Regge-pole description of rainbow scattering by means of the phase-integral method

Abraham Amaha
Blodstensvägen 2 230, S-752 44 Uppsala, Sweden

Karl-Erik Thylwe
Department of Mechanics, Royal Institute of Technology, S-100 44 Stockholm, Sweden
(Received 8 September 1993)

In the present paper we study the effects in the rainbow differential cross sections of using higher-order phase-integral residues in the pole sum of the scattering amplitude. We have recently found that already in the first-order approximation the uniform residue formula, derived by Fröman and Fröman, provides an important means for an accurate calculation of the rainbow differential cross section where reliable numerical quantum methods are not available. From the present investigation it is clear that the use of higher-order approximations is not the crucial step to further reveal the rainbow structures in the cross section. For that purpose, it is instead essential to increase the purely numerical precision (in any order) of the uniform phase-integral residue calculations.

PACS number(s): 34.40.+n, 03.65.Nk, 03.65.Sq

I. INTRODUCTION

The Regge-pole theory of atomic and molecular scattering was introduced two decades ago [1–4] and has, since then, gradually increased the understanding of prominent features of differential cross sections. The theory has recently been reviewed by Thylwe [5] and Connor [6]. It has been particularly successful in the analysis of diffraction effects and resonance structures in differential scattering cross sections. The strength of the Regge-pole theory in the cases mentioned is the appearance of just a few significant terms in the pole contribution to the scattering amplitude. The analysis of the structures in the differential scattering cross sections is then easy to do and leads to simple modified semiclassical interpretations; see Refs. [5] and [6], for details. The application of the semiclassical Regge-pole theory to rainbow collisions [7–10] has for a long time been shown to be less success. Only for very light particles with a weak long-range part of the interaction potential was the differential cross section accurately obtained. With larger reduced mass of the collision partners and larger well depth of the interaction potential the number of important terms in the pole sum increases. Although in some cases up to 50 poles, calculated both with numerical quantum and semiclassical methods, were included in the calculation the correct differential cross section could not be reproduced. It was soon realized that strong cancellations between exponentially large terms were present in the evaluation of the pole sum and that the residues were not accurately obtainable by methods existing at the time; see Ref. [9].

Pajunen [11] found a procedure based on the Prüfer phase function which indicated that the residue calculations could be more accurate than previous results with accurate Regge-pole positions. Recently, Fröman and Fröman [12] and the present authors [13,14] showed that the previous phase-integral residue formula is considerably improved by explicitly treating the two relevant complex turning points as lying at an arbitrary distance from each other, i.e., also allowing them to lie close together, but well isolated from other transition points. As demonstrated in Ref. [13] the residues were sufficiently accurate to drastically improve the semiclassical Regge-pole calculations of the rainbow scattering cross section already in the first-order approximation.

In the present paper, we go beyond the improved semiclassical Regge-pole theory just described and presented in Ref. [13], and study the effects in the differential scattering cross sections of using higher-order phase-integral approximations for the residues and positions of Regge poles. It should be pointed out, however, that the semiclassical (and improved semiclassical) approximations used in the Regge-pole theory involve two asymptotic methods: the saddle-point method and the first-order (nonuniform or uniform) phase-integral method. The latter method is applied not only for calculating the positions and residues of the Regge poles, but also for calculating the phase shift and Legendre functions of complex degree appearing in the expression for the scattering amplitude. Hence, we could not be certain to arbitrarily improve the differential cross section by merely improving the accuracy of residues alone. The idea to focus our rainbow study on the residue calculations alone is, however, motivated by the well-known presence of strong cancellations in the pole sum, where the residues are key quantities. Nevertheless, as explained in Sec. IV, the present investigation shows a remarkably simple recipe of how to improve the calculation of supernumerary rainbow features in the differential cross sections of Regge-pole theory.

Although we expected to be able to show that the much more accurate higher-order phase-integral calculations of pole positions and residues could cure the inaccurate Regge cross sections at lower scattering angles, it turned out that the use of first-order uniform phase-

integral calculations is sufficient for that purpose. The key to the resolution lies rather in the performance of *high-precision* calculations, either using the Fröman-Fröman residue formula, or using some numerical quantum method which seems to be very difficult to do for extremely large pole residues.

In Sec. II we review the basic Regge-pole theory and the approximations used in the present calculations. Section III contains a description of the ion-atom and atom-molecule collision systems investigated with the analytic potential parameters explicitly given. The results are discussed in Sec. IV and conclusions are given in Sec. V.

II. BRIEF REVIEW OF REGGE THEORY

We write the radial Schrödinger equation in the form

$$\frac{d^2\psi}{dr^2}+R(r)\psi=0 , \tag{2.1}$$

where, according to conventional notations,

$$R(r)=k^2-\frac{2\mu}{\hbar^2}V(r)-\frac{l(l+1)}{r^2} . \tag{2.2}$$

The quantity $V(r)$, which is the physical potential for two spinless particles, is assumed to satisfy the condition (for the Coulomb case see [15])

$$\lim_{r\to\infty} r^2V(r)=0 . \tag{2.3}$$

The wave function, which is to be a regular solution of the differential equation (2.1) fulfills, aside from a normalizing factor, the asymptotic condition [16]

$$\psi(r)\sim\exp\left[-i\left[kr-\frac{\pi}{2}l\right]\right] -S_l\exp\left[i\left[kr-\frac{\pi}{2}l\right]\right] , \quad r\to+\infty , \tag{2.4}$$

where the function

$$S_l=\exp(2i\delta_l) \tag{2.5}$$

is the scattering-matrix (S-matrix) element and δ_l is the phase shift dependent on both the angular-momentum quantum number l and the energy $E(=k^2\hbar^2/2\mu)$ of the relative motion of the interacting particles. A detailed analysis concerning (2.4) and (2.5) within the framework of the phase-integral technique developed by Fröman and Fröman [17], is given in [18] and [19].

With the knowledge of this S-matrix element the differential cross section $I(\theta)$ relevant in the analysis of scattering data can be obtained through the scattering amplitude $f(\theta)$ as

$$I(\theta)=|f(\theta)|^2 , \tag{2.6}$$

where θ is the scattering angle. The partial-wave representation of the scattering amplitude, expressed in terms of the Legendre polynomials of discrete values of l, is given by

$$f(\theta)=\frac{1}{ik}\sum_{l=0}^{\infty}(l+\tfrac{1}{2})(S_l-1)P_l(\cos\theta) . \tag{2.7}$$

It is a well-known problem, however, especially for heavy-particle scattering at relatively high energies, that the partial-wave representation converges very slowly. For potentials with a Coulombic tail the partial-wave series is even divergent [15]. To this effect the complex-angular-momentum (CAM) formalism introduced by Regge [20–22] seems to be adequate, at least for a large class of potentials.

When the Regge condition is imposed the regular solutions of (2.1) are set to behave as purely outgoing waves at infinity [22]. This condition is characteristic for the quasibound states of the colliding particles, and it is fulfilled if either the energy E or the angular-momentum quantum number l takes on complex values. With l allowed to take on complex values, the wave functions satisfying the pure-outgoing-wave boundary condition correspond to poles (Regge poles) of the S matrix as is evident from Eq. (2.4). The quantities associated with these Regge states are the Regge poles l_m and the corresponding residues r_m, where m is a non-negative integer that distinguishes between the different poles of the scattering matrix.

To express the scattering amplitude in an integral form [23], one introduces the Watson transformation which involves the residues of $1/\sin(\pi l)$ for a complex variable l. The underlying formula for the transformation is given by (e.g., Ref. [26])

$$\sum_{l=0}^{\infty}g(l)=-\tfrac{1}{2}\int_C g(l)\frac{\exp[-i\pi(l+\frac{1}{2})]}{\sin(\pi l)}dl , \tag{2.8}$$

where $g(l)$ is an analytic function in the neighborhood of the non-negative real l axis and C is the contour surrounding the non-negative real l axis in the clockwise sense. With the scattering matrix S_l now being a continuous function of the complex variable l, henceforth denoted as $S(l)$, the scattering amplitude $f(\theta)$ can therefore be written as

$$f(\theta)=\frac{1}{2k}\int_C\frac{(l+\frac{1}{2})[S(l)-1]P_l(-\cos\theta)}{\sin(\pi l)}dl , \tag{2.9}$$

where the identity $\exp(-i\pi l)P_l(\cos\theta)=P_l(-\cos\theta)$ has been used and $P_l(-\cos\theta)$ is now the Legendre function of complex degree l.

A. Basic formulas in the Regge-pole theory

By deforming the contour of integration in Eq. (2.9) one can include the residues of the scattering-matrix poles. No other singularities are assumed to be present in the half plane $\mathrm{Re}\,l>-\frac{1}{2}$. The scattering amplitude may thus be reproduced by a sum of terms containing pole positions l_m and associated residues r_m, known as the pole sum $f_P(\theta)$, and the remaining integral, also known as the background integral $f_B(\theta)$. In this way Eq. (2.9) can be written as

$$f(\theta)=f_P(\theta)+f_B(\theta) , \tag{2.10}$$

where

$$f_P(\theta)=\frac{\pi i}{k}\sum_{m=0}^{\infty}\frac{(l_m+\frac{1}{2})r_m}{\sin(\pi l_m)}P_{l_m}(-\cos\theta) \tag{2.11}$$

is the pole sum, and

$$f_B(\theta)=\frac{1}{2k}\int_\Gamma\frac{(l+\frac{1}{2})[S(l)-1]P_l(-\cos\theta)}{\sin(\pi l)}dl \tag{2.12}$$

is the background integral with Γ being a new contour lying to the left of the Regge poles in the right half plane $\mathrm{Re}\,l>-\frac{1}{2}$.

The actual path of integration in (2.12), with consideration of the properties of $S(l)$ for various potentials, is discussed in detail by Thylwe [5] and by Connor [24]. For practical purposes it starts along the positive imaginary axis of $l+\frac{1}{2}$, passes a saddle point and terminates in the fourth quadrant of the complex l plane such that $\mathrm{Re}\,l\to+\infty$ and $\mathrm{Im}\,l\to-\infty$. Here, we give only the essential formulas pertaining to the background integral given in [25] and [15]. For a singular potential of the Lennard-Jones type an exact expression for the background integral is

$$f_B(\theta)=-\frac{i}{k}\int_\Gamma(l+\tfrac{1}{2})Q_l^{(-)}(\cos\theta)\exp[2i\delta(l)]dl\ , \tag{2.13}$$

where the so-called regenerative-wave angular function [26] $Q_\nu^{(-)}(x)$ expressed in terms of the first and second kind of the Legendre functions is

$$Q_\nu^{(-)}(x)=\tfrac{1}{2}\left[P_\nu(x)+\frac{2i}{\pi}Q_\nu(x)\right]\ . \tag{2.14}$$

The Regge representation has been proven useful in the interpretation of structures in the differential cross sections as being caused by certain interfering physical phenomena in the collision processes; see Ref. [6].

For a more general, exact CAM representation of the scattering amplitude, namely, the *subamplitude-pole representation*, see Refs. [19] and [15].

B. Approximate formulas

In the higher-order phase-integral approximations the Regge-pole positions l_m can be calculated from the generalized Bohr-Sommerfeld formula

$$\bar\gamma=\frac{1}{2\pi}\int_{(t_1)}^{(t_2)}q(r)dr=m+\tfrac{1}{2}\ ,\quad m=0,1,2,\ldots\ , \tag{2.15}$$

where $q(r)$ is given by the asymptotic expansion of order $2N+1$:

$$q(r)=Q(r)\sum_{n=0}^{N}Y_{2n}\ . \tag{2.16}$$

The first term $Q(r)$ is the base function [corresponding to the reduced classical momentum $R^{1/2}(r)$] specified by

$$Q^2(r)=R(r)-\frac{1}{4r^2}\ . \tag{2.17}$$

The relevant higher-order corrections terms Y_{2n} in (2.16) are given by Eqs. (3.15a)–(3.15c) and (3.19) in Ref. [17]. Furthermore, t_1 and t_2 are the relevant transition zeros of $Q^2(r)$, and integration is performed along a closed contour surrounding t_1 and t_2 (with a cut joining them) in the positive sense. The corresponding residues are [12]

$$r_m=\left[\frac{f(\bar\gamma_0,\ldots,\bar\gamma_{2N})\exp\left\{2i\lim_{r\to+\infty}\left[w(r)-kr+(l+\frac{1}{2})\frac{\pi}{2}\right]\right\}}{2\pi i\,\partial\bar\gamma/\partial l}\right]_{l=l_m}\ , \tag{2.18}$$

where $f(\bar\gamma_0,\ldots,\bar\gamma_{2N})$ is the correction function that allows the transition zeros to lie arbitrarily close to each other with

$$\bar\gamma_{2n}=\frac{1}{2\pi}\int_{(t_1)}^{(t_2)}Q(r)Y_{2n}dr \tag{2.19}$$

and

$$w(r)=\tfrac{1}{2}\int_{\Gamma_{t_2}}q(r)dr\ , \tag{2.20}$$

Γ_{t_2} being a contour in the complex r plane which starts at the point corresponding to r on the lower Riemann sheet encircling t_2 as well as the associated zeros of $q(r)$ in (2.16) and ending at the point r itself. We remark that, for the first-order approximation, the above integrals become line integrals on suitable paths.

Formulas (2.15) and (2.18) are used in the first-order as well as higher-order phase-integral calculations of l_m and r_m in the pole sum (2.11). As for the Legendre function, also appearing in (2.11), we use only its leading (first-order) asymptotic form ($|l\sin\theta|\to\infty$)

$$P_l(-\cos\theta)\sim\left[\frac{2}{\pi(l+\frac{1}{2})\sin\theta}\right]^{1/2}\times\cos\left[(l+\tfrac{1}{2})(\pi-\theta)-\frac{\pi}{4}\right]\ , \tag{2.21}$$

which is given in [27], where the accuracy is also discussed in detail.

To single out and investigate the improvement of the differential cross section by improving the accuracy of the positions and residues with higher-order phase-integral calculations, we keep the background integral calculations strictly in the first order.

Hence, the regenerative-wave angular function is approximated by

$$Q_l^{(-)}(\cos\theta)\sim\left[\frac{1}{2\pi(l+\frac{1}{2})\sin\theta}\right]^{1/2}\times\exp\left\{-i\left[(l+\tfrac{1}{2})-\frac{\pi}{4}\right]\right\}, \tag{2.22}$$

so that formula (2.13) becomes

$$f_B(\theta)=\frac{\exp\left[-i\frac{\pi}{4}\right]}{k\sqrt{2\pi\sin\theta}}\int_\Gamma(l+\tfrac{1}{2})^{1/2}\times\exp\{i[2\delta(l)-(l+\tfrac{1}{2})\theta]\}dl\ . \tag{2.23}$$

By using the saddle-point method, one obtains for the leading-order asymptotic representation of the background integral the expression [25]

$$f_B(\theta)=-\frac{i}{k}\left[\frac{l_\theta+\frac{1}{2}}{\sin\theta|\partial\Theta(l_\theta)/\partial l|}\right]^{1/2}\times\exp\{i[2\delta(l_\theta)-(l_\theta+\tfrac{1}{2})\theta]\}\ , \tag{2.24}$$

where $\delta(l)$ is the semiclassical phase shift in terms of which the scattering-matrix element in (2.5) is defined with δ_l replaced by $\delta(l)$. The quantity l_θ in the above equation is the saddle point which fulfills

$$\theta=2\partial\delta(l)/\partial l|_{l=l_\theta}\equiv\Theta(l_\theta)\ , \tag{2.25}$$

where $\Theta(l)$ is the usual classical deflection function, if the first-order phase-integral approximation for the phase shift is used, i.e.,

$$\delta(l)=\lim_{r\to\infty}\left[\int_{t_1}^{r}Q(r')dr'-kr\right]+(l+\tfrac{1}{2})\frac{\pi}{2}\ , \tag{2.26}$$

where the classical turning point t_1 is, in a generalized sense [since $Q^2(r)\neq R(r)$], the radius of closest approach to the scatterer.

III. APPLICATION TO PARTICULAR POTENTIALS

We consider two scattering systems (H^+ + Ar and K + HBr) in our analysis of the Regge theory, where in each case the interaction potentials are of the Lennard-Jones type. The H^+ + Ar and K + HBr scattering have been studied recently in model calculations in Refs. [11] and [14]. In this investigation we take into account 25 Regge poles for each system to compute the differential cross sections. The saddle-point method and the first-order phase-integral approximations are used for the calculation of the background integrals, while both the first and fifth orders of the phase-integral approximations are used, as described above, to calculate the pole sums.

The computational procedure is the same as in our previous paper [13]. With dimensions and energies expressed in units of Å and eV, respectively, and with $\hbar=6.465\,416\,717\times10^{-2}$, the cross sections are given in units of $(\text{Å})^2$. The scattering cross sections are calculated in each system for three different energies converted to units of eV. As a reference, we also computed the differential cross sections from the partial-wave series, using an average of 8000 accurate phase shifts.

A. The H^+ + Ar System

Proton-argon scattering has been studied both theoretically and experimentally (see Toennies [28]). This system, which has a small reduced mass and a relatively strong long-range attraction in comparison with neutral systems, shows pronounced rainbow oscillations with the fast oscillations experimentally resolved even at quite high center-of-mass scattering energies. In our study, we have chosen a Lennard-Jones LJ(6,4) potential,

$$V(r)=\epsilon\left[2\left[\frac{r_{\min}}{r}\right]^6-3\left[\frac{r_{\min}}{r}\right]^4\right], \tag{3.1}$$

to represent the system. This potential has also been used in Refs. [11] and [14]. As in Ref. [30] the radial Schrödinger equation is initially transformed by the introduction of the dimensionless parameters

$$A=kr_{\min}\ ,\quad K=E/\epsilon\ ,\quad R=r/r_{\min}\ . \tag{3.2}$$

For the radial Schrödinger equation (2.1) thus transformed, the square of the base function is chosen in accordance with (2.17), which yields

$$Q^2(r)=A^2-\frac{A^2}{K}\left[\frac{2}{r^6}-\frac{3}{r^4}\right]-\frac{(l+\frac{1}{2})^2}{r^2}\ , \tag{3.3}$$

so that, apart from the use of the uniform residue formula (2.18), the first-order phase-integral approximation would agree with previous semiclassical results. In Fig. 1 the plots of the scattering cross section for energies 15, 5, and 3 eV and a plot of corresponding deflection functions are given. From Figs. 1(a)–1(c) we see that no apparent difference is observed in the differential cross sections between the first- and the fifth-order calculations for the positions and residues, except when the angle is small where both of the Regge calculations start to deviate from the partial-wave representation. Table I gives the values of the pole positions and residues (in the first and fifth order of the phase-integral approximation) at $E=5$ eV with the parameters given in [31]. We notice, in particular, that these residues are large compared to residues typical in diffraction scattering [5].

B. The K + HBr system

This system, which has a larger reduced mass and a weaker long-range attraction compared to the previous one, has also been studied by Eu [29] and Connor, Mackay, and Thylwe [30]. In the present paper, only the real part of the potential, given by

$$V(r)=4\epsilon\left[\left[\frac{\sigma}{r}\right]^{12}-\left[\frac{\sigma}{r}\right]^6\right], \tag{3.4}$$

is considered. As in the previous system, the transformed dimensionless parameters are (see Ref. [30])

$$A=k\sigma\ ,\quad K=E/\epsilon\ ,\quad R=r/\sigma\ , \tag{3.5}$$

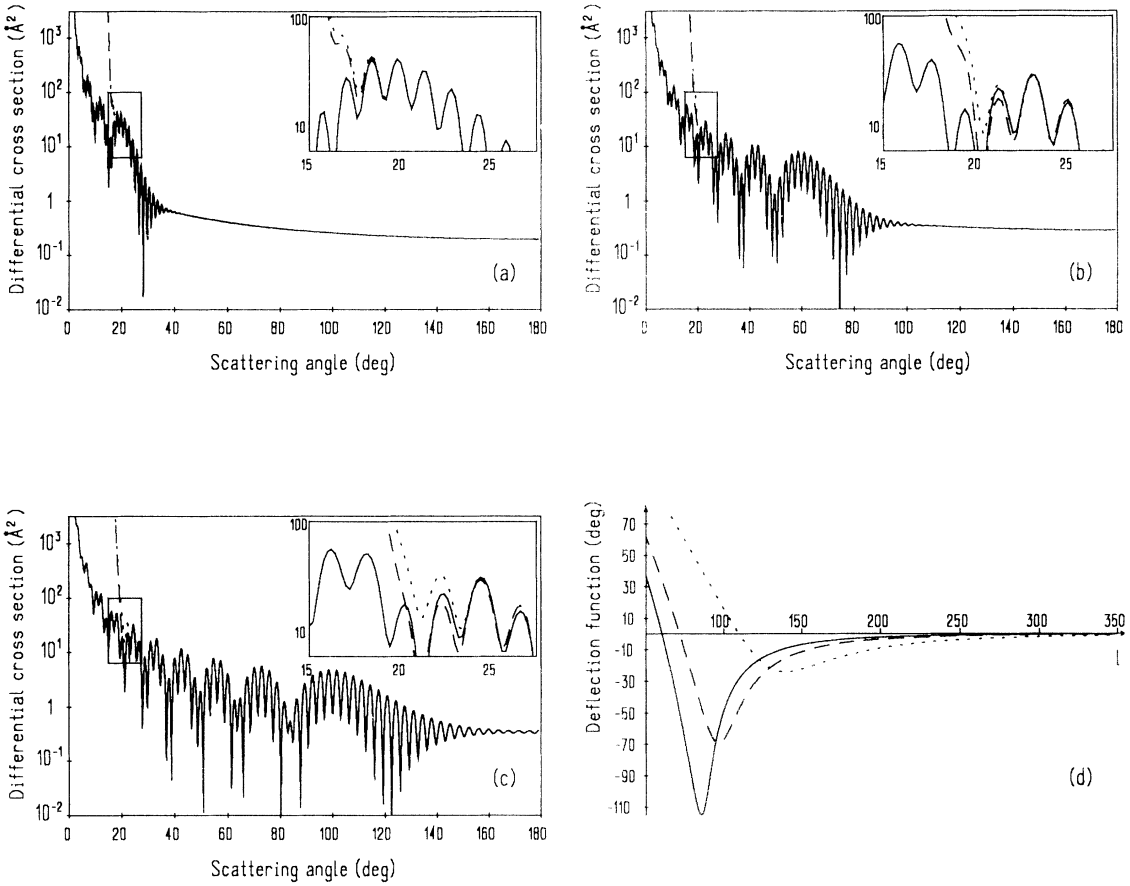

FIG. 1. (a)–(c) Logarithmic plots of the differential cross section $I(\theta)$ against the scattering angle θ in the $H^+ + Ar$ system represented by the potential (3.1) at energies (a) $E=15$, (b) $E=5$, and (c) $E=3$ eV. The solid curve represents the partial-wave results, the broken curve represents the fifth-order, and the dotted curve represents the first-order phase-integral calculations. It is seen that the plots coincide except at small scattering angles. The insets are magnifications in the plots $I(\theta)$ vs θ to reveal the differences between the partial-wave and the fifth- and first-order phase-integral results for small scattering angles. (d) Plot of corresponding deflection functions $\Theta(l)$ against the real variable l, where the dotted curve represents the deflection function corresponding to the energy $E=15$, broken curve to $E=5$, and solid curve to $E=3$ eV.

TABLE I. Positions and residues for the potential (3.1) calculated by the first- and fifth-order phase-integral approximation at $E=5$ eV for the parameter values given in [31], $\epsilon=6.97235\times10^{-19}/1.60219\times10^{-19}$ eV, $r_{\min}$ (denoted by r_m in [31]) $=1.3123$ Å, and $\mu=1.63178\times10^{-27}/1.66057\times10^{-27}$ u. The truncated numerical entries in l_m and r_m correspond to the first-order calculations while the quantities just below them are of the fith order.

m	$\mathrm{Re}\,l_m$	$\mathrm{Im}\,l_m$	$\mathrm{Re}\,r_m$	$\mathrm{Im}\,r_m$
0	97.4984	12.3961	3.503×10^{7}	-1.4110×10^{8}
	97.496 528 74	12.396 371 67	$3.456\,203\,692\,7\times10^{7}$	$-1.414\,950\,9717\times10^{8}$
1	96.7054	14.0227	-2.3020×10^{9}	1.749×10^{9}
	96.703 582 45	14.022 984 00	$-2.298\,955\,871\,4\times10^{9}$	$1.760\,141\,387\,5\times10^{9}$
5	93.7098	20.8748	1.228×10^{12}	-1.264×10^{12}
	93.708 161 18	20.875 320 67	$1.223\,991\,790\,7\times10^{12}$	$-1.269\,118\,819\,9\times10^{12}$
10	90.5619	30.1100	7.444×10^{12}	1.2686×10^{13}
	90.560 376 21	30.110 637 42	$7.485\,185\,481\,2\times10^{12}$	$1.265\,789\,108\,9\times10^{13}$
15	88.2959	39.8219	8.844×10^{11}	$-3.222\,279\times10^{12}$
	88.294 614 93	39.822 660 73	$8.741\,624\,769\,3\times10^{11}$	$-3.222\,178\,159\,8\times10^{12}$
20	86.9784	49.6679	3.487×10^{10}	-1.1210×10^{11}
	86.977 289 80	49.668 728 74	$3.454\,719\,033\,1\times10^{10}$	$-1.120\,484\,199\,4\times10^{11}$
24	86.5473	57.4415	-9.23×10^{7}	4.8048×10^{9}
	86.546 353 99	57.442 338 13	$-8.220\,114\,657\,2\times10^{7}$	$4.798\,208\,410\,1\times10^{9}$

and the corresponding base function is

$$Q^2(R)=A^2-4\frac{A^2}{K}\left[\frac{1}{R^{12}}-\frac{1}{R^6}\right]-\frac{(l+\frac{1}{2})^2}{R^2}\ . \quad (3.6)$$

Figure 2 shows the plots of the cross sections for energies of 0.3, 0.1, and 0.035 eV as well as the deflection functions corresponding to these energies. The slowly varying rainbow pattern is similar to that in Fig. 1 in this more massive system, but the fast oscillations clearly indicate that the real parts of the Regge poles are large because of the reduced mass. Again we see that the first- and the fifth-order results are in close agreement except at small scattering angles, where both Regge calculations start to deviate from the partial-wave results. The angular width of the deviation is considerably smaller, however, in this case. Pole positions and residues at $E=0.1$ eV are calculated and given in Table II. We observe in Table II that the largest residues are about five orders-of-magnitude smaller than in Table I.

IV. DISCUSSION OF RESULTS

We have already shown in a previous paper that without the use of the residue formula due to Fröman and Fröman [12] the semiclassical calculations of the Regge differential cross sections would fail completely to describe the rainbow oscillations, while this formula in the first-order approximation provides an important means for accurate calculation of the rainbow differential cross section. In the present investigation we find that the much more accurate higher-order phase-integral residues (cf. Ref. [14]) do not further improve the differential cross sections to the extent that we had expected. The higher-order phase-integral calculations simply do not reveal further supernumerary rainbow features in the differential cross sections.

To explain the results we first study Tables III and IV which illustrate the contribution of individual Regge poles in the pole sum. In Table III the first- and fifth-order individual terms and some of their partial sums at two different angles, $\theta=22$ and $32°$ are given. It is im-

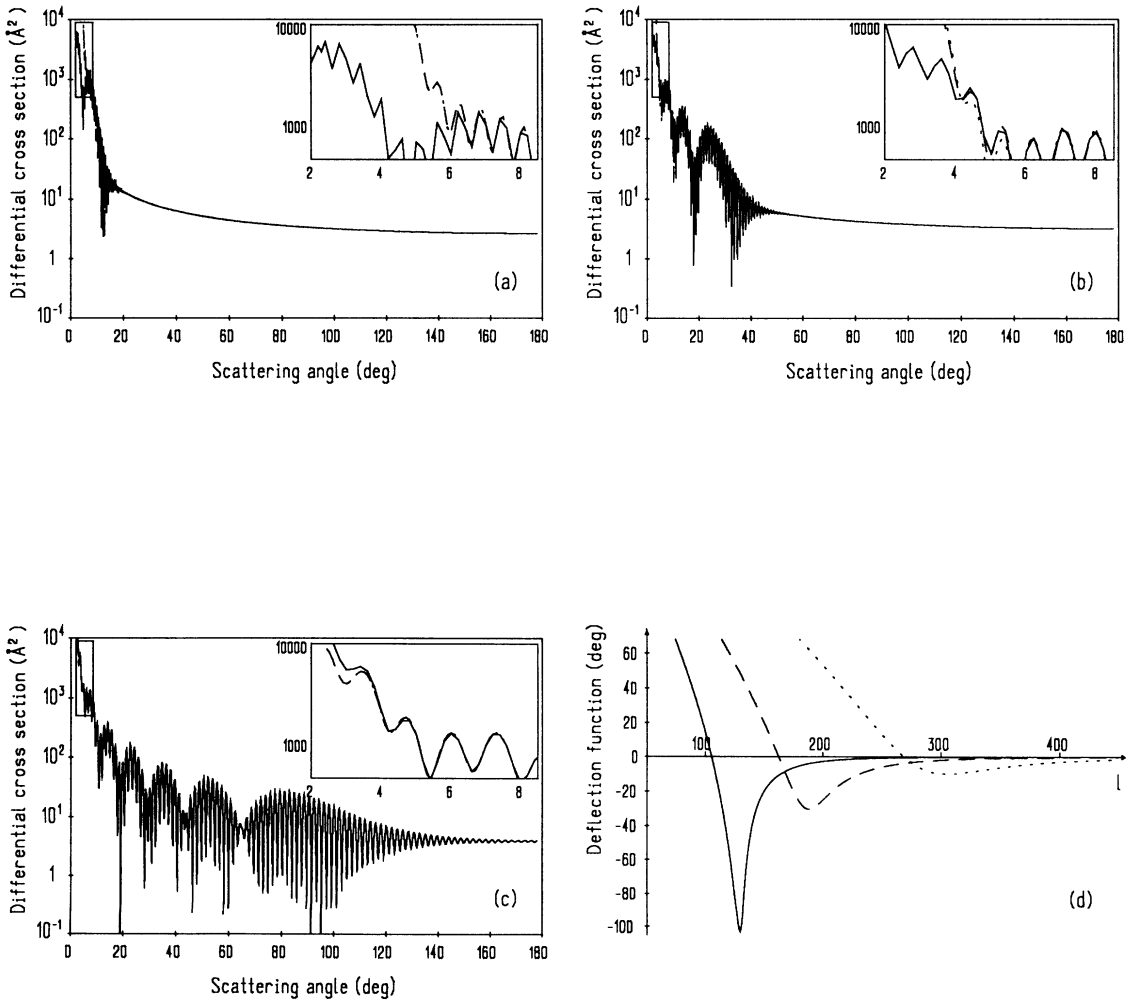

FIG. 2. Same as Fig. 1 but in the K + HBr system represented by the potential (3.4) at energies (a) $E=0.3$, (b) $E=0.1$, and (c) $E=0.035$ eV. Figure 2(d) shows the plot of the deflection functions with dotted curve corresponding to $E=0.3$, broken curve to $E=0.1$, and solid curve to $E=0.035$ eV.

TABLE II. Positions and residues for the potential (3.4) calculated by the first- and fifth-order phase-integral approximation at $E=0.1$ eV corresponding to the parameter values given in [31], $\epsilon=4.0\times10^{-21}/1.60219\times10^{-19}$ eV, σ (denoted by r_m in [31]) $=4.0$ Å, and $\mu=4.377\times10^{-26}/1.66057\times10^{-27}$ u. The truncated numerical entries in l_m and r_m correspond to the first-order calculations while the quantities just below them are of the fifth order.

m	$\mathrm{Re}\,l_m$	$\mathrm{Im}\,l_m$	$\mathrm{Re}\,r_m$	$\mathrm{Im}\,r_m$
0.	186.3363	19.1346	-1.7870×10^{6}	-4.597×10^{5}
	186.332 980 95	19.135 064 03	$-1.792\,365\,662\,1\times10^{6}$	$-4.522\,211\,014\,9\times10^{5}$
1	185.4888	21.8672	1.208×10^{7}	1.5336×10^{7}
	185.485 522 68	21.867 777 87	$1.216\,556\,609\,2\times10^{7}$	$1.530\,134\,678\,3\times10^{7}$
5	182.6329	33.2037	-3.087×10^{8}	-8.1483×10^{8}
	182.630 004 24	33.204 539 28	$-3.124\,059\,008\,0\times10^{8}$	$-8.136\,732\,118\,6\times10^{8}$
10	180.4288	47.9405	-4.19×10^{7}	3.7644×10^{8}
	180.426 191 04	47.941 626 05	$-4.035\,379\,151\,2\times10^{7}$	$3.763\,057\,395\,1\times10^{8}$
15	179.7828	62.7654	-4.985×10^{6}	1.00853×10^{7}
	179.780 518 61	62.766 741 94	$-4.944\,687\,398\,9\times10^{6}$	$1.008\,641\,521\,3\times10^{7}$
20	180.5087	77.2048	5.312×10^{4}	-1.4707×10^{5}
	180.506 706 51	77.206 243 92	$5.264\,090\,508\,9\times10^{4}$	$-1.469\,248\,873\,9\times10^{5}$
24	181.8683	88.2764	-4.37109×10^{3}	-4.304×10^{3}
	181.866 504 75	88.277 872 69	$-4.370\,602\,182\,7\times10^{3}$	$-4.285\,758\,489\,3\times10^{3}$

mediately clear that individual contributions are very large, becoming larger at smaller scattering angles, so that strong cancellations have to be mastered in the correct calculation of the pole sum, which is several orders of magnitude smaller than the individual terms. Considering now that terms in the pole sum corresponding to the first-order phase-integral approximation are accurate to about one percent, one would expect that the inaccuracy of the pole sum would be much longer than the correct value of the pole sum. However, in various test calculations, we find that the trailing decimals, which, in a sense, are not correct, cannot be simply neglected. They obviously play a significant role in the cancellation. In our scattering calculations all the root searching routines and quadratures are computed with a tolerance of 10^{-12}. If this precision is not set, then our calculations of Regge-pole cross sections would start to diverge from the partial-wave results at larger scattering angles.

Table III also shows that the number of terms in the pole sum must be larger the smaller the scattering angle needed in the calculations. To make the pole sum converge to the partial-wave value at $\theta\leq22$ we would have to include more pole contributions.

Similarly, in Table IV we show the first- and fifth-order individual terms and some of their partial sums at $\theta=7$ and 10. Individual terms in the pole sum are large also in this case, but the scattering angles are much smaller here. The Regge calculations cover a larger angular range of the differential cross section because the residues of the K + HBr scattering are smaller than those in our H^+ + Ar scattering.

We shall not attempt to explain, in this paper, how the trailing decimals can be relevant for the description of

TABLE III. Partial sums of the pole amplitude (2.11) for which $f_P^{(m=\infty)}(\theta)=f_P(\theta)$, where m is the highest pole number included in the calculation of the cross sections for the potential given in (3.1) at $\theta=22°$ and 32°. While the truncated numerical entries are calculated with the first-order phase-integral approximations, the quantities just below them are those with the fifth order.

m	$\mathrm{Re}\,f_P^{(m)}(22°)$	$\mathrm{Im}\,f_P^{(m)}(22°)$	$\mathrm{Re}\,f_P^{(m)}(32°)$	$\mathrm{Im}\,f_P^{(m)}(32°)$
0	-5.462×10^{5}	-8.9173×10^{5}	-7.5669×10^{4}	6.695×10^{4}
	$-5.511\,512\,954\,5\times10^{5}$	$-8.908\,192\,393\,3\times10^{5}$	$-7.547\,311\,199\,1\times10^{4}$	$6.743\,302\,270\,8\times10^{4}$
2	1.30×10^{6}	1.0055×10^{7}	6.4040×10^{5}	-3.065×10^{5}
	$1.351\,903\,720\,4\times10^{6}$	$1.006\,368\,459\,5\times10^{7}$	$6.397\,938\,951\,6\times10^{5}$	$-3.099\,947\,262\,1\times10^{5}$
5	2.1187×10^{8}	-4.505×10^{7}	-4.501×10^{6}	-3.343×10^{6}
	$2.118\,021\,326\,0\times10^{8}$	$-4.600\,621\,658\,5\times10^{7}$	$-4.518\,548\,827\,3\times10^{6}$	$-3.323\,596\,049\,0\times10^{6}$
10	7.7978×10^{7}	4.278×10^{7}	-2.944×10^{5}	-2.931×10^{5}
	$7.811\,396\,813\,5\times10^{7}$	$4.245\,953\,998\,0\times10^{7}$	$-2.954\,790\,932\,5\times10^{5}$	$-2.916\,802\,813\,0\times10^{5}$
15	-5.3271×10^{5}	-3.128×10^{5}	4.5757×10^{2}	1.946×10^{2}
	$-5.331\,991\,529\,5\times10^{5}$	$-3.106\,127\,563\,7\times10^{5}$	$4.577\,196\,021\,2\times10^{2}$	$1.926\,940\,924\,3\times10^{2}$
20	-5.64539×10^{2}	-91.9	-2.8429	-0.904
	$-5.646\,072\,715\,4\times10^{2}$	$-89.869\,720\,24$	$-2.840\,859\,447\,3$	$-0.890\,045\,319\,2$
25	2.4	3.24	-2.9216	-0.888
	1.731 735 594 0	3.461 061 482 5	$-2.919\,439\,119\,1$	$-0.873\,092\,570\,4$

TABLE IV. Partial sums of the pole amplitude (2.11) for which $f_P^{(m=\infty)}(\theta)=f_P(\theta)$, where m is the highest pole number included in the calculation of the cross sections for the potential given in (3.4) at $\theta=7°$ and 10°. While the truncated numerical entries are calculated with the first-order phase-integral approximations, the quantities just below them are those with the fifth order.

m	$\mathrm{Re}f_P^{(m)}(7°)$	$\mathrm{Im}f_P^{(m)}(7°)$	$\mathrm{Re}f_P^{(m)}(10°)$	$\mathrm{Im}f_P^{(m)}(10°)$
0	4.633×10^5	1.705×10^5	-1.151×10^5	-9.905×10^4
	$4.649\,120\,322\,3\times10^5$	$1.684\,349\,002\,3\times10^5$	$-1.158\,085\,247\,0\times10^5$	$-9.860\,992\,302\,9\times10^4$
2	-1.833×10^6	-2.7744×10^6	2.251×10^5	8.36605×10^5
	$-1.849\,399\,489\,8\times10^6$	$-2.768\,798\,453\,4\times10^6$	$2.297\,070\,717\,8\times10^5$	$8.365\,036\,282\,5\times10^5$
5	-2.2890×10^7	-8.822×10^6	3.209×10^6	2.165×10^6
	$-2.293\,939\,549\,3\times10^7$	$-8.715\,865\,332\,3\times10^6$	$3.220\,931\,602\,0\times10^6$	$2.149\,540\,113\,0\times10^6$
10	2.1905×10^6	1.933×10^6	-1.350×10^5	-1.486×10^5
	$2.196\,683\,265\,5\times10^6$	$1.922\,094\,629\,3\times10^6$	$-1.354\,986\,961\,5\times10^5$	$-1.478\,931\,484\,0\times10^5$
15	7.075×10^3	1.6576×10^4	-1.907×10^2	-5.0901×10^2
	$7.122\,301\,915\,9\times10^3$	$1.652\,434\,531\,7\times10^4$	$-1.924\,191\,278\,1\times10^2$	$-5.075\,823\,277\,6\times10^2$
20	-37.1	-42.0	-6.642	9.255
	$-35.966\,676\,71$	$-41.433\,364\,27$	$-6.790\,767\,924\,8$	$9.122\,996\,002\,0$
25	-25	6.43	-6.760	8.567
	$-23.482\,964\,58$	$6.857\,898\,076\,2$	$-6.910\,203\,900\,9$	$8.436\,920\,056\,2$

the overall rainbow scattering phenomenon. The explanation, as we see it, must be closely related to the analytic form of the underlying S-matrix formula, which is similar in different orders of approximation.

V. CONCLUSION

The pole positions and associated residues, calculated in the first and fifth orders of the phase-integral technique, have been used to compute the scattering cross sections for two, atomic and molecular, scattering systems. As shown in Ref. [13] the new phase-integral formula (for Regge-pole residues) which allows the relevant transition zeros of the base function to lie arbitrarily close to each other, while other zeros or poles are assumed to be sufficiently far away from this cluster, makes a dramatic improvement in the calculation of the cross sections.

The calculations in Ref. [13] were based on the first-order phase-integral approximations. From the present investigation we conclude that with higher-order phase-integral approximations, no further rainbow oscillations are revealed. On the other hand, one can expect that the higher-order phase-integral calculations of Regge-pole positions and residues do provide *numerically* more accurate values for the differential cross section than the first-order ones for scattering angles where they converge to the partial-wave result, but the improvement is not large enough to show up in the plots.

We would like to emphasize that if the first-order calculations based on the Fröman-Fröman formulas are to be carried out, sufficiently accurate evaluation of the poles and residues is important. The trailing terms in the positions and residues, which would seem to be unreliable, are also important and prove to contain (inherently) some physical information.

A consequence of our subtle result on "trailing figures" is the following: Let us say that we have a numerical method that is reliable and we choose a tolerance corresponding to six significant figures in the residues. These residues are far better than the first-order phase-integral residues even if the first-order residues are calculated in double precision and are very accurate first-order results.

Now we like to compare the corresponding differential cross sections and discover, to our surprise, that the first-order phase-integral cross section reveals much more of rainbow oscillations than the one with quantum numerical residues. Before the quantum numerical cross section diverges (i.e., before the scattering angle becomes too small) it is more accurate than the first-order phase-integral cross section (although one cannot see it in the graph), but when it finally diverges the pole sum cancellations require numerical figures beyond the first six positions. These trailing figures are random in the numerical quantum residues (that is the reason for the "divergence") but they are not random in the first-order phase-integral residues.

We conclude that the trailing figures in the first-order phase integral residues are important for the success of the corresponding differential cross section. Somehow the trailing figures in the terms of the pole sum are "synchronized" in such a way that cancellations are successful.

Finally, we would also like to hint that, with the inclusion of more terms in the pole sum, together with a suitable increase in the precision of the calculations, one could get better accuracy towards small scattering angles, if the correct residue formula is used.

ACKNOWLEDGMENTS

The authors are grateful to Professor N. Fröman and Professor P.O. Fröman for helpful discussions. One of the present authors (A.A.) would also like to acknowledge the financial support from the United Nations Development Program (UNDP) and the Commission for Higher Education of Ethiopia.

[1] E. A. Remler, Phys. Rev. A **3**, 1949 (1971).
[2] L. D. Doverspike, R. L. Champion, S. M. Bobbio, and W. G. Rich, Phys. Rev. Lett. **25**, 909 (1970).
[3] S. M. Bobbio, W. G. Rich, L. D. Doverspike, and R. L. Champion, Phys. Rev. A **4**, 957 (1971).
[4] W. G. Rich, S. M. Bobbio, R. L. Champion, and L. D. Doverspike, Phys. Rev. A **4**, 2253 (197).
[5] K.-E. Thylwe, in *Resonances—The Unifying Route Towards the Formulation of Dynamical Processes—Foundations and Applications in Nuclear, Atomic and Molecular Physics,* edited by E. Brändas and N. Elander (Springer, Berlin, 1989), p. 281.
[6] J. N. L. Connor, *New Theoretical Methods for Molecular Collisions: The Complex Angular Momentum Approach* [J. Chem. Soc. Faraday Trans. **86**, 1627 (1990)].
[7] C. V. Sukumar, S. L. Lin, and J. N. Bardsley, J. Phys. B **8**, 577 (1975).
[8] J. N. L. Connor and W. Jakubetz, Mol. Phys. **33**, 1619 (1977).
[9] J. N. L. Connor and W. Jakubetz, Mol. Phys. **35**, 949 (1978).
[10] S. Bosanac, Mol. Phys. **35**, 1057 (1978).
[11] P. Pajunen, J. Chem. Phys. **88**, 4268 (1988).
[12] N. Fröman and P. O. Fröman, Phys. Rev. A **43**, 3563 (1991).
[13] K.-E. Thylwe and A. Amaha, Phys. Rev. A **43**, 3567 (1991).
[14] A. Amaha and K.-E. Thylwe, Phys. Rev. A **44**, 4203 (1991).
[15] K.-E. Thylwe and J. N. L. Connor, J. Phys. A **18**, 2957 (1985).
[16] M. S. Child, *Molecular Collision Theory* (Academic, New York, 1974).
[17] N. Fröman and P. O. Fröman, *Phase-Integral Approximation of Arbitrary Order Generated From an Unspecified Base Function,* review article in Forty More Years of Ramifications: Spectral Asymptotics and Its Applications, edited by S. A. Fulling and F. J. Narcowich, Discourses in Mathematics and its Applications, No. 1 (Texas A & M University, Department of Mathematics, College Station, Texas, 1991).
[18] K.-E. Thylwe and N. Fröman, Ann. Phys. **150**, 413 (1983).
[19] K.-E. Thylwe, J. Phys. A **16**, 3325 (1983).
[20] T. Regge, Nuovo Cimento **14**, 951 (1959).
[21] A. Bottino, A. M. Longoni, and T. Regge, Nuovo Cimento **23**, 954 (1962).
[22] V. de Alfaro and T. Regge, *Potential Scattering* (North-Holland, Amsterdam, 1965).
[23] A. Sommerfeld, *Partial Differential Equations in Physics* (Academic, New York, 1949).
[24] J. N. L. Connor, in *Semiclassical Methods in Molecular Scattering and Spectroscopy,* Vol. 53 of *NATO Advanced Study Institute, Series B: Physics,* edited by M. S. Child (Reidel, Dordrecht, 1980), Chap. 2.
[25] J. N. L. Connor and D. C. Mackay., Chem. Phys. Lett. **59**, 163 (1978).
[26] R. Anni, L. Renna, and L. Taffara, Nuovo Cimento **55**, 456 (1980).
[27] J. N. L. Connor and D. C. Mackay, Mol. Phys. **37**, 1703 (1979).
[28] J. P. Toennies, *Semiclassical Descriptions of Atomic and Nuclear Collisions,* Proceedings of the Niels Bohr Centennial Conference, Copenhagen, edited by J. Bang and J. de Boer (North-Holland, Amsterdam, 1985).
[29] B. C. Eu, J. Chem. Phys. **52**, 3021 (1970).
[30] J. N. L. Connor, D. C. Mackay, and K.-E. Thylwe, J. Chem. Phys. **85**, 6368 (1986).
[31] J. N. L. Connor, W. Jakubetz, and C. V. Sukumar, J. Phys. B **9**, 1783 (1976).