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Regge-pole positions and residues calculated from phase-integral formulas

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Regge-pole positions and residues associated with real and complex optical potentials of the Lennard-Jones type are calculated by phase-integral formulas. Two relevant transition zeros are taken into account; they may lie at an arbitrary distance from each other, while the origin and the other transition points are assumed to lie far away from the two relevant transition zeros. The calculations are performed up to the 13th order of the phase-integral approximation. The results obtained are much more accurate than results published earlier.

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I. INTRODUCTION

The purpose of this paper is to calculate Regge-pole positions and associated residues by means of phase-integral formulas, which are derived by Fröman and Fröman [1] in a recent paper. The results in that paper have already been used by the present authors [2] for accurate calculation in the first-order approximation of the differential scattering cross section.

The Regge-pole theory, in which the positions and the residues of the Regge poles are key quantities, provides a powerful reformulation of atomic and molecular potential scattering theory. Differential cross sections can be described in terms of a small number of interfering, physically significant amplitudes, whereas the series of partial-wave amplitudes is slowly convergent and tedious in application. Recent research has led to an improved analysis of large-angle oscillatory structures in the differential cross sections of chemically reactive systems modeled by complex optical potentials [3–5]. Regge-pole theory has recently also dealt with the description of orbiting [6–11] and rainbow scattering [12], as well as diffraction scattering in elastic [13] and rotationally inelastic [14–16] collisions. See also a review by Connor [17] on earlier applications of Regge-pole theory.

In using the phase-integral method for calculating Regge-pole positions and corresponding residues, when there are two relevant transition zeros t_1 and t_2, one has so far assumed that they lie sufficiently far away from each other and from the origin and other transition points [18, 19]; see Fig. 1. The case where t_1 and t_2 may lie at an arbitrary distance from each other (i.e., even close together), which is highly relevant for elastic diffraction and rainbow scattering of atoms and molecules, has been treated for the first time in the paper by Fröman and Fröman [1]. It is shown in that paper that, when t_1 and t_2 approach each other, the earlier known formula for Regge-pole positions [17, 18] remains valid, while one needs a new formula, given in Ref. [1], for the corresponding residues; the latter formula goes over into the earlier known residue formula when the distance between t_1 and t_2 is sufficiently large. The phase-integral formulas now mentioned will be used in the present paper, and it will be seen that the use of the new residue formula makes it possible to attain a much higher accuracy than that attained earlier.

In Sec. II the basic formulas for the case of two relevant transition zeros are reviewed, and expressions up to the 13th order of approximation are obtained for the quantities $D^{(2n+1)}$ appearing in these formulas. Applications to particular real and complex potentials and comparison of the results with those obtained earlier by numerical calculations are given in Sec. III.

II. PHASE-INTEGRAL FORMULAS FOR REGGE-POLE POSITIONS AND RESIDUES FOR THE CASE OF A WELL ISOLATED CLUSTER OF TWO RELEVANT TRANSITION ZEROS

According to Ref. [1] the Regge-pole positions ℓ_m and residues r_m can be calculated from the $(2N+1)$th-order phase-integral formulas

$$\bar{\gamma} = m + \tfrac{1}{2}, \quad \ell = \ell_m \tag{2.1}$$

where m is any non-negative integer and

$$r_m = \left(\frac{f(\bar{\gamma}_0, \ldots, \bar{\gamma}_{2N}) \exp\left(2i \lim_{r\to+\infty} \left[w(r) - kr + (\ell + \tfrac{1}{2})\tfrac{\pi}{2}\right]\right)}{2\pi i \, \partial\bar{\gamma}/\partial\ell} \right)_{\ell=\ell_m} . \tag{2.2}$$

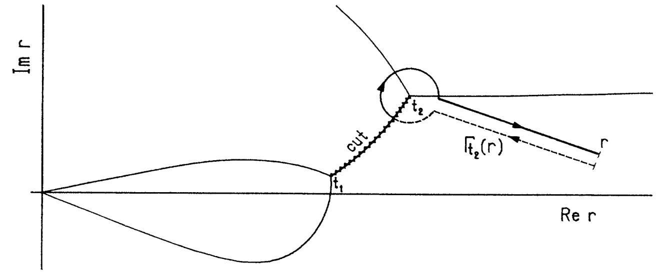

FIG. 1. The relevant transition zeros t_1 and t_2 and the integration contour $\Gamma_{t_2}(r)$ in (2.3). Note that although the contour $\Gamma_{t_2}(r)$ is drawn here in a different way than in Ref. [1], it gives the same value of the integral in (2.3). Solid thin curves indicate anti-Stokes lines associated with the transition zeros. The wavy line joining t_1 and t_2 indicates a cut in the complex r plane. The figure is drawn for the particular situation when the zeros t_1 and t_2 can be joined by an anti-Stokes line (coinciding with the cut joining t_1 and t_2). The phase of the base function $Q(r)$ is chosen such that $Q(r)/|Q(r)| \to 1$ as $r \to \infty$ along the real r axis.

The quantities in these formulas are obtained as we shall now describe. The function $w(r)$ is defined by

$$w(r) = \frac{1}{2} \int_{\Gamma_{t_2}(r)} q(r)dr \,, \tag{2.3}$$

where the contour of integration $\Gamma_{t_2}(r)$, as shown in Fig. 1, starts from the point corresponding to r but lying on an adjacent Riemann sheet, encircles the transition zero t_2, and ends at the point r in the complex r plane under consideration. The function $q(r)$ in (2.3) is given by

$$q(r) = Q(r) \sum_{n=0}^{N} Y_{2n} \,, \tag{2.4}$$

Y_{2n} being the quantities appearing in the theory of the arbitrary-order phase-integral approximation generated from an unspecified base function $Q(r)$, the phase of which is chosen as explained in the caption to Fig. 1. The quantity $\bar{\gamma}$ is defined by

$$\bar{\gamma} = \sum_{n=0}^{N} \bar{\gamma}_{2n} \tag{2.5}$$

with

$$\bar{\gamma}_{2n} = \frac{1}{2\pi} \int Y_{2n} Q(r) dr \,, \tag{2.6}$$

where the path of integration is a contour encircling in the positive sense the two transition zeros t_1 and t_2 but no other transition point. Note that the quantity γ used by previous authors [17, 18] is related to $\bar{\gamma}$ according to the formula $\gamma = \pi\bar{\gamma}$.

For the function $f(\bar{\gamma}_0, \ldots, \bar{\gamma}_{2N})$ in (2.2) we have the formula

$$f(\bar{\gamma}_0, \ldots, \bar{\gamma}_{2N}) = \frac{(2\pi)^{1/2}}{\Gamma\left(\frac{1}{2} + \bar{\gamma}\right)} \exp\left(\bar{\gamma} \ln \bar{\gamma}_0 + \sum_{n=0}^{N} D^{(2n+1)} \right) , \tag{2.7}$$

$D^{(2n+1)}$ being the coefficients in the formal expansion

$$\begin{aligned} \ln \Gamma\left(\tfrac{1}{2} + \bar{\gamma}\right) = {} & \ln (2\pi)^{1/2} \\ & + \left(\frac{\bar{\gamma}_0}{\lambda} + \bar{\gamma}_2 \lambda + \bar{\gamma}_4 \lambda^3 + \cdots \right) \ln \frac{\bar{\gamma}_0}{\lambda} \\ & + D^{(1)} \lambda^{-1} + D^{(3)} \lambda + D^{(5)} \lambda^3 + \cdots , \end{aligned} \tag{2.8}$$

where now

$$\bar{\gamma} = \frac{1}{\lambda} \left(\bar{\gamma}_0 + \bar{\gamma}_2 \lambda^2 + \bar{\gamma}_4 \lambda^4 + \cdots \right) \tag{2.9}$$

and λ is a formal expansion parameter. From (2.8) and (2.9) one can thus calculate $D^{(2n+1)}$, $n = 0, 1, 2, \ldots$. In Ref. [1] only the first three of these quantities were given, and therefore we have written a symbolic computer program for obtaining further expressions for these quantities. Collecting the expressions so far obtained, we have

$$D^{(1)} = -\bar{\gamma}_0, \tag{2.10a}$$

$$D^{(3)} = -\frac{1}{24\bar{\gamma}_0}, \tag{2.10b}$$

$$D^{(5)} = \frac{\bar{\gamma}_2^2}{2\bar{\gamma}_0} + \frac{\bar{\gamma}_2}{24\bar{\gamma}_0^2} + \frac{7}{2880\bar{\gamma}_0^3}, \tag{2.10c}$$

$$D^{(7)} = \frac{\bar{\gamma}_2\bar{\gamma}_4}{\bar{\gamma}_0} - \frac{1}{24\bar{\gamma}_0^2}(4\bar{\gamma}_2^3 - \bar{\gamma}_4) - \frac{\bar{\gamma}_2^2}{24\bar{\gamma}_0^3} - \frac{7\bar{\gamma}_2}{960\bar{\gamma}_0^4} - \frac{31}{40320\bar{\gamma}_0^5}, \tag{2.10d}$$

$$\begin{aligned} D^{(9)} = {} & \frac{1}{2\bar{\gamma}_0}(2\bar{\gamma}_2\bar{\gamma}_6 + \bar{\gamma}_4^2) - \frac{1}{24\bar{\gamma}_0^2}(12\bar{\gamma}_2^2\bar{\gamma}_4 - \bar{\gamma}_6) + \frac{1}{12\bar{\gamma}_0^3}(\bar{\gamma}_2^4 - \bar{\gamma}_2\bar{\gamma}_4) + \frac{1}{960\bar{\gamma}_0^4}(40\bar{\gamma}_2^3 - 7\bar{\gamma}_4) \\ & + \frac{7\bar{\gamma}_2^2}{480\bar{\gamma}_0^5} + \frac{31\bar{\gamma}_2}{8064\bar{\gamma}_0^6} + \frac{127}{215040\bar{\gamma}_0^7}, \end{aligned} \tag{2.10e}$$

$$
\begin{aligned}
D^{(11)} = {} & \frac{1}{\bar\gamma_0}(\bar\gamma_2\bar\gamma_8+\bar\gamma_4\bar\gamma_6)-\frac{1}{24\bar\gamma_0^2}(12\bar\gamma_2^2\bar\gamma_6+12\bar\gamma_2\bar\gamma_4^2-\bar\gamma_8)+\frac{1}{24\bar\gamma_0^3}(8\bar\gamma_2^3\bar\gamma_4-2\bar\gamma_2\bar\gamma_6-\bar\gamma_4^2)\\
& -\frac{1}{960\bar\gamma_0^4}(48\bar\gamma_2^5-120\bar\gamma_2^2\bar\gamma_4+7\bar\gamma_6)-\frac{1}{240\bar\gamma_0^5}(10\bar\gamma_2^4-7\bar\gamma_2\bar\gamma_4)-\frac{1}{8064\bar\gamma_0^6}(196\bar\gamma_2^3-31\bar\gamma_4)\\
& -\frac{31\bar\gamma_2^2}{2688\bar\gamma_0^7}-\frac{127\bar\gamma_2}{30720\bar\gamma_0^8}-\frac{511}{608256\bar\gamma_0^9},
\end{aligned}
\tag{2.10f}
$$

$$
\begin{aligned}
D^{(13)} = {} & \frac{1}{2\bar\gamma_0}(2\bar\gamma_2\bar\gamma_{10}+2\bar\gamma_4\bar\gamma_8+\bar\gamma_6^2)-\frac{1}{24\bar\gamma_0^2}(12\bar\gamma_2^2\bar\gamma_8+24\bar\gamma_2\bar\gamma_4\bar\gamma_6+4\bar\gamma_4^3-\bar\gamma_{10})\\
& +\frac{1}{12\bar\gamma_0^3}(4\bar\gamma_2^3\bar\gamma_6+6\bar\gamma_2^2\bar\gamma_4^2-\bar\gamma_2\bar\gamma_8-\bar\gamma_4\bar\gamma_6)-\frac{1}{960\bar\gamma_0^4}(240\bar\gamma_2^4\bar\gamma_4-120\bar\gamma_2^2\bar\gamma_6-120\bar\gamma_2\bar\gamma_4^2+7\bar\gamma_8)\\
& +\frac{1}{480\bar\gamma_0^5}(16\bar\gamma_2^6-80\bar\gamma_2^3\bar\gamma_4+14\bar\gamma_2\bar\gamma_6+7\bar\gamma_4^2)+\frac{1}{8064\bar\gamma_0^6}(336\bar\gamma_2^5-588\bar\gamma_2^2\bar\gamma_4+31\bar\gamma_6)\\
& +\frac{1}{1344\bar\gamma_0^7}(49\bar\gamma_2^4-31\bar\gamma_2\bar\gamma_4)+\frac{1}{92160\bar\gamma_0^8}(2840\bar\gamma_2^3-381\bar\gamma_4)+\frac{127\bar\gamma_2^2}{7680\bar\gamma_0^9}+\frac{511\bar\gamma_2}{67584\bar\gamma_0^{10}}+\frac{1414477}{738017280\bar\gamma_0^{11}}.
\end{aligned}
\tag{2.10g}
$$

For the first-order approximation we have $2N+1=1$ and $\bar\gamma=\bar\gamma_0$, and the function given by (2.7) and (2.10a) is

$$
f(\bar\gamma_0)=\frac{(2\pi)^{1/2}\exp[\bar\gamma_0\,(\ln\bar\gamma_0-1)]}{\Gamma(\frac{1}{2}+\bar\gamma_0)}. \tag{2.11}
$$

Figure 2 shows a graphical representation of this function when $\bar\gamma_0$ is real and positive.

When the two relevant transition zeros t_1 and t_2 lie far away from each other, $f(\bar\gamma_0,\ldots,\bar\gamma_{2N})$ is approximately equal to unity for $\ell=\ell_m$, and we obtain from (2.2) the less accurate formula

$$
r_m=\left(\frac{\exp\left(2i\lim\limits_{r\to+\infty}\left[w(r)-kr+(\ell+\frac{1}{2})\frac{\pi}{2}\right]\right)}{2\pi i\,\partial\bar\gamma/\partial\ell}\right)_{\ell=\ell_m}, \tag{2.12}
$$

which has earlier been given by Thylwe [18].

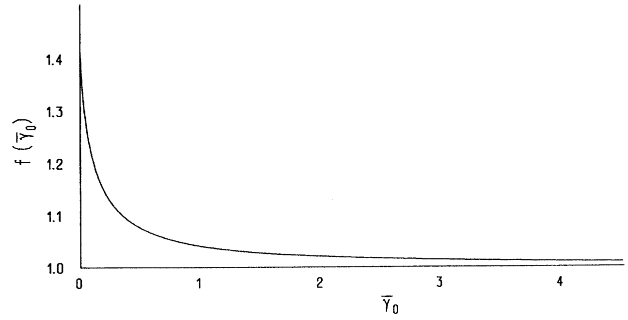

FIG. 2. Graphical representation of the function $\bar\gamma_0$ defined by (2.11).

III. APPLICATIONS TO PARTICULAR POTENTIALS

This section reports results of the arbitrary-order phase-integral calculation of Regge-pole positions and residues. We emphasize that the analysis of Fröman and Fröman [1] and the analysis of Thylwe [18] resulted in the same formula (2.1) for the pole positions. However, the corresponding formulas for the residues, i.e., (2.2) and (2.12), are different; we shall label them "uniform" and "nonuniform," respectively.

In our study we have chosen a complex perturbed Lennard-Jones (12,6) potential

$$
V(r)=4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right]-iW\left(\frac{\sigma}{r}\right)^{S} \tag{3.1a}
$$

and a real Lennard-Jones (6,4) potential

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

since results for these potentials have been published previously [3,20–22].

As in Ref. [4] the radial Schrödinger equation is transformed by the introduction of the dimensionless parameters

$$
A=k\sigma\,,\quad K=E/\epsilon\,,\quad C=2\mu W\sigma^2/\hbar^2\,,\quad R=r/\sigma\,, \tag{3.2a}
$$

for the potential (3.1a), and

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

for the potential (3.1b). For the radial Schrödinger equations thus transformed, the squares of the base functions are chosen to be

$$
Q^2(R)=A^2-4\frac{A^2}{K}\left(\frac{1}{R^{12}}-\frac{1}{R^6}\right)+i\frac{C}{R^S}-\frac{(\ell+\frac{1}{2})^2}{R^2} \tag{3.3a}
$$

and

TABLE I. Positions and residues of Regge poles for the potential (3.1a), specified by the reduced quantities $A = 141.425$, $K = 5$, $C = 0$, and $S = 0$. In the column labelled "order" the digits indicate the different orders of the phase-integral approximation, while Num. (Ref. [21]) and Num. (Ref. [22]) indicate the numerical results quoted from Refs. [21] and [22], respectively. (Note that the numerical results r_m are given in the "uniform" column.) The numbers in square brackets are the powers of 10 by which the entries are to be multiplied.

		Position		Residue (nonuniform)		Residue (uniform)	
m	Order	$\mathrm{Re}\,\ell_m$	$\mathrm{Im}\,\ell_m$	$\mathrm{Re}\,r_m$	$\mathrm{Im}\,r_m$	$\mathrm{Re}\,r_m$	$\mathrm{Im}\,r_m$
0	1	180.0153	21.21840	5.34[5]	4.24[5]	5.745[5]	4.554[5]
	3	180.0119479	21.21891562	5.84[5]	4.58[5]	5.774710[5]	4.5334723[5]
	5	180.011948024	21.218915128	5.73[5]	4.50[5]	5.77470703[5]	4.53347700[5]
	7	180.011948024	21.218915128	5.87[5]	4.61[5]	5.77470703[5]	4.53347700[5]
	9	180.011948024	21.218915128	5.4[5]	4.3[5]	5.77470703[5]	4.53347700[5]
	11	180.011948024	21.218915128	8.4[5]	6.5[5]	5.77470703[5]	4.53347700[5]
	13	180.011948024	21.218915128	0.2[5]	0.2[5]	5.77470703[5]	4.53347700[5]
	Num. (Ref. [21])	180.012	21.219			5.79[5]	4.52[5]
	Num. (Ref. [22])	180.01195	21.21892			5.7730[5]	4.5349[5]
2	1	178.5261	26.889	−1.423[7]	2.026[7]	−1.446[7]	2.0600[7]
	3	178.522893725	26.89009572	−1.43789[7]	2.06863[7]	−1.4376913[7]	2.0683181[7]
	5	178.522893751	26.890095348	−1.437683[7]	2.068303[7]	−1.43769254[7]	2.06831771[7]
	7	178.522893751	26.890095348	−1.437694[7]	2.068319[7]	−1.43769254[7]	2.06831771[7]
	9	178.522893751	26.890095348	−1.437692[7]	2.068317[7]	−1.43769254[7]	2.06831771[7]
	11–13	178.522893751	26.890095348	−1.437693[7]	2.068318[7]	−1.43769254[7]	2.06831771[7]
	Num. (Ref. [21])	178.522	26.890			−1.43[7]	2.08[7]
	Num. (Ref. [22])	178.52289	26.89010			−1.4382[7]	2.0677[7]
14	1	174.8832	62.4429	−1.2465[6]	1.527[6]	−1.250[6]	1.5318[6]
	3	174.880818084	62.4442070	−1.2430054[6]	1.5333823[6]	−1.24300479[6]	1.53338108[6]
	5–13	174.880818033	62.444206948	−1.24300490[6]	1.53338122[6]	−1.24300490[6]	1.53338122[6]
	Num. (Ref. [21])	174.881	62.444			−1.25[6]	1.52[6]
	Num. (Ref. [22])	174.88082	62.44421			−1.2431[6]	1.5328[6]

$$Q^2(R) = A^2 - \frac{A^2}{K}\left(\frac{2}{R^6} - \frac{3}{R^4}\right) - \frac{(\ell + \frac{1}{2})^2}{R^2}\,, \tag{3.3b}$$

respectively, in order that the first-order phase-integral approximation will agree with previous semiclassical results.

We consider for the potential (3.1a) three sets of the parameters A, K, C, and S (Tables I–III) and for the potential (3.1b) one set of the parameters A and K (Table IV).

The computational procedure follows closely that for the semiclassical approach [16, 17]. The notable exceptions are that Müller's method, rather than Newton and Raphson's method, is used in the present root searching routines [23], and that the quadratures along the complex paths are based on the Numerical Algorithms Group (NAG) Fortran library routine D01AHF instead of the Gauss-Mehler quadrature. The derivative $\partial\tilde{\gamma}/\partial\ell$ in (2.2) is calculated according to formula (23) in Ref. [24].

The numerical results quoted in our Tables I–IV are obtained by means of a method of Sukumar and Bardsley

TABLE II. Same as Table I but with $A = 141.425$, $K = 5$, $C = 2 \times 10^4$, and $S = 12$. The numerical results are taken from Refs. [3] and [22]. The numbers in square brackets are the powers of 10 by which the entries are to be multiplied.

		Position		Residue (nonuniform)		Residue (uniform)	
m	Order	$\mathrm{Re}\,\ell_m$	$\mathrm{Im}\,\ell_m$	$\mathrm{Re}\,r_m$	$\mathrm{Im}\,r_m$	$\mathrm{Re}\,r_m$	$\mathrm{Im}\,r_m$
0	1	192.3599	19.37305	1.94[3]	−1.38[3]	2.0875[3]	−1.484[3]
	3	192.35701674	19.37323342	2.11[3]	−1.51[3]	2.08395172[3]	−1.4921294[3]
	5	192.357016977	19.373233303	2.07[3]	−1.48[3]	2.08395156[3]	−1.49212863[3]
	7	192.357016977	19.373233303	2.12[3]	−1.52[3]	2.08395156[3]	−1.49212863[3]
	9	192.357016977	19.373233303	2.0[3]	−1.4[3]	2.08395156[3]	−1.49212863[3]
	11	192.357016977	19.373233303	3.0[3]	−2.2[3]	2.08395156[3]	−1.49212863[3]
	13	192.357016977	19.373233303	6.4[1]	−3.8[1]	2.08395156[3]	−1.49212863[3]
	Num. (Ref. [3])	192.357	19.373			2.08[3]	−1.50[3]
	Num. (Ref. [22])	192.35702	19.37323			2.0843[3]	−1.4913[3]
2	1	191.5636	24.89303	−2.263[4]	7.97[4]	−2.30[4]	8.103[4]
	3	191.56072704	24.89339594	−2.27280[4]	8.1157[4]	−2.2725200[4]	8.114470[4]
	5	191.560727210	24.893395803	−2.272506[4]	8.11441[4]	−2.27252092[4]	8.11446871[4]
	7	191.560727210	24.893395803	−2.272523[4]	8.11448[4]	−2.27252092[4]	8.11446871[4]
	9–13	191.560727210	24.893395803	−2.272521[4]	8.11447[4]	−2.27252092[4]	8.11446871[4]
	Num. (Ref. [3])	191.560	24.893			−2.25[4]	8.12[4]
	Num. (Ref. [22])	191.56073	24.89340			−2.2749[4]	8.1131[4]
14	1	190.7540	58.3915	7.5952[4]	−5.933[4]	7.62[4]	−5.951[4]
	3	190.751768469	58.39259283	7.5901989[4]	−5.9627976[4]	7.59019439[4]	−5.96279222[4]
	5–13	190.751768469	58.392592720	7.59019458[4]	−5.96279242[4]	7.59019458[4]	−5.96279242[4]
	Num. (Ref. [3])	190.751	58.393			7.57[4]	−5.98[4]
	Num. (Ref. [22])	190.75177	58.39259			7.5904[4]	−5.9595[4]

TABLE III. Same as Table I but with $A = 53.401$, $K = 2.462$, $C = 1 \times 10^4$, and $S = 20$. The numerical results are taken from Refs. [3] and [22]. The numbers in square brackets are the powers of 10 by which the entries are to be multiplied.

		Position		Residue (nonuniform)		Residue (uniform)	
m	Order	Reℓ_m	Imℓ_m	Rer_m	Imr_m	Rer_m	Imr_m
0	1	76.957	4.668	−3.96[1]	−0.98[1]	−4.253[1]	−1.053[1]
	3	76.936799	4.67775	−4.33[1]	−1.02[1]	−4.28772[1]	−1.01152[1]
	5	76.936749	4.6776483	−4.25[1]	−1.01[1]	−4.287374[1]	−1.011723[1]
	7	76.93675206	4.6776460	−4.35[1]	−1.02[1]	−4.2873723[1]	−1.0116974[1]
	9	76.936752359	4.677646201	−4.05[1]	−0.98[1]	−4.2873750[1]	−1.0116970[1]
	11	76.936752335	4.677646269	−6.1[1]	−1.1[1]	−4.28737520[1]	−1.01169750[1]
	13	76.936752312	4.677646268	−0.1[1]	−0.1[1]	−4.28737505[1]	−1.01169759[1]
	Num. (Ref. [3])	76.955	4.679			−4.30[1]	−0.977[1]
	Num. (Ref. [22])	76.93675	4.67764			−4.2873[1]	−1.0177[1]
2	1	76.575	10.359	3.524[2]	−2.67[2]	3.583[2]	−2.715[2]
	3	76.56192	10.369766	3.5624[2]	−2.7536[2]	3.56200[2]	−2.7532[2]
	5	76.56189838	10.3697723	3.562125[2]	−2.752955[2]	3.5621453[2]	−2.752975[2]
	7	76.56189832	10.3697729	3.562150[2]	−2.752970[2]	3.5621478[2]	−2.7529678[2]
	9	76.56189830	10.3697729	3.562147[2]	−2.752967[2]	3.5621480[2]	−2.7529673[2]
	11–13	76.56189830	10.369773005	3.562148[2]	−2.752967[2]	3.5621480[2]	−2.7529672[2]
	Num. (Ref. [3])	76.580	10.371			3.56[2]	−2.76[2]
	Num. (Ref. [22])	76.56190	10.36977			3.5624[2]	−2.7524[2]
14	1	81.5997	41.9016	−2.7503	−1.812	−2.7582	−1.817
	3	81.596082	41.9081033	−2.75158226	−1.802450	−2.7515811	−1.802450
	5–13	81.596079236	41.908102484	−2.75158295	−1.80244629	−2.75158295	−1.80244629
	Num. (Ref. [3])	81.613	41.910			−2.76	−1.80
	Num. (Ref. [22])	81.59608	41.90810			−2.7510	−1.8025

[20], also used by Connor and co-workers [3, 21], and by means of Prüfer's method used in a paper by Pajunen [22]; his Tables I–IV refer to the same cases as our Tables I–IV, respectively, although Pajunen does not give the correct values of the parameters C used in his Tables III and IV.

Apart from possible misprints [3, 4] concerning Imr_0 for the parameter values used in our Table III, the previously published phase-integral results [3, 4, 21] for the present potentials are in complete agreement with the first-order results for ℓ_m and the first-order "nonuniform" results for r_m in our tables.

Concerning the calculations of Regge-pole positions, we make the following observations. Comparing consecutive orders of the phase-integral approximation, we find consistent numerical values with at least nine correct decimals in our optimal results, except for the first three Regge poles in Table III, where there are at least seven correct decimals in the optimal results. The reason for this diminished accuracy is that the parameters of the potential in Table III are less favorable for phase-integral calculations, since the potential is very steep, and a large number of comparatively close-lying transition zeros are present.

Furthermore, the pole positions obtained by Pajunen [22] are seen to be in full agreement with our phase-

TABLE IV. Positions and residues of Regge poles for the real Lennard-Jones (6,4) potential (3.1b), specified by the reduced quantities $A = 63.641$ and $K = 1.1489$. The numerical results are taken from Refs. [20] and [22]. The numbers in square brackets are the powers of 10 by which the entries are to be multiplied.

		Position		Residue (nonuniform)		Residue (uniform)	
m	Order	Reℓ_m	Imℓ_m	Rer_m	Imr_m	Rer_m	Imr_m
0	1	97.5198	12.39810	3.38[7]	−1.31[8]	3.64[7]	−1.4133[8]
	3	97.517893910	12.39832484	3.63[7]	−1.43[8]	3.591641[7]	−1.4172938[8]
	5	97.517893925	12.398324519	3.56[7]	−1.41[8]	3.59165430[7]	−1.41729377[8]
	7	97.517893925	12.398324520	3.65[7]	−1.44[8]	3.59165429[7]	−1.41729377[8]
	9	97.517893925	12.398324520	3.40[7]	−1.34[8]	3.59165429[7]	−1.41729377[8]
	11	97.517893925	12.398324520	5.0[7]	−2.0[8]	3.59165429[7]	−1.41729377[8]
	13	97.517893925	12.398324520	0.1[7]	−0.4[7]	3.59165429[7]	−1.41729377[8]
	Num. (Ref. [20])	97.519	12.398			2.08[7]	−1.42[8]
	Num. (Ref. [22])	97.51789	12.39832			3.59233[7]	−1.41725[8]
2	1	95.9485	15.68662	2.628[10]	1.479[9]	2.6716[10]	1.50[9]
	3	95.946688763	15.68696369	2.6761[10]	1.40453[9]	2.6757163[10]	1.404472[9]
	5	95.946688714	15.686963459	2.67570[10]	1.404482[9]	2.67571696[10]	1.40448733[9]
	7	95.946688714	15.686963459	2.675719[10]	1.404488[9]	2.67571696[10]	1.40448733[9]
	9–13	95.946688714	15.686963459	2.675717[10]	1.404487[9]	2.67571696[10]	1.40448733[9]
	Num. (Ref. [20])	95.948	15.687			2.63[10]	−1.34[9]
	Num. (Ref. [22])	95.94669	15.68696			2.67567[10]	1.40573[9]
14	1	88.6931	37.85922	5.344[12]	1.31[12]	5.359034[12]	1.31[12]
	3	88.691761371	37.859942569	5.359071[12]	1.29169342[12]	5.3590669[12]	1.2916930[12]
	5–13	88.691761325	37.859942545	5.35906740[12]	1.29169325[12]	5.35906740[12]	1.29169325[12]
	Num. (Ref. [20])	88.693	37.860			5.33[12]	0.736[12]
	Num. (Ref. [22])	88.69176	37.85994			5.35883[12]	1.29184[12]

integral results to the five decimals given by him. However, the numerical results from Refs. [3], [20], and [21] agree with our phase-integral results to within a few units in the third decimal, except in Table III, where the results differ by approximately two units in the second decimal.

Concerning the calculations of the Regge-pole residues, we make the following observations. Comparing successive orders of approximation, one sees that the "nonuniform" formula (2.12) does not give very accurate results for low quantum numbers m, with only two significant digits for $m = 0$. However, the situation rapidly improves as m increases and the relevant complex transition zeros thus move apart.

As expected, the "uniform" residue formula (2.2) gives quite consistent and, according to our experience, accurate results for all quantum numbers m. The difference between uniform and nonuniform results, which is dramatic for low values of m, gradually decreases as m increases. Again we observe that the parameter values in Table III are less favorable for our phase-integral treatment than those in Tables I, II, and IV.

The Regge-pole residues obtained by Pajunen [22] agree with our optimal uniform results up to the third or fourth digit. This agreement is somewhat surprising, since the numerical procedure used by Pajunen for calculating the residues has not been theoretically justified.

In Tables I–III the numerical results quoted from Refs. [3], [20], and [21] differ from our optimal uniform results in the third digit. However, in Table IV the discrepancies are considerably larger. The reason for these discrepancies may partly be that the dimensionless form of the radial Schrödinger equation was not used in Ref. [20].

The reason for presenting the phase-integral results up to the 13th order of approximation in Tables I–IV is connected with our desire to illustrate in a lucid way the fact that one can in many cases obtain considerably more accurate results by the phase-integral method than by numerical methods. On the other hand, to reduce the size of the tables, we have presented the results only for a few values of m, which are chosen such that the tables are essentially as informative for the judgment of the power of the method as if the results for the interjacent values of m had also been included in the tables [25]. We have strong reason to believe that the results for the optimal orders of the phase-integral approximation (determined by the digits which remain unchanged when one changes the order of the phase-integral approximation) are quite correct and thus represent the results that are now known quantum mechanically. The results obtained by numerical methods by other authors and quoted as Num. (Ref. [3]), Num. (Ref. [20]), Num. (Ref. [21]) and Num. (Ref. [22]) in our tables show that it is difficult to obtain accurate results by numerical methods, that it has been desirable to increase the accuracy of the results, and that the most accurate results so far obtained by numerical methods, viz., those designated by Num. (Ref. [22]) in our tables, are not quite reliable. To obtain accurate results that are completely reliable we have used phase-integral approximations up to comparatively high orders. In our tables we have presented the results with the accuracy that we have obtained and have not speculated about which accuracy may be needed in particular applications, since this is a question that is currently under investigation.

From the present investigation we conclude that the new Fröman-Fröman phase-integral residue formula [1], which is highly relevant for the diffraction and rainbow scattering of atoms and molecules, provides an extremely accurate computational as well as analytical tool in the Regge-pole theory. We have strong reason to believe that the optimal uniform phase-integral results obtained in the present paper are much more accurate than previously published results for the same potentials.

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