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Effect of nonspherical distorting potentials in a first-order distorted-wave calculation

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The first-order distorted-wave approximation (DWB1) has proved to be one of the most successful approaches for the theoretical calculation of electron-atom scattering. It is now evident that one must perform multistate close-coupling calculations or second-order perturbation calculations to improve significantly upon the DWB1, but these calculations require enormous computational efforts. Consequently, it is of interest to investigate the possibility of improving the standard DWB1. One such possibility that has not been investigated for electron-atom scattering is the use of realistic nonspherical distorting potentials. In this paper, the DWB1 formalism is presented for nonspherical distorting potentials, and the effects of such a potential are investigated for electron-impact excitation of the $2p$ state of hydrogen.

I. INTRODUCTION

One of the current dilemmas in atomic physics is that the most sophisticated theoretical calculations are not in satisfactory agreement with experimental measurements of differential cross sections and angular-correlation parameters for electron scattering from even the most elementary atoms. This is particularly remarkable when one considers the present state of the art for theoretical calculations. For the close-coupling approach, for example, van Wyngaarden and Walters [1] have performed a 21-state calculation, where three of these states were exact and 18 were pseudostates. More recently, Scholz *et al.* [2] reported an improved "intermediate-energy R-matrix (IERM) calculation" in which the wave function in the inner region is expanded in terms of bound-bound, bound-continuum, and continuum-continuum orbital products. For the perturbation-series approach, Madison and Winters [3] and Madison, Winters, and Downing [4] have performed distorted-wave calculations exact to second order that included distortion not only in the wave function of the projectile electron, but also in the Green's function describing the second-order interaction. More recently, Madison, Bray, and McCarthy [5] reported a second-order calculation for hydrogen including second-order exchange that for the first time exhibited good agreement at all scattering angles for those experimental measurements that depended only on the magnitude of the scattering amplitude. Interestingly, this same calculation was not in agreement at large scattering angles with the measurements that depend on both the magnitude and the phase of the scattering amplitude.

One of the interesting observations resulting from these theoretical works is that the elementary first-order distorted wave (DWB1) results are typically in reasonable qualitative agreement with the experimental data, and it appears that an enormous computational effort is required to significantly improve on the DWB1 results. Consequently, in the interest of calculational simplicity, it has become important to consider the possibility of improving upon the standard DWB1 method. The DWB1 approximation can be derived from a two-state close-coupling calculation [6]. In the standard DWB1 method, two approximations are made: (1) the coupling between the two states is assumed to be weak enough that it can be neglected, and (2) the initial- and final-state distorting potentials are assumed to be spherically symmetric. For elastic scattering and processes involving s states, the distorting potentials will automatically be zero. However, if one is exciting a final p state, then the final-state distorting potential is clearly nonspherical. Since the cases for which the disagreement between the DWB1 results and experiment are largest involve non-s states, we have decided to investigate the effect of assumption (2) by calculating DWB1 results using proper nonspherical atomic distorting potentials.

The concept of using nonspherical distorting potentials in atomic scattering calculations is not new. Boardman, Hill, and Sampanthar [7] derived the general theory of elastic scattering for nonspherical potentials, and Lane and Geltman [8] and Geltman [9] discussed the use of nonspherical potentials for electron-molecule scattering. Today, nonspherical potentials are routinely used for molecular scattering, but to our knowledge the effects have not been investigated for electron-atom scattering.

In this paper, we will analyze the effect of nonspherical distorting potentials in a DWB1 calculation for electron-atom scattering. Section II contains the theoretical for-

mulation of the DWB1 for nonspherical distorting potentials, while results for electron impact excitation of the $1s \rightarrow 2p$ transition in hydrogen are given in Sec. III. The conclusions are drawn in Sec. IV.

II. THEORY

A. Form of the nonspherical distorting potential

In this paper, we shall restrict our considerations to quasi-one-electron atoms. If a one-electron atom is in the state ψ_{nlm} with nlm representing the principal quantum number, orbital angular momentum, and magnetic quantum number, respectively, the interaction between an incident electron and the charge distribution $\psi^*_{nlm}\,\psi_{nlm}$ is given by (in Rydberg energy units)

$$V^m_{nl}(\mathbf{r}) = -\frac{2Z}{r} + 2\int \frac{\psi^*_{nlm}(\mathbf{R})\psi_{nlm}(\mathbf{R})}{|\mathbf{R}-\mathbf{r}|} d^3R \ , \tag{1}$$

where Z is the charge of the nucleus, $\mathbf{r}$ is the position of the incident electron, and $\mathbf{R}$ is the position of the bound atomic electron. Next we express the atomic wave function as

$$\psi_{nlm}(\mathbf{R}) = \frac{R_{nl}(R)}{R} Y_{lm}(\hat{\mathbf{R}}) \ , \tag{2}$$

where $\hat{\mathbf{R}}$ designates the spherical angles (θ,ϕ) describing the direction of the vector $\mathbf{R}$. If a multipole expansion for the distance between the two electrons is made, Eq. (1) may be expressed as

$$V^m_{nl}(\mathbf{r}) = -\frac{2Z}{r} + 2\sum_{\lambda \text{ even}}^{\infty} U^{\lambda}_{nlm}(r) Y_{\lambda 0}(\hat{\mathbf{r}}) \ , \tag{3}$$

where

$$U^{\lambda}_{nlm}(r) = \left[\frac{4\pi}{2\lambda+1}\right]^{1/2} C(l\lambda l; m0m) \times C(l\lambda l; 000) \int R^2_{nl}(R) \frac{r^{\lambda}_<}{r^{\lambda+1}_>} dR \ . \tag{4}$$

Here $C(l_1 l_2 l_3; m_1 m_2 m_3)$ is a Clebsch-Gordan coefficient and $r_{<(>)}$ is the lesser (greater) of (r,R). The spherically symmetric distorting potential $W_{nl}(r)$ that is normally used in DWB1 calculations consists of the nuclear term plus the monopole term of the summation in Eq. (3), i.e.,

$$W_{nl}(r) = -\frac{2Z}{r} + U^0_{nl0}(r)/\sqrt{\pi} \ . \tag{5}$$

Consequently, we have

$$V^m_{nl}(\mathbf{r}) = W_{nl}(r) + 2\sum_{\substack{\lambda=2 \\ \lambda \text{ even}}}^{\infty} U^{\lambda}_{nlm}(r) Y_{\lambda 0}(\hat{\mathbf{r}}) \ . \tag{6}$$

For atomic s states there is no contribution from the summation in Eq. (6) and the distorting potential is spherically symmetric. For p states and higher-angular-momentum states, the summation in Eq. (6) will be nonzero, but these terms are ignored in the standard DWB1 approach. For the case of exciting the $2p$ state of hydrogen, which will be considered in the next section, only the $\lambda=2$ term in the summation contributes, and this term is given by

$$U^2_{2pm}(r) = \sqrt{16\pi/125}(-1)^m(|m|+1)^{-1} \times \int R^2_{2p}(R) \frac{r^2_<}{r^3_>} dR \ . \tag{7}$$

This quadrupole term falls off asymptotically as r^{-3} and is the leading term with nonspherical symmetry, since the atom does not have a permanent dipole moment. The incoming projectile will induce a dipole moment in the atom, but the potential from the induced dipole moment falls off asymptotically as r^{-4}. Potentials decreasing like r^{-4} have often been investigated since the pioneering work of O'Malley, Spruch, and Rosenberg [10]. Stewart and Madison [11] investigated the effect of including the induced dipole potential in a DWB1 calculation, and they found almost no effect from this potential even in the extreme adiabatic approximation.

B. Partial-wave expansion for distorted waves

In the DWB1 approach, partial-wave expansions are made for the initial and final projectile electron wave function. In this section we will examine these expansions for the case of nonspherical distorting potentials. For the case of the incident electron, we assume that the atom is initially in an s state such that the distorting potential is naturally spherically symmetric. The standard expansion may then be made for the initial-state distorted wave:

$$X^{(+)}_i(\mathbf{r}) = \left[\frac{2}{\pi}\right]^{1/2} \frac{1}{k_i r} \times \sum_{l_i, m_i} i^{l_i} \chi_{l_i}(k_i, r) Y^*_{l_i m_i}(\hat{\mathbf{k}}_i) Y_{l_i m_i}(\hat{\mathbf{r}}) \ , \tag{8}$$

which is normalized to $\delta(\mathbf{k}-\mathbf{k}')$. Here k_i is the magnitude of the momentum of the incident electron moving in the direction $\hat{\mathbf{k}}_i$. The radial function x_{l_i} is a solution of

$$\left[-\frac{d^2}{dr^2} + \frac{l_i(l_i+1)}{r^2} + W_i(r) - E\right] \chi_{l_i}(r) = 0 \ , \tag{9}$$

where W_i is the initial-state distorting potential. Asymptotically, the radial function behaves as

$$\lim_{r\rightarrow\infty} x_{l_i}(r) = j_{l_i}(k_i r) + T_{l_i}[n_{l_i}(k_i r) + i j_{l_i}(k_i r)] \ , \tag{10}$$

where j_{l_i} and n_{l_i} are the regular and irregular Riccati-Bessel functions, respectively and

$$T_{l_i} = e^{i\delta_{l_i}} \sin\delta_{l_i} \ , \tag{11}$$

where δ_{l_i} is the phase shift.

For the case of the final-state distorted wave that is scattering from a nonspherical distorting potential, the radial function will depend upon the magnetic state of the atom. Hence, a separate partial-wave expansion must

be made for each magnetic quantum number m. Consequently, the partial-wave expansion for the final-state distorted wave is given by

$$\Phi_f^{m(-)*}(\mathbf{r})=\left[\frac{2}{\pi}\right]^{1/2}\frac{1}{k_f r}\times\sum_{l_f,m_f} i^{-l_f}\phi_{l_f m_f}^{m}(k_f r)Y_{l_f m_f}^{*}(\hat{\mathbf{k}})Y_{l_f m_f}(\hat{\mathbf{r}})\ . \tag{12}$$

The differential equation for the radial function $\phi_{l_f m_f}^m$ is now coupled to other l_f values [see Eq. (14) below] and the set of coupled equations that one must solve depends on the choice of coordinate axes. The coordinate choice that produces the most elementary set of coupled equations is to pick the z axis along $\hat{\mathbf{k}}_f$ and the y axis perpendicular to the scattering plane. With this choice, the only nonzero contributions to the m_f sum occur for $m_f=0$; thus, it is convenient to set

$$\phi_{l_f}^m=\phi_{l_f,m_f=0}^m\ . \tag{13}$$

For a distorting potential of the form of Eq. (6), the coupled differential equations for the radial function $\phi_{l_f}^m$ are given by

$$\left[-\frac{d^2}{dr^2}+\frac{l_f(l_f+1)}{r^2}+W_f(r)-E\right]\phi_{l_f}^m(k_f,r)+\sum_{l_f'=0}^{\infty}B_{l_f l_f'}^m(r)\phi_{l_f'}^m(k_f,r)=0\ , \tag{14}$$

where

$$B_{l_f l_f'}^m(r)=\sum_{\substack{\lambda=2\\ \lambda\ \text{even}}}^{\infty}\frac{2l_f'+1}{2l_f+1}\left[\frac{2\lambda+1}{4\pi}\right]^{1/2}i^{l_f-l_f'}\times C(l_f'\lambda l_f;000)^2U_{nlm}^{\lambda}(r)\ . \tag{15}$$

Here W_f is the spherically symmetric final-state distorting potential. For the case of a final $2p$ state, the only nonzero term in the summation in Eq. (15) occurs for $\lambda=2$ with U_{2pm}^2 given by Eq. (7). From the above results, it is clear that the primary complication created by the nonspherical potentials is that one must solve a set of coupled radial differential equations, Eq. (14), for the final-state distorted wave, instead of an uncoupled set, such as that given by Eq. (9).

An equation equivalent to Eq. (14) was obtained by Boardman, Hill, and Sampanthar [7], and by Geltman [9] for the partial-wave treatment of elastic scattering. Numerical techniques for solving the set of coupled equations have been discussed, for example, by Lane and Geltman [8], Lester and Bernstein [12], Smith [13], and Burke and Seaton [14].

We have applied the generalized Numerov method described by Lane and Geltman [8]. In this method $(L_{\max}+1)$ independent solutions $\tilde{\phi}_{l_f}^m$ of Eq. (14) for partial-wave l_f values from 0 to $L_{\max}$ for a given m are determined. A linear combination of these independent solutions must then be constructed to satisfy the correct asymptotic boundary conditions. To achieve this, the $(L_{\max}+1)$ independent solutions $\tilde{\phi}_{l_f}^m$ are arranged as columns in a matrix $\tilde{F}_{l_f l_f'}^m$, with the l_f values designating the row index. The second subscript l_f' of the matrix $\tilde{F}_{l_f l_f'}^m$ is used to distinguish between the $(L_{\max}+1)$ independent solutions for a given l_f value. By matching both the radial function and its derivative at large r, the matrix $\tilde{F}_{l_f l_f'}^m$ can be transformed to the solution matrix $F_{l_f l_f'}^m$ that satisfies the asymptotic boundary condition

$$\lim_{r\to\infty}F_{l_f l_f'}^m=\delta_{l_f l_f'}j_{l_f}(k_f r)-R_{l_f l_f'}^m n_{l_f}(k_f r)\ . \tag{16}$$

The matrix $R_{l_f l_f'}^m$ is similar to the "reactance" matrix in the standard close-coupling scattering problem. Note, however, that this matrix is not symmetric, since the coupling matrix $B_{l_f l_f'}^m$ in Eq. (14) is not symmetric either. Instead, the symmetry requirement is such that

$$R_{l_f l_f'}^m=\frac{2l_f+1}{2l_f'+1}R_{l_f' l_f}^m\ . \tag{17}$$

While only the R matrix is needed in the close-coupling approach, an actual wave function is required to evaluate the radial integrals in the inelastic T matrix [see Eqs. (21) and (23) below]. This wave function [denoted by $\phi_{l_f m_f}^m$ in Eq. (12)] was taken to be the "diagonal" term $F_{l_f l_f}^m$ of the solution matrix. Recall that $m_f=0$ for our choice of coordinate system.

It was found that the off-diagonal $(l_f\neq l_f')$ coupling terms $B_{l_f l_f'}^m$ in Eq. (14) had very little effect on the final results. In fact, the coupled equations could be solved with $L_{\max}=10$, and the solutions joined smoothly to the solutions from the much simpler uncoupled equations for $l_f>10$ for all energies of interest, provided that the diagonal quadrupole coupling term $B_{l_f l_f}^m$ was retained in the uncoupled equations.

C. DWB1 T matrix

In the DWB1, the T matrix for excitation of a single-particle atom is given by

$$T_m^s=\left\langle\Phi_f^{m(-)}(0)\psi_f(1)\left|\frac{2}{r_{01}}\right|[1+(-1)^s P_{01}]\psi_i(1)X_i^{(+)}(0)\right\rangle, \tag{18}$$

where ψ_i and ψ_f are the initial and final wave functions for the atom. The projectile electron is arbitrarily labeled as 0 and the atomic electron as 1, r_{01} is the distance between the two electrons, and P_{01} is the operator which interchanges particles 0 and 1. The first term in Eq. (18) is the direct term and the second term is the exchange term, while $s=0$ corresponds to singlet scattering and $s=1$ corresponds to triplet scattering, respectively.

Using the standard multipole expansion for the Coulomb interaction and the partial-wave expansions,

Eqs. (8) and (12), for the initial- and final-state distorted waves, the DWB1 amplitude for excitation from an initial s state can be expressed as

$$T^s_m = \sum_{l_i,l_f} [D^m_{l_i l_f} + (-1)^s E^m_{l_i l_f}] \times C(l l_f l_i; m\,0\,m) Y^*_{l_i m}(\theta,\pi) , \quad (19)$$

where the D and E are the partial-wave amplitudes for the direct and exchange terms, while l is the angular momentum and m is the magnetic quantum number for the final atomic state. Recall that the z axis has been chosen parallel to $\hat{\mathbf{k}}_f$, while the y axis is parallel to $\hat{\mathbf{k}}_i \times \hat{\mathbf{k}}_f$; hence, the quantization axis for m is parallel to the direction of the outgoing electron instead of the incident electron, as is normally assumed. The angles (θ,π) represent the direction of the incoming beam relative to the outgoing beam in this coordinate system.

The partial-wave expression for the direct scattering amplitude is given by

$$D^m_{l_i l_f} = 2\pi^{-3/2}(k_i k_f)^{-1} \left[\frac{2l_f+1}{2l+1}\right]^{1/2} (-1)^l \times C(l_i l l_f; 000) i^{l_i - l_f} I^m_{l_i l_f} , \quad (20)$$

with

$$I^m_{l_i l_f} = \int\int \phi^m_{l_f}(k_f,r) R^*_{nl}(R) \frac{r^l_<}{r^{l+1}_>} \times R_{1s}(R) \chi_{l_i}(k_i,r) dR\, dr . \quad (21)$$

Here nl are the quantum numbers of the final atomic state with the initial state assumed to be the $1s$ state. For the exchange case, the partial-wave expression for the amplitude is given by

$$E^m_{l_i l_f} = 2\pi^{-3/2}(k_i k_f)^{-1}(-1)^{l_f} C(l_i l_f l; 000) \times i^{l_i - l_f} G^m_{l_i l_f} , \quad (22)$$

with

$$G^m_{l_i l_f} = \int\int \phi^m_{l_f}(k_f,r) R^*_{nl}(R) \frac{r^{l_f}_<}{r^{l_f+1}_>} \times R_{1s}(r) \chi_{l_i}(k_i,R) dR\, dr . \quad (23)$$

Once more, we point out the m dependence of the present radial matrix elements, which does not exist in the standard DWB1 approach.

To compare with experimental λ and R parameters, it is necessary to transform to a quantization axis parallel to the incident-beam direction. This can be accomplished as follows. For the above coordinate system, the atomic wave function after the collision can be written as

$$\psi^s = T^s_1 Y_{11}(\hat{\mathbf{R}}) + T^s_0 Y_{10}(\hat{\mathbf{R}}) + T^s_{-1} Y_{1-1}(\hat{\mathbf{R}}) , \quad (24)$$

where the s superscript designates either singlet or triplet scattering and the angles $\hat{\mathbf{R}}$ are measured relative to the $\hat{\mathbf{k}}_f$ direction. If we make a rotation through an angle θ about the y axis, Eq. (24) becomes

$$\psi^s = b^s_1 Y_{11}(\hat{\mathbf{R}}') + b^s_0 Y_{10}(\hat{\mathbf{R}}') + b^s_1 Y_{1-1}(\hat{\mathbf{R}}') , \quad (25)$$

with

$$b^s_1 = (\cos\theta) T^s_1 - [(\sin\theta)/\sqrt{2}] T^s_0 \quad (26a)$$

and

$$b^s_0 = \sqrt{2}(\sin\theta) T^s_1 + (\cos\theta) T^s_0 . \quad (26b)$$

The quantization axis is parallel to the $\hat{\mathbf{k}}_i$ direction, and the angles defining $\hat{\mathbf{R}}'$ are measured relative to this direction. The above b^s_m amplitudes can be used to calculate the standard λ and R parameters, which can then be compared with experiment.

III. RESULTS

We have written a computer code to solve the coupled equations given by Eq. (14), and have modified standard DWB1 codes to calculate the direct and exchange amplitudes given by Eqs. (20) and (22) and finally the b^s_m amplitudes given by Eqs. (26a) and (26b). These amplitudes were then used to evaluate cross sections as well as λ and R parameters for electron-impact excitation of the $2p$ state of hydrogen. Most of the experiments for this process have been performed for 54.4-eV incident electrons. At this energy, cross-section results calculated with the nonspherical distorting potential (DWB1NS) or with the standard DWB1 method would be indistinguishable on a journal figure.

One can expect, however, that the effect of the nonspherical distorting potential would be larger for the λ and R parameters, since these quantities are sensitive to the final magnetic state of the atom and the nonspherical potential is dependent on the final m state. Results for these parameters are shown in Figs. 1 and 2. Although

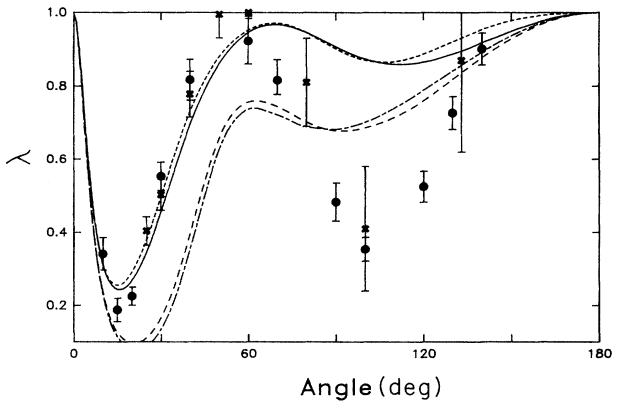

FIG. 1. λ parameter for 54.4-eV electron-impact excitation of the $2p$ state of atomic hydrogen. The experimental data are taken from Williams (●) (Ref. [15]) and Weigold, Frost, and Nygaard (×) (Ref. [16]). The theoretical calculations are ——, EP; - - -, EP-NS; –––, MM; and — — —, MM-NS.

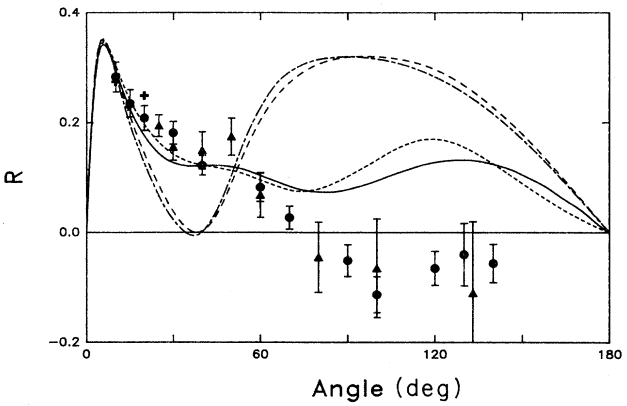

FIG. 2. R parameter for 54.4-eV electron-impact excitation of the $2p$ state of atomic hydrogen. The theoretical calculations are ——, EP; - - - , EP-NS; –––, MM; and — — —, MM-NS. The experimental data are taken from Williams (●), (Ref. [15]); and Weigold, Frost, and Nygaard (▲) (Ref. [16]).

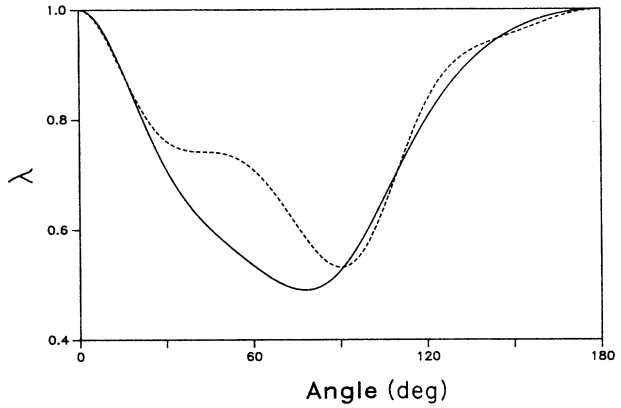

FIG. 3. λ parameter for 13.87-eV electron-impact excitation of the $2p$ state of atomic hydrogen. The theoretical curves are ——, EP; and - - -, EP-NS.

the nonspherical potential does have a somewhat larger influence on the results than it did for the cross section, the effect is still quite small for this energy.

Figures 1 and 2 contain two sets of nonspherical calculations that are each compared with equivalent standard DWB1 results. In the traditional distorted-wave method discussed by Mott and Massey (MM) the incoming electron is distorted by the spherically symmetric ground-state potential, and the outgoing electron is distorted by the spherically symmetric final-state potential. For the case labeled MM-NS, the incoming electron is distorted by the spherically symmetric ground state of the hydrogen atom, while the outgoing electron is distorted by the nonspherical potential of the excited $2p$ state. The curve labeled EP is a distorted-wave model for which both the incoming and outgoing electrons are distorted by the spherically symmetric excited-state potential. In this model, the excitation process happens early in the collision and the projectile is primarily influenced by the excited state of the atom. The EP model has given the best overall agreement with experiment for excitation of many different states of many different atoms. The nonspherical equivalent of the EP model would correspond to both the incoming and outgoing electrons being distorted by the nonspherical excited-state potential. However, we were not able to perform that calculation, since the coupled equations, Eq. (14), are valid only for the z axis parallel to either the incident-beam direction or the scattered particle's direction. Consequently, the present formalism can only be applied to the incoming electron or outgoing electron, but not both. For the results labeled EP-NS, the incoming electron is distorted by the spherically symmetric excited-state potential, and the outgoing electron is distorted by the nonspherically symmetric excited-state potential.

It is clear from Figs. 1 and 2 that the quadrupole potential has a small effect on the DWB1 results at 54 eV. The EP model continues to be in significantly better agreement with experiment than the MM model. For the EP model, the nonspherical quadrupole distorting potential did slightly improve the agreement between experiment and theory for scattering angles out to 60°, bringing the EP-NS results even closer to experiment in this angular range for both the λ and R parameters.

We also examined the effect of the nonspherical distorting potential as a function of incident electron energy. For energies greater than 54 eV, the effect decreased with increasing energy, but was qualitatively similar to Figs. 1 and 2. The largest effect of the nonspherical quadrupole potential was found for much lower incident electron energies. Figure 3 presents results for the λ parameter at an incident electron energy very near threshold in the EP model. For this case the DWB1NS and the standard DWB1 predict fairly different behavior near the 60° scattering angle. However, this observation is primarily

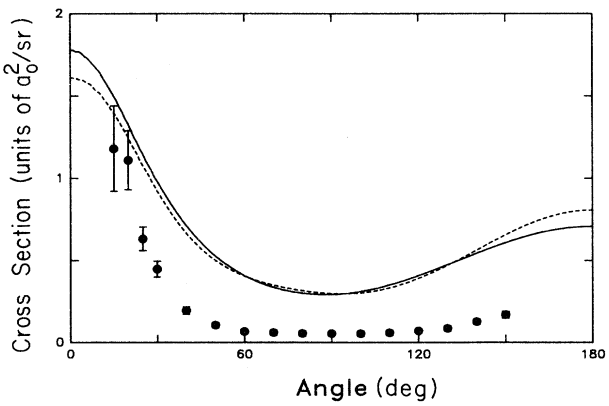

FIG. 4. Differential cross section in units of a_0^2/sr for 13.87-eV electron-impact excitation of the $2s+2p$ states of atomic hydrogen. The theoretical curves are ——, EP; and - - -, EP-NS. The experimental data are taken from Williams (●) (Ref. [17]).

of academic interest, since it is the well known that the standard DWB1 is unreliable for energies this low. This fact is demonstrated in Fig. 4, where experimental and theoretical cross sections for 13.87-eV excitation of the $2s+2p$ states of hydrogen are compared with the EP model. While there are no nonspherical contributions to the $2s$ part of the sum shown in Fig. 4, this sum is dominated by the $2p$ contribution. It is interesting to note that the nonspherical distorting potential continues to only have a small effect on the differential cross sections—even for energies near threshold. While the quadrupole potential is clearly important for the angular correlation parameters for low-incident-energy electrons, other effects not contained in the DWB1 are certainly important too. Hence, we would not expect the DWB1NS λ parameters of Fig. 3 to be highly reliable.

IV. CONCLUSIONS

In this paper we have investigated the effect of including a nonspherical distorting potential in a DWB1 calculation. For our test case of electron-impact excitation of the $2p$ state of atomic hydrogen, the quadrupole distortion produced changes in the differential cross section that were generally the same size or smaller than the experimental error. Hence, this effect can be ignored for all practical purposes if one is interested only in cross sections. For angular-correlation parameters, the nonspherical potential tended to slightly improve the agreement between experiment and theory for the higher incident electron energies (where the DWB1 is expected to be valid). However, the changes were fairly small, so it is questionable whether the additional effort required to solve the coupled differential equations is justifiable. For lower incident-electron energies, the nonspherical potentials are important for the angular correlation parameters and should certainly be included in an accurate calculation. However, additional physical effects neglected in the DWB1 are also important for these energies, so a DWB1NS calculation alone is not expected to agree well with experiment.

In conclusion, then, for energies where the DWB1 approximation is expected to be valid, the nonspherical distorting potentials produce a small effect, which, for practical purposes, can be neglected without producing too great an error. For lower energies where the DWB1 is not expected to be valid, the neglect of the nonspherical distorting potentials is part of the problem, but is by no means the entire problem. We therefore conclude that the standard practice of using spherically symmetric distorting potentials in the DWB1 is justifiable at the higher energies but not at the lower energies, where one will have to do something more than simply adding a quadrupole distorting potential to fix the problem.

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