Regge Oscillations in Integral Cross Sections for Proton Impact on Atomic Hydrogen

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The integral cross sections for elastic scattering and spin exchange for proton impact on atomic hydrogen show several oscillations in the energy range 0.01–1.0 eV that cannot be associated with resonances or the glory effect. A complex angular momentum analysis using computed Regge trajectories shows that each peak of the oscillatory structure is predominantly associated with at most three trajectories. In this way, the peaks are related to the $L = 0$ bound states of H_2^+. The complex angular momentum theory for integral cross sections that we introduce shows that such oscillations are a general feature of potential scattering.

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Potential scattering is the simplest collision process and has been extensively studied from a variety of perspectives. Numerous texts on quantum mechanics and scattering theory give an apparently complete description of the topic [1,2]. It would seem that the process is completely understood on the basis of standard theory, yet we show that there are oscillations in integral elastic scattering cross sections for proton impact on atomic hydrogen whose origin is not readily apparent using standard partial wave representations.

The oscillations show up more clearly in the spin exchange cross section; thus our report emphasizes this process. We show that a summation technique exploited by Vogt and Wannier [3] is able to isolate the oscillations and relate their number to the number of bound states N_b of the potential with orbital angular momentum $L = 0$. This association means that features identified by our analysis are expected for a wide variety of collision processes. Atomic units are used throughout unless explicitly noted otherwise.

Integral cross sections, i.e., cross sections integrated over scattering angles, are given by sums over partial waves of the form

$$S = \frac{2\pi}{k_i^2} \sum_{L=0}^{\infty} f(L + 1/2)(L + 1/2), \qquad (1)$$

where $f(L + 1/2)$ is proportional to the squared magnitude of the appropriate T-matrix element and k_i is the magnitude of the initial wave vector. Because the partial wave amplitudes are readily calculated, the partial wave sum is usually evaluated directly. Features of the sum are then identified with features, e.g., shape resonances, of the individual terms $f(L + 1/2)$.

In some cases, when there are a large number of partial waves and the phase shift η_L has an extremum as a function of L, a stationary phase approximation identifies oscillations that are not associated with a single partial wave but are a feature, known as the glory effect [4], of the sum over partial waves. In this work we analyze oscillations in $H^+ + H$ spin exchange and elastic scattering cross sections at energies in the range 0.01–1.0 eV [5–7] that are neither associated with specific partial waves nor are explained by stationary phase evaluations of the partial wave sum.

The spin exchange cross section for which $f(L + 1/2) = \sin^2[\eta_g(L) - \eta_u(L)]$ and $\eta_{g(u)}$ is the phase shift in the gerade (ungerade) channel [7,8] is shown in Fig. 1. A number of features are apparent. Some are well-understood narrow shape resonances with standard Fano line shapes, but the broad symmetric peaks cannot be identified with any of the standard potential scattering features [1,2]. In this connection, note that these features were seen in the hyperspherical calculations of Igarashi and Lin [9] for HD^+ where it was also shown that they could not be identified with resonances in the partial cross sections. Earlier calculations for $H^+ + H$ and $H^+ + D$

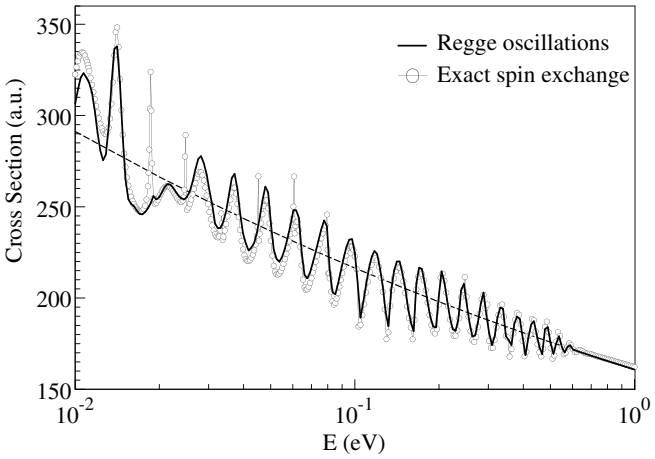

FIG. 1. Spin exchange cross section for proton impact on atomic hydrogen. The solid curve is the exact partial wave sum and the dashed curve is the sum of 20 pole contributions plus a smooth power law fit to the background cross section.

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also showed the oscillations but did not identify their origin [5,6]. The main point of our work is to show that these features cannot be identified with structures in the partial cross sections, and that a representation of integral cross sections alternative to the partial wave representation is needed. We introduce such a representation and show that it is able to separate the oscillations from the smooth part of the cross section.

To study the origin of the peaks we consider an alternative analytic representation of the sum due to Mulholland [10]. He shows that the partial wave sum of Eq. (1) may be written

$$S = \frac{2\pi}{k_i^2}\int_0^\infty f(\lambda)\lambda d\lambda - \mathrm{Re}\left\{\int_0^{i\infty}\frac{4\pi f(\lambda)/k_i^2}{1+\exp(-i2\pi\lambda)}\lambda d\lambda\right\} - \frac{2\pi}{k_i^2}\mathrm{Re}\left\{\sum_m \frac{4\pi i f_r(\lambda_m)\lambda_m}{1+\exp(-i2\pi\lambda_m)}\right\}, \quad (2)$$

where λ_m are the poles of $f(\lambda)$ in the upper right quadrant of the complex λ plane, and $f_r(\lambda_m)$ are the residues of $f(\lambda)$ at the poles. These poles are commonly referred to as Regge poles [11] and have been extensively used to analyze angular distributions [2]. The Sommerfeld-Watson transformation [12] used in the Regge analysis, however, does not apply to integral cross sections, but Eq. (2) does.

The Mulholland identity separates the sum into a smooth part, given by the first two terms in Eq. (2), from the pole contributions, given by the last term. The first term is recognized as a semiclassical, impact parameter-type contribution. Oscillations associated with the glory effect [4] originate with this term; thus Eq. (2) provides a natural way to identify oscillations that are unrelated to extrema of the phase shift.

The second term involving an integration along the imaginary axis is a correction that is small in the applications considered here. The third term, namely, a sum over pole contributions is associated with the low energy oscillations, as we show. Narrow shape resonances also appear in this term, but they are readily separated from the broad peaks seen in Fig. 1, except perhaps for relatively broad shape resonances that occur at low angular momenta and therefore low energy (below 0.03 eV).

To evaluate the last term, it is necessary to compute the positions of the poles and the residues at the poles. Upon writing

$$\sin^2(\eta_g - \eta_u) = (S_g S_u^* - 1)(S_g^* S_u - 1)/4, \quad (3)$$

where $S_{g(u)} = \exp[2i\eta_{g(u)}]$ is the gerade (ungerade) S matrix for $H^+ + H$ collisions, one sees that the poles of $S_{g(u)}$ are also the poles of $\sin^2(\eta_g - \eta_u)$. Only the poles of S_g play a significant role in our analysis.

We calculate the positions of the poles in the complex L plane by solving the nonrelativistic Schrödinger equation for complex angular momentum and searching numerically for the values of L for which the pole condition, namely $\tan\eta(L, E) = i$, is satisfied for a given E. The residues $f_r(L_m + 1/2)$ were then found by computing $\lim_{L\to L_m}(L - L_m)f(L + 1/2)$. Using the above procedure we found the Regge trajectories $L_m(E) = \lambda_m(E) - 1/2$ as a function of energy shown in Fig. 2.

Figure 2 shows that there are 20 Regge trajectories. They start at the bound states for the unphysical angular momentum $L = -1/2$, where $\lambda = 0$. As L increases to $L = 0$ the twentieth bound state moves into the continuum and the corresponding trajectory moves into the complex L plane so that the trajectory nearest the imaginary axis has a nonzero value of $\mathrm{Im}\{L\}$ for $\mathrm{Re}\{L\} = 0$. Each subsequent trajectory has $\mathrm{Re}\{L\} = \mathrm{Im}\{L\} = 0$ with a negative energy equal to the eigenenergy of one of the $L = 0$ vibrational bound states of H_2^+. There are $N_b = 19$ such trajectories for H_2^+, and we may use the vibrational quantum number ν to label them. As the parameter E increases, $\mathrm{Re}\{L_\nu\}$ increases and $\mathrm{Im}\{L_\nu\}$ remains equal to zero until the energy becomes positive. When E becomes positive $\mathrm{Im}\{L_\nu\}$ becomes nonzero but is exponentially small. In this case the νth bound state becomes a narrow shape resonance with an exponentially small width owing to tunneling through the angular momentum barrier. With a further increase of energy, the νth state is no longer confined by the angular momentum barrier so that its width and $\mathrm{Im}\{L_\nu\}$ abruptly increase. The increase of $\mathrm{Im}\{L_\nu\}$ is apparent in the trajectories shown in Fig. 2. Notice that the abrupt increase need not occur at a physical (integer) value of L.

As the energy increases further, $\mathrm{Im}\{L_\nu\}$ increases rapidly. The behavior of the corresponding pole term in Eq. (2) is shown in Fig. 3 for the trajectories corresponding to $\nu = 0$, 1, 2, and 3. The $\nu = 0$ contribution is vanishingly small below an energy of $E = E_0 = 0.425$ eV, except at the narrow shape resonances (not

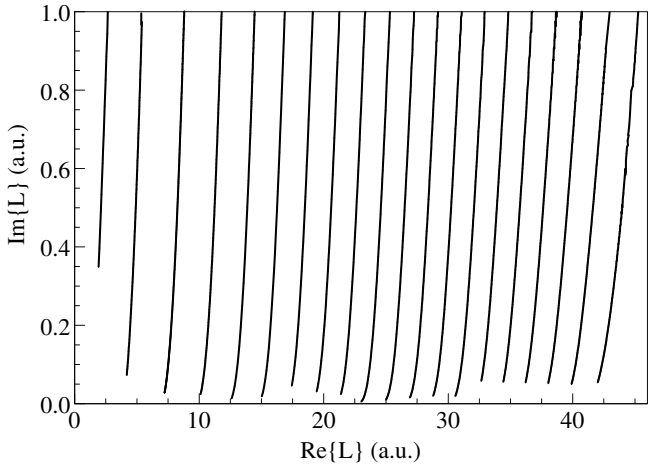

FIG. 2. Regge trajectories giving the pole positions for $0.01 < E < 1$ eV for proton impact on atomic hydrogen. The trajectories in the regions near the real axis are not shown for clarity.

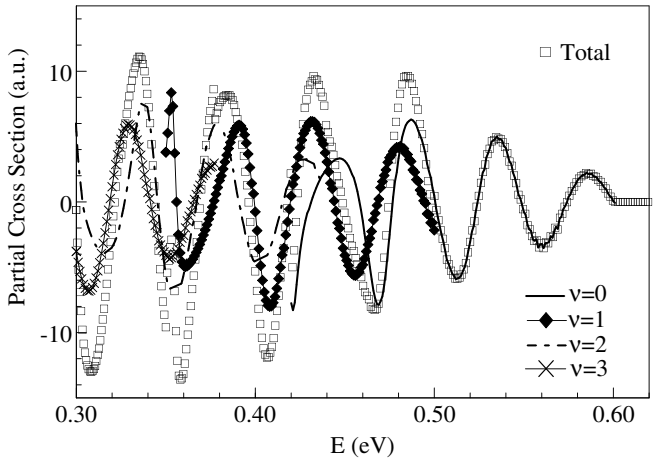

FIG. 3. Contributions to the integral spin exchange cross section for $\nu = 0$, 1, 2, and 3.

shown), but increases abruptly at E_0 owing to the increase of the partial cross section when the classical orbit can go over the angular momentum barrier. The pole contribution exhibits damped oscillations above that energy owing to the factor $1/[1 - \exp(i2\pi L_m)]$ in Eq. (2). Similarly, the $\nu = 1$ contribution has an apparent onset at $E = 0.35$ eV and shows damped oscillations that are in phase with the $\nu = 0$ oscillations. One can show on general grounds that the trajectories are approximately parallel and separated by $L_\nu - L_{\nu-1} = 2$ so all of the pole contributions are approximately in phase, although only two or three trajectories contribute to each prominent peak seen in the integral cross section.

The contributions from the pole terms are compared with the partial wave sum in Fig. 1. To facilitate the comparison a slowly varying fitted power law function was added to the pole terms. Also, the narrow resonance features in the pole contributions were not included, except at the lowest energy peak near 10^{-2} eV, where a top-of-barrier shape resonance [7] is superimposed on a broad structure. The agreement between the sum over pole terms and the exact sum over about 300–1000 partial waves is excellent.

The damped oscillations above $E > 0.525$ eV seen in the integral cross section in Fig. 1 correspond to the damped oscillations of the $\nu = 0$ contribution, the peak at 0.48 eV to $\nu = 0$ and 1, and the peak at 0.43 eV to $\nu = 0$, 1, and 2. The $\nu = 0$ term does not contribute below 0.42 eV. If we associate the lowest energy peak where the νth trajectory contributes, then one trajectory is associated with each broad peak in the energy range $0.02 < E < 0.43$ eV. Below an energy of 0.02 eV the pattern becomes less regular, but the peak just above 0.01 eV is associated with the $\nu = 16$ trajectory. The trajectories with $\nu = 17$ and 18 contribute to very broad structures below 0.01 eV that are mixed with resonances in both the g and u channels so that it is difficult to identify peaks uniquely associated with the highest two $L = 0$ vibrational levels or to the three Regge trajectories with $\mathrm{Re}L_m < 9$. With allowance for the damped oscillations from the penultimate trajectory and shape resonaces at low energies, we see that the number of broad peaks in the integral cross section approximately equals the number N_b of $L = 0$ bound states of the potential.

In our case, the number of trajectories actually equals the number of bound states for $L = -1/2$, namely, $N_b + 1 = 20$. The number of trajectories that contribute in the energy range considered here is less, namely, 17. The remaining three trajectories correlate with very broad structures below $E = 0.01$ eV, but this is compensated by the two additional peaks representing damped oscillations of the $\nu = 0$ contribution. The excellent quantitative agreement shows that the oscillations in the spin exchange cross section are indeed correlated, via the Regge trajectories, with the $L = 0$ vibrational bound states of H_2^+.

This association of the oscillations in the integral cross section with the $L = 0$ bound states of the potential is the new feature that emerges from our application of the Mulholland representation. This representation is computationally more involved than the partial wave sum, but it serves to separate a novel-type oscillatory structure from the expected smoothly varying potential scattering cross section.

There is some rough association of the computed structure in the integral cross section with broad "orbiting" resonances seen in the partial cross sections [4,9], but a quantitative picture does not emerge from that perspective. In fact, we find that there are broad resonaces for L as large as 150. For example, Fig. 4 shows our computed $L = 80$ phase shift and the corresponding partial wave term with three broad overlapping resonance oscillations for $2.0 < E < 6.0$ eV. The oscillations are present in the partial cross sections, yet there are no corresponding resonance oscillations in the integral cross sections. More spectacularly, there is no well in the effective potential to trap the particles, yet the phase increases through three multiples of π as if there were three broad shape resonances. The Mulholland representation gives a natural explanation for the absence of these oscillations, namely, there are no Regge trajectories near the real L axis for $L > 43$.

Since the detailed properties of the potential play no role in our analysis, it is expected that these oscillations are a general feature of potential scattering when the potential can support a large, but finite, number of bound states. The oscillations are in addition to glory oscillations [4] that appear when the integrand in the first term of Eq. (2) has a point of stationary phase [7] and those that are due to conventional shape resonances [1]. Because all three features are often present in elastic scattering cross sections, the novel nature of the oscillations identified

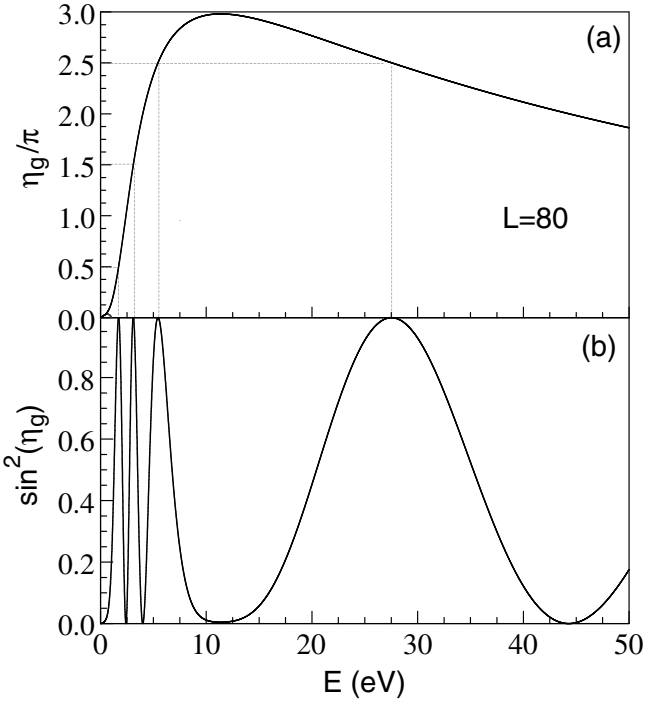

FIG. 4. Partial wave term for $L = 80$. (a) Phase shift η_g/π showing a rise of η_g through three multiples of π and (b) plot of $\sin^2\eta_g$ showing the corresponding broad overlapping resonance oscillations. The dotted lines correlate the points where η_g/π is a half integral number with the maxima of $\sin^2\eta_g$.

with the pole contributions is easily missed. The structure is most readily seen in the spin exchange cross section shown here since there is no point of stationary phase for the first term in Eq. (1), the narrow shape resonances are readily identified, and the pole contributions are of the order of 10% of the total. However, because poles of the S matrix occur in all channels, the oscillations identified here are present in the integral cross sections for all processes. Their importance, however, depends upon the magnitude of the residues at the poles, and this depends upon the specific reaction channel. For example, the computed elastic integral cross sections are much larger in absolute magnitude than the spin exchange cross sections so that the Regge oscillations are a much smaller fraction of the total. In addition the Regge oscillations are coherently superimposed on the glory oscillations; thus they are less easily identified in the elastic than the spin exchange channel.

We have shown that the standard partial wave representation is unable to identify the origin of some oscillations in atomic cross sections. To interpret these oscillations it is necessary to use an alternative representation of partial wave sums that splits off a smooth semiclassical part from purely quantal contributions that are related to the presence of bound states. Thus standard discussions of potential scattering in terms of partial waves must be supplemented by the alternative Mulholland representation to give a complete picture of potential scattering.

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