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Calculation of the Non Forward Scattering Amplitude for Long Range Potentials

C.R. Garibotti [1,*], F.F. Grinstein [2,**] and J.E. Miraglia [1,*]

[1] Centro Atómico Bariloche, Bariloche, Argentina***

[2] Instituto de Física, Universidade Federal Fluminense, Niterói, RJ, Brasil

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The regularization factor technique is considered as a summation method for divergent, oscillating and slowly convergent partial wave expansions of the non-forward scattering amplitude for long range central potentials. Its convergence properties are studied and its efficiency is compared with that of the Punctual Padé approximant method in the cases of the Kratzer and Lennard-Jones potentials.

I. Introduction

A usual method for the calculation of differential cross-sections is that based on the partial wave expansion of the scattering amplitude (PWESA). For two body potential scattering, and if we restrict ourselves to spherically symmetric interactions, this series is given by

$$f(\theta)=\sum_{\ell=0}^{\infty} a_\ell \mathbf{P}_\ell(\cos\theta) \tag{1.1}$$

where the $\{a_\ell\}$ are the partial wave amplitudes and the $\{\mathbf{P}_\ell\}$ are the Legendre polynomials. The number of terms in (1.1) which contribute significally to the series can be estimated by the semiclassical relation.

$$N_{\max} \sim k r_0$$

where r_0 is the effective range of the potential. Thus, the method is of great value when relatively low values of r_0, of the energy, and of the reduced mass of the system, are involved. Otherwise, the convergence of the PWESA is slow and a considerable number of partial wave amplitudes, and hence of phaseshifts, must be calculated in order to obtain accurate values for the scattering amplitude. Typical of these situations are atomic and molecular collision processes, where long range interactions are present, and nuclear systems described by short range potentials, in the intermediate energy region. In the former case, the convergence of the PWESA is, in principle, restricted to the physical interval $-1 \leqq \cos\theta \leqq 1$. Anomalous situations exist, however, for which the scattering amplitude has finite meaningful values, while its calculation is impossible by means of its PWESA. Such is the case when the dominant long range component of the potential is of the Coulombian or the inverse square type, which involve divergent (in the non-forward directions), and oscillating (in the backward direction) PWESA's respectively.

An interesting global approach can be proposed in order to deal with this type of problems. This idea consists in keeping the original PWESA, which is assumed to contain in its terms all the physical information required to solve the scattering problem, independently of its convergence properties, and to seek efficient mathematical methods capable of resuming that information.

Several such methods exist within the framework of Padé-type rational approximations, and some of them have been proposed for that purpose [1-4]. Of particular interest is the Punctual Padé Approximant (PPA) approach [2] which has the advantage, from the numerical point of view, of counting on algorithms which allow for the recurrent calculation of the successive approximations. Furthermore, the formal convergence properties of the PPA are quite well

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known [2, 3] for this type of applications, while their practical significance has been shown in typical examples of those situations where such a method for the summation of the PWESA is required [4].

Some years ago, the regularization factor (RF) method was proposed [5] in order to summate the divergent PWESA associated to Coulombian long range forces. In spite of its mathematical simplicity and the satisfactory results found in the particular application for which it was used, no attempt seems to have been done to extend its use to other cases where a convergence acceleration technique for the PWESA may be of value.

In this paper we prove the convergence of the sequences of approximations defined through the RF method and obtain asymptotic estimates for their errors. The proofs include all the long range potentials of interest in potential scattering, and are restricted to $\theta>0$, cases for which the method is capable of being applied. A numerical comparison is then made between the PPA and RF methods, when summating the non-forward PWESA corresponding to the Kratzer and Lennard-Jones potentials.

In Sect. 2 the asymptotic properties of the sequence of partial wave sums of the non-forward PWESA, corresponding to long range potentials, are recalled and discussed, those of the sequences defined through the RF method are proven, and the PPA method and the relevant formal results regarding its convergence are briefly reviewed; Section 3 deals with the numerical applications, and the final discussion of the results is presented in Sect. 4.

2. Summation of the Non-Forward PWESA for Long Range Potentials

Let us consider potentials with the long range behaviour

$$V(r) \underset{r\to\infty}{\sim} V_0 r^{-\alpha-2}, \quad \alpha \geqq -1, \tag{2.1}$$

where V_0 is a constant and α an integer. Here, usual interactions present in atomic and molecular collision processes are included, i.e., Coulombian ($\alpha=-1$), charge-dipole ($\alpha=0$), induced polarization ($\alpha=2$), and Van der Waals ($\alpha=4$). The asymptotic behaviour of the corresponding partial wave amplitudes for $\ell\to\infty$ depends only on the long range tail (2.1) of the potential, and can be found in the form*

$$a_\ell \underset{\ell\to\infty}{\sim} \sum_{i=1}^{J} B_i(\ell+\tfrac{1}{2})^{\beta_i} + \mathcal{O}[\ell^{\beta_{J+1}}], \tag{2.2}$$

where the parameters $\{B_i\}$ and $[\beta_i]$ are dependent on V_0 and α, and are defined, for relevant values of J, in Appendix I.

a) *The Sequence of Partial Sums of the PWESA*

By using (2.2) and well known properties of Legendre polynomials, the asymptotic behaviour of the sequence of partial wave sums

$$S_m(\theta) = \sum_{\ell=0}^{m} a_\ell \mathbf{P}_\ell(\cos\theta) \tag{2.3}$$

can also be obtained for $\theta>0$. It can be shown that [3]

$$S_m(\theta) \underset{m\to\infty}{\sim} \begin{cases} f(\theta) + B_1 A(\theta)(m+\tfrac{1}{2})^{\beta_1-\frac{1}{2}} \sin \Lambda_m(\theta), \\ \quad (0<\theta<\pi), & (2.4\text{a}) \\ f(\pi) + \dfrac{(-1)^m}{2} \sum_{i=1}^{J} B_i(m+\tfrac{1}{2})^{\beta_i}, \\ \quad (\theta=\pi), & (2.4\text{b}) \end{cases}$$

where

$$A(\theta) = -\left(2\pi \sin\theta \sin^2\frac{\theta}{2}\right)^{-\frac{1}{2}}$$

and

$$\Lambda_m(\theta) = (m+1)\,\theta - \frac{\pi}{4}.$$

By inspection of (2.4) it can be readily seen that $S_m(\theta)$ is divergent for all $\theta>0$ if $\alpha=-1$, and oscillatory for $\theta=\pi$ and $\alpha=0$, which correspond, respectively, to potentials having long range behaviour of the type $(1/r)$ and $(1/r^2)$, and convergent otherwise for $\theta>0$ and $\alpha\geqq 0$. The non-forward scattering amplitude is well defined, however, even for these anomalous cases, although its calculation is not possible by using $S_m(\theta)$ in the traditional way.

b) *The Regularizing Factor Method*

Let us consider $\theta>0$, and introduce the regularizing factor $(1-\cos\theta)$ in order to define, for $n\geqq 0$*

* Throughout this paper, we shall say that sequence $\{A_m\}$ tends asymptotically to sequence $\{B_m\}$, i.e., $A_m \sim B_m$, if given any small positive quantity ε an integer m_0 can be found such that $|A_m - B_m|/|A_m| < \varepsilon$ for $m \geqq m_0$

* By the symbol $\doteq$ we indicate that nothing is assumed with regards to the convergence of the expansion, which is nevertheless uniquely determined by the function involved

$$f^{(n)}(\theta)=(1-\cos\theta)^n f^{(0)}(\theta) \doteq \sum_{\ell=0}^{\infty} a_\ell^{(n)} \mathbf{P}_\ell(\cos\theta), \qquad (2.5)$$

where $f^{(0)}(\theta)\equiv f(\theta)$, $a_\ell^{(0)}\equiv a_\ell$, and the $a_\ell^{(n)}$ satisfy, for $n\geqq 1$, the following recurrence relation [5]

$$a_\ell^{(n)}=a_\ell^{(n-1)}-\frac{\ell+1}{2\ell+3}a_{\ell+1}^{(n-1)}-\frac{\ell}{2\ell-1}a_{\ell-1}^{(n-1)}, \qquad (2.6)$$

with $a_{-1}^{(n-1)}\equiv 0$.

In Appendix II we study the convergence properties of the sequences

$$S_m^{(n)}(\theta)=\sum_{\ell=0}^{m} a_\ell^{(n)} \mathbf{P}_\ell(\cos\theta)$$

with $a_\ell^{(0)}$ having an asymptotic representation of the type (2.2). As a particular consequence of our proofs it follows that a sequence of approximations to $f(\theta)$ can be constructed defined by

$$f_m^{(n)}(\theta)=(1-\cos\theta)^{-n} S_m^{(n)}(\theta), \qquad (2.7)$$

and having the asymptotic behaviour:

$$f_m^{(n)}(\theta) \underset{m\to\infty}{\sim} \begin{cases} f(\theta)+A^{(n)}(\theta)\, C_1^{(n)}(m+\tfrac{1}{2})^{\beta_1-\frac{1}{2}-2n} \cdot \sin A_m(\theta), \quad (0<\theta<\pi), & (2.8\text{a}) \\ f(\pi)+\frac{(-1)^m}{2^{n+1}}\, C_1^{(n)}(m+\tfrac{1}{2})^{\beta_1-2n}, \quad (\theta=\pi), & (2.8\text{b}) \end{cases}$$

with

$$A^{(n)}(\theta)=(1-\cos\theta)^{-n}A(\theta),$$

$$C_1^{(n)}=(-1)^n 2^{-n} B_1(\beta_1-1)^2(\beta_1-3)^2\ldots(\beta_1-2n-1)^2,$$

for $n>1$, and $C_1^{(0)}=B_1$.

By comparison of (2.8) and (2.4) it is seen that $f_m^{(n)}$ for $n>0$, has a greater asymptotic rate of convergence than that of the original sequence $S_m=f_m^{(0)}$, when convergent. Moreover, that rate is seen to increase rapidly with n by a factor of the order of $(1/m)^{2n}$. In particular, (2.8) also show that $f_m^{(n)}(\theta)$ converges for all $\theta>0$ and $n\geq 1$, even for the patological cases mentioned above, for which S_m is divergent or oscillating, while $f(\theta)$ has finite meaningful values.

c) The Punctual Padé Approximant Method

Associated to the PWESA given by (1.1) we can define the power series

$$F(\theta,z)=\sum_{\ell=0}^{\infty} a_\ell \mathbf{P}_\ell(\cos\theta)\, z^\ell, \qquad (2.9)$$

and the Padé approximant (PA) [8] to $F(\theta,z)$, $[N,M]_{F(\theta,z)}$, as

$$[N,M]_{F(\theta,z)}=\frac{r_0+r_1 z+\ldots+r_M z^M}{1+q_1 z+\ldots+q_N z^N},$$

satisfying the requirement:

$$[N,M]_{F(\theta,z)}-F(\theta,z)=\mathcal{O}[z^{M+N+1}].$$

Then, the Punctual Padé Approximant (PPA) [2] to $f(\theta)$, $[N,M]_{f(\theta)}$, is defined as the $[N,M]_{F(\theta,z)}$ (PA) to $F(\theta,z)$, calculated at $z=1$. In this way, a doubly infinite array of rational approximations to $f(\theta)$ are introduced, the so called PPA table.

The convergence of the row sequences of this table, i.e., sequences $[n,n+m]_{f(\theta)}$ with fixed n, has been studied in recent papers [2-4, 16]. For potentials satisfying (2.1), and for the non-forward scattering directions, it has been shown that [3]

$$[n,n+m]_{f(\theta)} \underset{m\to\infty}{\sim} f(\theta) + \frac{A(\theta)B_1(\sin\theta)^{2(n-N)}[\beta_1]_N\, N!\,(\sin A_{m+n})^{2(2N-n)+1}}{2^{2(n-N)}\left(\sin\frac{\theta}{2}\right)^{2n}(m+\frac{1}{2})^{2N-\beta_1+\frac{1}{2}}},$$

$$(0<\theta<\pi;\ \sin A_{m+n}\neq 0), \qquad (2.10\text{a})$$

$$[n,n+m]_{f(\pi)} \underset{m\to\infty}{\sim} f(\pi) + \begin{cases} \frac{B_1(-1)^{m+n} n!\,[\beta_1]_n}{2^{2n+1}(m+\frac{1}{2})^{2n-\beta_1}}, & \alpha\neq 0, \quad (2.10\text{b}) \\ \frac{B_1}{2}(-1)^m\delta_{n0}+\frac{B_2(-1)^m\gamma_n(n+1)!}{2^{2n+1}(m+\frac{1}{2})^{2n+1}}, & \alpha=0, \quad (2.10\text{c}) \end{cases}$$

where $[\beta_1]_n=(\beta_1-1)\ldots(\beta_1-n+1)$ and $\gamma_n=(n-1)!$ for $n\geqq 1$, $[\beta_1]_0=\gamma_0=1$, and $N=n/2$ (for even n) or $N=(n-1)/2$ (for odd n).

Comparing now the convergence properties of the non-trivial row sequences of the table ($n>0$) relative to those of the first ($[0,m]_f\equiv S_m(\theta)$), it is seen that they converge to the right values when $m\to\infty$ in all cases for which the PWESA is convergent, while their corresponding rates of convergence increase with n by factors of order $(1/m)^n$ $(0<\theta<\pi,\ \alpha\geqq 0)$ and $(1/m)^{2n}$ $(\theta=\pi,\ \alpha\geqq 1)$. Furthermore, they are also seen to be convergent when the PWESA is anomalous, i.e., for $0<\theta<\pi$ and $\alpha=-1$ (for $n\geqq 2$), and for $\theta=\pi$ and $\alpha=0$ (for $n\geqq 1$). Thus, the PPA method is also capable of regularizing the PWESA in those cases.

3. Numerical Examples

In the preceding section we have dealt with the asymptotic convergence properties of the RF and

PPA methods, when used for the summation of the PWESA corresponding to long range potentials. We shall now compare their practical significance in two examples where the calculation of the non-forward scattering amplitude is troublesome when based on its PWESA.

They are, the scattering by the Kratzer, and by the Lennard-Jones potentials, which give simple models of those interactions typically involved in the calculation of collision processes between ions, and between molecules, respectively. In both cases, we have studied the relative error ε of the approximations, as a function of the number of partial waves (NPW) involved, when calculating $|f(\theta)|^2$, for different values of the scattering angle $\theta>0$. We display, in particular, our results for $\theta=\pi/4$ and $\theta=\pi$, representatives of intermediate and large values of θ, respectively. The reference "exact" values $f_R(\theta)$ for $f(\theta)$ were calculated as indicated in each case below, and we have taken ε to be given by

$$\varepsilon_A=\{|f_A(\theta)|^2-|f_R(\theta)|^2|/|f_R(\theta)|^2 \tag{3.1a}$$

for the particular approximation A, which will be the resultant of using, alternatively, the RF, the PPA, or the traditional partial wave sums method. For the sake of comparison of the numerical results with those predicted by the formal asymptotic estimates, let us note that for relatively large values of NPW, ε_A is essentially given by

$$\varepsilon_A \simeq 2\frac{|\mathrm{Re} f_R(\theta)|}{|f_R(\theta)|^2}|\mathrm{Re} f_A(\theta)-\mathrm{Re} f_R(\theta)|. \tag{3.1b}$$

Since the contribution of the error of $\mathrm{Im} f_A(\theta)$ is negligible as compared to that of $\mathrm{Re} f_A(\theta)$, asymptotically.

a) Scattering by the Kratzer Potential

This potential played a rather large role in the early days of Quantum Mechanics, when investigating the rotation-vibration spectrum of diatomic molecules [10]. We shall here interpret it as describing the interaction between two ions, each of electrical charge e.

The Kratzer potential is given by the expression:

$$V(r)=-2D\left(\frac{a}{r}-\frac{1}{2}\frac{a^2}{r^2}\right), \quad (D, a>0) \tag{3.2}$$

having a minimum for $r=a$, with $V(a)=-D$.

Let us consider the potential expressed in the following way:

$$V(r)=\frac{\hbar^2}{2\mu}\left(\frac{2\xi}{r}+\frac{\lambda}{r^2}\right) \quad (\xi<0,\ \lambda>0) \tag{3.3}$$

where μ is the reduced mass of the system. Then, the non-forward PWESA is given by [10]:

$$f(\theta)\doteq\sum_{\ell=0}^{\infty}(2\ell+1)\exp(2i\delta_\ell)\mathbf{P}_\ell(\cos\theta)/(2ik) \tag{3.4}$$

with

$$\begin{aligned}&\delta_\ell=\eta_L-(L-\ell)\pi/2,\\ &\eta_L=\arg\Gamma(L+1+i\gamma), \qquad \gamma=\xi/k\\ &L=-\tfrac{1}{2}+\sqrt{\lambda+(\ell+1/2)^2}.\end{aligned} \tag{3.5}$$

Expansion (3.4) is divergent owing to the fact that the dominant long range component of the potential is Coulombian, but represents nevertheless $f(\theta)$. In practical calculations, the usual procedure to overcome this difficulty is to "substract" from $f(\theta)$ the divergent PWESA corresponding to the Coulombian scattering amplitude $f_c(\theta)$. With:

$$\begin{aligned}f_c(\theta)&=-\gamma^2\exp\{2i\eta_0-i\gamma\\ &\cdot\ln[(1-\cos\theta)/2]\}/(1-\cos\theta)\\ &\doteq\sum_{\ell=0}^{\infty}(2\ell+1)\exp(2i\eta_\ell)\mathbf{P}_\ell(\cos\theta)/(2ik),\end{aligned} \tag{3.6}$$

we may express $f(\theta)$ for $\theta>0$ in the form

$$\begin{aligned}f(\theta)\doteq f_c(\theta)+&\sum_{\ell=0}^{\infty}(2\ell+1)\exp(2i\eta_\ell)[\exp(2i\sigma_\ell)-1]\\ &\cdot\mathbf{P}_\ell(\cos\theta)/(2ik),\end{aligned} \tag{3.7}$$

where:

$$\sigma_\ell=\delta_\ell-\eta_\ell. \tag{3.8}$$

The calculations of the scattering amplitude corresponding to potentials for which Coulombian plus a shorter range (tending to zero at least as $1/r^2$ when $r\to\infty$) components are involved, are made with expansion (3.7), when based on the partial wave method. The expectation is that having substracted the divergent part of the series, the resulting one will be rapidly convergent. This is not necessarily the case when long range components are present, apart of the Coulombian one. In our case, for example, this series is slowly convergent for $0<\theta<\pi$ and oscillatory for $\theta=\pi$, owing to the $1/r^2$ part of the potential.

In the calculations that follow, the Kratzer potential has been taken to represent the interaction between the H^+ and Cl^- ions. Consequently, we have chosen a to be the molecular radius of HCl. Taking account of the rotational spectra data for HCl [11] we have $a=1.2746\times10^{-8}$ cm. For large separation we have an attractive Coulomb potential, then $2Da=e^2/4\pi\varepsilon_0$ and this implies $D=5.6488$ eV for the dissociation energy of HCl. By now fixing the wave vector magnitude k, the dimensionless parameters γ and λ may be uniquely determined by means of the relations $\gamma = -1/ka_0$ and $\lambda = a/a_0$. Here, we have chosen $k = 2/a_0$, which then fixes $\gamma = -0.5$ and $\lambda = 2.4086$; a_0 is the Böhr radius.

We have studied the calculation of $f(\theta)$ for $\theta > 0$, based on both its total (TS) and substracted (SS) series representations, given by (3.4) and (3.7), respectively, by using alternatively, the PPA and RF methods. The efficiency of the approximation schemes is compared to that of the traditional partial wave sums method, measured by the corresponding curves of ε_A, defined by (3.1a), as a function of NPW, which are plotted in Figs. 1–4 for the significant cases $\theta = \pi/4$ and $\theta = \pi$, and for representative low order approximants. The reference values for $f(\pi/4)$ and $f(\pi)$ were calculated with 8 and 9 significant figures, respectively, by using the first 150 partial waves with the $[4, 4+m]$ PPA and the corresponding 4 times iterated $f_m^{(4)}$ RF approximant.

By inspection of Figs. 1–2, which correspond to calculations based on the TS, the general features predicted by (2.8) and (2.10) are seen to be present. In particular, we note the divergence of the error of the sequence of partial wave sums of the TS, i.e., of the sequence $[0, 0+m] = f_m^{(0)} = S_m$. In the case $\theta = \pi/4$ (Fig. 1) we also note that the error of the $[n, n+m]$ PPA diverges for $n = 1$, while tending to zero quite rapidly for $n > 1$, showing a good agreement with the estimates of Eq. (2.10a), which improves with increasing NPW, for NPW > 10, approximately:

i) the positions of the dips for the $[0, 0+m]$ and the peaks for the $[1, 1+m]$ tend to coincide, as well as the values of the relative extrema between them;

ii) the period of the oscillations tends to be $\Delta\ell = 4$, and the set of positions of the relative maxima for the errors, associated to a given even value of n, shift correctly relative to those corresponding to other values of n considered;

iii) the global rate of convergence or divergence follows closely the corresponding power of $(m + \frac{1}{2})$ law.

Moreover, the curves for the $f_m^{(n)}$ $(\pi/4)$ approximants are seen to be convergent for $n \geq 1$, and the agreement is also good with (2.8a) in the sense discussed above, although the asymptotic conditions are approached for NPW > 20.

For $\theta = \pi$ (Fig. 2), no oscillations are present, as expected from (2.8b) and (2.10b), and all the non-trivial approximants converge. The asymptotic convergence pattern is approached as in the precedent case, for NPW greater than 10 and 20, for the PPA and RF methods, respectively.

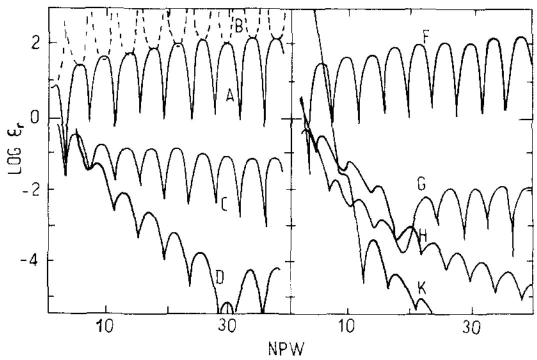

Fig. 1. Kratzer potential (TS), $\theta = \pi/4$; $\log_{10}\varepsilon_A$ as function of NPW; A: $[0, m] = S_m$; B: $[1, 1+m]$; C: $[2, 2+m]$; D: $[4, 4+m]$; F: $f_m^{(0)} = S_m$; G: $f_m^{(1)}$; H: $f_m^{(2)}$; K: $f_m^{(4)}$

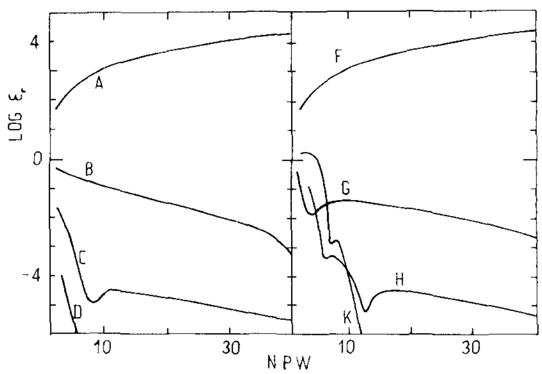

Fig. 2. Kratzer potential (TS), $\theta = \pi$; captions as in Fig. 1

In the case of the SS, displayed in Figs. 3 and 4, the sequence of partial wave sums converges very slowly for $\theta = \pi/4$, and oscillates for $\theta = \pi$, being these features typical of those associated to the $1/r^2$ component of the potential, which dominates the convergence of the SS. The same discussion above for the TS regarding the general convergence pattern, is proper here. Comparing with that case, however, the PPA to the SS are seen to converge faster, while the rate of convergence of the $f_m^{(n)}$ sequences turns out to be correspondingly, similar or poorer than that for the TS.

Finally, let us remark that according to the asymptotic formal predictions of Sects. 2b and c, the natural efficiency comparison should be set between the $f_m^{(n)}$ and the $[2n, 2n+m]$ sequences for $\theta = \pi/4$, and between the $f_m^{(n)}$ and $[n, n+m]$ sequences for $\theta = \pi$. The results of such a comparison in the case of the Kratzer potential, indicate that the PPA method is in general similar or better than the RF method.

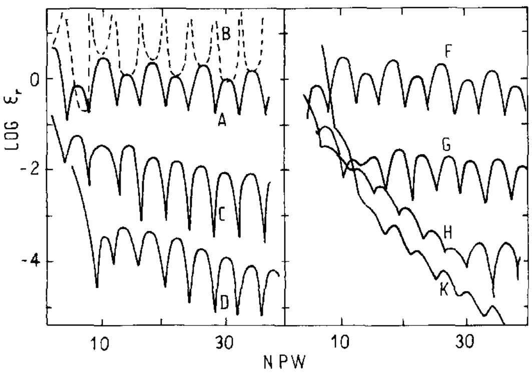

Fig. 3. Kratzer potential (SS), $\theta=\pi/4$; captions as in Fig. 1

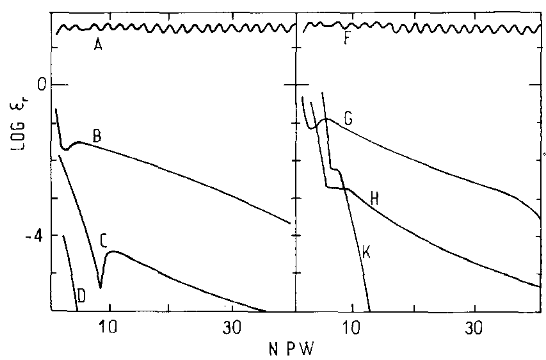

Fig. 4. Kratzer potential (SS), $\theta=\pi$; captions as in Fig. 1

b) Scattering by the Lennard-Jones Potential

The Lennard-Jones (LJ) potential gives a simple description of the interactions between neutral polarizable systems, and because of its mathematical simplicity it has been extensively used on the grounds of testing different approximation procedures in the calculations of atomic and molecular collision processes. It is given by the expression

$$V(r)=4V_0\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right] \tag{3.9}$$

having a minimum for $r_0=2^{\frac{1}{6}}\sigma$, with $V(r_0)=-V_0$. Aside of a normalization factor, we may parametrize its corresponding scattering amplitude by means of the de Boer parameter $\Omega=2\pi\hbar/(2\mu V_0\sigma^2)^{\frac{1}{2}}$ and the reduced energy $\epsilon=E/V_0$, where μ is the reduced mass of the particular system involved.

We are mainly interested in the range $\Omega<0.3$, where rainbow scattering occurs [12] and where the convergence of the PWESA is worst, owing to the fact that as $\Omega\to 0$ the classical conditions are approached. Moreover, the phase-shifts are well represented by the semiclassical JWKB approximation in this range [13] and we may use a compact expression for their evaluation [14]. In terms of ϵ, Ω, and reduced dimensionless quantities, the latter becomes

$$\delta_\ell=\frac{\pi\epsilon^{\frac{1}{2}}}{\Omega}\int_{x_m}^{\infty}\frac{x\,v'(x)F(x)\,dx}{\epsilon-v(x)} \tag{3.10}$$

where $x=r/\sigma$, $v(x)=V(x\sigma)/V_0$, x_m is the reduced classical turning point, i.e., the outermost zero of

$$F(x)=[1-v(x)/\epsilon-b^2/x^2]^{\frac{1}{2}}$$

and $b^2=\ell(\ell+1)\Omega^2/(4\pi^2\epsilon)$ is the square of the reduced impact parameter. As in [4] and [12], we have calculated the integral in (3.10) by Gauss-Melher quadratures, by considering the sequence

$$\delta_\ell(n)=\frac{\pi^2 x_m\epsilon^{\frac{1}{2}}}{2\Omega n}\sum_{j=1}^{n-1}\frac{x_j v'(x_j)F(x_j)}{\epsilon-v(x_j)}\cdot\frac{\sin(j\pi/2n)}{\cos^2(j\pi/2n)} \tag{3.11}$$

where $x_j=x_m/\cos(j\pi/2n)$, which converges quite rapidly to the exact JWKB phase-shifts as $n\to\infty$.

In our calculations we have fixed $\Omega=0.1$ and $\epsilon=4$. These are typical values involved when seeking a fit of the experimental rainbow oscillations of the differential cross-section for the K–Hg system, based on a description of the interactions by means of a *LJ* potential [12].

In Figs. 5 and 6 we have only plotted the maximum envelope of relative error ε_A as function of NPW. For the relatively large values of NPW here involved, and following the predictions of (2.8a) and (2.10a), the period of the oscillations for $\theta=\pi/4$, turn out to be too small to allow them to be displayed. Furthermore, in the case $\theta=\pi$, the sequence of partial wave sums is very slowly convergent and its corresponding curve falls out of Fig. 6. In this case the monotonic convergence predicted by (2.8b) and (2.10b) is attained when the NPW is larger than 180. The reference values were calculated with 7 significant figures, by using the first 400 partial waves, as in the previous example.

With both methods, PPA and RF, the curves are seen to step down rapidly in the neighbourhood of NPW=300. Moreover, for $\ell>298$ the phase-shifts satisfy $\delta_\ell<0.5$ and are well represented by a simple extension of the Massey-Möhr expression [15], $\delta_\ell=A/\ell^5-B/\ell^{11}$, with $A=24\pi^7\epsilon^2/\Omega^6$ and $B=1{,}008\,\pi^{13}\epsilon^5/\Omega^{12}$. Hence, when the δ_ℓ attain their asymptotic form, a few partial waves are enough for the PPA and RF methods to resume the information contained in the higher order ones. Thus, as noted previously [4] for the PPA, the relevant physical

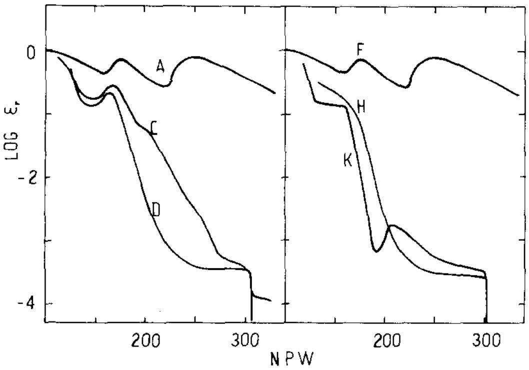

Fig. 5. Lennard-Jones potential, $\theta=\pi/4$; captions as in Fig. 1

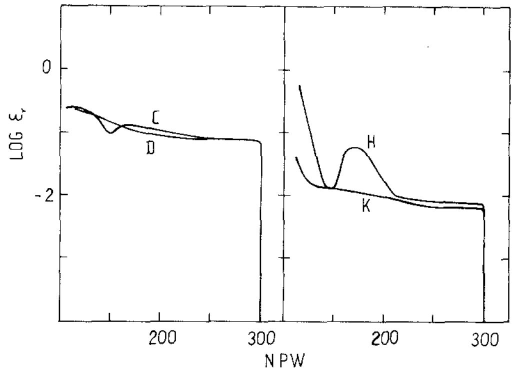

Fig. 6. Lennard-Jones potential, $\theta=\pi$; captions as in Fig. 1

information used is similar to that required by semi-classical approximation schemes. The efficiencies of the PPA and RF methods are essentially similar in this example.

4. Discussion

In the precedent section the practical importance of the PPA and RF methods has been shown for the calculation of the non-forward scattering amplitude corresponding to long range potentials, based on anomalous behaving or very slowly convergent PWESA's. Our comparative results also indicate that the PPA method seems to be preferable of the two. Further arguments can be given in behalf of the PPA as a summation method for the PWESA in the general case. In the first place, it is also useful in the case of forward scattering calculations [2, 4], whereas the RF method can only be applied for $\theta>0$. On the other hand, the efficiency of the approximation schemes is quite different in the case of short range potentials. Recently [16] the convergence proofs for the PPA have been extended to include potentials having the asymptotic representation.

$$V(r) \underset{r\to\infty}{\sim} V_0 r^{-\rho-1} \exp(-\mu r) \tag{4.1}$$

where V_0 is a constant, ρ an integer and $\mu>0$, thus including important potentials from the physical point of view, such as the Yukawa ($\rho=0$) and Exponential ($\rho=-1$). In this case, it can be shown that the partial wave amplitudes behave asymptotically as

$$a_\ell \underset{l\to\infty}{\sim} B(\ell+\tfrac{1}{2})^\beta q^{\ell+\frac{1}{2}} \tag{4.2}$$

where $q=\exp(-\alpha)$, $\beta=-\rho+\frac{1}{2}$

$$B=\frac{-V_0}{k^2}\left(\frac{\pi}{2}\right)^{\frac{1}{2}}(\mathrm{Sh}\,\alpha)^{-\beta}\left(\frac{k^2}{\mu}\right)^\rho,$$

and α is a positive quantity such that $\mathrm{Ch}\,\alpha=1+\mu^2/2k^2$. Owing to this behaviour, the PWESA converges within an elliptical domain in the complex $\cos\theta$ plane, the so called Lehmann ellipse, characterized by having focii at ± 1 and major axis equal to $2\,\mathrm{Ch}\,\alpha$. The same general qualitative features regarding the convergence of the row sequences of the PPA table for the case of long range potentials, were shown to be valid also in this case, when $\cos\theta$ is within the Lehmann ellipse. They were thus shown to be stable with respect to variations on the range of the potential. For example, restricting ourselves to fixed even $n>0$, to simplify the discussion, we have

$$\frac{|[n, n+m]-f(\theta)|}{|[0, 0+m]-f(\theta)|} \underset{m\to\infty}{\sim} \mathcal{O}[m^{-t}] \tag{4.3}$$

with $t\geqq 2n$.

Following the lines of Appendix II, we can also extend the convergence proofs for the RF method, for this type of applications. In particular, taking account of (4.2) and operating as in the proof of the Lemma, we can show that

$$a_\ell^{(n)} \underset{\ell\to\infty}{\sim} \frac{(-1)^n}{2}(q-1)^{2n} a_\ell. \tag{4.4}$$

Hence, we can expect, within the Lehmann ellipse, and for $\theta\neq 0$,

$$\frac{|f_m^{(n)}(\theta)-f(\theta)|}{|f_m^{(0)}(\theta)-f(\theta)|} \underset{m\to\infty}{\sim} \frac{(-1)^n}{2}(q-1)^{2n}(1-\cos\theta)^{-n} \tag{4.5}$$

with $f_m^{(0)}(\theta)\equiv S_m(\theta)$. Thus, the rate of convergence of sequence $f_m^{(n)}(\theta)$ is, aside of a constant factor dependent on θ, the same as that of $S_m(\theta)$ and the RF method appears to be of no value in the case of short range potentials. Furthermore, it is clear that because of (4.4), the domain of convergence of the $f_m^{(n)}$ sequences will also be restricted to within the Lehmann ellipse. Because of the rational nature of the PPA, however, we can expect them to converge in a much larger domain, and hence be an important procedure for the approximate analytical continuation of $f(\theta)$ in the complex $\cos\theta$ plane, starting from its PWESA.

Appendix I

The asymptotic behaviour of the partial wave amplitudes a_ℓ for $\ell\to\infty$ depends only on the long range tail (2.1) of the potential, and can be readily obtained [3]

$$a_\ell \underset{\ell\to\infty}{\sim} \sum_{i=1}^{J} B_i(\ell+\tfrac{1}{2})^{\beta_i}+\mathcal{O}[\ell^{\beta_{J+1}}], \tag{I.1}$$

where for $\alpha\geqq 0$, $J=2$, and

$$B_1=-V_0 k^{\alpha-1} I_\alpha, \qquad B_2=i V_0^2 k^{2\alpha-1} I_\alpha^2/2,$$
$$\beta_1=-\alpha, \quad \beta_2=-2\alpha-1, \quad \beta_3=-2\alpha-2,$$

while for $\alpha=-1$, $J=1$, and

$$B_1=-i/k,$$
$$\beta_1=1+i\kappa, \quad \beta_2=-1+i\kappa,$$

I_α is a numeric factor, dependent on α, defined by

$$I_\alpha=\begin{cases}\pi/2, & \alpha=0\\ (\pi/2)(\alpha-1)!!/\alpha!!, & \text{even } \alpha>0\\ (\alpha-1)!!/\alpha!!, & \text{odd } \alpha,\end{cases}$$

and $\kappa=V_0/k$.

Appendix II

Lemma. If $a_\ell^{(0)}$ has the asymptotic representation

$$a_\ell^{(0)} \underset{\ell\to\infty}{\sim} B(\ell+\tfrac{1}{2})^{\beta}, \tag{II.1}$$

where B is a constant, and β is a complex number different from an odd positive integer but otherwise arbitrary, then for $n\geqq 1$, we have

$$a_\ell^{(n)} \underset{\ell\to\infty}{\sim} C^{(n)}(\ell+\tfrac{1}{2})^{\beta-2n} \tag{II.2a}$$

with

$$C^{(n)}=(-1)^n 2^{-n} B(\beta-1)^2(\beta-3)^2\dots(\beta-2n-1)^2. \tag{II.2b}$$

Proof. Let us first consider the case $n=1$. By using (II.1) in (2.6), we have

$$a_\ell^{(1)} \underset{l\to\infty}{\sim} B[(\ell+\tfrac{1}{2})^{\beta}-\tfrac{1}{2}(\ell+1)(\ell+\tfrac{3}{2})^{\beta-1} -\tfrac{1}{2}\ell(\ell-\tfrac{1}{2})^{\beta-1}]$$
$$\underset{\ell\to\infty}{\sim} B\Big\{(\ell+\tfrac{1}{2})^{\beta}-\frac{\ell+1}{2}\Big[(\ell+\tfrac{1}{2})^{\beta-1}+(\beta-1)(\ell+\tfrac{1}{2})^{\beta-2} +\frac{(\beta-1)(\beta-2)}{2}(\ell+\tfrac{1}{2})^{\beta-3}\Big]-\frac{\ell}{2}\Big[(\ell+\tfrac{1}{2})^{\beta-1} -(\beta-1)(\ell+\tfrac{1}{2})^{\beta-2}+\frac{(\beta-1)(\beta-2)}{2}(\ell+\tfrac{1}{2})^{\beta-3}\Big]\Big\}$$
$$=-\frac{B}{2}(\beta-1)^2(\ell+\tfrac{1}{2})^{\beta-2}.$$

Assuming now that (II.2) are valid for $n-1$, and using them in (2.6), we prove, in the same way, that they are valid for n, and by induction the proof of the Lemma follows.

Theorem. Let $S_m^{(n)}(\theta)$ be the partial sum of order m corresponding to series (2.5) defining $f^{(n)}(\theta)$ for $n\geqq 1$, i.e.,

$$S_m^{(n)}(\theta)=\sum_{\ell=0}^{m} a_\ell^{(n)}\mathbf{P}_\ell(\cos\theta) \tag{II.3}$$

and let us assume that the behaviour of the $a_\ell^{(0)}$ are those of the Lemma.
Then, the sequence $\{S_m^{(n)}(\theta)\}$ is convergent for n such that

$$2n+\tfrac{1}{2}>\mathrm{Re}(\beta), \quad 0<\theta<\pi,$$
$$2n>\mathrm{Re}(\beta), \quad \theta=\pi \tag{II.4}$$

and has the following asymptotic behaviour

$$S_m^{(n)}(\theta) \underset{m\to\infty}{\sim} \begin{cases} f^{(n)}(\theta)+A(\theta)C^{(n)}(m+\tfrac{1}{2})^{\beta-\frac{1}{2}-2n}\sin\Lambda_m(\theta), \quad (0<\theta<\pi), & \text{(II.5a)}\\ f^{(n)}(\pi)+\dfrac{(-1)^m}{2}C^{(n)}(m+\tfrac{1}{2})^{\beta-2n}, \quad (\theta=\pi), & \text{(II.5b)}\end{cases}$$

where $A(\theta)$, $\Lambda_m(\theta)$ and $C^{(n)}$ are those previously defined.

Proof. Starting from (II.3), and assuming that sequence $\{S_m^{(n)}(\theta)\}$ is convergent, we may write

$$S_m^{(n)}(\theta)=\sum_{\ell=0}^{m} a_\ell^{(n)}\mathbf{P}_\ell(\cos\theta) =f^{(n)}(\theta)-\sum_{\ell=m+1}^{\infty} a_\ell^{(n)}\mathbf{P}_\ell(\cos\theta), \tag{II.6}$$

and evaluate $S_m^{(n)}$ asymptotically for large m, by replacing the terms of the series in the last equality by their large expression, to obtain

$$S_m^{(n)}(\theta) \underset{m\to\infty}{\sim} f^{(n)}(\theta) - \left(\frac{2}{\pi \sin\theta}\right)^{\frac{1}{2}} C^{(n)}$$
$$\cdot \sum_{\ell=m+1}^{\infty} (\ell+\tfrac{1}{2})^{\beta-2n-\frac{1}{2}} \cdot \cos\left[(\ell+\tfrac{1}{2})\theta - \frac{\pi}{4}\right],$$
$$(0<\theta<\pi) \tag{II.7a}$$

$$S_m^{(n)}(\pi) \underset{m\to\infty}{\sim} f^{(n)}(\pi) - C^{(n)} \sum_{\ell=m+1}^{\infty} (\ell+\tfrac{1}{2})^{\beta-2n} \cos \pi\ell \tag{II.7b}$$

where (II.2a) and well known properties of the Legendre polynomials have been used. When conditions (II.4) are satisfied, the series in (II.7) are convergent and may be summed up by using the Euler-McLaurin summation formula (7) as in the proof of Lemma 3.1 of [2], and thus (II.5) are obtained.

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C.R. Garibotti
J.E. Miraglia
Centro Atómico Bariloche
8400 Bariloche
Argentina

F.F. Grinstein
Instituto de Fisica
Universidade Federal Fluminense
Caixa Postal 296
Outeiro de São João Batista, S/N
24000 Niterói - RJ
Brasil