

# Schwinger variational principle

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The application of Schwinger's variational principle to problems involving discrete and continuous spectra, and also nonstationary problems, is considered. The results of numerical calculations are presented, and these suggest that the approach to few-body problems based on this principle is universal and effective.

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## INTRODUCTION

The majority of variational calculations contain a fortuitous element—the choice of the trial function. The situation is more favorable if the calculation employs an expansion with respect to a complete system of functions and one succeeds in observing practical convergence.

For the Schwinger variational principles considered here, one can give a criterion of accuracy for not only stationary quantities but also for the wave function, i.e., essentially this provides a dynamical approach. By Schwinger variational principles (SVPs) we shall in what follows mean stationary expressions for the corresponding quantities obtained by approximating the interaction or part of it by a finite-rank operator and then solving exactly the dynamical equations.

Since the entire treatment is based on the equivalence of the Schwinger variational principle and the method of separable representation of the potential, we briefly describe this method.

We consider the symbolic identity

$$V = VV^{-1}V = \sum_{ij} V|i\rangle \langle i|V^{-1}|j\rangle \langle j|V, \quad (1)$$

where  $V$  is the potential;  $|i\rangle$  and  $|j\rangle$  are in general different complete sets. Truncating in (1) the summation over the complete sets we obtain the separable approximation<sup>[1-3]</sup>

$$V^{(N)} = \sum_{i,j=1}^N V|\eta_i\rangle d_{ij}^{(N)} \langle \chi_j|V; \quad [d^{-1}]_{ij} = \langle \chi_i|V|\eta_j\rangle. \quad (2)$$

In reality, Eq. (2) represents an interpolation process since  $V^{(N)}|\eta_i\rangle = V|\eta_i\rangle$ ,  $\langle \chi_i|V^{(N)} = \langle \chi_i|V$ . One can show<sup>[3]</sup> that the well known Bubnov-Galerkin,<sup>[4]</sup> Hilbert-Schmidt,<sup>[5]</sup> and Bateman<sup>[6]</sup> methods are special cases of the expansion (2) for appropriate choice of the functions  $|\eta\rangle$  and  $|\chi\rangle$ . The approximation (2) is intimately related to Weinstein's method of intermediate problems in the formulation of Bazley and Fox.<sup>[7]</sup>

In the literature, two forms of Schwinger functional are given:

$$f_I(k, k') = -(1/2\pi) \langle k'|V|\chi_k^{(+)} \rangle \times \langle \chi_{k'}^{(-)}|V|k\rangle / \langle \chi_{k'}^{(-)}|V - VG_0V|\chi_k^{(+)} \rangle; \quad (3)$$

$$f_{II}(k, k') = -(1/2\pi) \langle k'|V|\eta_k^{(+)} \rangle + \langle \eta_{k'}^{(-)}|V|k\rangle - \langle \eta_{k'}^{(-)}|V - VG_0V|\eta_k^{(+)} \rangle, \quad (4)$$

where  $|\chi^{(+)}\rangle$ ,  $|\eta^{(+)}\rangle$  are trial functions and  $G_0$  is the free Green's function.

The functional (3) is obtained from (4) by a definite choice of  $|\eta^{(+)}\rangle$ . We set  $|\eta_k^{(+)}\rangle = c^{(+)}|\chi_k^{(+)}\rangle$ ,  $|\eta_{k'}^{(-)}\rangle = c^{(-)}|\chi_{k'}^{(-)}\rangle$ , and determine the coefficients  $c^{(\pm)}$  from the equations  $\partial f_{II}/\partial c^{(\pm)} = \partial f_{II}/\partial c^{(\pm)*} = 0$ . In this case,  $f_{II} = f_I$ .

In what follows, we shall use the Schwinger variational principle in the formulation (3). The convergence of the expansion (2) is ensured by a well known theorem: If  $V$  is a completely continuous operator, it can be approximated arbitrarily accurately in the norm by an operator of finite rank  $V^{(N)}$ .

Thus, the problem is solved by replacing  $V$  by  $V^{(N)}$ , and  $|V - V^{(N)}|$  characterizes the error. In this sense, the separable representation method is close to Lanczos's<sup>[8]</sup>  $\tau$  process, which is based on a fairly simple idea. Usually, it is difficult to find the error of a numerical solution to a problem, but it is easy to say for which similar problem the calculated answer is an exact solution.

In the present paper, I summarize the results of the investigations that I have carried out using the Schwinger variational principle in the quantum-mechanical few-body problem.<sup>[8-17]</sup>

We consider the problem of a quantum particle passing through potential barriers. Schwinger variational principles are constructed for the coefficients of reflection and transmission. In the nuclear two-body problem, this method is applied to construction of the off-shell amplitudes. The equations of the coupled-channel method are investigated. It is shown that virtual transitions in the continuum can be taken into account. The iterative process to which the Schwinger variational principle leads is studied.

For potentials containing repulsion, it is not convenient to formulate the Schwinger variational principle in the form (3). This case is investigated in detail. Examples are found ( $pd\mu$  scattering) for which the Schwinger variational-iterational method converges, but not to the exact solution. It is shown how the principle must be generalized for such potentials. Scattering at high energies is considered. "Dual" amplitudes are constructed, these coinciding with the exact ones at high and low energies.

Particular interest attaches to bound-state problems since the Schwinger variational principle has not been widely used for them. In the paper, we consider the corrections to the main approximation of the method of  $K$  harmonics for the example of the nucleus  $^{16}\text{O}$ .

Nonstationary problems are investigated. In this case, the Schwinger variational principle can serve as the theoretical basis for constructing approximate methods that go beyond the framework of perturbation theory. Resonance scattering of ultracold neutrons is considered as an example.

Since the Schwinger variational principle is obtained in an exact solution of dynamical equations with an approximate potential, it is obvious that the solution, irrespective of the choice of the trial functions, will give a qualitatively correct description of the quantum-mechanical effects. It is also clear that of all variational principles the best is the one that depends least on the choice of the trial function. Compared with the variational principles of Kohn, Hulthén, and Ritz, the Schwinger variational principle has this property.

## 1. SCATTERING PROBLEMS

**One-Dimensional Problem. Passage through a Potential Barrier.** Suppose the potential  $V(x)$  is nonvanishing in the interval  $(a, b)$  and particles move from the left, so that the unperturbed wave function is  $\exp(ikx)$ . In the standard method, to find the coefficients of reflection  $R$  and transmission  $D$  one either approximates the potential barrier by rectangular potentials and fits the solutions obtained in each of the regions to the Schrödinger equation

$$d^2\psi(x)/dx^2 + [k^2 - V(x)]\psi(x) = 0, \quad (5)$$

or one uses the variable phase approach. However, for potentials of fairly complicated form, it is difficult to estimate the error if these approaches are used.

We rewrite (5) in the integral form

$$\begin{aligned} \psi(x) &= \exp(ikx) + \int_{-\infty}^{+\infty} G(x, x') V(x') \psi(x') dx'; \\ G(x, x') &= (1/2ik) \exp(ik|x - x'|). \end{aligned} \quad (6)$$

Consequently,

$$\begin{aligned} \psi(x) &= \exp(ikx) + \exp(-ikx) \frac{1}{2ik} \int_{-\infty}^{+\infty} \exp(ikx') V(x') \psi(x') dx'; \\ \psi(x) &= \exp(ikx) + \exp(ikx) \frac{1}{2ik} \int_{-\infty}^{+\infty} \exp(-ikx') V(x') \psi(x') dx', \end{aligned}$$

i.e., the coefficients of reflection and transmission are determined by the equations

$$\left. \begin{aligned} R &= |f_r|^2; \quad f_r = \frac{1}{2ik} \int_{-\infty}^{+\infty} \exp(ikx') V(x') \psi(x') dx'; \\ D &= |f_d|^2; \quad f_d = 1 + \frac{1}{2ik} \int_{-\infty}^{+\infty} \exp(-ikx') V(x') \psi(x') dx', \end{aligned} \right\} \quad (7)$$

where  $f_r$  and  $f_d$  are the amplitudes of the reflected wave and the transmitted wave, respectively.

We introduce

$$\psi_k^{(1)}(x) = \exp(ik'x) + \int_{-\infty}^{+\infty} G^*(x, x') V(x') \psi_k^{(1)}(x') dx'. \quad (8)$$

In (2), we set  $N = 1$ . With the potential

$$(V^{(1)}\psi)(x) = V(x) \eta(x) \int_{-\infty}^{+\infty} \chi^*(x') V(x') \psi(x') dx' / \int_{-\infty}^{+\infty} \chi^*(y) V(y) \eta(y) dy,$$

Eq. (6) can be solved explicitly:

$$\left. \begin{aligned} \psi^{(1)}(x) &= \exp(ikx) + \int_{-\infty}^{+\infty} G(x, x') V(x') \eta(x') dx' \cdot C; \\ C &= \int_{-\infty}^{+\infty} \chi^*(x) V(x) \exp(ikx) dx / \left[ \int_{-\infty}^{+\infty} \chi^*(x') V(x') \eta(x') dx' - \int_{-\infty}^{+\infty} dx' \int_{-\infty}^{+\infty} dy \chi^*(x') V(x') G(x', y) \eta(y) V(y) \right]; \\ f_r^{(1)} &= \frac{1}{2ik} \int_{-\infty}^{+\infty} \exp(ikx) V(x) \eta(x) dx \cdot C; \\ f_d^{(1)} &= 1 + \frac{1}{2ik} \int_{-\infty}^{+\infty} \exp(-ikx) V(x) \eta(x) dx \cdot C. \end{aligned} \right\} \quad (9)$$

It is easy to show that if  $\eta = \psi + \delta\psi$ ; and  $\chi = \psi_k + \delta\psi$  then

$$f_r^{(1)} = f_r + O[(\delta\psi)^2],$$

and if

$$\eta = \psi + \delta\psi, \quad \chi = \psi_k + \delta\psi,$$

then

$$f_d^{(1)} = f_d + O[(\delta\psi)^2].$$

Similarly, one can consider an  $N$ -term factorization. As an example, let us consider reflection from the  $\delta$ -functional potential  $\alpha\delta(x)$ :

$$f_r^{(1)} = \alpha/(2ik - \alpha); \quad f_d^{(1)} = 2ik/(2ik - \alpha).$$

We see that the result agrees with the exact solution, and the dependence on the trial functions has disappeared. This is not fortuitous since the  $\delta$ -functional potential is a first-rank operator, i.e.,  $V^{(1)} = V$ . Choosing  $\eta = \chi = \exp(ikx)$ , we obtain the analog of the Born approximation:

$$\begin{aligned} f_d^{(1)} &= 1 + \frac{1}{2ik} \\ &\quad \times \frac{\left( \int_{-\infty}^{+\infty} V(x) dx \right)^2}{\int_{-\infty}^{+\infty} V(x) dx - \frac{1}{2ik} \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \exp(-ikx) V(x) \exp(ik|x-y|) V(y) \exp(iky)}. \end{aligned}$$

**Partial-Wave Two-Body Problem.** In (2) we set  $N = 1$  and  $|\eta\rangle = |\chi\rangle = |\eta_1\rangle$ ; then

$$V^{(1)} = V |\eta_1\rangle \langle \eta_1| / V |\eta_1\rangle \langle \eta_1|. \quad (10)$$

With the potential (10), the equation

$$\psi_l(r) = f_l(kr) + \int_0^\infty G_l(r, r', E) V(r') \psi_l(r') dr' \quad (11)$$

can be solved explicitly, and for the phase shift we obtain the expression

$$\text{tg } \delta_l^{(1)} = (1/k) \langle \eta_1 | V | \eta_1 \rangle / \langle \eta_1 | V - V G_l V | \eta_1 \rangle, \quad (12)$$

which coincides with the Schwinger variational functional. In the case of  $N$ -term separation  $|\eta_i\rangle = |\chi_i\rangle = |\eta_i^1\rangle$ , Eq. (11) can also be solved\*:

$$\begin{aligned} \text{tg } \delta_l^{(N)} &= -\frac{1}{k} \sum_{i,j=1}^N \langle \eta_i | V | \eta_j^1 \rangle C_{ij}^{(N)} \langle \eta_j | V | \eta_i^1 \rangle; \\ \{C^{-1}\}_{ij} &= \langle \eta_i^1 | V - V G_l V | \eta_j^1 \rangle. \end{aligned} \quad (13)$$

We show that (13) is the Schwinger variational functional. To prove this, we choose the trial function in (10) in the form

$$|\eta_i\rangle = \sum_{j=1}^N c_j |\eta_j^1\rangle. \quad (14)$$

\*The Russian notation for the trigonometric functions (tg, ctg, etc.) is retained in the displayed equations.

Substituting (14) in (12) and determining the coefficients  $c_i$  from the stationarity condition (12),

$$\partial \text{tg} \delta_l^{(N)} / \partial c_i = 0, \quad (15)$$

we obtain (13).

We turn to the construction of a variational principle for the off-shell amplitudes. The Lippmann-Schwinger equation for the off-shell wave function has the form

$$|\psi_l(q, E)\rangle = |q\rangle + G_l(E) V |\psi_l(q, E)\rangle. \quad (16)$$

Here  $|q\rangle \equiv j_l(qr); \langle r' | G_l(E) | r \rangle = G_l(r, r', E)$ . Using the solution (16), we can readily obtain an expression for the  $t$  matrix:

$$\begin{aligned} \langle k | t_l(E) | k' \rangle &= -(1/k) \langle k | V | \psi_l(k', E) \rangle; \\ \langle k | t_l(k^2/2\mu) | k \rangle &= \text{tg} \delta_l. \end{aligned}$$

In (2) we set  $N=1$  and  $|\eta\rangle = |\eta_l(k')\rangle$ ,  $|\chi\rangle = |\eta_l(k)\rangle$ . Then Eq. (16) can be solved as follows:

$$\begin{aligned} |\psi_l^{(1)}(k', E)\rangle &= |k'\rangle + G_l(E) V |\eta_l(k')\rangle \\ \times \langle \eta_l(k) | V | k' \rangle / \langle \eta_l(k) | V - V G_l V | \eta_l(k') \rangle, \end{aligned}$$

and for the  $t$  matrix we obtain the functional

$$\begin{aligned} \langle k | t_l^{(1)}(E) | k' \rangle &= -\frac{1}{k} \langle k | V^{(1)} | \psi_l^{(1)}(k', E) \rangle \\ &= -\langle k | V | \eta_l(k') \rangle \langle \eta_l(k) | V | k' \rangle / \langle \eta_l(k) | V - V G_l(E) V | \eta_l(k') \rangle, \end{aligned}$$

which is stationary with respect to variations of first order:

$$\begin{aligned} |\eta_l(k)\rangle &= |\psi_l(k, E)\rangle + |\delta\psi_l(k, E)\rangle; \\ |\eta_l(k')\rangle &= |\psi_l(k', E)\rangle + |\delta\psi_l(k', E)\rangle. \end{aligned}$$

An  $N$ -term separation can be considered in the same way as (13).

**Three-Dimensional Two-Body Problem.** In (2), we set

$$|\eta_i\rangle = |\chi_k^{(+)}\rangle, \quad |\chi_i\rangle = |\chi_k^{(-)}\rangle. \quad (17)$$

Substituting (17) in the equation

$$|\psi_k^{(\pm)}\rangle = |k\rangle + G_0^{(\pm)} V |\psi_k^{(\pm)}\rangle,$$

we obtain for the amplitude the expression

$$\begin{aligned} f^{(N)}(k, k') &= -\frac{1}{2\pi} \sum_{i,j=1}^N \langle k' | V | \chi_k^{(+)} \rangle C_{ij}^{(N)} \langle \chi_k^{(+)} | V | k \rangle; \\ [C^{-1}]_{ij} &= \langle \chi_k^{(-)} | V - V G_0^{(+)} V | \chi_k^{(+)} \rangle. \end{aligned} \quad (18)$$

For  $N=1$ , Eq. (18) reduces to a variational principle for the scattering amplitude, and therefore (18) is stationary with respect to first-order variations with respect to each trial function  $|\chi^{\pm}\rangle$ . Indeed, if

$$\begin{aligned} |\chi_k^{m(-)}\rangle &= |\psi_k^{(-)}\rangle + |\delta\psi_k^{(-)}\rangle, \\ |\chi_k^{n(+)}\rangle &= |\psi_k^{(+)}\rangle + |\delta\psi_k^{(+)}\rangle, \end{aligned}$$

then

$$f^{(N)}(k, k') = f(k, k') - \frac{1}{2\pi} \langle \delta\psi_k^{(-)} | W - W^{(N)} | \delta\psi_k^{(+)} \rangle; \quad W = V - V G_0 V.$$

Note that, in contrast to the partial-wave problem, even a short-range potential is not in the general case a completely continuous operator if, for example,  $V$  is a local operator. However,  $f^{(N)}$  converges to  $f$  since  $G_0 V$  for short-range potentials is a completely continuous operator.

We now point out a very important property of the Schwinger variational principle.<sup>[8]</sup>

We consider the case when the specified potential is already an operator of finite rank  $N$ , which can always be represented in the form

$$V = \sum_{i,j=1}^N A |z_i\rangle d_{ij}^{(N)} \langle y_j| A; \quad [d^{-1}]_{ij} = \langle y_i | A | z_j \rangle. \quad (19)$$

We replace  $V$  by  $V^{(N)}$  in accordance with Eq. (2):

$$\begin{aligned} V^{(N)} &= \sum_{\alpha, \beta=1}^N V | \eta_{\alpha} \rangle D_{\alpha\beta}^{(N)} \langle \chi_{\beta} | V; \\ [D^{-1}]_{\alpha\beta} &= \langle \chi_{\alpha} | V | \eta_{\beta} \rangle. \end{aligned} \quad (20)$$

Substituting (19) in (20), we readily see that

$$V^{(N)} \equiv V. \quad (21)$$

Therefore, if the original potential is an operator of finite rank  $N$ , the variational principle based on the Schwinger functional for a trial function of the form

$$\psi = \sum_{i=1}^N c_i \psi_i$$

leads to the exact solution for all  $\psi_i$  for the variational choice of  $c_i$ .

**Many-Channel Theory.** We now turn to the system of integral equations of the coupled-channel method:

$$|\psi_k^{(\pm)}\rangle = |\varphi_{k_v}\rangle + \sum_{\mu} G_{0v}^{(\pm)} V_{v\mu} |\psi_{k_{\mu}}^{(\pm)}\rangle, \quad (22)$$

where  $|\varphi_{k_v}\rangle$  is a plane wave in the ingoing channel. Since

$$(V\psi)_v = \sum_{\mu} V_{v\mu} \psi_{k_{\mu}},$$

Eq. (2) takes the form

$$\begin{aligned} (V^{(N)}\psi)_v &= \sum_{i,j=1}^N \sum_{\mu, l, n} V_{v\mu} |\eta_{\mu}^i\rangle d_{ij}^{(N)} \langle \chi_l^j | V_{ln} | \psi_{k_n} \rangle; \\ [d^{-1}]_{ij} &= \sum_{\mu} \langle \chi_l^i | V_{\mu\mu} | \eta_{\mu}^j \rangle. \end{aligned} \quad (23)$$

Substituting (23) in (22), we obtain, for example, for the elastic scattering amplitude the expression<sup>1)</sup>

$$\begin{aligned} f^{(N)} &= -\frac{1}{2\pi} \sum_{i,j=1}^N \sum_{m, l, l'} \langle k_i | V_{im} | \eta_m^i \rangle C_{ij}^{(N)} \langle \chi_l^j | V_{ll'} | \varphi_{k_{l'}} \rangle; \\ [C^{-1}]_{ij} &= \sum_{l, l'} \langle \chi_l^i | V_{ll'} - V_{ll'} G_{0l} V_{l'l} | \eta_{l'}^j \rangle. \end{aligned} \quad (24)$$

As in the case of the two-body problem, one can show that (24) is equivalent to the Schwinger variational principle. Suppose that

$$\eta_m^i = \psi_{k_m}^{(+)} + \delta\psi_{k_m}^{(+)}, \quad \chi_m^j = \psi_{k_m}^{(-)} + \delta\psi_{k_m}^{(-)};$$

then<sup>[8]</sup>

$$f^{(N)}(k, k') = f(k, k') - \frac{1}{2\pi} \sum_{\mu, \nu} \langle \delta\psi_{k_{\mu}}^{(-)} | (W_{\mu\nu} - W_{\mu\nu}^{(N)}) | \delta\psi_{k_{\nu}}^{(+)} \rangle, \quad (25)$$

where

$$W_{\mu\nu} = V_{\mu\nu} - \sum_l V_{\mu l} G_{0l}^{(+)} V_{l\nu}.$$

As in the two-body problem, the variational principle (24) can be obtained from the variational functional

<sup>1)</sup>The summation over  $m, l, l'$  includes integration over the continuum.



$$f^{(1)}(k, k') = -\frac{1}{2\pi} \sum_{l', ml} \langle k' | V_{lm} | \eta_m \rangle$$

$$\times \langle \chi_l | V_{ll'} | \varphi_{kl'} \rangle / \sum_{n, \mu, n'} \langle \chi_n | V_{nn} - V_{nn} G_{0n}^{(+)} V_{nn'} | \eta_{\mu} \rangle$$

for trial functions of the form

$$\eta_m = \sum_{i=1}^N b_i \eta_m^i; \quad \chi_i = \sum_{i=1}^N a_i \chi_i^i,$$

if  $b_i$  and  $a_i$  are chosen on the basis of the condition

$$\partial f^{(1)} / \partial b_i = \partial f^{(1)} / \partial a_i = 0.$$

If the interaction matrix  $V_{ij}$  is an operator of finite rank:

$$\left. \begin{aligned} V_{ij} &= \sum_{\alpha, \beta=1}^N \sum_{n, l} A_{ln} | z_n^\alpha \rangle d_{\beta\alpha}^{(N)} \langle y_l^\alpha | A_{lj}; \\ [d^{-1}]_{\alpha\beta} &= \sum_{i,j} \langle y_l^\alpha | A_{ij} | z_j^\beta \rangle, \end{aligned} \right\} \quad (26)$$

then, replacing  $V$  by  $V^{(N)}$ , we readily find on the basis of Eqs. (23) that  $V^{(N)} = V$ , i.e., in this case the variational principle obtained by an  $N$ -term separable representation leads to the exact value of the amplitude.

Let us consider in more detail the possibility of approximating  $V_{ij}$  by an operator of finite rank  $V_{ij}^{(N)}$  in many-channel theory. For simplicity, we consider a characteristic case of the three-body problem, namely, elastic scattering of particle 1 on a bound state of particles 2 and 3. Then

$$V_{ij}(\rho) = \int \psi_i^*(r_{23}) V(r_{23}, \rho) \psi_j(r_{23}) dr_{23}, \quad (27)$$

where

$$V(r_{23}, \rho) = V_{12} \left( \left| \rho - \frac{m_3}{m_2 + m_3} r_{23} \right| \right) + V_{31} \left( \left| \rho + \frac{m_2}{m_2 + m_3} r_{23} \right| \right).$$

We show that the approximation (23) is obtained by replacing  $V(r_{23}, \rho)$  by an operator of finite rank  $V^{(N)}(r_{23}, \rho)$  in accordance with formula (2):

$$V^{(N)} = \sum_{i,j=1}^N V | \eta_i \rangle d_{ij}^{(N)} \langle \eta_j | V;$$

$$[d^{-1}]_{ij} = \int \chi_i^*(r_{23}, \rho) V(r_{23}, \rho) \eta_j(r_{23}, \rho) dr_{23} d\rho.$$

We expand  $\chi$  and  $\eta$  with respect to the system of functions  $\psi_i(r_{23})$ :

$$\chi_i(r_{23}, \rho) = \sum_{\mu} \chi_{\mu}^i(\rho) \psi_{\mu}(r_{23}); \quad \eta_i(r_{23}, \rho) = \sum_{\mu} \eta_{\mu}^i(\rho) \psi_{\mu}(r_{23}).$$

Then

$$[d^{-1}]_{ij} = \sum_{\mu\nu} \int \chi_{\mu}^{i*}(\rho) V_{\mu\nu}(\rho) \eta_{\nu}^j(\rho) d\rho = \sum_{\mu\nu} \langle \chi_{\mu}^i | V_{\mu\nu} | \eta_{\nu}^j \rangle$$

and

$$\int \psi_i^*(r_{23}) V^{(N)}(r_{23}, \rho) \psi_j(r_{23}) dr_{23} = \sum_{m, n=1}^N \sum_{l, l'} V_{il'm} | \eta_{\mu}^m \rangle d_{mn}^{(N)} \langle \chi_{l'}^n | V_{lj},$$

i.e., we obtain exactly the expression (23).

It is, however, known that even after separation of the angular momentum  $V(r_{23}, \rho)$  is not a completely continuous operator, and therefore (23) is a formal equation. And therefore the Schwinger variational principle for many-channel problems is not a dynamical approach since one cannot invoke the smallness of  $|V - V^{(N)}|$ ; it would therefore seem that in this case the Schwinger variational principle has no real advantages over the expressions of Kohn and Hulthén. We show that in a

number of cases this is not so. In many problems, a good approximation is obtained by ignoring the strong coupling  $V_{\nu\mu}$  of the channels, and then both  $|\nu\rangle$  and  $|\mu\rangle$  correspond to the continuum.<sup>[18]</sup> If such an approximation is made, then the integration in (27) over  $r_{23}$  will be within finite limits, and  $V(r_{23}, \rho)$  can be replaced by the completely continuous operator  $V(r_{23}, \rho)\theta(R - r_{23})$ . It is clear that in the framework of this approximation one can describe not only elastic scattering but also disintegration processes. Thus, the Schwinger variational principle gives one the possibility of taking into account virtual transitions in the continuum.

**Variational-Iterational Method.** To solve quantum-mechanical problems, one very frequently uses an iterative method. The variational-iterational technique that we consider in the present subsection leads to not only a systematic improvement of the trial function but also to the possibility of estimating the error at each step.

The variational-iterational Schwinger method is based on integral equations for the wave function. In the partial-wave two-body problem, this method for the phase shift is formulated as follows<sup>[25]</sup>:

$$\left. \begin{aligned} |\psi_i^{(N+1)}\rangle &= \bar{G}_i^{(N)} V |\psi_i^{(N)}\rangle; \\ \bar{G}_i^{(N)}(r, r') &= G_i(r, r') - j_i(kr) j_i(kr') / k \operatorname{tg} \delta_i^{(N)}; \\ G_i(r, r') &= \begin{cases} k^{-1} j_i(kr) n_i(kr'), & r \leq r'; \\ k^{-1} n_i(kr) j_i(kr'), & r' \leq r; \end{cases} \\ \operatorname{tg} \delta_i^{(N)} &= -k^{-1} \langle j_i | V | \psi_i^{(N)} \rangle^2 \langle \psi_i^{(N)} | V - V G_i V | \psi_i^{(N)} \rangle, \end{aligned} \right\} \quad (28)$$

where  $|\psi_i^{(N)}\rangle$  is the trial wave function in the  $N$ -th iteration;  $V$  is the operator of the potential;  $j_i$  and  $n_i$  are Riccati-Bessel functions;  $k$  is the wave vector of the scattered particle; and  $\sigma_i^{(N)}$  is the phase shift in the  $N$ -th iteration.

In Ref. 19, an iteration-separation method was proposed. The essence of this method consists of replacing the exact operator of the potential  $V$  by a separable operator of first rank:

$$V^{(1)} = V | \varphi_i^{(0)} \rangle \langle \varphi_i^{(0)} | V / \langle \varphi_i^{(0)} | V | \varphi_i^{(0)} \rangle, \quad (29)$$

some approximate solution of Eq. (11) being chosen as the initial trial function  $|\varphi_i^{(0)}\rangle$ . With the potential (29), Eq. (11) is solved explicitly and the wave function  $|\varphi_i^{(1)}\rangle$  of the first approximation is found; this is then used as one of the functions in (29), etc. Thus, replacing  $V$  in (11) by the separable potential of the  $N$ -th approximation:

$$V^{(1)} = V | \varphi_i^{(N)} \rangle \langle \varphi_i^{(N)} | V / \langle \varphi_i^{(N)} | V | \varphi_i^{(N)} \rangle, \quad (30)$$

we obtain

$$|\varphi_i^{(N+1)}\rangle = |j_i\rangle + G_i V | \varphi_i^{(N)} \rangle C^{(N)}(k), \quad (31)$$

where

$$C^{(N)}(k) = \langle \varphi_i^{(N)} | V | \varphi_i^{(N+1)} \rangle / \langle \varphi_i^{(N)} | V | \varphi_i^{(N)} \rangle. \quad (32)$$

Substituting (31) in (32), we obtain an expression for  $C^{(N)}(k)$  in terms of functions of only the  $N$ -th iteration:

$$C^{(N)}(k) = \langle j_i | \bar{V} | \varphi_i^{(N)} \rangle / \langle \varphi_i^{(N)} | V - V G_i V | \varphi_i^{(N)} \rangle. \quad (33)$$

The phase shift in this method for the  $N$ -th iteration is also obtained by replacing the exact potential  $V$  by the

separable representation (30):

$$\text{tg } \delta_l^{(N)} = -k^{-1} \langle j_l | V | \varphi_l^{(N)} \rangle C^{(N)}. \quad (34)$$

In the construction by this method of (31) and (33) it was assumed that the following condition is satisfied at each step of the iteration:

$$\langle \varphi_l^{(N)} | V | \varphi_l^{(N)} \rangle \neq 0. \quad (35)$$

For potentials of fixed sign, this condition is always satisfied.

Despite the apparent difference in construction of this method and the variational-iterational Schwinger method, they lead to identical expressions for the phase shifts, as can be seen by comparing (28) and (34). Although the phase shifts at each iterative step are equal in the two methods, the wave functions  $|\varphi_l^{(N)}\rangle$  (31) and  $|\psi_l^{(N)}\rangle$  (28) differ, if  $|\varphi_l^{(0)}\rangle = |\psi_l\rangle$ , by a coefficient:

$$|\psi_l^{(N)}\rangle = [C^{(0)} C^{(1)} \dots C^{(N-1)}]^{-1} |\varphi_l^{(N)}\rangle.$$

One can show that

$$\text{tg } \delta_l - \text{tg } \delta_l^{(N)} \sim |C^{(N)} - 1|^2,$$

if  $|C^{(N)} - 1| \ll 1$ . This makes it possible to estimate the error of the results at each step.

It is easy to show that if the iteration-separation method converges, the series  $C_k^{(N)}$  must tend to unity:

$$\lim_{N \rightarrow \infty} C^{(N)}(k) = 1. \quad (36)$$

In its turn, the expression (36) is a necessary condition for convergence of the iteration-separation method. If the condition (36) is satisfied, then the integral equations for the function (31)

$$|\varphi_l\rangle = \lim_{N \rightarrow \infty} |\varphi_l^{(N)}\rangle$$

and the exact wave function  $|\psi_l\rangle$  (11) coincide. Thus, the iteration-separation method leads to a convergent procedure not only for the phase shifts, like the variational-iterational Schwinger method, but also for the wave functions, the phase shifts being determined, naturally, at each iteration step from the asymptotic behavior of the wave functions.

If the condition (35) for constructing the iteration-separation method is not satisfied and in the limit  $N \rightarrow \infty$  we have

$$\lim_{N \rightarrow \infty} \langle \varphi_l^{(N)} | V | \varphi_l^{(N)} \rangle = 0, \quad (37)$$

then for the exact wave function

$$\langle \psi_l | V | \psi_l \rangle \neq 0,$$

and in this case the relation (36) cannot be proved and the iteration-separation method may not converge. Moreover, the philosophy of the method is from the very start inapplicable.

Thus, from the convergence of the variational-iterational Schwinger method under the condition (37) it does not yet follow that the method converges to the exact phase shift. However, it should be pointed out that in the case of (37) it is in principle possible that the condition (36) is satisfied and then the variational-iterational Schwinger method will converge to the exact

solution (this is possible if  $\langle \psi_l | V | \psi_l \rangle = 0$ ).

As an illustration of the iteration-separation method for many-channel problems, let us consider the elastic scattering of the positron on the hydrogen atom and of the proton on the deuterium mesic atom<sup>[14]</sup>:

$$e^+ + H \rightarrow e^+ + H; \quad p + d\mu \rightarrow p + d\mu.$$

For these processes, the iteration-separation method in the case of zero total angular momentum of the system of particles is constructed as follows:

$$\left. \begin{aligned} |\varphi_{nl}^{(N+1)}\rangle &= j_0(k_n r) \delta_{n,1} \delta_{l,0} + \sum_{n', l'} G_{nl} V_{nl, n'l'} |\varphi_{n'l'}^{(N)}\rangle C^{(N)}(k_l); \\ C^{(N)}(k_l) &= \sum_{nl} \langle j_0 | V_{10nl} | \varphi_{nl}^{(N)} \rangle / \left\{ \sum_{n, l, n', l'} \langle \varphi_{nl}^{(N)} | V_{nl, n'l'} \right. \\ &\quad \left. - V_{nl, n'l'} G_{n'l'} V_{n'l', n''l''} | \varphi_{n''l''}^{(N)} \rangle \right\}; \end{aligned} \right\} \quad (38)$$

$$\text{tg } \delta_0^{(N)} = \sum_{nl} \langle k_l | j_0 | V_{10, nl} | \varphi_{nl}^{(N)} \rangle C^{(N)}(k_l), \quad (39)$$

where  $n$  and  $l$  are the quantum numbers characterizing the states of the hydrogen atom (mesic atom);  $k_n$  is the wave vector of the scattered particle in channel  $n$ . The variational-iterational Schwinger method gives an expression for the phase shift that agrees with (39).

A necessary condition of convergence of the iteration-separation method (38) for many-channel problems coincides with (36); one cannot construct (38) if a condition of the type (37) holds:

$$\lim_{N \rightarrow \infty} \sum_{nl, n'l'} \langle \varphi_{nl}^{(N)} | V_{nl, n'l'} | \varphi_{n'l'}^{(N)} \rangle = 0. \quad (40)$$

In this case, one may have a pathological convergence of the variational-iterational Schwinger method to a result which is not the exact phase shift if the condition (36) is not satisfied.

For convergence of the variational-iterational Schwinger method with accuracy governed by the accuracy with which the integrals in (39) are calculated, between three and 10 iterations were made. The results of the calculations showed that if the condition (40) is indeed satisfied (with the necessary accuracy) the necessary condition of convergence (36) of the iteration-separation method is not satisfied and there is pathological convergence of the variational-iterational Schwinger method. But if (40) is not satisfied, then the series  $C^{(N)}(k_l)$  tends to unity, the iteration-separation method converges, and correct convergence is also observed for the other method.

As zeroth approximations, we chose

$$|\varphi_{nl}^0\rangle = |j_0\rangle \delta_{n1} \delta_{l0} \quad (41)$$

and as the set of wave functions of the hydrogen atom (mesic atom) for the discrete spectrum

$$|\varphi_{nl}^0\rangle = |\psi_{nl}\rangle. \quad (42)$$

In the cases when pathological convergence of the variational-iterational Schwinger method was observed (the condition (36) was not satisfied) the series of  $C^{(N)}$  and  $\tan \delta_0^{(N)}$  values converged to quantities that did not change on the transition from the initial approximation (41) to (42). This shows that both the initial approximations in these cases are far from the exact wave function. We now show that if  $|\varphi_{nl}^0\rangle$  is chosen sufficiently close to the exact function the iteration-separation method ensures convergence of our iteration function

TABLE I.

E, eV	Channels allowed for	Total number of channels	C	$\tan \delta_0$ or scattering length	Type of process
0.000	$l=0; n=1,2$	2	1	0.562 (0.564)	$e^+H$
0.000	$l=0.1; (l+1) \leq n < 2$	3	0.373	0.1717	
0.544	$l=0.1; (l+1) \leq n < 2$	3	0.641	-0.0533 (-0.0426)	
2.476		3	0.908	-0.0584 (-0.1472)	
4.898		3	0.978	-0.2462 (-0.2460)	
4.898	$l=0.1; (l+1) \leq n \leq 3$	5	0.965	-0.231	$pd\mu$
4.898	$l=0.1; (l+1) \leq n \leq 6$	11	0.943	-0.218	
0.000	$l=0.1; (l+1) \leq n \leq 2$	3	0.145	0.339	
0.000		3	0.238	-0.0726	
10.000		3	0.238	-0.0726	

Note. In the table, the phase shifts and scattering lengths for  $e^+H$  and  $pd\mu$  elastic scattering are given in the atomic system of units for different energies and with allowance for different numbers of closed channels calculated in the variational-iterational Schwinger method. The values obtained by numerical integration of the corresponding system of coupled-channel equations<sup>20</sup> are given in brackets.

$\langle \varphi_{nl}^{(N)} \rangle$  to the exact function.

With allowance for a small number of closed channels (1S-2S), the initial approximation (41) is evidently fairly close to the exact wave function, so that the condition (36) is satisfied and the variational-iterational Schwinger method converges to the exact solution. If the number of closed channels is increased (1S-2S-2P), the approximation (41) is already so bad that the variational-iterational Schwinger method gives only pathological convergence when

$$\lim_{N \rightarrow \infty} C^{(N)} \neq 1.$$

It follows from physical considerations that when the energy of the scattered particles is increased the approximation (41) for (1S-2S-2P) may again become a sufficiently good initial approximation to ensure convergence of the variational-iterational Schwinger method to the exact phase shift (this can be seen in Table I). Therefore, if there is a large number of closed channels and the energies are sufficiently low both the initial approximations (41) and (42) are sufficiently bad for the variational-iterational Schwinger method not to converge to the exact phase shift. It can be seen from Table I that even in these cases the phase shifts and scattering lengths of the variational-iterational Schwinger method (39) differ from the exact results<sup>[20]</sup> by not more than 25%.

Thus, in the case of many-channel scattering the actual convergence of the variational-iterational Schwinger method does not yet mean that exact results have been obtained if the necessary condition (36) for convergence of the iteration-separation method is not satisfied; such a situation is realized in the case of  $e^+H$  and  $pd\mu$  elastic scattering with allowance for a finite number of closed channels.

**Potentials Containing Repulsion.** Hitherto, we have not considered the following question: Are all the Schwinger variational principles obtained for the approximation (2)? It is obvious that in the case of the finite-dimensional approximation  $V^{(N)}$  a variational principle is obtained if for at least one trial function the

following relation is satisfied:

$$V^{(N)}|\varphi\rangle = V|\varphi\rangle; \quad \langle\varphi|V^{(N)} = \langle\varphi|V. \quad (43)$$

In this sense, the Schwinger variational principles obtained on the basis of (2) are optimal since (43) is satisfied for the maximal number of trial functions, which is equal to  $N$ . However, in a number of cases it is also necessary to consider other possibilities.

We have seen that if the potential  $V$  is not an operator of fixed sign, then the convergence of the variational-iterational Schwinger method may be pathological. This is because  $\langle\varphi|V|\varphi\rangle$  vanishes, and therefore the factorization  $V^{(1)} = V|\varphi\rangle\langle\varphi|V/\langle\varphi|V|\varphi\rangle$  is not convenient.

We represent the potential in the form

$$V = V_1 + V_2, \quad (44)$$

where  $V_1 > 0$ ,  $V_2 < 0$ . Although  $\langle\varphi|V|\varphi\rangle$  may vanish,  $\langle\varphi|V_1|\varphi\rangle$  and  $\langle\varphi|V_2|\varphi\rangle$  do not. We replace  $V$  by a second-rank operator, but such that (43) is satisfied for only one trial function. Evidently, there are a great number of such substitutions; we consider only two—(45) and (50):

$$\begin{aligned} \tilde{V}^{(2)} = & (1/d) \left\{ \langle\eta_l|V_2 - V_2G_lV_1|\eta_l\rangle V_1|\eta_l\rangle \langle\eta_l|V_1 + \langle\eta_l|V_1 - V_1G_lV_2|\eta_l\rangle V_2|\eta_l\rangle \langle\eta_l|V_2 - \langle\eta_l|V_1G_lV_2|\eta_l\rangle V_1|\eta_l\rangle \langle\eta_l|V_2 - \langle\eta_l|V_2G_lV_1|\eta_l\rangle V_1|\eta_l\rangle \langle\eta_l|V_1 \right\} \\ & d = \langle\eta_l|V_1|\eta_l\rangle \langle\eta_l|V_2|\eta_l\rangle - \langle\eta_l|V_1|\eta_l\rangle \langle\eta_l|V_2G_lV_1|\eta_l\rangle - \langle\eta_l|V_2|\eta_l\rangle \langle\eta_l|V_1G_lV_2|\eta_l\rangle. \end{aligned} \quad (45)$$

With the potential (45), Eq. (11) is solved as follows:

$$\begin{aligned} \tilde{\psi}_l^{(2)} = & j_l(kr) + \int_0^\infty G_l(r, r', E) V_1(r') \eta_l(r') dr' \cdot C_1 \\ & + \int_0^\infty G_l(r, r', E) V_2(r') \eta_l(r') dr' \cdot C_2; \end{aligned} \quad (46)$$

$$\begin{aligned} C_1 = & \langle\eta_l|V_1|j_l\rangle / \langle\eta_l|V_1 - V_1G_lV_1 - V_1G_lV_2|\eta_l\rangle; \\ C_2 = & \langle\eta_l|V_2|j_l\rangle / \langle\eta_l|V_2 - V_2G_lV_2 - V_2G_lV_1|\eta_l\rangle, \end{aligned}$$

and for the phase shift we obtain the stationary expression

$$\begin{aligned} \text{tg } \delta_l^{(2)} = & -\frac{1}{k} \left[ \frac{\langle j_l|V_1|\eta_l\rangle \langle\eta_l|V_1|j_l\rangle}{\langle\eta_l|V_1 - V_1G_lV_1 - V_1G_lV_2|\eta_l\rangle} + \frac{\langle j_l|V_2|\eta_l\rangle \langle\eta_l|V_2|j_l\rangle}{\langle\eta_l|V_2 - V_2G_lV_2 - V_2G_lV_1|\eta_l\rangle} \right]. \end{aligned} \quad (47)$$

One can consider the  $2N$ -term approximation

$$\begin{aligned} \text{tg } \delta_l^{(2N)} = & -\frac{1}{k} \left[ \sum_{i,j=1}^N \langle j_l|V_1|\eta_i\rangle [W_1^{-1}]_{ij} \langle\eta_j|V_1|j_l\rangle + \langle j_l|V_2|\eta_i\rangle [W_2^{-1}]_{ij} \langle\eta_j|V_2|j_l\rangle \right]; \\ [W_1]_{ij} = & \langle\eta_i|V_1 - V_1G_lV_1 - V_1G_lV_2|\eta_j\rangle; \\ [W_2]_{ij} = & \langle\eta_i|V_2 - V_2G_lV_2 - V_2G_lV_1|\eta_j\rangle. \end{aligned} \quad (48)$$

We prove (48) is stationary. Suppose

$$|\eta_i^k\rangle = |\psi_i\rangle + |\delta\psi_i\rangle.$$

After simple transformations, we obtain

$$\begin{aligned} \text{tg } \delta_l^{(2N)} = & \text{tg } \delta_l - (1/k) \langle\delta\psi_l|W - W_1^{(N)} - W_2^{(N)}|\delta\psi_l\rangle; \\ W = & V_1 + V_2 - V_1G_lV_2 - V_2G_lV_1 - V_1G_lV_1 - V_2G_lV_2; \\ W_1 = & V_1 - V_1G_lV_1 - V_1G_lV_2; \quad W_2 = V_2G_lV_2 - V_2G_lV_1; \\ W_1^{(N)} = & \sum_{n,m=1}^N W_1|\eta_n^k\rangle [d_1^{-1}]_{nm} \langle\eta_m^k|W_1; \\ [d_1]_{nm} = & \langle\eta_n^k|W_1|\eta_m^k\rangle. \end{aligned}$$

As in the case of (31), we formulate the iterative process



$$\left. \begin{aligned} |\varphi_i^{(N+1)}\rangle &= |f_i\rangle + G_1 V_1 |\varphi_i^{(N)}\rangle C_1^{(N)} + G_1 V_2 |\varphi_i^{(N)}\rangle C_2^{(N)}; \\ C_1^{(N)} &= \frac{\langle f_i | V_1 | \varphi_i^{(N)} \rangle}{\langle \varphi_i^{(N)} | V_1 - V_1 G_1 V_1 - V_1 G_1 V_2 | \varphi_i^{(N)} \rangle}; \\ C_2^{(N)} &= \langle f_i | V_2 | \varphi_i^{(N)} \rangle / \langle \varphi_i^{(N)} | V_2 - V_2 G_1 V_2 - V_2 G_1 V_1 | \varphi_i^{(N)} \rangle. \end{aligned} \right\} \quad (49)$$

The following substitution that we consider is taken from Ref. 15:

$$\tilde{V}^{(3)} = V_1 |\eta_1\rangle \langle \eta_1| V_2 / \langle \eta_1 | V_1 | \eta_1 \rangle + V_2 |\eta_2\rangle \langle \eta_2| V_1 / \langle \eta_2 | V_2 | \eta_2 \rangle. \quad (50)$$

Further, one can show that the potential (50) leads to a phase shift that is stationary under first-order variations of the trial function  $|\eta_i\rangle$ , and one can formulate an iterative process. Note that the variational principles based on (45) have not been considered in the literature.

**High Energies.** Suppose that there is a set of trial functions that are close to the exact function in different energy intervals; substituting them in (2), we obtain the amplitude (25), for which one can assert that it describes the scattering in the complete energy region, i.e., formula (25) represents an interpolation procedure.

To construct "dual" amplitudes on the basis of the interpolation formulas it is natural to choose  $N=2$ , and as functions in the separable representation the S-wave solution  $\psi_s$  and the high-energy approximation.<sup>[11]</sup> In many-channel theory, the Glauber approximations are suitable<sup>[21]</sup>:

$$\left. \begin{aligned} \psi_{k_v}(r) &= \exp(ikz) \int \psi_v^*(R_1, \dots, R_A) \\ &\times \exp\left(-\frac{ik}{2E} \int_{-\infty}^z \sum_i V_i(r' - R_i) dz\right) \psi_{v_0}(R_1, \dots, R_A) d\tau; \\ d\tau &= dR_1, \dots, dR_A \end{aligned} \right\} \quad (51)$$

( $r$  is the coordinate of the projectile,  $V_i(r - R_i)$  is the potential of its interaction with nucleon  $i$ , and  $\psi_v$  is the wave function of the target nucleus), and also the S-wave solution obtained by integrating the Faddeev equations.<sup>[22]</sup>

It follows from (25) that the obtained amplitude at high and low energies is close to the exact amplitude because  $\delta\psi$  is small, and it is also so at medium energies because  $|W - W^{(N)}|$  is small.

We consider scattering on a potential of the rectangular well type with parameters that describe the experimental data on low-energy nucleon-nucleon scattering. We construct three types of amplitude:

$$N=1; \quad \eta_k^{(+)} = |k\rangle; \quad \eta_k^{(-)} = |k'\rangle; \quad (51a)$$

$$N=1; \quad \eta_k^{(+)} = \eta_k^{(-)} = \psi_s; \quad (51b)$$

$$N=2; \quad \eta_k^{(+)} = \eta_k^{(-)} = \psi_s; \quad \eta_k^{(+)} = |k\rangle; \quad \eta_k^{(-)} = |k'\rangle. \quad (51c)$$

In the case of (51a), the amplitude  $f^{(1)}$  is virtually equal to the exact amplitude at  $E \sim 100$  MeV, and in the region  $E < 100$  MeV the error is  $\sim 40\%$ . In the case of (51b), the amplitude  $f_s^{(1)}$  coincides with the exact one for  $E < 10$  MeV since at low energies the S wave makes the main contribution. At higher energies ( $\sim 150$  MeV),  $f_s^{(1)}$  differs from the exact amplitude by about an order of magnitude.

The "dual" amplitude  $f^{(2)}$  (51c) coincides with  $f^{(1)}$  in the high-energy region, and with  $f_s^{(1)}$  and with the exact

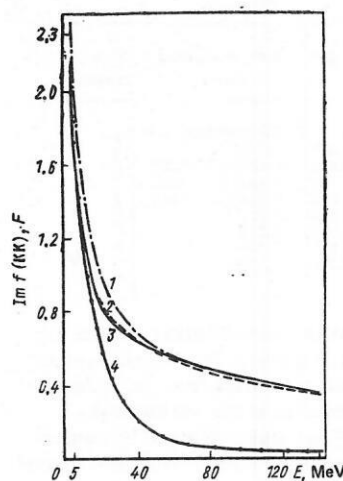


FIG. 1. Imaginary parts of the zero-angle scattering amplitudes as functions of the energy  $E$ : 1)  $f^{(1)}$ ; 2)  $f$ ; 3)  $f^{(2)}$ ; 4)  $f_s^{(1)}$ .

amplitude in the low energy region. In the region of medium energies,  $f^{(2)}$  is also fairly close to the exact amplitude  $f$  (deviation less than 10%).

In Fig. 1, we give the imaginary parts of the zero-angle scattering amplitudes  $f^{(1)}$ ,  $f_s^{(1)}$ ,  $f^{(2)}$ , and  $f$  (singlet scattering). It can be seen that  $\text{Im} f^{(2)}(k, k)$  has its largest deviation from the exact quantity in the energy range 20–80 MeV, but the deviation does not exceed 4%.

Thus, the interpolation formula (25) leads to an amplitude that with high accuracy describes elastic scattering at all energies.

On the basis of this approach, one can obtain the high energy amplitude in the region of both small and large angles. Indeed, taking the Glauber and Schiff approximations<sup>[23]</sup> as the functions in the separable representation, we obtain an amplitude that at small angles coincides with the eikonal amplitude and at large angles with the approximation obtained by summing the Born series by the method of stationary phase. In contrast to the quasiclassical amplitude constructed in Ref. 24, in our approach the scattering processes are described at lower energies.<sup>[9]</sup> Note that if the S-wave solution is not known exactly,  $\psi_s = \exp(-\beta r)$ , where  $\beta$  is a variational parameter (see, for example, Ref. 25), can serve as a suitable low-energy approximation.

We now turn to the calculation of the Fresnel corrections to the Glauber approximation. In deriving the Glauber expression for the scattering amplitude of a fast particle on a nucleus within the framework of potential theory we make the following approximations<sup>[26]</sup>: 1) we ignore the binding energy and the kinetic energy of the nucleons in the nucleus. This is frequently called the adiabatic approximation ( $G \rightarrow \tilde{G}$ ); 2) we use the approximation of geometrical optics ( $\tilde{G} \rightarrow \tilde{G}_2$ ). Here,  $G$  is the exact free Green's function. Since we are interested in the Fresnel corrections, we make the calculation in the framework of the adiabatic approximation, choosing the Glauber solution as the trial function. We consider the example of elastic  $\pi d$  scattering. In this

$$\tilde{G}(\mathbf{r}, \mathbf{R}) = \delta(\mathbf{r}) \int \frac{d^3p}{(2\pi)^3} \exp(i\mathbf{p}\mathbf{R}) \left[ \frac{k^2 - p^2}{2m} - \frac{(k-p)^2}{2M} + i\epsilon \right]^{-1}. \quad (52)$$

Here,  $k$  and  $m(k'$  and  $m')$  are the momentum and mass of the incident (respectively, scattered) meson;  $M$  is the deuteron mass. The difference between  $\tilde{G}$  and  $\tilde{G}_0$  has the form

$$g(\mathbf{k}, \mathbf{r}) = \delta(\mathbf{r}) \int \frac{d^3q}{(2\pi)^3} \exp[i(\mathbf{k}-\mathbf{q})\mathbf{r}] g(\mathbf{k}, \mathbf{q}), \quad (53)$$

where

$$g(\mathbf{k}, \mathbf{q}) = (m^2/2\mu) q^2/(k\mathbf{q} + i\epsilon)(k\mathbf{q} - q^2 + i\epsilon);$$

$$\mu = mM/(m+M).$$

With allowance for the results of the preceding sections, we arrive at an expression for the amplitude of scattering on fixed centers, the Fresnel corrections being allowed for:

$$\left. \begin{aligned} f^{(1)}(\mathbf{k}, \mathbf{k}', \mathbf{r}) &= C(\mathbf{k}, \mathbf{k}', \mathbf{r}) f_0(\mathbf{k}, \mathbf{k}', \mathbf{r}); \\ C &= f_0(\mathbf{k}, \mathbf{k}', \mathbf{r}) \left[ f_0(\mathbf{k}, \mathbf{k}', \mathbf{r}) \right. \\ &\quad \left. - \int \frac{d^3q}{(2\pi)^3} f_0(\mathbf{k}, \mathbf{k}-\mathbf{q}, \mathbf{r}) f_0(\mathbf{k}-\mathbf{q}, \mathbf{k}', \mathbf{r}) g(\mathbf{k}, \mathbf{q}) \right]^{-1}. \end{aligned} \right\} \quad (54)$$

Here,  $f_0$  is the amplitude in the eikonal (Glauber) approximation. Averaging then over the initial and the final wave functions, we obtain the expression for the amplitude of scattering on the deuteron with allowance for the Fresnel corrections.

For comparison with the results of other studies, we calculate approximately the expression (54). Assuming that the correction is small, we find

$$f_1 = f_0 + \int \frac{d^3q}{(2\pi)^3} f_0(\mathbf{k}, \mathbf{k}-\mathbf{q}, \mathbf{r}) f_0(\mathbf{k}-\mathbf{q}, \mathbf{k}', \mathbf{r}) g(\mathbf{k}, \mathbf{q}). \quad (55)$$

In the second term in (55), we take the amplitude  $f_0$  in the impulse approximation:

$$f_0 \approx \exp(i\Delta\mathbf{r}/2) f_{0\pi n}(\Delta) + \exp(-i\Delta\mathbf{r}/2) f_{0\pi p}(\Delta); \quad \Delta = \mathbf{k} - \mathbf{k}'. \quad (56)$$

Note that the  $\pi N$  amplitude must be taken in the eikonal approximation ( $f_{0\pi N}$ ). As a result, we obtain

$$\begin{aligned} f_1 &= f_0 + \exp(i\Delta\mathbf{r}/2) \int g(\mathbf{q}) f_{0\pi n}(\mathbf{q}) f_{0\pi n}(-\mathbf{q} + \Delta) \frac{d^3q}{(2\pi)^3} \\ &\quad + \exp(-i\Delta\mathbf{r}/2) \int g(\mathbf{q}) f_{0\pi p}(\mathbf{q}) f_{0\pi p}(-\mathbf{q} + \Delta) \frac{d^3q}{(2\pi)^3} \\ &\quad + \int g(\mathbf{q}) f_{0\pi p}(\mathbf{q}) f_{0\pi n}(-\mathbf{q} + \Delta) \exp[i(\mathbf{q} + \Delta/2)\mathbf{r}] \frac{d^3q}{(2\pi)^3} \\ &\quad + \int g(\mathbf{q}) f_{0\pi p}(\mathbf{q}) f_{0\pi p}(-\mathbf{q} + \Delta) \exp[i(\mathbf{q} - \Delta/2)\mathbf{r}] \frac{d^3q}{(2\pi)^3}. \end{aligned} \quad (57)$$

Note that the second and third terms simply renormalize the impulse approximation for  $f_0$ ; they correspond to the Fresnel corrections to the amplitudes of  $\pi N$  scattering; the fourth and fifth terms represent the Fresnel corrections, which renormalize the rescattering effects. These corrections have been considered on a number of occasions (see, for example, Refs. 26 and 28).

In any method of calculation, the parametrization of the off-shell amplitude causes difficulty.

To conclude this section, we consider the interesting choice of the trial functions of the Schwinger variational principle used in Ref. 29 to calculate above-threshold  $nd$  scattering. We illustrate the main idea of this approach by the example of the two-body problem. The expression (18) for  $N=1$  has the form

$$f^{(1)}(\mathbf{k}, \mathbf{k}') = -(1/2\pi) \langle \mathbf{k}' | V | \eta_{\mathbf{k}'}^{(+)} \rangle \langle \eta_{\mathbf{k}}^{(-)} | V | \mathbf{k} \rangle / \langle \eta_{\mathbf{k}}^{(-)} | V - V G_0 V | \eta_{\mathbf{k}}^{(+)} \rangle. \quad (57')$$

We introduce the new functions

$$|U_{\mathbf{k}'}^{(+)}\rangle = V | \eta_{\mathbf{k}'}^{(+)} \rangle; \quad |U_{\mathbf{k}}^{(-)}\rangle = V | \eta_{\mathbf{k}}^{(-)} \rangle.$$

Substituting  $U^{(\pm)}$  in (57'), we obtain for the functional (57') the expression

$$f^{(1)}(\mathbf{k}, \mathbf{k}') = -(1/2\pi) \langle \mathbf{k}' | U_{\mathbf{k}'}^{(+)} \rangle \langle U_{\mathbf{k}}^{(-)} | \mathbf{k} \rangle / \langle U_{\mathbf{k}}^{(-)} | V^{-1} | U_{\mathbf{k}'}^{(+)} \rangle - \langle U_{\mathbf{k}}^{(-)} | G_0 | U_{\mathbf{k}'}^{(+)} \rangle.$$

The functions  $U^{(\pm)}$  are introduced, first, to make it unnecessary to know the behavior of the functions at large  $r$  (under the condition that  $V(r)$  is a short-range potential) and, second, to avoid needing to calculate the integral  $\langle \eta | V G_0 V | \eta \rangle$ .

## 2. DISCRETE SPECTRUM

We consider the Lippmann-Schwinger equation for a bound state of a system of  $A$  nucleons:

$$\psi = -G_E V \psi, \quad (58)$$

where  $G_E$  is the Green's function of free motion. We replace  $V$  by an operator of finite rank  $V^{(N)}$  in accordance with Eq. (2) with  $|\eta\rangle = |\chi\rangle$ . Then Eq. (58) can be solved explicitly:

$$\left. \begin{aligned} |\tilde{\psi}\rangle &= -G_E V \sum_{i=1}^N c_i |\eta_i\rangle; \quad c_i = \sum_{k=1}^N B_{ik} c_k; \\ B_{ik} &= - \sum_{j=1}^N d_{ij}^{(N)} \langle \eta_j | V G_E V | \eta_k \rangle, \end{aligned} \right\} \quad (59)$$

and the binding energy  $E$  is determined from the condition of vanishing of the determinant of the matrix

$$D_{ik} = \delta_{ik} - B_{ik}. \quad (60)$$

For  $N=1$ ,

$$|\tilde{\psi}\rangle = G_E V |\eta\rangle; \quad (61)$$

$$\langle \eta | V G_E V | \eta \rangle / \langle \eta | V | \eta \rangle = -1. \quad (62)$$

We show that (62) leads for the binding energy  $E$  to a variational functional that is stable against first-order variation.<sup>[12]</sup> Indeed, suppose  $\eta = \psi + \delta\psi$  and  $\tilde{E} = E + \delta E$ ; then

$$\frac{\langle \psi | V G_E V | \psi \rangle + 2 \langle \delta\psi | V G_E V | \psi \rangle + O(\|\delta\psi\|^2) + \text{const } \delta E}{\langle \psi | V | \psi \rangle + 2 \langle \delta\psi | V | \psi \rangle + O(\|\delta\psi\|^2)} = -1,$$

i.e.,  $\delta E = O(\|\delta\psi\|^2)$ . Here,  $\psi$  is the exact solution (58) with energy  $E$ . In (61) and (62) we choose the trial function  $\psi$  in the form

$$|\eta\rangle = \sum_{i=1}^N c_i |\eta_i\rangle, \quad (63)$$

and we determine the coefficients  $c_i$  from the condition

$$\partial \tilde{E} / \partial c_i = 0. \quad (64)$$

Substituting (63) in (62) and taking into account (64), we see that  $c_i$  is determined by (59), and the binding energy by (60).

We consider the case when  $V$  in (58) is an operator of finite rank  $N$ . For such potentials, Eq. (2) becomes an identity and therefore the variational procedure for constructing the optimal combination of  $N$  trial functions based on the potential (62) always gives a result agreeing with the exact one for finite-rank potentials.<sup>[12]</sup>



The Schwinger variational principle for the scattering amplitude has just this property. We shall therefore call (62) the Schwinger variational principle for the binding energy. In contrast to the Ritz variational principle, (62) leads to one-sided bounds only for potentials that do not contain repulsion (irrespective of whether a ground or excited state is considered<sup>[3]</sup>). We show that nevertheless, using the variational principle (62), one can obtain a one-sided bound on the binding energy in the case of an arbitrary interaction. To this end, we consider the identity  $V \equiv V^{(N)} + (V - V^{(N)}) = V^{(N)} + V_1$ . Then in the first order of perturbation theory in  $V_1$ ,

$$E^{(1)} = \bar{E} + \frac{\langle \tilde{\psi} | V | \tilde{\psi} - \sum_{i=1}^N c_i \eta_i \rangle}{\langle \tilde{\psi} | \tilde{\psi} \rangle}, \quad (64a)$$

where  $\tilde{\psi}$  and  $\bar{E}$  are determined by (59) and (60). It is readily seen that  $E^{(1)}$  is the Ritz variational functional with trial function  $\tilde{\psi}$ , i.e.,  $E^{(1)}$  is an upper bound.

On the basis of the variational principle (62) one can formulate an iterative process:

$$|\psi_N\rangle = -G_{E_N} V |\psi_{N-1}\rangle; \quad \langle \psi_{N-1} | V G_{E_N} V | \psi_{N-1} \rangle / \langle \psi_{N-1} | V | \psi_{N-1} \rangle = -1,$$

and use it to improve the existing approximation. The convergence of this process was investigated in detail in Ref. 25.

The Ritz variational principle can also be obtained on the basis of the philosophy of the separable representation method. However, it is then necessary to approximate the complete Hamiltonian. Indeed, let us replace  $H^{(1)} = H | \chi \rangle \langle \chi | / \langle \chi | \chi \rangle$ . With this Hamiltonian, the equation  $H\psi = E\psi$  can be solved, and for the energy we obtain the Ritz variational principle:  $E = \langle \chi | H | \chi \rangle / \langle \chi | \chi \rangle$ . In this connection, the Schwinger principle is preferable to the Ritz one since the kinetic energy is not approximated, i.e., the asymptotic behavior of the solution for all trial functions is correct.

There exists an opinion that a finite-dimensional operator  $V^{(N)}$  gives not more than  $N$  bound states. This is so if the functions in the separable representation do not depend on the energy. In the general case, even  $V^{(1)}$  can lead to a complete spectrum. Consider, for example, the S-wave two-body problem:

$$(d^2/dr^2 + 2\mu E/\hbar^2 - 2\mu V/\hbar^2) \psi = 0. \quad (65)$$

In the case of a bound state,  $E = -\hbar^2 \kappa^2 / 2\mu$  and

$$\psi(r) = - \int G_E(r, r') V(r') \psi(r') dr'; \quad G_E(r, r') = \begin{cases} (\mu/\hbar^2 \kappa) \exp(-\kappa r) [\exp(\kappa r') - \exp(-\kappa r')], & r' \leq r, \\ (\mu/\hbar^2 \kappa) [\exp(\kappa r) - \exp(-\kappa r)] \exp(-\kappa r'), & r \leq r'. \end{cases} \quad (66)$$

Let  $R$  be the range of the potential  $V(r)$ , i.e.,  $V(r) = 0$  for  $r > R$ , and let  $\psi_1(E, r)$  be a regular solution of (65) within the range of the potential. In (59) we set  $N = 1$  and  $|\eta\rangle = |\psi_1\rangle$ , and then

$$|\psi\rangle = -G_E V |\psi_1\rangle; \quad \langle \psi_1 | V G_E V | \psi_1 \rangle / \langle \psi_1 | V | \psi_1 \rangle = -1. \quad (67)$$

Taking into account (66) and the fact that  $\psi_1$  is a solution of (65), we obtain from (67)

$$\psi_1'(R) / \psi_1(R) = -\kappa. \quad (68)$$

Equations (68) coincides with the exact fitting condition, from which the complete spectrum is determined. In the scattering problem, the trial function  $\psi_1$  also leads to the exact phase shift.

For a potential of rectangular well type, the solution of rectangular well type, the solution of the partial-wave Schrödinger equation has the form  $j_l(k_0 r)$ , where  $k_0^2 = (2\mu/\hbar^2)(E - V_0)$ . Therefore, a Bateman expansion with one of the nodes equal to  $k_0$  exactly describes the bound-state problem and the scattering problem for the half-off-shell case. It is clear that the function  $|\eta\rangle$  can be expressed in the form

$$|\eta\rangle = \sum_{i=1}^N c_i |\eta_i\rangle$$

and the variational principle for  $|\eta\rangle$  reformulated into one for  $|\eta_i\rangle$  with an appropriate choice of  $c_i$  for the Ritz variational principle as well. However, one then obtains an equation for the energy whose roots include unphysical values.<sup>[30]</sup> The sequence of the variational principle (59) does not have this shortcoming since it is found from the solution of (58) with the potential  $V^{(N)}$ .

With regard to the validity of the replacement of  $V$  by  $V^{(N)}$  in many-particle problems, i.e., the problem of giving a dynamical meaning to the Schwinger variational principle (in the sense that  $|V - V^{(N)}|$  is small), we point out that in bound-state problems  $V$  is defined on the class of square-integrable function and the replacement of  $V$  by  $V^{(N)}$  is justified. Calculations were made in Ref. 31 in accordance with this method for the three-body problem; rapid convergence was established.

Since the asymptotic behavior of the solution in the Schwinger method is correct for any choice of the trial functions, an oscillator basis is convenient. This basis is widely used in the Ritz variational principle, and a method has been developed for calculating matrix elements of the type

$$\langle \eta_i | V | \eta_j \rangle; \quad \langle \eta_i | G_E | \eta_j \rangle, \quad (69)$$

where  $|\eta_i\rangle$  are oscillator functions. We simplify the Schwinger variational principle in such a way that it is only necessary to calculate the matrix elements (69). We consider the case  $N = 1$  and replace (62) by the approximate expression

$$\sum_{i,j=1}^N \frac{\langle \eta_i | V | \eta_j \rangle \langle \eta_j | G_E | \eta_i \rangle \langle \eta_j | V | \eta \rangle}{\langle \eta | V | \eta \rangle} = -1. \quad (70)$$

Although the stationarity of (70) is approximate, this expression is convenient for practical calculations and, which is particularly important, is obtained by replacing  $V$  by a first-rank operator  $V^{(1)}$ :

$$V^{(1)} = \sum_{i,j=1}^N \frac{\langle \eta_i | V | \eta_j \rangle \langle \eta_j | V | \eta \rangle}{\langle \eta | V | \eta \rangle} |\eta_i\rangle \langle \eta_j|. \quad (71)$$

One can also consider the general case (59).

*Corrections to the Main Approximations in the Method of Multidimensional Harmonics.* Calculations of the binding energies of the lightest nuclei have shown that the method of  $K$  harmonics converges rapidly, i.e., the main contribution to the wave function and energy of low-

lying states is made by the first terms with  $K = K_{\min}$ .<sup>[32]</sup> However, it is not yet clear whether the method converges rapidly on the transition to heavy nuclei (for example, to  $^{16}\text{O}$ , etc).

We calculate the corrections to the basic approximation of the method of  $K$  harmonics.<sup>[10]</sup> For simplicity, we shall assume that the fundamental harmonic with total angular momentum  $J$  and projection  $J_z$  onto the  $z$  axis is unique:

$$U_{K_{\min} J, J_z}(\Omega_{3A-3}) \equiv U_{K_{\min}(\Omega_{3A-3})}.$$

in (62) we set

$$\eta = \rho^{-(3A-4)/2} \varphi(\rho) U_{K_{\min}(\Omega_{3A-3})} \quad (72)$$

and, using the approximation of Ref. 33, we find

$$\left. \begin{aligned} \tilde{\psi} &= -V\eta / \left( \frac{\kappa(\kappa+1)}{2m\rho^2} + |\tilde{E}| \right); \\ \int d\rho \left[ \varphi^2(\rho) \tilde{V}^2(\rho) / \left( \frac{\kappa(\kappa+1)}{2m\rho^2} + |\tilde{E}| \right) \right] / \int d\rho \varphi^2(\rho) \tilde{V}(\rho) &= -1, \end{aligned} \right\} \quad (73)$$

where

$$\begin{aligned} \kappa &= K_{\min} + (3A-6)/2; \\ \tilde{V}(\rho) &= \int U_{K_{\min}(\Omega_{3A-3})} V^a U_{K_{\min}(\Omega_{3A-3})} d\Omega_{3A-3}, \end{aligned}$$

and  $\varphi(\rho)$  for many-nucleon nuclei is close to the oscillator function<sup>[34]</sup>:

$$\varphi(\rho) = \exp \{ -(\rho - \bar{\rho})^2 / \Delta \rho^2 \}; \quad \Delta \rho \sim \bar{\rho} / \sqrt{A}. \quad (74)$$

It is obvious that the expansion of  $\tilde{\psi}$  with respect to the hyperspherical functions contains all potential harmonics besides the fundamental one.

Although (73) is obtained under the same approximations as the expression for the corrections in Ref. 33, our formulas are much simpler (the term with  $\tilde{V}^3$  is absent). This is one of the advantages of the present approach.

As an example, we estimate  $\tilde{E}$  for the nucleus  $^{16}\text{O}$  and a spinless two-particle potential of the form

$$V_{ij} = \lambda_1 \exp(-\rho_{ij}^2/\tau_1^2) - \lambda_2 \exp(-\rho_{ij}^2/\tau_2^2) \quad (75)$$

with the parameters<sup>2)</sup>

$$\lambda_1 = 10; \quad \tau_1 = 1; \quad \lambda_2 = 1.58; \quad \tau_2 = 2.5, \quad (76)$$

which lead to a  $^{16}\text{O}$  energy in the basic approximation:

$$E_0 = -6. \quad (77)$$

For  $\bar{\rho} = 10$ , calculation in accordance with (73) gives

$$E = -21.9. \quad (78)$$

[The expressions  $\tilde{V}^2$  for the nucleus  $^{16}\text{O}$  and the potential (75) are given in Ref. 33]. The accuracy of (78) can be estimated by using (64a). For the cases (75) and (76),

$$|\Delta \tilde{E}/E| \cdot 100\% \sim 30\%; \quad \Delta \tilde{E} = E^{(1)} - \tilde{E}. \quad (79)$$

Remembering that in reality the accuracy in the calculation of  $\tilde{E}$  is much better, since the upper bound for  $|\Delta \tilde{E}|$  was used to derive (79), we can assert that already in the first approximation of the method there is

significant improvement in the  $K_{\min}$  approximation. The value (78) is in qualitative agreement with the results of Ref. 33, in which the estimate  $E < -15$  was found for the same example.

*Problems with More Complicated Boundary Conditions.* To demonstrate the effectiveness of the Schwing-er variational principle in problems with a discrete spectrum, we consider the problem of microwave breakdown. The problem of breakdown of a gas in an inhomogeneous microwave field has been considered on many occasions.<sup>[35,36]</sup> In such a field, it is as a rule impossible to obtain an exact analytic solution for the nonstationary diffusion equation that describes the electron density:

$$\nabla(D\nabla n) + \nu_{\text{net}} n = \partial n / \partial t \quad (80)$$

( $\nu_{\text{net}} = \nu_i - \nu_a$  is the effective ionization frequency, which depends on the effective field  $E_{\text{eff}} = |E|/\sqrt{1 + \omega^2/\nu^2}$ ;  $|E|$  is the modulus of the microwave field;  $\nu$  is the frequency of collisions of electrons in the gas;  $\omega$  is the angular frequency;  $\nu_i$  and  $\nu_a$  are respectively the ionization and trapping frequencies;  $D$  is the diffusion coefficient).

To find the conditions of breakdown in the gas, methods based on the Ritz variational principle are usually used. In the first of them, which was proposed by Epstein,<sup>[35]</sup> the following variational principle is obtained from the condition of continuous breakdown  $\partial n / \partial t = 0$ :

$$\delta \langle \eta | L_0 - \nu_{\text{net}} | \eta \rangle = 0,$$

where  $L_0 = -\nabla(D\nabla)$ ;  $\eta$  is a trial function.

In the second approach proposed by Mayhan,<sup>[36]</sup> Eq. (80) leads to an eigenvalue problem. For this, one expands the electron density  $n(r, t)$  with respect to a complete system of functions:

$$n(r, t) = \sum_k N_k(r) T_k(t).$$

After this, (80) reduces to the system of equations

$$\left. \begin{aligned} (L_0 + \nu) N_k &= \lambda_k N_k; \\ \partial T_k / \partial t &= -\lambda_k T_k, \end{aligned} \right\} \quad (81)$$

where  $\lambda_k$  is the eigenvalue;  $L_0 = -\nabla(D\nabla)$ ;  $\nu = -\nu_{\text{net}}$ . It follows from (81) that the onset of continuous breakdown corresponds to a condition under which the minimal eigenvalue  $\lambda_k^{\min}$  is zero.

To find  $\lambda_k^{\min}$ , one used the Ritz variational principle

$$\lambda_k^{\min} = -\langle \eta | L_0 + \nu | \eta \rangle / \langle \eta | \eta \rangle$$

with trial function  $|\eta\rangle$  satisfying the following boundary conditions:  $\eta = 0$  on the surface of the emitter and  $\nabla\eta \rightarrow 0$  for the open part of space. A schwing-er variational principle is obtained by replacing  $\nu$  by an operator of finite rank in accordance with Eq. (2). It should be emphasized that the calculation of the Green's functions of the operator  $L_0$  for the majority of the models used does not present difficulties. In Refs. 35 and 36 the Ritz principle was demonstrated for some model problems whose exact solution is known. We show that the Schwing-er principle with the same trial functions leads to more accurate results.<sup>[17]</sup> For this, we introduce the notation

$$\nu = \nu_0 f(r); \quad D = D_0; \quad \mu = \nu_0 l^2 / D_0. \quad (82)$$

<sup>2)</sup>Here, the energies are measured in units of 20.6 MeV and the distances in fermis.

We consider microwave breakdown between two infinite parallel slabs. The boundary conditions are  $n(0) = n(1) = 0$ . We write down the diffusion equation for this case:

$$d^2n/dx^2 + \mu f(x)n = \partial n/\partial t. \quad (82')$$

The Green's function of the operator  $d^2/dx^2$  with appropriate boundary conditions has the form

$$G(x, x') = \begin{cases} x(1-x'), & x' > x; \\ x'(1-x), & x' < x. \end{cases} \quad (83)$$

If  $f(x) = 1$ , then the exact solution is

$$n = \sin \pi x; \quad \mu = \pi^2 = 9.869.$$

We give the values obtained by the variational methods with the trial functions

$$\eta = x(1-x); \quad (84)$$

$$\eta = x(1-x)(c_1 + c_2 x^2) \quad (85)$$

( $c_1$  and  $c_2$  are variational parameters).

For (84) the Ritz principle gives  $\mu = 10.0$  and the Schwinger principle  $\mu = 9.883$ , i.e., the latter is an order of magnitude more accurate than the former.

For (85) the Ritz principle gives  $\mu = 9.99$  and the Schwinger principle with the trial function (84) is much more accurate than the Ritz principle with the trial function (85). If the trial function  $\eta = 1$ , which does not satisfy the boundary conditions, is used in the Schwinger principle, the result  $\mu = 12.0$  is obtained, and this differs by only 20% from the exact result.

In the case  $f(x) = 1 - x$  (in the same problem) the exact value is  $\mu = 18.956$ .

Let us consider the results obtained by the variational methods with the trial function

$$\eta = x(1-x); \quad (86)$$

$$\eta = x(1-x)(c_1 + c_2 x^2). \quad (87)$$

For (86), the Ritz principle gives  $\mu = 20.0$  and the Schwinger principle gives  $\mu = 19.09$ .

For (87) the Ritz principle gives  $\mu = 19.02$  and the Schwinger principle gives  $\mu = 18.961$ . It can be seen that the Schwinger principle with the trial function (87) leads to a solution that is virtually the same as the exact one.

We now consider two-dimensional problems. We consider microwave breakdown in a cylindrical cavity of radius  $R$  and length  $L$ . The equation in this case has the form

$$\partial^2 n/\partial r^2 + (1/r) \partial n/\partial r + \partial^2 n/\partial z^2 + \mu f(r, z)n = \partial n/\partial t, \quad (88)$$

and the boundary conditions are  $n_{r=0} = 0$  and  $n_{r=R} = 0$ . If we choose  $f(r) = 1 - r^2$ , then the variables separate and the exact solution for  $\pi R/L = k = 1$  gives  $\mu = 8.5$ . The Green's function for the radial equation is

$$G(r, r') = \begin{cases} (1/c) I_0(kr) [I_0(kr') + cK_0(kr')], & r < r'; \\ (1/c) I_0(kr') [I_0(kr) + cK_0(kr)], & r > r', \end{cases} \quad (89)$$

where  $c = I_0(k)/K_0(k)$ ;  $I_0(kr)$  and  $K_0(kr)$  are Bessel and MacDonald functions of imaginary argument.

The results obtained by the variational methods with the trial function  $\eta = (1 - r^2) \sin \pi z$  for  $k = 1$  are as follows:

Ritz principle,  $\mu = 9.33$  and Schwinger principle  $\mu = 8.868$ . In this case too, the results obtained by the latter is much more accurate than for the former.

Summarizing the above examples, we can say that even in problems with complicated boundary conditions the Schwinger principle has the advantage over the Ritz principle.

### 3. SCHWINGER VARIATIONAL PRINCIPLE IN NONSTATIONARY THEORY

In a number of problems of atomic and nuclear physics (for example, in many-photon ionization of atoms<sup>[37]</sup> and in reactions induced by heavy ions<sup>[38]</sup>) it is necessary to go beyond the framework of standard perturbation theory. Although successes have been achieved in this direction (the quasienergy method<sup>[3]</sup> (Ref. 39), the Green's function method<sup>[40]</sup> etc.) the large number of channels that must be taken into account and also the special nature of the existing approximations have the consequence that one must investigate the general methods of theoretical description of such systems. It is obvious that variational principles can provide the basis of such an approach.<sup>[4]</sup>

**Basic Equations.** The wave function of the system satisfies the equation

$$i\partial\Psi(\zeta, t)/\partial t = [H_0(\zeta) + V(\zeta, t)]\Psi(\zeta, t), \quad (90)$$

and it is natural to seek a solution in the form of the expansion

$$\Psi(\zeta, t) = \sum_{\nu} a_{\nu}(t) \exp[-iE_{\nu}t] \psi_{\nu}$$

with respect to the eigenfunctions of the nucleus (atom) in the absence of an external field:

$$H_0|\psi_{\nu}\rangle = E_{\nu}|\psi_{\nu}\rangle.$$

Then for  $a_{\nu}$  we obtain the system of equations

$$i \frac{da_{\nu}}{dt} = \sum_{\nu'} \exp(i\omega_{\nu\nu'}t) \langle \psi_{\nu} | V(t) | \psi_{\nu'} \rangle a_{\nu'}, \quad (91)$$

where  $\omega_{\nu\nu'} = (E_{\nu} - E_{\nu'})$ ;  $a_{\nu}(t)$  is the probability amplitude for finding the system at time  $t$  in one of the states  $|\psi_{\nu}\rangle$ .

Suppose that at the initial time  $t_0$  the system is in the state  $|\psi_0\rangle$ ; then we have the following initial conditions for solving the system (91):

$$a_{\nu}(t_0) = \delta_{\nu\nu_0}.$$

We rewrite (91) in the integral form

$$a_{\nu}(t) = \delta_{\nu\nu_0} + \frac{i}{\hbar} \int_{t_0}^t \sum_{\nu'} V_{\nu\nu'}(t') a_{\nu'}(t') dt', \quad (92)$$

<sup>3)</sup>It is to be expected that the use of quasienergies will be fruitful in the theory of many-photon ionization although the practical use of quasienergies in the theory of many-quantum processes is apparently difficult.<sup>[41]</sup>

<sup>4)</sup>Note that an analogous variational principle for an infinite time interval was considered in Ref. 42, and a generalization of variational principles of the Kohn and Hult  n type to nonstationary problems was given in Ref. 43.



where

$$V_{vv'}(t) = \exp(i\omega_{vv'}t) \langle v | V(t) | v' \rangle.$$

We introduce

$$a_v(t, T) = \delta_{vv_0} + \frac{1}{i} \int_{t_0}^T \sum_{v'} V_{vv'}(t') \theta(t-t') a_{v'}(t', T) dt';$$

$$\theta(x) = \begin{cases} 1, & x > 0; \\ 0, & x < 0. \end{cases} \quad (93)$$

It is readily seen that

$$a_v(t, T) = a_v(t), \quad \text{if } t \leq T,$$

and for  $t > T$

$$a_v(t, T) = \delta_{vv_0} + \frac{1}{i} \int_{t_0}^T \sum_{v'} V_{vv'}(t') a_{v'}(t') dt',$$

i.e.,

$$a_v(t, T) = \begin{cases} a_v(t), & t \leq T; \\ a_v(T), & t > T. \end{cases} \quad (94)$$

Such a situation is realized if the potential is switched off at the time  $T$ ; in this sense, Eqs. (93) are analogous to the equations of the variables phase approach.

In what follows, we shall also require the functions  $a_v^{i(-)}(t, T)$ :

$$a_v^{i(-)}(t, T) = \delta_{vv_i} - \frac{1}{i} \int_{t_0}^T \sum_{v'} V_{vv'}(t') \theta(t'-t) a_{v'}^{i(-)}(t', T) dt'. \quad (95)$$

For  $T \leq t$ , the  $a_v^{i(-)}(t, T)$  are solutions of the system (92) with the initial conditions

$$a_v^{i(-)}(T, T) = \delta_{vv_i}.$$

**Separable Representation Method.** To solve the system (93), we generalize the method of separable representation of the potential in many-channel theory. We replace  $V$  by an operator  $V^{(N)}$  of finite rank in accordance with

$$\left. \begin{aligned} & \sum_{v'} V_{vv'}^{(N)}(t) b_{v'}(t) \\ &= \sum_{i,j=1}^N \sum_{\mu, \mu'} V_{\mu\mu'}(t) \eta_{\mu}^i(t) d_{ij}^{-1} \int_{t_0}^T (\eta_{\mu'}^{j(-)}(t'))^* V_{\mu'v'}(t') b_{v'}(t') dt'; \\ & d_{ij} = \sum_{\mu, \mu'} \int_{t_0}^T (\eta_{\mu}^{i(-)}(t))^* V_{\mu\mu'}(t) \eta_{\mu'}^j(t) dt. \end{aligned} \right\} \quad (96)$$

With the potential (96), the system (93) can be solved explicitly:

$$\left. \begin{aligned} & a_v^{(N)}(t, T) = \delta_{vv_0} + \frac{1}{i} \sum_{i,j=1}^N \sum_{\mu, \mu'} \int_{t_0}^T V_{\mu\mu'}(t') \theta(t-t') \eta_{\mu}^i(t') \\ & \times dt' [C^{-1}(T)]_{ij} \int_{t_0}^T (\eta_{\mu'}^{j(-)}(t''))^* V_{\mu'v_0}(t'') dt''; \\ & C_{ij}(T) = \sum_{\mu, \mu'} \left[ \int_{t_0}^T (\eta_{\mu}^{i(-)}(t))^* V_{\mu\mu'}(t) \eta_{\mu'}^j(t) dt \right. \\ & \left. - \frac{1}{i} \sum_{\mu'} \int_{t_0}^T dt' \int_{t_0}^T dt'' (\eta_{\mu}^{i(-)}(t'))^* V_{\mu\mu'}(t) \theta(t-t') V_{\mu'v'}(t') \eta_{\mu'}^j(t') \right]. \end{aligned} \right\} \quad (97)$$

We mention the specific features of the separation method with respect to the time. It can be seen from (97) that if  $t < T$  then  $a_v^{(N)}(t, T)$  has no meaning. Indeed, we have replaced the potential by one that is nonlocal with respect to the time. Therefore,  $a_v^{(N)}(t, T)$  depends

on the fields at times that are not only smaller than but are also larger than  $t$  right up to  $T$ . This obviously contradicts the causality condition. However, for  $a_v^{(N)}(T, T)$  there are not such contradictions. Using (94) and replacing  $T$  by  $t$ , we arrive at the solution of Eqs. (91) obtained by the separable representation method<sup>[16]</sup>:

$$a_v^{(N)}(t) = a_v^{(N)}(t, t); \quad (98)$$

$$a_v^{(N)}(t) = \delta_{vv_0} + \frac{1}{i} \sum_{i,j=1}^N \sum_{\mu, \mu'} \int_{t_0}^t V_{\mu\mu'}(t') \eta_{\mu}^i(t') dt' [C^{-1}(t)]_{ij} \times \int_{t_0}^t (\eta_{\mu'}^{j(-)}(t''))^* V_{\mu'v_0}(t'') dt''. \quad (99)$$

Let us consider briefly the convergence of (99). We consider the equations

$$\left. \begin{aligned} & \psi_v^{(+)}(t, T) = \exp(-iE_v t) | v_0 \rangle \\ & + \frac{1}{i} \int_{t_0}^T \exp[iH_0(t'-t)] \theta(t-t') V(t') \psi_v^{(+)}(t', T) dt'; \\ & \psi_v^{(-)}(t, T) = \exp(-iE_v t) | v \rangle \\ & - \frac{1}{i} \int_{t_0}^T \exp[iH_0(t'-t)] \theta(t'-t) V(t') \psi_v^{(-)}(t', T) dt', \end{aligned} \right\} \quad (100)$$

whose solutions satisfy (90). The amplitude is determined from the equation

$$a_v(t, T) = \langle \Phi_v(t) | \psi_v^{(+)}(t, T) \rangle; \quad \Phi_v(t) = \exp(-iE_v t) | v \rangle.$$

To solve (100), we use an identity that can be written symbolically as

$$V = V V^{-1} V = \sum_{i,j} V | i \rangle \langle i | V^{-1} | j \rangle \langle j | V; \quad (101)$$

here,  $| i \rangle$  and  $| j \rangle$  are complete sets also with respect to the time in the interval  $[t_0, T]$ ;

$$\langle i | V | j \rangle = \int_{t_0}^T dt \int \chi_i^*(\xi, t) V(\xi, t) \varphi_j(\xi, t) d\xi.$$

In (101), we truncate the summation over the complete sets, and then

$$\left. \begin{aligned} & V^{(N)} = \sum_{i,j=1}^N V | \varphi_i \rangle \langle \varphi_j | d_{ij}^{-1} \langle \chi_j | V; \\ & d_{ij} = \langle \chi_i | V | \varphi_j \rangle. \end{aligned} \right\} \quad (102)$$

With the potential (102), the system (100) can be solved, and for  $a_v^{(N)}(t)$  we arrive at (99) after appropriate transformations. It is clear from the argument we have given that if Eqs. (100) have solutions, in other words, if the kernels (100) are completely continuous, then (99) converges.

**Schwinger Variational Principle.** We show that (99) is stationary against first-order variations with respect to each of the trial functions  $\eta$ . We consider first the case  $N=1$ . Then

$$a_v^{(1)}(t) = \delta_{vv_0} + \frac{1}{i} \frac{\sum_{\mu, \mu'} \int_{t_0}^t V_{\mu\mu'}(t') \eta_{\mu'}(t') dt' \int_{t_0}^t (\eta_{\mu}^{(-)}(t''))^* V_{\mu'v_0}(t'') dt''}{\sum_{\mu, \mu'} \int_{t_0}^t dt' \int_{t_0}^t dt'' [(\eta_{\mu}^{(-)}(t'))^* V_{\mu\mu'}(t') \eta_{\mu'}(t')]} \rightarrow -\frac{1}{i} \int_{t_0}^t dt' \sum_{\mu} (\eta_{\mu}^{(-)}(t'))^* V_{\mu\mu}(t') \theta(t'-t'') V_{\mu\mu}(t'') \eta_{\mu}(t'') \quad (103)$$

We rewrite (103) in the form

$$a_v^{(1)}(t) = \delta_{vv_0} + \frac{\sum_{\mu\nu\mu'\nu'} \int_{t_0}^t \delta_{\mu\nu} V_{\mu\nu'}(t') \eta_{\nu'}(t') dt' \int_{t_0}^t (\eta_{\mu}^{(-)}(t''))^* V_{\mu'\nu''}(t'') \delta_{\nu''\nu_0} dt''}{\sum_{\sigma\rho} \int_{t_0}^t dt' [(\eta_{\sigma}^{(-)}(t'))^* V_{\sigma\rho}(t') \eta_{\rho}(t')]} \rightarrow -\frac{1}{i} \int_{t_0}^t dt'' \sum_{\sigma} (\eta_{\sigma}^{(-)}(t''))^* V_{\sigma\delta}(t'') \theta(t' - t'') V_{\delta\rho}(t'') \eta_{\rho}(t'')$$

Further, using (95) and (94), we obtain

$$\sum_{\mu\nu\nu'} \int_{t_0}^t \delta_{\mu\nu} V_{\mu\nu'}(t') \eta_{\nu'}(t') dt' = \sum_{\mu\nu\nu'} \int_{t_0}^t dt' [(\eta_{\mu}^{(-)}(t', t))^* V_{\mu\nu'}(t') \eta_{\nu'}(t')] - \frac{1}{i} \int_{t_0}^t dt'' \sum_{\mu} (a_{\mu}^{(-)}(t', t))^* V_{\mu\mu'}(t') \theta(t' - t'') V_{\mu'\nu''}(t'') \eta_{\nu''}(t'') \sum_{\mu'\nu''} \int_{t_0}^t (\eta_{\mu'}^{(-)}(t''))^* V_{\mu'\nu''}(t'') \delta_{\nu''\nu_0} dt'' = \sum_{\mu'\nu''} \int_{t_0}^t dt'' [(\eta_{\mu'}^{(-)}(t''))^* V_{\mu'\nu''}(t'') a_{\nu''}(t', t)] - \frac{1}{i} \int_{t_0}^t dt'' \sum_{\mu} (\eta_{\mu}^{(-)}(t''))^* V_{\mu\mu'}(t'') \theta(t' - t'') V_{\mu'\nu''}(t'') a_{\nu''}(t', t).$$

Therefore, if

$$\eta_{\mu}^{(-)}(t') = a_{\mu}^{(-)}(t', t) + \delta a_{\mu}^{(-)}; \quad \eta_{\mu}^{(+)}(t') = a_{\mu}^{(+)}(t', t) + \delta a_{\mu}^{(+)},$$

it follows that

$$a_v^{(1)}(t) = a_v(t) + O[(\delta a)^2],$$

i.e., (103) is a variational functional.

In (103), we choose the trial functions

$$\eta_{\nu}(t) = \sum_{i=1}^N a_i \eta_{\nu}^i(t); \quad \eta_{\mu}^{(-)}(t) = \sum_{i=1}^N b_i \eta_{\mu}^{(-)i}(t). \quad (104)$$

Substituting (104) in (103) and finding the coefficients  $a_i$  and  $b_i$  from the conditions

$$\partial a_v^{(1)}(t) / \partial a_i = \partial a_v^{(1)}(t) / \partial b_i = 0,$$

we find that  $a_v^{(1)}(t) = a_v^{(N)}(t)$ . Hence, if

$$\eta_{\mu}^{(+)}(t') = a_{\mu}^{(+)}(t', t) + \delta a_{\mu}^{(+)}; \quad \eta_{\mu}^{(-)}(t') = a_{\mu}^{(-)}(t', t) + \delta a_{\mu}^{(-)},$$

then

$$a_v^{(N)}(t) = a_v(t) + O[(\delta a)^2]$$

and we have proved our assertion.

As an example of the use of the variational principle (103), we choose

$$\eta_{\mu}(t') = \delta_{\mu\nu_0}; \quad \eta_{\mu}^{(-)}(t') = \delta_{\mu\nu}. \quad (105)$$

Substituting (105) in (103), we obtain for the amplitude the expression

$$a_v^{(1)}(t) = \delta_{vv_0} + \frac{\left( \int_{t_0}^t V_{vv_0}(t') dt' \right)^2}{\int_{t_0}^t V_{vv_0}(t') dt' - \frac{1}{i} \int_{t_0}^t dt' \int_{t_0}^t dt'' \sum_{\mu} V_{\mu\nu}(t') \theta(t' - t'') V_{\mu\nu_0}(t'')}, \quad (106)$$

which is an improved Born approximation and, to terms quadratic in the interaction, coincides with the second Born approximation.

We note further that if the Hamiltonian does not de-

pend explicitly on the time, then, replacing  $V$  by  $\exp(-\epsilon|t|)V$  and taking  $t_0 = -\infty$ , we obtain the ordinary Schwinger variational principle for  $a_v^{(1)}(\infty)$ .

#### Transmission of a Particle Through a Potential Barrier Varying Depth.

In Ref. 41, a study was made of the transmission of a particle through a narrow potential barrier with periodically varying depth and numerical calculations showed that the reflection of the particles from such a barrier has a resonance nature. In this section, we consider this problem on the basis of the Schwinger variational principle. Suppose the potential is

$$V(x, t) = -(\alpha + \lambda \cos \omega t) \delta(x). \quad (107)$$

We consider elastic scattering. Substituting the potential (107) in (106), we use the adiabatic hypothesis, i.e., we replace  $V(x, t)$  by  $\exp(-\epsilon|t|)V(x, t)$ , go to the limit  $t_0 = -\infty$ ,  $t \rightarrow \infty$  in (106), and obtain as a result for the reflection coefficient  $R$  the expression<sup>5)</sup>

$$R = |\alpha^2/2k(\lambda^2/8\sqrt{\omega - k^2} - \alpha) + i(\alpha^2 + 2k\lambda^2/8\sqrt{\omega + k^2})|^2, \quad (108)$$

which is valid if  $\omega \neq 0$ .

It can be seen from (108) that if  $\alpha > 0$ , i.e., if the system has a bound state for  $\lambda = 0$ , then for  $k^2 < \omega$  the reflection has a resonance nature, and near the resonance the expression for  $R$  has the form of the Breit-Wigner formula with a width that depends on the transfer. In the region of energies  $k^2 > \omega$  there are no resonances.

For  $\lambda = 0$ , the expression (108) goes over into the exact expression for the coefficient of reflection on a  $\delta$ -functional potential.

Let us consider briefly the physical picture of the phenomenon. For  $k^2 < \omega$ , the system can emit a quantum  $\omega$ , go over into the region of negative energies, and then absorb a quantum  $\omega$ ; for  $k^2 > \omega$ , the probability of absorption of a real quantum is small.<sup>6)</sup>

It is known<sup>[44]</sup> that ultracold neutrons provide, on account of their exceptionally low energy ( $\sim 10^{-7}$  eV), a unique possibility for investigating nonstationary quantum-mechanical effects.

Of particular interest is the case when the frequency of a nonstationary field bears the relation  $k^2 < \omega$  to the energy of the ultracold neutrons.

It is obvious that the field (107) for ultracold neutrons can be obtained, for example, by placing a ferromagnetic foil in an alternating magnetic field. Since the case  $\alpha > 0$  is realized in experiments with ultracold neutrons, their reflection has a resonance nature.

Since in reality there is an anomalously rapid leakage of ultracold neutrons from traps,<sup>[45]</sup> it appears to us

<sup>5)</sup>Here and in what follows we use a system of units with  $\hbar = 2m = 1$ .

<sup>6)</sup>Since (108) is obtained on the basis of the Schwinger variational principle, i.e., exact solution of the problem with approximate potential, it follows that this effect is not peculiar to  $\delta$ -functional forces.

very interesting to use high-frequency magnetic fields to confine ultracold neutrons.<sup>[16]</sup> In this case  $\omega \sim 10^8 - 10^{10} \text{ (sec)}^{-1}$ . Such frequencies are readily obtainable. In addition, it is of considerable interest to make an experimental study of the resonances. It is possible that this effect could be used to obtain monoenergetic ultracold neutrons.

To consider the interaction of the ultracold neutrons with the walls of the trap, it is necessary to take into account the acoustic vibrations of the trap. This interaction can be described by a potential of the form

$$V(x, t) = -\alpha \delta(x - \lambda \cos \omega t). \quad (109)$$

Using the approximation (106), we readily obtain a formula for the amplitude of the elastically reflected wave:

$$a_{-k} = \frac{1}{i} \frac{\alpha^2 J_0^2(2k\lambda)}{-\alpha J_0(2k\lambda) + \frac{\alpha^2}{2\pi i} \sum_{m=-\infty}^{\infty} \int dq \frac{J_m(\lambda(q-k)) J_m(\lambda(q+k))}{q^2 - k^2 + m\omega - i\varepsilon}}. \quad (110)$$

In contrast to (108), in (110) we have taken into account the virtual absorption and emission of infinitely many quanta.

To conclude this section, we consider the interesting although little investigated possibility of extending the results obtained in this section to the theory of nuclear reactions. The point is that almost all theoretical models are based in some sense on the concept of single-particle stationary motion. One such approximation—the optical potential—is widely used. We can complicate the simple single-particle motion by introducing into the potential a time dependence, which appears because of the motion of the nucleons in the nucleus. The suggestion is therefore to replace the many-channel system of equations describing the scattering of a particle on a bound complex by the problem of the scattering of the particle on an effective potential  $U_{\text{eff}}(r, t)$  which depends on the time.

It is known that at low energies nuclear reactions have a resonance nature, while direct processes are dominant at higher energies. This fact finds a simple explanation in a theory with time-dependent effective potential. Indeed, it follows from (108) that there are resonances when  $k^2 < \omega$  but these disappear at energies greater than  $\omega$ .

## CONCLUSIONS

Let us list the main properties of the Schwinger variational principle.

1. It enables one to describe in a unified manner bound-state problems, scattering, and nonstationary problems.
2. In reality, it is a dynamical approach since the problem is solved by replacing  $V$  by  $V^{(N)}$ , and  $|V - V^{(N)}|$  characterizes the error.
3. If  $V$  is a completely continuous operator, the convergence of the method is ensured by the well known theorem on the approximation of a completely continuous operator by an operator of finite rank.

4. If the original interaction is described by an operator of finite rank  $N$ , the variational principle obtained with an  $N$ -term separable representation leads to the exact value for all trial functions.

5. The Schwinger variational principle is obtained as a result of factorizing the interaction, while the kinetic energy, i.e., the asymptotic behavior of the solution, remains correct for all functions. Therefore, in calculations of the binding energies and wave functions of light nuclei with oscillator trial functions the method will converge rapidly, in contrast to the Ritz variational principle.

It should be noted that the Schwinger variational principle is somewhat more complicated than the Ritz, Kohn, and Hulthén principles since it contains an integral of the form  $\langle \eta | V G_0 V | \eta \rangle$ ; for this reason, the opinion has even been expressed (see, for example, Ref. 46) that the Schwinger variational principle is not particularly convenient in practical calculations. However, the advantages of the Schwinger formula, which we have considered in detail here, and also the possibility of choosing comparatively simple trial function encourage the belief that this principle is helpful in quantum-mechanical problems.<sup>[7]</sup>

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<sup>7</sup>In this paper, we have not considered the connection between the Schwinger variational principle and the method of Padé approximation<sup>[47]</sup> nor the application of it to the solution of the Faddeev equations<sup>[48]</sup> and relativistic equations.<sup>[49]</sup>

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