Variational scattering theory using a functional of fractional form. I. General theory

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We propose a variational method for scattering in which the functional is of a fractional form as for the Schwinger variational principle. However, our functional does not involve the Green's function, but the Hamiltonian and the potential function. This method shows features of both the Schwinger-type variational principles and the Kohn-type standard variational principles. As a result, our method can derive distinct advantages from both of these approaches. The resultant K matrix is symmetric and anomaly-free. Some other properties, including a minimum principle, which is useful in the selection of an optimum basis for the expansion of the scattering functions are also discussed.

I. INTRODUCTION

The Schwinger variational principle[1] for scattering, which is based on the Lippmann-Schwinger equation, has several potential advantages over other standard methods. Among them are (i) the variational functional is of fractional form or homogeneous (multiplication of a wave function involved in the functional by a constant does not change the results), (ii) no specific asymptotic form is required for the wave function (L^2 approaches are possible), (iii) no anomalous singularities are expected, and (iv) iterative computations to obtain scattering solutions of higher accuracy is possible.

On the other hand, the relative merits of the standard variational principles[2] such as the Kohn method,[3] which are based on Schrödinger's equation, include (a) the computation of the matrix elements is easy (no double integrations are involved), (b) the effect of polarization can be incorporated without the use of the optical potential formalism, (c) the extension to multichannel scattering is quite straightforward. However, the resultant K matrices are very often nonsymmetric, which can lead to nonunitary S matrices. Some special approaches[4] involving nonlinear iterative calculations have been proposed for obtaining a symmetric and anomaly-free K matrix.

In this paper, we propose a variational functional which has a fractional form but does not include the Green's function. This new method takes advantages of features (i)–(iii) of the Schwinger principle and (a)–(c) of the standard variational principle. Further, the resultant K matrix is symmetric. This is a natural consequence of the symmetric form of our variational functional. The formalism includes only linear computations as in the Schwinger and Kohn methods.

A family of variational functionals based on the Lippmann-Schwinger equation will be discussed in Sec. II. The simplest variational functional among the family is our starting point. It will be shown that under some special conditions our method reduces to the Kohn method (Sec. III). However, in several aspects our method goes beyond the Kohn and other standard methods. In Sec. IV, procedures for avoiding the singularities are discussed. Section V deals with the extension of the formulation to multichannel scattering. Finally, some aspects of the minimum principle for the selection of basis functions will be discussed in Sec. VI.

II. FRACTIONAL FUNCTIONALS

We will introduce a family of variational functionals, from which our working functional can be derived. We first consider only single-channel scattering, for which the Lippmann-Schwinger equation can be written as

$$\Psi = S + G_0 V \Psi , \tag{2.1}$$

where Ψ is a total wave function for a Hamiltonian $H = H_0 + V$. G_0 is the standing-wave Green's function associated with the zeroth-order Hamiltonian H_0. S is the regular solution of H_0 with the asymptotic form of $S \underset{r\to\infty}{\sim} (\mu/k)^{1/2} \sin(kr - \frac{1}{2} l\pi)$, where μ is a reduced mass.

A very important prototype of our approach is the Schwinger variational principle, for which the functional can be written as

$$-\tfrac{1}{2}[\lambda] = \frac{\langle \Psi | V | S \rangle \langle S | V | \Psi \rangle}{\langle \Psi | (V - VG_0 V) | \Psi \rangle} . \tag{2.2}$$

$[\lambda]$ (the tangent of the phase shift) is stationary under variation of Ψ about its exact value. With the expansion

$$\Psi = \sum_i a_i \chi_i , \tag{2.3}$$

one obtains the stationary value of λ

$$-\tfrac{1}{2}[\lambda]=\sum_{i,j}\langle S|V|\chi_i\rangle D_{ij}\langle\chi_j|V|S\rangle\,, \tag{2.4}$$

where

$$(D^{-1})_{ij}=\langle\chi_i|(V-VG_0V)|\chi_j\rangle\,. \tag{2.5}$$

It is well known[1,5] that if a separable potential

$$V^s=\sum_{i,j}V|\chi_i\rangle v_{ij}\langle\chi_j|V \tag{2.6}$$

with

$$(v^{-1})_{ij}=\langle\chi_i|V|\chi_j\rangle \tag{2.7}$$

is introduced into the Lippmann-Schwinger equation for the K operator, with K defined by $K\Psi=VS$,

$$K=V+VG_0K\,, \tag{2.8}$$

then Eq. (2.8) can be solved to give the same result in Eq. (2.4).

It is instructive to start our discussion by considering the functional of fractional form

$$F_0=\frac{\langle\Psi|VG_0V|S\rangle\langle S|VG_0V|\Psi\rangle}{\langle\Psi|(VG_0V-VG_0VG_0V)|\Psi\rangle}\,. \tag{2.9}$$

Although this functional itself is complicated, we can derive some very useful functionals from it. F_0 is stationary with respect to variation of the exact wave function, since $\delta F_0=0$ gives

$$VG_0V[(1-G_0V)|\Psi\rangle-|S\rangle]=0\,, \tag{2.10}$$

which is true since the term in the square bracket of Eq. (2.10) is just the Lippmann-Schwinger equation, Eq. (2.1). It is also convenient to introduce the operator f defined by

$$f=K-V\,, \tag{2.11}$$

and which satisfies the integral equation

$$f=VG_0V+VG_0f. \tag{2.12}$$

As with the Schwinger variational principle, f can be solved in closed form if a finite rank approximation is introduced for G_0 or V. We can evaluate the variational functional F_0 assuming an expansion such as Eq. (2.3) for either Ψ, $V\Psi$, or $G_0V\Psi$.

A. Expansion of $G_0V\Psi$

We first consider the expansion of $G_0V\Psi$. Let us define

$$\tilde{C}=G_0V\Psi\,. \tag{2.13}$$

Then F_0 becomes

$$F_1=\frac{\langle\tilde{C}|V|S\rangle\langle S|V|\tilde{C}\rangle}{\langle\tilde{C}|G_0^{-1}-V|\tilde{C}\rangle} \tag{2.14}$$

$$=\frac{\langle\tilde{C}|V|S\rangle\langle S|V|\tilde{C}\rangle}{\langle\tilde{C}|\hat{H}|\tilde{C}\rangle}\,, \tag{2.15}$$

where $\hat{H}=E-H$. Expansion of $\tilde{C}$ as in Eq. (2.3) and variation of the functional leads to

$$F_1=\sum_{i,j}\langle S|V|\chi_i\rangle A_{ij}\langle\chi_j|V|S\rangle\,, \tag{2.16}$$

where

$$(A^{-1})_{ij}=\langle\chi_i|\hat{H}|\chi_j\rangle\,. \tag{2.17}$$

This result is also obtained by inserting the approximation for G_0,

$$G_{01}^s=\sum_{i,j}|\chi_i\rangle B_{ij}\langle\chi_j|\,, \tag{2.18}$$

with

$$(B^{-1})_{ij}=\langle\chi_i|G_0^{-1}|\chi_j\rangle=\langle\chi_i|E-H_0|\chi_j\rangle \tag{2.19}$$

into the integral equation for f, Eq. (2.12), i.e.,

$$f_1=\sum_{i,j}V|\chi_i\rangle A_{ij}\langle\chi_j|V\,. \tag{2.20}$$

The functional F_1 of Eq. (2.15) is the basis of our proposed variational method and also serves as a starting point for some important theoretical developments. Some obvious characteristics of F_1 should first be stressed: (a) The functional has a fractional form. This fact will be important in the avoidance of singularities. (b) F_1 involves the Hamiltonian H and not the Green's function. Therefore, F_1 should be regarded as one of the standard variational principles. In fact, $\delta F_1=0$ requires

$$\hat{H}|\tilde{C}\rangle=V|S\rangle\,, \tag{2.21}$$

which is exactly the Schrödinger equation ($\hat{H}\Psi=0$). (c) F_1 does not require any specific asymptotic form for $\tilde{C}$. This feature allows us to develop various methods for the solution of Eq. (2.15).

B. Expansion of Ψ

Before proceeding with some further developments from Eq. (2.15), we will obtain two additional functionals stemming from Eq. (2.9). Insertion of the expansion, Eq. (2.3), for Ψ in the functional F_0 gives

$$F_2=\sum_{i,j}\langle S|VG_0V|\chi_i\rangle\mathfrak{a}_{ij}\langle\chi_j|VG_0V|S\rangle\,, \tag{2.22}$$

where

$$(\mathfrak{a}^{-1})_{ij}=\langle\chi_i|(VG_0V-VG_0VG_0V)|\chi_j\rangle\,. \tag{2.23}$$

The same result is obtained if G_0 in Eq. (2.12) is replaced by the finite rank form

$$G_{02}^s=\sum_{i,j}G_0V|\chi_i\rangle\mathfrak{B}_{ij}\langle\chi_j|VG_0\,, \tag{2.24}$$

where

$$(\mathfrak{B}^{-1})_{ij}=\langle\chi_i|VG_0V|\chi_j\rangle\,. \tag{2.25}$$

Equation (2.12) can be solved for f to obtain

$$f_2=\sum_{i,j} VG_0V|\chi_i\rangle\alpha_{ij}\langle\chi_j|VG_0V, \tag{2.26}$$

where α is the same as defined in Eq. (2.23). Since G_0 is always associated with V in Eq. (2.9), it is important that G_{02}^s has a property

$$G_{02}^sV|\chi_i\rangle=G_0V|\chi_i\rangle \tag{2.27}$$

and

$$\langle\chi_i|VG_{02}^s=\langle\chi_i|VG_0, \tag{2.28}$$

provided χ_i is used in G_{02}^s. The F_2 should lead to very accurate results. However, as stated above, F_2 should be viewed as having merely formal significance, since it is quite complicated.

C. Expansion of $V\Psi$

Let us define the form factor $V\Psi$ as ψ. F_0 then reduces to another functional

$$F_3=\frac{\langle\psi|G_0V|S\rangle\langle S|VG_0|\psi\rangle}{\langle\psi|(G_0-G_0VG_0)|\psi\rangle}. \tag{2.29}$$

The stationary value of F_3 with respect to the variation of ψ, expanded in terms of the χ_i's, becomes

$$F_3=\sum_{i,j}\langle S|VG_0|\chi_i\rangle a_{ij}\langle\chi_j|G_0V|S\rangle, \tag{2.30}$$

where

$$(a^{-1})_{ij}=\langle\chi_i|(G_0-G_0VG_0)|\chi_j\rangle. \tag{2.31}$$

The latter form of F_3, Eq. (2.30), was originally obtained by Sloan and Brady[6] through a different variational approach proposed by Newton.[7]

From a general study of finite rank approximations for the T matrix, Sloan and Adhikari[8] showed that the form of F_3 of Eq. (2.30) is also obtained with a particular separable potential. Equivalently, this can be restated using a finite rank Green's function

$$G_{03}^s=\sum_{i,j} G_0|\chi_i\rangle b_{ij}\langle\chi_j|G_0, \tag{2.32}$$

where

$$(b^{-1})_{ij}=\langle\chi_i|G_0|\chi_j\rangle. \tag{2.33}$$

G_{03}^s gives a finite rank operator for f, i.e.,

$$f_3=\sum_{i,j} VG_0|\chi_i\rangle a_{ij}\langle\chi_j|G_0V. \tag{2.34}$$

The separable Green's function of Eq. (2.32) corresponds to the separable potential of the Schwinger principle Eq. (2.6). As for V^s in Eq. (2.6), one finds

$$G_{03}^s|\chi_i\rangle=G_0^s|\chi_i\rangle. \tag{2.35}$$

This property is favorable for f_3 to be very effective. In fact, Adhikari and Sloan have shown numerically[8b] that F_3 gives very accurate results with small basis set.

In comparing the operators f_1, f_2, and f_3, one should note that G_{01}^s does not have the properties of Eqs. (2.27), (2.28), or (2.35). This means that F_1 may give a worse K matrix than F_2 and F_3. However, we will show, in the following paper,[9] that one can apply F_1 very effectively.

Before closing this section, we would like to identify another type of variational functional for $\tilde{C}$. In addition to the Schrödinger equation, Eq. (2.21), $\tilde{C}$ also satisfies a following integral equation (Lippmann-Schwinger equation for $\tilde{C}$),

$$\tilde{C}=G_0VS+G_0V\tilde{C} \tag{2.36}$$

[insert $\Psi=S+\tilde{C}$ into Eq. (2.1)]. Analogously to the Schwinger principle for Ψ, the functional F_C,

$$F_C=\frac{\langle\tilde{C}|VG_0V|S\rangle\langle S|VG_0V|\tilde{C}\rangle}{\langle\tilde{C}|V-VG_0V|\tilde{C}\rangle} \tag{2.37}$$

is stationary with respect to variations in $\tilde{C}$. Thus, our variational functional F_1 is closely related to the Schwinger principle for $\tilde{C}$, Eq. (2.37), rather than the original Schwinger principle, Eq. (2.2). Incidentally, by the expansion technique, we have

$$-\tfrac{1}{2}[\lambda]=\langle S|V|S\rangle+\langle S|VG_0V|S\rangle+\sum_{i,j}\langle S|VG_0V|\chi_i\rangle D_{ij}\langle\chi_j|VG_0V|S\rangle, \tag{2.38}$$

where D is the same as that of Eq. (2.5). The variational principle of $\tilde{C}$, Eq. (2.37), should give better results than the original Schwinger principle, Eq. (2.2), although Eq. (2.37) involves more work. It should be noted, however, that the numerical evaluation of the Schwinger principle, Eq. (2.2), requires the calculation of the terms $G_0V|\Psi\rangle$ which are just the ones which are needed in the numerator of Eq. (2.37). The increase in effort should not be significant in going from the original Schwinger principle, Eq. (2.2), to the variational expression for $\tilde{C}$, Eq. (2.37).

III. THE KOHN VARIATIONAL PRINCIPLE

With the variational condition $\delta F_1=0$ it may seem that F_1 coincides with the Kohn method.[10] This is not true in general, since F_1 does not require the correct asymptotic form. This will become clearer in the multichannel formulation. However, if we impose the same asymptotic form on $\tilde{C}$ as that of the Kohn method, F_1 coincides exactly with the Kohn method,[10] for single-chan-

nel scattering. This can be shown as follows: The total wave function Ψ of the Kohn method can be written as

$$\Psi = S + \lambda C + \sum_i a_i \eta_i , \tag{3.1}$$

where λ is the tangent of the phase shift δ. C is a long-range function which has the same asymptotic form as the irregular solution of H_0 and $C=0$ at $r=0$. η_i's are short-range basis functions. The coefficients λ and a_i's are determined through the requirement

$$\delta[\lambda] = 0 , \tag{3.2}$$

where

$$[\lambda] = \lambda + 2\langle \Psi | \hat{H} | \Psi \rangle . \tag{3.3}$$

Now we can connect $[\lambda]$ with F_1. Defining

$$\tilde{C} = \lambda C + \sum a_i \eta_i , \tag{3.4}$$

one can write

$$[\lambda] = 2\langle \tilde{C} | \hat{H} | \tilde{C} \rangle + 2\langle \tilde{C} | \hat{H} | S \rangle + 2\langle S | \hat{H} | S \rangle + (\lambda + 2\langle S | \hat{H} | \tilde{C} \rangle) . \tag{3.5}$$

The use of an identity[2]

$$\langle C | \hat{H} | S \rangle - \langle S | \hat{H} | C \rangle = \tfrac{1}{2} , \tag{3.6}$$

leads to

$$[\lambda] = 2\langle \tilde{C} | \hat{H} | \tilde{C} \rangle - 2\langle \tilde{C} | V | S \rangle - 2\langle S | V | \tilde{C} \rangle - 2\langle S | V | S \rangle . \tag{3.7}$$

We now define

$$F_4 = \langle \tilde{C} | V | S \rangle + \langle S | V | \tilde{C} \rangle - \langle \tilde{C} | \hat{H} | \tilde{C} \rangle . \tag{3.8}$$

F_4 is stationary[13] with respect to $\delta\tilde{C}$, since $[\lambda] + 2F_4$ is a constant. We next replace $|\tilde{C}\rangle$ and $\langle \tilde{C}|$ with $p|\tilde{C}\rangle$ and $p^*\langle \tilde{C}|$, respectively. With the condition $\partial F_4/\partial p = 0$ and $\partial F_4/\partial p^* = 0$, F_4 reduces to F_1. This shows that, for single-channel scattering, the functional F_1 is identical with the Kohn method, if $\tilde{C}$ is defined as Eq. (3.4).

One major defect of the Kohn method, as is well known,[2] is that it is not free from anomalous singularities which arise from the inverse matrix of Eq. (2.17). The flexibility of our proposed variational method overcomes the defect quite easily.

IV. AVOIDANCE OF THE ANOMALOUS SINGULARITIES

For both cases of the complete set and a truncated set of basis functions for $\tilde{C}$, one should have poles in the diagonal representation of the A matrix of Eq. (2.17). Hence, the poles which have nothing to do with true resonances[2(d),2(e),2(f),12] will lead to divergences in F_1. Moreover, the true resonances cannot be distinguished from those singularities, since both of them contribute to F_1 in the same manner. These singularities are known[2] to be inherent in some of the standard variational principles. In order to avoid the singularities a number of theories have been proposed.[2(d),2(e),2(f),12]

It is quite easy to avoid these spurious singularities in our scheme. Let us go back to the Schrödinger equation in the inhomogeneous form, Eq. (2.21). We recall that the functional F_1 has a fractional form and hence F_1 is invariant if $\tilde{C}$ is replaced by $x\tilde{C}$ (x: constant, $\neq 0$). So we now consider the new functional

$$F_1^t = \frac{\langle \tilde{C}_t | V | S \rangle \langle S | V | \tilde{C}_t \rangle}{\langle \tilde{C}_t | (\hat{H} - tX) | \tilde{C}_t \rangle} , \tag{4.1}$$

where an operator X is defined as

$$X = V|S\rangle\langle S|V , \tag{4.2}$$

and t is an arbitrary parameter. By variation of F_1^t ($\delta F_1^t = 0$), we have

$$(\hat{H} - tX)|\tilde{C}_t\rangle = V|S\rangle \tag{4.3}$$

or

$$\hat{H}|\tilde{C}_t\rangle = (1 + t\langle S|V|\tilde{C}_t\rangle)V|S\rangle . \tag{4.4}$$

Comparing this equation with the Schrödinger equation we see

$$|\tilde{C}_t\rangle = x_t|\tilde{C}\rangle , \tag{4.5}$$

with

$$x_t = (1 - t\langle S|V|\tilde{C}\rangle)^{-1} . \tag{4.6}$$

Therefore, the $\tilde{C}_t$ determined from F_1^t should be proportional to $\tilde{C}$. However, the constant factor x_t should be canceled out from the F_1^t, Eq. (4.1).

Using the expansion technique, the stationary value of F_1^t becomes

$$F_1^t = \frac{\langle \tilde{C} | V | S \rangle \langle S | V | \tilde{C} \rangle}{\langle \tilde{C} | (\hat{H} - tX) | \tilde{C} \rangle} \tag{4.7}$$

$$= \sum_{i,j} \langle S | V | \chi_i \rangle A_{ij}^t \langle \chi_j | V | S \rangle , \tag{4.8}$$

where

$$(A^{t-1})_{ij} = \langle \chi_i | (\hat{H} - tX) | \chi_j \rangle . \tag{4.9}$$

Since X is a positive semidefinite operator, it can shift the position of poles which induce the singularities. The resultant value of F_1^t is

$$F_1^t = \frac{\langle S | V | \tilde{C} \rangle}{1 - t\langle S | V | \tilde{C} \rangle} . \tag{4.10}$$

So,

$$-\tfrac{1}{2}\tan\delta = \langle S | V | S \rangle + \frac{F_1^t}{1 + tF_1^t} . \tag{4.11}$$

Thus we have avoided these singularities.

On the other hand, for the true resonances, we must always have (not depending on t)

$$|\langle S|V|\tilde{C}\rangle| = \infty \tag{4.12}$$

in Eq. (4.10). This means

$$F_1^t = -1/t . \tag{4.13}$$

So, the true resonance is characterized by this expression.

V. EXTENSION TO MULTICHANNEL SCATTERING

A. Simple extension

A straightforward and simple extension of the single-channel theory to the multichannel case is to define a functional

$$F_{mn} = \frac{\langle \tilde{C}_m|V|S_n\rangle\langle S_m|V|\tilde{C}_n\rangle}{\langle \tilde{C}_m|\hat{H} - tX_{nm}|\tilde{C}_n\rangle} , \tag{5.1}$$

where

$$X_{nm} = V|S_n\rangle\langle S_m|V . \tag{5.2}$$

From the condition $\delta F_{mn} = 0$, we have

$$F_{mn} = \sum_{i,j} \langle S_m|V|\chi_i\rangle (A^t_{nm})_{ij}\langle \chi_j|V|S_n\rangle , \tag{5.3}$$

where

$$(A^{t^{-1}}_{nm})_{ij} = \langle \chi_i|(\hat{H} - tX_{nm})|\chi_j\rangle . \tag{5.4}$$

Note that all the functions S_m, $\tilde{C}_m$, χ_i's have been redefined so that they can describe many-particle systems. Since F_{mn} is symmetric, the resultant K matrix

$$-\tfrac{1}{2}K_{mn} = \langle S_m|V|S_n\rangle + \frac{F_{mn}}{1+tF_{mn}} \tag{5.5}$$

will be symmetric. This situation is quite different from the other standard variational principles.[2,4] The functional F_{mn} requires the construction of the matrix A^t_{mn} for the calculation of each K_{mn}. This can be a time-consuming procedure.

B. General extension

Let us start from the equation for the multichannel wave functions,

$$\hat{H}|\tilde{C}_m\rangle = V|S_m\rangle \quad (m = 1, 2, \ldots, N_C) . \tag{5.6}$$

As mentioned in the single-channel case, $\hat{H}$ is a Hermitian operator in a domain of $\{C_m; \eta_i | m = 1, \ldots, N_C; i = 1, \ldots\}$. Hence, we can introduce new channel functions (denoted by $\tilde{C}_\alpha$) which diagonalize $\hat{H}$,

$$\langle \tilde{C}_\alpha|\hat{H}|\tilde{C}_\beta\rangle = \delta_{\alpha\beta}\langle \tilde{C}_\alpha|\hat{H}|\tilde{C}_\alpha\rangle . \tag{5.7}$$

These new channel functions $\tilde{C}_\alpha$ are related to the functions $\tilde{C}_m$'s by a unitary transformation

$$\tilde{C}_\alpha = \sum_{m=1}^{N_C} \tilde{C}_m U_{m\alpha} , \tag{5.8}$$

and also

$$S_\alpha = \sum_{m=1}^{N_C} S_m U_{m\alpha} . \tag{5.9}$$

So, the Schrödinger equation for $\Psi_\alpha = S_\alpha + \tilde{C}_\alpha$ is

$$\hat{H}|\tilde{C}_\alpha\rangle = V|S_\alpha\rangle . \tag{5.10}$$

Using this, we also have the orthogonality condition

$$\langle \tilde{C}_\alpha|V|S_\beta\rangle = \delta_{\alpha\beta}\langle \tilde{C}_\alpha|V|S_\alpha\rangle . \tag{5.11}$$

Note that the new wave functions Ψ_α are not the so-called eigenchannel wave functions,[2,7] since the K matrix is not diagonal in the Ψ_α's.

Now we define X as

$$X = \sum_{\alpha}^{N_C} V|S_\alpha\rangle\langle S_\alpha|V . \tag{5.12}$$

From Eq. (5.9), X can also be written as

$$X = \sum_{m}^{N_C} V|S_m\rangle\langle S_m|V . \tag{5.13}$$

From the orthogonality condition of Eq. (5.11) we have

$$x^t_\alpha(\hat{H} - tX)|\tilde{C}_\alpha\rangle = V|S_\alpha\rangle , \tag{5.14}$$

where

$$x^t_\alpha = \frac{1}{1 - t\langle S_\alpha|V|C_\alpha\rangle} . \tag{5.15}$$

Therefore, in analogy to the single-channel case one can construct a variational functional

$$G^t_{\alpha\alpha} = \frac{\langle \tilde{C}_\alpha|V|S_\alpha\rangle\langle S_\alpha|V|\tilde{C}_\alpha\rangle}{\langle \tilde{C}_\alpha|(\hat{H} - tX)|\tilde{C}_\alpha\rangle} . \tag{5.16}$$

If $\tilde{C}_\alpha$ and $\tilde{C}_\beta$ are the exact solutions,

$$G^t_{\alpha\beta} = \delta_{\alpha\beta}x^t_\alpha\langle S_\alpha|V|\tilde{C}_\alpha\rangle . \tag{5.17}$$

As usual, the expansion technique gives

$$G^t_{\alpha\beta} = \sum_{i,j}\langle S_\alpha|V|\chi_i\rangle\Delta^t_{ij}\langle \chi_j|V|S_\beta\rangle , \tag{5.18}$$

where

$$(\Delta^{t^{-1}})_{ij} = \langle \chi_i|(\hat{H} - tX)|\chi_j\rangle . \tag{5.19}$$

Now the inverse matrix $\Delta^{t^{-1}}$ is common to all channels.

We have to return to the physical channel functions to get the K matrix. To do so, we define a matrix g^t, with elements

$$g^t_{mn} = \sum_{i,j}\langle S_m|V|\chi_i\rangle\Delta^t_{ij}\langle \chi_j|V|S_n\rangle . \tag{5.20}$$

All integrals required in g^t_{mn} are known, since X is given by Eq. (5.13). From the discussion of the above paragraph, it is clear that the eigenvalues of g^t must be identical with $G^t_{\alpha\alpha}$'s and the unitary matrix composed of the eigenvectors is just the U of Eq. (5.8). That is,

$$U^\dagger g^t U = \mathrm{diag}(G^t_{11} \cdots G^t_{N_C N_C}) . \tag{5.21}$$

On the other hand, by Eqs. (5.15) and (5.17), $\langle S_\alpha | V | \tilde{C}_\alpha \rangle$ can be written as

$$\langle S_\alpha | V | \tilde{C}_\alpha \rangle = \frac{G^t_{\alpha\alpha}}{1 + tG^t_{\alpha\alpha}} . \tag{5.22}$$

So, using the inverse transformation of Eqs. (5.8) and (5.9), we get

$$\langle S_m | V | \tilde{C}_n \rangle = \sum_\alpha \langle S_\alpha | V | \tilde{C}_\alpha \rangle U^\dagger_{\alpha m} U^\dagger_{\alpha n} . \tag{5.23}$$

And finally, the K matrix is

$$-\tfrac{1}{2} K_{mn} = \langle S_m | V | S_n \rangle + \langle S_m | V | \tilde{C}_n \rangle . \tag{5.24}$$

The K matrix thus obtained is again symmetric and anomaly-free. The matrix inversion process is done only once. The price one pays is the diagonalization of g^t matrix. However, in general, g^t will not be a large matrix as long as the energy under study is not too high.

IV. MINIMUM PRINCIPLE

The role played by the Rayleigh-Ritz variational principle[2(c)] in the bound-state quantum theory cannot be overemphasized. The situation in scattering theory is much more complicated. There are many theories which try to obtain simple variational bounds.[14] However, most of them are quite complicated. Hence it may be worthwhile to show a very simple aspect of a minimum principle for a functional which can help in the selection of an optimum basis for the expansion of the trial scattering wave function within the fractional functional approach.

To begin with, we refer to the classical work of Kato[15] on the Schwinger variational principle. If the potential V is non-negative everywhere, the Schwinger functional can be rewritten in a form

$$-2K^{-1} = \frac{\langle \upsilon | A | \upsilon \rangle}{\langle \upsilon | f \rangle \langle f | \upsilon \rangle} \tag{6.1}$$

where $\upsilon = V^{1/2}\Psi$, $f = V^{1/2}S$, and $A = 1 - V^{1/2} G_0 V^{1/2}$. Kato stated the necessary and sufficient condition under which K^{-1} will have an extremum value. It is obvious, however, that the constraint on V (i.e., $V \geq 0$ everywhere) is too strong for general purpose. We now observe that the inverse of $G^t_{\alpha\alpha}$, namely,

$$G^{t-1}_{\alpha\alpha} = \frac{\langle \tilde{C}_\alpha | (\hat{H} - tX) | \tilde{C}_\alpha \rangle}{\langle \tilde{C}_\alpha | V | S_\alpha \rangle \langle S_\alpha | V | \tilde{C}_\alpha \rangle} , \tag{6.2}$$

already has the same form as Eq. (6.1), if we identify $\upsilon = \tilde{C}_\alpha$, $f = VS_\alpha$, and $A = \hat{H} - tX$. We can thus apply Kato's theorem[15] to our case without regard to the sign of V. That is, if all eigenvalues of the Hermitian operator $\hat{H} - tX + cV | S_\alpha \rangle \langle S_\alpha | V$ are negative for some constant c, then $G^{t-1}_{\alpha\alpha}$ is the maximum, and vice versa. So, the problem is one of finding t sufficiently large which allows some constant c to satisfy the theorem.

Another simple discussion of the variational bound can be based on the Schwarz inequality.[16] If the basis set used for $G^t_{\alpha\alpha}$ is complete, $G^t_{\alpha\alpha}$ can be written formally as

$$G^t_{\alpha\alpha} = \langle S_\alpha | V (\hat{H} - tX)^{-1} V | S_\alpha \rangle . \tag{6.3}$$

(Note again that $H - tX$ is a Hermitian operator in the domain for $\tilde{C}_\alpha$.) Since $\hat{H}$ has an upper bound, one can keep $\hat{H} - tX$ negative semidefinite by a suitable choice of the parameter t. Owing to the general form of the Schwarz inequality,[16] we have

$$(\hat{H} - tX)^{-1} \leq \sum_{i,j}^{N} | \chi_i \rangle [(\hat{H} - tX)^{-1}]_{ij} \langle \chi_j | \leq 0 \tag{6.4}$$

if $\hat{H} - tX$ is negative semidefinite. Moreover, the finite rank approximation of Eq. (6.4) decreases monotonically as the basis set size N increases. Hence a basis giving a smaller $G^t_{\alpha\alpha}$ should be regarded as better. Thus we have obtained the variational upper bound of the true $G^t_{\alpha\alpha}$. Unfortunately, the variational bound obtained is not the bound for the K matrix. It is likely, however, that better $G^t_{\alpha\alpha}$'s will lead to improved K matrices.

A striking feature of our minimum principle is, beside its simplicity, that it does not have to care about the existence of bound states below E. In the theories which are based on the spectral structure of $\langle \Psi | \hat{H} | \Psi \rangle$ in Eq. (3.3), the subtraction[17] of such bound states is necessary. However, this is not always possible. In our minimum principle, such a subtraction procedure is not necessary as long as the bound states are not orthogonal to VS (or equivalently to S), since $\hat{H} - tX$ can always be fixed to be negative semidefinite by selecting t properly.

VII. CONCLUDING REMARKS

In this paper we have proposed a variational method with a functional of fractional form as in the Schwinger's functional. Our variational principle can be derived from the Lippmann-Schwinger equation but does not contain the Green's function. Our theory is related to both the standard variational principle and also to the Schwinger-type principle.

We have presented the general properties of the new functional. The method is anomaly-free and gives symmetric K matrices. The correct asymptotic form of the trial wave function is not neces-

sary. Its implementation should be relatively easy. An example of the application will be shown in a following paper.[9] We have also discussed a minimum principle for a functional which can lead to the selection of an optimum basis for the expansion of the scattering functions.

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