A convergence proof for the Schwinger variational method for the scattering amplitude

1975 J. Phys. A: Math. Gen. 8 1379

(http://iopscience.iop.org/0305-4470/8/9/005)

J. Phys. A: Math. Gen., Vol. 8, No. 9, 1975. Printed in Great Britain. © 1975

A convergence proof for the Schwinger variational method for the scattering amplitude

S R Singh and A D Stauffer

Physics Department, York University, Downsview, Ontario, Canada, M3J 1P3

Received 12 May 1975

Abstract. We show that with certain restrictions on the trial functions the Schwinger variational method yields a convergent process for computing the scattering amplitude in scattering from short-range potentials.

1. Introduction

Various forms of variational methods have been used extensively in computing scattering data involving a variety of interactions (see eg Mott and Massey 1965). Most of these methods reduce to either the Schwinger method (SV) or the Kohn method (Singh 1973). Recently we have rigorously studied both these methods when they are used to compute the tangent of the phase shift for the case of partial wave scattering from a potential $zV(r)$ (Singh and Stauffer 1974a). The potential was assumed to satisfy the following conditions:

$$\int |zV(\boldsymbol{r})|\,\mathrm{d}\boldsymbol{r} < \infty; \qquad \iint \frac{|zV(\boldsymbol{r})|\,|zV(\boldsymbol{r}_1)|}{|\boldsymbol{r}-\boldsymbol{r}_1|^2}\,\mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}_1 < \infty \tag{1}$$

and to be of definite sign so that, by absorbing the sign in the potential strength z, $V(\boldsymbol{r})$ can be taken to be positive. In the present paper we extend the treatment to the case where SV is used to compute the scattering amplitude. We show that, with certain restrictions on the trial functions, SV yields a convergent process for determining the wavefunction and the scattering amplitude. These restrictions will be seen not only to assure the convergence but also to reduce the computational labour.

2. Preliminary remarks

In potential scattering one is interested in solving the Lippmann–Schwinger equation

$$\psi_\pm(\boldsymbol{r}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}_\pm\cdot\boldsymbol{r}} - \frac{z}{4\pi}\int G_\pm(\boldsymbol{r},\boldsymbol{r}_1)V(\boldsymbol{r}_1)\psi_\pm(\boldsymbol{r}_1)\,\mathrm{d}\boldsymbol{r}_1 \tag{$2_\pm$}$$

where

$$G_\pm(\boldsymbol{r},\boldsymbol{r}_1) = \frac{\exp(\pm\mathrm{i}k|\boldsymbol{r}-\boldsymbol{r}_1|)}{|\boldsymbol{r}-\boldsymbol{r}_1|} \tag{2a}$$

are the free particle Green functions with energy $E = \frac{1}{2}k^2$ and $\boldsymbol{k}_+$ and $\boldsymbol{k}_-$ are the momenta of the incident and the scattered particle respectively. We consider the case of $\psi_+(\boldsymbol{r})$. The case of $\psi_-(\boldsymbol{r})$ is treated similarly. The scattering amplitude T is given by:

$$T = -\frac{z}{4\pi}\int \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_-\cdot\boldsymbol{r}}V(\boldsymbol{r})\psi_+(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}. \tag{3}$$

By multiplying (2_+) by $\psi^*_-(\boldsymbol{r})V(\boldsymbol{r})$, integrating and adding the resultant identity to (3) we get an alternate expression, T_s, for T, namely

$$T_s(\psi_\pm) = -\frac{z}{4\pi}\bigg[\int \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_-\cdot\boldsymbol{r}}V(\boldsymbol{r})\psi_+(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} + \int \psi^*_-(\boldsymbol{r})V(\boldsymbol{r})\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}_+\cdot\boldsymbol{r}}\,\mathrm{d}\boldsymbol{r}$$
$$-\int \mathrm{d}\boldsymbol{r}\psi^*_-(\boldsymbol{r})V(\boldsymbol{r})\bigg(\psi_+(\boldsymbol{r}) + \frac{z}{4\pi}\int G_+(\boldsymbol{r},\boldsymbol{r}_1)V(\boldsymbol{r}_1)\psi_+(\boldsymbol{r}_1)\,\mathrm{d}\boldsymbol{r}_1\bigg)\bigg] \tag{4}$$

The advantage in dealing with T_s, instead of T, is that considered as a functional of $\psi_\pm$ it is stationary with respect to arbitrary and independent variations of $\psi_\pm$ about their exact values (Mower 1955).

In SV one constructs $T_s(\psi^t_\pm)$ by replacing $\psi_\pm$ on the right-hand side of (4) by some trial functions $\psi^t_\pm$ containing arbitrary parameters. These parameters are then varied to obtain the stationary value T_n of $T_s(\psi^t_\pm)$ which is taken to be the approximate value of T. Because of computational advantages, $\psi^t_\pm$ are often chosen to be linear combinations of some 'basis functions'. As we have shown previously (Singh and Stauffer 1974b) ψ^t_+ and ψ^t_- must contain the same number of terms and for best results be constructed from the same basis functions ψ_i, ie

$$\psi^t_\pm = \sum_{i=1}^{n} \alpha_i^\pm \psi_i. \tag{5}$$

By setting the derivatives of $T_s(\psi^t_\pm)$ with respect to the $\alpha_i^\pm$ equal to zero one obtains the following sets of algebraic equations:

$$\sum_{j=1}^{n} \alpha_j^\pm \int \mathrm{d}\boldsymbol{r}\psi_i^*(\boldsymbol{r})V(\boldsymbol{r})\bigg(\psi_j(\boldsymbol{r}) + \frac{z}{4\pi}\int G_\pm(\boldsymbol{r},\boldsymbol{r}_1)V(\boldsymbol{r}_1)\psi_j(\boldsymbol{r}_1)\,\mathrm{d}\boldsymbol{r}_1\bigg)$$
$$= \int \psi_i^*(\boldsymbol{r})V(\boldsymbol{r})\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}_\pm\cdot\boldsymbol{r}}\,\mathrm{d}\boldsymbol{r} \qquad i = 1,\ldots,n. \tag{$6_\pm$}$$

With these restrictions on the trial functions, it is sufficient to solve only the set given by (6_+) and T_n is given by:

$$T_n = -\frac{z}{4\pi}\int \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_-\cdot\boldsymbol{r}}V(\boldsymbol{r})\psi^t_+(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}. \tag{7}$$

It is pertinent to remark here that the original stationary expression $\tilde{T}_s$ for T given by Schwinger (1947, Lectures on Nuclear Physics, unpublished) was

$$\tilde{T}_s(\psi_\pm) = -\frac{z}{4\pi}\,\frac{\int \mathrm{e}^{-\mathrm{i}\boldsymbol{k}_-\cdot\boldsymbol{r}}V(\boldsymbol{r})\psi_+(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}\int \psi^*_-(\boldsymbol{r})V(\boldsymbol{r})\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}_+\cdot\boldsymbol{r}}\,\mathrm{d}\boldsymbol{r}}{\int \mathrm{d}\boldsymbol{r}\,\psi^*_-(\boldsymbol{r})V(\boldsymbol{r})[\psi_+(\boldsymbol{r}) + (z/4\pi)\int G_+(\boldsymbol{r},\boldsymbol{r}_1)V(\boldsymbol{r}_1)\psi_+(\boldsymbol{r}_1)\,\mathrm{d}\boldsymbol{r}_1]} \tag{8}$$

It can be shown that, with the forms of $\psi^t_\pm$ given above, the stationary values of $\tilde{T}_s(\psi^t_\pm)$ and $T_s(\psi^t_\pm)$ are identical. Hence in our terminology SV implies the solution of (6_+) followed by the evaluation of T_n via (7). In the following section we show there are further restrictions on $\{\psi_i\}$ to ensure the convergence of SV.

3. Convergence of the Schwinger method

We denote by $\mathscr{H}$ the Hilbert space of square integrable functions of $\boldsymbol{r}$. Let $f^{\pm} = V^{1/2}\psi_{\pm}$, $g^{\pm} = V^{1/2}\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}_{\pm}\cdot\boldsymbol{r}}$ and $K^{\pm}$ be the operators defined by:

$$(K^{\pm}u)(\boldsymbol{r}) = \frac{1}{4\pi}\int V^{1/2}(\boldsymbol{r})G_{\pm}(\boldsymbol{r},\boldsymbol{r}_1)V^{1/2}(\boldsymbol{r}_1)u(\boldsymbol{r}_1)\,\mathrm{d}\boldsymbol{r}_1 \tag{9}$$

for each u in $\mathscr{H}$. With a V which satisfies the conditions given by (1), $K^{\pm}$ are Hilbert–Schmidt operators and $f^{\pm}$, $g^{\pm}$ are in $\mathscr{H}$ (see, eg Scadron *et al* 1964). Instead of $(2_{\pm})$ we consider the transformed equations

$$(1+zK^{\pm})f^{\pm} = g^{\pm} \tag{10}$$

$T = T_{\mathrm{s}}(\psi_{\pm})$ is given by

$$4\pi z^{-1}T = -\langle g^{-}|f^{+}\rangle = \langle f^{-}|(1+zK^{+})f^{+}\rangle - \langle f^{-}|g^{+}\rangle - \langle g^{-}|f^{+}\rangle \tag{11}$$

where $\langle u|v\rangle = \int u^{*}(\boldsymbol{r})v(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}$ is the scalar product in $\mathscr{H}$.

After this preparation we are in a position to prove the following theorem.

Theorem

If the 'basis set' $\{\phi_i\} = \{V^{1/2}\psi_i\}$ is an orthonormal basis in $\mathscr{H}$, then: (i) SV yields a convergent process to determine ψ_{+} and T; (ii) the error in T_n is of second order in the error in ψ^{t}_{+}.

We remark that for computational purposes it is sufficient that $\{\phi_i\}$ be linearly independent rather than strictly orthonormal.

Proof

(i) With the conditions of the theorem, (6_{+}) reduces to:

$$\sum_{j=1}^{n} \alpha_j^{+}\langle\phi_i|(1+zK^{+})\phi_j\rangle = \langle\phi_i|g^{+}\rangle, \qquad i = 1,\ldots,n. \tag{12}$$

It is straightforward to show that $f_n^{+} = \Sigma_{j=1}^{n}\alpha_j^{+}\phi_j \to f^{+}$ in the norm of $\mathscr{H}$ (Mikhlin 1964). In brief, the argument is based on the fact that, since K^{+} is compact,

$$K_n^{+} = P_nK^{+}P_n \underset{\mathrm{u}}{\rightarrow} K^{+}$$

where $P_n = \Sigma_{i=1}^{n}|\phi_i\rangle\langle\phi_i|$ and $\underset{\mathrm{u}}{\rightarrow}$ denotes uniform convergence. Since $(1+zK^{+})^{-1}$ exists it follows that $(1+zK_n^{+})^{-1}$ also exists for each n greater than some N, and $(1+zK_n^{+})^{-1} \underset{\mathrm{u}}{\rightarrow} (1+zK^{+})^{-1}$. (12) is equivalent to

$$(1+zK_n^{+})f_n^{+} = P_ng \tag{13}$$

and since $\|P_ng^{+}-g^{+}\| \to 0$, it follows that $\|f_n^{+}-f^{+}\| \to 0$, where $\|\ldots\|$ denotes the norm in $\mathscr{H}$. It is now obvious that $T_n = -(z/4\pi)\langle g^{-}|f_n^{+}\rangle \to T$.

(ii) Following the same line of argument as in the proof of (i) one observes that

$$\sum_{j=1}^{n} \alpha_j^{-}\langle\phi_i|(1+zK^{-})\phi_j\rangle = \langle\phi_i|g^{-}\rangle \qquad i = 1,\ldots,n \tag{14}$$

has a solution for sufficiently large n and that

$$f_n^- = \sum_{j=1}^{n} \alpha_j^- \phi_j \rightarrow f^-. \tag{14a}$$

From (11) we have that

$$\begin{aligned} 4\pi z^{-1} T_n &= \langle f_n^- |(1+zK^+) f_n^+\rangle - \langle f_n^- | g^+\rangle - \langle g^- | f_n^+\rangle \\ &= 4\pi z^{-1} T + \langle (1+zK^-) f^- - g^- | f_n^+ - f^+\rangle \\ &\quad + \langle f_n^- - f^- |(1+zK^+) f^+ - g^+\rangle + \langle f_n^- - f^- |(1+zK^+)(f_n^+ - f^+)\rangle. \end{aligned} \tag{15}$$

That is

$$\begin{aligned} |4\pi z^{-1}(T_n - T)| &= |\langle f_n^- - f^- |(1+zK^+)(f_n^+ - f^+)\rangle| \\ &\leqslant \|1+zK^+\| \, \|f_n^- - f^-\| \, \|f_n^+ - f^+\|. \end{aligned}$$

Thus the error in T_n is $\mathrm{O}\|f_n^- - f^-\| \, \|f_n^+ - f^+\|$. Since f_n^- is accurate to the same order as f_n^+ the error in T_n is of second order in the error in f_n^+.

In the following we prove the existence of a potential for which T_n is the exact scattering amplitude.

Proposition

T_n is the exact scattering amplitude corresponding to the potential $zV_n = zV^{1/2}P_nV^{1/2}$. (Note that V_n is a non-local potential while V is local.)

Proof

From (13) one has that

$$f_n^+ + zP_nV^{1/2}G_+V^{1/2}P_nf_n^+ = P_ng^+. \tag{16}$$

The detailed meaning of (16) is as given by (9). Let $\tilde{\psi}_n = G_+V^{1/2}P_nf_n^+$. It is obvious that $\psi_n^{\mathrm{s}} = \mathrm{e}^{\mathrm{i}\boldsymbol{k}_+\cdot\boldsymbol{r}} - z\tilde{\psi}_n$ is a scattering state function. Further $\tilde{\psi}_n$ is a particular solution of

$$(H_0 - E)\tilde{\psi}_n = V^{1/2}P_nf_n^+ = V^{1/2}f_n^+ = V^{1/2}P_ng^+ - zV^{1/2}P_nV^{1/2}\tilde{\psi}_n \tag{17}$$

where H_0 is the free particle Hamiltonian. That is

$$(H_0 - E + zV_n)\psi_n^{\mathrm{s}} = 0. \tag{18}$$

It follows from (18) that ψ_n^{s} is the exact scattering state solution of the Schrödinger equation with potential zV_n. From the asymptotic behaviour of ψ_n^{s} it follows that T_n is the exact scattering amplitude corresponding to the potential zV_n.

In spite of its simplicity the proposition has useful consequences. For example it is now obvious that T_n satisfies the optical theorem (see, eg, Prugovecki 1971). Hence the approximate total cross section in SV can be determined from the knowledge of the imaginary part of the approximate forward scattering amplitude.

4. Discussion

To assure the convergence of SV in computing the scattering amplitude we require $\{V^{1/2}\psi_i\}$ to be a basis set in $\mathscr{H}$. One such basis is obtained from the perturbation expansion of ψ^+, ie $\psi_i = (G_+V)^{i-1}\,e^{i\boldsymbol{k}_+\cdot\boldsymbol{r}}$, $i = 1, 2, \ldots$. With this particular choice SV becomes the method of moments. If one considers partial wave scattering and replaces G_+ by its principal value, one can formulate SV for $\tan\delta$ where δ is the usual scattering phase shift. In this case the method of moments reduces to the method of Padé approximants (Singh and Stauffer 1974a).

We have proved the convergence of the Kohn variational method for $\tan\delta$ (Singh and Stauffer 1974a). However, since the symmetry of K plays an important role in that case, we have been unable to extend it to the case of the scattering amplitude.

Acknowledgments

One of us (SRS) would like to thank the National Research Council of Canada for a scholarship. As well, ADS is grateful to Royal Holloway College for the provision of facilities during a sabbatical leave.

This research was supported in part by the National Research Council of Canada under grant A-4632.

References

Mikhlin S G 1964 *Variational Methods in Mathematical Physics* (New York: Academic Press) chap 9
Mott N F and Massey H S W 1965 *The Theory of Atomic Collisions*, 3rd edn (London: Oxford University Press)
Mower L 1955 *Phys. Rev.* **99** 1065–9
Prugovecki E 1971 *Quantum Mechanics in Hilbert Space* (New York: Academic Press) pp 479–80
Scadron M, Weinberg S and Wright J 1964 *Phys. Rev.* B **135** 202–7
Singh S R 1973 *Lett. Nuovo Cim.* **6** 482–4
Singh S R and Stauffer A D 1974a *Nuovo Cim.* B **22** 139–52
—— 1974b *J. Phys.* B: *Atom. Molec. Phys.* **7** 782–7