Application of Variational Principles to Scattering Problems*

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The Schwinger and Kohn-Hulthén variational principles are adapted to scattering problems in which only a part of the scattering potential is small.

I. INTRODUCTION

SEVERAL authors[1-3] have discussed the problem of scattering by a potential, only part of which is to be considered small. It is found that the scattering operator can be written as the sum of two terms: the first is the scattering operator which would be obtained if the small part of the potential vanished and the second is a term involving the eigenfunction of the entire Hamiltonian. The first term is assumed known. Hence to find the scattering operator of the problem one needs to find the second term only. In the present paper it is our objective to show how the Schwinger and Kohn-Hulthen variational principles can be used to find approximate expressions for this term.

II. THE VARIATIONAL PRINCIPLES

We shall briefly review the scattering operator formalism and indicate the usual form of the variational expressions. In scattering problems the total Hamiltonian H is broken up into two parts,

$$H=K+V, \tag{1}$$

where K is the unperturbed Hamiltonian and V is the scattering potential. Usually the eigenvalues of K are degenerate. It will thus be convenient to introduce additional operators collectively denoted by B which together with K form a complete set of commuting variables. Using a slightly modified form of Dirac's bra and ket notation[4] we denote the eigenvector of K and B belonging to the eigenvalue E of K and a of B by $|K,B;E,a\rangle$. Hence,

$$K|K,B;E,a\rangle=E|K,B;E,a\rangle. \tag{2}$$

Assuming the eigenfunctions normalized we have

$$\langle K,B;F,b|K,B;E,a\rangle=\delta(E-F)\delta(a,b), \tag{3}$$

where $\delta(a,b)$ is a suitably generalized δ function defined by

$$\int_R f(a)\delta(a,b)da=f(b),$$

if the range of integration R includes b;

$$\int_R f(a)\delta(a,b)da=0,$$

if R does not include b. Integration over a is to be interpreted as summation when a lies in a discrete spectrum.

The completeness of the set of eigenfunctions $|K,B;E,a\rangle$ is expressed by the relation

$$\int|K,B;E,a\rangle dEda\langle K,B;E,a|=I, \tag{4}$$

where I is the identity operator.

We shall assume that the continuous spectrum of H coincides with that of K and hence that the degeneracy of the continuous spectrum of H is the same as that of K. We can therefore introduce operators, collectively denoted by A, which together with H form a complete set of commuting variables such that the eigenvalues of A have the same range as those of B. We shall concern ourselves with two sets of eigenfunctions belonging to the continuous spectrum of H. One set is commonly called the set of "outgoing eigenfunctions." Eigenfunctions of this set are denoted by $|H,A;E,a\rangle_-$. They satisfy the equation

$$|H,A;E,a\rangle_-=|K,B;E,a\rangle+\gamma_-(E-K)V|H,A;E,a\rangle_-, \tag{5}$$

where

$$\gamma_-(x)=\lim_{\epsilon\to 0}[1/(x+i\epsilon)]=-i\pi\delta(x)+(P/x). \tag{6}$$

Here P/x means the principal part should be used in integrations over x. The second set of eigenfunctions which we denote by $|H,A;E,a\rangle_+$ are called the "incoming eigenfunctions." They satisfy the equation

$$|H,A;E,a\rangle_+=|K,B;E,a\rangle+\gamma_+(E-K)V|H,A;E,a\rangle_+, \tag{7}$$

where

$$\gamma_+(x)=\lim_{\epsilon\to 0}[1/(x-i\epsilon)]=+i\pi\delta(x)+(P/x). \tag{6a}$$

The operators $\gamma_-(E-K)$ and $\gamma_+(E-K)$ are the

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[1] K. Watson, Phys. Rev. **88**, 1163 (1952).
[2] M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 403 (1953).
[3] G. Breit and H. A. Bethe, Phys. Rev. **93**, 888 (1954).
[4] The author is indebted to Professor K. O. Friedrichs for suggesting this notation.

Hermitian adjoints of each other. We note the identity,

$$\lim_{t\to\pm\infty} e^{i(K-E)t}\gamma_\pm(E-K)=0, \quad (8)$$

$$\lim_{t\to\mp\infty} e^{i(K-E)t}\gamma_\pm(E-K)=\pm 2\pi i\delta(E-K). \quad (9)$$

We should note that we have reversed the usual convention of denoting outgoing and incoming eigenfunctions. In the usual convention outgoing eigenfunctions are denoted by $+$ and incoming eigenfunctions by $-$. We have reversed the convention because in a more rigorous treatment[5] the outgoing and incoming eigenfunctions are specified in a time-dependent fashion by conditions at $t=-\infty$ and $t=+\infty$, respectively. It can be shown from (8) and (5) and (6) that

$$\lim_{t\to\pm\infty} e^{iKt}e^{-iHt}|H,A;E,a\rangle_\pm=\lim_{t\to\pm\infty} e^{i(K-E)t}|H,A;E,a\rangle_\pm$$
$$=|K,B;E,a\rangle. \quad (10)$$

This means that for values of $t\to-\infty$ we have

$$e^{-iHt}|H,A;E,a\rangle_-\cong e^{-iKt}|K,B;E,a\rangle.$$

Thus the outgoing eigenfunction $|H,A;E,a\rangle_-$ is specified by the condition that the solution $e^{-iHt}|H,A;E,a\rangle_-$ of the time-dependent Schroedinger equation with the Hamiltonian H shall behave at $t=-\infty$ like the solution $e^{-iKt}|K,B,E,a\rangle$ of the equation with the Hamiltonian K. A similar statement can be made with respect to the relation

$$e^{-iHt}|H,A;E,a\rangle_+\cong e^{-iKt}|K,A;E,a\rangle$$

for $t=+\infty$.

The scattering operator S is defined by

$$\lim_{t\to+\infty} e^{iKt}e^{-iHt}|H,A,E,a\rangle_-=\lim_{t\to+\infty} e^{i(K-E)t}|H,A;E,a\rangle_-$$
$$=S|K,B;E,a\rangle. \quad (11)$$

The state $e^{-iKt}S|K,B;E,a\rangle$ represents the final state (which like the initial state is an eigenstate of K) when the initial state is $e^{-iKt}|K,B;E,a\rangle$. From (9) and (5) it is clear that

$$\lim_{t\to+\infty} e^{i(K-E)t}|H,A;E,a\rangle_-$$
$$=|K,B;E,a\rangle-2\pi i\delta(E-K)V|H,A;E,a\rangle_-, \quad (12)$$

and hence from (11) the scattering operator in the K representation is given by

$$\langle K,B;F,b|S|K,B;E,a\rangle=\delta(E-F)\delta(a,b)$$
$$-2\pi i\delta(E-F)\langle K,B;E,b|V|H,A;E,a\rangle_-. \quad (13)$$

Similarly, the inverse scattering operator S^{-1} is defined by

$$\lim_{t\to-\infty} e^{i(K-E)t}|H,A;E,a\rangle_+=S^{-1}|K,B;E,a\rangle, \quad (14)$$

and

$$\langle K,B;F,b|S^{-1}|K,B;E,a\rangle=\delta(E-F)\delta(a,b)$$
$$+2\pi i\delta(E-F)\langle K,B;E,b|V|H,A;E,a\rangle_+. \quad (15)$$

It can also be shown that

$$\langle K,B;E,b|V|H,A;E,a\rangle_+=\langle K,B;E,a|V|H,A;E,b\rangle_-^*, \quad (16)$$

where the asterisk means complex conjugate. Equation (16) is called the reciprocity theorem. A final identity which might be noted is

$$_+\langle H,A;F,b|H,A;E,a\rangle_-=\langle K,B;F,b|S|K,B;E,a\rangle, \quad (17)$$

$$_-\langle H,A;E,a|H,A;F,b\rangle_+=\langle K,B;F,b|S|K,B;E,a\rangle^*$$
$$=\langle K,B;E,a|S^{-1}|K,B;F,b\rangle. \quad (18)$$

From Eq. (13) it is seen that if we knew $\langle K,B;E,b|V|H,A;E,a\rangle_-$, we should know the scattering operator. Both the Schwinger and the Kohn-Hulthén variational principles are concerned with finding this quantity.

The Schwinger variational principle is based upon the two equations

$$a=Ry,\quad a'=R'y', \quad (18)$$

where a and a' are given vectors, y and y' unknown vectors, and R and R' are given operators which are the Hermitian adjoints of each other. We define λ and $\lambda(v',v)$ by

$$\lambda=1/(a',y)=1/(y',a) \quad (19)$$

and

$$\lambda(v',v)=(v',Rv)/(a',v)(v',a), \quad (19a)$$

respectively, where (w,v) indicates the Hermitian inner product of the vectors w and v. It can be shown that the first variation of $\lambda(v',v)$ due to variations of v' about y' and v about y is zero. Hence, since $\lambda(y',y)=\lambda$ we have

$$1/(a',y)\cong(v',Rv)/(a',v)(v',a), \quad (20)$$

where v' and v approximate y' and y, respectively.

We can write (5) and (7) as

$$V|K,B;E,a\rangle=V|H,A;E,a\rangle_-$$
$$-V\gamma_-(E-K)V|H,A;E,a\rangle_- \quad (21)$$

and

$$V|K,B;E,b\rangle=V|H,A;E,b\rangle_+$$
$$-V\gamma_+(E-K)V|H,A;E,b\rangle_+. \quad (22)$$

We identify a and a' with $V|K,B;E,a\rangle$ and $V|K,B;E,b\rangle$, respectively; y and y' with $|H,A;E,a\rangle_-$ and $|H,A;E,b\rangle_+$, respectively; and R and R' with $V-V\gamma_-(E-K)V$ and $V-V\gamma_+(E-K)V$, respectively.

[5] H. E. Moses, New York University, Institute of Mathematical Sciences, Research Report CX-12, 13, 1953 (unpublished).

Hence relation (20) becomes

$$[\langle K,B;E,b|V|H,A;E,a\rangle_-]^{-1} \cong \frac{{}_{+t}\langle H,A;E,b|V|H,A,E,a\rangle_{-t} - {}_{+t}\langle H,A;E,b|V\gamma_-(E-K)V|H,A;E,a\rangle_{-t}}{\langle K,B;E,b|V|H,A;E,a\rangle_{-t} \; {}_{+t}\langle H,A;E,b|V|K,B;E,a\rangle}, \tag{23}$$

where $|H,A;E,b\rangle_{+t}$ and $|H,A;E,a\rangle_{-t}$ are states which approximate $|H,A;E,b\rangle_+$ and $|H,A;E,a\rangle_-$, respectively.

In the Kohn-Hulthén variational principle one introduces the functional $A(|H,A,E,a\rangle_{-t},|H,A;E,b\rangle_{+t})$ defined by

$$A(|H,A;E,a\rangle_{-t},|H,A;E,b\rangle_{+t}) = \lim_{F\to E} {}_{+s}\langle H,A;F,b|H-E|H,A;E,a\rangle_{-s} + \langle K,B;E,b|V|H,A;E,a\rangle_{-t}. \tag{24}$$

Here

$$|H,A;E,a\rangle_{\pm s} = |K,B;E,a\rangle + \gamma_\pm(E-K)V|H,A;E,a\rangle_{\pm t}.$$

It can be shown[6] that the first variation of $A(|H,A;E,a\rangle_{-t},|H,A;E,b\rangle_{+t})$ due to variations of $|H,A;E,a\rangle_{-t}$ and $|H,A;E,b\rangle_{+t}$ about $|H,A;E,a\rangle_-$ and $|H,A;E,b\rangle_+$, respectively, is zero. Hence, as can be shown, since

$$A(|H,A;E,a\rangle_-,|H,A;E,b\rangle_+) = \langle K,B;E,b|V|H,A;E,a\rangle_-,$$

we have

$$\langle K,B;E,b|V|H,A;E,a\rangle_- \cong A(|H,A;E,a\rangle_{-t},|H,A;E,b\rangle_{+t}), \tag{25}$$

where $|H,A;E,a\rangle_{-t}$ and $|H,A;E,b\rangle_{+t}$ approximate $|H,A;E,a\rangle_-$ and $|H,A;E,b\rangle_+$, respectively. By rewriting the expression for A one can get a more useful expression, namely:

$$\begin{aligned}\langle K,B;E,b|V|H,A;E,a\rangle_- &\cong \langle K,B;E,b|V|K,B;E,a\rangle \\ &+ {}_{+t}\langle H,A;E,b|V\gamma_-(E-K)V|K,B;E,a\rangle \\ &+ \langle K,B;E,b|V\gamma_-(E-K)V|H,A;E,a\rangle_{-t} \\ &- {}_{+t}\langle H,A;E,b|V\gamma_-(E-K)V|H,A;E,a\rangle_{-t} \\ &+ {}_{+t}\langle H,A;E,b|V\gamma_-(E-K)V\gamma_-(E-K)V|H,A;E,a\rangle_{-t}.\end{aligned} \tag{26}$$

III. FINAL FORM OF THE VARIATIONAL PRINCIPLES

We shall now give the form of the variational principles for the case discussed in the introduction, namely, when the scattering potential is the sum of two parts, one of which is to be considered small. Accordingly we write

$$V = V_1 + V_2, \tag{27}$$

where V_2 is to be considered the small part of the potential. We define L by

$$L = K + V_1. \tag{28}$$

Hence H, as defined in (1), is also given by

$$H = L + V_2. \tag{29}$$

Let us denote the incoming and outgoing eigenvectors of L with respect to K by $|L,C;E,a\rangle_\pm$, where

$$|L,C;E,a\rangle_\pm = |K,B;E,a\rangle + \gamma_\pm(E-K)V_1|L,C;E,a\rangle_\pm. \tag{30}$$

We assume these eigenvectors are known. In reference 2, it is shown that the quantity $\langle K,B;E,b|V|H,A;E,a\rangle_-$ which we seek can be written as

$$\langle K,B;E,b|V|H,A;E,a\rangle_- = \langle K,B;E,b|V_1|L,C;E,a\rangle_- + {}_+\langle L,C;E,b|V_2|H,A;E,a\rangle_-. \tag{31}$$

Equation (31) is the decomposition of the scattering operator referred to in the introduction. It is our objective to obtain variational expressions for ${}_+\langle L,C;E,b|V_2|H,A;E,a\rangle_-$ only, instead of the entire quantity $\langle K,B;E,b|V|H,A;E,a\rangle_-$. The possibility of obtaining such expressions is based on the fact that the eigenvectors $|H,A;E,a\rangle_\pm$ which satisfy (5) and (7) can be shown also to satisfy the equations,

$$|H,A;E,a\rangle_\pm = |L,C;E,a\rangle_\pm + \gamma_\pm(E-L)V_2|H,A;E,a\rangle_\pm. \tag{32}$$

The equation of (32) with the minus subscript is proved in reference 2. The equation with the plus subscript is proved analogously.

The Schwinger variational principle for

$${}_+\langle L,C;E,b|V_2|H,A;E,a\rangle_-$$

is obtained by rewriting (32) as follows:

$$\begin{aligned}V_2|L,C;E,a\rangle_- &= V_2|H,A;E,a\rangle_- - V_2\gamma_-(E-L)V_2|H,A;E,a\rangle_-, \\ V_2|L,C;E,b\rangle_+ &= V_2|H,A;E,b\rangle_+ - V_2\gamma_+(E-L)V_2|H,A;E,b\rangle_+.\end{aligned} \tag{32a}$$

We identify a and a' of Eq. (18) with $V_2|L,C;E,a\rangle_-$ and $V_2|L,C;E,b\rangle_+$, respectively; the vectors y and y' with $|H,A;E,a\rangle_-$ and $|H,A;E,b\rangle_+$; and R and R' with $V_2 - V_2\gamma_-(E-L)V_2$ and $V_2 - V_2\gamma_+(E-L)V_2$. Then Schwinger's variational principle yields

$$[{}_+\langle L,C;E,b|V_2|H,A;E,a\rangle_-]^{-1} \cong \frac{{}_{+t}\langle H,A;E,b|V_2|H,A;E,a\rangle_{-t} - {}_{+t}\langle H,A;E,b|V_2\gamma_-(E-L)V_2|H,A;E,a\rangle_{-t}}{{}_+\langle L,C;E,b|V_2|H,A;E,a\rangle_{-t} \; {}_{+t}\langle H,A;E,b|V_2|L,C;E,a\rangle_-}, \tag{33}$$

[6] H. E. Moses, Phys. Rev. 92, 817 (1953).

where $|H,A;E,a\rangle_{\pm t}$ approximate $|H,A;E,a\rangle_{\pm}$ respectively. Incidently, equations (32a) yield a reciprocity theorem, namely,

$$_{+}\langle L,C;E,b|V_2|H,A;E,a\rangle_{-} = {}_{+}\langle H,A;E,b|V_2|L,C;E,a\rangle_{-} = {}_{-}\langle L,C;E,a|V_2|H,A;E,b\rangle_{+}^{*}. \quad (34)$$

Borowitz and Friedman[7] use this form of the Schwinger variational principle in a special case.

The Kohn-Hulthén variational principle uses the functional $\tilde{A}(|H,A;E,a\rangle_{-t},|H,A;E,b\rangle_{+t})$ defined by

$$\tilde{A}(|H,A;E,a\rangle_{-t},|H,A;E,b\rangle_{+t}) = \lim_{F\to E} {}_{+s}\langle H,A;F,b|H-E|H,A;E,a\rangle_{-s} + {}_{+}\langle L,C;E,b|V_2|H,A;E,a\rangle_{-t}, \quad (35)$$

where $|H,A;E,a\rangle_{\pm s}$ are defined by

$$|H,A;E,a\rangle_{\pm s} = |L,C;E,a\rangle_{\pm} + \gamma_{\pm}(E-L)V_2|H,A;E,a\rangle_{\pm t}. \quad (35a)$$

As in reference 6, it can be shown that the first variations of $\tilde{A}$ due to variations of $|H,A;E,a\rangle_{\pm t}$ about $|H,A;E,a\rangle_{\pm}$, respectively, vanish. Since also

$$\tilde{A}(|H,A;E,a\rangle_{-},|H,A;E,b\rangle_{+}) = {}_{+}\langle L,C;E,b|V_2|H,A;E,a\rangle_{-}, \quad (36)$$

we have

$$_{+}\langle L,C;E,b|V_2|H,A;E,a\rangle_{-} \cong A(|H,A;E,a\rangle_{-t},|H,A;E,b\rangle_{+t}), \quad (37)$$

where $|H,A;E,a\rangle_{\pm t}$ approximates $|H,A;E,a\rangle_{\pm}$ respectively. Using an alternative form for $\tilde{A}$ obtained by substituting (35a) into (35) we have

$$\begin{aligned} {}_{+}\langle L,C;E,b|V_2|H,A;E,a\rangle_{-} \cong {}& {}_{+}\langle L,C;E,b|V_2|L,C;E,a\rangle_{-} \\ &+ {}_{+t}\langle H,A;E,b|V_2\gamma_{-}(E-L)V_2|L,C;E,a\rangle_{-} \\ &+ {}_{+}\langle L,C;E,b|V_2\gamma_{-}(E-L)V_2|H,A;E,a\rangle_{-t} \\ &- {}_{+t}\langle H,A;E,b|V_2\gamma_{-}(E-L)V_2|H,A;E,a\rangle_{-t} \\ &+ {}_{+t}\langle H,A;E,b|V_2\gamma_{-}(E-L)V_2\gamma_{-}(E-L)V_2|H,A;E,a\rangle_{-t}. \end{aligned} \quad (38)$$

If we assume that $V_1=0$, that is $V=V_2$, then the Kohn-Hulthén and the Schwinger variational principles (38) and (33) reduce to (26) and (23), respectively, as required, for in this case $L=K$ and

$$|L,C;E,a\rangle_{\pm} = |K,A;E,a\rangle.$$

[7] S. Borowitz and B. Friedman, Phys. Rev. **89**, 441 (1953).