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On a fitting technique approach in potential scattering theory

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Abstract. A straightforward uniform estimate has been made of the difference between the Jost functions corresponding to scattering of one particle by two close potentials within the region Im $k \geqslant 0$. The Jost function for an approximating piecewise potential was found by developing a very simple technique of fitting. The exact solution of the original problem can be represented as a uniform limit of the n-fold product of 2×2 matrices at $n \to \infty$.

Let $f_l^{(\pm)}(k, r)$ and $\phi_l(k, r)$ be the solutions of the Schrödinger equation $u''(r)+[k^2-V(r)+l(l+1)/r^2]u(r)=0$ which are normalised by the conditions $\lim_{r\to\infty}(f_l^{(\pm)}\,\mathrm{e}^{\mp ikr})=1$ and $\lim_{r\to 0}(\phi_l/r^{l+1})=1$. Let us define, in accordance with Newton (1964), the Jost function $\mathscr{F}_l(k)$ by $\mathscr{F}_l(k)=(2l+1)\lim_{r\to 0}(r^l f_l^{(+)})$. Denoting by tilde the same quantities corresponding to another potential $\tilde{V}(r)$ which, just as $V(r)$, is assumed to satisfy the condition for the existence of $\int_0^\infty |V(r)|r\,\mathrm{d}r$, one can derive the integral representation for $\mathscr{F}_l(k)$ given by

$$\mathscr{F}_l(k)-\tilde{\mathscr{F}}_l(k)=\int_0^\infty \Delta V(r)\tilde{\phi}_l(k, r)f_l^{(+)}(k, r)\,\mathrm{d}r; \qquad \Delta V \equiv V-\tilde{V}. \tag{1}$$

We estimate the right-hand side of equation (1). It is known (Newton 1964) that the functions $\tilde{\phi}_l$ and $f_l^{(+)}$ satisfy the inequalities

$$|\tilde{\phi}_l|<\tilde{C}_l\,\mathrm{e}^{|\nu|r}\left(\frac{|k|r}{1+|k|r}\right)^{l+1}\exp\left(\tilde{C}_l\int_0^r|\tilde{V}(r)|r\,\mathrm{d}r\right)$$

where $\nu=\operatorname{Im} k$ and

$$|f_l^{(+)}|\leqslant C_l\,\mathrm{e}^{-\nu r}\left(\frac{|k|r}{1+|k|r}\right)^{-l}\exp\left(C_l\int_r^\infty|V(r)|r\,\mathrm{d}r\right).$$

We readily come to the following proposition having denoted $\bar{C}=\max\{\tilde{C}_l, C_l\}$, $\bar{V}(r)=\max\{|V|, |\tilde{V}|\}$ and $M=(\bar{C})^2\exp\{\bar{C}\int_0^\infty r\bar{V}(r)\,\mathrm{d}r\}$.

Proposition 1. In the half-plane Im $k\geqslant 0$, the Jost functions $\mathscr{F}_l(k)$ and $\tilde{\mathscr{F}}_l(k)$ satisfy the following uniform estimate:

$$|\mathscr{F}_l(k)-\tilde{\mathscr{F}}_l(k)|<\epsilon M \tag{2}$$

where

$$\epsilon=\int_0^\infty|\Delta V(r)|\,\mathrm{d}r.$$

It is interesting to mention that the theorem reveals the exact meaning of the well known statement that the scattering amplitude depends solely on the global properties of the potential (e.g. Newton 1964).

Now we divide the region $(0, \infty)$ into intervals $\Omega_j = (r_{j-1}, r_j)$, where $0 = r_0 < r_1 < \ldots < r_{n+1} = \infty$ and for $\tilde{V}(r)$ we take the piecewise potential to be of the form $\tilde{V}(r) = V_j(r)$ when $r \in \Omega_j$ and $j = 1, 2, \ldots, n+1$. Let the function $\phi_1(k, r)$, normalised to r^{l+1} when $r \to 0$, be the regular solution of the Schrödinger equation involving the potential $V_1(r)$ for $r \in \Omega_1$. Let us denote by $\phi_j^{(\alpha)}$, for $j = 2, \ldots, n+1$ and $\alpha = 1, 2$, a set of pairs of linear independent solutions of the Schrödinger equations involving the potentials $V_j(r)$ in the regions Ω_j. Here the normalisation of the functions $\phi_j^{(1)}(k, r)$ may be arbitrary but $\phi_j^{(2)}(k, r)$ should be normalised by the conditions

$$W[\phi_j^{(1)}\phi_j^{(2)}] = 1, \qquad r \in \Omega_j, \quad j > 1 \tag{3}$$

where $W[\phi\psi]$ is the Wronskian of the functions ϕ and ψ.

If the functions $\phi_{n+1}^{(1)}(k, r)$ and $\phi_{n+1}^{(2)}(k, r)$ are normalised in exactly the same way as $f_l^{(-)}$ and $f_l^{(+)}$ respectively, one can write the regular (physical) wavefunction $\psi^{(+)}(k, r)$ corresponding to scattering by potential $\tilde{V}(r)$ in the form

$$\psi^{(+)} = \begin{cases} a_1(k)\phi_1(k, r), & r \in \Omega_1 \\ \hat{a}_j^{\mathrm{T}}\hat{\phi}_j(k, r), & r \in \Omega_j,\ j > 1 \end{cases} \tag{4}$$

where

$$\hat{a}_j = \begin{pmatrix} a_j^{(1)} \\ a_j^{(2)} \end{pmatrix}, \quad j > 1; \qquad \hat{a}_{n+1} = \frac{\mathrm{i}\,\mathrm{e}^{-\mathrm{i}\pi l/2}}{2}\begin{pmatrix} \mathrm{e}^{\mathrm{i}\pi l} \\ \tilde{S}(k) \end{pmatrix}; \qquad \hat{\phi}_j = \begin{pmatrix} \phi_j^{(1)} \\ \phi_j^{(2)} \end{pmatrix} \tag{5}$$

and the superscript T means that $\hat{a}_j$ is transposed.

Let us introduce the 2×2 matrices U_j whose elements are the Wronskians of the functions $\phi_j^{(\alpha)}$ and $\phi_{j+1}^{(\alpha')}$ calculated at $r = r_j$:

$$U_j = \begin{pmatrix} W[\phi_{j+1}^{(1)}\phi_j^{(2)}] & W[\phi_{j+1}^{(2)}\phi_j^{(2)}] \\ W[\phi_j^{(1)}\phi_{j+1}^{(1)}] & W[\phi_j^{(1)}\phi_{j+1}^{(2)}] \end{pmatrix}, \quad j > 1; \qquad U_1 = \begin{pmatrix} W[\phi_1\phi_2^{(2)}] & 0 \\ 0 & W[\phi_2^{(1)}\phi_1] \end{pmatrix}^{-1}. \tag{6}$$

The system of fitting equations for the coefficients $a_j^{(\alpha)}$, a_1, and $\tilde{S}$, which is rather cumbersome in other approaches, can now be represented in the compact form

$$a_1\begin{pmatrix} 1 \\ 1 \end{pmatrix} = U_1\hat{a}_2; \qquad \hat{a}_j = U_j\hat{a}_{j+1}, \qquad 2 \leqslant j \leqslant n. \tag{7}$$

Thus, the set of fitting equations has been reduced to a chain of recurrence relations, which permits us to find immediately an equation connecting $a_1(k)$ with $\tilde{S}(k)$:

$$a_1(k)\begin{pmatrix} 1 \\ 1 \end{pmatrix} = U\hat{a}_{n+1}; \qquad U = U_1 \,.\, U_2 \ldots U_n. \tag{8}$$

Hence, for the Jost function $\tilde{\mathscr{F}}_l(k) \equiv k\,\mathrm{e}^{\mathrm{i}\pi l/2}/a_1(k)$ (Newton 1964), using equation (5), one can obtain at once

$$\tilde{\mathscr{F}}_l(k) = 2\mathrm{i}k\,\frac{u_{12}(k) - u_{22}(k)}{\Delta(k)} \tag{9}$$

where

$$\Delta = \det U = \Pi \det U_j \tag{10}$$

while the quantities $u_{\alpha\beta}(k)$ are the elements of matrix U defined by equation (8). This completes the proof of the following proposition.

Proposition 2. The relations (9) and (10) give the exact expression for the Jost function $\tilde{\mathscr{F}}_l(k)$ corresponding to the approximate potential $\tilde{V}(r)$.

Let us consider a sequence of approximating potentials $\tilde{V}^{(m)}(r)$ of the above form, which is convergent to $V(r)$. Since the sequence $\tilde{V}^{(m)}$ can be adopted in such a way that $|\tilde{V}^{(m)}(r)|$ tends monotonically to $|V(r)|$ and therefore the corresponding sequence $M^{(m)}$ is uniformly bounded, we obtain the following proposition.

Proposition 3. If a sequence $\tilde{V}^{(m)}(r)$ tends to $V(r)$ at each point $r \in (0, \infty)$ such that $|\tilde{V}^{(m)}(r)| \to |V(r)|$ monotonically and $\int_0^\infty |V(r) - \tilde{V}^{(m)}(r)|\, dr \to 0$ then the Jost function $\mathscr{F}_l(k)$ corresponding to the potential $V(r)$ can be represented as a uniform limit:

$$\mathscr{F}_l(k) = \lim_{m\to\infty} \tilde{\mathscr{F}}_l^{(m)}(k), \qquad \operatorname{Im} k \geqslant 0.$$

There are various potentials $V_j(r)$ for which the exact solutions $\phi_j^{(\alpha)}$ are known. By choosing different kinds of V_j, it is possible to develop fairly interesting approximations especially in the limit $m \to \infty$; in particular as follows.

(a) When $V \leqslant 0$ (no turning points) one may choose a piecewise constant potential as $\tilde{V}^{(m)}$ (here m is the number of the intervals) and then show that for $\alpha \neq \beta$ $(u_{\alpha\beta})_j = o((u_{\alpha\alpha})_j)$ and $(u_{\alpha\alpha})_j = O(1)$ where $(u_{\alpha\beta})_j$ are matrix elements of U_j. The smallness parameter is here just the reciprocal classical momentum $k^{-1} \sim (E - V)^{-1/2}$ so an appropriate treatment of the matrix product in (8) at $m \to \infty$ would lead to the whole quasi-classical series whose nth term is an n-fold quadrature. This is a natural development of the layer approach used by Rayleigh (1912) to obtain the two first terms of the similar expansion for the wave equation.

(b) Using piecewise linear potentials as $\tilde{V}^{(m)}$ we would deal with the Airy functions as $\phi_j^{(\alpha)}$. Similarly to case (a) one can derive (at $m \to \infty$) both far more powerful approximate integral representations of the Jost function as well as exact series.

(c) The same can be done by means of quadratic interpolations of $V(r)$. Integral representations that arise would now involve the parabolic cylinder functions. Some approximations of that kind are conventional in the theory of diffraction.

As a matter of course equations like (8) are suitable for finding Green functions as well. The latter can be expressed in terms of Feynman's path integrals so it is very important that approximations (a), (b), (c) which we have outlined, at finite m, are thought to be analogous with the standard one-dimensional approximate integration formulae of rectangles, trapeziums and the Simpson formula, respectively.

In order to apply the approach developed to some concrete problems of atomic physics it should be mentioned that factors $(f_l(k))^{-1}$ corresponding to the exit and entrance channels are inserted in any matrix elements of inelastic processes. Each of them gives the amplitude of relative probability for the particle being near $r = 0$. The simplest example dealing with K-shell ionisation has been carried out by Chernyak and Nikolaev (1976). For a more realistic model it is reasonable to bear in mind that the expansion of the local part of the Hartree–Fock effective potential may be written in the form

$$V_{\mathrm{HF}}(R) = \frac{l(l+1)}{r^2} - \frac{Z}{r} + \left\langle \frac{Z-1}{r} \right\rangle + O(r^2).$$

Hence, all the given terms can be taken into account exactly in $V_1(r)$. Similarly, it is sufficient to put the Coulomb tail and the centrifugal term into $V_{n+1}(r)$ within the region Ω_{n+1}. With such choices the following estimates are true:

$$V_{\mathrm{HF}}(r) - V_1(r) = o(r) \qquad \text{at } r \to 0$$

and

$$V_{\mathrm{HF}}(r) - V_{n+1}(r) = O(e^{-|\lambda| r}) \qquad \text{at } r \to \infty$$

with a constant $\lambda = O(1)$. Thus, the appropriate piecewise potential can readily be introduced in the infinite region $(0, \infty)$ such that sensible preciseness for $\mathscr{F}(k)$ may be guaranteed due to the estimates noted and equation (2).

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