Commun. Theor. Phys. **69** (2018) 28–30 Vol. 69, No. 1, January 1, 2018

# Note on Resonant and Non-resonant Peaks in Electron-Atom Total Scattering Cross Sections

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(Received August 14, 2017; revised manuscript received November 17, 2017)

***Abstract*** *Certain broad low-energy peaks caused by a single partial wave in total cross sections are explained in terms of phase shifts. Such peaks have been associated with the real part of a Regge pole trajectory, having a maximum near an integer value of the angular momentum quantum number. At the peak energies, the pertinent partial-wave phase shift was shown to have a local maximum near a value $\pi/2$ modulo $\pi$. This implies no time delay in the semiclassical context. The phenomenon is a quantum effect, lacking a semiclassical interpretation.*

**PACS numbers:** 03.65.-w, 03.65.Nk **DOI:** 10.1088/0253-6102/69/1/28
**Key words:** scattering, resonances, quantum mechanics, cross sections

## 1 Introduction

In an earlier publication[1] the authors showed that certain broad peaks in the total cross section could not be explained as resonance phenomena in the sense of long-lived quasi-bound states. One could see a correlation with complex-angular momentum pole positions (Regge poles) behaviors as functions of the energy (Regge trajectories).[1−2] The pole trajectories were seen to turn in the complex angular momentum $l$-plane, with Re $l$ having a maximum close to an integer value as function of energy. Regge trajectories turning in the complex angular momentum $l$-plane were studied in Ref. [2].

Resonances in single-channel scattering are difficult to detect and identify experimentally for collision systems with large masses; see e.g. Toennies *et al.* in Ref. [3]. Scattering experiments with atomic particles are most sensitive to the broader resonances in a total cross section, with energies near the top of the centrifugal barrier. Such resonances may be mixed with non-resonance states of the type mentioned in Ref. [1]. Sharp resonances due to tunneling through the barrier and back again give negligible contribution to the cross sections but play a dominant role in predissociation spectroscopy; see e.g. Kolos and Peek, Bernstein.[3] In ion-atom systems the number of partial waves increases in comparison with atom-atom scattering; see Konrad and Linder in Ref. [3].

Recent experiments on electron-atom resonances, forming negative ions (anions), focus on electron affinities; see Walter *et al.* (2011) in Ref. [4]. Laser spectroscopy techniques seem to be the primary tools (Calbrese *et al.* (2005) in Ref. [4]). Electron transfer via (somewhat more complex) anions is among the most fundamental of chemical reactions and features prominently in all branches of chemistry; see Bull *et al.* (2015) in Ref. [4].

In the present note a potential model relevant for electron-atom scattering is used. The relevant "resonance" peaks in total scattering cross section are explained in terms of scattering phase shifts. The partial-wave analysis of scattering cross sections associate the scattering dynamics with phase shifts, one for each partial wave. The phase shift can be obtained from the regular solutions of the Schrödinger equation. Resonance phenomena are explained in terms of phase shift behaviors in many text books.[5−8] In the low-energy limit resonant phase shifts, due to attractive potentials, typically approach positive values $n\pi$ (Levinson's theorem), where $n$ is the maximal number of bound states existing in that potential. Typical resonances in a partial wave (integer orbital angular momentum $l$) are related to relatively rapid changes, or jumps, in the phase shifts, $\delta_l(E)$, as function of energy. In potential scattering with a single potential the phase shift defines the so-called scattering matrix expressed as $S_l = \exp(2\mathrm{i}\delta_l)$, and also the transition matrix element defined here as $T_l = S_l - 1$. Note that each $|T_l|^2$ is multiplied by a factor $2(2l+1)\pi/E$, where $E$ is the scattering energy, in order to compute the total cross section from significant $l$-contributions. Therefore the contribution from a single partial-wave can be large at low scattering energies, where only the few first values of $l$ are expected to be important.[7]

The rational function Thomas-Fermi potential (RTF) used for illustration of phase-shift behaviors has two adjustable parameters which can be adjusted to confirm a couple of experimentally measurable resonances in a reasonable way. It has been applied with some success in various calculations of electron-atom total cross sections.[1−2] Several anion states, identified by laser spectroscopy techniques,[4] have been interpreted as scattering

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resonances.[2] However, relevant scattering cross section measurements showing clearly resolved sharp resonances are hard to find in the literature.

The main purpose of this note is to make clear that certain broad peaks in the total cross section as function of scattering energy may not be proper resonances. There is a similarity between such broad peaks and so-called zero-momentum (quasi-) resonances appearing in connection with Levinson's theorem,[6−8] saying that for particular potentials the zero-energy phase shift approaches an odd (rather than an even) multiple of $\pi/2$. This note confirms the existence of certain peaks in the total cross-section that differ from sharp and broad resonances by having no time delays. The notion of time delay relies here on its definition $2\hbar \mathrm{d}\delta_l(E)/\mathrm{d}E$.[5−6] It turns out that these particular peaks occur at maxima of the phase shifts as functions of energy, and these maxima are close to an odd integral multiple of $\pi/2$.

Section 2 briefly describes a scattering wave function satisfying the radial Schrödinger equation. Computations and illustrations are in Sec. 3 and conclusions in Sec. 4.

## 2 Radial Schrödinger Equation

By introducing a dimensionless radial variable $r/a_0 \to r$ with $a_0$ being the Bohr radius, one obtains the radial Schrödinger equation

$$\frac{\mathrm{d}^2\Psi_l}{\mathrm{d}r^2} + \left(2[E - V(r)] - \frac{l(l+1)}{r^2}\right)\Psi_l = 0\,, \qquad (1)$$

with a dimensionless energy and a potential function defined as

$$ma_0^2 E/\hbar^2 \to E\,, \qquad (2)$$

$$ma_0^2 V(r)/\hbar^2 \to V(r)\,. \qquad (3)$$

"$\hbar$" is Planck's constant divided by $2\pi$ and $m$ the reduced mass of the collision system.

The regular solution $\Psi_l$ satisfies the scattering boundary conditions that define the scattering matrix elements $S_l$,[8] i.e.

$$\Psi_l(r) \sim \mathrm{e}^{-\mathrm{i}(kr - l\pi/2)} - S_l\,\mathrm{e}^{\mathrm{i}(kr - l\pi/2)}, \quad r \to +\infty\,, \qquad (4)$$

where $k$ is the scattering wave number

$$k = \sqrt{2E}\,. \qquad (5)$$

The transition matrix elements $T_l$ are given by

$$T_l = S_l - 1 = 2\mathrm{i}\,\mathrm{e}^{\mathrm{i}\delta_l}\sin\delta_l\,. \qquad (6)$$

The phase shifts $\delta_l$ are real and the maxima of $|T_l|$ are given by the condition $\delta_l = (n + 1/2)\pi$, $n = 0, 1, 2, \ldots$ for which $T_l = -2$.

## 3 Computations and Illustrations

The rational function Thomas-Fermi (RTF) potential[1−2] used for illustrating an electron-atom interaction has a Coulomb attraction near the origin but adopts an attractive polarization interaction at long range. The dimensionless form of the RTF potential used here is given by[2]:

$$V(r) = \frac{-Z}{r\,(1 + aZ^{1/3}r)\,(1 + bZ^{2/3}r^2)}\,, \qquad (7)$$

with the long-range behavior

$$V(r) \approx -\frac{1}{abr^4}, \text{ as } r \to +\infty\,. \qquad (8)$$

Three sets of potential parameters are used. All of them correspond to the nuclear core charge $Z = 63$ and all with the same long-range polarization property defined by $ab = 0.015$. These potentials are used to illustrate both non-resonant and resonant behaviors of phase shifts and squared moduli of the transition matrix elements ($|T_l|^2$).

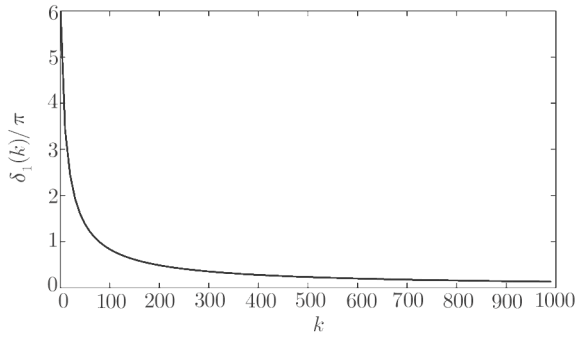


**Fig. 1** A typical phase shift behavior for a wide range of $k$-values. The RTF potential is defined by $a = 0.19$, with $Z = 63$ and $l = 1$.

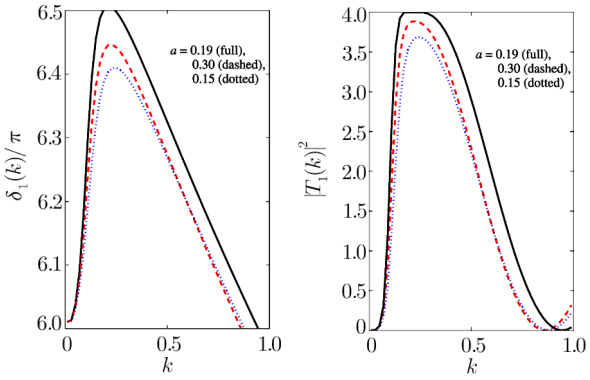


**Fig. 2** Particular low-energy phase shifts as functions of $k$. The RTF potentials are defined by $a = 0.15, 0.19$, and $0.30$, with $Z = 63$ and $l = 1$.

A phase shift behavior in the range $0 < k < 1000$ is illustrated for $l = 1$ and the RTF-potential with $a = 19$ (and $b = 0.015/a$) and is shown in Fig. 1. The effective potential is seen to support six bound states according to Levinson's theorem, since the phase shift tends to $6\pi$ in the low-energy limit. Since the potential is neither strongly singular nor repulsive at the origin (in contrast to a Lennard-Jones potential) any partial-wave phase shift tends to zero in the (non-relativistic) high-energy limit.

On a more detailed level, for scattering wave numbers in the range $0 < k < 1$ and $l = 1$ one sees a local maximum of the phase shift. In the left subplot of Fig. 2 this

maximum exists for the three potentials corresponding to $a = 0.15$, $0.19$, and $0.30$. All three maxima are in the neighborhood of an odd integral multiple of $\pi/2$, although for $a = 0.19$ it is closest. The effect on $|T_1(k)|^2$ is shown in the right subplot of Fig. 2. All three curves describe peaks although the energy derivatives of the corresponding phase shifts are zero at the peak positions. Obviously, the concept of "time delay" cannot be applied in this case.

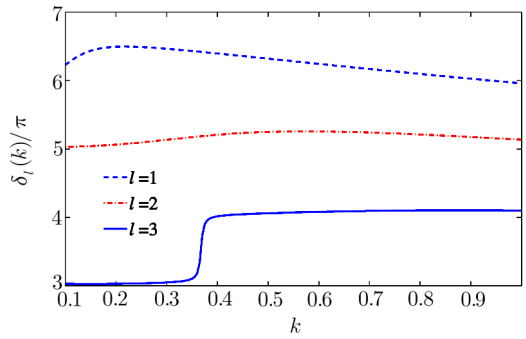


**Fig. 3** Comparison of the phase shifts corresponding to $l = 1$ (as in Fig. 2) and $l = 2$ and $l = 3$ as functions of $k$. The RTF potential is defined by $a = 0.19$, with $Z = 63$. For $l = 3$ the phase shift passes through an odd integral multiple of $\pi/2$ in value, while for $l = 1, 2$ it does not.

By fixing the value $a = 0.19$ for the RTF potential and comparing the phase shifts for $l = 1$, 2, and 3, one obtains Fig. 3. The corresponding behaviors of $|T_l(k)|^2$ are seen in Fig. 4. Firstly, one observes that the effective potential for $l = 2$ supports five bound states and that for $l = 3$ supports three bound states. The phase shift curve $\delta_2(k)$ does not pass through an odd integral multiple of $\pi/2$ in this energy range. It has a similar smooth behavior to $\delta_1(k)$, but is not as close to an odd integral multiple of $\pi/2$ as $\delta_1(k)$.

The phase shift $\delta_3(k)$ shows a typical resonance behavior. It jumps across an odd integral multiple of $\pi/2$ and adds to its value one unit of $\pi$. In this case the slope $\mathrm{d}\delta_3(k)/\mathrm{d}E$ is comparatively large so that the semiclassical notion of time delay applies (or may apply). The energy is low ($k^2 \ll 1$) and the partial cross section from $l = 3$ may be significantly large. The effect on $|T_3(k)|^2$ in Fig. 4 indicates a narrow peak and elsewhere small contributions.

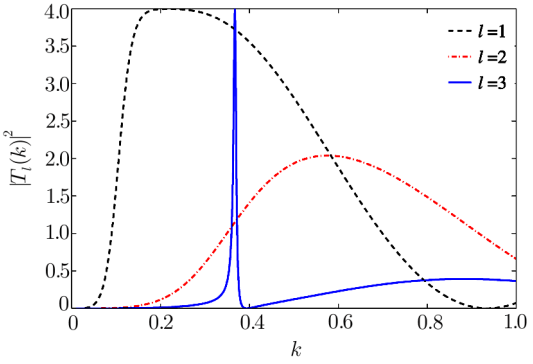


**Fig. 4** $|T_l|^2$ as function of $k$. The RTF potential is defined by $a = 0.19$, with $Z = 63$ and $l = 1, 2$, and 3.

## 4 Conclusions

Significant, low-energy peaks in the total cross section may be observed that are not resonances. This is explained in terms of particular phase shift behaviors, not generally seen for arbitrary potential parameters. The responsible phase shift stays close to an odd integral multiple value of $\pi/2$ for a range of scattering energies. At low energies contributions from $l = 1$ or $l = 2$ in the cross sections may be significant. In contrast, a typical resonance phase shift passes through an odd integral multiple value of $\pi/2$ completely, like that for $l = 3$ in Fig. 3, and in a relatively small energy region.

## References

[1] K. E. Thylwe and P. McCabe, Eur. Phys. J. D **68** (2014) 323.

[2] S. M. Belov, N. B. Avdonina, Z. Felfli, *et al.*, J. Phys. A **37** (2004) 6943; Z. Felfli, A. Z. Msezane, and D. Sokolovski, Phys. Rev. A **79** (2009) 012714; S. M. Belov, K. E. Thylwe, M. Marletta, *et al.*, J. Phys. A **43** (2010) 365301.

[3] J. P. Toennies, W. Welz, and G. Wolf, J. Chem. Phys. **61** (1974) 2461; J. P. Toennies, W. Welz, and G. Wolf, J. Chem. Phys. **71** (1979) 614; R. B. Bernstein, Chem. Phys. Lett. **25** (1974) 1; W. Kolos and J. M. Peek, Chem. Phys. **12** (1976) 381; M. Konrad and F. Linder, J. Phys. B **15** (1982) L405.

[4] C. W. Walter, N. D. Gibson, Y. G. Li, *et al.*, Phys. Rev. A **84** (2011) 032514; D. Calabrese, A. M. Covington, W. W. Williams, *et al.*, Phys. Rev. A **71** (2005) 042708; J. N. Bull, C. W. West, and J. R. R. Verlet, Phys. Chem. Chem. Phys. **17** ( 2015) 16125.

[5] C. J. Joachain, *Quantum Collision Theory*, North-Holland, Amsterdam (1975).

[6] M. S. Child, *Molecular Collision Theory*, Dover Publications, New York (1996).

[7] H. A. Bethe and R. Jackiw, *Intermediate Quantum Mechanics*, 3rd ed., Benjamin/Cummings, Menlo Park (California, US) (1986).

[8] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions*, 3rd ed., Oxford University Press, London, Ch. 9 (1965).