Rearrangement Collisions

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(Received December 12, 1955)

We discuss the quantum-mechanical theory of rearrangement collisions. In particular, we consider: (a) the transformation of the state vector from the original basis to the basis of the rearranged system; (b) the conditions for the equivalence of the "post" and "prior" interactions when computing matrix elements; and, (c) the extension of Schwinger's variational principle to rearrangement collisions.

1. INTRODUCTION

VARIATIONAL principles for scattering processes have been devised by Schwinger, and have been discussed, for direct collisions, previously.[1] In this paper, we wish to treat rearrangement collisions.

The distinction between the two is as follows. In a *direct* collision, the scattered and the incident particles are the same; only their states may change. In a *rearrangement* collision, the particles scattered differ from those incident, either in identity, as in an exchange collision, or in intrinsic structure, as in a stripping or pickup reaction.[2]

Borowitz and Friedman have already described a variational principle for rearrangement scattering.[3] In form, this variational principle is rather unexpected. For, although it is an essential feature of Schwinger's variational principle—as formulated for direct scattering—that the initial and final states appear symmetrically, in the expression given by Borowitz and Friedman this is not so; the original and the rearranged systems enter quite unsymmetrically.

The same variational principle is derived here, but in a context that clearly shows it to be one of a pair of dissymmetrical stationary expressions. In the present treatment, the other member of the pair is exhibited, and the two expressions are then averaged; the result is a variational principle that is symmetrical in the original and rearranged systems.

In the course of the preliminary development, it is necessary to examine the transformation of the state vector from the original basis to the basis of the rearranged system, a question which has also been considered in the recent literature.[4,5] Here, our formalism permits a concise, and at the same time rather general, derivation of the essential results.[5]

The "post-prior" discrepancy is also discussed briefly. We remark, first, that the vanishing of the discrepancy for the exact wave functions implies that it also vanishes in the Born approximation, and conversely. Second, we note that the discrepancy vanishes if the "post" and "prior" unperturbed Hamiltonians are Hermitian between the initial and final states. Thus, the elimination of the "post-prior" discrepancy imposes a restriction only on the formal representation used for the wave functions: for the continuum states it may be necessary to use wave packets, or an analytical equivalent.

Our method, and notation, differ somewhat from I.[1] To explain them most simply, we first review the familiar case of direct scattering.

2. DIRECT COLLISIONS

We limit ourselves, in this section, to collisions in which the scattered particles are the same as those incident. That is, in both the initial and final states, the two separated parts of the system are characterized by the unperturbed Hamiltonian H_0, and their interaction by the operator V:

$$H=H_0+V. \tag{2.1}$$

Let λ be a complex number, the imaginary part of which is arbitrarily small and positive:

$$\lambda=E+i\epsilon; \quad \epsilon\to 0^+. \tag{2.2}$$

Then, since both H_0 and H are Hermitian, $\lambda-H_0$ and $\lambda-H$ are nonsingular operators. Their inverses, the operator Green's functions,[6]

$$G_0(\lambda)=1/(\lambda-H_0)=G_0(\lambda^*)^\dagger, \tag{2.3}$$

$$G(\lambda)=1/(\lambda-H)=G(\lambda^*)^\dagger, \tag{2.4}$$

[1] B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950). References to this paper will be preceded by I.

[2] Stripping or pick-up reactions appear as exchange processes relative to the particle that is stripped-off or picked-up.

[3] S. Borowitz and B. Freidman, Phys. Rev. **91**, 398 (1953). A slight error appears in this paper. Although the kernels encountered here are not self-adjoint, the variational principle is discussed in the form appropriate for a self-adjoint kernel. The correction involves replacing the kernels appearing in Eqs. (15b), (19), and (31) by their adjoints.

[4] T. Y. Wu, Phys. Rev. **87**, 1010 (1952); L. E. H. Trainor and T. Y. Wu, Phys. Rev. **89**, 273 (1953).

[5] H. E. Moses, Phys. Rev. **91**, 185 (1953); S. Altschuler, Phys. Rev. **91**, 1167 (1953); **92**, 1157 (1953).

[6] In a coordinate representation, $G(\lambda)$ and $G(\lambda^*)$ become the Green's functions satisfying an outgoing and an incoming wave condition, respectively. For example, in one dimension, let $H=-d^2/dx^2$, and $\lambda=E+i\epsilon=(\kappa+i\alpha)^2$. Then,

$$\langle x|G(\lambda)|x'\rangle=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dk\,\exp[ik(x-x')]}{(\kappa+i\alpha)^2-k^2}$$

$$=\frac{\exp[i(\kappa+i\alpha)|x-x'|]}{2i(\kappa+i\alpha)} \quad (\alpha\to 0).$$

Similarly,

$$\langle x|G(\lambda^*)|x'\rangle=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dk\,\exp[ik(x-x')]}{(\kappa-i\alpha)^2-k^2}$$

$$=\frac{\exp[i(-\kappa+i\alpha)|x-x'|]}{2i(-\kappa+i\alpha)} \quad (\alpha\to 0).$$

Observing that $\lambda^*=(-\kappa+i\alpha)^2$, we see that (2.4) is satisfied.

therefore exist, and, as shown, are unaffected by Hermitian conjugation, provided λ is also replaced by its complex conjugate. This latter property is frequently of use in deducing or checking equations.

For example, simple operator algebra applied to (2.3) and (2.4) shows that

$$\begin{aligned} G(\lambda)&=G_0(\lambda)[1+VG(\lambda)] \\ &=[1+G(\lambda)V]G_0(\lambda), \end{aligned} \tag{2.5}$$

where the last equation may be deduced directly or by hermitian conjugation plus $\lambda\rightarrow\lambda^*$ applied to the first equation.

We shall also need the operators

$$T(\lambda)=V+VG(\lambda)V=T(\lambda^*)^\dagger \tag{2.6}$$

and

$$U(\lambda)=1+G(\lambda)V. \tag{2.7}$$

The latter equation, according to (2.5), may also be written:

$$[1-G_0(\lambda)V]U(\lambda)=1. \tag{2.8}$$

Comparing the last three equations, we see that

$$\begin{aligned} T(\lambda)&=VU(\lambda)=U(\lambda^*)^\dagger V \\ &=U(\lambda^*)^\dagger[V-VG_0(\lambda)V]U(\lambda). \end{aligned} \tag{2.9}$$

We turn now to the physical interpretation. The initial and final states of the system are described by the eigenvectors of H_0:

$$H_0\Phi_a=E_a\Phi_a. \tag{2.10}$$

As the two parts of the system approach one another, during the collision, the interaction becomes effective and induces transitions from the given initial state to those final states that are accessible to the system. In particular, if the system is initially in the state Φ_a, the probability of ultimately finding it in the state Φ_b increases with time at the rate [(I-1.68) to (I-1.72)]:

$$w_{ba}=\frac{2\pi}{\hbar}|(\Phi_b,V\Psi_a^{(+)})|^2\delta(E_a-E_b), \tag{2.11}$$

where, according to (I-1.61),

$$\Psi_a^{(\pm)}=\Phi_a+\frac{1}{E_a\pm i\epsilon-H_0}V\Psi_a^{(\pm)}. \tag{2.12}$$

The delta function in (2.11) insures that transitions only occur between states of equal energy, while the plus (minus) sign in (2.12) corresponds to the choice of outgoing (incoming) scattered waves.

From (2.8) and (2.12),

$$\Psi_a^{(\pm)}=U(E_a\pm i\epsilon)\Phi_a, \tag{2.13}$$

thereby establishing the connection between the theory of I and the operators introduced here.

For example, if E is the energy common to states a and b, it follows from (2.9) and (2.11) that the matrix element required to compute the transition rate $a\rightarrow b$ is

$$T_{ba}(E+i\epsilon)=(\Phi_b,T(E+i\epsilon)\Phi_a)=[T(E-i\epsilon)^\dagger]_{ba}. \tag{2.14}$$

This is the familiar result (I-1.63):

$$(\Phi_b,V\Psi_a^{(+)})=(\Psi_b^{(-)},V\Phi_a). \tag{2.15}$$

Using (2.9), we may now write the variational principle (I-1.78) in operator form:

$$\begin{aligned} '\!T(\lambda)'&=VU(\lambda)+U(\lambda^*)^\dagger V \\ &\quad -U(\lambda^*)^\dagger[V-VG_0(\lambda)V]U(\lambda). \end{aligned} \tag{2.16}$$

The variation of $U(\lambda)$ in this expression leads to

$$\begin{aligned} '\delta T(\lambda)'&=\{1-[1-G_0(\lambda^*)V]U(\lambda^*)\}^\dagger V\delta U(\lambda) \\ &\quad +\delta U(\lambda^*)^\dagger V\{1-[1-G_0(\lambda)V]U(\lambda)\}. \end{aligned} \tag{2.17}$$

As expected, this is zero, and therefore (2.16) is stationary, for variations about the solution of (2.8).

Finally, according to (2.9), the stationary value of $'\!T(\lambda)'$ is $T(\lambda)$. Thus, (2.16) is the Schwinger variational principle[7] for the operator $T(\lambda)$.

This completes our review of the theory of direct scattering.

3. REARRANGEMENT COLLISIONS

We now assume that the separated parts of the system can exist, in the initial and final states, in two different arrangements ("channels") corresponding to the "original" and "rearranged" systems.

For the original system,

$$H=H_0'+V', \tag{3.1}$$

while for the rearranged system,

$$H=H_0''+V''. \tag{3.2}$$

If we stay in the same channel initially and finally, the discussion of Sec. 2 requires only the addition of primes or double primes. Thus, for direct scattering among the states of the original system, we introduce

$$G_0'(\lambda)=\frac{1}{\lambda-H_0'}=G_0'(\lambda^*)^\dagger, \tag{3.3}$$

and

$$[1-G_0'(\lambda)V']U'(\lambda)=1. \tag{3.4}$$

Direct scattering in the original system is then described by (2.11) with the matrix element replaced by

$$(\Phi_b',V'\Psi_a^{(+)'}), \tag{3.5}$$

where

$$H_0'\Phi_a'=E_a'\Phi_a', \tag{3.6}$$

and

$$\Psi_a^{(\pm)'}=\Phi_a'+\frac{1}{E_a'\pm i\epsilon-H_0'}V'\Psi_a^{(\pm)'}. \tag{3.7}$$

Using (3.4), the last equation implies that

$$\Psi_a^{(\pm)'}=U'(E_a'\pm i\epsilon)\Phi_a'. \tag{3.8}$$

[7] The relation of (2.16) to the more conventional forms of the Schwinger variational principle is discussed in the Appendix.

For the discussion of direct scattering in the rearranged system, all the equations above hold with the primes replaced by double primes. The variational principle (2.16) may also be transcribed to hold in either the original ($'$) or the rearranged ($''$) system.

For rearrangement scattering, from the original to the rearranged system, or conversely, an additional discussion is required. We now consider these transitions.

In (3.4), $U'(\lambda)$ is defined in terms of the operator Green's function of the original system, $G_0'(\lambda)$. This has the consequence, when used in (3.8), that the scattered wave is expanded most naturally in the basis of the original system. For scattering from the original to the rearranged system, however, it is preferable to express the scattered wave in the basis of the rearranged system. (3.4) should therefore be rewritten so that G_0' is replaced by G_0''.

To do this, we multiply (3.4) on the left, first by $\lambda-H_0'$, then by $G_0''(\lambda)$. This yields, first

$$(\lambda-H)U'(\lambda)=\lambda-H_0'=\lambda-H_0''+(V'-V''), \quad (3.9)$$

and then

$$[1-G_0''(\lambda)V'']U'(\lambda)=G_0''(\lambda)(\lambda-H_0') \\ =1+G_0''(\lambda)(V'-V''). \quad (3.10)$$

If this is used in (3.8), the state vector becomes

$$\Psi_a^{(\pm)'}=\frac{\pm i\epsilon}{E_a'\pm i\epsilon-H_0''}\Phi_a' \\ +\frac{1}{E_a'\pm i\epsilon-H_0''}V''\Psi_a^{(\pm)'}. \quad (3.11)$$

In (3.7), the direct scattering was explicit. Since rearrangement scattering also occurs, this possibility was contained implicitly in (3.7). By the transformation to (3.11), the presence of a scattered wave belonging to the rearranged system has been exhibited more directly.

For example, if (3.11) is expanded in terms of the eigenvectors of H_0'', (defined by (3.6) with $'\rightarrow''$),

$$\Psi_a^{(\pm)'}=\sum_b \frac{\pm i\epsilon\Phi_b''(\Phi_b'',\Phi_a')}{E_a'-E_b''\pm i\epsilon} \\ +\sum_b \frac{\Phi_b''(\Phi_b'',V''\Psi_a^{(\pm)'})}{E_a'-E_b''\pm i\epsilon}. \quad (3.12)$$

It is clear that the second term provides a natural description of rearrangement scattering. The first term will also contribute to the rearrangement scattering, unless it vanishes asymptotically. We therefore must examine the asymptotic form of this term. Only those states for which E_b'' is in the continuum need be considered, since discrete values of E_b'' correspond to states that vanish asymptotically.

In the first term of (3.12), as $\epsilon\rightarrow 0$, the ϵ-dependent factor approaches zero for $E_b''\neq E_a'$ and unity for $E_b''=E_a'$. Thus, in this term, the state Φ_a' is first expanded in terms of the eigenstates Φ_b''; the ϵ-dependent factor then acts as a projection operator that limits the b states to those states, say "b", on the energy shell $E_b''=E_a'$. That is, if we split the sum over b into an integral over the energy E_b'' and a sum over states "b" of equal energy, E_b'', the first term of (3.12) becomes

$$\lim_{\epsilon\rightarrow 0}\int_{E_a'-\epsilon}^{E_a'+\epsilon} dE_b'' \sum_{\text{"}b\text{"}} \rho(E_b'')\Phi_b''(\Phi_b'',\Phi_a'), \quad (3.13)$$

where $\rho(E_b'')$ is the number of states of type "b" per unit energy range. Since the integral is over a vanishingly small interval, (3.13) is zero unless the integrand contains a delta function in energy.

To analyze (3.13) further, let us consider an exchange collision. We suppose two independent particles, 1 and 2, collide. In state a, the energies are E_1' and E_2'; in state b, they are E_1'' and E_2''. In the transition $a\rightarrow b$, energy is conserved.

Because 1 and 2 are uncoupled in both states a and b, the scalar product in (3.13) factors into a scalar product of the wave vectors of 1 times a similar product of the wave vectors of 2. (A similar factorization occurs for the integration over E_b'' and the sum over states of equal energy, "b".) Now, the scalar product of the 1 vectors is independent of the variables of 2, in particular of E_2' and E_2''. It follows, that if an energy-dependent delta function results from this factor, it must be $\delta(E_1''-E_1')$. Similarly, if the scalar product of the state vectors of particle 2 produces a delta function in energy, it must be $\delta(E_2''-E_2')$. We conclude that (3.13) vanishes unless particles 1 and 2 individually have the same energy in state b that they have in state a.

If, for example, E_1' and E_2'' are in the (positive) continuum, (3.13) vanishes if E_1'' and E_2' take on (negative) discrete values. Or, (3.13) is different from zero only if, in going from a to b, neither particle changes from an unbound, or continuum, state to a bound state, or conversely.

Ordinarily, this requirement is not satisfied in rearrangement scattering. The customary exchange situation corresponds to the particle that is bound in state a becoming free in state b, while the other particle behaves oppositely. The first term of (3.12) then reduces, asymptotically, to zero.

We shall limit ourselves to such cases. When using (3.11) to expand $\Psi_a^{(\pm)'}$ asymptotically in terms of eigenvectors of H_0'', the first term of (3.11) therefore may be ignored. In an exact expression, however, this term is essential: it relates $\Psi_a^{(\pm)'}$ to its source. Only when this term is retained, may (3.7) be derived unambiguously from (3.11).

In the light of these remarks, the probability that a system, originally in state Φ_a', will finally be found in state Φ_b'' may be obtained by considering only the

second term of (3.12):

$$|(\Phi_b'',\Psi_a^{(+)\prime})|^2=\frac{|(\Phi_b'',V''\Psi_a^{(+)\prime})|^2}{(E_a'-E_b'')^2+\epsilon^2}. \quad (3.14)$$

The transition rate for rearrangement scattering, $w_{ba}^{(r)}$, follows by taking the time derivative of (3.14). To do this, we note that (3.7) implies that $\Psi_a^{(+)\prime}$ has the complex energy $E_a'+i\epsilon$, and therefore that the time dependence $\exp[i(E_a'+i\epsilon)t/\hbar]$ must be associated with this stationary state. That is, (3.14) has the time dependence $\exp[(-2\epsilon t)/\hbar]$ and[8]

$$w_{ba}^{(r)}=\frac{\partial}{\partial t}|(\Phi_b'',\Psi_a^{(+)\prime})|^2$$

$$=\frac{2\pi}{\hbar}|(\Phi_b'',V''\Psi_a^{(+)\prime})|^2\delta(E_a'-E_b''), \quad (3.15)$$

where we have used (I-1.58):

$$\lim_{\epsilon\to 0}\int_{-\infty}^{\infty}\frac{\epsilon}{\epsilon^2+x^2}f(x)dx=\pi f(0). \quad (3.16)$$

Clearly, (3.15) plays the same role in rearrangement scattering that (2.11) does in direct scattering. The matrix element required, according to (3.8) and (3.15), is

$$(\Phi_b'',V''\Psi_a^{(+)\prime})=(\Phi_b'',V''U'(E_a'+i\epsilon)\Phi_a'), \quad (3.17)$$

where $E_a'=E_b''$.

We have already remarked that $U'(\lambda)$ and $U''(\lambda)$ follow by putting primes and double primes on (2.7):

$$U'(\lambda)=1+G(\lambda)V', \quad (3.18)$$

$$U''(\lambda)=1+G(\lambda)V''. \quad (3.19)$$

In fact, (3.4) follows from (3.18) and (3.3). A similar equation holds for $U''(\lambda)$ if we replace primes by double primes:

$$[1-G_0''(\lambda)V'']U''(\lambda)=1. \quad (3.20)$$

In the same way, the substitution $'\leftrightarrow''$ in (3.10) leads to

$$[1-G_0'(\lambda)V']U''(\lambda)=G_0'(\lambda)(\lambda-H_0'')$$
$$=1+G_0'(\lambda)(V''-V'). \quad (3.21)$$

From (3.18) and (3.19) we infer that

$$V''[U'(\lambda)-1]=[U''(\lambda^*)-1]^\dagger V'. \quad (3.22)$$

Taking matrix elements as in (3.17), we have

$$(\Phi_b'',V''\Psi_a^{(+)\prime})-(\Psi_b^{(-)\prime\prime},V'\Phi_a')$$
$$=(\Phi_b'',[V''-V']\Phi_a')$$
$$=(\Phi_b'',[H_0'-H_0'']\Phi_a'), \quad (3.23)$$

where we have used (3.1), (3.2), and the analog of (3.8):

$$\Psi_b^{(\pm)\prime\prime}=U''(E_b''\pm i\epsilon)\Phi_b''. \quad (3.24)$$

We now wish to impose the condition that H_0' and H_0'' are Hermitian over the domain of states a and b. For the case to which we have restricted ourselves—where one particle is bound in Φ_a', and the other is bound in Φ_b''—the Hermitian condition is already satisfied. For other pairs of states, involving only continuum states of both particles, H_0' and H_0'' may be made Hermitian by the use of wave packets or an analytical equivalent.

Assuming, then, that the Hermitian condition holds, (3.23) is zero on the energy shell. That is, either of the two matrix elements on the left of (3.23) may be used[8] in computing $w_{ba}^{(r)}$:

$$(\Phi_b'',V''\Psi_a^{(+)\prime})=(\Psi_b^{(-)\prime\prime},V'\Phi_a'); E_b''=E_a'. \quad (3.25)$$

We also note from (3.23) that whenever (3.25) holds for the exact state vectors, it also holds in the Born approximation:

$$(\Phi_b'',V''\Phi_a')=(\Phi_b'',V'\Phi_a'); E_b''=E_a'. \quad (3.26)$$

Equations (3.23)–(3.26) confirm the remarks, made in the Introduction, regarding the "post-prior" discrepancy: If H_0' and H_0'' are both hermitian, the discrepancy vanishes when either the exact wave functions or their Born approximations are used in the matrix elements.

If we put $V'=V''=V$ in these equations, (3.25) reduces to (2.15) while (3.26) becomes an empty identity.

We turn now to the consideration of variational principles for rearrangement scattering. The first one, involving $G_0''(\lambda)$ only, is based on (3.20) and (3.10). These equations imply that

$$U(\lambda^*)^\dagger[V''-V''G_0''(\lambda)V'']U'(\lambda)-1]$$
$$=U''(\lambda^*)^\dagger V''G_0''(\lambda)V'$$
$$=V''[U'(\lambda)-1]. \quad (3.27)$$

It therefore follows that the expression

$$'F_1'=U''(\lambda^*)^\dagger V''G_0''(\lambda)V'+V''[U'(\lambda)-1]$$
$$-U''(\lambda^*)^\dagger[V''-V''G_0''(\lambda)V'']U'(\lambda)-1] \quad (3.28)$$

is stationary for arbitrary variations of $U''(\lambda)$ and $U'(\lambda)$ about the solutions of (3.20) and (3.10), respectively:

$$\delta'F_1'=\delta U''(\lambda^*)^\dagger V''\{G_0''(\lambda)V'$$
$$-[1-G_0''(\lambda)V'']U'(\lambda)-1]\}$$
$$+\{1-[1-G_0''(\lambda^*)V'']U''(\lambda^*)\}^\dagger$$
$$\times V''\delta[U'(\lambda)-1]. \quad (3.29)$$

The exact value of $'F_1'$ is given by either side of (3.22). This is the variational principle given by Borowitz and Friedman.[3] It is clearly unsymmetrical in the prime and double prime quantities.

[8] Equations (3.15) and (3.25) have previously been derived by M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 398 (1953).

A dissymmetrical variational principle may be derived from (3.28) by the transformations $'\leftrightarrow''$ and $\lambda\leftrightarrow\lambda^*$ followed by Hermitian conjugation:

$$'F_2'=V''G_0'(\lambda)V'U'(\lambda)+[U''(\lambda^*)-1]^\dagger V' -[U''(\lambda^*)-1]^\dagger[V'-V'G_0'(\lambda)V']U'(\lambda). \quad (3.30)$$

Equations (3.4) and (3.21) bear the same relation to (3.30) that (3.10) and (3.20) do to (3.28). That is, $'F_2'$ is stationary for independent variations of $U'(\lambda)$ and $U''(\lambda)$ about the solutions of (3.4) and (3.21). The stationary value of $'F_2'$ is the same as that of $'F_1'$, namely (3.22).

Since (3.4) is equivalent to (3.10), and (3.21) to (3.20), the independent variations of U' and U'' that leave $'F_1'$ stationary also leave $'F_2'$ stationary. We may therefore construct a symmetrical variational principle by averaging $'F_1'$ and $'F_2'$:

$$'F_3'=\tfrac{1}{2}['F_1'+'F_2'], \quad (3.31)$$

where the stationary value of $'F_3'$ is given by (3.22).

Another symmetrical variational principle, actually another form of $'F_3'$, is

$$2'F_4'=2U''(\lambda^*)^\dagger V'+2V''U'(\lambda)-U''(\lambda^*)^\dagger \times[1-V''G_0''(\lambda)][V''U'(\lambda)+(V'-V'')] -[U''(\lambda^*)^\dagger-(V'-V'')][1-G_0'(\lambda)V']U'(\lambda). \quad (3.32)$$

Vary U' and U'' independently; the result is

$$2\delta'F_4'=\delta U''(\lambda^*)^\dagger\{V'[1-(1-G_0'(\lambda)V'')U'(\lambda)]+V' -(1-V''G_0''(\lambda))[V''U'(\lambda)+(V'-V'')]\} +\{[1-(1-G_0''(\lambda^*)V'')U''(\lambda^*)]^\dagger V'' +V''-[U''(\lambda^*)^\dagger-(V'-V'')] \times(1-G_0'(\lambda)V')\}\delta U'(\lambda), \quad (3.33)$$

or, $'F_4'$ is stationary if U' and U'' are varied independently about the solutions of (3.4) and (3.20), provided that we also have

$$\begin{aligned} V'&=[1-V''G_0''(\lambda)][V''U'(\lambda)+(V'-V'')] \\ V''&=[U''(\lambda^*)^\dagger V'-(V'-V'')][1-G_0'(\lambda)V']. \end{aligned} \quad (3.34)$$

When (3.4) and (3.20) apply, however, the last two equations, if multiplied on the left by $U''(\lambda^*)^\dagger$ and on the right by $U'(\lambda)$, respectively, reduce to (3.22). The latter, of course, may be derived from (3.4) and (3.20). Therefore, $'F_4'$ is stationary for independent variations of U' and U'' about the solutions of (3.4) and (3.20).

Using (3.4) and (3.20), we find the exact value of $'F_4'$:

$$['F_4']_{\text{exact}}=\tfrac{1}{2}\{U''(\lambda^*)^\dagger V'+V''U'(\lambda)\}. \quad (3.35)$$

Or, according to (3.25), the matrix elements of $'F_4'$, formed by using the state vectors Φ_a' and Φ_b'', are precisely the matrix elements required in $w_{ba}^{(r)}$.

$'F_3'$ and $'F_4'$ are related by

$$'F_3'='F_4'-\tfrac{1}{2}(V'+V''). \quad (3.36)$$

If $V'=V''=V$, $'F_4'$ reduces directly to $'T(\lambda)'$, as given by (2.16), while $'F_1'$ and $'F_2'$ each become $'T(\lambda)'-V$.

ACKNOWLEDGMENTS

In developing the formalism presented here, we have benefited from discussions with S. Borowitz, N. Marcuvitz, and H. Moses. We have also found the methods used in the recent literature[8,9] very suggestive.

APPENDIX

The operator variational principle, (2.16), may be related to the more customary expressions as follows.

Taking matrix elements of (2.16) between two states, a and b, of equal energy, E, leads to (I-1.78):

$$'T_{ba}(E+i\epsilon)'=(\Psi_b^{(-)},V\Phi_a)+(\Phi_b,V\Psi_a^{(+)}) -(\Psi_b^{(-)},\{V-VG_0(E+i\epsilon)V\}\Psi_a^{(+)}). \quad (A\text{-}1)$$

This is the *bilinear* form of the Schwinger variational principle. Another form, which appears more frequently in the literature, is obtained by putting

$$\begin{aligned} \Psi_a^{(+)}&=A\Psi_a^{(+)'}, \\ \Psi_b^{(-)}&=B\Psi_b^{(-)'} \end{aligned} \quad (A\text{-}2)$$

in (A-1) and varying the amplitudes A and B, subject to the requirement that $'T'$ be stationary. This leads to the best choice of amplitudes for the wave functions:

$$\begin{aligned} A(\Psi_b^{(-)'},\{V-VG_0(E+i\epsilon)V\}\Psi_a^{(+)'}) &=(\Psi_b^{(-)'},V\Phi_a), \\ B(\Psi_b^{(-)'},\{V-VG_0(E+i\epsilon)V\}\Psi_a^{(+)'}) &=(\Phi_b,V\Psi_a^{(+)'}). \end{aligned} \quad (A\text{-}3)$$

Using (A-2) and (A-3) in (A-1), and dropping primes, produces the *fractional* form of the Schwinger variational principle:

$$'T_{ba}(E+i\epsilon)'=\frac{(\Psi_b^{(-)},V\Phi_a)(\Phi_b,V\Psi_a^{(+)})}{(\Psi_b^{(-)},\{V-VG_0(E+i\epsilon)V\}\Psi_a^{(+)})}. \quad (A\text{-}4)$$

Thus, the fractional form, (A-4), is independent of the amplitudes of the wave functions because the amplitudes have been adjusted to their most favorable values, (A-3).

For numerical calculations, the fractional form is preferable, since it is unaffected by the normalization of the trial functions. For theoretical discussions, the bilinear form is usually more convenient, since the functional dependence on the quantities of interest, trial functions, potential, etc., is simpler.

[9] G. F. Chew and M. L. Goldberger, Phys. Rev. **87**, 778 (1952); K. M. Watson, Phys. Rev. **89**, 575 (1953).