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Notes

A Numerical Approach to Principal Value Integrals in Dispersion Relations

In this note we describe a convenient and rapidly convergent numerical procedure for the evaluation of principal value integrals, which arise in a dispersion theoretical treatment of the coupled channel scattering problem.

The knowledge of the set of partial wave phaseshifts $\delta_l(E)$ suffices for the construction of the total scattering amplitude $T(E)$ [1]. The causality principle and plausible behavior of the potential $V(r)$ guarantee analyticity of the partial wave phaseshifts in the upper half plane of complex energy. This permits the use of the powerful theory of analytic functions and establishes integral relations between the real and imaginary parts of the phaseshifts, $\delta_l(E)$, which correspond to dispersive and absorptive effects, respectively.

We are presently working on a novel approach [2] to the scattering problem for n coupled two body channels. In the course of the analysis repeated integrals of the form

$$\begin{aligned} \delta_R^{(l)}(k^2) &= \frac{k}{\pi} P \int_0^\infty \frac{\delta_I^{(l)}(k'^2)\, dk'^2}{k'(k'^2 - k^2)} \\ \delta_I^{(l)}(k^2) &= -\frac{k^2}{\pi} P \int_0^\infty \frac{\delta_R^{(l)}(k'^2)\, dk'^2}{k'^2(k'^2 - k^2)} \end{aligned} \tag{1}$$

appear. Here $\delta_R(k^2)$, $\delta_I(k^2)$ stand for the real and imaginary parts of the l-th partial wave phaseshift, $\delta^{(l)}(k^2) = \delta_R^{(l)}(k^2) + i\delta_I^{(l)}(k^2)$. In the following we suppress the partial wave label l, and will confine ourselves to s wave ($l = 0$) phaseshifts. Relations (1) areknown as Hilbert transforms in the mathematical literature and follow from the analytic properties of the phaseshift. If, for example, the absorptive part $\delta_I(k^2)$ is given over the whole range of scattering energies from the inelastic threshold (taken to be 0 in (1)) to infinite energy, the total phaseshift is given immediately by

$$\delta(k^2 + i\epsilon) = \frac{k}{\pi} \int_0^\infty \frac{\delta_I(k'^2)\, dk'^2}{k'(k'^2 - k^2 - i\epsilon)} \tag{1a}$$

We note $k = +(k^2 + i\epsilon)^{1/2}$ takes care of the elastic branch-cut $0 \leqslant k^2 \leqslant \infty$ while the integral contains the branch-cut due to the inelastic channel, opening up at the inelastic threshold. Relation (1a) was given and applied by Frazer and Ball [3] to correct the elastic scattering amplitude for inelastic effects, which were assumed known in the form of the total inelastic cross-section. Use of the formal identity

$$\frac{1}{k'^2 - k^2 - i\epsilon} = i\pi\delta(k'^2 - k^2) + P\frac{1}{k'^2 - k^2} \tag{2}$$

then leads to the separation of the real and imaginary parts of the phaseshifts, i.e.,

$$\delta(k^2 + i\epsilon) = \frac{k}{\pi} P \int^{\infty} \frac{\delta_I(k'^2)\, dk'^2}{k'(k'^2 - k^2)} + i\delta_I(k^2) \tag{1b}$$

We note here, that similar principal value integrals occur in the Feynman formulation of perturbation theory in terms of propagators and in the solution of the Lippman–Schwinger [4] equations.

In our approach to the many coupled channel problem, an initial approximation is made for the integrands $\delta_I^{(0)}(k'^2)$, $\delta_R^{(0)}(k'^2)$, in (1), which is based on perturbation theory (e.g. 1st Born approximation $T = V$). Equations (1) are then solved iteratively until stability is reached. As a consequence of our basic equations (1), repeated principal value integrations have to be performed numerically.

A simpleminded attempt to use Laguerre integration for the semiinfinite integration interval fails due to the asymmetric distribution of the Laguerre roots with respect to the apparent singularity at $k'^2 = k^2$. After some experimentation with rescaling the roots, which did not much improve the accuracy of the result, we discovered a much more straightforward and satisfactory procedure.

As mentioned, our difficulty with finite numbers of gridpoints stem from the dominant influence of the factor $1/k'^2 - k^2$, which should be treated symmetrically We therefore divide the integration interval after normalizing variables by $x = k'/k$ into two regions $0 \leqslant x \leqslant 1 - \epsilon$, $1 + \epsilon \leqslant x \leqslant \infty$ as in the definition of the Cauchy principal value. Next we map the second interval by inversion $y = 1/x$ into the first to obtain

$$\delta_R(k^2) = \frac{2}{\pi} \lim_{\epsilon \to 0} \int_0^{1-\epsilon} \frac{dx}{x^2 - 1} \left[\delta_I^{(0)}(k^2 x^2) - \delta_I^{(0)}\left(\frac{k^2}{x^2}\right)\right] \tag{5}$$

We note with satisfaction, that the integrand is manifestly well-behaved at the singularity $x = 1$ and tends to $2k\delta_I^{(0)\prime}(k^2)$. (In this connection see the recent note by I. H. Sloan [5] in this journal).

In order to use Gaussian quadrature we once again change variables to obtain a symmetric integration interval.

Our final result is then obtained in the form

$$\delta_R(k^2) = \frac{4}{\pi}\int_{-1}^{1}\frac{dy}{(y+1)^2-4}\left[\delta_I^{(0)}\left(\frac{k^2(y+1)^2}{4}\right)-\delta_I^{(0)}\left(\frac{4k^2}{(y+1)^2}\right)\right]$$
$$= \frac{4}{\pi}\sum_{i=1}^{2n}\frac{w_i}{(y_i+1)^2-4}\left[\delta_I^{(0)}\left(\frac{k^2(y_i+1)^2}{4}\right)-\delta_I^{(0)}\left(\frac{4k^2}{(y_i+1)^2}\right)\right] \quad (6)$$

The w_i, y_i are the weights and roots used for a $2n$ point Gaussian quadrature [6].
In Table I we demonstrate our use of (6) for two cases:

$$\text{I.} \quad \delta_I^{(0)}(k^2) = \frac{\mu}{k^2+b^2}$$
$$\text{II.} \quad \delta_I^{(0)}(k^2) = -\frac{1}{4}\log\left[1-\left(\frac{\mu}{k}\right)^2\log\left(1+\frac{4k^2}{b^2}\right)\right] \quad (7)$$

TABLE I

Case I: $\delta_I^{(0)}(k^2) = \dfrac{\mu}{k^2+b^2}$ $(\mu = 0.1;\ b^2 = 1.01)$;

n Number of Gridpoints in Gaussian Quadrature;

$\delta_R(k^2)\times 10^2$ $\quad \delta_R(k^2) = \dfrac{k}{\pi}P\displaystyle\int_0^\infty \frac{\delta_I^{(0)}(k'^2)\,dk'^2}{k'(k'^2-k^2)} = -\frac{\mu}{2b(k^2+b^2)}$

k	$n = 2$	$n = 4$	$n = 8$	Exact
.3	−1.375881	−1.336933	−1.337852	−1.337851
.6	−2.175505	−2.152076	−2.152233	−2.152233
.9	−2.440125	−2.434552	−2.434536	−2.434537
1.5	−2.286489	−2.270760	−2.270799	−2.270800
2.4	−1.796622	−1.751299	−1.752361	−1.752362

Case II: $\delta_I^{(0)}(k^2) = -0.25\log\left[1+\left(\frac{\mu}{k}\right)^2\log\left(1+\frac{4k^2}{b^2}\right)\right]$ $(\mu = 0.1;\ b^2 = 1.01)$

$\delta_R(k^2)\times 10^3$ $\quad \delta_R(k^2) = \dfrac{k}{\pi}P\displaystyle\int_0^\infty \frac{\delta_I^{(0)}(k'^2)\,dk'^2}{k'(k'^2-k^2)}$

k	$n = 2$	$n = 4$	$n = 8$	$n = 20$
.3	3.45803	3.24849	3.26072	3.26111
.6	2.47818	2.47410	2.47790	2.47803
.9	7.54994	7.14626	7.17044	7.17104
1.5	−1.46368	−1.56638	−1.56166	−1.56163
2.4	−2.74110	−2.66423	−2.67511	−2.67518

For Case I, we can calculate the principal value integral trivially by contour integration. In both cases, we note the rapid convergence for very small numbers of gridpoints. The calculations were performed on the Call/360 remote terminal system, utilizing simple programs written in BASIC CODE and took negligible time. More detailed results on the coupled many channel problem will be published elsewhere in the near future.

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