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Off-shell variational bounds

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Abstract. The Schwinger variational principle is shown to lead to upper and lower bounds for the off-shell scattering amplitude for local potentials satisfying $\int_0^A r|V(r)| dr < \infty$ and $\int_A^\infty |V(r)| dr < \infty$.

1. Introduction

In a recent paper (Warburton 1983, hereafter referred to as I) the Hellmann–Feynman theorem was proved for local potentials satisfying the conditions

$$\int_0^A r|V(r)| dr < \infty, \quad \int_A^\infty |V(r)| dr < \infty \quad (1.1)$$

and corresponding bounds deduced for the R -matrix elements, both on and off the energy shell. However, an important application of the theorem, to which the above proof does not apply, is to obtain bounds using the Schwinger variational principle, where a local potential is approximated by a sum of separable terms (Bessis *et al* 1977). The purpose of the present paper is to extend the results of I to a sum of local and separable potentials, thereby justifying the Schwinger principle bounds, both on and off the energy shell.

Specifically, we consider a potential $V = V_1 + V_2$, where V_2 is a solvable potential and $V_1(r) \geq 0$ (or $V_1(r) \leq 0$), both V_1 and V_2 satisfying (1.1). As shown by Sugar and Blankenbecler (1964):

$$V_1 \geq \sum_{ij} V_1 |q_i\rangle V_{ij}^{-1} \langle q_j| V_1 \quad (1.2)$$

where $V_{ij} = \langle q_i | V_1 | q_j \rangle$ and $q_1 \dots q_L$ is any given set of momenta. We thus have a bound for V which we use to prove corresponding bounds for the R -matrix elements.

For a rigorous proof we need to express all quantities in terms of square integrable wavefunctions and Hilbert–Schmidt kernels. This is done for $V_1 + V_2$ in § 2, and for the (local plus separable) bounding potential in § 3, where the Hellmann–Feynman theorem is also proved.

The relation to the Schwinger variational principle is given in § 4, and the bounds discussed. It should be noted that in practical calculations several stationary points may be found, so that having definite bounds enables one to choose between these. Also, the functions $\langle r | q_i \rangle = q_i r j_i(q_i r)$ may be replaced by other functions (with similar bounds as $r \rightarrow 0$ and $r \rightarrow \infty$) provided the matrix $[V_{ij}]$ is invertible.

2. The R-matrix for the sum of two potentials

We consider here the potential $V = V_1 + V_2$, where V_1 and V_2 both satisfy (1.1), $V_1(r) \geq 0$, and V_2 is a solvable potential. The off-shell Lippmann-Schwinger equation is

$$\Phi_q = qrj_l(qr) + G_0^0 V \Phi_q \tag{2.1}$$

where $\langle r | G_0^0 | r' \rangle = krr' j_l(kr) n_l(kr)$.

In order to obtain equations involving only square integrable wavefunctions and Hilbert-Schmidt kernels, we introduce (for $m, n = 1, 2$)

$$\Psi_q^m = |V_m|^{1/2} \Phi_q, \tag{2.2}$$

$$\phi_q^m = |V_m|^{1/2} \langle r | q \rangle = |V_m|^{1/2} qrj_l(qr),$$

and

$$K_{mn} = |V_m|^{1/2} G_0^0 |V_n|^{1/2} \text{sgn } V_n,$$

which is Hilbert-Schmidt by the arguments in I.

Then (2.1) gives

$$\Psi_q^m = \phi_q^m + \sum_{n=1}^2 K_{mn} \Psi_q^n \tag{2.3}$$

(the solutions of which can be substituted back into (2.1) to give Φ_q , even where $V_m = 0$).

Also,

$$\begin{aligned} \langle p | R | q \rangle &= \langle \Phi_p | V | q \rangle \\ &= \sum_{m=1}^2 (\text{sgn } V_m \Psi_p^m, \phi_q^m). \end{aligned} \tag{2.4}$$

On-shell $\langle k | R | k \rangle = -k \tan \delta$.

Provided $\cos \delta_2 \neq 0$ (see I) we can invert $(1 - K_{22})$ in (2.3) to obtain

$$\Psi_q^2 = (1 - K_{22})^{-1} \phi_q^2 + (1 - K_{22})^{-1} K_{21} \Psi_q^1$$

whence

$$\Psi_q^1 = \psi_q + K \Psi_q^1 \tag{2.5}$$

with

$$\psi_q = \phi_q^1 + K_{12} (1 - K_{22})^{-1} \phi_q^2 = V_1^{1/2} \Phi_q^{(2)} \tag{2.6}$$

and

$$K = K_{11} + K_{12} (1 - K_{22})^{-1} K_{21} = K^+. \tag{2.7}$$

Here $\Phi_q^{(2)}$, the wavefunction for V_2 alone, is supposedly known. Hence $\Psi_q^1 = (1 - K)^{-1} \psi_q$ and $\Psi_q^2 = (1 - K_{22})^{-1} \phi_q^2 + (1 - K_{22})^{-1} K_{21} (1 - K)^{-1} \psi_q$, so that

$$\langle p | R | q \rangle = \langle p | R | q \rangle^{(2)} + (\psi_p, (1 - K)^{-1} \psi_q) = \langle p | R | q \rangle^{(2)} + (\psi_p, \Psi_q^1) \tag{2.8}$$

provided that $(1 - K)$ is invertible, i.e. provided $\cos \delta \neq 0$. Note that the wavefunctions are only needed where $V_1 \neq 0$.

3. The Hellmann–Feynman theorem

We now consider the potential (see § 1)

$$V(\lambda) = V_2 + \lambda V_1 + (1 - \lambda) \sum_{ij} V_1 |q_i\rangle V_{ij}^{-1} \langle q_j| V_1$$

as λ increases from 0 to 1. With the notation of § 2, (2.3) is replaced by

$$\Psi_q^m = \phi_q^m + \lambda K_{m1} \Psi_q^1 + K_{m2} \Psi_q^2 + (1 - \lambda) \sum_{ij} K_{m1} \phi_i V_{ij}^{-1} (\phi_j, \Psi_q^1) \tag{3.1}$$

while (2.4) becomes, recalling $V_1 \geq 0$,

$$\langle p|R|q\rangle^{(\lambda)} = \lambda (\Psi_p^1, \phi_q^1) + (\text{sgn } V_2 \Psi_p^2, \phi_q^2) + (1 - \lambda) \sum_{ij} (\Psi_p^1, \phi_i) V_{ij}^{-1} (\phi_j, \phi_q^1) \tag{3.2}$$

where we put $\phi_i = \phi_q^1$.

We now eliminate ϕ_q^m from (3.2) by means of (3.1) with λ replaced by λ' , to obtain an expression homogeneous in the functions Ψ_p^m and Ψ_q^m , the dash on the latter indicating evaluation at λ' . We find

$$\langle p|R|q\rangle^{(\lambda)} = \lambda (\Psi_p^1, \Psi_q^1) + (1 - \lambda) \sum_{ij} (\Psi_p^1, \phi_i) V_{ij}^{-1} (\phi_j, \Psi_q^1) + S \tag{3.3}$$

where S represents certain terms which are invariant under the simultaneous interchange $p \leftrightarrow q$, $\lambda \leftrightarrow \lambda'$. Choosing $\lambda' = \lambda$ in (3.3) reveals that $\langle p|R|q\rangle^{(\lambda)} = \langle q|R|p\rangle^{(\lambda)}$ whence subtracting from (3.3) the same equation with $p \leftrightarrow q$ and $\lambda \leftrightarrow \lambda'$ yields

$$\begin{aligned} \frac{d}{d\lambda} \langle p|R|q\rangle^{(\lambda)} &= \lim_{\lambda' \rightarrow \lambda} \left\{ (\Psi_p^1, \Psi_{p'}^1) - \sum_{ij} (\Psi_p^1, \phi_i) V_{ij}^{-1} (\phi_j, \Psi_{q'}^1) \right\} \\ &= (\Psi_p^1, \Psi_q^1) - \sum_{ij} (\Psi_p^1, \phi_i) V_{ij}^{-1} (\phi_j, \Psi_q^1) \end{aligned} \tag{3.4}$$

provided that Ψ_q^1 is continuous in λ , which we now prove. The kernel K_λ of (3.1), a 2×2 matrix of integral operators, depends linearly on λ , and hence is continuous (in the norm) in λ . Hence, provided $M_\lambda = (1 - K_\lambda)^{-1}$ exists, we can (as in I) use the identity

$$M_{\lambda'} - M_\lambda = M_\lambda [1 - (K_{\lambda'} - K_\lambda) M_\lambda]^{-1} (K_{\lambda'} - K_\lambda) M_\lambda \tag{3.5}$$

to prove that there is a neighbourhood of λ in which $M_{\lambda'}$ is defined and continuous in the norm. It follows from (3.1) that Ψ_q^1 is continuous in λ .

If $(1 - K_\lambda)$ is not invertible, then we can show, by a similar argument to that in I, that $\cos \delta = 0$. The essence of the argument is that the corresponding T -matrix kernel must be invertible, or there would be a positive energy bound state. Since the complex on-shell wavefunction in that case is $e^{i\delta} \cos \delta$ times our real wavefunction, it must satisfy (3.1) with $e^{i\delta} \cos \delta \phi_k^m$ as inhomogeneous term. Hence the homogeneous form of (3.1) can only have a non-trivial solution if $\cos \delta = 0$.

Now choose $p = q$. By virtue of (1.2) and (2.2), (3.4) gives

$$(d/d\lambda) \langle q|R|q\rangle^{(\lambda)} \geq 0.$$

Integrating from 0 to 1 we see that

$$\langle q|R|q\rangle^{(1)} \geq \langle q|R|q\rangle^{(0)} \tag{3.6}$$

provided $\cos \delta$ never vanishes for $0 \leq \lambda \leq 1$. In the context of variational approximations we may presume that our approximate potential $V(0)$ is sufficiently close to $V(1) = V_1 + V_2$ that this is so.

4. The Schwinger variational principle

The inequality we have obtained may be related to the Schwinger variational principle. Consider the functional

$$F(\Psi', \Psi) = \langle p|R|q \rangle^{(2)} + (\psi_p, \Psi) + (\Psi', \psi_q) - (\Psi', (1-K)\Psi) \quad (4.1)$$

where the R -matrix for V_2 is given, ψ_p and ψ_q are defined by (2.6), and K by (2.7).

This is stationary when

$$\Psi = \psi_q + K\Psi \quad \Psi' = \psi_p + K\Psi' \quad (4.2)$$

so that, from (2.5), $\Psi = \Psi_q^1$ and $\Psi' = \Psi_p^1$ and

$$F = \langle p|R|q \rangle^{(2)} + (\psi_p, \Psi_p^1) = \langle p|R|q \rangle \quad (4.3)$$

the exact R -matrix element for $V = V_1 + V_2$, by (2.8). For $p = q$ we need only consider $\Psi' = \Psi$.

In practice, (see, for example, Bessis *et al* 1977), Ψ and Ψ' are restricted to the space E_L spanned by the $\phi_1 \dots \phi_L$ defined in § 3. In this case we find a stationary value

$$F = \langle p|R|q \rangle^{(2)} + \sum_{ij} (\psi_p, \phi_i) N_{ij}^{-1} (\phi_j, \psi_q) \quad (4.4)$$

where $N_{ij} = (\phi_i, (1-K)\phi_j) = N_{ji}$. (4.4) is the exact off-shell R -matrix element for

$$V(0) = V_2 + \sum_{ij} V_1|q_i\rangle V_{ij}^{-1} \langle q_j| V_1 \quad (4.5)$$

as may be seen, for example, by solving the equations (3.1) with $\lambda = 0$. (Note, however, that the wavefunction Ψ_0 produced by the variational method will differ, in general, from the function Ψ_q^1 for $V(0)$.) We thus deduce from (3.6) that, for $p = q$, the variational method leads to a lower bound for $\langle p|R|p \rangle$, in the sense that the stationary value $F(\Psi_0, \Psi_0)$ on E_L is such a bound. From (4.1) with $\Psi' = \Psi$ we see that only if $\|K\| < 1$ can we guarantee that F is a maximum for arbitrary variations in Ψ . The set q_i ($i = 1, L$) is now varied for fixed L , and we seek a maximum of the stationary value $F(\Psi_0, \Psi_0)$, giving the optimal lower bound to the R -matrix element for the given L . By choosing a V_2 such that $V_1 \leq 0$, upper bounds may similarly be found.

For $p \neq q$ we see, by replacing q by $\alpha q + \beta p$ in (3.6), where α and β are arbitrary, that

$$(\langle p|R|q \rangle^{(1)} - \langle p|R|q \rangle^{(0)})^2 \leq (\langle p|R|p \rangle^{(1)} - \langle p|R|p \rangle^{(0)}) (\langle q|R|q \rangle^{(1)} - \langle q|R|q \rangle^{(0)}). \quad (4.6)$$

This enables us to deduce upper and lower bounds for the off-diagonal R -matrix elements from those for the on-diagonal elements. If we seek an approximating potential $V(0)$ which is independent of the off-shell momenta then (4.6) tells us that the greatest error will be for the on-diagonal elements, so that we choose $q_1 \dots q_L$ to minimise the on-diagonal errors.

References

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