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Dependence of the Phase Shift on Energy and Atomic Number for Electron Scattering by Atomic Fields

Steven Trent Manson*

National Bureau of Standards, Washington, D. C. 20234

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Phase shifts of *s*, *p*, *d*, and *f* electrons scattered elastically by a potential appropriate to singly-charged positive ions have been calculated for energies ranging up to 2 Ry above threshold and for selected elements throughout the periodic system. The results are discussed in terms of characteristics of the model potential.

I. INTRODUCTION

Although the low-energy elastic scattering of electrons from singly-ionized positive ions is important in plasmas, the upper atmosphere, and astrophysics, its experimental and theoretical study has not been extensive. For exploratory purposes we have computed scattering phase shifts extensively using a simple theoretical model, not so much to obtain accurate quantitative results, but rather to get order of magnitude estimates and to understand the systematics of phase shifts near threshold as functions of both energy and atomic number. In a sense this work represents a continuation of Rau and Fano's[1] investigation of the systematics of the potential we are using.

II. METHOD OF CALCULATION

The continuum solutions employed in this calculation pertain to the unrelaxed Herman-Skillman[2] (Hartree-Fock-Slater) potential for the ground state of a given atom: specifically we consider solutions of

$$\left(\frac{d^2}{dr^2}+V(r)+\epsilon-\frac{l(l+1)}{2}\right)P_{\epsilon l}(r)=0\ , \qquad (1)$$

where $V(r)$ is the Herman-Skillman (HS) potential,

$$V(r)\to 2Z/r, \quad \text{as } r\to 0\ ;$$
$$\to 2/r, \quad \text{as } r\to\infty\ ;$$

with r in units of a_0 $(=5.29\times10^{-9}\text{ cm})$, and ϵ is the electron energy in Rydbergs. The asymptotic (large r) form of $P_{\epsilon l}(r)$ is

$$P_{\epsilon l}(r)\to \epsilon^{-1/4}\sin[\epsilon^{1/2}r-\tfrac{1}{2}l\pi - \epsilon^{-1/2}\ln 2\epsilon^{1/2}r+\sigma_l(\epsilon)+\delta_l(\epsilon)]\ , \qquad (2)$$

where $\delta_l(\epsilon)$ is the phase shift (with respect to Coulomb waves) and

$$\sigma_l(\epsilon)=\arg\Gamma(l+1-i\epsilon^{-1/2}).$$

Phase shifts were obtained from the numerical continuum wave functions by the Seaton and Peach method.[3]

III. RESULTS AND DISCUSSION

Calculations have been carried out from threshold ($\epsilon=0$) to $\epsilon=2$ Ry for $s, p, d,$ and f waves ($l=0,1,2,3$) for various elements. The results are shown in Figs. 1–4. Phase shifts for $l\geq 4$ are negligible in the energy range we are considering. The s- and p-wave phase shifts decrease monotonically from threshold for all ϵ. The d-wave phase shifts are increasing or decreasing at threshold, depending on the element's position in the periodic table. Considering that with the HS potential[2] the $3d$ orbital first becomes occupied in the ground state of the atom at $Z=21$ (scandium), the $4d$ at $Z=39$ (yttrium), the $5d$ at $Z=57$ (lanthanum), and the $6d$ at $Z=89$ (actinium), we see from Fig. 3 that the phase shift changes slope at threshold from positive to negative in the Z range just before these points, i.e., in the vicinity of the rare gases. We also note that no d phase shift rises by 2π; the largest phase shift rise is for argon ($Z=18$), and amounts to $\pi/2$. Figure 4 shows that the f-wave phase shift is always increasing at threshold. In our potential the $4f$ and $5f$ orbitals become occupied at $Z=58$ and 91, respectively, and the shape of the δ_f versus ϵ curve changes greatly just below these points. In fact for Z values of 54, 55, 86, and 87 we predict changes of the phase shift by π. It is well to reiterate at this point, that these phase shifts are for a model potential and will predict general trends well, but need not be quantitatively accurate.

The shapes of these phase shift curves can be explained in terms of the combination of HS and centrifugal potentials which have been discussed in detail elsewhere.[4] The relation between the phase shift and the potential is[5]

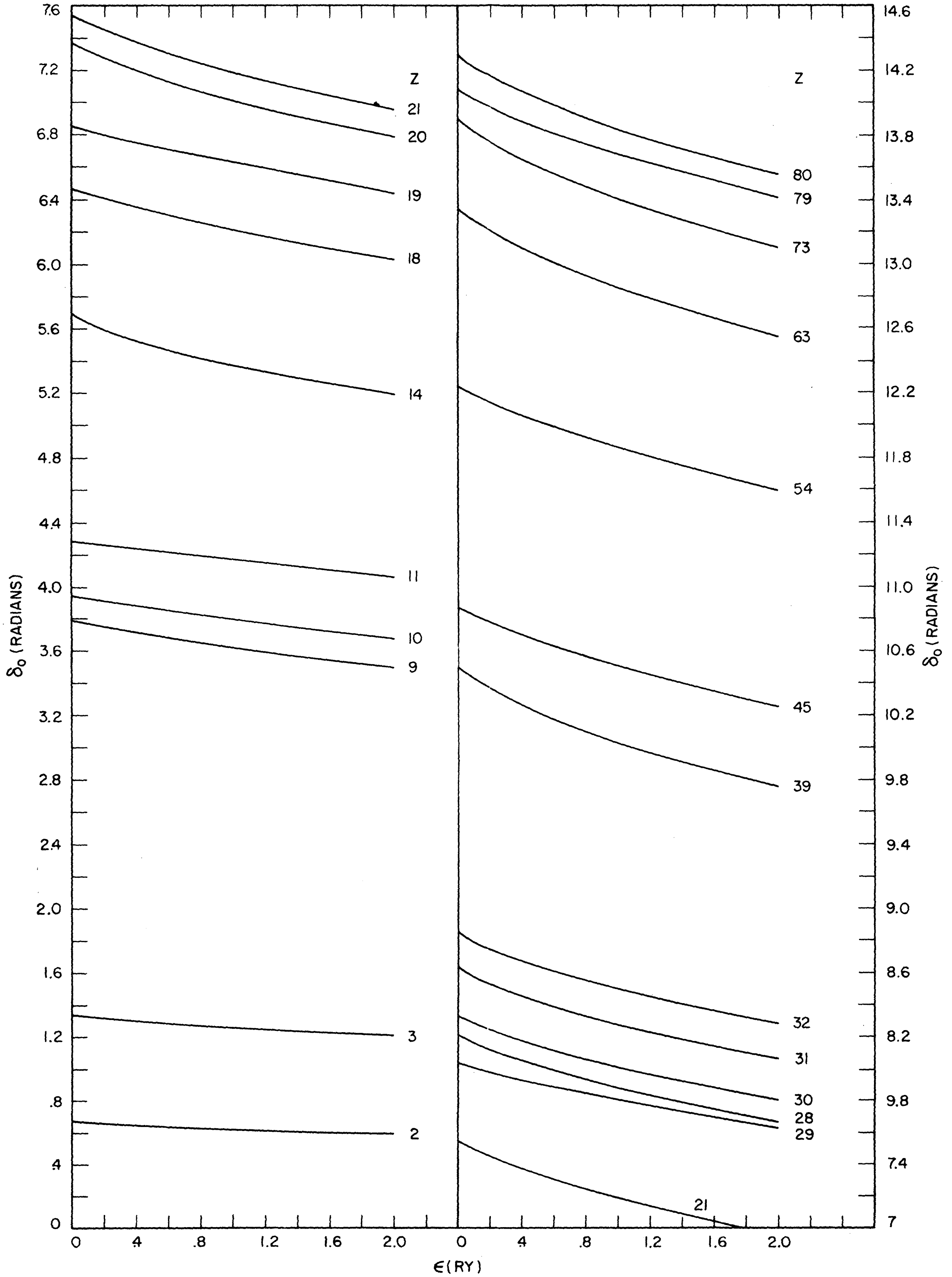

FIG. 1. The *s*-wave phase shifts for various elements as a function of energy above threshold ϵ. Z is the atomic number.

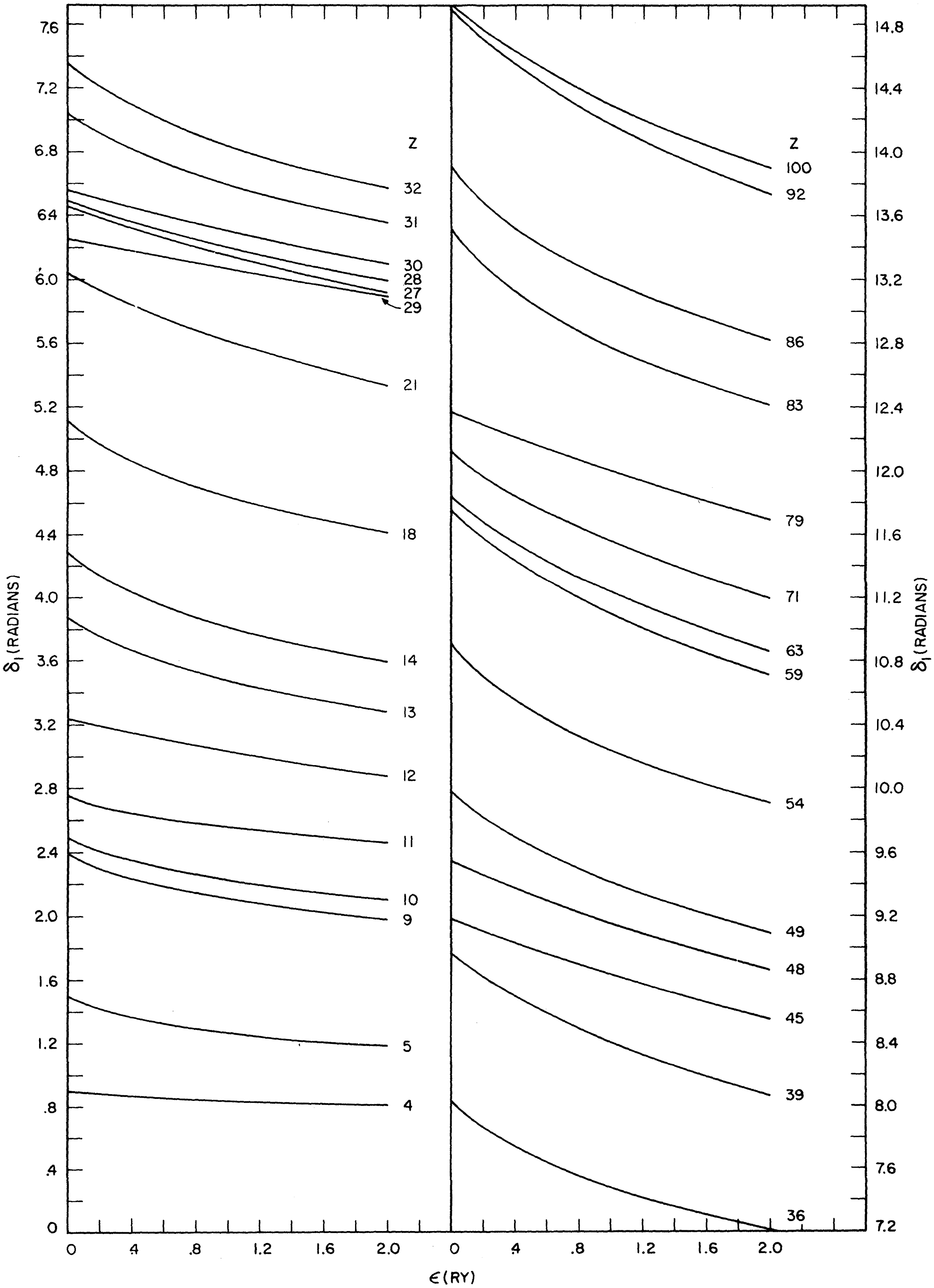

FIG. 2. The p-wave phase shifts for various elements as a function of energy above threshold ϵ. Z is the atomic number.

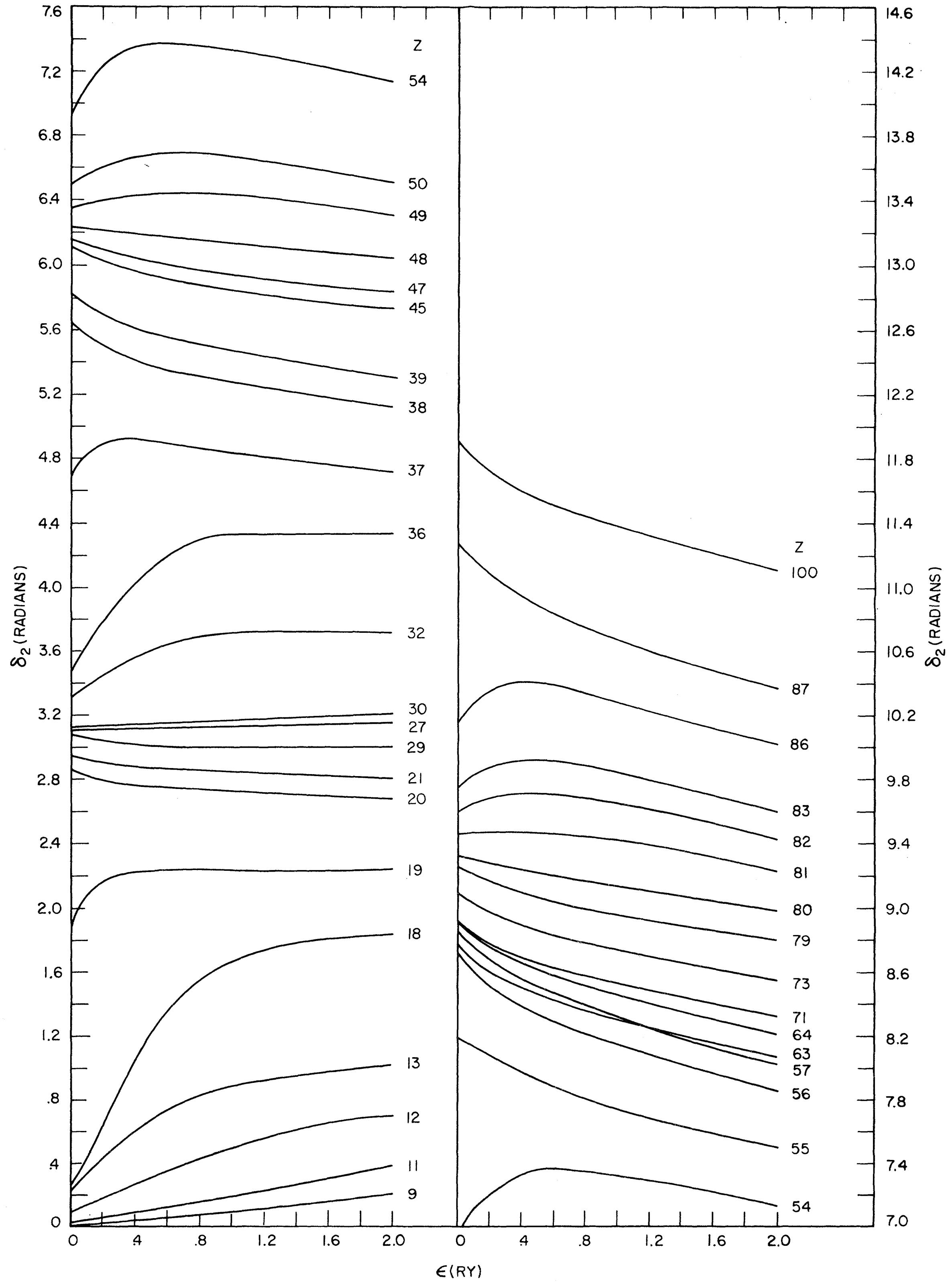

FIG. 3. The d-wave phase shifts for various elements as a function of energy above threshold ϵ. Z is the atomic number.

$$\sin\delta_l(\epsilon) = \int_0^\infty g_{\epsilon l}(r)\,[V(r)P_{\epsilon l}(r) - (2/r)P_{\epsilon l}(r)]\,dr\,, \qquad (3)$$

where $g_{\epsilon l}(r)$ is the solution to Eq. (1) with $V=0$ and $\bar{P}_{\epsilon l}(r)$ is the hydrogenic continuum solution, both normalized like $P_{\epsilon l}$ in Eq. (2). Thus, since $P_{\epsilon l}(r)$ and $\bar{P}_{\epsilon l}(r)$ vary relatively slowly with energy for s and p waves because the $\epsilon=0$ solutions are so penetrating, the only effect of increasing the energy is to make $g_{\epsilon l}$, $P_{\epsilon l}$, and $\bar{P}_{\epsilon l}$ oscillate with shorter wavelength so that the integral decreases and the phase shifts decrease monotonically from threshold. The situation is substantially different for d waves because the potential (HS plus centrifugal) now has two wells separated by a barrier.[1,4] This barrier tends to keep low-energy d waves from penetrating very much at low Z, but higher-energy waves through the barrier, thus increasing $\delta_d(\epsilon)$ with ϵ. Increasing Z, the inner well gets deep enough to support a bound d state so that the first loop of the continuum wave function is in the inner region even at $\epsilon=0$. The phase shift is then relatively flat as a function of energy until Z is increased to near where the next d state gets bound; this cycle is repeated for the 5d and 6d states as well. The same thing happens for f waves: here, however, the barrier is wider and higher, so it is more effective in keeping $\epsilon=0$ waves essentially completely nonpenetrating up to the values of Z around where the first f state becomes bound in the inner well. At high enough ϵ, of course, the effect of increased oscillations of the various functions in (3) takes over in all cases, and the phase shift then decreases with energy.

In Fig. 5, $\delta_l(\epsilon)$ is plotted against Z for $l=0$, 1, 2, 3, and $\epsilon=0$, 2 Ry. For f waves it is seen that at $\epsilon=0$, the curve is a step function since it depends essentially only on the outer region of the potential and on the number of bound states the inner well can support; however, the curve profile differs already at $\epsilon=2$ Ry since it now depends on the details of the potential in the inner region. The d state curves at $\epsilon=0$ and $\epsilon=2$ also sample different regions of the potential and, thus, are seen to be rather different. The p wave curves are much the same, the $\epsilon=0$ always being above the $\epsilon=2$ curve, and the same is true for s waves. This is because the s and p waves, being very penetrating, are determined by the potential over the entire range of r at both $\epsilon=0$ and $\epsilon=2$.

Finally, since the threshold value of $\delta_l(\epsilon)$ equals π times the $n=\infty$ quantum defect σ_l for the atom,[6] we can assess the accuracy of our calculations by computing quantum defects and comparing with the corresponding experimental values derived from atomic energy levels.[7] This is shown, for a few cases, in Table I. This com-

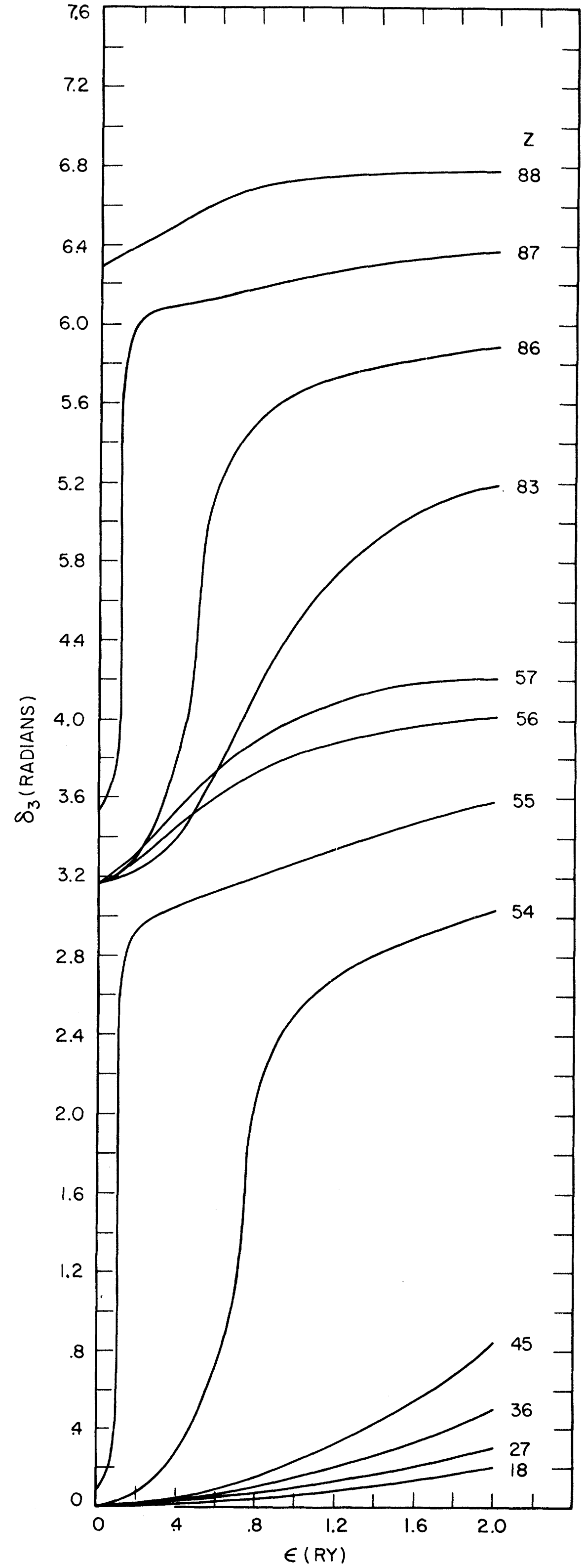

FIG. 4. The f-wave phase shifts for various elements as a function of energy above threshold ϵ. Z is the atomic number.

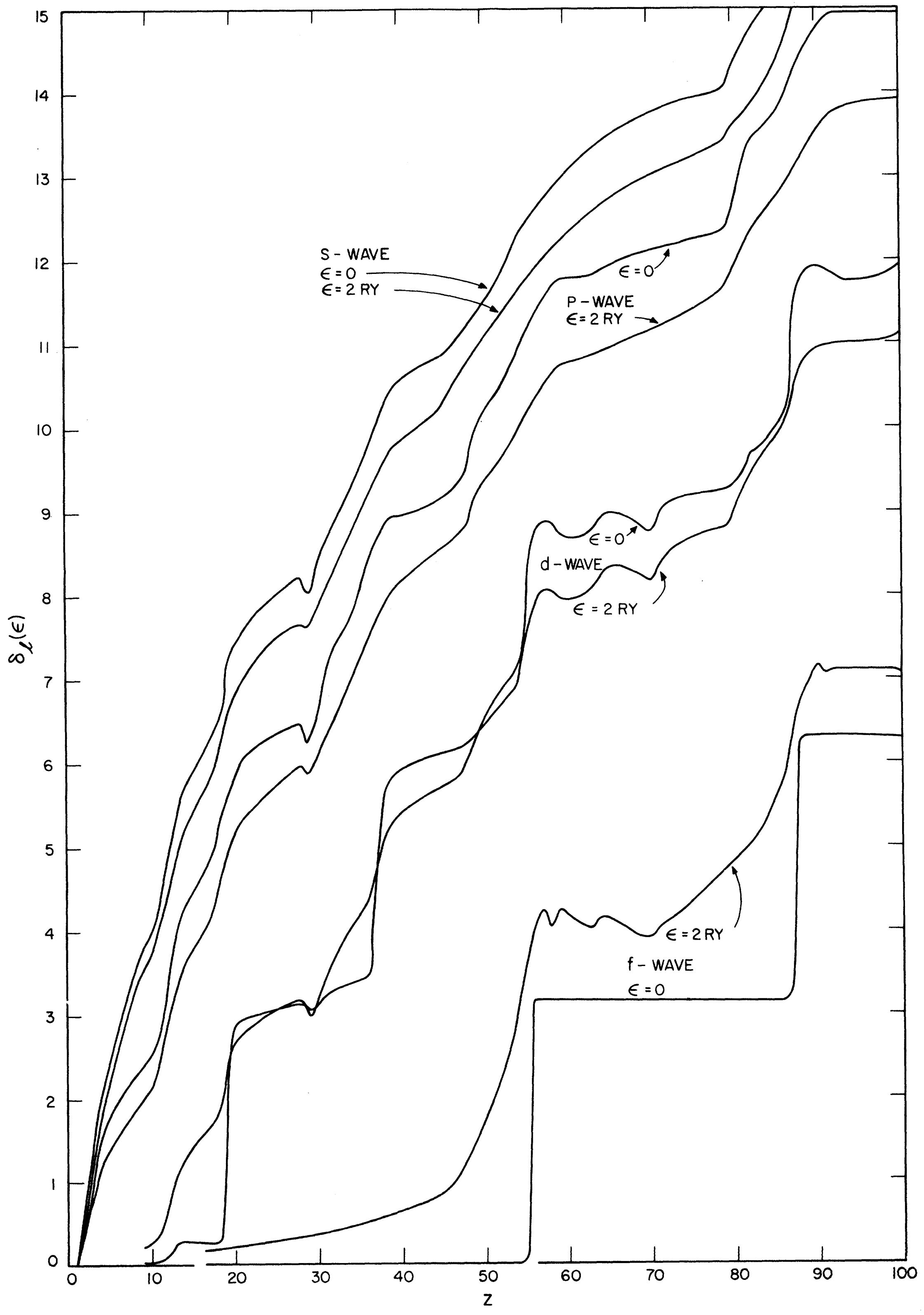

FIG. 5. Phase shifts at threshold and at $\epsilon = 2$ Ry for *s*, *p*, *d*, and *f* waves as a function of atomic number *Z*.

TABLE I. Experimental and theoretical quantum defects for s, p, d, and f waves in Rb and Xe.

Element	Angular momentum	Experimental	Calculated
Rb	0	3.14	3.15
Rb	1	2.66	2.74
Rb	2	1.35	1.47
Rb	3	0.01	0.00
Xe	0	4.02	3.90
Xe	1	3.56	3.46
Xe	2	2.43	2.22
Xe	3	0.03	0.00

parison, as well as a similar comparison of other quantities calculated from HS potentials such as the photo-ionization calculations of Ref. 4, gives an assessment of the accuracy of the HS potentials. The question can then be asked – can one replace systematically the HS by a substantially better central potential? If not, comparison of experimental phase shifts with those given in this paper provide an experimental characterization of nonlocal exchange effects.

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*Present Address: Department of Physics, Georgia State College, Atlanta, Georgia 30303.

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Cross Sections for Electron Capture into the Excited Level $n = 6$ of Hydrogen by 5- to 70-keV Protons in Mg Vapor and in Neon*

Klaus H. Berkner, William S. Cooper III, Selig N. Kaplan, and Robert V. Pyle
Lawrence Radiation Laboratory, University of California, Berkeley, California 94720

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An optical technique has been used to investigate electron capture into the excited level $n=6$ of hydrogen by 5- to 70-keV protons passing through magnesium vapor or neon. Photons from the Balmer H_δ transition which are emitted downstream of the target were analyzed with a grating spectrometer and counted. From these the population of the level $n=6$ and the cross section for electron capture into $n=6$ have been obtained. Cross-section estimates for ionization of the level $n=6$ collisions with Mg atoms are also presented. The electron-capture cross sections are consistent with n^{-3} extrapolations of electric-gap measurements for capture into higher quantum levels ($n \approx 9$ to 15) reported by Il'in and co-workers, Futch and Moses, and Riviere. The results are compared with those of various theoretical models.

I. INTRODUCTION

At proton energies between about 5 and 30 keV, cross sections for electron capture from metal vapors are much larger than those for capture from common gases. We have investigated one particular vapor, magnesium, and report here cross-section measurements for electron capture into