Critical points in low-energy positron-atom scattering

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Critical points, which represent minima in differential scattering cross sections as a function of scattering angle and incident projectile energy, are theoretically predicted for elastic scattering of low-energy positrons by Ar, Kr, and Xe. It is demonstrated that these points arise due to low-energy positron diffraction effects.

It is well known that in elastic scattering of low-energy electrons by heavy atoms, the angular distribution exhibits several minima which are attributed to low-energy-electron-diffraction effects. Similar minima are also observed when the incident electron energy is varied for a fixed angle of scattering. These points of minimum scattering, where a small change in either the incident electron energy or the scattering angle is associated with an appreciable increase in the differential scattering cross section, are called critical points of the electron-atom system.[1] The purpose of this paper is to present, for the first time, predictions of critical points for various positron-atom systems. These critical points, as we will later demonstrate, arise due to low-energy-positron diffraction. The clue for assigning the pattern to the diffraction phenomena comes from some empirical relationships satisfied by various phase shifts at the critical energy.

The standard partial-wave decomposition of the elastic-scattering amplitude[2] for positron- (or electron-) atom collisions

$$f(k,\theta)=(1/2ik)\sum_{l=0}^{\infty}(2l+1)(e^{2i\delta_l}-1)P_l(\cos\theta) \tag{1}$$

introduces energy-dependent phase shifts $\delta_l(k)$ for each relative angular momentum $l\hbar$ of the system. Here θ is the angle of scattering and $\hbar^2k^2/2m$ is the impact energy of the positron. The differential cross section obtained by

$$I(k,\theta)=|f(k,\theta)|^2$$

contains interference terms which lead to a diffraction pattern in the differential cross section as a function of the incident projectile energy and as a function of scattering angle. The exact shape of this pattern, of course, depends upon the nature of the phase shifts which, in turn, depend upon the potential experienced by the positron due to the target atom. A determination of the critical points, therefore, could provide a sensitive test for the atomic potential used in the calculations, and an experimental verification of the critical points for heavier atoms could provide a means for improving our knowledge of the atomic potentials for these atoms which are generally not known very accurately. In this investigation we have considered the heavier rare-gas atoms Ar, Kr, and Xe, for which the low-energy positron-atom scattering phase shifts for the first few partial waves are available.[3] It is possible to write the differential cross section $I(k,\theta)$ in terms of sums over the partial waves. The most general form for $I(k,\theta)$ turns out to be

$$k^2I(k,\theta)=\left[\sum_l(2l+1)\cos(\delta_l-b)\sin(\delta_l-a)P_l(\cos\theta)\right]^2+\left[\sum_l(2l+1)\sin(\delta_l-b)\sin(\delta_l-a)P_l(\cos\theta)\right]^2$$
$$+2\sin(a)\left[\sum_l(2l+1)\cos(\delta_l)\sin(\delta_l-a)P_l(\cos\theta)\right]\left[\sum_{l'}(2l'+1)P_{l'}(\cos\theta)\right]+\sin^2a\left[\sum_l(2l+1)P_l(\cos\theta)\right]^2, \tag{2}$$

where a and b are *arbitrary* and *real* constants. A judicious choice of a and b can lead to convenient expressions for the differential cross sections.

At low energies, only the first few terms in expansion (1) are important. If only the first two terms ($l=0,1$) are important and the contributions of other terms are negligible, then choosing $a=0$ and $b=\delta_1$ in (2) gives

$$I(k,\theta)=(1/k^2)\{[\sin\delta_0\cos(\delta_0-\delta_1)+3\sin\delta_1\cos\theta]^2+\sin^2\delta_0\sin^2(\delta_0-\delta_1)\}\ .$$

Note that the differential cross section assumes a minimum value of

$$I_{\min}(k,\theta)=(1/k^2)\sin^2\delta_0\sin^2(\delta_0-\delta_1) \tag{3a}$$

when the angle of scattering is

$$\cos\theta=-\tfrac{1}{3}\cos(\delta_0-\delta_1)[\sin(\delta_0)/\sin(\delta_1)]\ . \tag{3b}$$

Furthermore, at this angle no scattering occurs when

$$\delta_0-\delta_1=m\pi,\quad m=0,1,2,\ldots\ . \tag{4}$$

Condition (4), that the phase difference of the two interfering partial waves should be zero or a multiple of π for no scattering, is analogous to (but not the same as) the interference condition encountered in wave optics. From the numerical values of the phase shifts[3] it should be noted that in the low-energy scattering region, where the contributions of the d wave and the higher partial waves are completely insignificant, the condition (4) for no scattering is satisfied only for $m=0$. It is only at higher positron energies that the difference between the phase shifts of the s and p waves is a nonzero multiple of π; however, at such energies the contributions of higher partial waves to the differential cross section become significant. Furthermore, relation (4) provides guidelines for obtaining conditions for interference leading to minimum scattering when more than two partial waves contribute. The algebra involved when three or more partial waves contribute becomes prohibitive; however, the following *empirical* relationship among various phase shifts appears to hold at the critical point of minimum scattering:

$$\delta_0-\delta_1+\delta_2-\delta_3+\cdots=0\ . \tag{5}$$

In the case of two partial waves the angle at which no scattering occurs is obtained by substituting from (4) into (3), which leads to

$$\cos\theta=-\tfrac{1}{3}\ \text{or}\ \theta=109.5^\circ\ . \tag{6}$$

This value of θ is independent of the parameter m introduced in Eq. (4). However, in the energy region where the two-wave approximation is good, only $m=0$ is important. Interestingly, in this two-wave approximation θ is independent of the system under consideration. Of course, when more than two partial waves contribute there may be more than one angle of minimum scattering. In fact, in the case of elastic electron scattering by various atoms, more than one critical point has been discovered[4] for Ar, Kr, and Xe. However, in our investigation of critical points for positron-rare-gas-atom scattering at low incident positron energies, we have found only one critical point for each system. In our work we have used the phase shifts of the first seven partial waves for elastic scattering of positrons by Ar, Kr, and Xe, which have been numerically calculated by McEachran, Ryman, and Stauffer,[3] while for higher partial waves we used the Born approximation with known polarization potentials to obtain the phase shifts.[5] For higher partial waves it is also possible to obtain a more reliable set of phase shifts from expressions (in terms of the coefficients of the long-range potentials) obtained[6] by a solution of the Schrödinger equation by the variable phase method. However, for the conclusions of the present work, the Born approximation for the higher phase shifts is deemed sufficient. In the vicinity of a critical point, the numerical phase shifts are least-squares fitted to a polynomial of the form

$$\delta_l(k)=\sum_{n=0}^{3}a_{nl}(ka_0)^n\ .$$

Within the accuracy specified by such fits, the empirical relationship (5) among phase shifts appears to hold approximately at the critical energy. In all calculations of the differential cross sections, only the first 20 partial waves were summed since the effect of higher partial waves was negligible.

A three-dimensional perspective of the angular distributions for Ar is shown in Fig. 1, and the presence of only one critical point is clear in the low-energy region. The three-dimensional perspectives for Kr and Xe (not shown) are very similar to that of Ar. Figures 2 and 3 show the differential cross section as a function of positron energy (at the critical scattering angles) and scattering angle (at the critical energies), respectively, for Ar, Kr, and Xe, with the critical-point parameters given in Table I. It is rather curious that the angle of minimum scattering is almost independent of the rare-gas atom under investigation and is not too far from the two-wave approximation given by (6). There are, however, small shifts toward larger critical angles and lower critical energies, respectively, as one moves from the smaller to the larger atoms. The trends of these shifts are consistent with simple considerations of diffraction effects

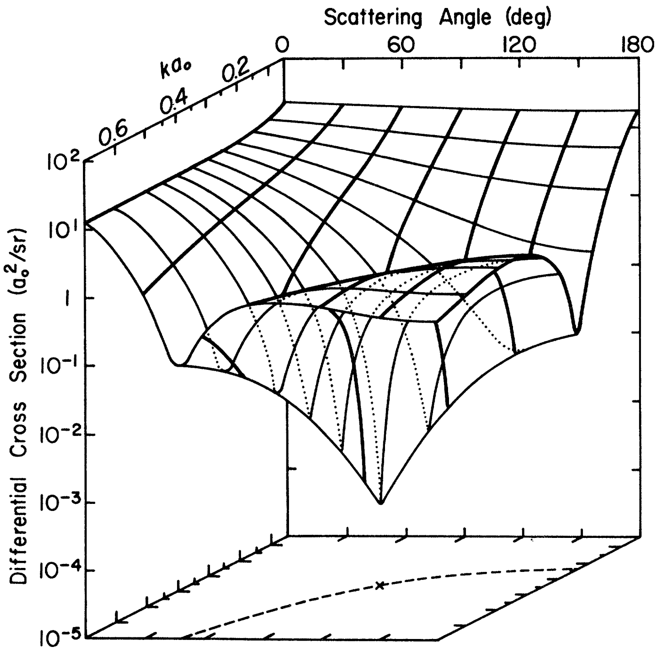

FIG. 1. Three-dimensional perspective of the differential cross section for positron-Ar collisions plotted vs ka_0 (where k is the projectile wave number and a_0 is the Bohr radius) and vs the scattering angle. The dashed curve represents the projection of the locus of the differential cross-section minima onto the projective-wave-number (ka_0)–scattering-angle plane with the × representing the critical point.

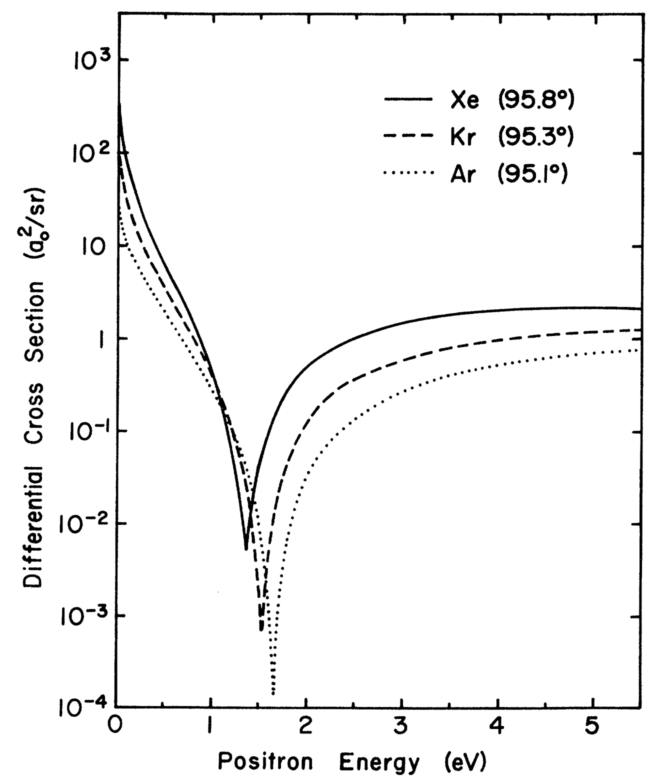

FIG. 2. Differential cross section for positrons colliding with Ar, Kr, and Xe plotted vs energy at their respective critical scattering angles.

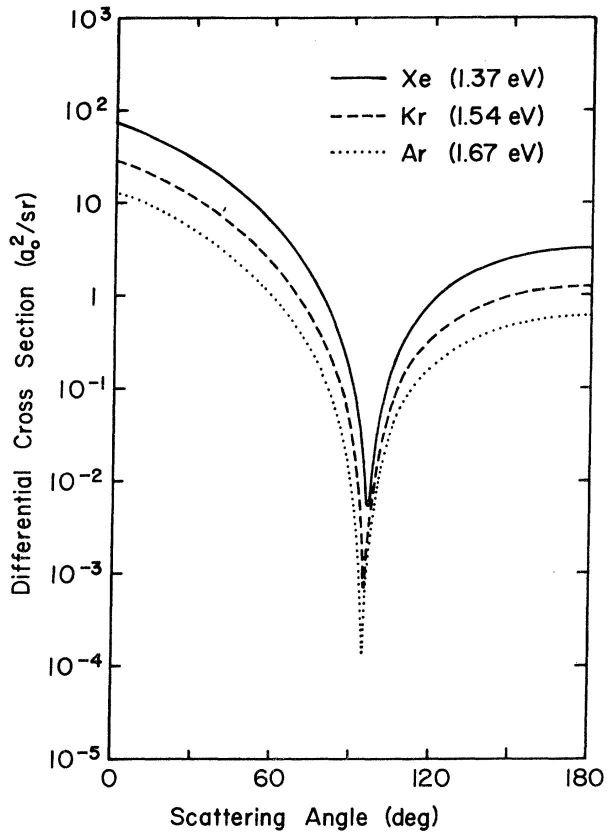

FIG. 3. Differential cross section for positrons colliding with Ar, Kr, and Xe plotted vs scattering angle at their respective critical energies.

TABLE I. Critical angle of scattering and the critical impact energy corresponding to minimum elastic scattering of positrons by various rare-gas atoms. I_{cr} is the differential cross section corresponding to the critical parameters.

Gas	θ_{cr} (deg)	E_{cr} (eV)	I_{cr} (a_0^2/sr)
Ar	95.1	1.67	0.137×10^{-3}
Kr	95.3	1.54	0.741×10^{-3}
Xe	95.8	1.37	0.540×10^{-2}

when the de Broglie wavelength of the incident positron is compared with the sizes of the respective target atoms. The curves indicate the extreme sensitivity of the differential cross sections to the projectile energies and scattering angles, respectively, in the vicinities of the respective critical points. One should be aware that the extent of the variations of the differential cross section that could be observed experimentally as a function of either scattering angle or positron energy would depend sensitively on the angular discrimination of the apparatus and the beam energy width. An additional experimental consideration is that the drop in the differential cross section near a critical point is so sharp (decreasing by several orders of magnitude) that the probability of a positron, scattered a few degrees away from the critical angle, undergoing multiple scattering and still reaching the detector, may become comparable with a positron reaching the detector after single scattering at the critical angle. Such multiple-scattering effects have been partially accounted for in electron scattering experiments.[7]

Experimentally, differential cross sections have only been measured[8] (with a time-of-flight approach) for positrons colliding with one gas (Ar) in a very limited angular and energy range (20°–60° and 2–9 eV, respectively), but there are other groups[9,10] preparing experiments for measurements of differential cross sections for positrons colliding with gas atoms using crossed atomic and positron beams. With the prospect of much more intense low-energy positron beams in the near future,[11] searches for critical points in positron-atom scattering may be feasible.

Finally, it is interesting to note that the positrons scattered at critical points may be fully polarized. In the case of electron scattering, an analysis[12] by Buhring shows that the elastically scattered electrons are fully polarized when the impact energy and the scattering angle correspond to the critical values. The origin of this polarization effect is spin-orbit coupling which has the same magnitude for positrons and electrons.

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