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THREDHOLD BEHAVIOR OF INELASTIC COLLISION CROSS SECTIONS

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The behavior of scattering cross sections near an excitation threshold is examined for the case of long range potentials. The theory is confirmed by computations of e-Li scattering. Recent observations of threshold structure in e-Na collisions are ascribed to a ^1D resonance of Na^-. A true cusp can occur only in the ^1P partial cross section.

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THRESHOLD BEHAVIOR OF INELASTIC SCATTERING CROSS SECTIONS

by

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The effects of long range potentials on the threshold behavior of elastic scattering cross sections were studied some time ago, principally by O'Malley, Spruch and Rosenburg[1] and by Levy and Keller.[2] However, there has been little analysis of the effects of such potentials on inelastic collisions. The purpose of this paper is to extend the analysis of Levy and Keller[2] to inelastic scattering, and to relate the results to recent experiments involving alkali atoms. One particular feature that we will examine is the appearance of Wigner cusps at excitation thresholds. Our analysis will be applicable to any atom except hydrogen, for which special problems arise due to the ℓ-degeneracy. These special problems have been studied by Gailitis and Damburg[3] and others.

The analysis of Levy and Keller[2] is based on the variable phase method, which has been extended to multi-channel problems by several authors.[4,5] For each channel α, the associated single-particle function $\phi_{\alpha\beta}(r)$ is written

$$\phi_{\alpha\beta}(r) = w_{0\alpha}(r)\delta_{\alpha\beta} + w_{1\alpha}(r)t_{\alpha\beta}(r) \quad . \tag{1}$$

The index β denotes the incident channel; $w_{0\alpha}(r)$ and $w_{1\alpha}(r)$ are independent functions which have the asymptotic form appropriate for the channel α. If there is no unscreened Coulomb interaction in the asymptotic region, these can be expressed in terms of spherical Bessel functions. For open channels we take

$$w_{0\alpha}(r) = k_\alpha^{\frac{1}{2}} r j_{\ell_\alpha}(k_\alpha r) \quad ; \tag{2}$$

$$w_{1\alpha}(r) = - k_\alpha^{\frac{1}{2}} r n_{\ell_\alpha}(k_\alpha r) \quad . \tag{3}$$

The scattering information is contained in the matrix $t_{\alpha\beta}(r)$. The limit of $t_{\alpha\beta}(r)$, as $r \to \infty$, is the reactance matrix, $K_{\alpha\beta}$, whose eigenvalues are are the tangents of the eigenphases.

By substitution in the Schrödinger equation we obtain an integral equation for $t_{\alpha\beta}(r)$, of the form[4]

$$t_{\alpha\beta}(r) = - 2 \int_0^r \sum_\gamma \sum_\delta (\delta_{\alpha\gamma} w_{0\gamma}(r') + t_{\alpha\gamma}(r') w_{1\gamma}(r')) V_{\gamma\delta}(r')$$

$$(w_{0\delta}(r') \delta_{\delta\beta} + w_{1\delta} t_{\delta\beta}(r')) dr' \quad , \tag{4}$$

where $V_{\gamma\delta}(r)$ is the interaction potential, expressed in matrix form. The K-matrix Born Approximation[6] can be obtained by neglecting the terms involving $t(r')$ on the RHS of Eq. (4). Substituting for $w_{0\beta}(r)$, we obtain

$$K_{\alpha\beta} \equiv t_{\alpha\beta}(\infty) = - k_\alpha^{\frac{1}{2}} k_\beta^{\frac{1}{2}} \int_0^\infty 2V_{\alpha\beta}(r) j_{\ell_\alpha}(k_\alpha r) j_{\ell_\beta}(k_\beta r) r^2 dr \quad . \tag{5}$$

As shown for single channel scattering by Levy and Keller,[2] the dominant term in the threshold behavior is given by Eq. (5).

Let us suppose that we have one or more old channels labelled α, β, ..., and one or more new channels labelled p, q, ... We will assume that the new channels share a common threshold so that $k_q = k_p$, and wish to determine the dependence of the elements of the reactance matrix

upon k_p. Let us first consider K_{pq} which corresponds to elastic scattering in the new channels. For any short range interaction the integral is dominated, as $k_p \to 0$, by small r and we find

$$K^S_{pq} = - k_p^{\ell_p+\ell_q+1} \left\{ \int_0^\infty 2V_{pq}(r) r^{\ell_p+\ell_q+2} dr + O(k_p^2) \right\} . \tag{6}$$

However, if the interaction contains a long range component, say Cr^{-s}, this leads to a contribution of the form

$$K^L_{pq} = - 2Ck_p \int_0^\infty r^{2-s} j_{\ell_p}(k_p r) j_{\ell_q}(k_p r) dr . \tag{7}$$

If $s < (\ell_p + \ell_q + 3)$, this integral is well defined and gives

$$K^L_{pq} = \frac{-\pi C}{2^{s-1}} k_p^{s-2} \frac{\Gamma(s-1)\Gamma\left(\frac{\ell_p+\ell_q-s+3}{2}\right)}{\Gamma\left(\frac{\ell_p-\ell_q+s}{2}\right)\Gamma\left(\frac{\ell_p+\ell_q+s+1}{2}\right)\Gamma\left(\frac{\ell_q-\ell_p+s}{2}\right)} . \tag{8}$$

Since, given the inequality above, $(s-2) < (\ell_p + \ell_q + 1)$, this term is dominant for small k. Thus we confirm the conclusion of Levy and Keller that the threshold behavior of the matrix elements K_{pq} can be changed by the presence of long range forces. If, however, $s \geq (\ell_p + \ell_q + 3)$ the potential must be modified at small r, and the dominant term remains $k^{\ell_p+\ell_q+1}$, since the integral is made finite by the short range behavior of the potential.

Let us next consider the term $K_{\alpha p}$, corresponding to inelastic scattering. For any short range interaction we obtain a result similar to

Eq. (6) with a dominant term proportional to $k_p^{\ell_p+\frac{1}{2}}$. From our long range component, Cr^{-s}, we find that if $s < (\ell_\alpha + \ell_p + 3)$

$$K^L_{\alpha p} = -2C\, k_\alpha^{\frac{1}{2}} k_p^{\frac{1}{2}} \int_0^\infty r^{2-s}\, j_{\ell_\alpha}(k_\alpha r)\, j_{\ell_p}(k_p r)\, dr$$

$$\simeq -\frac{\pi C}{2^{s-1}}\, k_\alpha^{s-\ell_\alpha-5/2}\, k_p^{\ell_p+\frac{1}{2}}\, \frac{\Gamma\left(\frac{\ell_\alpha+\ell_p-s+3}{2}\right)}{\Gamma(\ell_p+\frac{3}{2})\,\Gamma\left(\frac{\ell_\alpha-\ell_p+s}{2}\right)}$$

$$\times \left[1 + O\left(\frac{k_p^2}{k_\alpha^2}\right)\right] . \qquad (9)$$

For small k_p this has the same form as $K^S_{\alpha p}$. Thus we conclude that the long range interactions do not change the power of the dominant term for K-matrix elements in which the initial and final wave numbers are different. In this conclusion we confirm the analysis of Geltman,[7] but differ from the result of Mott and Massey[8] who state that $K_{\alpha p} \propto k_p^{s-\frac{1}{2}}$ when $s < \ell_p + 2$.

In order to examine the physical cross sections we must construct the T-matrix, given by $K(1 - iK)^{-1}$. By analytic continuation of the T-matrix, the behavior of the K-matrix below the threshold can be deduced.[9,10] It is well known[9,10] that if an element $K_{\alpha p}$ is proportional to $k_p^{\frac{1}{2}}$, then the elastic scattering T-matrix element $T_{\alpha\alpha}$ will, in general, have infinite slope at the threshold. This can lead to a cusp in $T_{\alpha\alpha}$ and in the corresponding partial wave cross section $\sigma_{\alpha\alpha}$. From our previous analysis we see that $K_{\alpha p} \propto k_p^{\frac{1}{2}}$ if, and only if, $\ell_p = 0$, that is, if the angular momentum of the scattered electron is zero.

Let us apply these ideas to electron scattering by alkalis in the ground ^2S state, at energies close to the threshold for excitation of the lowest ^2P state. For collisions in which the ^2P state is excited the initial and final values of the electronic angular momentum, ℓ_α and ℓ_p, are linked through the selection rule

$$\ell_p = \ell_\alpha \pm 1 \quad . \tag{10}$$

Thus ℓ_p can be zero only if $\ell_\alpha = 1$, so that cusps can appear at the excitation threshold only for incident p-waves.

Although through this type of analysis we can show that cusps may exist, we are unable to predict their magnitude except through an explicit calculation. We have, therefore, performed numerical computations of the reactance matrix and partial wave cross sections for electron scattering by lithium. We have used a variational method, used previously by Sinfailam and Nesbet[11] and by Oberoi and Nesbet,[12] which has been described in detail by Lyons et al.[13] The basis set of square integrable functions included 8 s-wave functions, 7 p-wave functions, 5 d-wave functions and 4 f-wave functions, supplemented by continuum functions with asymptotic forms given by Eq. (2).

At energies just above the inelastic threshold each of the elements of the reactance matrix varied with energy in a manner consistent with our previous analysis. However, some of the elements could be fitted by a simple power law only over a very small range of energies ($\sim 10^{-3}$ eV). The calculated partial wave cross sections for elastic scattering are shown in Fig 1. The s- and d-wave contributions pass smoothly through

the threshold energy. There is a very clear cusp in the ^1P contribution, which falls from 19 πa_0^2 at threshold to 9.5 πa_0^2 at an energy 0.02 eV above threshold. The total cross section decreases by approximately 6% over this energy range. The ^1P contribution should have an infinite slope on both sides of the threshold energy. The finite slope that we find at energies below threshold is probably due to an inadequacy in our trial wave function. The basis set does not include any terms which have exactly the proper asymptotic form required for closed channels. We do, however, have continuum functions with the proper asymptotic form for the open channels, and so obtain the correct analytic form of the cross sections just above threshold.

The ^3P contribution to elastic scattering also has an infinite slope at the threshold energy. However, the cross section derivative ($d\sigma/dE$) is negative on both sides of the threshold, so there is not a cusp, but a point of inflexion. In spite of the infinite derivative the magnitude of the change in the ^3P contribution near threshold is negligible. This is because the elastic scattering phase shift, $\eta_{\alpha\alpha}$, is very close to $(n + \frac{1}{2})\pi$ (we find $\sin \eta_{\alpha\alpha} = 0.999$). In this situation a change of 10% in the K-matrix element $K_{\alpha\alpha}$ leads to a change of only 0.04% in the cross section.

From comparison with previous calculations[11,14] of elastic electron-alkali scattering at lower energies and from exploratory calculations at higher energies it is clear that there are resonances in the ^1P and ^1D cross sections. These are presumably associated with the $(1s)^2(2s)(2p)\,^1P$ and $(1s)^2(2p)^2\,^1D$ states of Li^-. The effect of the resonances can be seen, for example, in the fact that the ^1P and ^1D contributions to

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inelastic scattering are considerably greater than the ^3P and ^3D contributions. The presence of the ^1P resonance enhances the effect of the cusp in that channel, and the maximum value of the ^1P partial cross section occurs at the threshold energy. The ^1D resonance causes the ^1D partial cross section also to peak at an energy very close to the threshold.

The existence of these resonances was previously noted by Burke and Taylor.[15] These authors also studied the sum of the scattering eigenphases, and found a discontinuity of slope at the threshold energy in each partial wave. We have confirmed this feature and find that for s-waves and d-waves this discontinuity is consistent with a smooth variation of the elastic scattering partial cross section.

Observations of cusps in e-Na differential scattering cross sections have been reported by Andrick et al.[16] and by Gehenn and Reichert.[17] The structure observed by Andrick et al.[15] is weak near 60°, and strong near 90°. However, the threshold cusps should vanish at 90°, since they are confined to incident p-waves. Since the qualitative features of e-Li scattering and e-Na scattering are very similar[11,14] it seems plausible that the observed structure is due predominantly to a ^1D resonance of Na^-. For many scattering angles the p-wave cusps should be masked by the ^1D resonance. However, the fact that there is no observed structure near 60° must still be explained.

The effects of the cusps may be more easily observed in photodetachment of the alkali negative ions, since the final state must have ^1P symmetry. From the calculations of Moores and Norcross[18] it is clear that the detachment cross section peaks very close to the threshold

energy for the production of excited neutral atoms. Using Na^- and K^-, Patterson et al.[19] have observed such peaks and from their observations have derived accurate values for the electron affinities of these alkalis.

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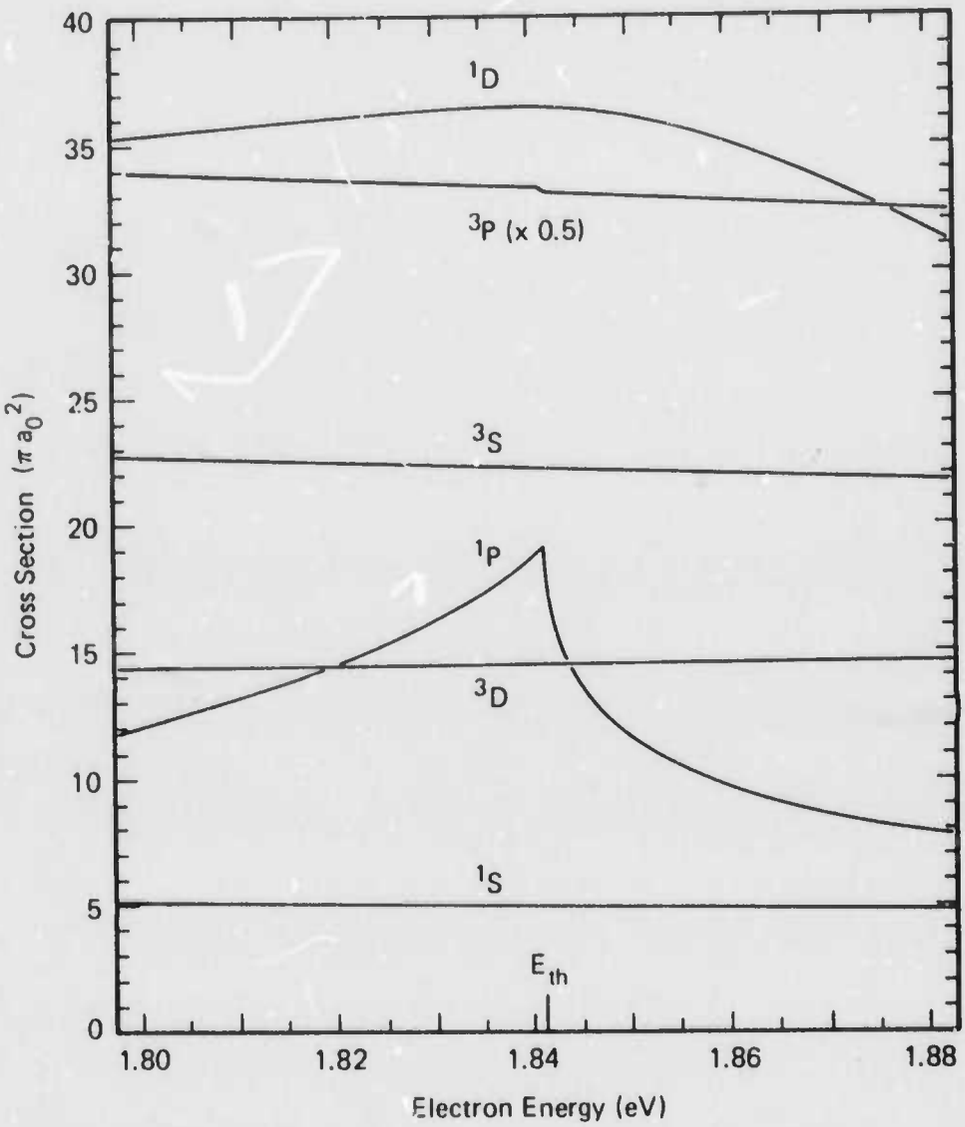

Figure 1. Partial wave contributions to the elastic scattering cross section in electron collisions with lithium atoms at energies close to the excitation threshold, E_{th}, which is calculated to be 1.8411 eV.