Inverse scattering for inelastic atomic processes at thresholds

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Abstract. We have observed resonance structures in detached electron spectra arising from fast collisions of Li° with gas targets and from photo-detachment of Li°. Using a generalization of the Wigner threshold law, we were able to fit the experimental data to a high degree of accuracy. Moreover, we were able to extract numerical values of different electron-atom parameters as the scattering length, the effective range of the potential and the number of supported bound states. Results for the scattering length obtained from this two differentiated experiments agree with each other within a maximum error of 2%.

1. Introduction

One of the ultimate purposes of studying scattering processes in Physics is the determination of the effective interactions between the components of a system. Usually these effective interactions are assumed known and cross sections and other observables are computed by means of scattering theory. Then, comparison with experiments let us know to what extend we succeeded in approximating all fundamental but otherwise intractable interactions or, at least, if we could manage to include all the necessary contributions to describe a given process. A more direct –although less used– method to determine the interactions would instead start from the experiments themselves. In elastic scattering, for example, phase-shift information at fixed angular momentum as function of energy (or alternatively, fixed-energy observations as a function of the angular momentum) can be used to feed a mathematical algorithm which would produce a potential that reproduces such observations [1, 2]. Potential ambiguities can be eliminated if additional data is known, such as the bound state energies and wave functions normalization factors. For inelastic processes, on the other hand, the multichannel inverse scattering theory is still under development [3, 4, 5]. Of particular interest are the energy regions where new (e.g., excitation, ionization or dissociation) channels open. At these thresholds, the interactions act over space scales greater than those usually found in Atomic or Molecular Physics [6]; and only a few low-energy parameters are expected to govern the cross sections. The energy dependence of cross sections near the threshold of opening reaction channels has been of great interest for years. A complete description of the two-body threshold behavior for the opening of an inelastic channel is given by \( \sigma_{inel} \propto k^{2\ell+1} \) where \( k \) and \( \ell \) stand for the relative linear and
angular momentum, respectively. This formula was proposed by Wigner more than 50 years ago [7], showing that the longest-range forces determine the energy dependencies near threshold. To go further than the leading energy dependence of the Wigner threshold law, one may proceed through the well-known multi-channel effective-range expansions [8, 9]. In the simpler case of the elastic scattering for an $s-$wave, it simply reads [10]

$$k \cot \delta_0 = -1/a_0 + r_0 k^2/2 + \ldots,$$

where $a_0$ is the scattering length and $r_0$ is the effective range. When the interaction behaves as $V(r) \sim r^{-s}$ for large $r$, $k \cot \delta_0$ is not longer analytic around $k = 0$ and the effective range expansions have to be modified [11, 12, 13].

On the other hand, in practice Wigner’s law usually describes the observations only over a very small range of energies above threshold. Rapid deviations have been observed for energies as low as a few meV when an electron and a neutral atom interact above threshold, and even for $s-$wave final states [14]. This shortcoming is of great theoretical and practical interest. In photodetachment of negative ions, for example, the knowledge of the threshold behavior is critical for the determination of electron affinities. At a first sight, it might seem that only the data that are closer to the threshold are useful. However, since the experimental observations in the close vicinity of the threshold usually have the worst signal-to-noise ratio, the proper procedure is to extrapolate the data down to the threshold, thereby making use of all the experimental information. It is therefore important to know the correct functional form that has to be employed in the extrapolation process. One can expect that an extended threshold law will depend on the interaction of the two-body fragments. In this sense, a threshold law in a broader energy range can be regarded as a useful tool to extract different interaction properties as the scattering length, the number of supported bound states, the long range behavior, etc.

In this work we propose an inverse scattering fitting technique based on the elastic $\ell-$wave Jost function of the final continuum electronic state. In section 2 we will analyze how the Wigner law has to be modified at threshold to take into account resonances effects and the presence of long range potentials. With this generalized threshold law, in section 3 we are able to represent observations on the full energy range for different kind of experiments and, moreover, to extract numerical values of interaction properties as the scattering length. Finally, in section 4 we present our conclusions and outlook for future works.

2. Theoretical description

During the last years [15, 16, 17, 18], we showed that the $\ell-$wave Jost functions establish a clear link between a resonant structure in a multichannel collision and the low-energy elastic dispersion by the same final-state interaction. In this context, for a system composed of an arbitrary number of particles, two of them moving with small relative velocities with respect to the threshold of an opening channel, we propose to generalize the Wigner law as

$$\sigma_{\text{inel}} \propto k^{2\ell+1} g_{\text{inel}}(k) \left| f_\ell(k) \right|^2,$$

In (1), $f_\ell(k)$ is the elastic $\ell-$wave Jost function for the two-body system in the final state continuum, as given by the $r \to 0$ limit of the corresponding normalized radial wave function

$$\psi_{\ell,k}(r) \approx \frac{(kr)^{\ell+1}}{(2\ell + 1)!!} \frac{1}{f_\ell(k)^2}.$$

Here $\ell$ represents the lowest final angular momentum allowed by selection rules, or the quantum number of a resonant wave at threshold. Meanwhile, the well behaved function $g_{\text{inel}}(k)$ accounts
for the transition from the initial to the final state. If the potential is short-ranged and the 
system is far from a resonance, the Jost function is nearly constant and the prefactor of Eq. (1) 
provides the usual Wigner law for the threshold of an opening reaction channel [7]. However, in 
the near presence of resonances, the Jost function strongly depends on \( k \) and the denominator 
produces a sharp a deviation of \( \sigma_{\text{inel}} \) from the usual \( k^{2l+1} \) dependence. At the same time, the 
small-\( k \) behavior of the \( \ell \)-wave Jost function is dominated by such parameters as the scattering 
length \( a_{\ell} \) in the corresponding effective range expansion of the Jost function about \( k = 0 \) 
[19]. Precisely, this dependence of \( \sigma_{\text{inel}} \) on the parameters that are characteristic of the elastic 
two-body scattering at low energies is the key element of the proposed method for obtaining 
information about them from an inelastic cross section. The underlying idea is that the small-\( k \) 
behavior of the cross section in an inelastic collision reproduces many aspects of the elastic cross 
section for the same two-body system of relative momentum \( k \). In principle, these parameters 
can be obtained by fitting the cross section at threshold with a suitable parametrization. For 
this reason Eq. (1) provides an alternative approach for the study of a two-particle continuum at 
extremely low-energies that might not be easily accessible in direct elastic scattering experiments. 
For example, for an \( s \)-wave scattering on a short-range potential, it is usually assumed that 
[13]

\[
\frac{1}{|f_0(k)|^2} \propto \frac{1}{1 + (a_0 k)^2}.
\] (2)

However, when the active interactions are long ranged, the Jost functions are not analytical 
at \( k = 0 \) (as occurs with the phase shifts \( \delta_\ell \)) and the above expression is not longer valid. 
In these cases a specifically constructed Jost function for the long-range potential is needed. 
Furthermore, even in the case of a short range interaction, the parameter accompanying \( k^2 \) in 
Eq. (2) is not necessarily equal to \( a_0^2 \), and it can even become negative [19].

As one of many systems for which Eq. (1) can be applied, in this work we will study threshold 
reactions for an electron-atom system, more specifically the electron-Lithium system. The four 
electrons of the Li\(^+\) ion make of it an interesting system to study, because of the significant role 
played by electron correlation in the binding of the outermost electron in this weakly bound 
system. In this case, the electron-atom interaction is dominated at large distances by the 
polarization potential \( V(r) \sim -\beta/(2mr^4) \), where \( \beta \) is the dipole polarizability of the system. 
One decade ago we demonstrated that the validity of effective range expansions for potentials 
with large polarizabilities is limited to a very small energy range, and does not provide a reliable 
starting point for the parametrization of resonant structures in multichannel collisions [19]. It is 
important to point out that switching to a modified effective range theory [20] or to a quantum 
defect multichannel approach [21] does not guarantee a solution to this shortcoming, since they 
also include some approximations in powers of \( k \). However, it can be shown that for the analysis 
of the Jost function at threshold, the intricate polarization effects of the electron-atom interaction 
can be cast in terms of a very simple model potential

\[
V(r) = -\left[ 1 - \Theta(R - r) \left( 1 - \frac{r^4}{R^4} \right) \right] \frac{\beta^2}{2mr^4},
\]

where \( \Theta(r) \) is the Heaviside’s step function. For this model potential, the Jost functions have 
been analytically obtained [19]. Thus, instead of dealing with a very complicated generalized 
effective range expansion with many parameters, this analytical expression, with at most two free 
parameter, the range \( R \) and the polarizability \( \beta \), can be used to fit the experimental data. Once 
these parameters are adjusted, the other coefficients in the expansion can be easily obtained 
[19]. For instance,

\[
a_0 = \frac{\beta}{2 \sin (\beta/R)} \left( \frac{(2\beta/R) \cos (2\beta/R) - \sin (2\beta/R)}{(2\beta/R) \cos (\beta/R) - \sin (\beta/R)} \right).
\]
3. Determination of electron - atom low energy interaction parameters

Negative alkali-metal ions as Li\(^{-}\) have valence electronic configurations \(ns^2\). Thus the first excited state in Li\(^{-}\) photodetachment occurs as \(h\nu + \text{Li}^{-}\ (2s^2 1S) \rightarrow \text{Li}^{-}\ (2p^2 P) + e\). In this case, above threshold we consider

\[
\sigma_{\text{inel}} = \sigma_{\text{bg}} + k - \frac{g(k^2)}{|f_0(k; R)|^2},
\]

(3)

where \(\sigma_{\text{bg}}\) is an experimental background, and \(k\) is the relative momentum \(k = \sqrt{E_\gamma - E_{\text{th}}}\) with \(E_\gamma\) and \(E_{\text{th}}\) the photon and threshold energy, respectively. Here, \(g(k)\) is a function which does not depend sensibly on \(k\). In this work we keep the polarizability fixed at the tabulated value \([22]\) and vary only the polarization potential range \(R\) whose explicit dependence is showed in the Jost function \(f_0(k; R)\). A quadratic expression on \(k\) for the function \(g(k)\) was also considered.

In figure 1, we show the fitting with our theoretical model of Li\(^{-}\) photodetachment data in the vicinity of the Li(2\(^2\)P) threshold measured by Sandström et al\([23]\). As can be seen, our method provides a perfect match over the whole energy range, well beyond the scope of the Wigner law. We obtained a threshold energy \(E_{\text{th}} = 2.465856(65)\) eV and a scattering length \(a_0 = -26.0 \pm 2.7\) au. We note that this result does not agree with the value \(a_0 = 61 \pm 6\) au obtained in \([23]\) using a modified effective range theory \([20]\) or a single channel version of a many channel quantum defect theory \([21]\). A number of reasons might explain this difference. First, in our fit we use all the available data points. In \([23]\), on the other hand, the \(s\)–wave cross section was fitted to only two experimental data points near threshold. This \(s\)–wave cross section falls below the experimental data after an energy around \(E = 2.47\) eV. It was assumed that this difference might be due to the neglect of the \(d\)–wave cross section. However, this assumption seems to be at odds with the fact that a continuum electron with only \(\sim 4\) meV above threshold should be very-well described by an \(s\)–wave alone. Secondly, the presence of a virtual state close to the threshold advises to be extremely cautious on the fitting model employed in a region where, as it is the case here, the experimental cross section exhibits a sharp variation. In our case, we do not approximate the denominator of Eq.(3). Meanwhile in \([23]\) a zero order approximation of \(K_{20}^P(\ell)\) was employed in the denominator of Eq.(A3).

![Figure 1](image-url). Cross section for the photodetachment of Li\(^{-}\) above the Li(2\(^2\)P\(_1/2\)) threshold. Symbols: experiments of Ref.[23]. Solid line: Least-squared fit of experimental data using Eq.(3)
In this work, we also consider the electron loss experiment of 100 KeV Li\(^{-}\) ions colliding with He atoms measured by Lee et al [24]. Although very few bound states of negative ions exist, many unstable excited states have been found embedded in the continuum of the neutral atom. Hence, several channels might contribute to the measured double differential cross section (DDCS) in the forward direction. First, an electron is ionized leaving the Lithium atom in the Li(2\(p^2P\)) state as in the previous photodetachment experiment. But here the atom can also reach the Li(2\(s^2S\)) state. This could be achieved in a direct way or through the shape resonance given by the Li\(^{-}\)(2\(s^2p^3P\)) state. Therefore, these two last contributions should be added coherently. We do this by using the standard method of Balashov [25] modified to include Wigner’s law at threshold. We fit the electron loss to the continuum using the following model for the projectile frame DDCS

\[
\frac{d\sigma^{Li}}{dE'd\Omega} = \frac{d(k')}{f_0(k';R)} + k'c(k') + k^2 \frac{a(k')e + b(k')}{1 + e^2},
\]

where \(k'\) is the electron momentum in the projectile frame with modulus \(k'\) and angle \(\theta'\). The reduced energy \(\epsilon = 2(E' - E_R)/\Gamma\) measures the departure from the resonant energy \(E_R\) and \(\Gamma\) is the half lifetime of the metastable resonant state. The functions \(a(k')\), \(b(k')\), \(c(k')\) and \(d(k')\) are supposed to be well-behaved. We expand them up to first order in \(k'\) and in terms of Legendre polynomials in \(\cos \theta'\). In figure 2 we show the fitting of the experimental data of Ref. [24] employing Eq.(4) after transforming it to the laboratory frame and convoluting it with the reported detector resolution. As can be seen in the figure, the fitted model shows a very good agreement over the whole energy range. Furthermore, by varying the polarization potential range \(R\) in the \(s\)-wave Jost function \(f_0(k';R)\), we managed to determine a scattering length \(a_0 = -26.6 \pm 5\) au for the electron in the continuum of the atom in the Li(2\(p^2P\)) state. This result is in complete agreement with the value previously obtained from the photodetachment experiment. We also find that the electron in the continuum of the Li(2\(p^2S\)) atom has a resonance at \(E_R = 0.0058(9)\) eV with half life \(\Gamma = 0.0059(7)\) eV, corresponding to the configuration Li\(^{-}\)(2\(s^2p^3P\)) which is in agreement with the experimental determinations [24].

**Figure 2.** Electron-loss energy spectrum for 100 keV Li\(^{-}\) ions incident on He targets. Symbols: experiments of Ref.[24]. Solid line: Least-squared fit of experimental data using Eq.(1)

4. Conclusions
In this work, we presented a physical motivated model to fit inelastic atomic processes at threshold. This model is based on the determination of the polarization potential range \(R\)
which parameterizes the elastic $\ell-$wave Jost function for an electron ending in the continuum of a neutral atom. To test our model we considered experimental data corresponding to two different inelastic atomic processes leading to the same final electron-atom interaction, namely, the Li$^-$ photodetachment in the vicinity of the Li($2^2P$) threshold [23] and the electron loss of 100 KeV Li$^-$ ions colliding with He atoms [24]. Our fitting technique provides a kind of inverse scattering method giving values for the scattering lengths which impressively agree within 2 percent, even though they were extracted from two different kinds of experiment. These results seem to validate our technique and encourage us to pursue its future application to other systems, as for instance, Li$^-$ photodetachment experiments with Li($2s\ 2S$) in the final state close to the opening of the Li($2p\ 2P$) threshold [14], and benchmark computations for electron Li($2s$)$\rightarrow$Li($2p$) excitation close to threshold [26]. Finally, we want to emphasize that starting from the fitted value of the range $R$ it would be possible, in principle, to determine the number of bound states of the negative ion. Furthermore, it would be also feasible to acquire the electron-atom dipole polarizability by treating $\beta$ as another adjustable parameter.

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