As mentioned earlier, terms inside [ ] contribute only if A and H are identical atoms. The identification of A or H has been dropped on the right-hand side of the equations since the only manner in which the A system affects the equations is through the single parameter $\epsilon(A)$. A similar conclusion has been given by Grossetête.[7] This substantiates the suspicion that it is, after all, only the expectation value of the electron spin polarization that is important in spin exchange. The nuclear spin only increases the number of hyperfine spin states among which this polarization is distributed. The appearance of $\epsilon(A)$ in Eqs. (8) also indicates the manner in which spin exchange serves as a "polarization detector" between two types of atoms. This effect has already been used extensively.[3,5,8] Furthermore, the off-diagonal part of Eqs. (8) enables one to readily determine the form of the spin-exchange shift for a particular resonant atomic system.

III. CONCLUSIONS

As shown by the form of the equations for the diagonal and off-diagonal elements, the only manner in which the A system affects the time evolution of $\rho(H)$ is through the particular combination of density-matrix elements $\epsilon(A)$ and not through the specific population of each hyperfine level. Although the final equations appear complex at first glance, they are much easier to deal with than the matrix equation that was the starting point. Only the matrix elements of σ_x, σ_y, and σ_z for the systems of interest are needed to give quickly the equations of motion for spin exchange. For example, since Rb^{87} has eight hyperfine levels, using Eq. (3) directly would mean manipulating 64×64 matrices, and the simplification of this calculation is particularly evident.[9] Equation (8), of course, reproduces previously published results for the cases of hydrogen-hydrogen spin exchange,[3,5,10] hydrogen-deuterium spin exchange,[3] deuterium-deuterium spin exchange,[3] rubidium-rubidium spin exchange,[9] and rubidium-hydrogen spin exchange.[6] The matrix elements of $\vec{\sigma}$ for these calculations are displayed in Tables I–III.[11]

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[*] Work supported in part by the National Science Foundation and the Office of Naval Research.

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PHYSICAL REVIEW A VOLUME 3, NUMBER 1 JANUARY 1971

Addendum to "Potential-Scattering Model for Electrons on Helium and Other Atoms"*

R. A. Berg, J. E. Purcell, and A. E. S. Green
Department of Physics and Astronomy, University of Florida, Gainesville, Florida 32601

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It is shown, as an extension to Ref. 1, that a relatively simple analytic potential, which was obtained from studies of bound electron states in atoms, gives differential cross sections in good agreement with experimental values for the rare gases Ar, Kr, and Xe.

A relatively simple analytic potential for describing the elastic scattering of electrons by atoms was proposed by the present authors.[1] The model is based on a single-particle model for bound states of electrons in atoms.[2]

The purpose of the work done in Ref. 1 was to study the feasibility of the approach by considering the case of electrons on helium, although the more general problem was discussed somewhat. In this paper, the results of applying the model to argon, krypton, and xenon are shown and compared with recent experimental data. Our main purpose is to show that the simple modification given in Ref. 1 of the analytical form used in Ref. 2 is sufficient to account for the main features of the observed cross sections without further adjustment of the parameters involved.

The solid curves shown in Fig. 1 for Ar, Fig. 2

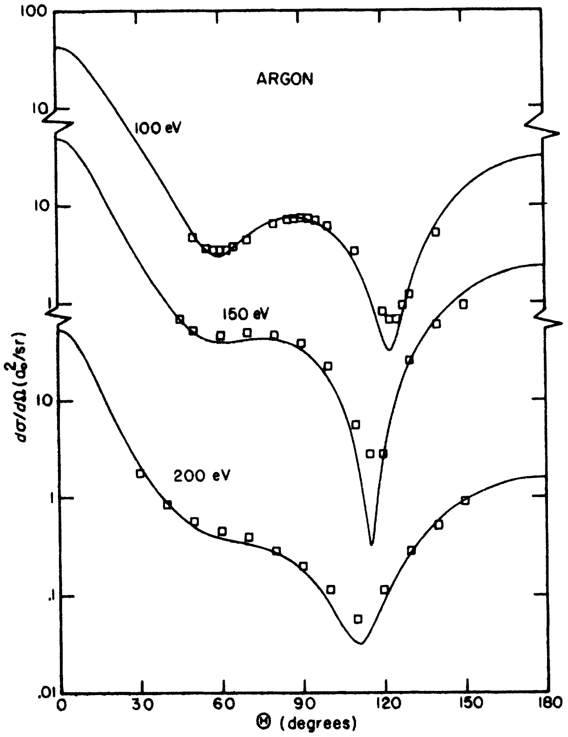

FIG. 1. Comparison of differential cross sections for electron scattering by argon. The boxes are normalized experimental results (see text). The vertical axis is logarithmic. The energy of the incident electron is listed next to the curve.

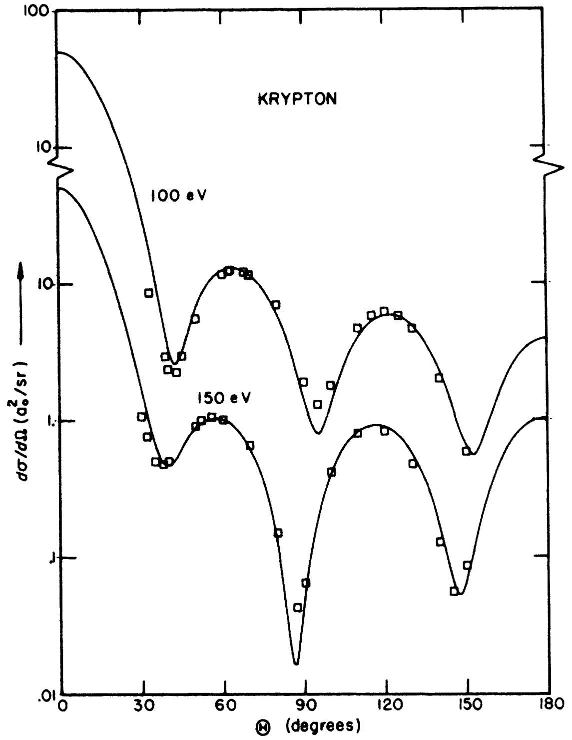

FIG. 2. Comparison of differential cross sections for electron scattering by krypton. See Fig. 1 for details.

for Kr, and Fig. 3 for Xe were obtained using just the potential V_s given in Eq. (5) of Ref. 1, namely,

$$V_s = -2Zr^{-1}\Omega(r)\,, \qquad (1)$$

where

$$\Omega(r) = [H(e^{r/D} - 1) + 1]^{-1}.$$

The constant D is tabulated in Ref. 2 and H is given in terms of D and Z by[3]

$$H = DZ^{0.4}\,. \qquad (2)$$

Hence, the screening function $\Omega(r)$ is determined by the single parameter D which fluctuates around the value $D \simeq 0.8$ a.u. as a function of Z. The values of D used here as given in Table II of Ref. 2 are 0.862 (Ar), 0.689 (Kr), and 0.940 (Xe).

The data plotted in Figs. 1–3 were obtained from graphs given in the literature[4] and do not have absolute values assigned to them. The normalization process used here was to require that the areas under the parts of the angular distribution which were common to both experiment and theory should be equal. It is clear that the calculations agree quite well with the observations both in detail of structure and in relative magnitude. Since the data

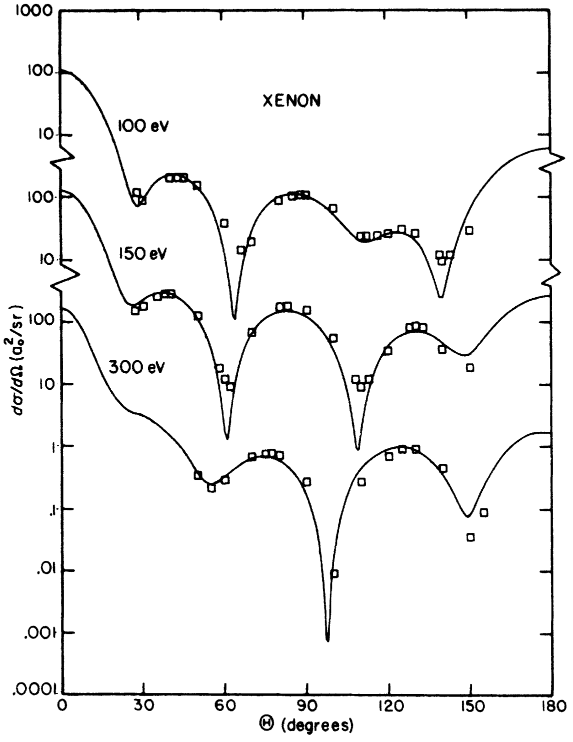

FIG. 3. Comparison of differential cross sections for electron scattering by xenon. See Fig. 1 for details.

do not extend to angles less than about 30°, no special treatment of small angles was necessary.

We have also considered the elastic scattering of electrons by mercury and bismuth, for which some data is available. Again, only real potentials are used.

In order to obtain the correct small-angle behavior for $d\sigma/d\Omega$, it is necessary to include a polarization term in the potential. It was found that a polarization term of the form used in Ref. 1 is quite adequate to correctly give $d\sigma/d\Omega$ for small-angle scattering of electrons from Hg. Also, the position of the first diffraction peak is correctly predicted by the model, but the magnitude of the calculated diffraction maximum was larger than the observed. Data for this atom were obtained from Bromberg.[5]

There are also recent relative differential cross-section data[6] for electrons on Bi, an atom with a similar and relatively high value of Z. Again the results obtained correctly predict the positions of maxima and minima but do not show the correct behavior for the relative magnitudes of the peaks. The results for Hg and Bi are not shown since there is reason to think that one should use a completely relativistic approach for larger-Z atoms.[7] This may account for some of the discrepancies mentioned above. However, the simple independent particle model potential characterized by Eq. (1) with parameters determined by bound-state studies in conjunction with Schrödinger's equation seems to characterize the available scattering data for small and middle values of Z quite well.

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[3] In Refs. 1 and 2, H was given as $H=\alpha D(Z-1)^{0.4}$. It was found that α could be fixed essentially at unity. Also the interpretation given to the factor $(Z-1)$ was that it represented one less than the total number of electrons in the problem, which in this case is $[(Z+1)-1]=Z$. At any rate, the difference in the two forms is very minor in most cases of interest.

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Use of Nonlinear Sequence-to-Sequence Transformations in High-Order Perturbation Theory Calculations*

James H. Renken
Sandia Laboratories, Albuquerque, New Mexico 87115

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The sequences of partial sums for quantities such as bound-state energies that one obtains from high-order perturbation theory often have poor convergence qualities. Here it is pointed out that use of nonlinear sequence-to-sequence transformations may dramatically improve the convergence properties of the perturbation theory results. This technique is illustrated by application to data from a recent paper.

I. INTRODUCTION

In some recent papers, high-order perturbation theory has been applied to the determination of bound-state energies of atomic systems. The results are often less than satisfactory because either the sequence of energy values converges very slowly or the sequence is generated by an asymptotic expansion which begins to diverge before the desired value for the energy is revealed.

The purpose of this paper is to point out the existence of a family of nonlinear sequence-to-sequence transformations which, in some cases, is effective in accelerating the convergence of slowly convergent sequences and inducing convergence in divergent sequences. Data from a paper by Iafrate and Mendelsohn[1] (IM) are used to illustrate the use of these transformations; the results are quite encouraging. In view of the ease with which many of these transformations are performed, it seems that their use should be explored in any high-order perturbation calculation.

II. TRANSFORMATIONS

Shanks[2] describes several types of nonlinear