

Variational Scattering Theory in Momentum Space I. Central Field Problems

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(Received July 23, 1951)

Variational principles for scattering problems in a central field are formulated in momentum space and studied in detail. The method allows of generalization to collisions of composite particles, including disintegrations, into more than two end products, which will be discussed in a forthcoming paper.

I. INTRODUCTION

THE variational method has for many years been a valuable tool for the solution of the Schrodinger equation in bound state problems. But only rather recently Hulthén¹ has pointed out that it may also be applied to a study of scattering phenomena. Following Hulthén's work, which dealt with one-dimensional equations, the method was slightly modified by the author and extended to more general problems.² These included calculation of the scattering amplitude in three-dimensional collision problems, and of the elements of the scattering matrix in elastic or inelastic collisions of composite particles, with the limitation that no disintegrations into three or more units were energetically allowed.

Such methods were applied by the author² and more extensively by Verde and Troesch³ to the collisions of neutrons and deuterons, and by Huang⁴ and Massey and Moiseiwitsch⁵ to the scattering of electrons by a hydrogen atom.

A different approach, based on an integral equation formulation of the Schrodinger equation, has been developed by Schwinger⁶ and extensively applied to collisions of two elementary particles. However, no useful generalization of this method to yield the elements of the scattering matrix in collisions of composite particles has so far been found.

Variational methods have already been so useful in collision theory that for some time it has seemed very desirable to generalize them further, so as to cover the many physically interesting processes in which two composite particles collide and break up into three or more units. Examples are the disintegration of a deuteron by a fast neutron or the ionization of a hydrogen atom by a high energy electron. The difficulty in carrying out this generalization lay in the fact that when a disintegration into three or more particles can take

place, the form of the wave function in the asymptotic region is very complicated due to the involved correlation of the positions and momenta of the particles. On the other hand it was to be expected that such a generalization is in principle possible.

Meanwhile, the clue for overcoming these difficulties had been given quite a long time ago by Heisenberg⁷ in his work on the S -matrix. It was shown there that the asymptotic behavior of the wave function in coordinate space is reflected in the singularities of the momentum wave function. Generalizing a result obtained by Dirac,⁸ Heisenberg showed that the asymptotic behavior of several outgoing particles is described, in momentum space, quite simply by a singularity of the form $\delta_+(E - \sum_i p_i^2/2m_i)$, where $\delta_+(x) = (2\pi ix)^{-1} + \frac{1}{2}\delta(x)$, E is the total energy and p_i , m_i are the momenta and masses of the particles.

This suggested investigating the entire variational theory of collision processes in momentum space. Indeed it is somewhat surprising that this was not done earlier, since the momentum representation is probably the most natural one for a description of scattering.

In bound state problems, one does not find any essentially new features by going into the momentum space. In fact the coordinate and momentum wave functions have a rather similar character since they are both finite and both vanish as their arguments approach infinity.

On the other hand, in collision theory the coordinate wave function extends over infinite regions of space but is finite everywhere, while the momentum wave function vanishes at infinity but has very significant singularities. It is not surprising then that the formulation of variational principles in momentum space differs considerably from the corresponding formulation in coordinate space. In particular, the greater simplicity of the momentum wave function suggests directly a variational formulation of disintegration processes.

The present paper introduces the momentum space method in the simple case of central field problems. Such problems have been studied in great detail in coordinate space so that one has considerable familiarity with them. Just for this reason they afford a good practice ground to get acquainted with the characteristic features of

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¹ L. Hulthén, *Arkiv Mat. Astron. Fysik*, **35A**, No. 25 (1948); references to Hulthén's earlier work may be found in this paper.

² W. Kohn, *Phys. Rev.* **74**, 1763 (1948).

³ M. Verde, *Helv. Phys. Acta* **22**, 339 (1949). A. Troesch and M. Verde, *Helv. Phys. Acta* **24**, 39 (1951).

⁴ S. S. Huang, *Phys. Rev.* **76**, 477 (1949).

⁵ H. S. W. Massey and B. L. Moiseiwitsch, *Proc. Roy. Soc. (London)* **205**, 483 (1951).

⁶ J. Schwinger, mimeographed lecture notes (Harvard, 1947).

⁷ W. Heisenberg, *Z. Physik* **120**, 513 (1943).

⁸ P. A. M. Dirac, *Quantum Mechanics* (Clarendon Press, Oxford, 1947), third edition, Sec. 50.

variational scattering theory in the somewhat "unanschaulich" momentum space. The generalization to three-dimensional problems and to collisions of composite particles will be given in a forthcoming paper.

II. THE SINGULARITIES OF THE MOMENTUM WAVE FUNCTION

It is well known that in the case of a single particle scattered by a spherically symmetrical center of force and in the case of two particles interacting through a central potential, the Schroedinger equation can be separated and leads to a radial equation for each angular momentum, l . For S -scattering, $l=0$, one obtains the equation,

$$[-(\partial^2/\partial x^2) + V(x) - k^2]\psi(x) = 0, \quad (2.1)$$

where $V(x)$ and k^2 are proportional to the potential and total energy respectively. We shall confine ourselves to the case of $l=0$ until Sec. VII, when we shall make the obvious extension to higher angular momenta.

If the potential falls off more rapidly than x^{-1} , the wave function ψ satisfies the boundary conditions,

$$\psi(0) = 0, \quad \lim_{x \rightarrow \infty} \psi(x) = \sin kx + \tan \eta \cos kx, \quad (2.2)$$

where η is the phase shift whose evaluation is the object of a theoretical scattering calculation.

Passing to the momentum representation, we note that the eigenfunctions of the square of the momentum satisfying the first of the boundary conditions (2.2) are $\sin px$. Hence we expand $\psi(x)$ as

$$\psi(x) = \int_0^\infty \varphi(p) \sin px dp \quad (2.3)$$

with the understanding that if $\varphi(p)$ is singular, the principal value of the integral is to be taken. Substituting (2.3) into (2.1) and defining

$$V(p, p') = V(p', p) = (2/\pi) \int_0^\infty \sin p'x V(x) \sin px dx \quad (2.4)$$

we obtain the usual momentum space equation,

$$(p^2 - k^2)\varphi(p) + \int_0^\infty V(p, p')\varphi(p')dp' = 0, \quad (2.5)$$

where again the principal value of the integral is understood.

We are interested in the behavior of $\psi(x)$ for large values of x and therefore must examine how this behavior is reflected in the momentum space function $\varphi(p)$. Now it is well known that if $g(p)$ is a function free from singularities, then $\int_0^\infty g(p) \sin px dp \rightarrow 0$ as $x \rightarrow \infty$; for, due to the highly oscillatory character of $\sin px$, the positive and negative contributions to the integral tend to cancel. It follows that if we transform back from momentum to coordinate space by means of (2.3) only

the singularities of $\varphi(p)$ will determine the asymptotic behavior of $\psi(x)$.

To examine the singular behavior of $\varphi(p)$, we replace (2.5) by the integral equation,

$$\varphi(p) = \delta(p - k) - \frac{1}{p^2 - k^2} \int_0^\infty V(p, p')\varphi(p')dp'. \quad (2.6)$$

Actually the inhomogeneous term, $\delta(p - k)$ should be multiplied by an arbitrary constant; however, choosing this constant equal to 1 merely fixes a convenient normalization of the wave function. Now since $V(p, p')$ is a regular function of p and p' , the integral in (2.6) is also a regular function of p , even though $\varphi(p)$ has singularities. Thus we see that the singular behavior of $\varphi(p)$ can be described by the expression,

$$\varphi(p) = \delta(p - k) - B(p)/(p^2 - k^2), \quad (2.7)$$

with the understanding that $B(p)$ is free from singularities.

Our previous considerations already indicated that the phase shift η is determined by the value of B at the singular point $p = k$. To show this in detail we transform (2.7) back to coordinate space by means of (2.3), giving

$$\psi(x) = \sin kx - \int_0^\infty \frac{B(p)}{p^2 - k^2} \sin px dp. \quad (2.8)$$

We separate out the singular part of $B(p)/(p^2 - k^2)$ by writing

$$\frac{B(p)}{p^2 - k^2} = \frac{B(k)}{2k} \frac{1}{p - k} + \left[\frac{B(p)}{p^2 - k^2} - \frac{B(k)}{2k(p - k)} \right]. \quad (2.9)$$

For large x the term in square brackets which is regular gives no contribution, so that we only require the improper integral $\int_0^\infty (p - k)^{-1} \sin px dp$ whose principal value approaches $\pi \cos kx$ as $x \rightarrow \infty$. Hence

$$\lim_{x \rightarrow \infty} \psi(x) = \sin kx - \frac{B(k)\pi}{2k} \cos kx, \quad (2.10)$$

so that by definition of the phase-shift η , we find the required connection,

$$\tan \eta = -\pi B(k)/2k, \quad (2.11)$$

between η and $B(k)$.

III. FORMULATION OF THE VARIATIONAL PRINCIPLE IN MOMENTUM SPACE

In reference 2 a variational principle for the phase shift was developed in the coordinate representation. Calling now η_0 the correct phase shift, η the phase shift of a trial function satisfying the boundary conditions (2.2), and I the functional

$$I \equiv - \int_0^\infty \psi(x) [-(\partial^2/\partial x^2) + V(x) - k^2] \psi(x) dx \quad (3.1)$$

it was found that the expression,

$$k \tan \eta_0 = k \tan \eta + I, \tag{3.2}$$

was stationary relative to variations of ψ . In other words the integral I , which vanishes for the correct ψ , plays the role of a first-order correction to the tangent of the trial phase shift.

It is of course possible to express $\tan \eta$ and I in terms of the momentum wave function. However, because of the nonintegrability of ψ , such a procedure is somewhat delicate and in fact does not lead to a very desirable formulation. We prefer therefore to postpone this development (see Sec. IV) and meanwhile formulate variational principles based directly on the Schrodinger equation in momentum space.

In the case of a bound state problem one knows that the first variation of the functional

$$\int_0^\infty \varphi(p) \left[(p^2 - E) \varphi(p) + \int_0^\infty V(p, p') \varphi(p') dp' \right] dp \tag{3.3}$$

vanishes for the correct wave function and one can use this fact for a determination of the energy E and the wave function φ . This is just the momentum analog of the statement that if $\psi(\infty) = 0$ the first variation of I , Eq. (3.1), is zero. It is thus natural also in the case of a collision problem, to investigate the expression,

$$J \equiv \int_0^\infty \varphi(p) \left[(p^2 - k^2) \varphi(p) + \int_0^\infty V(p, p') \varphi(p') dp' \right] dp. \tag{3.4}$$

We consider this J as a functional of $\varphi(p)$'s, whose singularities are described by the form (2.7). In particular this includes functions for which $B(k) = 0$ and which therefore have only the δ -function singularity.

The integrand in (3.4) contains singular terms. Thus, to give a definite meaning to the integral, we must agree on how to deal with such terms. We therefore make the following conventions:

$$\int_0^\infty \delta(p - k) (p^2 - k^2) \delta(p - k) dp = 0, \tag{3.5}$$

$$\int_0^\infty \frac{F(p)}{p^2 - k^2} dp = \lim_{\delta \rightarrow 0} \left[\int_0^{k-\delta} \frac{F(p)}{p^2 - k^2} dp + \int_{k+\delta}^\infty \frac{F(p)}{p^2 - k^2} dp \right]. \tag{3.5^1}$$

Equation (3.5) is obtained when $\delta(p - k)$ is approximated by a nonsingular function because of the antisymmetry about the point $p = k$. It is therefore reasonable to postulate a similar relationship for the δ -functions themselves. Integrals of the type (3.5¹) are usually evaluated either by by-passing the singularity in the complex plane, which gives a complex result, or by taking the principal value. Since our problem is entirely real we have chosen the latter alternative. We could, of course, have adopted different conventions,

but it should be remarked that they all lead to the same final results.

Let us now first evaluate J for the correct wave function, $\varphi_0(p)$. Although for this function the square bracket in (3.4) is zero, we shall see that the corresponding value of J , denoted by J_0 , does not vanish. For, substituting for $\varphi_0(p)$ on the left of (3.4) the form (2.7), we find

$$J_0 = J_0^{(1)} + J_0^{(2)}, \tag{3.6}$$

where

$$J_0^{(1)} = \int_0^\infty \delta(p - k) \left[(p^2 - k^2) \varphi_0(p) + \int_0^\infty V(p, p') \varphi_0(p') dp' \right] dp, \tag{3.7}$$

$$J_0^{(2)} = \int_0^\infty -B_0(p) \left[\varphi_0(p) + \frac{1}{p^2 - k^2} \int_0^\infty V(p, p') \varphi_0(p') dp' \right] dp. \tag{3.7^1}$$

Now $J_0^{(1)}$ contains the term $\delta(p - k)(p^2 - k^2)\delta(p - k)$ whose integral we equate to zero. Thus we are left with

$$J_0^{(1)} = -B_0(p) + \int_0^\infty V(k, p') \varphi_0(p') dp' = 0, \tag{3.8}$$

as a comparison of (2.6) and (2.7) shows. On the other hand, by (2.6), the square bracket in (3.7¹) equals $\delta(p - k)$ so that

$$J_0 = J_0^{(2)} = -B_0(k). \tag{3.9}$$

Thus the expression J_0 , which vanishes in bound state problems, equals, in the present case, a constant times $\tan \eta_0$.

It is important for our later work to see clearly the origin of this nonvanishing result. It comes from the term $\varphi_0(p)(p^2 - k^2)\varphi_0(p)$ in (3.4). The $\varphi_0(p)$ on the right contains a term $\delta(p - k)$ which when multiplied by $(p^2 - k^2)$ vanishes and hence gives no contribution to the square bracket in (3.4). However, when this term is further premultiplied by the factor $-B_0/(p^2 - k^2)$, contained in $\varphi_0(p)$, it becomes $-B_0(p)\delta(p - k)$, resulting in $-B_0(k)$ on integration.

Next we calculate the first variation of J . Since we consider only trial functions of the form (2.7), the variation of φ may be written as $\delta\varphi(p) = -\delta B(p)/(p^2 - k^2)$ and we obtain

$$\begin{aligned} \delta J &= 2 \int_0^\infty -\frac{\delta B(p)}{p^2 - k^2} \left[(p^2 - k^2) \varphi_0(p) + \int_0^\infty V(p, p') \varphi_0(p') dp' \right] dp \\ &= -2\delta B(k). \end{aligned} \tag{3.10}$$

Hence the combination $J+2B(k)$ is stationary. This means that to the first order in $\delta\varphi$ we have the equation,

$$J+2B(k)=J_0+2B_0(k)=B_0(k) \\ =-(2k/\pi)\tan\eta_0, \quad (3.11)$$

which provides the desired stationary expression for $\tan\eta_0$.

As a simple check we can obtain the Born approximation from (3.11), by setting $\varphi(p)=\delta(p-k)$ so that $B(k)=0$. This gives, correctly,

$$V(k, k) = -(2k/\pi)\tan\eta_0. \quad (3.12)$$

When the functional J in (3.11) is written out in full using the form (2.7) of $\varphi(p)$, one obtains among other terms

$$2\int_0^\infty -\frac{B(p)}{p^2-k^2}(p^2-k^2)\delta(p-k)dp = -2B(k)$$

which precisely cancels the $2B(k)$ in (3.11). If we now for convenience replace (2.7) by

$$\varphi(p) = \delta(p-k) + \chi(p) \quad (3.13)$$

where $\chi(p)$ may have only a $(p^2-k^2)^{-1}$ singularity, (3.11) becomes in full

$$\int_0^\infty \chi(p)(p^2-k^2)\chi(p)dp + V(k, k) + 2\int_0^\infty V(k, p)\chi(p)dp \\ + \int_0^\infty \chi(p)V(p, p')\chi(p')dpdp' \\ = -(2k/\pi)\tan\eta_0. \quad (3.14)$$

Remarks on Regularization

We have seen that the extra term $2B(k)$ in (3.11) just removes the contributions to J coming from the singular point of $\chi(p)$. It follows that if $\chi(p)$ is replaced by a "regularized" function, in which the singularity at $p=k$ has been smeared out, the term $2B(k)$ in (3.11) will not occur. This allows one to write (3.11) in a more compact, though entirely equivalent form.

Thus let us define, corresponding to a function $\varphi(p)$, the regularized functions,

$$\varphi_\epsilon(p) = \delta(p-k) + \chi_\epsilon(p), \quad (3.15)$$

depending on the parameter ϵ . We assume that for all nonvanishing values of ϵ , $\chi_\epsilon(p)$ is a nonsingular function; but that as $\epsilon \rightarrow 0$, $\chi_\epsilon(p)$ approaches the singular $\chi(p)$ in the sense that if $F(p)$ is any smooth function,

$$\lim_{\epsilon \rightarrow 0} \int_0^\infty F(p)\chi_\epsilon(p)dp \\ = \text{principal value of } \int_0^\infty F(p)\chi(p)dp. \quad (3.16)$$

An example of such a regularized function is

$$\chi_\epsilon(p) = -\text{Re}[B(p)/(p^2-k^2-i\epsilon)].$$

Next we define

$$J'(\varphi) = \lim_{\epsilon \rightarrow 0} J(\varphi_\epsilon). \quad (3.17)$$

Then, clearly, $J'(\varphi) = J(\varphi) + 2B(k)$, so that (3.11) may be put into the form,

$$J'(\varphi) = B_0(k) = -(2k/\pi)\tan\eta_0, \quad (3.18)$$

or in full

$$\lim_{\epsilon \rightarrow 0} \int_0^\infty \varphi_\epsilon(p) \left[(p^2-k^2)\varphi_\epsilon(p) \right. \\ \left. + \int_0^\infty V(p, p')\varphi_\epsilon(p')dp' \right] dp \\ = B_0(k) = -(2k/\pi)\tan\eta_0. \quad (3.19)$$

When this is written out in terms of $\chi_\epsilon(p)$ and the limit $\epsilon \rightarrow 0$ is taken, one is of course led back to (3.14). The interesting feature of (3.19) is, however, that it shows that the expectation value of $(H-E)$ evaluated by suitable regularization is stationary even in scattering problems; but in contrast to bound state problems the stationary value is not zero but a constant times $\tan\eta_0$.

IV. RELATION TO THE VARIATIONAL FORMULATION IN COORDINATE SPACE

Both forms in which we have expressed the variational principle [Eqs. (3.11) and (3.18)] are apparently not simple transcripts of the coordinate space principle (3.2). For if one formally expresses I in terms of the momentum wave function, (3.2) becomes

$$\int_0^\infty \varphi(p) \left[(p^2-k^2)\varphi(p) \right. \\ \left. + \int_0^\infty V(p, p')\varphi(p')dp' \right] dp + B(k) = B_0(k). \quad (4.1)$$

It is really not surprising that we seem to have here yet another form of the variational principle, since by handling the singularities in different ways we obtained the two different forms (3.11) and (3.18). In fact we may already guess that the coordinate space principle is equivalent, in momentum space, to regularizing just one of the two wave functions occurring in the functional J .

To clarify this point, let us re-write carefully the definition (3.1) of I as

$$I = -\lim_{a \rightarrow \infty} \int_a^a \psi(x) \left[-\frac{d^2}{dx^2} + V(x) - k^2 \right] \psi(x) dx. \quad (4.2)$$

Passing into momentum space, this becomes

$$I = -\lim_{a \rightarrow \infty} \int_0^a dx \int_0^\infty dp \int_0^\infty dp' \varphi(p) \sin px \times \left[(p'^2 - k^2) \varphi(p') + \int_0^\infty V(p', p'') \varphi(p'') dp'' \right] \times \sin p'x. \quad (4.3)$$

The integration over x gives

$$\int_0^a \sin px \sin p'x dx = \frac{1}{2} \left[\frac{\sin(p-p')a}{(p-p')} - \frac{\sin(p+p')a}{(p+p')} \right] = \frac{1}{2} \pi \Delta_a(p, p') \quad (4.4)$$

where for $p, p' > 0$, $\lim_{a \rightarrow \infty} \Delta_a(p, p') = \delta(p-p')$, i.e., $\Delta_a(p, p')$ is a regularized δ -function. We now conveniently introduce the regularized function,

$$\varphi_a(p') = \int_0^\infty \Delta_a(p, p') \varphi(p) dp. \quad (4.5)$$

Then the variational principle (3.2) can be written as

$$\lim_{a \rightarrow \infty} \int_0^\infty \varphi_a(p') \left[(p'^2 - k^2) \varphi(p') + \int_0^\infty V(p', p'') \varphi(p'') dp'' \right] dp' + B(k) = B_0(k), \quad (4.6)$$

which confirms our expectation that one of the φ 's is regularized. The stationary character of (4.6) may also be checked directly in momentum space.

V. BILINEAR FORM OF THE VARIATIONAL PRINCIPLE; SCHWINGER'S VARIATIONAL PRINCIPLE IN MOMENTUM SPACE

In our later work, we shall have occasion to use bilinear forms $J(\varphi_1, \varphi_2)$ in order to discuss transition between two asymptotic states. It is therefore convenient to introduce such forms already in the one-dimensional case. Moreover, the bilinear forms show clearly the connection with Schwinger's variational principle.

We consider then the bilinear functional,

$$J(1, 2) = J(2, 1) = \int_0^\infty \varphi_1(p) \left[(p^2 - k^2) \varphi_2(p) + \int_0^\infty V(p, p') \varphi_2(p') dp' \right] dp, \quad (5.1)$$

for functions of the form,

$$\varphi_i(p) = \delta(p-k) - B_i(p)/(p^2 - k^2), \quad i = 1, 2. \quad (5.2)$$

As before we find that if $\varphi_1 = \varphi_2 = \varphi_0$,

$$J_0(1, 2) = -B_0(k) \quad (5.3)$$

and

$$\delta J(1, 2) = -\delta B_1(k) - \delta B_2(k). \quad (5.4)$$

Hence we have, in analogy with (3.11), the variational principle,

$$J(1, 2) + B_1(k) + B_2(k) = B_0(k), \quad (5.5)$$

and, in analogy with (3.18),

$$J'(1, 2) = B_0(k). \quad (5.6)$$

We may note in passing that the corresponding expression in coordinate space has the less symmetrical form,

$$I(1, 2) + k \tan \eta_2 = k \tan \eta_0. \quad (5.7)$$

Already, in reference 2, Schwinger's variational principle was derived in coordinate space from a bilinear expression such as (5.7). We can also derive it in momentum space, most easily from (5.5).

For $\varphi_2(p)$ we use any trial function of the form,

$$\varphi_2(p) = \delta(p-k) - B_2(p)/(p^2 - k^2). \quad (5.8)$$

The function $\varphi_1(p)$ is constructed from $\varphi_2(p)$ according to the equation,

$$\varphi_1(p) = \delta(p-k) - \frac{B_0(k) \int_0^\infty V(p, p') \varphi_2(p') dp'}{p^2 - k^2 \int_0^\infty V(k, p') \varphi_2(p') dp'}; \quad (5.9)$$

here $B_0(k)$ is the unknown correct value of B at $p=k$, given by

$$B_0(k) = \int_0^\infty V(k, p') \varphi_0(p') dp'.$$

It may be seen, from the integral equation (2.6), that if $\varphi_2 = \varphi_0$, then φ_1 as defined by (5.9) also equals φ_0 . Furthermore, however, φ_1 has the correct singular behavior,

$$\varphi_1(p) = \delta(p-k) - B_0(k)/(p^2 - k^2), \quad p \approx k, \quad (5.10)$$

regardless of the correctness of φ_2 . Thus, in general, if φ_2 is some approximation to φ_0 , φ_1 will be a better approximation, which is the reason for the practical success of this method.

Using now the fact that $B_1(k) = B_0(k)$ and substituting φ_2 and φ_1 into (5.5), one obtains after some simplification

$$B_0(k) = \left[\int_0^\infty V(k, p) \varphi_2(p) dp \right]^2 / \left[\int_0^\infty \varphi_2(p) V(p, p') \varphi_2(p') dp dp' + \int_0^\infty \varphi_2(p') V(p', p) (p^2 - k^2)^{-1} \times V(p, p'') \varphi_2(p'') dp dp' dp'' \right]. \quad (5.11)$$

This is just the momentum transcript of the stationary expression for $\cot\eta_0$ given by Schwinger in coordinate space.

VI. PRACTICAL APPLICATION

As usual, the stationary expressions which we have derived enable us to obtain approximate values for the stationary quantity, $\tan\eta_0$, as well as the wave function $\varphi_0(p)$. Practical procedures for accomplishing this in coordinate space have been described by Hulthén¹ and the author.² They may be directly taken over into momentum space and therefore will be only briefly outlined here.

Following reference 2, we use as trial function a linear combination of the type,

$$\varphi(p) = A\delta(p-k) + \chi(p), \quad (6.1)$$

where $\chi(p)$ is a superposition of a finite number of functions:

$$\chi(p) = \sum_0^n c_k \chi_k(p). \quad (6.2)$$

Because of the extra factor A in (6.1), compared to (3.13), Eq. (3.14) must be replaced by

$$\begin{aligned} & \int_0^\infty \chi(p)(p^2 - k^2)\chi(p)dp + A^2V(k, k) \\ & + 2A \int_0^\infty V(k, p)\chi(p)dp + \int_0^\infty \chi(p)V(p, p') \\ & \times \chi(p')dpdp' = -(2k/\pi)A^2 \tan\eta_0. \end{aligned} \quad (6.3)$$

The stationary character of this equation may be directly verified by dividing through by A^2 and calling $\chi/A = \chi'$, which leads one back to the form (3.14).

The condition that (6.3) be stationary with respect to variations of the parameters A and c_k leads to $(n+1)$ homogeneous linear equations for the $(n+1)$ parameters. They are compatible only if the determinant of the coefficients vanishes. This determinant is a function of $\tan\eta_0$ and, as in reference 2, it may be shown that its vanishing fixes a unique value for $\tan\eta_0$, in contrast to the $(n+1)$ eigenvalues in bound state problems. The values of c_k/A may be obtained by substituting the value of $\tan\eta_0$ into n of the linear equations for A and c_k and solving.

If one wants to evaluate the integrals of (6.3) in momentum space it is important to note that, while the correct $\chi_0(p)$ has a singularity of the type $-B_0(p)/(p^2 - k^2)$, it is not necessary to work with singular trial χ 's. For it is clear from (6.3) that slight regularization of $\chi_0(p)$ does not materially effect the value of $\tan\eta_0$. This is a fortunate circumstance since analytical work with singular wave functions is generally very difficult.

Alternatively, one may of course go back to the coordinate space for the evaluation of the integrals. There, calling

$$\int_0^\infty \chi(p) \sin px dp = f(x) \quad (6.4)$$

one finds, the stationary equation,

$$\begin{aligned} & \int_0^\infty f(x) [-(d^2/dx^2) + V(x) - k^2] f(x) dx \\ & + 2A \int_0^\infty \sin kx V(x) f(x) dx \\ & + A^2 \int_0^\infty \sin^2 kx V(x) dx = -A^2 k \tan\eta_0. \end{aligned} \quad (6.5)$$

The condition that $\chi(p)$ may only have a singularity of the type $-B(p)/(p^2 - k^2)$ means that $f(x)$, if it extends to infinity, must be asymptotically proportional to $\cos kx$. Incidentally (6.5) may be considered as an alternative and perhaps useful form of the variational principle (3.2) to which it is equivalent.

VII. EXTENSION TO HIGHER ANGULAR MOMENTA

The radial Schroedinger equation, corresponding to angular momentum l , is

$$\left(-\frac{d^2}{dx^2} + V(x) + \frac{l(l+1)}{x^2} - k^2 \right) \psi(x) = 0. \quad (7.1)$$

There are now two types of "momentum"-representations to which one may transform. The first is the space of solutions of the equations,

$$[-(d^2/dx^2) - p^2] \psi_p(x) = 0, \quad (7.2)$$

which, in view of the boundary condition $\psi(0) = 0$, are just the $\sin px$ considered before. In this case $V(x) + l(l+1)/x^2$ is to be regarded as the total potential $V'(x)$, but otherwise the treatment is exactly analogous to that of S -scattering.

Alternatively, one may transform to the space of solutions of the equations,

$$\left(-\frac{d^2}{dx^2} + \frac{l(l+1)}{x^2} - p^2 \right) \psi_p(x) = 0, \quad (7.3)$$

namely, the functions

$$\psi_p(x) = (px) j_l(px). \quad (7.4)$$

These obey the orthonormality relations,

$$\int_0^\infty \psi_p(x) \psi_{p'}(x) dx = \frac{1}{2} \pi \delta(p - p'). \quad (7.5)$$

Expanding $\psi(x)$ in (7.1) as

$$\psi(x) = \int_0^\infty \varphi(p) \psi_p(x) dp, \quad (7.6)$$

one finds the equation,

$$(p^2 - k^2) \varphi(p) + \int_0^\infty V(p, p') \varphi(p') dp' = 0 \quad (7.7)$$

where now

$$V(p, p') = V(p', p) = (2/\pi) \int_0^\infty \chi_p(x) V(x) \psi_{p'}(x) dx. \quad (7.8)$$

It is easily verified that the function, which in coordinate space has the asymptotic behavior

$$\psi(x) \rightarrow (kx) [j_l(kx) - \tan \eta_l n_l(kx)] \quad (7.9)$$

satisfies the integral equation,

$$\varphi(p) = \delta(p - k) - (p^2 - k^2)^{-1} \int_0^\infty V(p, p') \varphi(p') dp' \quad (7.10)$$

and that for the correct $\varphi_0(p)$

$$\int_0^\infty V(k, p') \varphi_0(p') dp' = -(2k/\pi) \tan \eta_0. \quad (7.11)$$

A variational principle for η_0 is now established just as before. Using functions of the form,

$$\varphi(p) = \delta(p - k) - B(p)/(p^2 - k^2) \quad (7.12)$$

and defining J as in (3.4), with the new meaning (7.8) for $V(p, p')$, we find, corresponding to (3.11), the equation,

$$J + 2B(k) = B_0(k) = -(2k/\pi) \tan \eta_0. \quad (7.13)$$

The rest of the development is entirely parallel to that of S -scattering.

VIII. DISCUSSION

We have seen how, in the simple case of scattering by a central field, a consideration of the basic integral,

$$J \equiv \int_0^\infty \varphi(p) \left[(p^2 - k^2) \varphi(p) + \int_0^\infty V(p, p') \varphi(p') dp' \right] dp$$

leads to a stationary expression for the tangent of the phase shift. To establish this variational principle, it was essential to know beforehand the form of the singularities of the momentum wave function. This was very easy in the simple case considered. But quite generally it is clear that the form of the singularities is independent of the details of the interaction, and thus one expects that it can be established without actually solving the Schroedinger equation.

This expectation is borne out by the work of Dirac⁸ and Heisenberg.⁷ It enables one to cast more complicated scattering problems, particularly also those involving disintegrations, into variational form. A discussion of such problems will be given in a forthcoming paper.

ACKNOWLEDGMENTS

This work was carried out during the author's tenure of a postdoctoral fellowship from the National Research Council, whose financial assistance is gratefully acknowledged. It is a great pleasure to thank Professor N. Bohr for the privilege of working in his institute and Professor C. Møller for his kind interest in this work.

Note added in proof: Dr. G. J. Kynch of the University of Birmingham has informed me that some time ago he has done similar unpublished work on the two body problem.