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Derivation of Schwinger variational principles

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Abstract

We present systematic derivations of bilinear and fractional Schwinger variational principles for matrix elements of a generalized transition operator in the context of quantum mechanical potential scattering. The employed method is based on a generalization of the method of Lagrange multipliers.

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1. Introduction

In standard presentations of Schwinger variational methods for quantum potential scattering theory relevant functionals appear as if they were guessed [1–5]. The question arises: is it possible to *derive* these functionals in some way? It is a purpose of this Letter to show that the answer is affirmative. We present systematic derivations of bilinear and fractional Schwinger variational principles for matrix elements of a generalized transition operator by employing a generalization of the method of Lagrange multipliers [6].

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2. Preliminaries

Let Φ_a and Φ_b be arbitrary (assumed to be known) solutions to the Schrödinger equation

$$\big[\hat{H}_0 - E\big]\Phi = 0, \tag{2.1}$$

both belonging to *the same* energy E from the continuous spectrum of the free-particle Hamiltonian $\hat{H}_0$. Further, let $\hat{G}_0$ be a particular Green operator associated with the operator $\hat{H}_0 - E$. We define Ψ_b as a solution to the Lippmann–Schwinger integral equation

$$\Psi_b = \Phi_b - \hat{G}_0 \hat{V} \Psi_b \tag{2.2}$$

with a Hermitian potential operator $\hat{V}$. Obviously, the function Ψ_b obeys the Schrödinger equation

$$\big[\hat{H}_0 + \hat{V} - E\big]\Psi_b = 0. \tag{2.3}$$

We shall assume that E is in the continuous part of the spectrum of $\hat{H}_0 + \hat{V}$ and define a generalized on-shell transition operator $\hat{A}$ so that

$$\langle \Phi_a | \hat{A} \Phi_b \rangle = \langle \Phi_a | \hat{V} \Psi_b \rangle. \tag{2.4}$$

It follows from Eqs. (2.4) and (2.2) that the operator $\hat{A}$ depends implicitly on $\hat{G}_0$.

There are two special choices of $\hat{G}_0$ which result in operators $\hat{A}$ commonly used in the scattering theory. If one chooses $\hat{G}_0$ as the 'outgoing' Green operator

$$\hat{G}_0^{(+)} = \lim_{\varepsilon \downarrow 0} \big[\hat{H}_0 - E - \mathrm{i}\varepsilon \big]^{-1}, \tag{2.5}$$

the resulting operator $\hat{A}$ is the standard on-shell transition operator $\hat{T}$. If, in turn, $\hat{G}_0$ is taken as the 'standing' (or the 'principal value') Green operator

$$\hat{G}_0^{(\mathrm{P})} = \frac{1}{2} \big[\hat{G}_0^{(+)} + \hat{G}_0^{(-)} \big], \tag{2.6}$$

where

$$\hat{G}_0^{(-)} = \hat{G}_0^{(+)\dagger} = \lim_{\varepsilon \downarrow 0} \big[\hat{H}_0 - E + \mathrm{i}\varepsilon \big]^{-1} \tag{2.7}$$

(here and henceforth the dagger denotes the Hermitian conjugation), the operator $\hat{A}$ is the on-shell reactance (or reaction) operator $\hat{K}$.[1]

3. Bilinear variational principle

Assume at first that it is our goal to derive a variational principle for the matrix element $\langle \Phi_a | \hat{A} \Phi_b \rangle$. We rewrite Eqs. (2.4) and (2.2) in the forms

$$\langle \Phi_a | \hat{A} \Phi_b - \hat{V} \Psi_b \rangle = 0, \tag{3.1}$$

$$\big[1 + \hat{G}_0 \hat{V} \big] \Psi_b - \Phi_b = 0, \tag{3.2}$$

respectively, and proceeding in the spirit of the generalized Lagrange method [6] start with the functional

$$F_1 \big[\bar{\hat{A}}, \bar{\Psi}_b, \bar{\eta}, \bar{\Lambda} \big] = \langle \Phi_a | \bar{\hat{A}} \Phi_b \rangle + \bar{\eta} \langle \Phi_a | \bar{\hat{A}} \Phi_b - \hat{V} \bar{\Psi}_b \rangle + \langle \bar{\Lambda} | \big[1 + \hat{G}_0 \hat{V} \big] \bar{\Psi}_b - \Phi_b \rangle, \tag{3.3}$$

in which $\bar{\hat{A}}$ and $\bar{\Psi}_b$ are some trial estimates of $\hat{A}$ and Ψ_b, respectively. The first term on the right-hand side is the most primitive estimate of $\langle \Phi_a | \hat{A} \Phi_b \rangle$, obtained by replacing in the latter $\hat{A}$ with $\bar{\hat{A}}$. The second and the third terms on the right-hand side of Eq. (3.3) incorporate, with the aid of the Lagrange *multiplier* $\bar{\eta}$ and the Lagrange *function* $\bar{\Lambda}$, Eqs. (3.1) and (3.2) as *constrains*. It is evident that the functional (3.3) possesses the property

$$F_1 \big[\hat{A}, \Psi_b, \bar{\eta}, \bar{\Lambda} \big] = \langle \Phi_a | \hat{A} \Phi_b \rangle \tag{3.4}$$

for *arbitrary* $\bar{\eta}$ and $\bar{\Lambda}$.

The first variation of the functional (3.3) due to small and sufficiently smooth but otherwise *unconstrained* variations in $\bar{\hat{A}}$, $\bar{\Psi}_b$, $\bar{\eta}$, and $\bar{\Lambda}$ around $\hat{A}$, Ψ_b, η, and Λ (with η and Λ at this stage chosen arbitrarily) is

$$\begin{aligned} \delta F_1 \big[\hat{A}, \Psi_b, \eta, \Lambda \big] &= \langle \Phi_a | \delta \hat{A} \Phi_b \rangle + \delta\eta \langle \Phi_a | \hat{A} \Phi_b - \hat{V} \Psi_b \rangle \\ &\quad + \eta \langle \Phi_a | \delta \hat{A} \Phi_b - \hat{V} \delta \Psi_b \rangle \\ &\quad + \langle \delta \Lambda | \big[1 + \hat{G}_0 \hat{V} \big] \Psi_b - \Phi_b \rangle \\ &\quad + \langle \Lambda | \big[1 + \hat{G}_0 \hat{V} \big] \delta \Psi_b \rangle. \end{aligned} \tag{3.5}$$

In virtue of Eqs. (3.1) and (3.2), the second and the fourth terms on the right-hand side of Eq. (3.5) vanish yielding

$$\begin{aligned} \delta F_1 \big[\hat{A}, \Psi_b, \eta, \Lambda \big] &= \langle \Phi_a | \delta \hat{A} \Phi_b \rangle + \eta \langle \Phi_a | \delta \hat{A} \Phi_b - \hat{V} \delta \Psi_b \rangle \\ &\quad + \langle \Lambda | \big[1 + \hat{G}_0 \hat{V} \big] \delta \Psi_b \rangle \end{aligned} \tag{3.6}$$

and further

$$\begin{aligned} \delta F_1 \big[\hat{A}, \Psi_b, \eta, \Lambda \big] &= [\eta + 1] \langle \Phi_a | \delta \hat{A} \Phi_b \rangle \\ &\quad + \langle \big[1 + \hat{V} \hat{G}_0^\dagger \big] \Lambda - \eta^* \hat{V} \Phi_a | \delta \Psi_b \rangle \end{aligned} \tag{3.7}$$

with the asterisk denoting the complex conjugate.

So far η and Λ have been arbitrary. At this moment, however, we stipulate that

$$\delta F_1 \big[\hat{A}, \Psi_b, \eta, \Lambda \big] = 0 \tag{3.8}$$

for *any* $\delta \hat{A}$ and $\delta \Psi_b$. From Eq. (3.7) it is clear that this is possible if and only if η and Λ are solutions of the

[1] In some texts, particularly older ones (e.g., Ref. [2]) the reactance operator is denoted by $\hat{R}$. In this connection, it should be pointed out that in the scattering theory there exists *another* integral operator $\hat{R}$, a matrix representation of which is Wigner's R-matrix [7]. Occasionally this notational coincidence causes confusions (e.g., [8]).

following equations:

$$\eta + 1 = 0, \tag{3.9}$$

$$\big[1 + \hat{V}\hat{G}_0^{\dagger}\big]\Lambda - \eta^* \hat{V}\Phi_a = 0. \tag{3.10}$$

From Eq. (3.9) we have

$$\eta = -1, \tag{3.11}$$

while Eqs. (3.10) and (3.11) imply that Λ obeys

$$\big[1 + \hat{V}\hat{G}_0^{\dagger}\big]\Lambda + \hat{V}\Phi_a = 0. \tag{3.12}$$

Let us define a function $\Psi_a^{(\dagger)}$ as a solution to the equation

$$\big[1 + \hat{G}_0^{\dagger}\hat{V}\big]\Psi_a^{(\dagger)} - \Phi_a = 0 \tag{3.13}$$

(the *parenthesized* dagger at $\Psi_a^{(\dagger)}$ is an *index* serving to emphasize that this function is a solution to the Lippmann–Schwinger equation (3.13) with the adjoint Green operator $\hat{G}_0^{\dagger}$). Then, it is clear that a solution to Eq. (3.12) is

$$\Lambda = -\hat{V}\Psi_a^{(\dagger)}. \tag{3.14}$$

Eqs. (3.11) and (3.14) suggest that in the functional (3.3) one chooses

$$\bar{\eta} = -1, \tag{3.15}$$

$$\bar{\Lambda} = -\hat{V}\bar{\Psi}_a^{(\dagger)}, \tag{3.16}$$

where $\bar{\Psi}_a^{(\dagger)}$ is some trial estimate of $\Psi_a^{(\dagger)}$. This yields the functional

$$\mathcal{F}_1\big[\bar{\Psi}_a^{(\dagger)}, \bar{\Psi}_b\big] = \big\langle \Phi_a \big| \hat{V}\bar{\Psi}_b \big\rangle + \big\langle \hat{V}\bar{\Psi}_a^{(\dagger)} \big| \Phi_b \big\rangle - \big\langle \bar{\Psi}_a^{(\dagger)} \big| \big[\hat{V} + \hat{V}\hat{G}_0\hat{V}\big]\bar{\Psi}_b \big\rangle, \tag{3.17}$$

which has the advantage of being independent of $\hat{\hat{A}}$. It follows from the method of its construction, presented above, and may be also easily verified directly, on employing Eq. (3.2), that the functional (3.17) possesses the properties

$$\mathcal{F}_1\big[\Psi_a^{(\dagger)}, \Psi_b\big] = \big\langle \Phi_a \big| \hat{V}\Psi_b \big\rangle, \tag{3.18}$$

hence (cf. Eq. (2.4))

$$\mathcal{F}_1\big[\Psi_a^{(\dagger)}, \Psi_b\big] = \big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle, \tag{3.19}$$

and

$$\delta\mathcal{F}_1\big[\Psi_a^{(\dagger)}, \Psi_b\big] = 0. \tag{3.20}$$

Eqs. (3.17), (3.19), and (3.20) may be summarized as the *bilinear* Schwinger variational principle

$$\big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle = \underset{\bar{\Psi}_a^{(\dagger)}, \bar{\Psi}_b}{\text{stat}} \Big\{ \big\langle \Phi_a \big| \hat{V}\bar{\Psi}_b \big\rangle + \big\langle \hat{V}\bar{\Psi}_a^{(\dagger)} \big| \Phi_b \big\rangle - \big\langle \bar{\Psi}_a^{(\dagger)} \big| \big[\hat{V} + \hat{V}\hat{G}_0\hat{V}\big]\bar{\Psi}_b \big\rangle \Big\} \tag{3.21}$$

with the stationary point attained for

$$\bar{\Psi}_a^{(\dagger)} = \Psi_a^{(\dagger)}, \qquad \bar{\Psi}_b = \Psi_b. \tag{3.22}$$

Concluding this section, it is worth noticing that from Eq. (3.17), with the aid of Eq. (3.13), we have

$$\mathcal{F}_1\big[\Psi_a^{(\dagger)}, \Psi_b\big] = \big\langle \hat{V}\Psi_a^{(\dagger)} \big| \Phi_b \big\rangle. \tag{3.23}$$

From this and from Eq. (3.19) we infer that, in addition to Eq. (2.4), it holds

$$\big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle = \big\langle \hat{V}\Psi_a^{(\dagger)} \big| \Phi_b \big\rangle. \tag{3.24}$$

We shall make use of Eq. (3.24) in Section 4.

4. Fractional variational principles

A different variational principle for $\langle \Phi_a | \hat{A}\Phi_b \rangle$ may be obtained by constructing at first a principle for $\langle \Phi_a | \hat{A}\Phi_b \rangle^{-1}$. The relevant starting functional

$$F_2\big[\hat{\hat{A}}, \bar{\Psi}_b, \bar{\eta}, \bar{\Lambda}\big] = \big\langle \Phi_a \big| \hat{\hat{A}}\Phi_b \big\rangle^{-1} + \bar{\eta}\big\langle \Phi_a \big| \hat{\hat{A}}\Phi_b - \hat{V}\bar{\Psi}_b \big\rangle + \big\langle \bar{\Lambda} \big| \big[1 + \hat{G}_0\hat{V}\big]\bar{\Psi}_b - \Phi_b \big\rangle, \tag{4.1}$$

incorporating the constraints (3.1) and (3.2), possesses the property

$$F_2\big[\hat{A}, \Psi_b, \bar{\eta}, \bar{\Lambda}\big] = \big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle^{-1}. \tag{4.2}$$

Varying this functional and making use of the constraints (3.1) and (3.2), we obtain

$$\delta F_2\big[\hat{A}, \Psi_b, \eta, \Lambda\big] = -\big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle^{-2}\big\langle \Phi_a \big| \delta\hat{A}\Phi_b \big\rangle + \eta\big\langle \Phi_a \big| \delta\hat{A}\Phi_b - \hat{V}\delta\Psi_b \big\rangle + \big\langle \Lambda \big| \big[1 + \hat{G}_0\hat{V}\big]\delta\Psi_b \big\rangle, \tag{4.3}$$

hence

$$\delta F_2\big[\hat{A}, \Psi_b, \eta, \Lambda\big] = \Big[\eta - \big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle^{-2}\Big]\big\langle \Phi_a \big| \delta\hat{A}\Phi_b \big\rangle + \big\langle \big[1 + \hat{V}\hat{G}_0^{\dagger}\big]\Lambda - \eta^* \hat{V}\Phi_a \big| \delta\Psi_b \big\rangle. \tag{4.4}$$

On stipulating

$$\delta F_2\big[\hat{A}, \Psi_b, \eta, \Lambda\big] = 0, \tag{4.5}$$

in virtue of arbitrariness of $\delta\hat{A}$ and $\delta\Psi_b$, we find the following equations defining η and Λ:

$$\eta - \big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle^{-2} = 0, \tag{4.6}$$

$$\big[1 + \hat{V}\hat{G}_0^\dagger\big]\Lambda - \eta^* \hat{V}\Phi_a = 0. \tag{4.7}$$

Hence, we infer that

$$\eta = \big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle^{-2}, \tag{4.8}$$

$$\Lambda = \big\langle \hat{A}\Phi_b \big| \Phi_a \big\rangle^{-2} \hat{V}\Psi_a^{(\dagger)}, \tag{4.9}$$

or equivalently, in virtue of Eqs. (2.4) and (3.24),

$$\eta = \big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle^{-1} \big\langle \Phi_a \big| \hat{V}\Psi_b \big\rangle^{-1}, \tag{4.10}$$

$$\Lambda = \big\langle \hat{V}\Psi_b \big| \Phi_a \big\rangle^{-1} \big\langle \Phi_b \big| \hat{V}\Psi_a^{(\dagger)} \big\rangle^{-1} \hat{V}\Psi_a^{(\dagger)}, \tag{4.11}$$

with $\Psi_a^{(\dagger)}$ defined by Eq. (3.13).

Guided by Eqs. (4.10) and (4.11), in the functional (4.1) we substitute

$$\bar{\eta} = \big\langle \Phi_a \big| \hat{\bar{A}}\Phi_b \big\rangle^{-1} \big\langle \Phi_a \big| \hat{V}\bar{\Psi}_b \big\rangle^{-1}, \tag{4.12}$$

$$\bar{\Lambda} = \big\langle \hat{V}\bar{\Psi}_b \big| \Phi_a \big\rangle^{-1} \big\langle \Phi_b \big| \hat{V}\bar{\Psi}_a^{(\dagger)} \big\rangle^{-1} \hat{V}\bar{\Psi}_a^{(\dagger)}, \tag{4.13}$$

with $\bar{\Psi}_a^{(\dagger)}$ and $\bar{\Psi}_b$ having the same meaning as in Section 3. This seemingly artificial choice of $\bar{\eta}$ and $\bar{\Lambda}$ yields a remarkably simple, independent of $\hat{\bar{A}}$, fractional functional

$$\mathcal{F}_2\big[\bar{\Psi}_a^{(\dagger)}, \bar{\Psi}_b\big] = \frac{\big\langle \bar{\Psi}_a^{(\dagger)} \big| [\hat{V} + \hat{V}\hat{G}_0\hat{V}]\bar{\Psi}_b \big\rangle}{\big\langle \Phi_a \big| \hat{V}\bar{\Psi}_b \big\rangle \big\langle \hat{V}\bar{\Psi}_a^{(\dagger)} \big| \Phi_b \big\rangle} \tag{4.14}$$

with the required properties

$$\mathcal{F}_2\big[\Psi_a^{(\dagger)}, \Psi_b\big] = \big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle^{-1}, \tag{4.15}$$

$$\delta\mathcal{F}_2\big[\Psi_a^{(\dagger)}, \Psi_b\big] = 0. \tag{4.16}$$

Actually, the functional (4.14) offers even *more* than we might expect from the procedure of its construction. A glance at Eq. (4.14) shows that for any $\alpha, \beta \in \mathbb{C}\backslash\{0\}$ it holds

$$\mathcal{F}_2\big[\alpha\bar{\Psi}_a^{(\dagger)}, \beta\bar{\Psi}_b\big] = \mathcal{F}_2\big[\bar{\Psi}_a^{(\dagger)}, \bar{\Psi}_b\big]. \tag{4.17}$$

Consequently, Eqs. (4.15) and (4.16) may be replaced by

$$\mathcal{F}_2\big[\alpha\Psi_a^{(\dagger)}, \beta\Psi_b\big] = \big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle^{-1}, \tag{4.18}$$

$$\delta\mathcal{F}_2\big[\alpha\Psi_a^{(\dagger)}, \beta\Psi_b\big] = 0, \tag{4.19}$$

i.e., we have

$$\big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle^{-1} = \operatorname*{stat}_{\bar{\Psi}_a^{(\dagger)}, \bar{\Psi}_b} \frac{\big\langle \bar{\Psi}_a^{(\dagger)} \big| [\hat{V} + \hat{V}\hat{G}_0\hat{V}]\bar{\Psi}_b \big\rangle}{\big\langle \Phi_a \big| \hat{V}\bar{\Psi}_b \big\rangle \big\langle \hat{V}\bar{\Psi}_a^{(\dagger)} \big| \Phi_b \big\rangle}, \tag{4.20}$$

with the stationary point attained for

$$\bar{\Psi}_a^{(\dagger)} = \alpha\Psi_a^{(\dagger)}, \qquad \bar{\Psi}_b = \beta\Psi_b, \tag{4.21}$$

where $\alpha, \beta \in \mathbb{C}\backslash\{0\}$.

From Eq. (4.22) we deduce the following *fractional* Schwinger variational principle for the matrix element $\langle \Phi_a | \hat{A}\Phi_b \rangle$:

$$\big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle = \operatorname*{stat}_{\bar{\Psi}_a^{(\dagger)}, \bar{\Psi}_b} \frac{\big\langle \Phi_a \big| \hat{V}\bar{\Psi}_b \big\rangle \big\langle \hat{V}\bar{\Psi}_a^{(\dagger)} \big| \Phi_b \big\rangle}{\big\langle \bar{\Psi}_a^{(\dagger)} \big| [\hat{V} + \hat{V}\hat{G}_0\hat{V}]\bar{\Psi}_b \big\rangle}, \tag{4.22}$$

with the stationary point attained for $\bar{\Psi}_a^{(\dagger)}$ and $\bar{\Psi}_b$ given in Eq. (4.21).

Before concluding this section, we mention that other choices of $\bar{\eta}$ and $\bar{\Lambda}$, alternative to these in Eqs. (4.12) and (4.13), are also possible. For instance, have we chosen in the functional (4.1)

$$\bar{\eta} = \big\langle \Phi_a \big| \hat{V}\bar{\Psi}_b \big\rangle^{-2}, \tag{4.23}$$

$$\bar{\Lambda} = \big\langle \hat{V}\bar{\Psi}_b \big| \Phi_a \big\rangle^{-2} \hat{V}\bar{\Psi}_a^{(\dagger)}, \tag{4.24}$$

$$\big\langle \Phi_a \big| \hat{\bar{A}}\Phi_b \big\rangle = \big\langle \Phi_a \big| \hat{V}\bar{\Psi}_b \big\rangle, \tag{4.25}$$

as suggested by Eqs. (4.8), (4.9), and (2.4), we would arrive at the variational principle

$$\begin{aligned} \big\langle \Phi_a \big| \hat{A}\Phi_b \big\rangle &= \operatorname*{stat}_{\bar{\Psi}_a^{(\dagger)}, \bar{\Psi}_b} \Big\{ \big\langle \Phi_a \big| \hat{V}\bar{\Psi}_b \big\rangle^2 \big[\big\langle \Phi_a \big| \hat{V}\bar{\Psi}_b \big\rangle - \big\langle \hat{V}\bar{\Psi}_a^{(\dagger)} \big| \Phi_b \big\rangle \\ &\quad + \big\langle \bar{\Psi}_a^{(\dagger)} \big| \big[\hat{V} + \hat{V}\hat{G}_0\hat{V}\big]\bar{\Psi}_b \big\rangle \big]^{-1} \Big\}, \end{aligned} \tag{4.26}$$

with the stationary point attained for

$$\bar{\Psi}_a^{(\dagger)} = \Psi_a^{(\dagger)}, \qquad \bar{\Psi}_b = \Psi_b. \tag{4.27}$$

Still another choice:

$$\bar{\eta} = \big\langle \hat{V}\bar{\Psi}_a^{(\dagger)} \big| \Phi_b \big\rangle^{-2}, \tag{4.28}$$

$$\bar{\Lambda} = \langle \Phi_b | \hat{V} \bar{\Psi}_a^{(\dagger)} \rangle^{-2} \hat{V} \bar{\Psi}_a^{(\dagger)}, \tag{4.29}$$

$$\langle \Phi_a | \hat{\bar{A}} \Phi_b \rangle = \langle \hat{V} \bar{\Psi}_a^{(\dagger)} | \bar{\Phi}_b \rangle, \tag{4.30}$$

suggested by Eqs. (4.8), (4.9), and (3.24), results in the principle

$$\begin{aligned} \langle \Phi_a | \hat{A} \Phi_b \rangle &= \operatorname*{stat}_{\bar{\Psi}_a^{(\dagger)}, \bar{\Psi}_b} \Big\{ \langle \hat{V} \bar{\Psi}_a^{(\dagger)} | \Phi_b \rangle^2 \\ &\quad \times \big[\langle \hat{V} \bar{\Psi}_a^{(\dagger)} | \Phi_b \rangle - \langle \Phi_a | \hat{V} \bar{\Psi}_b \rangle \\ &\quad + \langle \bar{\Psi}_a^{(\dagger)} | [\hat{V} + \hat{V} \hat{G}_0 \hat{V}] \bar{\Psi}_b \rangle \big]^{-1} \Big\}, \end{aligned} \tag{4.31}$$

with the stationary point attained for the same $\bar{\Psi}_a^{(\dagger)}$ and $\bar{\Psi}_b$ as in the case of the principle (4.26). However, because of simplicity of the functional involved, the principle (4.22) is evidently superior to the principles (4.26) and (4.31); in fact, this principle is also superior to all other fractional principles which may be obtained with alternative (but still consistent with Eqs. (4.8), (4.9), and either (2.4) or (3.24)) choices of $\bar{\eta}$, $\bar{\Lambda}$, and $\langle \Phi_a | \hat{\bar{A}} \Phi_b \rangle$.

5. Two examples

As the first example, consider

$$\hat{A} = \hat{T}, \tag{5.1}$$

where $\hat{T}$ is the standard on-shell transition operator. In this case, the Green operator $\hat{G}_0$, to be used in the Lippmann–Schwinger equation (3.2), is the 'outgoing' one (2.5), while its Hermitian adjoint, to be used in Eq. (4.7), is the 'ingoing' one (2.7). Following the common notation and denoting by $\Psi_c^{(\pm)}$ solutions to the Lippmann–Schwinger equations

$$[1 + \hat{G}_0^{(\pm)} \hat{V}] \Psi_c^{(\pm)} - \Phi_c = 0, \tag{5.2}$$

we have

$$\Psi_a^{(\dagger)} = \Psi_a^{(-)}, \qquad \Psi_b = \Psi_b^{(+)}. \tag{5.3}$$

Adopting the analogous notation for the estimates:

$$\bar{\Psi}_a^{(\dagger)} = \bar{\Psi}_a^{(-)}, \qquad \bar{\Psi}_b = \bar{\Psi}_b^{(+)}, \tag{5.4}$$

from Eqs. (3.21) and (4.22), as particular cases, we obtain the well-known Schwinger variational principles [1–5]:

$$\begin{aligned} \langle \Phi_a | \hat{T} \Phi_b \rangle = \operatorname*{stat}_{\bar{\Psi}_a^{(-)}, \bar{\Psi}_b^{(+)}} \Big\{ &\langle \Phi_a | \hat{V} \bar{\Psi}_b^{(+)} \rangle + \langle \hat{V} \bar{\Psi}_a^{(-)} | \Phi_b \rangle \\ &- \langle \bar{\Psi}_a^{(-)} | [\hat{V} + \hat{V} \hat{G}_0^{(+)} \hat{V}] \bar{\Psi}_b^{(+)} \rangle \Big\}, \end{aligned} \tag{5.5}$$

$$\langle \Phi_a | \hat{T} \Phi_b \rangle = \operatorname*{stat}_{\bar{\Psi}_a^{(-)}, \bar{\Psi}_b^{(+)}} \frac{\langle \Phi_a | \hat{V} \bar{\Psi}_b^{(+)} \rangle \langle \hat{V} \bar{\Psi}_a^{(-)} | \Phi_b \rangle}{\langle \bar{\Psi}_a^{(-)} | [\hat{V} + \hat{V} \hat{G}_0^{(+)} \hat{V}] \bar{\Psi}_b^{(+)} \rangle}. \tag{5.6}$$

In the principle (5.5) the stationary value is attained for

$$\bar{\Psi}_a^{(-)} = \Psi_a^{(-)}, \qquad \bar{\Psi}_b^{(+)} = \Psi_b^{(+)}, \tag{5.7}$$

and in the principle (5.6) for

$$\bar{\Psi}_a^{(-)} = \alpha \Psi_a^{(-)}, \qquad \bar{\Psi}_b^{(+)} = \beta \Psi_b^{(+)}, \tag{5.8}$$

with $\alpha, \beta \in \mathbb{C} \backslash \{0\}$. Eqs. (2.4) and (3.24), specialized to the case considered here, yield

$$\langle \Phi_a | \hat{T} \Phi_b \rangle = \langle \Phi_a | \hat{V} \Psi_b^{(+)} \rangle = \langle \hat{V} \Psi_a^{(-)} | \Phi_b \rangle. \tag{5.9}$$

In the second example, we take

$$\hat{A} = \hat{K}, \tag{5.10}$$

where $\hat{K}$ is the on-shell reactance operator. The relevant Green operator $\hat{G}_0$ is now the 'principal-value' one (2.6); evidently, it is self-adjoint:

$$\hat{G}_0^{(\mathrm{P})\dagger} = \hat{G}_0^{(\mathrm{P})}. \tag{5.11}$$

If we denote by $\Psi_c^{(\mathrm{P})}$ a solution to the equation

$$[1 + \hat{G}_0^{(\mathrm{P})} \hat{V}] \Psi_c^{(\mathrm{P})} - \Phi_c = 0, \tag{5.12}$$

in virtue of the hermiticity of $\hat{G}_0^{(\mathrm{P})}$ we have

$$\Psi_c^{(\mathrm{P})(\dagger)} = \Psi_c^{(\mathrm{P})}, \tag{5.13}$$

hence, in this example:

$$\Psi_a^{(\dagger)} = \Psi_a^{(\mathrm{P})}, \qquad \Psi_b = \Psi_b^{(\mathrm{P})}. \tag{5.14}$$

Again, adopting the analogous notation for estimates:

$$\bar{\Psi}_a^{(\dagger)} = \bar{\Psi}_a^{(\mathrm{P})}, \qquad \bar{\Psi}_b = \bar{\Psi}_b^{(\mathrm{P})}, \tag{5.15}$$

Eqs. (3.21) and (4.22) yield the Schwinger variational principles [2,4]:

$$\begin{aligned} \langle \Phi_a | \hat{K} \Phi_b \rangle = \operatorname*{stat}_{\bar{\Psi}_a^{(\mathrm{P})}, \bar{\Psi}_b^{(\mathrm{P})}} \Big\{ &\langle \Phi_a | \hat{V} \bar{\Psi}_b^{(\mathrm{P})} \rangle + \langle \hat{V} \bar{\Psi}_a^{(\mathrm{P})} | \Phi_b \rangle \\ &- \langle \bar{\Psi}_a^{(\mathrm{P})} | [\hat{V} + \hat{V} \hat{G}_0^{(\mathrm{P})} \hat{V}] \bar{\Psi}_b^{(\mathrm{P})} \rangle \Big\}, \end{aligned} \tag{5.16}$$

$$\langle \Phi_a | \hat{K} \Phi_b \rangle = \operatorname*{stat}_{\bar{\Psi}_a^{(\mathrm{P})}, \bar{\Psi}_b^{(\mathrm{P})}} \frac{\langle \Phi_a | \hat{V} \bar{\Psi}_b^{(\mathrm{P})} \rangle \langle \hat{V} \bar{\Psi}_a^{(\mathrm{P})} | \Phi_b \rangle}{\langle \bar{\Psi}_a^{(\mathrm{P})} | [\hat{V} + \hat{V} \hat{G}_0^{(\mathrm{P})} \hat{V}] \bar{\Psi}_b^{(\mathrm{P})} \rangle}. \tag{5.17}$$

The functional on the right-hand side of Eq. (5.16) is stationary for

$$\bar{\Psi}_a^{(\mathrm{P})} = \Psi_a^{(\mathrm{P})}, \qquad \bar{\Psi}_b^{(\mathrm{P})} = \Psi_b^{(\mathrm{P})}, \tag{5.18}$$

while for the functional in Eq. (5.17) this occurs when

$$\bar{\Psi}_a^{(\mathrm{P})} = \alpha \Psi_a^{(\mathrm{P})}, \qquad \bar{\Psi}_b^{(\mathrm{P})} = \beta \Psi_b^{(\mathrm{P})}, \tag{5.19}$$

with $\alpha, \beta \in \mathbb{C} \setminus \{0\}$. From Eqs. (2.4) and (3.24) we have

$$\langle \Phi_a | \hat{K} \Phi_b \rangle = \langle \Phi_a | \hat{V} \Psi_b^{(\mathrm{P})} \rangle = \langle \hat{V} \Psi_a^{(\mathrm{P})} | \Phi_b \rangle = \langle \hat{K} \Phi_a | \Phi_b \rangle, \tag{5.20}$$

i.e., the operator $\hat{K}$ is Hermitian.

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Appendix A. An alternative derivation of the fractional principle (4.22)

The fractional variational principle (4.22) may be obtained [3,9] in a way alternative to that presented in Section 4. To show this, we consider the bilinear functional (3.17) with trial functions

$$\bar{\Psi}_a^{(\dagger)} = \bar{\alpha} \bar{\psi}_a^{(\dagger)}, \qquad \bar{\Psi}_b = \bar{\beta} \bar{\psi}_b, \tag{A.1}$$

where $\bar{\alpha}, \bar{\beta} \in \mathbb{C}$ are adjustable scalars while $\bar{\psi}_a^{(\dagger)}$ and $\bar{\psi}_b$ are new trial functions. On defining

$$F_3[\bar{\alpha}, \bar{\beta}, \bar{\psi}_a^{(\dagger)}, \bar{\psi}_b] = \mathcal{F}_1[\bar{\alpha} \bar{\psi}_a^{(\dagger)}, \bar{\beta} \bar{\psi}_b], \tag{A.2}$$

we have explicitly

$$\begin{aligned} F_3[\bar{\alpha}, \bar{\beta}, \bar{\psi}_a^{(\dagger)}, \bar{\psi}_b] &= \bar{\beta} \langle \Phi_a | \hat{V} \bar{\psi}_b \rangle + \bar{\alpha}^* \langle \hat{V} \bar{\psi}_a^{(\dagger)} | \Phi_b \rangle \\ &\quad - \bar{\alpha}^* \bar{\beta} \langle \bar{\psi}_a^{(\dagger)} | [\hat{V} + \hat{V} \hat{G}_0 \hat{V}] \bar{\psi}_b \rangle. \end{aligned} \tag{A.3}$$

Keeping $\bar{\psi}_a^{(\dagger)}$ and $\bar{\psi}_b$ fixed and varying $\bar{\alpha}$ and $\bar{\beta}$ around some α and β, respectively, yields

$$\begin{aligned} \delta F_3[\alpha, \beta, \bar{\psi}_a^{(\dagger)}, \bar{\psi}_b] &= \delta\alpha^* [\langle \hat{V} \bar{\psi}_a^{(\dagger)} | \Phi_b \rangle - \beta \langle \bar{\psi}_a^{(\dagger)} | [\hat{V} + \hat{V} \hat{G}_0 \hat{V}] \bar{\psi}_b \rangle] \\ &\quad + \delta\beta [\langle \Phi_a | \hat{V} \bar{\psi}_b \rangle - \alpha^* \langle \bar{\psi}_a^{(\dagger)} | [\hat{V} + \hat{V} \hat{G}_0 \hat{V}] \bar{\psi}_b \rangle]. \end{aligned} \tag{A.4}$$

Stipulation

$$\delta F_3[\alpha, \beta, \bar{\psi}_a^{(\dagger)}, \bar{\psi}_b] = 0 \tag{A.5}$$

gives

$$\alpha^* = \frac{\langle \Phi_a | \hat{V} \bar{\psi}_b \rangle}{\langle \bar{\psi}_a^{(\dagger)} | [\hat{V} + \hat{V} \hat{G}_0 \hat{V}] \bar{\psi}_b \rangle}, \tag{A.6}$$

$$\beta = \frac{\langle \hat{V} \bar{\psi}_a^{(\dagger)} | \Phi_b \rangle}{\langle \bar{\psi}_a^{(\dagger)} | [\hat{V} + \hat{V} \hat{G}_0 \hat{V}] \bar{\psi}_b \rangle}. \tag{A.7}$$

Choosing

$$\bar{\alpha} = \alpha, \qquad \bar{\beta} = \beta, \tag{A.8}$$

with α and β defined in Eqs. (A.6) and (A.7), the functional (A.3) becomes

$$\mathcal{F}_3[\bar{\psi}_a^{(\dagger)}, \bar{\psi}_b] = \frac{\langle \Phi_a | \hat{V} \bar{\psi}_b \rangle \langle \hat{V} \bar{\psi}_a^{(\dagger)} | \Phi_b \rangle}{\langle \bar{\psi}_a^{(\dagger)} | [\hat{V} + \hat{V} \hat{G}_0 \hat{V}] \bar{\psi}_b \rangle}. \tag{A.9}$$

It is evident that, apart from unimportant notational differences, the functional (A.9) is identical with the one used in the principle (4.22).

It has to be emphasized, however, that in some variational problems [10] (in fact, more involved than these discussed in this Letter) the method presented in this appendix leads to fractional variational principles *different* from those which may be obtained by applying the Lagrange procedure in the manner analogous to that outlined in Section 4.

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