

# Near/far-side angular decompositions of Legendre polynomials using the amplitude-phase method

Karl-Erik Thylwe<sup>1</sup> · Patrick McCabe<sup>2</sup>

Received: 7 January 2017 / Accepted: 11 April 2017 / Published online: 5 May 2017  
© The Author(s) 2017. This article is an open access publication

**Abstract** A decomposition of Legendre polynomials into propagating angular waves is derived with the aid of an amplitude-phase method. This decomposition is compared with the 'Nussenzweig/Fuller' so called near/far-side decomposition of Legendre polynomials. The latter decomposition requires the Legendre function of the second kind. This is not the case with the amplitude-phase decomposition. Both representations have the same asymptotic expressions for large values of  $(l + 1/2) \sin \theta$ , where  $l$  and  $\theta$  are the polynomial degree and the angle respectively. Furthermore, both components of both representations satisfy the Legendre differential equation. However, we show the two representations are not identical.

**Keywords** Scattering · Legendre polynomials · Amplitude-phase method · Differential cross section · Chemical reaction theory

## 1 Introduction

Differential cross sections measure angular distributions of nuclear, atomic and molecular scattering events and are expressed in terms of angular eigenfunction expansions, typically involving several, tens or hundreds of terms [1,2]. Various approximations, like the infinite-order-sudden approximation in rotationally inelastic molecular scattering, may express differential cross sections in terms of Legendre polynomials  $P_l(\cos \theta)$ , where  $l$  and  $\theta$  are the (non-negative integer) polynomial degree and the scattering angle respectively. The analysis in terms of single Legendre polynomials

---

✉ Karl-Erik Thylwe  
ket@mech.kth.se

<sup>1</sup> KTH-Mechanics, Royal Institute of Technology, 10044 Stockholm, Sweden

<sup>2</sup> CCDC, 12 Union Road, CB2 1EZ Cambridge, UK

may be complicated. Usually semiclassical theories involving quantum interferences of semi-classical trajectories are of great help, but they involve further approximations of the partial-wave expansion [2]. An alternative, yet exact, way is to use a near/far-side decomposition. This approach collects terms in the differential cross sections corresponding to semiclassical contributions originating from repelled and attracted classical trajectories. In this way one has a complementary computational tool explaining interference structures valid beyond the semiclassical view in terms of near(repulsive)/far(attractive) trajectories [3–8].

The near/far-side analysis of differential cross sections of radially symmetric interactions based on partial-wave expansions uses decompositions of the Legendre polynomials  $P_l(\cos \theta)$  into propagating angular wave functions. The propagating angular waves are required to satisfy the Legendre differential equation and also to satisfy semiclassical expressions as  $(l + 1/2) \sin \theta \rightarrow \infty$  [3–8]. Advantages of the near/far-side decomposition of a partial-wave expansion of scattering amplitudes have been pointed out by several authors in molecular scattering [3–8], and in nuclear scattering [9–15].

An amplitude-phase method for solving second-order ordinary differential equations was recently applied to obtain Legendre functions and associated Legendre functions of the first kind [16], in particular for complex values of the degree  $l$ . The method provides numerically 'exact' solutions from analytically exact boundary conditions, in particular for calculating the Legendre polynomials. It expresses any Legendre function in terms of two fundamental amplitude-phase solutions [16]. Fundamental amplitude-phase solutions allow direct exponential representations of Legendre polynomials, without requiring linear combinations with Legendre functions of the second kind. Therefore it suggests an alternative way to separate near/far-side angular contributions in differential cross sections.

The amplitude-phase representation of the Legendre polynomial turns out to be different from the typically used propagating angular waves as defined by Nussenzveig and Fuller [17–20]. The differences are however not manifested, as shown in this study, under semiclassical conditions where scattering involves significant contributions from large angular momentum quantum numbers.

Section 2 deals with the real-valued fundamental amplitude-phase solutions of the Legendre differential equation and their behaviors as  $(l + 1/2) \sin \theta \rightarrow \infty$ . The particular linear combinations of amplitude-phase solutions representing the Legendre polynomials are presented in Sect. 3, where also the semiclassical expression of the Legendre polynomials is derived. Section 4 deals with the near/far-side components of the Legendre polynomials in terms of the amplitude-phase solutions and in the Nussenzveig/Fuller approach. In Sect. 5 the propagating angular functions of the Nussenzveig/Fuller- and the amplitude-phase types corresponding to Legendre polynomials are compared numerically. Conclusions are in Sect. 6.

## 2 Fundamental amplitude-phase solutions of the Legendre differential equation

The Legendre functions  $P_l(\cos \theta)$  and  $Q_l(\cos \theta)$  satisfy the Legendre differential equation [21]

$$y''(\theta) + \cot \theta y'(\theta) + [l(l+1)]y(\theta) = 0, \quad (1)$$

where the prime,  $'$ , denotes differentiation with respect to the angle  $\theta$  ( $0 \leq \theta \leq \pi$ ). The degree  $l$  is assumed to be a non-negative integer, although the amplitude-phase formulas presented are still valid without this assumption. By introducing a new angular function

$$\chi(\theta) = (\sin \theta)^{1/2} y(\theta) \quad (2)$$

in (1), one finds

$$\chi''(\theta) + \left( (l+1/2)^2 + \frac{1}{4 \sin^2 \theta} \right) \chi(\theta) = 0. \quad (3)$$

The amplitude-phase method [16] is applied to Eq. (3) by assuming fundamental solutions of either exponential form

$$\chi_{\pm}(\theta) = u(\theta) \exp(\pm i \phi(\theta)), \quad (4)$$

or trigonometric form

$$\begin{pmatrix} \chi_s(\theta) \\ \chi_c(\theta) \end{pmatrix} = u(\theta) \begin{pmatrix} \sin \phi(\theta) \\ \cos \phi(\theta) \end{pmatrix}, \quad (5)$$

where in both cases the phase  $\phi(\theta)$  depends on the amplitude  $u(\theta)$  via

$$\phi'(\theta) = u^{-2}(\theta). \quad (6)$$

The amplitude function  $u(\theta) > 0$  is any solution of the non-linear Milne-type differential equation [16]

$$u''(\theta) + \left( (l+1/2)^2 + \frac{1}{4 \sin^2 \theta} \right) u(\theta) = u^{-3}(\theta). \quad (7)$$

Since the coefficient in (3) is symmetric with respect to  $\theta = \pi/2$  it is possible to use a symmetrical amplitude function  $u(\theta) = u(\pi - \theta)$ .

From (2), the fundamental amplitude-phase solutions of Eq. (1) are:

$$\begin{pmatrix} y_s(\theta) \\ y_c(\theta) \end{pmatrix} = (\sin \theta)^{-1/2} u(\theta) \begin{pmatrix} \sin \phi(\theta) \\ \cos \phi(\theta) \end{pmatrix}, \quad \phi'(\theta) = u^{-2}(\theta). \quad (8)$$

An unspecified integration constant in (6) defining  $\phi(\theta)$  completely will be introduced so that

$$\phi(\pi/2) = 0. \quad (9)$$

This choice is based on the presence of particular values for  $P_l(\cos \theta)$  and  $Q_l(\cos \theta)$  for  $\theta = \pi/2$  [22], where the boundary conditions of  $u(\theta)$  are defined [16].

## 2.1 Asymptotic behaviors of the fundamental amplitude-phase solutions

Equation (7) is solved algebraically for the amplitude  $u$  by assuming  $u$  is sufficiently slowly varying that  $u'$  and  $u''$  can be neglected, leading to

$$u^{-2} = \left( (l + 1/2)^2 + \frac{1}{4 \sin^2 \theta} \right)^{1/2} \approx (l + 1/2) \left( 1 + \frac{1}{8(l + \frac{1}{2})^2 \sin^2 \theta} + \dots \right). \quad (10)$$

The approximation is valid provided  $(l + 1/2) \sin \theta \gg 1$ . The phase  $\phi$  in (8) then has an asymptotic (large- $l$ ) approximation

$$\phi \approx (l + 1/2)\theta - (l + 1/2)\pi/2, \quad (l + 1/2) \sin \theta \gg 1, \quad (11)$$

where the integration constant  $-(l + 1/2)\pi/2$  is chosen so that  $\phi = 0$  for  $\theta = \pi/2$ .

The fundamental amplitude-phase solutions of (8) thus have the large- $l$  approximations:

$$\begin{pmatrix} y_s \\ y_c \end{pmatrix} \approx ((l + 1/2) \sin \theta)^{-1/2} \begin{pmatrix} \sin \left[ \left( l + \frac{1}{2} \right) \left( \theta - \frac{\pi}{2} \right) \right] \\ \cos \left[ \left( l + \frac{1}{2} \right) \left( \theta - \frac{\pi}{2} \right) \right] \end{pmatrix}, \quad (l + 1/2) \sin \theta \gg 1. \quad (12)$$

When analyzed with the aid of trigonometric relations one obtains

$$\begin{pmatrix} y_s \\ y_c \end{pmatrix} \approx ((l + 1/2) \sin \theta)^{-1/2} \begin{pmatrix} -\sin \left( \frac{\pi l}{2} \right) \cos \left[ \left( l + \frac{1}{2} \right) \theta - \frac{\pi}{4} \right] \\ \cos \left( \frac{\pi l}{2} \right) \cos \left[ \left( l + \frac{1}{2} \right) \theta - \frac{\pi}{4} \right] \end{pmatrix}, \quad (l + 1/2) \sin \theta \gg 1. \quad (13)$$

Asymptotic expressions of  $P_l(\cos \theta)$  and  $Q_l(\cos \theta)$  are obtained by appropriate linear combinations of  $y_s$  and  $y_c$  in (12). They are discussed in the subsequent section.

## 3 Amplitude-phase expressions of Legendre polynomials

Values for  $\chi(\theta)$  (and  $\chi'(\theta)$ ) satisfying Eq. (3) and relevant for computing Legendre functions of the *first* kind are given for  $\theta = \pi/2$  (see [22])

$$\chi_{\pi/2}^{(1)} = \frac{1}{\sqrt{\pi}} \cos \left( \frac{\pi l}{2} \right) \frac{\Gamma \left( \frac{1}{2} + \frac{l}{2} \right)}{\Gamma \left( 1 + \frac{l}{2} \right)}, \quad (14)$$

$$\chi'_{\pi/2}^{(1)} = -\frac{2}{\sqrt{\pi}} \sin \left( \frac{\pi l}{2} \right) \frac{\Gamma \left( 1 + \frac{l}{2} \right)}{\Gamma \left( \frac{1}{2} + \frac{l}{2} \right)}. \quad (15)$$

The superscript '(1)' refers to 'the *first* kind' and  $\chi_{\pi/2}^{(1)}$  is shorthand for  $\chi^{(1)}(\pi/2)$ , as for the corresponding derivative  $\chi'^{(1)}(\pi/2)$ . The minus sign in Eq. (15) comes from the differential relation  $d \cos \theta = -d \sin \theta$ .

By fitting the fundamental amplitude-phase solutions  $y_s$  and  $y_c$  to the specific values (14) and (15), exact representations of the Legendre polynomials can be obtained as [16]

$$P_l(\cos \theta) = (\sin \theta)^{-1/2} u(\theta) \left( \chi'_{\pi/2}{}^{(1)} u_{\pi/2} \sin \phi(\theta) + \chi_{\pi/2}^{(1)} / u_{\pi/2} \cos \phi(\theta) \right), \quad (16)$$

where  $\chi'_{\pi/2}{}^{(1)} u_{\pi/2}$  and  $\chi_{\pi/2}^{(1)} / u_{\pi/2}$  are the appropriate factors of the amplitude-phase fundamental solutions. The notation  $u_{\pi/2}$  is defined by

$$u_{\pi/2} = \left[ l(l+1) + \frac{1}{2} \right]^{-1/4}, \quad (17)$$

which is obtained from the boundary conditions of the symmetric amplitude function  $u(\theta)$  for  $\theta = \pi/2$  [16].

For odd integer values of  $l$  the amplitude-phase expression (16) is

$$P_l(\cos \theta) = (\sin \theta)^{-1/2} \chi'_{\pi/2}{}^{(1)} u_{\pi/2} u(\theta) \sin \phi(\theta), \quad (\text{odd } l) \quad (18)$$

$$= \chi'_{\pi/2}{}^{(1)} u_{\pi/2} y_s, \quad (19)$$

and for even integer values of  $l$

$$P_l(\cos \theta) = (\sin \theta)^{-1/2} \chi_{\pi/2}^{(1)} / u_{\pi/2} u(\theta) \cos \phi(\theta), \quad (\text{even } l) \quad (20)$$

$$= \chi_{\pi/2}^{(1)} / u_{\pi/2} y_c. \quad (21)$$

Near the angle  $\theta = \pi/2$ , used in the boundary conditions of the amplitude function, the representations (18) and (20) can be expanded as

$$P_l(\cos \theta) \approx \chi'_{\pi/2}{}^{(1)} (\theta - \pi/2) + O\left((\theta - \pi/2)^3\right) \quad (\text{odd } l) \quad (22)$$

and

$$P_l(\cos \theta) \approx \chi_{\pi/2}^{(1)} + O\left((\theta - \pi/2)^2\right) \quad (\text{even } l) \quad (23)$$

respectively. These expansions are exact to the explicit order shown and based on the even symmetry of  $u(\theta)$  with respect to  $\theta = \pi/2$ .

### 3.1 Asymptotic expression of Legendre polynomials

For large integer values of  $l$  it is possible to compare formulas of the present amplitude-phase approach with standard asymptotic expressions for the Legendre polynomials (see e.g. [18, 19] and/or McCabe and Connor [3–8]), given by

$$P_l(\cos \theta) \approx \sqrt{\frac{2}{\pi(l+1/2)\sin \theta}} \cos((l+1/2)\theta - \pi/4), \quad (l+1/2)\sin \theta \gg 1, \quad (24)$$

valid for all large non-negative integers  $l$ . The two amplitude-phase expressions to compare with are

$$P_l(\cos \theta) \approx -\sin\left(\frac{\pi l}{2}\right) \left(\chi_{\pi/2}^{(1)}/u_{\pi/2}\right) \sqrt{\frac{1}{(l+1/2)\sin \theta}} \cos((l+1/2)\theta - \pi/4), \quad (l+1/2)\sin \theta \gg 1, \quad (25)$$

for odd integers of  $l$ , and

$$P_l(\cos \theta) \approx \cos\left(\frac{\pi l}{2}\right) \left(\chi_{\pi/2}^{(1)}/u_{\pi/2}\right) \sqrt{\frac{1}{(l+1/2)\sin \theta}} \cos((l+1/2)\theta - \pi/4), \quad (l+1/2)\sin \theta \gg 1, \quad (26)$$

for even integers of  $l$ .

From (25), (26) in comparison with (24), one observes the different factors in asymptotic expressions. By hypothesis, the following asymptotic relations hold

$$-\sin\left(\frac{\pi l}{2}\right) \chi_{\pi/2}^{(1)}/u_{\pi/2} \sim \sqrt{\frac{2}{\pi}}, \quad (l+1/2) \gg 1 \quad (\text{odd } l), \quad (27)$$

$$\cos\left(\frac{\pi l}{2}\right) \chi_{\pi/2}^{(1)}/u_{\pi/2} \sim \sqrt{\frac{2}{\pi}}, \quad (l+1/2) \gg 1 \quad (\text{even } l). \quad (28)$$

From (14) and (15) one obtains

$$-\sin\left(\frac{\pi l}{2}\right) \chi_{\pi/2}^{(1)}/u_{\pi/2} = \frac{2}{\sqrt{\pi}} \frac{\Gamma(1 + \frac{l}{2}) u_{\pi/2}}{\Gamma(\frac{1}{2} + \frac{l}{2})}, \quad (29)$$

$$\cos\left(\frac{\pi l}{2}\right) \chi_{\pi/2}^{(1)}/u_{\pi/2} = \frac{1}{\sqrt{\pi}} \frac{\Gamma(\frac{1}{2} + \frac{l}{2})}{\Gamma(1 + \frac{l}{2}) u_{\pi/2}}. \quad (30)$$

so the key asymptotic relation to be proved in order to derive the well-known semi-classical expression (24) is

$$\frac{\Gamma(\frac{1}{2} + \frac{l}{2})}{\Gamma(1 + \frac{l}{2}) u_{\pi/2}} \approx \sqrt{2}, \quad l \rightarrow \infty. \quad (31)$$

In fact, with the use of the asymptotic formula (5) on page 32 in [23], i.e.

$$\ln \Gamma\left(\frac{1}{2} + z\right) \approx z \ln z - z + \frac{1}{2} \ln(2\pi), \quad z \rightarrow \infty, \quad (32)$$

one obtains

$$\ln \left[ \frac{\Gamma\left(\frac{1}{2} + \frac{l}{2}\right)}{\Gamma\left(1 + \frac{l}{2}\right) u_{\pi/2}} \right] \approx \frac{1}{2} \ln 2, \quad (33)$$

which proves the semiclassical formula (24) for large  $l$  based on the amplitude-phase approach.

## 4 Near/far-side decompositions

### 4.1 The amplitude-phase near/far-side decomposition

This decomposition is the one introduced in Ref. [16] for complex values of  $l$  with  $\text{Re } l > -1/2$ . From (16) there is an obvious decomposition of  $P_l(\cos \theta)$  in terms of Jost-type propagating angular functions

$$P_l^{(\pm)}(\cos \theta) = \frac{1}{2} (\sin \theta)^{-1/2} u(\theta) \left( \chi_{\pi/2}^{(1)} / u_{\pi/2} \mp i \chi_{\pi/2}'^{(1)} u_{\pi/2} \right) \exp(\pm i \phi(\theta)), \quad (34)$$

satisfying

$$P_l(\cos \theta) = P_l^{(+)}(\cos \theta) + P_l^{(-)}(\cos \theta). \quad (35)$$

The solutions  $P_l^{(\pm)}(\cos \theta)$  satisfy the Legendre differential equation, since they are linear combinations of the real-valued fundamental solutions  $y_s$  and  $y_c$ . For odd integer values of  $l$  the amplitude-phase expressions (34) simplify to

$$P_l^{(\pm)}(\cos \theta) = \mp i \frac{1}{2} (\sin \theta)^{-1/2} \chi_{\pi/2}'^{(1)} u_{\pi/2} u(\theta) \exp(\pm i \phi(\theta)), \quad (\text{odd } l). \quad (36)$$

For even integer values of  $l$  expressions (34) simplify to

$$P_l^{(\pm)}(\cos \theta) = \frac{1}{2} (\sin \theta)^{-1/2} \chi_{\pi/2}^{(1)} / u_{\pi/2} u(\theta) \exp(\pm i \phi(\theta)), \quad (\text{even } l). \quad (37)$$

Using Euler's formula for the exponential factor in (34), one obtains

$$\begin{aligned} P_l^{(\pm)}(\cos \theta) = & \frac{1}{2} (\sin \theta)^{-1/2} u(\theta) \left( \chi_{\pi/2}^{(1)} / u_{\pi/2} \sin \phi(\theta) + \chi_{\pi/2}'^{(1)} / u_{\pi/2} \cos \phi(\theta) \right) \\ & \mp i \frac{1}{2} (\sin \theta)^{-1/2} u(\theta) \left( \chi_{\pi/2}'^{(1)} / u_{\pi/2} \cos \phi(\theta) - \chi_{\pi/2}^{(1)} / u_{\pi/2} \sin \phi(\theta) \right), \end{aligned} \quad (38)$$

valid for all non-negative integers  $l$ . Equation (38) can be written

$$P_l^{(\pm)}(\cos \theta) = \frac{1}{2} (P_l(\cos \theta) \mp i R_l(\cos \theta)), \quad (39)$$

with the real function  $R_l(\cos \theta)$  being defined by

$$R_l(\cos \theta) = (\sin \theta)^{-1/2} u(\theta) \left( \chi'_{\pi/2} u_{\pi/2} \cos \phi(\theta) - \chi_{\pi/2}^{(1)} / u_{\pi/2} \sin \phi(\theta) \right). \quad (40)$$

$R_l(\cos \theta)$  is a solution of the Legendre differential equation since it is a linear combination of exact (amplitude-phase) solutions.

## 4.2 Nussenzveig/Fuller near/far-side decomposition

The propagating angular functions used in the Nussenzveig/Fuller decomposition involve both  $P_l(\cos \theta)$  and  $Q_l(\cos \theta)$ , and are defined as [18–20, 22]

$$Q_l^{(\pm)}(\cos \theta) = \frac{1}{2} \left( P_l(\cos \theta) \mp \frac{2i}{\pi} Q_l(\cos \theta) \right). \quad (41)$$

This decomposition can also be expressed in terms of the same amplitude-phase fundamental solutions, which is done for the first time in this paper. With the analogical approach to Sects. 2 and 3 one finds for  $Q_l(\cos \theta)$

$$Q_l(\cos \theta) = (\sin \theta)^{-1/2} u(\theta) \left( \chi'_{\pi/2} u_{\pi/2} \sin \phi(\theta) + \chi_{\pi/2}^{(2)} / u_{\pi/2} \cos \phi(\theta) \right), \quad (42)$$

where  $\chi'_{\pi/2} u_{\pi/2}$  and  $\chi_{\pi/2}^{(2)} / u_{\pi/2}$  are the new factors in the linear combinations of the amplitude-phase fundamental solutions. While  $u_{\pi/2}$  is the same as in (17), values for  $\chi_{\pi/2}^{(2)}$  and  $\chi'_{\pi/2}$  relevant for computing Legendre functions of the second kind at  $\theta = \pi/2$  are

$$\chi_{\pi/2}^{(2)} = -\frac{\sqrt{\pi}}{2} \sin \left( \frac{\pi l}{2} \right) \frac{\Gamma \left( \frac{1}{2} + \frac{l}{2} \right)}{\Gamma \left( 1 + \frac{l}{2} \right)}, \quad (43)$$

$$\chi'_{\pi/2} = -\sqrt{\pi} \cos \left( \frac{\pi l}{2} \right) \frac{\Gamma \left( 1 + \frac{l}{2} \right)}{\Gamma \left( \frac{1}{2} + \frac{l}{2} \right)}, \quad (44)$$

which are also obtained from reference [22].

## 5 Numerical comparison

The amplitude-phase method provides ways of calculating Legendre functions of the first or second kind in terms of fundamental solutions of Legendre's differential equation. It is then possible to compare the two near/far-side representations presented in Sect. 4. Hence, Eqs. (39) and (41) are the two (exact) near/far-side representations compared numerically in the present section.

Differences in  $Q_l^{(\pm)}(\cos \theta)$  and  $P_l^{(\pm)}(\cos \theta)$  occur only in the imaginary parts. In a series of tables the differences of the imaginary parts can be seen for small, medium

**Table 1** Numerical comparison of the imaginary parts of  $Q_3^{(+)}(\cos \theta)$  and  $P_3^{(+)}(\cos \theta)$  for selected values of the angle  $\theta$ 

$\theta/^\circ$	$\text{Im } Q_3^{(+)}(\cos \theta)$	$\text{Im } P_3^{(+)}(\cos \theta)$
5	−0.396551939796008	−0.396412615667989
15	0.011252516825386	0.011248563378341
25	0.200897859221705	0.200827275985947
35	0.268338287533512	0.268244009850886
45	0.235275455754521	0.235192794331319
55	0.130350634271783	0.130304837021450
65	−0.006178921957558	−0.006176751061825
75	−0.129825363966732	−0.129779751264299
85	−0.202571714339455	−0.202500543013258

**Table 2** Numerical comparison of the imaginary parts of  $Q_{30}^{(+)}(\cos \theta)$  and  $P_{30}^{(+)}(\cos \theta)$  for selected values of the angle  $\theta$ 

$\theta/^\circ$	$\text{Im } Q_{30}^{(+)}(\cos \theta)$	$\text{Im } P_{30}^{(+)}(\cos \theta)$
5	0.234615351459853	0.234615368359349
15	0.111215921672006	0.111215929682961
25	−0.005817186004943	−0.005817186423959
35	−0.080725653595215	−0.080725659409937
45	−0.079219865834323	−0.079219865834323
55	−0.017049671863151	−0.017049673091250
65	0.051365737103799	0.051365740803706
75	0.072855536558358	0.072855541806189
85	0.033393747988477	0.033393750393851

and large integer values of  $l$ , and a sequence of  $\theta$ . MatLab (version 10a) was used for the computations and the relative and absolute errors are controlled by the 'tol' parameter, set to  $2.3 \times 10^{-14}$ .

Tables 1, 2 and 3 show values of the imaginary parts of  $Q_l^{(+)}(\cos \theta)$  and  $P_l^{(+)}(\cos \theta)$ . Values of  $Q_l^{(-)}(\cos \theta)$  and  $P_l^{(-)}(\cos \theta)$  are obtained by complex conjugate symmetry. The real parts agree to all significant figures.

Table 1 shows results for  $l = 3$  and a restricted sequence of angles in the range  $5 \leq \theta/^\circ \leq 85$ . The polynomials exhibit exact symmetries about  $\theta = 90^\circ$ . The entries for a given angle agree to about 3 decimal positions. Low values of the angular momentum quantum number are relevant in electron- and in other sub-atomic scattering problems. For such values the semiclassical condition  $(l + 1/2) \sin \theta \gg 1$  may not be satisfied.

Table 2 shows results for  $l = 30$  and the same restricted angular region. The entries for a given angle agree to about 7 decimal positions. This value of  $l$  represents typical angular momenta in atomic orbiting and rainbow scattering of hydrogen.

Table 3 shows results for  $l = 300$  and the same angles. The entries for a given angle agree to about 12 decimal positions. Large values of  $l$  are typical for atomic collisions with large reduced masses compared to the case of hydrogen scattering. Further results (not shown) indicate that the agreements are independent of the parity of  $l$ .

**Table 3** Numerical comparison of the imaginary parts of  $Q_{300}^{(+)}(\cos \theta)$  and  $P_{300}^{(+)}(\cos \theta)$  for selected values of the angle  $\theta$ 

$\theta/^\circ$	$\text{Im } Q_{300}^{(+)}(\cos \theta)$	$\text{Im } P_{300}^{(+)}(\cos \theta)$
5	0.023085715194327	0.023085715194494
15	0.027593673426331	0.027593673426530
25	−0.035365628346761	−0.035365628347017
35	0.016311824755513	0.016311824755631
45	0.010483837095221	−0.235275455754521
55	−0.024826451939561	−0.024826451939741
65	0.017819818789656	0.017819818789785
75	0.003059009369289	0.003059009369311
85	−0.020452790176916	−0.020452790177063

**Table 4** Numerical comparison of the imaginary parts of  $Q_l^{(+)}(\cos \theta)$  and  $P_l^{(+)}(\cos \theta)$  for the angle  $\theta = 10^{-7}$  and two values of  $l$ 

$l$	$\text{Im } Q_l^{(+)}(\cos \theta)$	$\text{Im } P_l^{(+)}(\cos \theta)$
1	−6.32146	−6.28012
10	−5.70746	−5.70748

At forward angles close to  $\theta = 0$ , and backward angles close to  $\theta = 180^\circ$ , both angular functions diverge with similar numerical agreements depending mainly on the magnitude of  $l$ . Table 4 shows the numerical values of the imaginary parts of  $Q_l^{(+)}(\cos \theta)$  and  $P_l^{(+)}(\cos \theta)$ , for  $\theta = 10^{-7}$  and  $l = 1, 10$ . At larger values of  $l$  the agreement improves.

There are problems with the separation of a Legendre polynomial into its natural propagating angular functions at such small values of  $l$ . Since the asymptotic condition  $((l + 1/2) \sin \theta \gg 1)$  is not satisfied for small values of  $l$ ; how can two near/far-side methods with the same asymptotic condition satisfied be seen as 'exact methods'? Explicitly, for  $l = 0$  one has  $P_0(\cos \theta) = 1$  and it is not clear how to separate unity into two near/far-side angular waves other than in a symmetric way; for  $l = 1$  one has  $P_1(\cos \theta) = \cos \theta = \frac{1}{2} (e^{i\theta} + e^{-i\theta})$ , where the *natural* propagating angular functions ( $e^{\pm i\theta}$ ) do not satisfy the Legendre equation separately. At present the near/far-side analysis of scattering seems to be an analysis slightly more useful than the semiclassical trajectory method mentioned in the introduction [2].

## 6 Conclusion

A near/far-side decomposition of Legendre polynomials is derived with the aid of an amplitude-phase method. For large values of  $(l + 1/2) \sin \theta$  expressions of the Legendre polynomial and its near/far-side components are shown to agree with the well-known semiclassical expressions. The 'Nussenzveig/Fuller' near/far-side components of Legendre polynomials are also known to satisfy the semiclassical expressions.

On account of similar numerical and asymptotic (semiclassical) properties, the Legendre polynomials can be represented by both types of complex conjugate pairs of propagating angular functions, (39) and (41), compared in this paper.

However, it is shown that the amplitude-phase and the Nussenzweig/Fuller representations are not identical. The amplitude-phase decomposition uses only functional properties of the Legendre polynomial itself, while the Nussenzweig/Fuller decomposition also uses properties of the corresponding Legendre function of the second kind. Non-negligible numerical differences occur for Legendre polynomials of degrees  $l = 1$  (and to a lesser extent for  $l = 2$  and 3). Such a difference would possibly affect near/far-side analysis of (sub-)nuclear scattering at low energies, but not near/far-side analysis of non-resonant very low energy heavy-particle scattering.

**Acknowledgements** The authors thank Professor JNL Connor for inspiring discussions, and the referees for their careful reading of the original manuscript.

**Open Access** This article is distributed under the terms of the Creative Commons Attribution 4.0 International License (<http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted use, distribution, and reproduction in any medium, provided you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license, and indicate if changes were made.

## References

1. C.J. Joachain, *Quantum Collision Theory* (Elsevier Science Publishers B.V., North-Holland, Amsterdam, 1975)
2. M.S. Child, *Molecular Collision Theory* (Dover, New York, 1996)
3. G. Guillon, T. Stoecklin, Eur. Phys. J. D At. Mol. Opt. Plasma Phys. **39**(3), 359 (2006)
4. P. McCabe, J.N.L. Connor, D. Sokolovski, J. Chem. Phys. **114**, 5194 (2001)
5. J.J. Hollifield, J.N.L. Connor, Mol. Phys. **97**(1–2), 293 (1999)
6. P. McCabe, J.N.L. Connor, J. Chem. Phys. **104**, 2297 (1996)
7. H. Carsten, S. Schmatz, Phys. Chem. Chem. Phys. **17**(40), 2667076 (2015)
8. M. Hankel, J.N.L. Connor, Nearside-farside, local angular momentum and resummation theories: useful tools for understanding the dynamics of complex-mode reactions. AIP Adv. **5**(7), 077160 (2015)
9. R. Anni, J.N.L. Connor, C. Noli, Phys. Rev. C **66**, 044610 (2002)
10. R. Anni, Phys. Rev. C **67**, 057601 (2003)
11. K.W. Mcvay, G.R. Satchler, Nucl. Phys. Sect. A **581**(3), 665 (1995)
12. Y. Sakuragi, J. Phys. G Nucl. Phys. **16**(4), 639 (1990)
13. A. Farooq, G. Ra, S. Roman, Nucl. Phys. Sect. A **469**(2), 313 (1987)
14. K. Heck, G. Grawert, D. Mukhopadhyay, Nucl. Phys. Sect. A **437**(1), 226 (1985)
15. D.R. Dean, J. Phys. G Nucl. Phys. **10**(4), 493 (1984)
16. K.-E. Thylwe, P. McCabe, Commun. Theor. Phys. J. **64**, 9 (2015)
17. K.-E. Thylwe, J. Phys. A: Math. Gen. **16**, 1141 (1983)
18. H.M. Nussenzweig, J. Math. Phys. **10**, 82 (1969)
19. H.M. Nussenzweig, *Causality and Dispersion Relations* (Academic, New York, 1972)
20. R.C. Fuller, Phys. Rev. C **12**, 1561 (1975)
21. L.D. Landau, E.M. Lifschitz, *Quantum Mechanics (Non-Relativistic Theory)* (Pergamon, Oxford, 1965), Ch VII
22. M. Abramowitz, I.A. Stegun (eds.), *Handbook of Mathematical Functions* (Dover, New York, 1972)
23. Y.L. Luke, *The Special Functions and Their Approximations*, vol. I (Academic Press, New York, 1969)