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Functionals of fractional form in variational scattering theory

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We present a sequence of variational principles for scattering problems consisting of functionals of fractional form. Schwinger's variational principle and the functional recently proposed by Takatsuka and McKoy are discussed as special cases. For high scattering energies a correspondence to the Born series is established.

I. INTRODUCTION

Variational methods are a powerful tool in the treatment of scattering problems. In general, these methods can be divided into two groups: one is based on the Schrödinger equation and contains, e.g., the classical principles of Hulthén[1] and Kohn[2]; the other is based on the Lippmann-Schwinger equation and contains the Schwinger variational principle.[3] The first group of variational methods, usually referred to as "standard variational principles," requires trial functions which satisfy the standard scattering boundary conditions. For the second group, the boundary conditions are taken into account through the Green's function and, for this reason, need not be incorporated in the trial functions. Therefore, these variational methods allow for L^2 approaches. The corresponding functionals can further be cast into a fractional form which has the advantage that multiplication of the trial function by a constant does not change the value of the functional. For these reasons (and others as well), the second group of variational principles is intrinsically superior to the corresponding standard principles. However, their applicability is limited by numerical problems: The matrix elements involving the Green's function are extremely tedious to compute.

In two recent publications,[4,5] Takatsuka and McKoy have proposed a functional of the second group which does not contain the Green's function. This functional thus combines the merits of the variational principles based on the Lippmann-Schwinger equation with the advantage of computational simplicity.

The method of Takatsuka and McKoy has been formulated as a variational principle for the phase shifts. In Sec. II of this paper we will formulate a generalization of the method for the scattering amplitude which contains no partial-wave expansion. On the basis of this formulation we will then discuss the behavior of the functional for high scattering energies. It will be shown explicitly that the functional reproduces at least the third Born approximation if plane waves are inserted as trial functions.

Finally, in Sec. III, we will discuss a hierarchy of variational functionals which contains the Schwinger principle and the method of Takatsuka and McKoy as special cases.

This paper is concerned only with potential scattering, i.e., the simplest situation in scattering theory. Extension to more general cases is possible, e.g., following the application of Schwinger's variational principle to multichannel scattering.[6] As usual, exact quantities are denoted by a bar throughout this paper; wave functions without a bar are always variational trial functions. Thus, the Lippmann-Schwinger equation which determines the exact wave functions reads

$$|\bar{\psi}_i^{(+)}\rangle = |\vec{k}_i\rangle + G_o^{(+)} V |\bar{\psi}_i^{(+)}\rangle \tag{1}$$

for "outgoing wave" boundary conditions, and

$$\langle\bar{\psi}_f^{(-)}| = \langle\vec{k}_f| + \langle\bar{\psi}_f^{(-)}| V G_o^{(+)} \tag{2}$$

for "incoming wave" boundary conditions. The Green's operator is defined by

$$G_o^{(+)} = \lim_{\epsilon\to 0+} \frac{1}{E - H_0 + i\epsilon} \tag{3}$$

with the kinetic energy operator H_0 and the scattering energy E. The "normalization" of plane waves is chosen such that $\langle\vec{r}|\vec{k}\rangle = e^{i\vec{k}\cdot\vec{r}}$.

II. VARIATIONAL PRINCIPLE OF TAKATSUKA AND MCKOY

We first consider the functional

$$F[\psi_f^{(-)},\psi_i^{(+)}]=\langle\psi_f^{(-)}\,|\,VG_o^{(+)}V\,|\,\vec{k}_i\rangle+\langle\vec{k}_f\,|\,VG_o^{(+)}V\,|\,\psi_i^{(+)}\rangle -\langle\psi_f^{(-)}\,|\,VG_o^{(+)}V-VG_o^{(+)}VG_o^{(+)}V\,|\,\psi_i^{(+)}\rangle\;. \tag{4}$$

For small variations around the exact wave functions we find F to be stationary, i.e., $\delta F=0$. By inserting the exact wave functions in the functional F we can establish a relation to the exact scattering amplitude; using the Lippmann-Schwinger equations (1) and (2) we find

$$\bar{F}=F[\bar{\psi}_f^{(-)},\bar{\psi}_i^{(+)}]=\langle\vec{k}_f\,|\,V\,|\,\bar{\psi}_i^{(+)}\rangle-\langle\vec{k}_f\,|\,V\,|\,\vec{k}_i\rangle=-\frac{2\pi\hbar^2}{m}\bar{f}-\langle\vec{k}_f\,|\,V\,|\,\vec{k}_i\rangle\;.$$

Thus we can formulate a bilinear variational principle for the scattering amplitude by

$$[\tilde{f}]=-\frac{m}{2\pi\hbar^2}(F[\psi_f^{(-)},\psi_i^{(+)}]+\langle\vec{k}_f\,|\,V\,|\,\vec{k}_i\rangle)\;. \tag{5}$$

Transition to a variational principle of fractional form is easily made by replacing $|\,\psi_i^{(+)}\rangle\to\alpha\,|\,\psi_i^{(+)}\rangle$, $\langle\psi_f^{(-)}\,|\to\beta\langle\psi_f^{(-)}\,|$ and subsequently inserting the variationally optimized parameters α and β. This yields

$$[f]=-\frac{m}{2\pi\hbar^2}\left[\frac{\langle\vec{k}_f\,|\,VG_o^{(+)}V\,|\,\psi_i^{(+)}\rangle\langle\psi_f^{(-)}\,|\,VG_o^{(+)}V\,|\,\vec{k}_i\rangle}{\langle\psi_f^{(-)}\,|\,VG_o^{(+)}V-VG_o^{(+)}VG_o^{(+)}V\,|\,\psi_i^{(+)}\rangle}+\langle\vec{k}_f\,|\,V\,|\,\vec{k}_i\rangle\right]\;. \tag{6}$$

If a partial-wave decomposition of $|\,\psi_i^{(+)}\rangle$, $\langle\psi_f^{(-)}\,|$, and f is carried through, then the functional (6) reduces to the expression for the phase shifts given in Ref. 4.

In actual computations it is most convenient to construct trial functions not for the functions $|\,\psi_i^{(+)}\rangle$ and $\langle\psi_f^{(-)}\,|$ but, instead, for the functions

$$|\,\phi_i\rangle:=G_o^{(+)}V\,|\,\psi_i^{(+)}\rangle\;, \tag{7a}$$

$$\langle\phi_f\,|:=\langle\psi_f^{(-)}\,|\,VG_o^{(+)}\;. \tag{7b}$$

By use of the identity

$$\langle\psi_f^{(-)}\,|\,VG_o^{(+)}V-VG_o^{(+)}VG_o^{(+)}V\,|\,\psi_i^{(+)}\rangle=\langle\phi_f\,|\,(G_o^{(+)})^{-1}-V\,|\,\phi_i\rangle=\langle\phi_f\,|\,E-H\,|\,\phi_i\rangle \tag{8}$$

(which is correct provided $|\,\phi_i\rangle$ and $\langle\phi_f\,|$ are not plane waves on the energy shell), we finally obtain the following expression:

$$[f]=-\frac{m}{2\pi\hbar^2}\left[\frac{\langle\vec{k}_f\,|\,V\,|\,\phi_i\rangle\langle\phi_f\,|\,V\,|\,\vec{k}_i\rangle}{\langle\phi_f\,|\,E-H\,|\,\phi_i\rangle}-\langle\vec{k}_f\,|\,V\,|\,\vec{k}_i\rangle\right]\;. \tag{9}$$

This variational principle does not require the trial functions $|\,\phi_i\rangle$ and $\langle\phi_f\,|$ to satisfy any particular boundary conditions even though the functional does not contain the Green's function. Besides this advantage, Takatsuka and McKoy have been able to show that anomalous singularities can be avoided in a simple way and that a minimum principle can be formulated under certain conditions.[4] First applications of the functional (9) have yielded extremely encouraging results.[5]

It should be noted that the exact solutions $|\,\bar{\phi}_i\rangle$ and $\langle\bar{\phi}_f\,|$ are given by

$$|\,\bar{\phi}_i\rangle=G_o^{(+)}V\,|\,\bar{\psi}_i^{(+)}\rangle=|\,\bar{\psi}_i^{(+)}\rangle-|\,\vec{k}_i\rangle$$

and

$$\langle\bar{\phi}_f\,|=\langle\bar{\psi}_f^{(-)}\,|-\langle\vec{k}_f\,|\;.$$

This means that the functional (9) essentially represents a variational principle for *only* the scattered wave.

Let us now investigate the behavior of the functional for high scattering energies. By inserting plane waves as trial functions

$$|\psi_i^{(+)}\rangle \to |\vec{k}_i\rangle, \quad \langle\psi_f^{(-)}| \to \langle\vec{k}_f| ,$$

i.e.,

$$|\phi_i\rangle \to G_o^{(+)}V|\vec{k}_i\rangle, \quad \langle\phi_f| \to \langle\vec{k}_f|VG_o^{(+)} , \tag{10}$$

we obtain for the scattering amplitude

$$[f]^{(\mathrm{pw})} = -\frac{m}{2\pi\hbar^2}\left[\langle\vec{k}_f|VG_o^{(+)}V|\vec{k}_i\rangle\cdot\left[1-\frac{\langle\vec{k}_f|VG_o^{(+)}VG_o^{(+)}V|\vec{k}_i\rangle}{\langle\vec{k}_f|VG_o^{(+)}V|\vec{k}_i\rangle}\right]^{-1}+\langle\vec{k}_f|V|\vec{k}_i\rangle\right].$$

If the quantity

$$|\langle\vec{k}_f|VG_o^{(+)}VG_o^{(+)}V|\vec{k}_i\rangle/\langle\vec{k}_f|VG_o^{(+)}V|\vec{k}_i\rangle|$$

is considered to be small (this should be the case for high scattering energies), the term in the inner brackets can be expanded, yielding

$$[f]^{(\mathrm{pw})} = -\frac{m}{2\pi\hbar^2}(\langle\vec{k}_f|V|\vec{k}_i\rangle+\langle\vec{k}_f|VG_o^{(+)}V|\vec{k}_i\rangle+\langle\vec{k}_f|VG_o^{(+)}VG_o^{(+)}V|\vec{k}_i\rangle+\cdots)\approx f_{B3} . \tag{11}$$

The series agrees with the Born series up to third order. This result promises a high reliability of the variational principle (9) for high scattering energies as well.

III. HIERARCHY OF VARIATIONAL PRINCIPLES

In this section we investigate the sequence of functionals

$$\begin{aligned} F_n[\psi_f^{(-)},\psi_i^{(+)}] = {} & \langle\psi_f^{(-)}|(VG_o^{(+)})^nV|\vec{k}_i\rangle+\langle\vec{k}_f|(VG_o^{(+)})^nV|\psi_i^{(+)}\rangle \\ & -\langle\psi_f^{(-)}|(VG_o^{(+)})^n(V-VG_o^{(+)}V)|\psi_i^{(+)}\rangle, \quad n\in N_0 . \end{aligned} \tag{12}$$

Following the arguments of Sec. II, we find

$$\delta F_n = 0$$

and

$$\bar{F}_n = -\frac{2\pi\hbar^2}{m}\bar{f} - \sum_{j=0}^{n-1}\langle\vec{k}_f|(VG_o^{(+)})^jV|\vec{k}_i\rangle .$$

Thus we can formulate a sequence of bilinear variational principles by

$$[\tilde{f}]_n = -\frac{m}{2\pi\hbar^2}\left[F_n[\psi_f^{(-)},\psi_i^{(+)}]+\sum_{j=0}^{n-1}\langle\vec{k}_f|(VG_o^{(+)})^jV|\vec{k}_i\rangle\right] . \tag{13}$$

The corresponding variational principles of fractional form are given by

$$[f]_n = -\frac{m}{2\pi\hbar^2}\left[\frac{\langle\vec{k}_f|(VG_o^{(+)})^nV|\psi_i^{(+)}\rangle\langle\psi_f^{(-)}|(VG_o^{(+)})^nV|\vec{k}_i\rangle}{\langle\psi_f^{(-)}|(VG_o^{(+)})^n(V-VG_o^{(+)}V)|\psi_i^{(+)}\rangle}+\sum_{j=0}^{n-1}\langle\vec{k}_f|(VG_o^{(+)})^jV|\vec{k}_i\rangle\right] . \tag{14}$$

For $n=0$ we obtain the Schwinger variational principle

$$[f]_0 = -\frac{m}{2\pi\hbar^2}\frac{\langle\vec{k}_f|V|\psi_i^{(+)}\rangle\langle\psi_f^{(-)}|V|\vec{k}_i\rangle}{\langle\psi_f^{(-)}|V-VG_o^{(+)}V|\psi_i^{(+)}\rangle} . \tag{15}$$

For $n=1$, Eq. (14) yields the variational principle discussed in Sec. II.

For practical purposes it may be advantageous to express the functionals $[f]_n$ in terms of the trial functions $|\phi_i\rangle$ and $\langle\phi_f|$ [see Eq. (7)]. This yields the following sequence of variational principles:

$$[f]_n=-\frac{m}{2\pi\hbar^2}\left[\frac{\langle\vec{k}_f\,|\,(VG_o^{(+)})^{n-1}V\,|\,\phi_i\rangle\langle\phi_f\,|\,(VG_o^{(+)})^{n-1}V\,|\,\vec{k}_i\rangle}{\langle\phi_f\,|\,(VG_o^{(+)})^{n-1}(E-H)\,|\,\phi_i\rangle}+\sum_{j=0}^{n-1}\langle\vec{k}_f\,|\,(VG_o^{(+)})^jV\,|\,\vec{k}_i\rangle\right]. \tag{16}$$

All these functionals are of fractional form, and no specific asymptotic form is required for the trial functions. For higher values of n, these variational principles are clearly of little practical value. However, it is interesting to note that each $[f]_n$ contains the Born series to nth order in the interaction potential. Therefore, the remaining fractional part can be interpreted as a variational estimate for the higher orders of the Born series (at least in the case of high scattering energies). In fact, if plane waves are inserted as trial functions, the fractional expression yields two more orders of the Born series so that the variational estimate for the scattering amplitude agrees with the Born series up to order $(n+2)$ in the interaction potential:

$$\begin{aligned}[f]_n^{(\mathrm{pw})}&=-\frac{m}{2\pi\hbar^2}\left[\langle\vec{k}_f\,|\,(VG_o^{(+)})^nV\,|\,\vec{k}_i\rangle\cdot\left[1-\frac{\langle\vec{k}_f\,|\,(VG_o^{(+)})^{n+1}V\,|\,\vec{k}_i\rangle}{\langle\vec{k}_f\,|\,(VG_o^{(+)})^nV\,|\,\vec{k}_i\rangle}\right]^{-1}\right.\\&\qquad\left.+\sum_{j=0}^{n-1}\langle\vec{k}_f\,|\,(VG_o^{(+)})^jV\,|\,\vec{k}_i\rangle\right]\\&\approx-\frac{m}{2\pi\hbar^2}\sum_{j=0}^{n+1}\langle\vec{k}_f\,|\,(VG_o^{(+)})^jV\,|\,\vec{k}_i\rangle=f_{B(n+2)}\,.\end{aligned} \tag{17}$$

In conclusion, we note that the functional $[f]_1$ proposed by Takatsuka and McKoy is distinguished from all other functionals $[f]_n$ by the absence of the Green's function. Therefore, it permits the use of more elaborate trial functions. If the particular trial functions (and the available computer storage) allow the calculation of matrix elements containing *one* Green's function, then either Schwinger's functional $[f]_0$ or the new functional

$$[f]_2=-\frac{m}{2\pi\hbar^2}\left[\frac{\langle\vec{k}_f\,|\,VG_o^{(+)}V\,|\,\phi_i\rangle\langle\phi_f\,|\,VG_o^{(+)}V\,|\,\vec{k}_i\rangle}{\langle\phi_f\,|\,VG_o^{(+)}(E-H)\,|\,\phi_i\rangle}+\langle\vec{k}_f\,|\,V\,|\,\vec{k}_i\rangle+\langle\vec{k}_f\,|\,VG_o^{(+)}V\,|\,\vec{k}_i\rangle\right] \tag{18}$$

may be used. For low-energy scattering it is difficult to decide which functional should be preferred. In the case of high scattering energies, $[f]_2$ is definitely superior to Schwinger's functional since it reproduces the Born series to fourth order in the limit of plane-wave trial functions while the Schwinger principle yields only the second Born approximation.

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