Improved semiclassical Regge-pole description of rainbow scattering

Karl-Erik Thylwe* and Abraham Amaha[†]

Department of Theoretical Physics, University of Uppsala, Thunbergsvägen 3, S-752 38 Uppsala, Sweden
(Received 30 July 1990)

A phase-integral formula for calculating Regge-pole residues, which has recently been derived by Fröman and Fröman [preceding paper, Phys. Rev. A **43**, 3563 (1991)], promises to be a powerful tool in the complex angular-momentum description of scattering. The present authors demonstrate the power, simplicity, and usefulness of that formula already in the first-order approximation. Application to proton-neon elastic scattering reveals that the new residue formula considerably improves the existing semiclassical Regge-pole description of the prominent rainbow oscillations in the differential cross section.

The well-known two-turning-point Wentzel-Kramers-Brillouin (WKB) formulas for Regge-pole positions and residues, which have been widely applied in theoretical studies of atomic and molecular collisions (see Refs. 1, 2, and references therein), date back more than 20 years to the papers by Brander[3] and by Dombey and Jones.[4] The latter authors successfully applied the WKB theory in the study of the asymptotic distribution of Regge poles in the complex angular-momentum plane for pure inverse-power potentials. Like Brander,[3] who used an asymptotic theory due to Olver,[5] Dombey and Jones[4] correctly showed that infinitely many Regge poles extend out to infinity along almost vertical strings in the first and third quadrants of the complex angular-momentum plane. The WKB formulas give correct approximate results for Regge-pole positions and residues in the large quantum number limit.

A decade ago, one of the present authors[6] showed that the error in the Bohr-Sommerfeld-type quantization condition for the Regge-pole *positions* vanishes in the large-wave-number limit for any quantum number of the Regge pole, i.e., even for low quantum numbers. It was not possible to show that the error in the formula for the Regge-pole *residues* vanishes in the large-wave-number limit; a discussion is given in Ref. 7. In the context of elastic atom-atom and atom-molecule scattering extensive numerical data[8-10] on the results of exact and WKB calculations clearly show that WKB residues have systematically a relative error of as much as 7–8 % for the leading pole, i.e., the pole with quantum number zero. The error gradually decreases as the quantum number becomes larger. In contrast to this, the WKB pole positions are in general very accurate.

It is highly desirable that accurate formulas for the properties of the Regge poles be available. The leading Regge pole, for example, plays a dominant role in the detailed interpretation of elastic and inelastic Fraunhofer diffraction in atomic and molecular collisions.[2,11-13] A new arbitrary-order phase-integral residue formula derived by Fröman and Fröman[14] and numerically applied

by Amaha and Thylwe[15] has proved to be extremely accurate. It differs from the previously derived arbitrary-order phase-integral residue formula[16] by a factor, which corrects for a possible proximity of the two relevant turning points. The analysis of Fröman and Fröman is uniformly valid with respect to the positions of the two relevant complex turning points, whereas this is not the case with the analysis in Ref. 16.

The purpose of the present paper is to demonstrate the power, simplicity, and usefulness of the residue formula already in the first-order approximation. The Bohr-Sommerfeld quantization condition for the Regge pole l_m is still valid in the uniform Fröman-Fröman[14] theory, i.e., we have

$$\bar{\gamma} = (m + \tfrac{1}{2}), \quad m = 0,1,2,\ldots, \tag{1}$$

where

$$\bar{\gamma} = \frac{1}{\pi} \int_{t_1}^{t_2} [k^2 - U(r) - (l + \tfrac{1}{2})^2 / r^2]^{1/2} dr . \tag{2}$$

In (2), t_1 and t_2 are the two relevant complex turning points, k is the wave number, and $U(r) = 2\mu V(r)/\hbar^2$, where $V(r)$ is the physical interaction potential. For the corresponding Regge-pole residues the phase-integral formula reads, in the first-order approximation,

$$r_m = f(m + \tfrac{1}{2}) \left[2\pi i \left[\frac{\partial \bar{\gamma}}{\partial l} \right]_{l = l_m} \right]^{-1} \exp(2i\eta_{l_m}) \tag{3}$$

with

$$f(m + \tfrac{1}{2}) = \frac{(2\pi)^{1/2}}{m!} \left[\frac{m + \tfrac{1}{2}}{e} \right]^{m + 1/2} , \tag{4}$$

η_{l_m} being the usual complex asymptotic WKB phase with respect to the outer turning point t_2; see Ref. 1 for details.

Equation (3) is recognized as the familiar residue formula multiplied by $f(m + \tfrac{1}{2})$, a function only of the

TABLE I. Numerical values of the first-order correction factor $f(m + \frac{1}{2})$ for $m = 0, 1, \ldots, 15$.

m	$f(m + \frac{1}{2})$
0	1.075 048
1	1.027 508
2	1.016 655
3	1.011 920
4	1.009 276
5	1.007 590
6	1.006 422
7	1.005 565
8	1.004 910
9	1.004 393
10	1.003 974
11	1.003 628
12	1.003 338
13	1.003 090
14	1.002 877
15	1.002 691

proton-neon ($\mu = 0.952$ atomic mass units) elastic scattering at 2.5-eV center-of-mass energy studied experimentally by Konrad.[18] A Lennard-Jones (8,4) potential was taken to approximate the ion-atom interaction with well depth $\epsilon = 2.28$ eV at an internuclear distance of $r_{min} = 0.996$ Å. Table II reports the positions and residues of the 16 Regge poles used in the calculation. Apart from the fact that we use the new first-order phase-integral residue formula instead of the old one, our calculation of the differential cross section follows the usual semiclassical procedure.[1,2,13] The exact Regge representation of the scattering amplitude is thus written in terms of two subamplitudes, viz., the *background integral* and the *residue series*. The background integral is evaluated by the saddle-point method, and at the end one replaces the exact phase shift by its first-order phase-integral approximation and a Legendre function by its leading asymptotic expression. In the residue series one inserts

Regge-pole quantum number m and not depending on any details of the physical potential. For the leading Regge-pole residue, i.e., for $m = 0$, we have $f(\frac{1}{2}) = (\pi/e)^{1/2} \approx 1.075$, which accounts for the previously observed relative error of 7–8 %. We also see that the error in the semiclassical residue is essentially associated with its absolute value but not with its argument. This fact has not been pointed out before in the literature. The uniform residue formula explains the universal character of the error caused by the proximity of the two relevant turning points.

The residue formula is as simple to use for computations as the old semiclassical formula. In fact, the only difference is the correction factor $f(m + \frac{1}{2})$, which for the first-order approximation can be calculated for any quantum number m by a pocket calculator, once and for all, and is given in Table I for $m = 0, 1, \ldots 15$. A comparison of results obtained by means of the uniform arbitrary-order residue formula[14] and previously published numerical and nonuniform phase-integral results are planned to be presented by Amaha and Thylwe.[15] The first-order uniform results are found to agree within an error of about 1% with the best available numerical results.

In recent applications the Regge-pole theory has successfully described various interference phenomena occurring in elastic differential cross sections. However, with the approximations used until now, the theory has failed to reproduce the angular distribution on the bright side of atomic and molecular scattering rainbows.[1] Severe numerical difficulties are involved in summing up the terms in the residue series.[17] Typically, several Regge-pole residues of widely varying magnitudes give significant contributions, and delicate cancellations are present. With the Fröman-Fröman residue formula the situation has improved considerably.

Using the residue formula in first-order approximation to calculate the differential cross section, we consider the
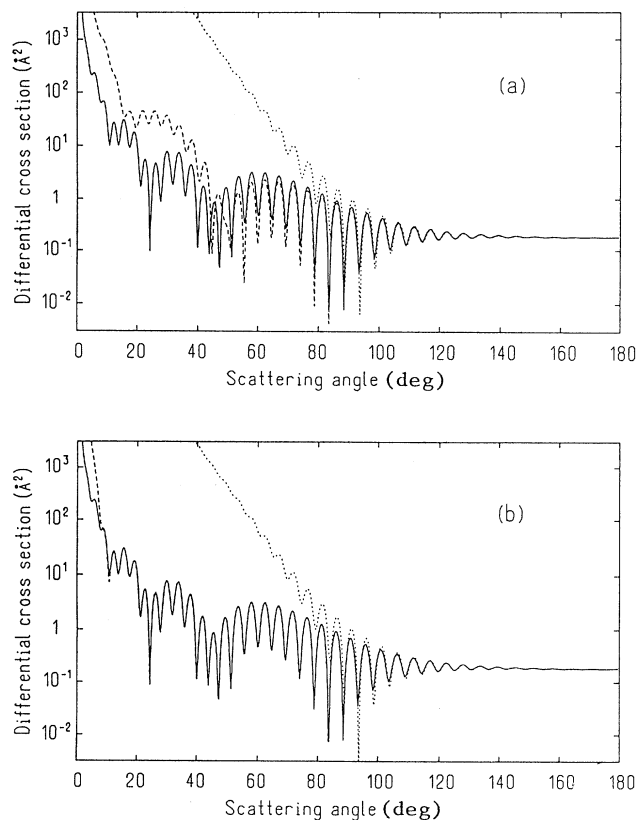

FIG. 1. Differential cross section for proton-neon elastic scattering at 2.5-eV center-of-mass energy. The solid lines in (a) and (b) represent the same accurate partial wave calculations. The dashed lines represent semiclassical and improved semiclassical Regge-pole calculations in (a) and (b), respectively, with 16 poles considered in the residue sum. The dotted lines illustrate semiclassical and improved semiclassical calculations in (a) and (b), respectively, with only the leading pole, i.e., $m = 0$, considered in the residue sum.

TABLE II. For the proton-neon elastic scattering at 2.5 eV, first-order Regge-pole positions are calculated from the Bohr-Sommerfeld quantization condition (1), and first-order residues are calculated from the nonuniform formula obtained from (3) when $f(m + \frac{1}{2})$ is replaced by unity, and from the uniform formula (3) with (4). The digits within parentheses indicate powers of 10.

	Position		Residue (nonuniform)		Residue (uniform)	
m	$\mathrm{Re}l_m$	$\mathrm{Im}l_m$	$\mathrm{Re}r_m$	$\mathrm{Im}r_m$	$\mathrm{Re}r_m$	$\mathrm{Im}r_m$
0	50.6796	4.8528	−6.1858(2)	−2.0511(3)	−6.6500(2)	−2.2050(3)
1	49.8625	6.6555	−9.2766(3)	2.0598(4)	−9.5317(3)	2.1165(4)
2	49.0942	8.5509	8.7491(4)	−3.6246(4)	8.8949(4)	−3.6850(4)
3	48.3915	10.5288	−1.9584(5)	−9.5718(4)	−1.9818(5)	−9.6859(4)
4	47.7678	12.5760	4.0998(4)	3.1494(5)	4.1378(4)	3.1786(5)
5	47.2332	14.6773	2.7732(5)	−1.6504(5)	2.7942(5)	−1.6629(5)
6	46.7937	16.8161	−1.6727(5)	−1.8258(5)	−1.6835(5)	−1.8375(5)
7	46.4514	18.9761	−1.1460(5)	1.0263(5)	−1.1524(5)	1.0320(5)
8	46.2045	21.1413	3.9484(4)	7.2172(4)	3.9678(4)	7.2526(4)
9	46.0485	23.2982	3.9837(4)	−2.3926(3)	4.0012(4)	−2.4031(3)
10	45.9764	25.4350	1.0001(4)	−1.5371(4)	1.0041(4)	−1.5433(4)
11	45.9801	27.5429	−1.4808(3)	−8.1246(3)	−1.4862(3)	−8.1541(3)
12	46.0507	29.6153	−2.6348(3)	−2.6534(3)	−2.6436(3)	−2.6623(3)
13	46.1795	31.6478	−1.6451(3)	−5.4716(2)	−1.6502(3)	−5.4885(2)
14	46.3582	33.6380	−8.3267(2)	2.8087(1)	−8.3507(2)	2.8168(1)
15	46.5792	35.5846	−4.0007(2)	1.2132(2)	−4.0115(2)	1.2165(2)

the first-order phase-integral pole positions and the nonuniform [to obtain Fig. 1(a)] and uniform [to obtain Fig. 1(b)] residues, respectively, and replaces a Legendre function by its leading asymptotic expression.

In Fig. 1 we compare the proton-neon scattering differential cross section, obtained by accurate partial wave calculations, with (a) semiclassical and (b) improved semiclassical Regge-pole results. The improved semiclassical results with 16 poles included are in very good agreement with the partial wave calculations at scattering angles $\theta > 10°$ and reproduce the supernumerary rainbows very well. However, the corresponding semiclassical calculations are of the same accuracy only for $\theta > 80°$, and therefore not even the primary rainbow is accurately de-

scribed.

In calculating differential cross sections, we have demonstrated the significance of the uniform residue formula already in the first-order approximation. The Regge-pole treatment has thus obviously been much improved with very little extra computational efforts.

*Present address: Department of Mechanics, Royal Institute of Technology, S-100 44 Stockholm, Sweden.

†Permanent address: Department of Physics, Asmara University, Box 1220, Asmara, Ethiopia.

[1]J. N. L. Connor, in Semiclassical Methods in Molecular Scattering and Spectroscopy, Vol. 53 of Proceedings of NATO Advanced Study Institute, Cambridge, 1979, Series C, edited by M. S. Child (Reidel, Dordrecht, 1980), Chap. 2.

[2]K. -E. Thylwe and J. N. L. Connor, J. Chem. Phys. 91, 1668 (1989).

[3]O. Brander, Ark. Fys. 32, 131 (1966).

[4]N. Dombey and R. H. Jones, J. Math. Phys. 9, 986 (1968).

[5]F. W. J. Olver, Asymptotics and Special Functions (Academic, New York, 1974).

[6]K. -E. Thylwe, Ph.D. thesis, University of Uppsala, Sweden, 1981.

[7]K. -E. Thylwe, J. Phys. A 18, 3445 (1985).

[8]J. N. L. Connor, W. Jakubetz, and C. V. Sukumar, J. Phys. B 9, 1783 (1976).

[9]J. N. L. Connor, D. C. Mackay, and C. V. Sukumar, J. Phys. B 12, L515 (1979).

[10]C. V. Sukumar, S. L. Lin, and J. N. Bardsley, J. Phys. B 8, 577 (1975).

[11]J. N. L. Connor, D. Farrelly, and D. C. Mackay, J. Chem. Phys. 74, 3278 (1981).

[12]K. -E. Thylwe and J. N. L. Connor, J. Phys. B 21, L597 (1988).

[13]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 Brändas and N. Elander (Springer, Berlin, 1989), p. 281.

[14]N. Fröman and P. O. Fröman, preceding paper, Phys. Rev. A 43, 3563 (1991).

[15]A. Amaha and K. -E. Thylwe (unpublished).

[16]K. -E. Thylwe, J. Phys. A 16, 3325 (1983).

[17]J. N. L. Connor and W. Jakubetz, Mol. Phys. 35, 949 (1978).

[18]M. Konrad, Ph.D. thesis, University of Kaiserslautern, Federal Republic of Germany, 1983.