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LETTER TO THE EDITOR

Analytical treatment of the Green function singularity in integral equations of scattering theory

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Abstract. A technique for solving the Lippmann–Schwinger equation in momentum space based on Chebyshev polynomials is proposed. It is found that exact results are obtained for standard low-energy nuclear separable potentials with an extremely low number of meshpoints. The technique naturally leads to a class of analytically solvable separable potentials. The application of the Chebyshev technique to two local standard N–N potentials, Yukawa and Reid, is discussed.

1. Introduction

In many areas of physics we are often faced with the problem of evaluating singular integrals of the Green function type [1]

$$I(E) = \lim_{\epsilon \to 0_+} \int_{E_T}^{\infty} \frac{|\psi(E')\rangle\langle\psi(E')|\,\mathrm{d}E'}{E' - E - \mathrm{i}\epsilon} \tag{1}$$

where $|\psi(E)\rangle$ is the wavefunction for the system at energy E and the integration is along the real axis above a threshold at E_T. Much more complicated integrals of this type appear in the theory of resonance [2, 3], in optical potential calculations [4] and in many other areas of physics, see for example [5].

When solving the Lippmann–Schwinger (LS) equation in momentum representation [6]

$$t_l(p, p') = V_l(p, p') + \frac{2}{\pi} \int_0^{\infty} \frac{q^2 V_l(p, q) t_l(q, p')}{E - q^2 + \mathrm{i}\epsilon}\,\mathrm{d}q \tag{2}$$

one usually transforms the integral on the right-hand side of (2) to a principal value integral

$$\mathrm{P} \int_0^{\infty} \frac{q^2 V_l(p, q) t_l(q, p')}{E - q^2}\,\mathrm{d}q \tag{3}$$

and treats the principal value integral numerically, substracting for example, the singularity [6]. Since the numerical treatment of the singularity may cause problems we adopt another approach here, which is based on the following identities [7]

$$\mathrm{P} \int_{-1}^{1} \frac{T_n(x)}{x - y} \frac{\mathrm{d}x}{\sqrt{1 - x^2}} = \begin{cases} \pi U_{n-1}(y) & n \geqslant 1, n \in \mathcal{N} \\ 0 & n = 0 \ (|y| < 1) \end{cases} \tag{4}$$

$$\mathrm{P} \int_{-1}^{1} \frac{U_n(x)}{x - y} \sqrt{1 - x^2}\,\mathrm{d}x = -\pi T_{n+1}(y) \qquad n \in N_0 \ \ (|y| < 1) \tag{5}$$

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where T_n and U_n are Chebyshev polynomials of the first and second kind. If the integrals (1) or (3) can be transformed to a sum of terms of the type (4) and (5), the singular integrals may be evaluated analytically in terms of the respective Chebyshev polynomials and the problems with the correct treatment of the singularity avoided. Moreover, as will be shown below, this approach allows us to solve the LS equation analytically for a class of separable potentials, including those widely used in nuclear physics. In addition, examples of physical anomalies of non-local potentials can be displayed.

It is hoped that the present method may find applications in treating multichannel scattering problems as well as other related areas.

2. Analytic treatment of the singularity

For simplicity we shall consider the partial wave K-matrix defined by the equation

$$K_l(q,q';E) = V_l(q,q') + \frac{2}{\pi}\ \mathrm{P}\int_0^\infty q''^2 \frac{V_l(q,q'')K_l(q'',q';E)}{E-E(q'')}\,\mathrm{d}q''. \tag{6}$$

The phase shift $\delta_l(E)$ is related to the K-matrix as

$$\tan\delta_l(E) = -kK_l(k,k;E) \tag{7}$$

where

$$E = k^2$$

(we use units $\hbar = 1,\ 2\mu = 1$). In order to apply our technique, the infinite range of integration in equation (6) must be transformed to the compact interval $\langle -1, 1\rangle$. There exist several ways of transforming (6) to a finite interval [6]. Here we propose to use the following transformation

$$q'' = C\sqrt{\frac{1+y''}{1-y''}} \qquad y'' = \frac{q''^2 - C''^2}{q''^2 + C^2} \tag{8}$$

where C is a positive constant. This transformation yields

$$K(y,y';y_0) = V(y,y') + \kappa\,\mathrm{P}\int_{-1}^{1} \frac{V(y,y'')K(y'',y';y_0)}{y''-y_0}\frac{(1+y'')^{1/2}}{(1-y'')^{3/2}}\,\mathrm{d}y'' \tag{9}$$

where

$$\kappa = -\frac{2}{\pi}\frac{C^3}{C^2+E} \tag{10}$$

$$y_0 = \frac{E-C^2}{E+C^2}. \tag{11}$$

Let us define

$$F(y,y'') = V(y,y'')\frac{(1+y'')^{1/2}}{(1-y'')^{3/2}} \tag{12}$$

then we can write

$$K(y,y';y_0) = V(y,y') + \kappa\,\mathrm{P}\int_{-1}^{1} \frac{F(y,y'')K(y'',y';y_0)}{y''-y_0}\,\mathrm{d}y''. \tag{13}$$

A word of caution is now in order: the integral kernel $F(y,y'')$ contains a term, $(1-y'')^{-3/2}$, which is singular at $y'' \to 1$ (i.e. at $q'' \to \infty$). However, the potential $V(q,q')$ is a decreasing function of q' and q behaving typically as q^{-2} as $q \to \infty$. If we assume this

asymptotic behaviour we get that as $y'' \to 1$, $F(y, y'') \sim (1-y'')^{-1/2}$. Hence equation (13) as it stands is not useful for numerical integration. However, the quantity $\sqrt{1-y''^2}F(y, y'')$ is regular as $y'' \to 1$ and the following expansion makes sense

$$f(y''; y, y') = \sqrt{1-y''^2}F(y, y'')K(y'', y'; y_0) \approx \sum_1^N a_n(y, y'; y_0)T_n(y''). \tag{14}$$

The expansion coefficients a_n are determined by the standard relation

$$a_n(y, y'; y_0) = \frac{2}{\pi}\int_{-1}^{1} F(y, y'')K(y'', y'; y_0)T_n(y'')\,\mathrm{d}y''. \tag{15}$$

Let us assume that the coefficient a_n are known (they depend on the unknown function $K(y'', y'; y_0)$). Then inserting (14) into (13) we get

$$K(y, y'; y_0) = V(y, y') + \kappa \sum_1^N a_n(y, y'; y_0)\,\mathrm{P}\int_{-1}^{1} \frac{T_n(y'')\,\mathrm{d}y''}{\sqrt{1-y''^2}(y''-y_0)} \tag{16}$$

and finally, by making use of (4)

$$K(y, y'; y_0) = V(y, y') + \kappa \sum_1^N a_n(y, y'; y_0)\pi U_{n-1}(y_0) \tag{17}$$

thus performing the principal value integration analytically. The problem now reduces to the calculation of the expansion coefficient a_n.

This can be done as follows. Since the integrand in equation (15) contains the term $(1-y''^2)^{-1/2}$ it can be evaluated by means of the Chebyshev quadrature with the weight function

$$w(x) = \frac{1}{\sqrt{1-x^2}}$$

i.e.

$$a_n(y, y'; y_0) = \frac{2}{\pi}\sum_1^M w_i \tilde{F}(y, x_i)K(x_i, y'; y_0)T_n(x_i) \tag{18}$$

where

$$w_i = w = \pi/M \qquad x_i = \cos((\mathrm{i} - \tfrac{1}{2})w)$$
$$\tilde{F}(y, x) = \frac{1}{\sqrt{1-x^2}}F(y, x) = V(y, x)\frac{1+x}{1-x}.$$

Inserting (18) into (17) we get

$$K(y, y'; y_0) = V(y, y') + \kappa \sum_1^M m(y, x_i; y_0)K(x_i, y'; y_0) \tag{19}$$

where

$$m(y, x, y_0) = \frac{\pi^2}{M}\tilde{F}(y, x)\sum_{n=1}^{N} T_n(x)U_{n-1}(y_0). \tag{20}$$

Equation (19) can be solved either by collocation or by the Bubnov–Galerkin method [13]. Both methods reduce to solving a set of linear equations.

3. Separable potentials

Before we proceed to the application of the proposed method to realistic potentials we find it worthwhile to discuss separable interactions first. Separable potentials of the form

$$V(k,k') = V_0 g(k) g(k') \tag{21}$$

play an essential role in many applications of low-energy nuclear and atomic physics and are of vital importance for three-body calculations [6, 4]. A widely used potential of this form is the Yamaguchi potential [15]

$$V(k,k') = V_0 \frac{1}{c^2+k^2}\frac{1}{c^2+k'^2}. \tag{22}$$

The LS equation with the potential (22) reduces to an algebraic equation. The K-matrix for a separable potential (21) can be writen as

$$K(k,k';E) = \frac{V_0 g(k) g(k')}{1-(2V_0/\pi)}\,\mathrm{P}\int_0^\infty q^2 g^2(q)/(E-q^2)\,\mathrm{d}q. \tag{23}$$

In order to obtain the K-matrix the principal value integral $I(E)$

$$I(E) = V_0\,\mathrm{P}\int_0^\infty \frac{q^2 g^2(q)\,\mathrm{d}q}{E-q^2} \tag{24}$$

must be evaluated. After performing the transformation (8) with $C = c$ in (22) we get

$$I(y_0) = \underbrace{-\frac{V_0 C^3}{C^2+E}}_{\rho}\,\mathrm{P}\int_{-1}^{1}\frac{g^2(y)(1+y)^{1/2}\,\mathrm{d}y}{(1-y)^{3/2}}. \tag{25}$$

Let us assume that the form factor $g(y)$ can be expanded as follows:

$$g(y) = \sqrt{1-y}\sum_{n=0}^{N} v_n T_n(y). \tag{26}$$

The integrals on the right-hand side of equation (25) can be calculated analytically using equation (4) since the product in the numerator in equation (26) is a polynomial in y. If only the zero-order term in the expansion (26) is retained, i.e.

$$g(y) = \sqrt{1-y}T_0(y) \qquad T_0(y) = 1 \tag{27}$$

then

$$v(q,q') = \frac{1}{\sqrt{1+q^2}}\frac{1}{\sqrt{1+q'^2}} \qquad (C=1). \tag{28}$$

This potential was introduced a long time ago by Bander [14]. In a complete analogy we can expand the potential $g(y)$ in the Chebyshev polynomials of the second kind

$$g(y) = (1-y)\sum_{n=0}^{N} v_n U_n(y). \tag{29}$$

Then

$$I(y_0) = \rho\sum v_n v_m\,\mathrm{P}\int_{-1}^{1}\frac{U_n(y)U_m(y)\sqrt{1-y^2}}{y-y_0}\,\mathrm{d}y. \tag{30}$$

This integral can be reduced to the basic integral (5). Again if only the zero-order term in equation (29) is taken, i.e. $g(y) = (1-y)$ then

$$v(q,q'') = \frac{1}{1+q^2}\frac{1}{1+q''^2} \tag{31}$$

which is the well known Yamaguchi potential [15].

With the potential (31), the function $f(y''; y, y')$ defined in equation (14) can be calculated analytically and, as can easily be shown, it reduces to a second-order polynomial in y''. This means that expansion (14) is exact for $N = 2$. Hence only three coefficients a_0, a_1, a_2 are non-zero and, as can easily be seen, these coefficient are accurately given by equation (18) with $M = 3$. This means that with just three meshpoints, exact results for the Yamaguchi potential are obtained. An analogous consideration for the Bander potential, equation (28) implies that the exact results are obtained with $M = 2$, i.e. only two meshpoints yield the exact results for all energies. This is a very remarkable property, indicating that for potentials that do not differ much from this type of potential, a very low number of mesh points may yield very accurate results.

Let us now consider higher terms in equations (27) and (29), taking into account one more polynomial, i.e.

$$g_1(y) = \sqrt{1-y}(a_0 T_0(y) + a_1 T_1(y)) \tag{32}$$

and

$$g_2(y) = (1-y)(b_0 U_0(y) + b_1 U_1(y)). \tag{33}$$

In momentum space we get

$$g_1(k) = \frac{1}{\sqrt{C^2+k^2}}\left(1 + \beta\frac{k^2-C^2}{k^2+C^2}\right) \tag{34}$$

and

$$g_2(k) = \frac{1}{C^2+k^2}\left(1 + \beta\frac{k^2-C^2}{k^2+C^2}\right). \tag{35}$$

For potentials $g_1(k)$ and $g_2(k)$ the principal value integrals in equation (24) can easily be evaluated with the results

$$I_1(E(y_0)) = -\frac{\pi V_0 C}{2(C^2+k_0^2)}\left(\beta^2 y_0^2 + \beta(\beta+2)y_0 + \frac{\beta^2}{2} + 2\beta + 1\right) \tag{36}$$

$$I_2(E(y_0)) = \frac{\pi V_0}{4C(C^2+k_0^2)}\left(\beta^2 y_0^3 + 2\beta y_0^2 + y_0\left(1 - \frac{\beta^2}{2}\right) - \beta\right) \tag{37}$$

$$y_0 = y(E).$$

In the coordinate representation, the 'generalized' Yamaguchi potential (35) has the form

$$g_2(r) = \sqrt{\frac{\pi}{2}}\mathrm{e}^{-Cr}(1 + \beta - \beta C r). \tag{38}$$

This potential has very interesting properties. Since it may change sign (for $\beta \notin \langle -1, 0\rangle$) in dependence on β and C, it describes a broader class of potential functions than the simple Yamaguchi potential. Moreover, it clearly displays certain anomalies pertinent to non-local interactions. Generally, the bound-state energy ($E < 0$) in the potential (21) is obtained from the equation

$$1 - \frac{2V_0}{\pi}\int_0^\infty \frac{q^2 g^2(q)\,\mathrm{d}q}{E - q^2} = 0. \tag{39}$$

The integral in (39) is no longer singular for negative and complex E and can be calculated by using the residue theorem. In our case the bound state must exist, provided

$$-V_0 > \frac{2C^3}{\frac{1}{2}\beta^2 - \beta + 1} \tag{40}$$

for the potential (35) and

$$-V_0 > \frac{C}{1+\frac{1}{2}\beta^2} \tag{41}$$

for the potential (34). Its energy is implicitly given by

$$-\frac{2C}{V_0}(C+k_0)^4 = k_0^2\left(\frac{\beta^2}{2}+\beta+1\right)+2Ck_0+C^2\left(\frac{\beta^2}{2}-\beta+1\right) \tag{42}$$

for the potential (35) and

$$-\frac{1}{V_0}(C+k_0)^3 = k_0^2(1+\beta)^2+2Ck_0\left(1+\frac{\beta}{2}\right)^2+C^2\left(1+\frac{\beta^2}{2}\right) \tag{43}$$

for the potential (34). The bound-state wavefunction ($E=-k_0^2$) for the potential (35) in the coordinate representation reads

$$u_{k_0}(r) = \mathrm{e}^{-Cr}-\mathrm{e}^{-k_0 r}+\beta\left[\mathrm{e}^{-Cr}(1-Cr)+\frac{1}{k_0^2-C^2}(2C^2\,\mathrm{e}^{-Cr}-(C^2+k_0^2)\,\mathrm{e}^{-k_0 r})\right]. \tag{44}$$

At first sight we see that this is a very peculiar bound-state wavefunction.

(1) First of all, we observe that the bound-state wavefunction $u_{k_0}(r)$ may change sign for some $r \neq 0$ (extra node). This is a very interesting feature since it is known that no ground-state wavefunction in any local potential is allowed to change sign.

(2) The wavefunction $u_{k_0}(r)$ is regular at the origin, as it should be. It can easily be shown that for a special choice of k_0 and C we can also have $u'_{k_0}(0)=0$. Such states are known as spurious states [10].

(3) If k_0 is smaller than C, the asymptotic behaviour of the bound-state function $u_{k_0}(r)$ is not determined by the energy of the bound state, as it must be in the case of local interactions, but is fully determined by the parameter C of the potential.

(4) It is well known [10] that under certain conditions non-local separable interactions may create zero-width resonances, the so-called continuum bound states (CBS), i.e. states with a quadratically integrable wavefunction at real k. When such potentials, which describe the N–N phase shifts surprisingly well [11], are used in three-body bound-state calculations an unphysically large value for the triton binding energy is obtained and the collapse of the bound-state wavefunction observed [12]. For CBS to exist, two conditions must be simultaneously fulfilled,

$$I(k_0) = \frac{\pi}{2} \tag{45}$$

$$g(k_0) = 0 \tag{46}$$

which ensure that the complex energy dependent denominator of the T-matrix vanishes for real k_0. The wavefunction of the CBS generated by the potential (35) does not depend on the energy of the CBS ($E_{\mathrm{CBS}}=k_0^2$) and has the simple form

$$u_{\mathrm{CBS}}(r) = Nr\,\mathrm{e}^{-Cr}. \tag{47}$$

The CBS exists when

$$-V_0 = \frac{4C}{(\beta+1)(\beta+2)} \tag{48}$$

for potential (34) and when

$$-V_0 = \frac{8C^3}{\beta+1} \tag{49}$$

for potential (35), provided $|\beta| > 1$ (for both potentials). Thus the existence of the CBS may easily be controlled. More complicated potentials may be created by increasing the number of terms in (26) and (29).

4. Results

In this section we apply the technique just described to local potentials designated to describe low-energy N–N interaction. We shall consider two standard local potentials widely used in the literature, namely the Yukawa potential [8]

$$V(r) = -V_0 \frac{e^{-\lambda r}}{r} \tag{50}$$

and the Reid soft-core potential [9], which equals a sum of three Yukawa-type terms. In momentum representation we have

$$V_{l=0}(k, k') = -\frac{V_0}{4kk'} \ln\left(\frac{(k+k')^2 + \lambda^2}{(k-k')^2 + \lambda^2}\right) \tag{51}$$

where $\lambda = 0.6329$ fm^{-1} and $V_0 = 65.246$ MeV fm for the Yukawa potential and

$$V_{l=0}(k, k') = \frac{1}{4\lambda_1 kk'} \sum_{i=1}^{3} v_i \ln\left(\frac{(k+k')^2 + \lambda_i^2}{(k-k')^2 + \lambda_i^2}\right) \tag{52}$$

with

$$\lambda_1 = 0.7 \text{ fm}^{-1} \qquad v_1 = -10.436 \text{ MeV}$$
$$\lambda_2 = 2.8 \text{ fm}^{-1} \qquad v_2 = -1650.6 \text{ MeV}$$
$$\lambda_3 = 4.9 \text{ fm}^{-1} \qquad v_3 = +6484.2 \text{ MeV}$$

for the Reid potential. Here we use $\hbar^2/(2\mu) = 41.47$ MeV (fm)^2.

Table 1. Phase shifts for the Yukawa potential.

	Number of Chebyshev polynomials				
E (MeV)	$N = 10$	$N = 15$	$N = 20$	$N = 30$	$N = 40$
12	1.5108	1.5062	1.5072	1.5057	1.5053
24	1.2847	1.2840	1.2827	1.2818	1.2819
48	1.0803	1.0813	1.0805	1.0803	1.0803
72	0.9689	0.9726	0.9727	0.9726	0.9725
104	0.8775	0.8804	0.8812	0.8810	0.8810
152	0.7874	0.7921	0.7928	0.7929	0.7928
176	0.7537	0.7593	0.7603	0.7604	0.7604

The LS equation in the form (6) was solved by expanding the function $f(y''; y, y')$, equation (14), into Chebyshev polynomials with various numbers of terms, N, in this expansion. The results are summarized in table 1 for the Yukawa potential and in table 2 for the Reid soft-core potential. The entries in the tables are phase shifts calculated at several energies E_i ranging from 12–176 MeV.

From both tables we see that a very low number, 10–15, of Chebyshev polynomials gives very accurate results exceeding in accuracy the most elaborated experimental values. It must also be stressed that all the calculations were performed with one fixed energy-independent

Table 2. Phase shifts for the Reid potential.

	Number of Chebyshev polynomials				
E (MeV)	$N = 10$	$N = 15$	$N = 20$	$N = 30$	$N = 40$
12	0.9164	0.8675	0.8605	0.8608	0.8607
24	0.7163	0.6776	0.6860	0.6846	0.6846
48	0.4127	0.4460	0.4398	0.4402	0.4402
72	0.2551	0.2597	0.2637	0.2632	0.2630
104	0.0964	0.0807	0.0800	0.0803	0.0803
152	−0.1225	−0.1276	−0.1292	−0.1297	−0.1296
176	−0.2193	−0.2183	−0.2164	−0.2163	−0.2164

constant C in the transformation formula, equation (8). Often the transformation of the infinite range to the finite one is performed with an energy-dependent parameter $C(E)$ in order to get the fastest convergence. However, this means that if the calculation is to be repeated for another energy the momentum representation of the potential $V(p, p')$ must be recalculated at each energy and in many practical applications the evaluation of the function $V(p, p')$ is the most time consuming part of the calculation. Here this nuisance is totally avoided. It is also interesting to note that expanding in Chebyshev polynomials means that the maximum absolute deviation between given and fitting functions is minimized—the minimax best-fit criterion [16]. This feature may be of importance when fitting the potentials to real data.

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