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Expansion of continuum wave solutions in terms of standing natural functions

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Abstract. It is shown that in the interior region of a finite-range potential a continuum outgoing wave solution may be expressed as an infinite sum involving standing natural functions, which are defined as the residues at the poles, real and complex, of the corresponding standing Green function of the problem. The above representation is valid provided the elastic scattering by the potential is known.

1. Introduction

It is the aim of this paper to show that standing natural functions may be used to expand continuum outgoing wave solutions of the radial Schrödinger equation along the internal region of the potential for an interaction of finite range provided the elastic scattering dependence on momentum is known.

In recent years there have been a number of works (García-Calderón 1976, García-Calderón and Rubio 1981, Bang *et al* 1978, 1980) concerning this problem. All of them are based on expansions in terms of the poles of the outgoing Green function of the problem, which are complex. In the present work we should like to explore such expansions by using the poles of the standing Green function. The residues at the poles of this function are solutions to the corresponding Schrödinger equation obeying the so called natural standing boundary conditions (Vitturi and Zardi 1974, García-Calderón and Berrondo 1979a). Though in general the corresponding eigenvalues are complex, a finite number of them stand on the real axis. These real poles correspond to a situation where the elastic phaseshift attains a value $\frac{1}{2}\pi$ and are essentially related to the presence of either resonances or antiresonances (echoes) in the elastic cross section (García-Calderón and Berrondo 1979a, Humblet 1970, 1972). It is this fact which provides a distinctive feature to the real poles of the standing Green function, which has mainly instigated the present work.

The poles and corresponding eigenfunctions, which we call standing natural functions, of the standing natural Green function have been used in the expansion of the K or Q matrices (Vitturi and Zardi 1974, García-Calderón and Berrondo 1979a, Humblet 1970, 1972) in scattering theory. Actually, since the K or Q matrices depend only on the momentum or the energy, standing natural functions enter into such expansions for a given value of the relative distance r , which is usually taken at the surface of the interaction potential. In the present discussion there is, in addition to the

energy, a dependence on the radial coordinate r along the internal region of the potential.

The paper is organised as follows. In § 2 the expansion of the continuum wave solution in terms of standing natural functions is derived. Section 3 deals with an exactly solvable problem, the repulsive delta shell potential, and there a comparison is made between the exact results for the continuum wavefunction and its approximate values using the expansion in terms of real standing solutions. Finally § 4 draws the conclusions to be made from this paper.

2. Expansion

Let us write the Schrödinger equation for the continuum outgoing solution $\Psi_l^+(k, r)$, associated with a given angular momentum l , as

$$\frac{d^2}{dr^2}\Psi_l^+(k, r) + \left(k^2 - V(r) - \frac{l(l+1)}{r^2}\right)\Psi_l^+(k, r) = 0 \quad (1)$$

where $k^2 = E$ is the energy in units where $\hbar = 2m = 1$ and $V(r)$ is a central potential of range a . The corresponding boundary conditions are

$$\begin{aligned} \Psi_l^+(k, r=0) &= 0 \\ \Psi_l^+(k, r) &= \frac{1}{2i}[h_l^{(-)}(kr) - S_l(k)h_l^{(+)}(kr)] \quad r \geq a \end{aligned} \quad (2)$$

where $S_l(k) = \exp(2i\delta_l(k))$ is the S matrix of the problem, $\delta_l(k)$ the corresponding phaseshift, and $h_l^{(-)}(kr)$ and $h_l^{(+)}(kr)$ are respectively the ingoing and outgoing Riccati-Hankel functions (Taylor 1972).

The standing Green function of the problem satisfies

$$\frac{\partial^2}{\partial r^2}G_l(r, r'; k^2) + \left(k^2 - V(r) - \frac{l(l+1)}{r^2}\right)G_l(r, r'; k^2) = \delta(r - r') \quad (3)$$

with boundary conditions at $r = 0$ and $r = a_+$ given by†

$$\begin{aligned} G_l(r=0, r'; k^2) &= 0 \\ \left(\frac{\partial}{\partial r}G_l(r, r'; k^2) - b_l(k, r)G_l(r, r'; k^2)\right)_{r=a_+} &= 0 \quad r' \leq a \end{aligned} \quad (4)$$

where $b_l(k, r)$ is defined as

$$b_l(k, r) = \frac{\eta_l'(k, r)}{\eta_l(k, r)} \quad (5)$$

here the prime denotes derivative with respect to r and $\eta_l(k, r)$ is an irregular solution of equation (4) which for $r \geq a$ becomes the Riccati-Neumann function (Taylor 1972). Using Green's theorem between equations (1) and (3), integrating from $r = 0$ to $r = a$, and the corresponding boundary conditions leads after simple manipulations to the expression

$$\Psi_l^+(k, r) = -\frac{k(1 + S_l(k))}{2\eta_l(ka)}G_l(r, a; k^2) \quad r \leq a. \quad (6)$$

† We define $a_+ = \lim_{\epsilon \rightarrow 0} a + \epsilon$.

The standing Green function $G_l(r, a; k^2)$ is a meromorphic function of the complex variable k^2 . Its only singularities are poles, real and complex, distributed in the k^2 plane. They are the same as those of the K and Q functions (García-Calderón and Berrondo 1979, Humblet 1970). We shall assume that the poles are simple. This is not a very strong assumption because poles of second or higher order occur only in special circumstances and can be treated as limiting cases of simple poles (García-Calderón and Berrondo 1979a, Humblet 1970).

Therefore, as one sees from equation (6), the expansion of $\Psi_l^+(k, r)$ results from the expansion of $G_l(r, a; k^2)$ in terms of its poles. The expansion may be obtained by using Cauchy's theorem. The interesting point (García-Calderón and Berrondo 1979b) is that for $r' = a$ and $r < a$, i.e. equation (6), the standing Green function has the behaviour

$$G_l(r, a; k^2) \rightarrow 0 \quad \text{as } |k^2| \rightarrow \infty \quad (7)$$

in all directions of the k^2 plane and therefore no integral or subtractions terms result in the Cauchy expansion. Hence

$$G_l(r, a; k^2) = \sum_n \frac{\rho_{nl}(r, a)}{k^2 - k_{nl}^2} \quad r < a. \quad (8)$$

The expression for the residues $\rho_{nl}(r, r')$ has been derived elsewhere (García-Calderón 1976, García-Calderón and Rubio 1981). For $r' = a$ it reads

$$\rho_{nl}(r, a) = \omega_{nl}(r)\omega_{nl}(a) \quad (9)$$

provided the standing natural functions $\omega_{nl}(r)$, which satisfy the Schrödinger equation with eigenvalue k_{nl}^2 and boundary conditions $\omega_{nl}(0) = 0$ and $[\omega'_{nl}(r) - b_l(k_n, r)\omega_{nl}(r)]_{r=a+} = 0$, are normalised according to the condition (García-Calderón and Berrondo 1979a, Vitturi and Zardi 1974)

$$\int_0^a \omega_{nl}^2(r) dr + \left(\frac{d}{dk^2} b_l(k, r) \right)_{k^2=k_{nl}^2} \omega_{nl}^2(a) = 1. \quad (10)$$

The normalisation condition is independent of the energy and can also be shown to be independent of the value of a provided this is taken at or beyond the range of the potential (García-Calderón and Berrondo 1979a). Therefore, using equation (8) in equation (6) leads to the expansion

$$\Psi_l^+(k, r) = \sum_n C_{nl}(k)\omega_{nl}(r) \quad r < a \quad (11)$$

where the expansion coefficients $C_{nl}(k)$ are given by

$$C_{nl}(k) = \frac{k\omega_{nl}(a)(1 + S_l(k))}{2\eta_l(ka)(k_{nl}^2 - k^2)}. \quad (12)$$

Hence for a given value of k we have obtained an expansion of the continuum outgoing solution $\Psi_l^+(k, r)$ in terms of a discrete summation over the standing natural functions of the problem, valid in the interior region of the potential.

It follows from equation (12) that the expansion coefficient for a given value of k , $C_{nl}(k)$, depends on elastic scattering by the potential through the scattering matrix $S_l(k)$. This situation, which is absent in expansions involving the outgoing Green function of the problem (García-Calderón 1976, García-Calderón and Rubio 1981), is the price one has to pay if one intends to use standing natural functions. Alternatively

one may write equation (12) in terms of the Q matrix by using the relationship (García-Calderón and Berrondo 1979a, Humblet 1970)

$$Q_l(k) = \frac{S_l(k) - 1}{S_l(k) + 1} \frac{1}{ik^{2l+1}}. \quad (13)$$

The above expression is particularly useful if one is very near a real pole k_{nl}^2 since then (Humblet 1970)

$$Q_l(k) \approx -\frac{\omega_{nl}^2(a)}{k^2 - k_{nl}^2} \frac{1}{k_{nl}^{2l} \eta_l^2(k_{nl}a)}, \quad (14)$$

consequently, using (12), (13) and (14) one obtains for $\Psi^+(k, r)$ at a pole k_{nl}^2

$$\Psi^+(k_{nl}, r) \approx i \frac{\eta_l(k_{nl}a)}{\omega_{nl}(a)} \omega_{nl}(r) \quad r \leq a. \quad (15)$$

We observe the interesting fact that at a given pole, either a resonance or an antiresonance pole, the continuum wave solution may be written as the corresponding standing natural eigenfunction times a coefficient which depends on the value at the radius $r = a$. Furthermore, we observe also that the resulting expression is independent of the normalisation condition for the standing natural functions.

3. Solvable model

In order to illustrate the expansion presented in the previous section, we consider in this section an exactly solvable problem, namely a repulsive delta shell potential of range a and strength λ , i.e. $V(r) = \lambda \delta(r - a)$. For the sake of simplicity we take angular momentum $l = 0$.

The exact continuum solution to the radial Schrödinger equation of the problem may be written as in equation (6) or equivalently in terms of the regular solution and the Jost function (Taylor 1972), i.e.

$$\Psi^+(k, r) = \frac{\sin kr}{1 + (\lambda/k) \sin ka e^{ika}}. \quad (16)$$

The expansion of $\Psi^+(k, r)$ in terms of standing natural functions requires the scattering matrix $S(k)$, which is given by (García-Calderón and Herrera Mote 1980, Gottfried 1966)

$$S(k) = \frac{1 + (\lambda/k) \sin ka e^{-ika}}{1 + (\lambda/k) \sin ka e^{ika}}. \quad (17)$$

The standing eigenfunctions $\omega_n(r)$ of the problem along the interior region of the potential are given by

$$\omega_n(r) = \alpha_n \sin k_n r \quad r \leq a \quad (18)$$

where the normalisation coefficient α_n is obtained from equation (10), i.e.

$$\alpha_n^2 = \frac{2k_n \cos k_n a}{2k_n a \cos k_n a + (\lambda a - 1) \sin k_n a}. \quad (19)$$

It is well known that for sufficiently large values of λ , the delta shell potential possesses both resonances and antiresonances in the elastic cross section (García-Calderón and Herrera Mote 1980, Gottfried 1966). They may be seen as related to the presence of real poles of the standing Green function which for the present problem correspond to the zeros of the function (Berrondo and García-Calderón 1979)

$$1 + (\lambda/2k) \sin 2ka = 0. \tag{20}$$

In table 1, the first 20 real values of k_n are given for $\lambda = 100 \text{ fm}^{-1}$ and $a = 1 \text{ fm}$. In table 2, the exact and the expanded values of $\Psi^+(k, r)$ are presented. The calculation was made for a number of values of the wavenumber k and of the distance r .

The delta shell potential has been used also by Bang *et al* (1978). In their approach they consider the Mittag-Leffler expansion of a function $\Psi^G(k, r)$ which, for $l = 0$, is related to $\Psi^+(k, r)$ as

$$\Psi^G(k, r) = k^{-1} e^{ika} \Psi^+(k, r). \tag{21}$$

Table 1. Values of k_n for the delta shell potential with $\lambda = 100 \text{ fm}^{-1}$ and $a = 1 \text{ fm}$.

n	k_n	n	k_n
1	1.586 065 05	11	17.457 087 12
2	3.110 467 88	12	1218.658 343 87*
	4.760 061 8	13	20.633 038 86
4	6.220 815 53	14	21.705 952 26
5	7.933 654 92	15	23.810 110 25
6	9.330 918 50	16	24.87 413 83
7	11.107 584 67	17	26.988 620 92
8	12.440 643 42	18	27.977 413 55
9	14.282 004 08	19	30.168 996 58
10	15.549 842 41	20	31.080 528 0

Table 2. Exact and expanded Ψ^+ for $\lambda = 100$, $a = 1$ and $N = 11$ poles.

k	r	Exact		Expanded	
		Re Ψ^+	Im Ψ^+	Re Ψ^+	Im Ψ^+
1.0	0.2	0.001 286 99	-0.001 961 23	0.001 140 90	-0.001 738 60
	0.4	0.002 522 67	-0.003 844 27	0.002 834 71	-0.004 319 79
	0.6	0.003 657 78	-0.005 574 06	0.003 112 32	-0.004 742483
	0.8	0.004 647 07	-0.007 081 62	0.005 693 06	-0.008 675 60
	1.0	0.005 45	-0.008 306 86	-0.000 193 92	0.000 295 52
3.11	0.2	-7.016 915 7	-14.844 545 9	-7.016 762 04	-14.842 207 8
	0.4	-11.405 301 9	-24.128 763 1	-11.405 830 37	-24.129 457 91
	0.6	-11.521 923 8	-24.375 057	-11.521 351 20	-24.373 846 51
	0.8	-7.322 573	-15.491 175	-7.323 665 16	-15.493 485 74
	1.0	-0.380 402 71	-0.804 560 7	-0.374 042 46	-0.792 570 05
4.0	0.2	0.024 990	-0.026 769	0.025 779 94	-0.027 615 55
	0.4	0.034 822	-0.037 301	0.033 137 44	-0.035 496 93
	0.6	0.023 530 9	-0.025 206 4	0.026 466 03	-0.028 350 50
	0.8	-0.002 033	0.002 178	-0.007 603 89	0.008 145 31
	1.0	-0.026 364 58	0.028 241 83	0.002 528 73	-0.002 708 79

Clearly $\Psi^G(k, r)$ is just, except for a minus sign, the outgoing Green function of the problem (García-Calderón 1976, Bang *et al* 1978). In table 3 a number of real values of k_n are given for $\lambda = 40 \text{ fm}^{-1}$ and $a = 1 \text{ fm}$. These values for the strength and range of the delta shell potential are the same as those chosen by Bang *et al* (1978). The above values of k_n are used to calculate the exact and the expanded values of $\Psi^+k, r)$. The results are presented in table 4.

Table 3. Values of k_n for $\lambda = 40 \text{ fm}^{-1}$ and $a = 1 \text{ fm}$.

n	k_n	n	k_n
1	1.611 117 97	6	9.186 169 69
2	3.064 672 79	7	11.295 659 41
3	4.834 459 53	8	12.237 166 66
4	6.127 494 18	9	14.544 294 67
5	8.061 416 56	10	15.273 471 15

Table 4. Exact and expanded $\Psi^G(k, r)$ for $\lambda = 40 \text{ fm}^{-1}$, $a = 1 \text{ fm}$ and $N = 10$ poles.

k	r	Exact		Expanded	
		Re Ψ^G	Im Ψ^G	Re Ψ^G	Im Ψ^G
1.0	0.2	0.005 805 68	0.000 142 8	0.005 363 97	0.000 142 85
	0.4	0.011 379 90	0.000 28	0.012 379 05	0.000 304 59
	0.6	0.016 500 44	0.000 405 99	0.145 859 3	0.000 358 89
	0.8	0.020 903 16	0.000 515 8	0.025 095 5	0.000 617 48
	1.0	0.024 590 15	0.000 605 040	-0.000 911 73	-0.000 022 43
3.0	0.2	0.205 936 31	0.032 594 76	0.205 518 11	0.032 528 57
	0.4	0.339 933 15	0.053 803 23	0.340 878 22	0.053 952 81
	0.6	0.355 181 56	0.056 216 68	0.353 375 01	0.055 930 75
	0.8	0.246 354 83	0.038 992 03	0.250 229 61	0.039 605 32
	1.0	0.051 469 27	0.008 146 35	0.028 047 39	0.004 439 23
3.0648 (res)	0.2	0.184 166 16	2.429 006 85	0.184 166 74	2.429 014 51
	0.4	0.301 282 04	3.973 673 26	0.301 282 83	3.973 083 69
	0.6	0.308 708 69	4.071 624 97	0.308 709 77	4.071 639 26
	0.8	0.203 742 26	2.687 200 22	0.203 742 47	2.687 203 06
	1.0	0.024 598 38	0.324 433 0	0.024 600 76	0.324 464 66
4.0	0.2	-0.021 029 7	-0.001 991 01	-0.022 124 01	-0.002 030 51
	0.4	-0.030 139 11	-0.002 774 3	-0.029 023 04	-0.002 671 57
	0.6	0.020 366 55	-0.001 874 74	-0.022 495 19	-0.002 070 68
	0.8	0.001 760 10	0.000 162 02	0.006 299 64	0.000 579 88
	1.0	0.022 819 09	0.002 100 49	-0.004 120 20	-0.000 379 26

In table 5 the exact and the expanded results for the wave solution are presented for a fixed value of the distance r and several values of the strength λ , the wavenumber k and the number of poles N .

It follows from tables 2, 4 and 5 that the expanded solution gives excellent agreement with the exact solution at resonance and antiresonance values of k for values of r along the interior region $r < a$. For other values of the wavenumber, the results, although reasonable, indicate that more terms, i.e. complex contributions, must be taken into account.

Table 5. Exact and expanded values of k for $r = 0.6$ fm and $a = 1$ fm. * and ** indicate, respectively, resonance and antiresonance values of k .

N	k	λ	Exact		Expanded	
			Re Ψ^+	Im Ψ^+	Re Ψ^+	Im Ψ^+
2	2.0	10	-0.046 48	-0.215 42	-0.045 31	-0.209 99
10	2.0	40	-0.019 34	-0.048 68	-0.018 12	-0.045 61
20	2.0	1000	-0.000 85	-0.001 87	-0.000 81	-0.001 78
1	*2.839 61	10	0.000 20	-3.181 9	0.000 20	-3.181 9
1	**1.611 11	40	0.000 00	-0.012 775	0.000 00	-0.127 84
1	*3.138 46	1000	133.61	-225.01	133.61	-225.01

For values of the distance at the radius $r = a$, the expansion obviously fails. However it gives excellent agreement at resonance or antiresonance values. This is not surprising. Actually it has been proved (García-Calderón and Berrondo 1979a, b) that at the radius $r = a$, a convergent expansion of the standing Green function in terms of its poles requires one subtraction term. At resonance energy the corresponding pole term is so dominant that all other contributions including the subtraction term remain negligible. The scattering matrix may be obtained from (2) and (6). For $l = 0$ it reads

$$S(k) \approx \frac{1 + ik(-(\tan ka)/k - (\cos^2 ka)^{-1}G(a, a; k))}{1 - ik(-(\tan ka)/k - (\cos^2 ka)^{-1}G(a, a; k))} \tag{22}$$

where the expression inside the brackets of equation (22) corresponds to the Q matrix of the problem (García-Calderón and Berrondo 1979a). The one-pole approximation for $G(a, a; k)$ follows from (8) with $r = a$, and the corresponding one involving one subtraction at $k = 0$ reads

$$G(a, a; k) \approx -\frac{a}{1 + \lambda a} + \frac{k^2}{k_n^2} \frac{\omega_n^2(a)}{k^2 - k_n^2} \tag{23}$$

In order to illustrate the above points, in table 6 the exact value of the partial elastic cross section for the delta shell potential ($l = 0$) is compared with the one-pole and one-pole plus subtraction approximations, for several values of k near the first resonance pole.

Table 6. Exact and one-pole approximations with and without subtraction term for the partial wave elastic cross section ($l = 0$) for the delta shell potential with $\lambda = 40$ fm⁻¹ and $a = 1$ fm around the resonance value $k_n = 3.064\ 672\ 79$.

k	$\sigma(k)^{\text{Exact}}$	$\sigma(k)^{\text{1-pole}}$	$\sigma(k)^{\text{1-pole+sub}}$
2.8	0.276 7	0.201 9	0.272 0
3.0	0.120 8	0.071 9	0.118 0
3.05	0.326 1	0.260 7	0.322 7
3.064 6 (res)	1.337 9	1.337 9	1.337 9
3.07	0.630 5	0.535 6	0.633 1
3.141 59	0.000 0	0.007 3	0.000 0
3.2	0.000 0	0.012 7	0.000 0
3.4	0.040 5	0.801 0	0.041 6

4. Conclusions

The main results of this paper are appropriately represented by equations (11) and (15). The first of these equations shows that a continuum wave solution of the Schrödinger equation for a potential of range a may be expanded in terms of an infinite set of standing natural functions along the interior region of the potential $r < a$. The second equation, i.e. equation (15), indicates that for a value of the wavenumber corresponding to a real pole, i.e. at resonance or antiresonance values, the continuum wave solution may be written approximately as the corresponding standing wave solution times a purely imaginary coefficient which makes the whole expression independent of the normalisation condition of the standing natural function. Though the expansion of the continuum wave solution at $r = a$ in terms of standing wave solutions requires one subtraction term (García-Calderón and Berrondo 1979a, b), it is well known that for values of the energy around resonance the corresponding pole term dominates and therefore around resonance it is possible to provide a prescription which discretises the continuum wave solution for $r \leq a$. This prescription may provide some advantages in comparison with others which involve complex quantities as in expansions of the outgoing Green function (García-Calderón 1976, García-Calderón and Rubio 1981, Bang *et al* 1978, 1980). At present, extension of the ideas discussed here to potentials behaving differently as a function of distance are in progress.

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