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Threshold Behavior of Inelastic-Scattering 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 should occur only in the ^1P partial cross section.

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 Rosenberg[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 owing 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 multichannel problems by several authors.[4,5] For each channel α, the associated single-particle function $\phi_{\alpha\beta}(r)$ is written

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

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

$$w_{0\alpha}(r) = k_\alpha^{1/2} r j_{l_\alpha}(k_\alpha r), \tag{2}$$

$$w_{1\alpha}(r) = -k_\alpha^{1/2} r n_{l_\alpha}(k_\alpha r). \tag{3}$$

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 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]

$$t_{\alpha\beta}(r) = -2\int_0^r \sum_\gamma \sum_\delta [\delta_{\alpha\gamma} w_{0\gamma}(r') + t_{\alpha\gamma}(r') w_{1\gamma}(r')] \times V_{\gamma\delta}(r')[w_{0\delta}(r')\delta_{\delta\beta} + w_{1\delta} t_{\delta\beta}(r')]\, dr', \tag{4}$$

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 right-hand side of Eq. (4). Substituting for $w_{0\beta}(r)$, we obtain

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

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 labeled $\alpha, \beta, \ldots$, and one or more new

channels labeled $p, q, \ldots$. We will assume that the new channels share a common threshold so that $k_q = k_p$, and we 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

$$K^S_{pq} = -k_p^{l_p+l_q+1}\left[\int_0^\infty 2V_{pq}(r) r^{l_p+l_q+2}\,dr + O(k_p^2)\right]. \quad (6)$$

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

$$K^L_{pq} = -2Ck_p \int_0^\infty r^{2-s} j_{l_p}(k_p r) j_{l_q}(k_p r)\,dr. \quad (7)$$

If $s < (l_p + l_q + 3)$, this integral is well defined and gives

$$K^L_{pq} = \frac{-\pi C}{2^{s-1}} k_p^{s-2} \frac{\Gamma(s-1)\Gamma[\frac{1}{2}(l_p + l_q - s + 3)]}{\Gamma[\frac{1}{2}(l_p - l_q + s)]\Gamma[\frac{1}{2}(l_p + l_q + s + 1)]\Gamma[\frac{1}{2}(l_q - l_p + s)]}. \quad (8)$$

Since, given the inequality above, $(s-2) < (l_p + l_q + 1)$, 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, $s \geq (l_p + l_q + 3)$, the potential must be modified at small r, and the dominant term remains $k^{l_p+l_q+1}$, 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 $k_p^{l_p+1/2}$. From our long-range component Cr^{-s}, we find that, if $s < (l_\alpha + l_p + 3)$,

$$\begin{aligned} K^L_{\alpha p} &= -2Ck_\alpha^{1/2} k_p^{1/2} \int_0^\infty r^{2-s} j_{l_\alpha}(k_\alpha r) j_{l_p}(k_p r)\,dr \\ &= -\frac{\pi C}{2^{s-1}} k_\alpha^{s-l_p-5/2} k_p^{l_p+1/2} \\ &\quad \times \frac{\Gamma[\frac{1}{2}(l_\alpha + l_p - s + 3)]}{\Gamma(l_p + \frac{3}{2})\Gamma[\frac{1}{2}(l_\alpha - l_p + s)]}\left[1 + O\left(\frac{k_p^2}{k_\alpha^2}\right)\right]. \end{aligned} \quad (9)$$

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 $K_{\alpha p} \propto k_p^{s-3/2}$ when $s < l_p + 2$.

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 $k_p^{1/2}$, 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 $K_{\alpha p} \propto k_p^{1/2}$ if and only if $l_p = 0$, that is, if the angular momentum of the scattered electron is zero.

Let us apply these ideas to electron scattering by alkali-metal atoms 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

$$l_p = l_\alpha \pm 1. \quad (10)$$

Thus l_p can be zero only if $l_\alpha = 1$, 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 eight s-wave functions, seven p-wave functions, five d-wave functions, and four 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 con-

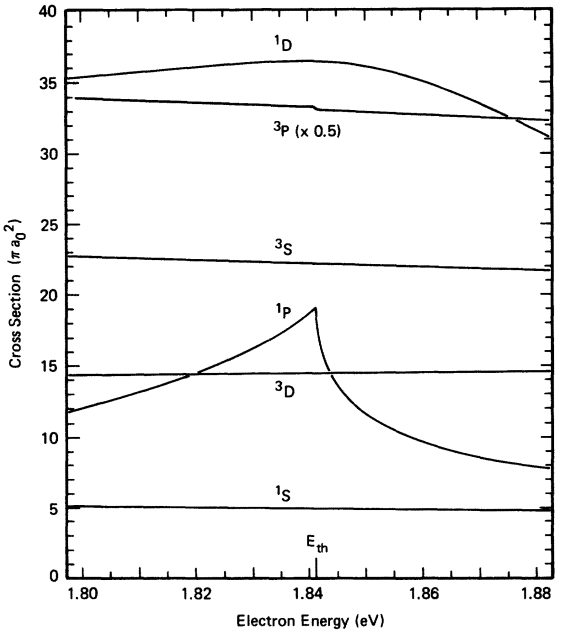

FIG. 1. Partial-wave contributions to the elastic-scattering cross section in electron collisions with lithium atoms at energies close to the excitation threshold E_{th}, which is calculated to be 1.8411 eV.

tribution, which falls from $19\pi a_0^2$ at threshold to $9.5\pi a_0^2$ 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-metal-atom 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 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.*[16] 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 Norcross and Moores[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 alkali metals.

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Rearrangement Collisions at Very High Energies*†

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The energy dependence of the charge-exchange cross section in proton–hydrogen-atom collisions at very high energies, within the framework of the Schrödinger equation, has long been a subject of controversy. We attempt to determine the energy dependence of the forward-scattering cross section at very high energies in an arbitrary rearrangement collision involving two heavy particles of masses M_a and M_b and a light particle of mass m, with m initially bound to M_a and finally bound to M_b. In the limits m/M_a, $m/M_b \to 0$ the scattering is entirely in the forward direction and the cross section σ for forward capture is given exactly by the impact-parameter treatment. A Born-type expansion is developed in the impact-parameter treatment for the forward-capture amplitude A. Thus, A is written as a sum of a finite number of Born terms plus a remainder R. The Schwarz inequality can be used to bound R since there are no non-normalizable plane-wave functions—the motion of M_a and M_b is treated classically. We can thereby show that for a certain class of nonsingular interactions the *second* Born term provides the dominant contribution to σ at high energies, whether or not the Born series converges. (This may be the first example for which it has been shown that the second Born term dominates.) This result makes plausible the dominance of the second Born term in p-H forward charge exchange.

I. INTRODUCTION

Within the framework of the Schrödinger equation, the determination of the energy dependence of the ground state to ground-state charge-transfer cross section in proton–hydrogen-atom collisions, as the relative kinetic energy E goes to infinity, is a vintage problem which continues to attract interest.[1] Capture into the backward direction is thought to dominate[2] for E sufficiently large, the main contribution coming from the first Born approximation[3] and being proportional to $(m_e/M_p)^2E^{-3}$, with m_e and M_p the electron and proton masses, respectively. However, back scattering is unobservably small due to the $(m_e/M_p)^2$ factor, and we will concern ourselves with the result obtained by first letting $m_e/M_p \to 0$ and *then* considering arbitrarily large E. Capture into the forward direction then dominates, and it is the energy dependence of the forward-capture cross section which is of greatest interest and which is the subject of this paper.

The first quantum-mechanical calculation of the proton-hydrogen charge-transfer cross section was performed in 1930 by Brinkmann and Kramers.[4] Neglecting the proton-proton interaction and using the first Born approximation, they found that the forward-capture cross section behaved as C/E^6 for sufficiently high energy. (The rapid decrease with E is a consequence of the