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R-matrix bounds for local potentials

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Abstract. The continuum form of the Hellmann–Feynman theorem is proved, both on and off the energy shell, for potentials satisfying $\int_0^A r|V(r)|\,\mathrm{d}r<\infty$ and $\int_A^\infty |V(r)|\,\mathrm{d}r<\infty$. The corresponding bounds for the phase shifts and off-shell amplitudes are deduced.

1. Introduction

Use of the Faddeev equations for three-body scattering calculations requires a reliable approximation to the two-body amplitudes off the energy shell. In view of the arbitrariness of the off-shell extrapolation in the absence of three-body data it seems safest to extrapolate, if possible, via a central local potential. These results could then be approximated by more manageable amplitudes. Because of their simplicity, separable potentials have often been used for the extrapolation, but suffer from theoretical and practical difficulties in that (i) for a local potential the T-matrix cannot be compact (Osborn 1973), and hence cannot be well approximated by a separable potential for all momenta, (ii) phase shifts which change sign cannot be approximated by a single separable term, so that the approximation loses its simplicity, while gaining undetermined parameters (see, for example, Ahmed and Beghi 1982).

The Hellmann–Feynman theorem, originally derived for the bound state problem (Feynman 1939), but later extended to the scattering problem (Sugar and Blankenbecler 1964), gives definite bounds for the off-shell amplitudes in terms of bounding potentials, and so can be used, for example with variational principles, to obtain potentials which approximate well both on- and off-shell. However, no rigorous derivation of the theorem has been given for local potentials. The on-shell form of the theorem, that $V_2(r)\leqslant V_1(r)$ implies $\delta_2\geqslant\delta_1$, has, of course, many direct applications.

We consider potentials satisfying the conditions, with $A>0$,

$$\int_0^A r|V(r)|\,\mathrm{d}r<\infty,\qquad \int_A^\infty |V(r)|\,\mathrm{d}r<\infty. \tag{1.1}$$

For such potentials Rajagopal and Shastry (1971) have shown that multiplication of the partial-wave Lippmann–Schwinger equation by $|V|^{1/2}$ gives a compact kernel K. Thus we have the partial-wave equivalent of the Rollnik class of potentials discussed by Simon (1971), although the latter class is more restricted as $r\to\infty$.

The Hellmann–Feynman theorem is most easily expressed in terms of the R-matrix and the corresponding real wavefunction. In § 2 we give the relevant formalism, establishing compactness (provided $\cos\delta \neq 0$), and reconstructing the 'usual' wavefunction, i.e. that without the $|V|^{1/2}$ factor. The advantages of the R-matrix approach are:

(i) all wavefunctions and amplitudes are real;

(ii) we avoid the complication of letting the energy approach the real axis from complex values, as discussed by Lovitch (1982);

(iii) full off-shell unitarity of the T-matrix is guaranteed for any approximation giving a real symmetric R-matrix.

The main disadvantage is that when $\cos\delta = 0$ the R-matrix diverges. This makes it difficult to establish a uniform bound for $(1-K)^{-1}$. However, in § 3 we show that, for a potential linearly dependent on a parameter λ, if $\cos\delta \neq 0$ for some λ, there is a neighbourhood of λ in which $\cos\delta \neq 0$ and $(1-K)^{-1}$ is uniformly bounded. It follows that the R-matrix is a differentiable function of λ, and the Hellmann–Feynman theorem follows.

Finally, in § 4, we derive the corresponding relations between the R-matrix elements for potentials $V_2 \geq V_1$. For the on-diagonal elements these are simple inequalities. For the off-diagonal elements we establish that these do not differ by more than the on-diagonal elements, so that the usefulness of an approximation need only be checked on-diagonal, i.e. for equal initial and final momenta.

2. *R*-matrix theory

The Lippmann–Schwinger equation reads, for the (real) off-shell wavefunction modified by the factor $|V(r)|^{1/2}$,

$$\Psi_q(r) = \phi_q(r) + \int_0^\infty K(r, r')\Psi_q(r')\,\mathrm{d}r' \tag{2.1}$$

where

$$\phi_q(r) = |V(r)|^{1/2} qrj_l(qr), \tag{2.2}$$

$$K(r, r') = |V(r)|^{1/2} G_0^0(r, r')|V(r')|^{1/2}\,\mathrm{sgn}\,V(r'), \tag{2.3}$$

with

$$G_0^0(r, r') = krr'j_l(kr)n_l(kr') = G_0^0(r', r) \qquad (r \leq r')$$

$$= G_0(r, r') + \mathrm{i}krr'j_l(kr)j_l(kr') \tag{2.4}$$

where G_0 is the (complex) T-matrix Green function.

The R-matrix elements are then given by

$$\langle p|R|q\rangle = (\Psi_p, \mathrm{sgn}\,V\phi_q) \tag{2.5}$$

so that

$$\langle k|R|k\rangle = -k\tan\delta. \tag{2.6}$$

For potentials satisfying (1.1) we see that $\phi_q \in L^2$ while

$$\mathrm{Tr}(K^+K) = \int_0^\infty \mathrm{d}r \int_0^\infty \mathrm{d}r'\,|V(r')|(krr'j_l(kr_<)n_l(kr_>))^2|V(r)|.$$

The only difference from the T-matrix calculation of Shastry and Rajagopal (1971) is that here n_l replaces $h_l^{(1)}$. But $|h_l^{(1)}|^2 = |j_l + in_l|^2 = j_l^2 + n_l^2 \geq n_l^2$, so that, since we are considering real positive energies, $\mathrm{Tr}(K^+K) < \infty$ by the same arguments.

Now, since K is Hilbert–Schmidt, we see by the Fredholm alternative that either

(i) K has a normalisable eigenfunction Ψ with unit eigenvalue, or

(ii) Ψ_q is uniquely defined (in L^2) by (2.1), whence $\langle p|R|q\rangle$ is well defined by (2.5) for all p and q.

In the case (i) we see, using (2.4), that

$$\Psi(r) = \int_0^\infty K(r, r')\Psi(r')\,\mathrm{d}r'$$

$$= \mu\phi_k(r) + \int_0^\infty |V(r)|^{1/2} G_0(r, r')|V(r')|^{1/2} \operatorname{sgn} V(r')\Psi(r')\,\mathrm{d}r'. \tag{2.7}$$

Apart from the constant μ this is just the on-shell equation for the complex wavefunction $\Psi_k^T(r)$ from T-matrix theory. Thus

$$\Psi(r) = \mu\Psi_k^T(r). \tag{2.8}$$

(We are assuming here that the energy k^2 does not correspond to a positive energy bound state, if any such exist. See, for example, Simon (1971).) Now from (2.7) we have

$$\mu = (\mathrm{i}/k)(\phi_k, \operatorname{sgn} V\Psi) = (\mathrm{i}\mu/k)(\phi_k, \operatorname{sgn} V\Psi_k^T) = -\mathrm{i}\mu\,\mathrm{e}^{\mathrm{i}\delta}\sin\delta.$$

Since $\mu \neq 0$ we see that we must have

$$\cos\delta = 0. \tag{2.9}$$

Thus at any energy such that $\cos\delta \neq 0$, $(1-K)^{-1}$ exists as a bounded operator, and the R-matrix is well defined. Given the solution $\Psi_q(r)$ of (2.1) we can define

$$\Phi_q(r) = qrj_l(qr) + \int_0^\infty G_0^0(r, r')|V(r')|^{1/2} \operatorname{sgn} V(r')\Psi_q(r')\,\mathrm{d}r' \tag{2.10}$$

since the integral is easily shown to be convergent for any r. This is the 'usual' wavefunction (satisfying the Schrödinger equation if suitably differentiable) and clearly

$$\Psi_q(r) = |V(r)|^{1/2}\Phi_q(r) \tag{2.11}$$

although (2.10) holds even where $V(r) = 0$.

Hence

$$\Phi_q(r) = qrj_l(qr) + \int_0^\infty G_0^0(r, r')V(r')\Phi_q(r')\,\mathrm{d}r' \tag{2.12}$$

although the kernel here is not Hilbert–Schmidt, and nor does $\Phi_q \in L^2$. Using (2.4) the T-matrix may be expressed in terms of the R-matrix by

$$\langle p|T|q\rangle = \langle p|R|q\rangle - (\mathrm{i}/k)\,\mathrm{e}^{\mathrm{i}\delta}\cos\delta\langle p|R|k\rangle\langle q|R|k\rangle \tag{2.13}$$

so that

$$\langle k|T|k\rangle = -k\,\mathrm{e}^{\mathrm{i}\delta}\sin\delta. \tag{2.14}$$

Any approximation yielding a real symmetric R will then give T satisfying the full off-shell unitarity condition

$$-k\,\mathrm{Im}\langle p|T|q\rangle = \langle p|T|k\rangle^*\langle q|T|k\rangle, \tag{2.15}$$

and

$$\langle p|T|q\rangle = \langle q|T|p\rangle. \tag{2.16}$$

Finally, we shall need the inverse of (2.13), which is

$$\langle p|R|q\rangle = \langle p|T|q\rangle + (\mathrm{i}/k)(\mathrm{e}^{-\mathrm{i}\delta}/\cos\delta)\langle p|T|k\rangle\langle q|T|k\rangle. \tag{2.17}$$

3. The Hellmann–Feynman theorem

Let V_1 and V_2 be two potentials satisfying (1.1). Define

$$K_{21} = \operatorname{sgn} V_2 |V_2|^{1/2} G_0^0 |V_1|^{1/2} \operatorname{sgn} V_1 = K_{12}^{+} \tag{3.1}$$

and

$$\Psi_q^{21} = \operatorname{sgn} V_2 |V_2|^{1/2} \Phi_q^{(1)} = \operatorname{sgn} V_2 \phi_q^{(2)} + K_{21}\Psi_q^{(1)} \tag{3.2}$$

using (2.10). K_{21} is Hilbert–Schmidt, by the same arguments as for K, whence $\Psi_q^{21} \in L^2$. Then

$$\int_0^\infty \Phi_p^{(2)}(r) V_2(r) \Phi_q^{(1)}(r)\,\mathrm{d}r = (\Psi_p^{(2)}, \Psi_q^{21}) = \langle p|R|q\rangle^{(2)} + (\Psi_p^{(2)}, K_{21}\Psi_q^{(1)}), \tag{3.3}$$

by (2.5), (2.11) and (3.2). Note that this formula, with $V_2 = V_1$, shows that R is symmetric in p and q.

Subtracting from (3.3) the same result with $1 \leftrightarrow 2$, $p \leftrightarrow q$, using (3.1) and the symmetry of R, we find

$$\langle p|R|q\rangle^{(2)} - \langle p|R|q\rangle^{(1)} = \int_0^\infty \Phi_p^{(2)}(r)(V_2(r) - V_1(r))\Phi_q^{(1)}(r)\,\mathrm{d}r. \tag{3.4}$$

Now let

$$V_\lambda = V_1 + \lambda(V_2 - V_1) = V_1 + \lambda V_0 \qquad (0 \leqslant \lambda \leqslant 1). \tag{3.5}$$

Then (3.4) gives, with V_λ and $V_{\lambda'}$ replacing V_1 and V_2,

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle p|R|q\rangle = \lim_{\lambda'\to\lambda} \int_0^\infty \Phi_p^{\lambda'}(r) V_0(r) \Phi_q^{\lambda}(r)\,\mathrm{d}r = \lim_{\lambda'\to\lambda} (\Psi_p^{0\lambda'}, \operatorname{sgn} V_0 \Psi_q^{0\lambda}) \tag{3.6}$$

where

$$\Psi_q^{0\lambda} = |V_0|^{1/2}\Phi_q^{\lambda} = \phi_q^0 + K_{0\lambda}\Psi_q^{\lambda} \tag{3.7}$$

and $K_{0\lambda} = |V_0|^{1/2} G_0^0 |V_\lambda|^{1/2} \operatorname{sgn} V_\lambda$ is Hilbert–Schmidt. To show the existence of the limit (3.6) we first show that $K_{0\lambda}$ is continuous in the norm as a function of λ. Suppose, for a given r, that $V_{\lambda'}(r)$ and $V_\lambda(r)$ are of the same sign (or one of them is zero). Then, since $V'_\lambda - V_\lambda = (\lambda' - \lambda)V_0$,

$$\big||V_{\lambda'}|^{1/2} \operatorname{sgn} V_{\lambda'} - |V_\lambda|^{1/2} \operatorname{sgn} V_\lambda\big| = \big||V_{\lambda'}|^{1/2} - |V_\lambda|^{1/2}\big| \leqslant |\lambda' - \lambda|^{1/2} |V_0|^{1/2} \tag{3.8}$$

(here and in (3.9) we use the fact that if a, b, c are non-negative numbers such that $a = b + c$, then $a^{1/2} \leqslant b^{1/2} + c^{1/2} \leqslant (2a)^{1/2}$).

On the other hand, if $V_{\lambda'}(r)$ and $V_\lambda(r)$ are of opposite sign then there exists λ_0 between λ and λ' such that $V_{\lambda_0}(r) = 0$. Therefore

$$V_\lambda(r) = (\lambda - \lambda_0) V_0(r)$$

so that

$$\|V_{\lambda'}|^{1/2}\,\mathrm{sgn}\,V_{\lambda'}-|V_\lambda|^{1/2}\,\mathrm{sgn}\,V_\lambda|=(|V_{\lambda'}|^{1/2}+|V_\lambda|^{1/2})$$
$$=(|\lambda-\lambda_0|^{1/2}+|\lambda'-\lambda_0|^{1/2})|V_0|^{1/2}\leqslant\sqrt{2}|\lambda'-\lambda|^{1/2}|V_0|^{1/2}. \tag{3.9}$$

Thus for fixed r, r'

$$|K_{0\lambda'}(r,r')-K_{0\lambda}(r,r')|\leqslant\sqrt{2}|V_0|^{1/2}|G_0^0||V_0|^{1/2}|\lambda'-\lambda|^{1/2}. \tag{3.10}$$

Hence

$$\|K_{0\lambda'}-K_{0\lambda}\|\leqslant A|\lambda'-\lambda|^{1/2} \tag{3.11}$$

where A is independent of λ, λ'.

In a similar way we may prove that

$$\|K_{\lambda'}-K_\lambda\|\leqslant B|\lambda'-\lambda|^{1/2} \tag{3.12}$$

where

$$K_\lambda=|V_\lambda|^{1/2}G_0^0|V_\lambda|^{1/2}\,\mathrm{sgn}\,V_\lambda$$

is the Lippmann–Schwinger kernel for the potential V_λ. (For this result we also use the fact that $|V_\lambda(r)|\leqslant\max(|V_1(r)|,|V_2(r)|)$, from which we can also see that $K_{0\lambda}$ and K_λ are uniformly bounded for $\lambda\in(0,1)$.)

Now choose a fixed λ such that $\cos\delta\neq 0$. Then $M_\lambda=(1-K_\lambda)^{-1}$ exists bounded and we may use the identity

$$M_{\lambda'}-M_\lambda=M_\lambda[1-(K_{\lambda'}-K_\lambda)M_\lambda]^{-1}(K_{\lambda'}-K_\lambda)M_\lambda \tag{3.13}$$

to prove:

(i) there is a neighbourhood of λ in which $M_{\lambda'}$ is defined and uniformly bounded, although the bound may depend on λ;

(ii) M_λ is continuous in the norm at such λ.

Since $K_{0\lambda}$ also has these properties, so does

$$N_\lambda=K_{0\lambda}M_\lambda=K_{0\lambda}(1-K_\lambda)^{-1}. \tag{3.14}$$

Returning to (3.7), we see that $\Psi_q^{0\lambda}$ is (strongly) continuous in λ. For $\Psi_q^{0\lambda}=\phi_q^0+N_\lambda\phi_q^\lambda$ so that

$$\|\Psi_q^{0\lambda'}-\Psi_q^{0\lambda}\|=\|N_{\lambda'}\phi_q^{\lambda'}-N_\lambda\phi_q^\lambda\|$$
$$\leqslant\|N_{\lambda'}\|\cdot\|\phi_q^{\lambda'}-\phi_q^\lambda\|+\|N_{\lambda'}-N_\lambda\|\cdot\|\phi_q^\lambda\|$$
$$\to 0 \qquad \text{as } \lambda'\to\lambda,$$

since $\phi_q^\lambda=|V_\lambda|^{1/2}qrj_l(qr)$ also has properties (i) and (ii) above.

It follows that the limit in (3.6) exists, giving

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle p|R|q\rangle=\int_0^\infty\Phi_p(r)V_0(r)\Phi_q(r)\,\mathrm{d}r. \tag{3.15}$$

4. Bounds on amplitudes

We now consider potentials such that, for all r,

$$V_0(r)=V_2(r)-V_1(r)\geqslant 0. \tag{4.1}$$

Case (i) $p = q = k$

On-shell, (3.15) gives

$$(\mathrm{d}/\mathrm{d}\lambda)\langle k|R|k\rangle \geqslant 0. \tag{4.2}$$

Integrating from $\lambda = 0$ to $\lambda = 1$, so that V_λ runs from V_1 to V_2, we see that $\langle k|R|k\rangle^{(2)} \geqslant \langle k|R|k\rangle^{(1)}$, i.e. that

$$\tan \delta^{(2)} \leqslant \tan \delta^{(1)}, \tag{4.3}$$

provided that $\cos \delta \neq 0$ for any V_λ with $0 \leqslant \lambda \leqslant 1$. Now our results show that $\tan \delta$ varies continuously with λ except where $\cos \delta = 0$, so it is possible to choose δ to vary continuously with λ even where $\cos \delta = 0$. (We do not consider $k = 0$.) Then we have

$$\delta^{(2)} \leqslant \delta^{(1)} \tag{4.4}$$

even if δ passes through an odd multiple of $\frac{1}{2}\pi$.

Case (ii) $p = q \neq k$.

As in the above we find

$$\langle q|R|q\rangle^{(2)} \geqslant \langle q|R|q\rangle^{(1)} \tag{4.5}$$

subject to $\cos \delta$ never vanishing. We can see from (3.13) that this can be guaranteed if V_0 is suitably small, for example, if V_2 were to be a variational approximation to V_1. If not, it is useful to introduce an off-shell phase shift by

$$\langle q|R|q\rangle = -k \tan \delta_q$$

together with the requirement that δ_q lies in the same interval $((r-\frac{1}{2})\pi, (r+\frac{1}{2})\pi)$ as δ. Then

$$\delta_q^{(2)} \leqslant \delta_q^{(1)} \tag{4.6}$$

without the restriction that $\cos \delta$ never vanishes.

If $\cos \delta = 0$ we see from the unitarity condition (2.15) that $\langle q|T|k\rangle$ is pure imaginary. Near such a point we see from (2.17) that

$$\tan \delta_q \approx C \tan \delta \tag{4.7}$$

where C is a positive constant unless $\langle q|T|k\rangle = 0$. This latter condition would imply that ϕ_q was orthogonal to sgn $V\Psi_k^T$, i.e. to the only eigenvector of K^+ with unit eigenvalue (see § 2). Hence (2.1) would have infinitely many solutions, but all would give the same value for $\langle q|R|q\rangle$. In this case alone δ_q would be discontinuous, but (4.6) would still apply.

Case (iii) $p \neq q$

In the off-diagonal case we see, by replacing q by $\alpha q + \beta p$ in (4.5), where α and β are arbitrary, that

$$(\langle p|R|q\rangle^{(2)} - \langle p|R|q\rangle^{(1)})^2 \leqslant (\langle p|R|p\rangle^{(2)} - \langle p|R|p\rangle^{(1)})(\langle q|R|q\rangle^{(2)} - \langle q|R|q\rangle^{(1)}). \tag{4.8}$$

This tells us that the off-diagonal elements do not differ by more than the on-diagonal elements. Thus the adequacy of an approximation need only be tested for the on-diagonal elements, subject of course to $V_2(r) \geqslant V_1(r)$.

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