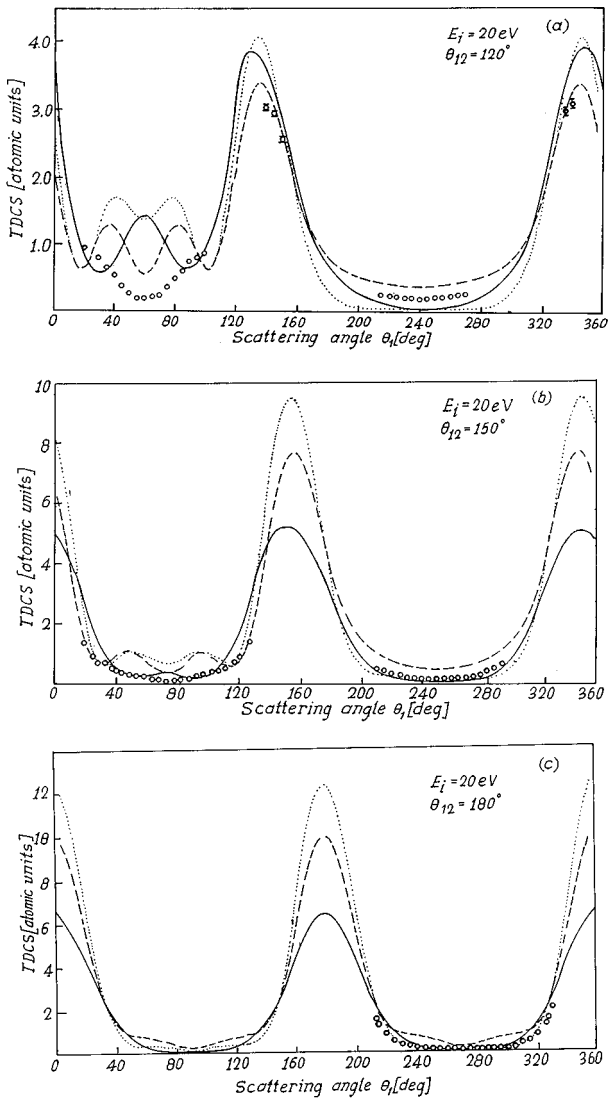

FIG. 2. Same as in Fig. 1, except for $E_i = 20$ eV.

obtained completely. So the peaks correspond to scattering of electrons with a larger angular momentum. Elsewhere, although fewer partial waves contribute, the convergence is slightly oscillatory. In the figures we present results based on calculations with l_{mx} $(=l_{1mx}=l_{2mx})$ up to 6, where there is rapid convergence, and up to 9, where convergence is slow.

In Fig. 1 we present our results for (a) $\Theta_{12}=90°$, (b) $\Theta_{12}=100°$, (c) $\Theta_{12}=120°$, and (d) $\Theta_{12}=150°$ for an incident energy of 30 eV. Here we compare our results with the measurements of Röder *et al.* [3] and with their two sets of DWBA calculations, one with the PCI and polarization included and the other with only the PCI included (see [3]). For $\Theta_{12}=90°$, 100°, and 120° there are four peaks. For the two peaks away from $\theta_1=\Theta_{12}$ there is good agreement between results of all these theories and experiments. In between these peaks there is also generally good agreement, particularly in the shapes, especially with the present calculation. Here it may be remarked that our results are in absolute units, whereas the results of Röder *et al.*, both experimental and theoretical, are not absolute. Incidentally the numbers they presented, when replaced by atomic units, coincide with those of our results in atomic units. In this way we made a comparison between our results and the results of Röder *et al.* Next we look to the region close to $\Theta_{12}/2$. For $\Theta_{12}=90°$ [Fig. 1(a)], the values of the peaks near $\Theta_{12}/2$ are nicely reproduced in our calculation and also in the calculation of Röder *et al.* with only the PCI included. Peak positions shift little and the deep area between the peaks is not well reproduced. However, calculation of Röder *et al.* with both the PCI and polarization included gives a better value for the deep area. With the increase of Θ_{12}, our calculated values for the deep area improve considerably, whereas the peak values deteriorate and the shape of the curves changes. In any case, the overall agreement of our results with experiments becomes better than those of the calculation of Röder *et al.* This is also understandable because our calculation becomes more accurate for larger Θ_{12}.

Next we consider Fig. 2, where we present results for an incident energy of 20 eV. For Θ_{12} large, say, 150° or 180°, our results are in good agreement with the experiments, except at about $\theta_1=\Theta_{12}/2$, where in place of a deep area we have a slight upward bulge [see Figs. 2(b) and 2(c)]. For $\Theta_{12}=120°$ the bulge at $\Theta_{12}/2$ develops into a peak. Except for this, there is good agreement between our present theory and the experiments. It may be noted here that the agreement between our calculation and the experiments is less satisfactory for an energy of 20 eV than for an energy of 30 eV. This is also understandable since the effects of coupling among different partial waves are neglected in the present calculation. This effect is increasingly important at lower energies because of the factor $1/P$ with the coupling potentials [see Eq. (5)]. Moreover, rejection of coupling terms affects results at different angles differently. In any case, gross features of the experimental results are nicely reproduced in the present calculation. Moreover, our results are in absolute units. Recently, we also made a calculation for the asymmetric geometry of Ehrhardt for an energy of 54.4 eV, where we find [28] a little better agreement with the experiment with our calculation than with the CCC calculation. So we have confidence in the absolute values of our cross-section results. Here it may also be remarked that the experiments by Röder *et al.* yield absolute cross sections.

IV. CONCLUSION

The kinematic condition of the above experimental setup for the constant Θ_{12} geometry (with Θ_{12} large) is specially suitable for our present theoretical treatment in which the effect of coupling among different partial waves (in hyperspherical radial variables) is neglected, the angular separation of the two outgoing electrons being large. The resulting calculation may be called the *weak correlation approximation*. For higher energies this approximation should also generally hold. One may need to include only a larger number of partial waves in such cases. For very low energies, close to threshold, or Θ_{12} small, the effect of coupling among different partial waves will no longer be negligible. The calculation will be more involved, but will remain manageable. The number of contributing partial waves then will be even smaller. Such calculations for various kinematic conditions are expected to shed more light on low-energy ionization problems. In any case, the present calculation already dis-

plays the power and strength of the hyperspherical partial-wave method and exhibits that it is a promising formalism for treating atomic ionization problems.

The calculations reported here were done on a Hewlett-Packard personal computer, Model No. 486, with Linux as the operating system (thanks to all at SYBEX who contributed to the development of Linux, a free operating system). For a single point (i.e., for fixed energy and angles) it took about 30 min of computer time for a double precision calculation for $l_{mx}=6$, $l_{1mx}=l_{2mx}=7$, and $n_{mx}=6$ and about 75 min for $l_{mx}=l_{1mx}=l_{2mx}=9$ and $n_{mx}=6$.

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