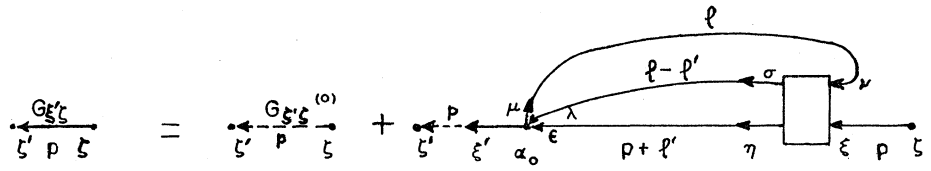

FIG. 6. Graphical representation of Eq. (9).

(the graphical equivalent of which is shown in Fig. 6), they are a closed system, making it possible to express Γ and G in terms of Γ_0.

In conclusion the author wishes to acknowledge his indebtedness to I. Y. Pomeranchuk for valuable discussions.

PHYSICAL REVIEW VOLUME 111, NUMBER 3 AUGUST 1, 1958

Variational Methods in Scattering Problems

MILDRED MOE* AND DAVID S. SAXON†
University of California, Los Angeles, California
(Received April 9, 1958)

Modifications of the Hulthén-Kohn variational principle are introduced with the hope of increasing the usefulness of variational methods. Although no simple formulation of general utility is found, it is shown that there exists a great variety of stationary expressions which make possible a greater freedom in the choice of variational principles than has hitherto been demonstrated. Some criteria for the selection of special forms are discussed.

I. INTRODUCTION

CONSIDERABLE attention has been given in the past to the development of variational principles for scattering problems.[1–4] However, the utility of these principles is limited by the difficulty of finding good trial functions and evaluating the necessary integrals, particularly so for the total scattering amplitude. In Schwinger's variational principle, the impediment is the evaluation of the double integral containing the Green's function. Even for plane waves, which are the simplest trial functions, this integral is not easy. On the other hand, the Hulthén-Kohn variational principle, which involves simpler integrations, is limited by the difficulty of finding adequate trial functions. The structure of this variational principle is such that it requires better trial functions than Schwinger's principle. For example, plane wave trial functions, which give a result similar to the second Born approximation in the Schwinger case, yield merely the first Born approximation in the Hulthén-Kohn case.

Our main purpose in the present paper is to discuss what might be done to overcome these difficulties. As we shall show, the Hulthén-Kohn and Schwinger principles are not the only stationary expressions for the scattering amplitude. There is a limitless number of other forms which may be obtained in a simple way. However, we have been unable to exploit this freedom sufficiently to construct variational principles entirely free of the troubles mentioned above. In any case, the existence of this great variety of forms is of independent interest.

II. FORMS OF THE VARIATIONAL PRINCIPLE

Schrödinger's equation for a two-body interaction can be written in the dimensionless form

$$[\nabla^2+k^2-V(\mathbf{x})]\psi(\mathbf{x})=0, \tag{1}$$

where

$$\mathbf{x}=\mathbf{r}/a, \quad k^2=2ma^2E/\hbar^2,$$

and

$$V(\mathbf{x})=(2ma^2/\hbar^2)V_0(a\mathbf{x}).$$

Here m is the reduced mass, E is the energy in the center-of-mass system, V_0 is the potential energy of interaction, and a is a characteristic length associated with the range of the potential.

The well-known integral equation corresponding to Eq. (1) is

$$\psi_k(\mathbf{x})=e^{i\mathbf{k}\cdot\mathbf{x}}-\int G(\mathbf{x},\mathbf{x}')V(\mathbf{x}')\psi_k(\mathbf{x}')d\mathbf{x}', \tag{2}$$

* Present address, The Ramo-Wooldridge Corporation, Los Angeles, California.

† Supported in part by the National Science Foundation.

[1] L. Hulthén, Kgl. Fysiograf. Sällskap. hund Förh. **14**, 257 (1944); Den 10 Skandinaviske Matematiker Kongres (1946), p. 201; Arkiv Mat. Astron. Fysik **35A**, No. 25 (1948).

[2] J. Schwinger, lectures on nuclear physics, Harvard University, 1947 (unpublished); H. Levine and J. Schwinger, Phys. Rev. **74**, 958 (1948).

[3] W. Kohn, Phys. Rev. **74**, 1763 (1948); **84**, 495 (1951).

[4] H. Feshbach and S. I. Rubinow, Phys. Rev. **88**, 484 (1952); S. I. Rubinow, Phys. Rev. **98**, 183 (1955).

where the Green's function is

$$G(\mathbf{x},\mathbf{x}')=\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}.$$

The subscript $\mathbf{k}$ on $\psi_{\mathbf{k}}(\mathbf{x})$ means that the incident wave is along the direction of $\mathbf{k}$. At large distances from the scattering center, we have

$$\psi_{\mathbf{k}}(\mathbf{x})\simeq e^{i\mathbf{k}\cdot\mathbf{x}}+f(\mathbf{k}\to\mathbf{k}')\frac{e^{ikx}}{x}, \tag{3}$$

where $\mathbf{k}'$ is the propagation vector of the scattered wave. The amplitude for scattering from the direction along $\mathbf{k}$ to that along $\mathbf{k}'$ is given by

$$f(\mathbf{k}\to\mathbf{k}')=-\frac{1}{4\pi}\int e^{-i\mathbf{k}'\cdot\mathbf{x}'}V(\mathbf{x}')\psi_{\mathbf{k}}(\mathbf{x}')d\mathbf{x}'. \tag{4}$$

When the potential is spherically symmetric, expansion of the wave function in spherical harmonics yields

$$\left[\frac{d^2}{dx^2}+k^2-V(x)-\frac{l(l+1)}{x^2}\right]u_l(kx)=0, \tag{5}$$

where the $u_l(kx)$ are the radial wave functions. The corresponding integral equation is

$$u_l(kx)=kxj_l(kx)-\int_0^\infty G_l(x,x')V(x')u_l(kx')dx', \tag{6}$$

where

$$G_l(x,x')=-kxx'j_l(kx_<)n_l(kx_>).$$

Here $x_<$ is the smaller and $x_>$ the larger of x and x' and j_l and n_l are the spherical Bessel and Neumann functions. The function $u_l(kx)$ must satisfy the usual boundary condition

$$u_l(0)=0,$$

and, for $x\to\infty$,

$$u_l(kx)\simeq\sin(kx-\tfrac{1}{2}l\pi)+\tan\delta_l\cos(kx-\tfrac{1}{2}l\pi), \tag{7}$$

where δ_l is the phase shift of the lth partial wave. The usual expression for $\tan\delta_l$ is found by letting x approach infinity in Eq. (6),

$$\tan\delta_l=-\int_0^\infty xj_l(kx)V(x)u_l(kx)dx. \tag{8}$$

Instead of starting from the differential equation (5) to form (6), one can start from the integral equation (2) and, by expanding the wave function in spherical harmonics, obtain an integral equation for a slightly different radial function, w_l, namely,

$$w_l(kx)=kx\left[j_l(kx)-\frac{1}{k}\times\int_0^\infty g_l(x,x')V(x')w_l(kx')x'dx'\right], \tag{9}$$

where

$$g_l(x,x')=ikj_l(kx_<)h_l^{(1)}(kx_>),$$

and where $h_l^{(1)}(kx)$ is the spherical Hankel function. The function $w_l(kx)$ satisfies Eq. (5) and the condition

$$w_l(0)=0,$$

and, for $x\to\infty$,

$$w_l(kx)\simeq\sin(kx-\tfrac{1}{2}l\pi)+\frac{\tan\delta_l}{1-i\tan\delta_l}e^{i(kx-\frac{1}{2}l\pi)}. \tag{10}$$

The relationship between the two radial functions is thus seen to be

$$u_l(kx)=(1-i\tan\delta_l)w_l(kx). \tag{11}$$

In either case, the scattering amplitude is given in terms of the phase shifts by

$$f(\mathbf{k}\to\mathbf{k}')=\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\frac{\tan\delta_l}{1-i\tan\delta_l}P_l(\cos\theta), \tag{12}$$

where θ is the scattering angle; that is, the angle between $\mathbf{k}$ and $\mathbf{k}'$.

The Hulthén-Kohn principle is based directly on the Schrödinger equation (1). In Kohn's form of the principle, it is required that the trial wave functions have the correct asymptotic form; that is, that

$$\psi_{\mathbf{k}}(\mathbf{x})\simeq e^{i\mathbf{k}\cdot\mathbf{x}}+f_1(\mathbf{k}\to\mathbf{k}'')e^{ikx}/x, \tag{13}$$

and

$$\psi_{-\mathbf{k}'}(\mathbf{x})\simeq e^{-i\mathbf{k}'\cdot\mathbf{x}}+f_2(-\mathbf{k}'\to\mathbf{k}'')e^{ikx}/x,$$

where f_1 and f_2 are trial scattering amplitudes in the indicated directions. Then Kohn's variational principle states that the expression

$$4\pi f(\mathbf{k}\to\mathbf{k}')=4\pi f_1(\mathbf{k}\to\mathbf{k}')+I, \tag{14}$$

where

$$I=\int\psi_{-\mathbf{k}'}(\mathbf{x})[\nabla^2+k^2-V(x)]\psi_{\mathbf{k}}(\mathbf{x})d\mathbf{x} \tag{15}$$

is stationary for independent variations of $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$ about their correct values as given by Eq. (1).

Observe that this variational principle depends on the amplitudes of $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$. Evidently, it might be advantageous to rewrite this result in such a way that it is independent of the amplitudes of the unknown trial fields. One way of accomplishing this is the following: let the trial functions be expressed as

$$\begin{aligned}\psi_{\mathbf{k}}(\mathbf{x})&=e^{i\mathbf{k}\cdot\mathbf{x}}+U(\mathbf{x}),\\ \psi_{-\mathbf{k}'}(\mathbf{x})&=e^{-i\mathbf{k}'\cdot\mathbf{x}}+W(\mathbf{x}),\end{aligned} \tag{16}$$

where $U(\mathbf{x})$ and $W(\mathbf{x})$ are scattered waves which must have the asymptotic forms given in Eq. (13). Notice that U and W then become the trial quantities which enter into Kohn's principle. To find a form which is independent of the amplitudes of U and W, assign amplitudes a and b, respectively, to them. The integral

(15) may then be expressed as

$$I=4\pi f_B(\mathbf{k}\to\mathbf{k}')-4\pi a f_1(\mathbf{k}\to\mathbf{k}')+aA'+bB'-abC',$$

where f_B is the Born approximation scattering amplitude,

$$4\pi f_B(\mathbf{k}\to\mathbf{k}')=-\int e^{-i\mathbf{k}'\cdot\mathbf{x}}V(x)e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{x}, \quad (17a)$$

and where

$$-4\pi f_1(\mathbf{k}\to\mathbf{k}')=\int e^{-i\mathbf{k}'\cdot\mathbf{x}}[\nabla^2+k^2]U(\mathbf{x})d\mathbf{x}, \quad (17b)$$

$$A'=-\int e^{-i\mathbf{k}'\cdot\mathbf{x}}V(x)U(\mathbf{x})d\mathbf{x}, \quad (17c)$$

$$B'=-\int W(\mathbf{x})V(x)e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{x}, \quad (17d)$$

$$C'=-\int W(\mathbf{x})[\nabla^2+k^2-V(x)]U(\mathbf{x})d\mathbf{x}. \quad (17e)$$

Then Eq. (14) becomes

$$4\pi f(\mathbf{k}\to\mathbf{k}')=4\pi f_B(\mathbf{k}\to\mathbf{k}')+aA'+bB'-abC'.$$

Making this stationary with respect to independent variations of a and b, we obtain

$$4\pi f(\mathbf{k}\to\mathbf{k}')-4\pi f_B(\mathbf{k}\to\mathbf{k}')=A'B'/C', \quad (18)$$

which we shall call the amplitude independent form of Kohn's principle.[5]

Now, as has been mentioned, the difficulty in using the Hulthén-Kohn principle is that of constructing adequate trial functions. The utility of amplitude-independent forms in this connection is indicated for the Schwinger principle by Gerjuoy and Saxon.[6] For convenience we briefly describe the method. Recall that Schwinger's principle is

$$4\pi f(\mathbf{k}\to\mathbf{k}')=A_sB_s/C_s, \quad (19)$$

where

$$A_s=-\int e^{-i\mathbf{k}'\cdot\mathbf{x}}V(x)\psi_{\mathbf{k}}(\mathbf{x})d\mathbf{x},$$
$$B_s=-\int e^{i\mathbf{k}\cdot\mathbf{x}}V(x)\psi_{-\mathbf{k}'}(\mathbf{x})d\mathbf{x}, \quad (20)$$

and

$$C_s=-\int\psi_{\mathbf{k}}(\mathbf{x})V(x)\psi_{-\mathbf{k}'}(\mathbf{x})d\mathbf{x}$$
$$-\int\int\psi_{\mathbf{k}}(\mathbf{x})V(x)G(\mathbf{x},\mathbf{x}')V(x')\psi_{-\mathbf{k}'}(\mathbf{x}')d\mathbf{x}d\mathbf{x}'.$$

Instead of choosing $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$ simply as plane waves, one can construct more elaborate trial functions from generalized sets of partial waves as follows: expand $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$ in a set of functions $\phi_n{}^{\mathbf{k}}$ and $\phi_n{}^{-\mathbf{k}'}$ which are eigenfunctions of some symmetry operator which commutes with the Hamiltonian[7]; for example, the spherical harmonics or the eigenfunctions of the parity operator. When it is required that Eq. (19) be stationary with respect to variations of the coefficients of the ϕ's, Schwinger's principle takes the form

$$4\pi f(\mathbf{k}\to\mathbf{k}')=\sum_{n=1}^{N}\frac{A_{sn}B_{sn}}{C_{sn}}, \quad (21)$$

where A_{sn}, B_{sn}, and C_{sn} are the same as A_s, B_s, and C_s but with $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$ replaced by $\phi_n{}^{\mathbf{k}}$ and $\phi_n{}^{-\mathbf{k}'}$. In case the ϕ's are the spherical harmonics, (21) becomes the usual infinite sum (12) over the angular momentum states in which the phase shifts, δ_l, are to be evaluated by Schwinger's principle for the phase shifts:

$$k(\cot\delta_l-i)=\frac{-\int_0^\infty V(x)w_l{}^2(kx)dx-\int_0^\infty\int_0^\infty w_l(kx)V(x)g_l(x,x')V(x')w_l(kx')xx'dxdx'}{\left[-\int_0^\infty j_l(kx)V(x)w_l(kx)xdx\right]^2}. \quad (22)$$

Now, if such generalized sets of partial waves are to be utilized in Kohn's formulation, it is helpful to establish the connection between the principles for the scattering amplitude and phase shifts as was done in the Schwinger case.[6] The Kohn principle for the phase shifts requires that the radial trial functions u_l have the correct asymptotic form

$$u_l(kx)\simeq\sin(kx-\tfrac{1}{2}l\pi)+\tan\delta_{l1}\cos(kx-\tfrac{1}{2}l\pi), \quad (23)$$

where δ_{l1} is a trial phase shift. Then one obtains the expression

$$k\tan\delta_l=k\tan\delta_{l1}+I, \quad (24)$$

where

$$I=\int_0^\infty u_l(kx)\left[\frac{d^2}{dx^2}+k^2-V(x)-\frac{l(l+1)}{x^2}\right]u_l(kx)dx$$

is stationary for variations of u_l about its correct value. The amplitude-independent form of this, corresponding

[5] This form was found independently by H. E. Moses, New York University Report CX-27, July, 1956 (unpublished).

[6] E. Gerjuoy and D. S. Saxon, Phys. Rev. **94**, 478 (1954).

[7] R. J. Finkelstein and M. Moe, Phys. Rev. **100**, 1775 (1955).

to Eq. (18) for the scattering amplitude, is

$$k\tan\delta_l = k\tan\delta_{lB} - \frac{\left[\int_0^\infty kx j_l(kx)V(x)u_{sl}(kx)dx\right]^2}{\int_0^\infty u_{sl}(kx)\left[\frac{d^2}{dx^2}+k^2-V(x)-\frac{l(l+1)}{x^2}\right]u_{sl}(kx)dx}, \tag{25}$$

where

$$k\tan\delta_{lB} = -\int_0^\infty [kxj_l(kx)]^2 V(x)dx, \tag{26}$$

which is just the Bonn approximation, and where

$$u_{sl}(kx) = u_l(kx) - kxj_l(kx) \tag{27}$$

is the scattered part of the radial wave function.

To find the relationship between Kohn's principles for the amplitude and phase shifts consider first Eq. (15). Expand the trial functions in spherical harmonics; *viz.*,

$$\begin{aligned}\psi_{\mathbf{k}}(\mathbf{x}) &= \sum_{l=0}^\infty \alpha_l \frac{w_l(kx)}{kx} P_l(\cos\theta_1),\\ \psi_{-\mathbf{k}'}(\mathbf{x}) &= \sum_{l=0}^\infty \beta_l \frac{w_l(kx)}{kx} P_l(\cos\theta_2),\end{aligned} \tag{28}$$

where

$$\cos\theta_1 = (\mathbf{k}\cdot\mathbf{x})/kx,$$

and

$$\cos\theta_2 = (-\mathbf{k}'\cdot\mathbf{x})/kx.$$

The condition that the wave functions must approach the correct asymptotic form (13) means that the radial wave function w_l must satisfy (10) with δ_l replaced by δ_{l1} and that the constants α_l and β_l must be $i^l(2l+1)$. Equating coefficients of the spherical harmonics in Eq. (14), we obtain

$$\frac{k\tan\delta_l}{1-i\tan\delta_l} = \frac{k\tan\delta_{l1}}{1-i\tan\delta_{l1}} + \int_0^\infty w_l(kx) \times\left[\frac{d^2}{dx^2}+k^2-V(x)-\frac{l(l+1)}{x^2}\right]w_l(kx)dx. \tag{29}$$

In terms of u_l, this is

$$\tan\delta_l = \frac{I_l + (1-i\tan\delta_{l1})k\tan\delta_{l1}}{iI_l + k(1-i\tan\delta_{l1})}. \tag{30}$$

This is a stationary form for $\tan\delta_l$, but it is not the same as Kohn's form (24). Thus, we have two different variational principles for $\tan\delta_l$ in terms of the same quantities, $\tan\delta_{l1}$ and I_l. Note also that Eq. (30) has the undesirable feature that it gives complex approximations to the phase shifts. This means that probability is not conserved. How can we arrive at a more satisfactory variational principle for the phase shifts? An obvious procedure is to try the amplitude-independent form (18), rather than Eq. (14), as the basis for the expansion of the scattered fields in spherical harmonics. After some manipulation, it can be seen, however, that there again results a (different) complex approximation for the phase shifts. To obtain a method which does work, it is first necessary to construct a modified amplitude independent form of Kohn's principle as follows: let us choose trial functions $\psi_{-\mathbf{k}'}(\mathbf{x})$ and $U(\mathbf{x})$ and make Eq. (14) stationary with respect to independent variations of their amplitudes. We obtain then

$$4\pi f(\mathbf{k}\to\mathbf{k}') = AB/C, \tag{31}$$

where

$$\begin{aligned}A &= 4\pi f_1(\mathbf{k}\to\mathbf{k}'),\\ B &= -\int \psi_{-\mathbf{k}'}(\mathbf{x})V(x)e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{x},\\ C &= -\int \psi_{-\mathbf{k}'}(\mathbf{x})[\nabla^2+k^2-V(x)]U(\mathbf{x})d\mathbf{x}.\end{aligned} \tag{32}$$

Now the expansions in spherical harmonics can be written in the form

$$\psi_{-\mathbf{k}'}(\mathbf{x}) = \sum_{l=0}^\infty b_l \frac{w_{l2}(kx)}{kx} P_l(\cos\theta_2), \tag{33}$$

$$U(x) = \sum_{l=0}^\infty i^l(2l+1)a_l \frac{w_{sl1}(kx)}{kx} P_l(\cos\theta_1), \tag{34}$$

where the trial function w_{l2} does not have to approach the correct asymptotic form,[8] but w_{sl1} must asymptotically approach

$$\gamma_{l1}e^{i(kx-\frac{1}{2}l\pi)},$$

where

$$\gamma_{l1} = \frac{\tan\delta_{l1}}{1-i\tan\delta_{l1}}. \tag{35}$$

The requirement that Eq. (31) be stationary with respect to arbitrary independent variations of a_l and b_l

[8] It is easy to show that in the Kohn variational principle, only the function appearing on the right of the differential operator, namely $\psi_{\mathbf{k}}$, need satisfy the correct boundary condition at infinity. Here we take advantage of this freedom in the choice of $\psi_{-\mathbf{k}'}$.

leads to Eq. (12) in which the phase shifts are given by

$$\frac{\tan\delta_l}{1-i\tan\delta_l}=\frac{k\gamma_{l1}\int_0^\infty xj_l(kx)V(x)w_{l2}(kx)dx}{\int_0^\infty w_{l2}(kx)\left[\frac{d^2}{dx^2}+k^2-V(x)-\frac{l(l+1)}{x^2}\right]w_{sl1}(kx)dx},$$

or, in terms of the u_l,

$$k\cot\delta_l=\frac{\int_0^\infty u_{l2}(kx)\left[\frac{d^2}{dx^2}+k^2-V(x)-\frac{l(l+1)}{x^2}\right]u_{sl1}(kx)dx}{\tan\delta_{l1}\int_0^\infty xj_l(kx)V(x)u_{l2}(kx)dx}. \tag{37}$$

This gives real approximations to the phase shifts. Furthermore, this variational principle for the phase shifts may be obtained from Kohn's principle (24) by making it independent of the amplitudes of u_{l2} and u_{sl1}. Another interesting observation is that Schwinger's principles for the total amplitude and phase shifts may be obtained directly from Eqs. (31) and (36) by choosing trial functions

$$\psi_{-\mathbf{k}'}(\mathbf{x})=\psi_{-\mathbf{k}'}(\mathbf{x}),$$
$$U(\mathbf{x})=-\int G(\mathbf{x},\mathbf{x}')V(x')\psi_{\mathbf{k}}(\mathbf{x}')d\mathbf{x}', \tag{38}$$

and

$$w_{l2}(kx)=w_l(kx),$$
$$w_{sl1}(kx)=-x\int_0^\infty g_l(x,x')V(x')w_l(kx')x'dx'. \tag{39}$$

III. MORE GENERAL VARIATIONAL PRINCIPLES

We have seen in the above discussion that there are different stationary expressions for $\tan\delta_l$ in terms of the same quantities. For example, Eqs. (24) and (30) are completely different variational principles for $\tan\delta_l$ in terms of the specific quantities $k\tan\delta_{l1}$ and I_l. To see how this is possible, note first that the stationary property of Kohn's principle (24) is a consequence of the relation

$$\delta(k\tan\delta_{l1})=-\delta I_l \tag{40}$$

for permissible variations of u_l about the correct wave function, that is, variations such that u_l has the correct asymptotic form. Now consider a functional $H(k\tan\delta_{l1}, I_l)$ which satisfies the conditions that for the correct u_l, H reduces to $k\tan\delta_l$, and that H is stationary for permissible variations of u_l. Evidently, such a functional provides a stationary expression for $k\tan\delta_l$. The second condition means that

$$\delta H=\left.\frac{\partial H}{\partial(k\tan\delta_{l1})}\right|_0\delta(\tan\delta_{l1})+\left.\frac{\partial H}{\partial I_l}\right|_0\delta I_l=0, \tag{41}$$

where the subscript zero denotes evaluation at the correct wave function. Upon using Eq. (40), this condition becomes

$$\left.\frac{\partial H}{\partial(k\tan\delta_{l1})}\right|_0=\left.\frac{\partial H}{\partial I_l}\right|_0. \tag{42}$$

Since there are many functionals H which satisfy these conditions, it is to be expected that different starting points could well lead to different variational principles for the phase shifts.

The preceding remarks apply equally well to the scattering amplitude. To make them more general, let us consider variational principles for a quantity Q which we write

$$Q=H(z_1,z_2,\cdots,z_n). \tag{43}$$

The quantities z_i are usually integrals which are linear or bilinear in the trial functions. These might be the $k\tan\delta_{l1}$ and I_l which appear in Kohn's principle, or they might be the A', B', C', A, B, or C which appear in the amplitude independent forms for the scattering amplitude. For variations of the trial functions about their correct values, the z_i will have corresponding variations δz_i. Let H be chosen such that, for the correct trial functions,

$$H(z_{10},z_{20},\cdots,z_{n0})=Q_0, \tag{44}$$

where Q_0 is the correct value of Q. If, now, it is required that

$$\delta Q=\sum_{i=1}^n\left(\left.\frac{\partial H}{\partial z_i}\right|_0\delta z_i\right)=0, \tag{45}$$

H becomes a stationary expression for Q. Of course, the δz_i are not all independent and it is just the relations between them which provide conditions for the determination of H, as in Eq. (42), for example.

We now show how to construct some generalized variational principles using these ideas. Consider first the total scattering amplitude, $Q=4\pi f(\mathbf{k}\to\mathbf{k}')$. One way of choosing the z_i is to take

$$z_1=g=4\pi f_1(\mathbf{k}\to\mathbf{k}'),$$

and

$$z_2=I=\int\psi_{-\mathbf{k}'}(\mathbf{x})[\nabla^2+k^2-V(x)]\psi_{\mathbf{k}}(\mathbf{x})d\mathbf{x}.$$

The variations of g and I are related by $\delta g=-\delta I$. It is easy to verify that a general form for H, satisfying Eqs. (44) and (45), is

$$H=g+I+I^{1+\alpha}F_1(g,I)+F_2(I), \tag{46}$$

provided that $\alpha>0$, $F_1(g, I=0)$ is bounded, and that

$$\lim_{I\to 0}[F_2(I)/I=0].$$

A special case of Eq. (46) is

$$H=4\pi f(\mathbf{k}\to\mathbf{k}')=g+I,$$

which is just Kohn's form (14). Equally possible forms, however, are for example,

$$H=g^2/(g-I), \tag{47}$$

or

$$H=ge^{I/g}, \tag{48}$$

and, of course, there is no *a priori* basis for choosing among them.

Other variational principles for the scattering amplitude may be found by taking the z_i to be the quantities A, B, and C of Eqs. (32). It is easy to show that, for the correct wave functions, we have

$$A_0=B_0=C_0=4\pi f_0(\mathbf{k}\to\mathbf{k}'),$$

and that for variations about these values, we have

$$\delta A+\delta B=\delta C. \tag{49}$$

Thus we seek functionals H such that

$$H(A_0,B_0,C_0)=4\pi f_0(\mathbf{k}\to\mathbf{k}'),$$

where, from Eqs. (45) and (49),

$$\left.\frac{\partial H}{\partial A}\right|_0=\left.\frac{\partial H}{\partial B}\right|_0=-\left.\frac{\partial H}{\partial C}\right|_0.$$

A general form for H which satisfies these requirements is

$$H(A,B,C)=G_1(A,B,C)+(A-C)G_2(B)+(B-C)G_3(A), \tag{50}$$

where G_1 can be any function which reduces to $4\pi f_0$ for the correct fields, and where G_2 and G_3 are given by

$$G_2(B)=\left.\frac{\partial G_1}{\partial B}\right|_{A=B;\,C=B}+\left.\frac{\partial G_1}{\partial C}\right|_{A=B;\,C=B}, \tag{51}$$

and

$$G_3(A)=\left.\frac{\partial G_1}{\partial A}\right|_{B=A;\,C=A}+\left.\frac{\partial G_1}{\partial C}\right|_{B=A;\,C=A}.$$

Some simple special cases are

$$H=A+B-C,$$

which is again Kohn's form, and

$$H=AB/C,$$

which is the amplitude independent form (31).

Still other principles can be constructed in the same way from A', B', and C' which have the properties

$$A_0'=B_0'=C_0'=4\pi f_0(\mathbf{k}\to\mathbf{k}')-f_B(\mathbf{k}\to\mathbf{k}'), \tag{52}$$

and

$$\delta A'+\delta B'=\delta C'.$$

The amplitude-independent form of Kohn's principle,

$$H=4\pi[f(\mathbf{k}\to\mathbf{k}')-f_B(\mathbf{k}\to\mathbf{k}')]=A'B'/C', \tag{18}$$

is an example.

Even more complicated variational principles can be constructed by introducing additionally the trial scattering amplitude $f_1(\mathbf{k}\to\mathbf{k}')$. A particularly interesting example is the form

$$H=4\pi f(\mathbf{k}\to\mathbf{k}')=-\frac{(4\pi f_1B')^2}{C'[4\pi f_BC'+B'(A'-8\pi f_1)]}, \tag{53}$$

which is stationary and independent of the amplitudes of the trial scattered waves, U and W. The existence of more than one amplitude independent form is a new feature; the amplitude-independent form of the Schwinger principle is unique.

Variational principles for the phase shifts are completely analogous to those for the scattering amplitude. For example, the form for the phase shifts corresponding to Eq. (53) is

$$k\tan\delta_l=-\frac{[k\tan\delta_{l1}B_l']^2}{C_l'[C_l'k\tan\delta_{lB}+B_l'(A_l'-2k\tan\delta_{l1})]}, \tag{54}$$

where

$$A_l'=-\int_0^\infty kxj_l(kx)V(x)u_{sl1}(kx)dx,$$

$$B_l'=-\int_0^\infty kxj_l(kx)V(x)u_{sl2}(kx)dx,$$

and

$$C_l'=-\int_0^\infty u_{sl2}(kx)\left[\frac{d^2}{dx^2}+k^2-V(x)-\frac{l(l+1)}{x^2}\right]u_{sl1}(kx)dx.$$

IV. CRITERIA FOR THE SELECTION OF SPECIAL FORMULATIONS

It is clear from the preceding discussion that we are free to choose among many variational expressions. We now consider the possibility of exploiting this freedom. Ideally, one would like to find forms which, in some sense, give the best possible approximation for given trial functions. An obvious measure of the accuracy of an approximation is the size of the higher variations. Can one control these quantities by choosing suitable stationary expressions? As far as we can tell, the answer is no. We have been unable to find any variational principles which decrease the higher variations

for any physically reasonable class of trial functions.[9] As an alternative, one might look at just the second variation with the hope that it could be made positive (or negative) definite. If so, a systematic approach to the correct solution, which would be an extremum, would be possible as in the Rayleigh-Ritz method. Unfortunately, the quantities z_i which enter into the construction of the variational principles are such that the second variations cannot be made to take on a definite sign.[9]

A second approach to the problem of choosing appropriate variational principles for the scattering amplitude is the following: one can try to select them in such a way that the general characteristics of scattering processes are not violated. Specifically, it seems reasonable to require that reciprocity and the unitarity of the scattering be maintained. The former is automatically built in to many of the variational expressions and in no case does it cause a serious problem. As far as the latter is concerned, the situation is more complicated. We have already seen that unitarity is generally not satisfied. Indeed, we found it difficult to construct variational principles, for appropriate trial functions, which gave real phase shifts and therefore conserved probability. By appropriate, we mean trial functions which are expanded in spherical harmonics, the coefficients of which are variationally determined—as in the derivation of Eq. (37). Since such functions contain a set of parameters, each of which is variationally determined, they must be regarded as very special trial functions. We shall call these trial functions "variationally best." Actually, it is possible to construct formal expressions for the scattering amplitude which satisfy unitarity regardless of the form of the trial functions, as discussed by Lippmann and Schwinger.[10] This was accomplished by introducing the so-called reactance matrix. However, the relation between the reactance matrix and the scattering amplitude is sufficiently complicated that the method cannot be easily used.[11] About the best we can do is to choose a variational form, like that of Eq. (31), which conserves probability at least for those trial functions which are "variationally best." Presumably such a form is better than one which violates unitarity under all conditions.

This seems to be about as far as one can go with criteria based on the general properties of scattering. Further criteria might, however, be based on more practical considerations. The property of amplitude independence is obviously useful in this respect, as has already been discussed in connection with the Schwinger principle.[6] Incidently, we might remark on why the Schwinger form is such a good one. Besides being amplitude-independent, it preserves probability when the "variationally best" trial functions are used and it automatically satisfies reciprocity. In addition, if regarded as a special case of Eq. (31), it uses the Schrödinger equation itself to generate the trial fields. From the practical standpoint, however, the Schwinger form has a serious disadvantage, the difficulty of evaluating the integral containing the Green's function. Thus, only the simplest trial functions can be used. This brings us to our final consideration in the choice of a variational principle, the ease of evaluating the integrals. A formulation which is theoretically inferior to Schwinger's but which allows more complicated trial functions might still give a more useful approximation to the scattering amplitude. For example, if we wish to calculate a correction to the Born approximation, the form

$$4\pi f=4\pi f_B+A'B'/C'$$

is a good one because it is amplitude-independent. It does not, however, preserve probability when the "variationally best" trial functions are used. Equation (31) which does preserve probability for such trial functions might be a better form to use. Of course, we must find trial functions which are simpler than those of Eq. (38) which lead to Schwinger's form. For instance, we might try choosing

$$\psi_{-\mathbf{k}'}(\mathbf{x})=e^{-i\mathbf{k}'\cdot\mathbf{x}},$$

and a trial scattered field U which behaves asymptotically like the Born scattered wave, namely,

$$U(\mathbf{x})\simeq f_B(\mathbf{k}\to\mathbf{k}'')\frac{e^{ikx}}{x},\quad x\to\infty.$$

Then (31) becomes

$$f(\mathbf{k}\to\mathbf{k}')=\frac{4\pi f_B^2(\mathbf{k}\to\mathbf{k}')}{4\pi f_B(\mathbf{k}\to\mathbf{k}')+\int e^{-i\mathbf{k}'\cdot\mathbf{x}}V(x)U(\mathbf{x})d\mathbf{x}}. \quad (55)$$

The advantage of this form is that, next to the first Born approximation, it is one of the simplest formulas for calculating the scattering amplitude. In general, it gives a nonzero imaginary part in the forward direction (unlike first Born) and so may be used with the cross-section theorem to provide a simple estimate of the total cross section. We have tested the utility of this form by calculating scattering amplitudes for neutron-proton scattering by the Yukawa potential at intermediate energies. With a trial scattered wave of the form

$$U(\mathbf{x})=(1-e^{-\mu x})f(\mathbf{k}\to\mathbf{k}'')\frac{e^{ikx}}{x},$$

the numerical results[9] appear roughly comparable to those obtained in the second Born.

We have also tried using other modifications of the Kohn principle. The results of some systematic though

[9] M. Moe, thesis, January, 1957, University of California at Los Angeles (unpublished).
[10] B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950).
[11] See reference 9 for discussion of a high-energy approximation to the reactance matrix formulation.

crude calculations show that it is difficult to obtain good approximations from the formulations for the total scattering amplitude. The formulations for the phase shifts are much easier to use and, as noted by others, give fairly good answers. Scattering amplitudes calculated from these phase shifts automatically conserve probability. The only disadvantage in using the phase shifts is that, at intermediate and high energies, one must calculate large numbers of them to obtain the scattering amplitude.

In closing, it might be worth mentioning a method which removes some of this difficulty and gives good results in an essentially closed form. It can be obtained by combining the Born scattering amplitude with a few variationally determined phase shifts. This is done by re-writing the Born scattering amplitude, f_B, given in Eq. (17a), in the form

$$f_B(\theta)=\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\tan\delta_{lB}P_l(\cos\theta), \qquad (56)$$

where $\tan\delta_{lB}$ is given by Eq. (26). Subtracting Eq. (56) from the usual phase shift expansion, Eq. (12), we have

$$f(\theta)-f_B(\theta)=\frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\left[\frac{\tan\delta_l}{1-i\tan\delta_l}-\tan\delta_{lB}\right]P_l(\cos\theta).$$

Since the Born phase shifts are not far from the correct ones for the higher l values when the phase shifts become small for most potentials, the right side converges satisfactorily. Even if only one or two terms are retained in the sum, the results are surprisingly good.[9] Consequently, only one or two phase shifts need be determined and for that purpose, variational methods are quite satisfactory.

ACKNOWLEDGMENT

We wish to thank Professor E. Gerjuoy for suggesting the possible utility of an amplitude-independent form of the Hulthén-Kohn variational principle.

PHYSICAL REVIEW VOLUME 111, NUMBER 3 AUGUST 1, 1958

Two-Component Fermion Theory*

LAURIE M. BROWN
Northwestern University, Evanston, Illinois
(Received March 4, 1958)

The relativistic generalization of Pauli's equation for the electron has recently motivated Feynman and Gell-Mann to propose a specific form of universal Fermi interaction. Particles satisfying this equation are studied from the viewpoint of their electromagnetic interaction. It is found that an anomalous magnetic moment similar to the Pauli moment violates the Hermiticity of the theory, and that only vector and axial vector interactions lead to simple two-component equations, even with parity conservation. Rules for calculation in quantum electrodynamics are developed which have definite advantages over the usual Dirac formulation.

BY considering a description of the known fermions in terms of two-component spinors satisfying the relativistic generalization of the Pauli equation and requiring that only direct (nonderivative) couplings act in the weak interactions, Feynman and Gell-Mann[1] have been led to a universal Fermi interaction which is essentially unique[2] and which has a considerable measure of agreement with experiment. While the solutions of the Dirac equation even in the presence of the electromagnetic field are exactly equivalent to those of the relativistic Pauli equation, the latter equation is more restrictive in several useful ways: it is CP-invariant, but not separately C- and P-invariant (though electromagnetic *effects* have the full invariance); it does not permit the simple addition of an anomalous intrinsic magnetic moment; it leads to a unique Fermi interaction when derivative couplings are excluded. It leads to *simple* interaction forms only of the vector and axial vector types, even for parity-conserving interactions (though this is not certain to be an advantage).

The present work is mainly concerned with a detailed formulation of the electromagnetic interaction of the two-component fermion and its relation to the Dirac formalism. New physical results do not, and should not, appear since the present predictions of quantum electrodynamics are in substantial agreement with experiment. However, one is led to calculational methods which are simpler; also, well-known results can be exhibited with a transparency which is sometimes clouded in the Dirac formalism. For example, the parity-conserving property of electromagnetic interactions will be seen to follow from a symmetry between the fermion spinor and a certain derivative spinor or,

* Work supported in part by the National Science Foundation.
[1] R. P. Feynman and M. Gell-Mann, Phys. Rev. **109**, 193 (1958).
[2] R. E. Marshak and G. Sudarshan, as well as J. J. Sakurai, and others, have also proposed this interaction.