Application of Variational Methods to Intermediate and High-Energy Scattering*

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The application of Schwinger's variational principle to scattering by a Yukawa potential is studied. A detailed comparison of the Born approximation, variational, and exact results is given in the energy region from 20 to 150 Mev for a potential strength and range appropriate to the ^3S neutron-proton interaction. Comparison with the second Born approximation is also made. The utility of the variational principle is discussed and consideration is given to the high-energy limit. It is judged that for most potentials, the variational formulation without elaborate trial functions will be better than the Born approximation.

The relation between the variational principles for the total scattering amplitude and for the phase shifts is analyzed. A new formulation intermediate between these two is presented as a compromise between the simplicity of the former and the accuracy of the latter. With the potential studied, use of this formulation leads to considerably better results for the total amplitude than does the original principle.

I. INTRODUCTION

IN the simplest and most fundamental quantum-mechanical scattering problem, the scattering of a particle by a fixed potential, which also yields the scattering of one particle by another in the center-of-mass frame, there exists an important energy region where no entirely suitable methods are available for the calculation of differential cross sections. We refer of course to those intermediate energies for which expansion in partial waves requires the determination of numerous phase shifts, and for which on the other hand, such high-energy approximations as the Born approximation are inadequate for estimating these phase shifts and, therefore, for estimating unexpanded or closed form approximations to the differential cross section. Consequently in this intermediate energy range the computations are tedious even for the simplest potentials, involving as they do numerical integration of the radial differential equation for each of the numerous partial waves. Moreover the resultant cross sections vary with energy and other parameters in so complicated a fashion, and in a manner so tenuously related to the detailed shape of the potential, that such calculations are actually not very enlightening qualitatively. The result is that the admittedly inadequate Born approximation, which has the virtue of simplicity, is frequently used in the hope that it can serve as a not entirely incorrect qualitative guide.

For the case of neutron-proton scattering this intermediate energy region begins at a laboratory energy E_L of about 20 Mev, where the contributions of higher (than S) partial waves become significant.[1] With a Yukawa well the validity of the Born approximation has seemed questionable at energies as high as 250 Mev "where the potential picture is getting to be quite far-fetched," since the second Born approximation is significantly different from the first, even up to these energies.[2] In the present paper we investigate the utility of Schwinger's variational expression for the total scattering amplitude[3] in bridging this gap for central field neutron-proton scattering with Yukawa wells, including exchange forces. The calculations have been performed for a potential $(V_0a/r)e^{-r/a}$ such that $V_0=53.8$ Mev and $a=1.35\times10^{-13}$ cm, corresponding to the ^3S neutron-proton interaction. In subsequent sections we describe in detail the comparison of the variational results for several varieties of trial functions with the "exact" differential cross sections obtained by numerical integration of Schrödinger's equation,[4] and with the results in Born approximation.[5] Briefly we may state that the Born approximation turns out to be quite good, particularly in the absence of exchange forces. As described in detail below, with an improved formulation and appropriately chosen wave function, the variational method is superior to Born approximation, rather more so when exchange forces are included. Naturally the variational results are achieved at the expense of considerably increased computational effort. It is our belief, to be elaborated in a later section, that the Yukawa case is especially and accidentally favorable for the Born approximation, while simultaneously unfavorable for the variational principle. We feel therefore, although we are in no position to guarantee, that for other well shapes the Schwinger formulation usually will prove superior to Born approximation with relatively less complicated machinery and trial functions than those we have found necessary,[6] as confirmed

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[1] G. Snow, Phys. Rev. **87**, 21 (1952).

[2] R. Jost and A. Pais, Phys. Rev. **82**, 840 (1951).

[3] J. Schwinger, "Lectures on Nuclear Physics," Harvard University, 1947 (unpublished).

[4] Futterman, Osborne, and Saxon (to be published).

[5] By Born approximation we mean always first Born approximation, unless otherwise stated.

[6] It must be remarked however that our choice of well shape, Yukawa, was motivated not merely by its obvious theoretical interest, but also by the fact that for the Yukawa well the integrals

by previously reported calculations of the total cross sections for a square well.[7]

Irrespective of the degree of generality of our particular numerical results, our method of application of Schwinger's variational principle has independent theoretical interest. As originally introduced, this variational principle was written in two forms. In one, the usual expansion in spherical harmonics was made, leading to an infinite set of independent integral equations and thence to a corresponding sets of variational expressions for the phase shifts. In the other, the entire scattering amplitude was expressed in stationary form, thus giving the scattering cross section directly, without necessitating summing over the individual phase shifts. These two modes of expressing the variational principle are formally equivalent, of course. Regarded as the basis for approximate calculations, however, they have quite different attributes: The expansion is intrinsically more accurate, whereas a direct estimate of the entire scattering amplitude is intrinsically simpler. Our method has been to develop a formulation intermediate between Schwinger's two alternatives by expanding in a finite set of "partial waves" using the eigenfunctions of finite rotation and reflection operators. This, we believe, represents a useful compromise between the requirements of accuracy and simplicity.

These introductory remarks are amplified in the following sections.

II. THE VARIATIONAL PRINCIPLES

In the coordinate system in which the center of mass is at rest, Schrödinger's equation for two particles interacting according to the central potential $V(r)$ can be written in the dimensionless form

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

where $\mathbf{x}=\mathbf{r}/a$, with a being a characteristic length (say the range), associated with the potential, and where

$$k^2=(2mE/\hbar^2)a^2, \quad u(x)=-(2m/\hbar^2)a^2V(ax), \tag{2}$$

with m the reduced mass, and E the energy in the center-of-mass system. Derivations of the variational formulation can be found, both in terms of the phase shifts[8] and of the entire scattering amplitude.[9] For convenience in describing our method, we very briefly recapitulate these derivations.

We first obtain a stationary expression for the amplitude $A(\mathbf{k}\to\mathbf{k}')$ of a wave scattered in the direction $\mathbf{k}'$, when the incident wave is in the direction $\mathbf{k}$. For this purpose Eq. (1) is re-expressed as an integral equation incorporating the proper boundary conditions, namely,

$$\psi_{\mathbf{k}}(\mathbf{x})=e^{i\mathbf{k}\cdot\mathbf{x}}+\int d\mathbf{x}'G(\mathbf{x},\mathbf{x}')u(x')\psi_{\mathbf{k}}(\mathbf{x}'), \tag{3}$$

where

$$G(\mathbf{x},\mathbf{x}')=e^{i\mathbf{k}|\mathbf{x}-\mathbf{x}'|}/4\pi|\mathbf{x}-\mathbf{x}'|, \tag{4}$$

and where the subscript $\mathbf{k}$ on ψ denotes the incident wave is in the direction $\mathbf{k}$. Examination of the asymptotic form of $\psi_{\mathbf{k}}$ for Eq. (3) then yields the rigorous expression for the amplitude of the scattered wave in the direction $\mathbf{k}'$,

$$A(\mathbf{k}\to\mathbf{k}')=\frac{1}{4\pi}\int d\mathbf{x}e^{-i\mathbf{k}'\cdot\mathbf{x}}u(x)\psi_{\mathbf{k}}(\mathbf{x})\equiv B(\mathbf{k}\to\mathbf{k}'). \tag{5}$$

From Eq. (5) the amplitude $A(-\mathbf{k}'\to-\mathbf{k})$ of the time reversed solution is

$$A(-\mathbf{k}'\to-\mathbf{k})=\frac{1}{4\pi}\int d\mathbf{x}e^{i\mathbf{k}\cdot\mathbf{x}}u(x)\psi_{-\mathbf{k}'}(\mathbf{x})\equiv B(-\mathbf{k}'\to-\mathbf{k}). \tag{6}$$

Moreover, from Eq. (3) and the corresponding time reversed integral equation it is shown that

$$A(\mathbf{k}\to\mathbf{k}')=A(-\mathbf{k}'\to-\mathbf{k})=\frac{1}{4\pi}\int d\mathbf{x}\psi_{\mathbf{k}}(\mathbf{x})u(x)\psi_{-\mathbf{k}'}(\mathbf{x})-\frac{1}{4\pi}\int\int d\mathbf{x}d\mathbf{x}'\psi_{\mathbf{k}}(\mathbf{x})u(x)G(\mathbf{x},\mathbf{x}')u(x')\psi_{-\mathbf{k}'}(\mathbf{x}')\equiv C(\mathbf{k}\to\mathbf{k}'). \tag{7}$$

Thereby it follows that

$$A(\mathbf{k}\to\mathbf{k}')=\frac{B(\mathbf{k}\to\mathbf{k}')B(-\mathbf{k}'\to-\mathbf{k})}{C(\mathbf{k}\to\mathbf{k}')}=\frac{1}{4\pi}\frac{\left[\int d\mathbf{x}e^{-i\mathbf{k}'\cdot\mathbf{x}}u\psi_{\mathbf{k}}\right]\left[\int d\mathbf{x}e^{i\mathbf{k}\cdot\mathbf{x}}u\psi_{-\mathbf{k}'}\right]}{\int d\mathbf{x}\psi_{\mathbf{k}}u\psi_{-\mathbf{k}'}-\int\int d\mathbf{x}d\mathbf{x}'\psi_{\mathbf{k}}(\mathbf{x})u(x)Gu(x')\psi_{-\mathbf{k}'}(\mathbf{x}')}. \tag{8}$$

Finally it is observed that, regarded as a functional of $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$, the expression on the right side of Eq. (8)

occurring in the variational principle can be evaluated in closed form for reasonable trial functions such as plane waves. The possibility of this evaluation appears to stem from the relatively simple form of the Fourier transform of the Yukawa potential. For other well shapes the variational principle need not yield closed form expressions for the scattering amplitude. In particular we have been unable to evaluate the integrals in closed form for square wells (except in the forward direction). Unless the integrals can be at least approximately evaluated in closed form, computations using the Schwinger variational formulation can be so tedious as to offer insufficient or no advantage over exact numerical integration of the differential equation. L. Mower [Phys. Rev. 89, 947 (1953)] lists some special cases for which the integrals can be evaluated in closed form.

[7] E. Gerjuoy and D. S. Saxon, Phys. Rev. **85**, 939 (1952).

[8] The S wave shift has been discussed in detail in reference 3 and in the more readily available article by J. M. Blatt and J. D. Jackson, Phys. Rev. **76**, 18 (1949). A discussion for general L values has been given by B. P. Lippman and J. Schwinger, Phys. Rev. **79**, 469 (1950) and F. Rohrlich and J. Eisenstein, Phys. Rev. **75**, 705 (1949).

[9] See, e.g., H. Levine and J. Schwinger, Phys. Rev. **74**, 958 (1948).

is stationary[10] with respect to arbitrary independent variations of $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$ about their true values as determined by Eq. (3), and the corresponding equation for $\psi_{-\mathbf{k}'}$. Furthermore the right side of Eq. (8) is independent of the amplitudes of $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$.

Stationary expressions for the phase shifts are obtained in a similar fashion. The standard expansion in spherical harmonics leads to a set of independent differential equations for the partial waves $\psi_L(x)$, from which are constructed a set of integral equations incorporating the boundary conditions, namely,

$$\psi_L(x)=j_L(kx)+\int_0^\infty dx'x'^2 g_L(x,x')u(x')\psi_L(x'), \quad (9)$$

where

$$g_L(x,x')=ikj_L(kx_<)h_L^{(1)}(kx_>). \quad (10)$$

Here $x_<$ denotes the smaller, $x_>$ the larger, of x and x'; and j_L and $h_L^{(1)}$ are the standard spherical Bessel and Hankel functions. It then follows that the phase shifts can be expressed in the form

$$k(\cot\delta_L-i)=\frac{1}{\left[\int_0^\infty dxx^2 j_L u\psi_L\right]^2}\left\{\int_0^\infty dxx^2 u\psi_L{}^2 - \int_0^\infty\int_0^\infty dxdx'x^2x'^2\psi_L(x)u(x)g_L u(x')\psi_L(x')\right\}\equiv Q_L. \quad (11)$$

The expression on the right side of Eq. (11) is stationary with respect to arbitrary variation of ψ_L about its true value, as determined from Eq. (9), and is independent of the amplitude of ψ_L.

We now compare some of the features of the formally equivalent results expressed by Eqs. (8) and (11). We observe first, that Eq. (11) can be derived directly from Eq. (8). This is effected by expanding the unknown functions $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$ in spherical harmonics. We write

$$\psi_{\mathbf{k}}=\sum_{L,m}\alpha_L{}^m\psi_L(x)Y_L{}^m(\theta,\phi), \quad (12)$$

$$\psi_{-\mathbf{k}'}=\sum_{L,m}\beta_L{}^m\psi_L(x)Y_L{}^{m*}(\theta,\phi). \quad (13)$$

Substituting in Eqs. (5)–(7) we find

$$B(\mathbf{k}\to\mathbf{k}')=\sum_{L,m}\alpha_L{}^m(-i)^L Y_L{}^m(\theta_{\mathbf{k}'},\phi_{\mathbf{k}'})\times\int_0^\infty dxx^2 j_L u\psi_L\equiv\sum_{L,m}\alpha_L{}^m A_{1L}{}^m,$$

$$B(-\mathbf{k}'\to-\mathbf{k})=\sum_{L,m}\beta_L{}^m i^L Y_L{}^{m*}(\theta_{\mathbf{k}},\phi_{\mathbf{k}})\times\int_0^\infty dxx^2 j_L u\psi_L\equiv\sum_{L,m}\beta_L{}^m A_{2L}{}^m, \quad (14)$$

$$C(\mathbf{k}\to\mathbf{k}')=\sum_{L,m}\alpha_L{}^m\beta_L{}^m\left[\frac{1}{4\pi}\int_0^\infty dxx^2 u\psi_L{}^2 - \frac{1}{4\pi}\int_0^\infty\int_0^\infty dxdx'x^2x'^2\times\psi_L(x)u_L(x)g_L u_L(x')\psi_L(x')\right]\equiv\sum_{L,m}\alpha_L{}^m\beta_L{}^m A_{3L}{}^m,$$

where the quantities $A_{1L}{}^m$, $A_{2L}{}^m$, $A_{3L}{}^m$ are defined by Eq. (14).

$A(\mathbf{k}\to\mathbf{k}')$, Eq. (8), is stationary with respect to arbitrary independent variations of $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$, which means, using Eqs. (12) and (13) in Eq. (8), that $A(\mathbf{k}\to\mathbf{k}')$ must be stationary with respect to arbitrary independent variations of the parameters $\alpha_L{}^m$ and $\beta_L{}^m$ about their correct values. We note that

$$\delta A(\mathbf{k}\to\mathbf{k}')=\frac{B_1}{C}\delta B_2+\frac{B_2}{C}\delta B_1-\frac{B_1B_2}{C^2}\delta C, \quad (15)$$

where we have condensed the notation, with $B_1=B(\mathbf{k}\to\mathbf{k}')$, $B_2=B(-\mathbf{k}'\to-\mathbf{k})$. Using Eq. (14) in Eq. (15), and equating to zero the coefficients of $\delta\alpha_L{}^m$ and $\delta\beta_L{}^m$, we then obtain

$$\alpha_L{}^m=\frac{C}{B_2}\frac{A_{2L}{}^m}{A_{3L}{}^m}, \quad (16)$$

$$\beta_L{}^m=\frac{C}{B_1}\frac{A_{1L}{}^m}{A_{3L}{}^m}. \quad (17)$$

These variationally determined values of $\alpha_L{}^m$ and $\beta_L{}^m$, when substituted into Eq. (8), yield

$$A(\mathbf{k}\to\mathbf{k}')=\sum_L(2L+1)P_L(\cos\theta)(1/Q_L), \quad (18)$$

where θ is the angle between $\mathbf{k}'$ and $\mathbf{k}$. Moreover we observe that Eq. (18) has been deduced without making use of any of the properties of $\psi_L(x)$. Hence, by virtue of Eq. (11), Eq. (18) is seen to be equivalent to the standard form[11]

$$A(\mathbf{k}\to\mathbf{k}')=\frac{1}{2ik}\sum_L(2L+1)(e^{2i\delta_L}-1)P_L(\cos\theta), \quad (19)$$

where in Eq. (19) the phase shifts are now defined in terms of the unknown functions ψ_L, by the stationary expression Eq. (11), and are of course identical with the exact phase shifts when ψ_L are the correct radial functions. Thus in spite of their formal equivalence, there is considerable difference in the use of Eqs. (18)

[10] Some discussion of the general formal requirements for constructing stationary expressions like Eq. (8) is given in E. Gerjuoy and D. S. Saxon, "Variational principles for the acoustic field" (to be published).

[11] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), p. 105.

and (11) as the basis for actual approximations to the cross section. Obviously, if the integrals can be evaluated in closed form for suitable trial functions, Eq. (8) is much more convenient than Eq. (11), which necessarily involves tedious sums over spherical harmonics. On the other hand, Eq. (11) is inherently more accurate than Eq. (8) in the sense of the variational principle, since Eq. (11) corresponds to the use of the "best" or variationally determined set of parameters $\alpha_L{}^m$, $\beta_L{}^m$ in Eq. (8), for the particular set of radial trial functions $\psi_L(x)$ which is being used. Or, to put it another way, use of, say, the incident plane wave as a trial function in Eq. (11), i.e., using $\psi_L(x)=j_L(kx)$, corresponds to using in Eq. (8) not the incident wave, but rather an expression in which the plane wave expansion coefficients have been replaced by a corresponding set of variationally determined coefficients.

At this point we interpolate a remark concerning the reliability of variational methods in general as applied to scattering problems. Inasmuch as no minimum principle has been established for these problems, one cannot guarantee that the use of a sequence of trial functions containing an increasing number of variationally determined parameters will uniformly improve the estimated scattering amplitude or cross section.[12] What is desired is a trial function which approximates as closely as possible the correct wave function. When physical reasoning points to a certain trial function, this choice of trial function probably should be favored over a variationally determined trial function. In the absence of physical indications, however, it is reasonable to expect that a variationally determined trial function will not be a very bad choice, and that it is likely to be better to choose the parameters variationally than to choose them purely arbitrarily. It is in this sense that the variationally determined set of parameters $\alpha_L{}^m$, $\beta_L{}^m$ are said to be the "best" set.

III. PROJECTION OPERATOR FORMULATION

We now seek a somewhat different expression of the variational principle which represents a compromise between the greater complexity of Eq. (11) and the lesser accuracy of Eq. (8). We proceed by analogy to the angular momentum eigenfunction expansion which leads from Eq. (8) to Eq. (11). Namely we expand $\psi_{\mathbf{k}}$ in the eigenfunctions of operators which commute with the Hamiltonian but which are so chosen that they generate only a finite complete set. In particular, we shall choose the parity operator and some suitable finite rotation operator for this purpose. We first develop the properties of the associated projection operators, in terms of which the desired expansion is conveniently obtained.

Consider initially the parity operator P, eigenvalues ± 1. We denote the corresponding eigenfunctions by ψ_+ and ψ_- and observe that

$$P_+=\tfrac{1}{2}(1+P), \tag{20}$$

$$P_-=\tfrac{1}{2}(1-P), \tag{21}$$

are the corresponding projection operators since for any function ψ:

$$P_+\psi=\psi_+, \quad P_-\psi=\psi_-. \tag{22}$$

That is to say,

$$PP_+\psi=P_+\psi, \quad PP_-\psi=-P_-\psi. \tag{23}$$

Next, introduce the rotation operator R denoting rotation through the angle $2\pi/N$ about some arbitrary fixed axis. Then $R^N=1$ and the eigenvalues λ_n of R are

$$\lambda_n=e^{2\pi n i/N}, \quad n=0, 1, \cdots, N-1. \tag{24}$$

The corresponding projection operators are

$$P_n=\frac{1}{N}\sum_{p=0}^{N-1}\lambda_n{}^{N-p}R^p, \tag{25}$$

since

$$RP_n=\lambda_nP_n, \tag{26}$$

as is easily demonstrated. Also

$$\sum_{n=0}^{N-1}P_n=1. \tag{27}$$

For any function ψ we define ψ_n by

$$\psi_n\equiv P_n\psi. \tag{28}$$

Then ψ_n is an eigenfunction of R with the eigenvalue λ_n.

In the preceding equations $R\psi(\mathbf{x})$ is understood to define a new function $\psi'(\mathbf{x})$ such that

$$\psi'(\mathbf{x})=R\psi(\mathbf{x})\equiv\psi(R\mathbf{x}), \tag{29}$$

where $R\mathbf{x}$ is the new vector (in some specified fixed coordinate system) into which $\mathbf{x}$ rotates under R. For any integral over all solid angles (along $\mathbf{x}$), with ϕ and ψ arbitrary functions,

$$\int\phi(\mathbf{x})[R\psi(\mathbf{x})]=\int\phi(\mathbf{x})\psi(R\mathbf{x})=\int\phi(R^{-1}\mathbf{x})\psi(\mathbf{x})$$

$$=\int[R^{-1}\phi(\mathbf{x})]\psi(\mathbf{x}). \tag{30}$$

Of course the second equality in Eq. (30) is a consequence of the introduction of new rotated polar and azimuth axes, or equivalently of the introduction of new primed variables of integration defined by $\mathbf{x}'=R\mathbf{x}$, $\mathbf{x}=R^{-1}\mathbf{x}'$. Thus Eq. (30) demonstrates that the definition of $R\psi$, Eq. (29), retains the orthogonality of R,

[12] Indeed one cannot even guarantee that for a given trial function the variational principle will increase the accuracy over less sophisticated approximation techniques. Thus, for example, calculation of the Coulomb scattering cross section in Born approximation gives the correct cross section, as is well known, while use of the incident plane wave as a trial function in the variational principle does not. For further details see the discussion of this point in Sec. IV.

i.e., that

$$\tilde{R}=R^{-1} \tag{31}$$

in integrals like those of Eq. (30).

From Eq. (31), using relations like $\lambda_n{}^{-1}=\lambda_{N-n}$, $R^{-1}=R^{N-1}$, it is simple to show

$$\tilde{P}_n=P_{N-n}. \tag{32}$$

It is also true that if ϕ_n is an eigenfunction of R with eigenvalue λ_n,

$$P_{n'}\phi_n=\frac{1}{N}\sum_{p=0}^{N-1}\lambda_{n'}{}^{N-p}\lambda_n{}^p\phi_n=\frac{1}{N}\sum_{p=0}^{N-1}e^{2\pi i(n-n')/N}\phi_n$$
$$=\delta_{nn'}\phi_n, \tag{33}$$

and therefore, by Eq. (28), that

$$P_{n'}P_n=\delta_{nn'}P_n. \tag{34}$$

Hence if ϕ_n is any eigenfunction with eigenvalue λ_n, and ψ_{N-n} is defined as in Eq. (28), then, by Eqs. (32) and (33),

$$\int\psi_{N-n}\phi_n=\int[P_{N-n}\psi]\phi_n$$
$$=\int\psi[\tilde{P}_{N-n}\phi_n]=\int\psi\phi_n. \tag{35}$$

Similarly, using Eq. (34), one obtains

$$\int\phi_m\phi_n=0, \quad m\neq N-n \tag{36}$$

for any two eigenfunctions ϕ_m, ϕ_n with eigenvalues λ_m, λ_n. It should be noted that in Eqs. (32)–(36) we have extended the definitions so that $\lambda_N=\lambda_0=1$, whence also $P_N=P_0$, $\psi_N=\psi_0$, etc.

We are now in a position to derive readily the desired variational expressions in terms of the simultaneous eigenfunctions of P and R. Such functions, we denote by $\phi_{n,\pm}$. They satisfy the relations

$$P\phi_{n,\pm}=\pm\phi_{n,\pm}, \quad R\phi_{n,\pm}=\lambda_n\phi_{n,\pm}, \tag{37}$$

and can be constructed from any arbitrary function ψ via the defining equation

$$P_\pm P_n\psi=P_nP_\pm\psi\equiv\psi_{n,\pm}. \tag{38}$$

In analogy to Eqs. (12) and (13), we write

$$\psi_{\mathbf{k}}=\sum_n\sum_{i=\pm}\alpha_{n,i}\phi_{n,i}{}^{\mathbf{k}},$$
$$\psi_{-\mathbf{k}'}=\sum_n\sum_{i=\pm}\beta_{n,i}\phi_{n,i}{}^{-\mathbf{k}'}, \tag{39}$$

where the superscripts indicate that $\phi_{n,i}{}^{\mathbf{k}}$ and $\phi_{n,i}{}^{-\mathbf{k}'}$ need not be the same functions. Corresponding to Eq. (14), we have:

$$B(\mathbf{k}\to\mathbf{k}')=\sum_{n,i}\frac{1}{4\pi}\alpha_{n,i}\int d\mathbf{x}e^{-i\mathbf{k}'\cdot\mathbf{x}}u(x)\phi_{n,i}{}^{\mathbf{k}}$$
$$\equiv\sum_{n,i}\alpha_{n,i}A_{n,i}{}^{(1)},$$
$$B(-\mathbf{k}'\to-\mathbf{k})=\sum_{n,i}\frac{1}{4\pi}\beta_{n,i}\int d\mathbf{x}e^{i\mathbf{k}\cdot\mathbf{x}}u(x)\phi_{n,i}{}^{-\mathbf{k}'}$$
$$\equiv\sum_{n,i}\beta_{n,i}A_{n,i}{}^{(2)}, \tag{40}$$
$$C(\mathbf{k}\to\mathbf{k}')=\sum_{n,i}\alpha_{n,i}\beta_{N-n,i}\Big[\frac{1}{4\pi}\int d\mathbf{x}\phi_{n,i}{}^{\mathbf{k}}u(x)\phi_{N-n,i}{}^{-\mathbf{k}'}$$
$$-\frac{1}{4\pi}\int d\mathbf{x}d\mathbf{x}'\phi_{n,i}{}^{\mathbf{k}}(\mathbf{x})u(x)$$
$$\times G(\mathbf{x},\mathbf{x}')u(x')\phi_{N-n,i}{}^{-\mathbf{k}'}(\mathbf{x}')\Big]$$
$$\equiv\sum_{n,i}\alpha_{n,i}\beta_{N-n,i}A_{n,i}{}^{(3)}.$$

The expression for $C(\mathbf{k}\to\mathbf{k}')$ in Eq. (40) is justified with the aid of Eqs. (32), (33), and (36), using obvious properties of the parity operator and noting that

$$R(\mathbf{x})R(\mathbf{x}')G(\mathbf{x},\mathbf{x}')=G(\mathbf{x},\mathbf{x}'), \tag{41}$$

where $R(\mathbf{x})$ rotates $\mathbf{x}$ only, all of which yields

$$P_{N-n}(\mathbf{x})G=N^{-1}\textstyle\sum_p\lambda_{N-n}{}^{N-p}R^p(\mathbf{x})G$$
$$=N^{-1}\textstyle\sum_p\lambda_{N-n}{}^{N-p}R^{-p}(\mathbf{x}')G=P_n(\mathbf{x}')G. \tag{42}$$

We require $A(\mathbf{k}\to\mathbf{k}')$, Eq. (8), to be stationary with respect to arbitrary independent variations of the parameters $\alpha_{n,i}$ and $\beta_{n,i}$. Then, using Eq. (15) we find that, for variationally determined values of $\alpha_{n,i}$ and $\beta_{n,i}$,

$$A(\mathbf{k}\to\mathbf{k}')=\sum_n\sum_{i=\pm}A_{n,i}(\mathbf{k}\to\mathbf{k}'),$$
$$A_{n,i}(\mathbf{k}\to\mathbf{k}')=A_{n,i}{}^{(1)}A_{N-n,i}{}^{(2)}/A_{n,i}{}^{(3)}. \tag{43}$$

This derivation of Eq. (43) is wholly analogous to the derivation of Eq. (11) from Eq. (8), for arbitrary ψ_L in Eq. (12), via variation of $\alpha_L{}^m$ and $\beta_L{}^m$. Alternatively we can use the expansions Eq. (39) in Eq. (1) to obtain

$$\nabla^2\phi_{n,\pm}{}^{\mathbf{k}}+[k^2+u(x)]\phi_{n,\pm}{}^{\mathbf{k}}=0, \tag{44}$$

and similarly for $\phi_{n,\pm}{}^{-\mathbf{k}'}$. The function $\phi_{n,\pm}{}^{\mathbf{k}}$ obeys the integral equation

$$\phi_{n,\pm}{}^{\mathbf{k}}(\mathbf{x})=P_nP_\pm e^{i\mathbf{k}\cdot\mathbf{x}}+\int d\mathbf{x}'G(\mathbf{x},\mathbf{x}')u(x')\phi_{n,\pm}{}^{\mathbf{k}}(\mathbf{x}'). \tag{45}$$

From Eq. (45) and the corresponding equation for $\phi_{n,\pm}{}^{-\mathbf{k}'}$, it is not difficult to determine that Eq. (43) is valid for the exact scattering amplitude, for which in fact

$$A_{n,i}(\mathbf{k}\to\mathbf{k}')=A_{n,i}{}^{(1)}(\mathbf{k}\to\mathbf{k}')$$
$$=A_{N-n,i}{}^{(2)}(\mathbf{k}\to\mathbf{k}')=A_{n,i}{}^{(3)}(\mathbf{k}\to\mathbf{k}'), \tag{46}$$

when, in Eq. (40), $\phi_{n,i}{}^{\mathbf{k}}$ and $\phi_{n,i}{}^{-\mathbf{k}'}$ take on their true values, i.e., $\phi_{n,i}{}^{\mathbf{k}}$ satisfies Eq. (45). Moreover, the expression for $A_{n,i}(\mathbf{k}\to\mathbf{k}')$, Eq. (43) is stationary with respect to arbitrary variation of $\phi_{n,i}{}^{\mathbf{k}}$ and $\phi_{n,i}{}^{-\mathbf{k}'}$ about their true values. This second derivation of Eq. (43) is of course analogous to the customary derivation of Eq. (11) from Eq. (9).

Equation (43) is the variational formulation we have been seeking. It can be expressed in a simpler form by the following device. We first specify that the functions $\phi_{n\pm}{}^{\mathbf{k}}$ and $\phi_{n,\pm}{}^{-\mathbf{k}'}$ are constructed from given trial functions $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$ by means of Eq. (38). We make the further restriction that $\psi_{\mathbf{k}}(\mathbf{x})$ is a function only of the angle between $\mathbf{k}$ and $\mathbf{x}$, i.e., that it does not depend on the azimuth of $\mathbf{x}$ about $\mathbf{k}$. This condition is certainly satisfied for the true $\psi_{\mathbf{k}}(\mathbf{x})$ which solves Eq. (3). Similarly, $\psi_{-\mathbf{k}'}(\mathbf{x})$ is independent of the azimuth of $\mathbf{x}$ relative to $-\mathbf{k}'$. This means that for any rotation R, in the notation of Eq. (41),

$$R(\mathbf{k})R(\mathbf{x})\psi_{\mathbf{k}}(\mathbf{x})=\psi_{\mathbf{k}}(\mathbf{x}), \tag{47}$$

and therefore just as Eq. (42) followed from Eq. (41)

$$P_n(\mathbf{x})\psi_{\mathbf{k}}(\mathbf{x})=P_{N-n}(\mathbf{k})\psi_{\mathbf{k}}(\mathbf{x}). \tag{48}$$

From Eq. (48), and also Eq. (42) we infer that

$$\begin{aligned}A_{n,\pm}{}^{(1)}&=\frac{1}{4\pi}\int d\mathbf{x}e^{-i\mathbf{k}'\cdot\mathbf{x}}u(x)[P_n(\mathbf{x})P_{\pm}(\mathbf{x})\psi_{\mathbf{k}}(\mathbf{x})]\\&=P_{N-n}(\mathbf{k})P_{\pm}(\mathbf{k})B(\mathbf{k}\to\mathbf{k}'),\\A_{N-n,\pm}{}^{(2)}&=\frac{1}{4\pi}\int d\mathbf{x}e^{i\mathbf{k}\cdot\mathbf{x}}u(x)[P_{N-n}(\mathbf{x})P_{\pm}(\mathbf{x})\psi_{-\mathbf{k}'}(\mathbf{x})]\\&=\frac{1}{4\pi}\int d\mathbf{x}[P_n(\mathbf{x})P_{\pm}(\mathbf{x})e^{i\mathbf{k}\cdot\mathbf{x}}]u(x)\psi_{-\mathbf{k}'}(\mathbf{x})\\&=P_{N-n}(\mathbf{k})P_{\pm}(\mathbf{k})B(-\mathbf{k}'\to-\mathbf{k}),\end{aligned} \tag{49}$$

and, by slightly more complicated manipulations, using Eq. (34) as well, that

$$A_{n,\pm}{}^{(3)}=P_{N-n}(\mathbf{k})P_{\pm}(\mathbf{k})C(\mathbf{k}\to\mathbf{k}'), \tag{50}$$

where $B(\mathbf{k}\to\mathbf{k}')$, $B(-\mathbf{k}'\to-\mathbf{k})$, and $C(\mathbf{k}\to\mathbf{k}')$ are defined by Eqs. (5)–(7).

Equations (49) and (50) make Eq. (43) particularly convenient, since they merely involve linear combinations of the same functions B and C which enter into the more familiar stationary expression Eq. (8). We further note that the extension of our result to the situation in which space exchange forces are involved is trivial, since space exchange merely introduces different interactions in even and odd states. The point here is of course that Eq. (43) is already decomposed into sums over even and odd states. Hence one need only use the corresponding even and odd interactions in computing the contribution of each to the total scattering amplitude.[13] Thus, for example, for the Serber type of exchange, wherein the interaction vanishes in odd states, Eq. (43) becomes simply

$$A(\mathbf{k}\to\mathbf{k}')=\textstyle\sum_n A_{n,+}(\mathbf{k}\to\mathbf{k}'). \tag{51}$$

To this point, R has representated a rotation about a fixed but arbitrary axis. In the actual application of Eq. (43), together with Eqs. (49) and (50), it is necessary to make some definite choice of the orientation of this axis, with respect to $\mathbf{k}$ for instance. For the true solutions $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$ the results are entirely independent of the orientation of this axis of rotation. In this event, $B(\mathbf{k}\to\mathbf{k}')=B(-\mathbf{k}\to-\mathbf{k})=C(\mathbf{k}\to\mathbf{k}')$ so that, using Eqs. (49) and (50) in Eq. (43), and noting that $P_{\pm}$ obviously sums to unity, as does P_{N-n}, by Eq. (27), we have, for the true $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$,

$$A(\mathbf{k}\to\mathbf{k}')=\sum_{n,i}P_{N-n}(\mathbf{k})P_i(\mathbf{k})B(\mathbf{k}\to\mathbf{k}')=B(\mathbf{k}\to\mathbf{k}'), \tag{52}$$

and $B(\mathbf{k}\to\mathbf{k}')$ does not involve R.

When $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$ are merely some suitable trial functions however, the results using Eq. (43) do depend on the axis of rotation of R. As an illustration, if the axis of rotation is chosen to lie along $\mathbf{k}$, the quantities B and C in Eqs. (49) and (50) are seen to be eigenfunctions of $R(\mathbf{k})$ with eigenvalue unity. Then only the terms with $n=0$ fail to vanish in Eq. (43), recalling Eq. (33), and we are left with the not unexpected result that with this choice of axis

$$A(k\to k')=A_+(k\to k')+A_-(k\to k'), \tag{53}$$

where A_+ and A_-, the even and odd parts of the scattering amplitude, are given by

$$A_{\pm}=\frac{[P_{\pm}(\mathbf{k})B(\mathbf{k}\to\mathbf{k}')][P_{\pm}(\mathbf{k})B(-\mathbf{k}'\to-\mathbf{k})]}{P_{\pm}(\mathbf{k})C(\mathbf{k}\to\mathbf{k}')}. \tag{54}$$

On the other hand, suppose R corresponds to a rotation through an angle of $\frac{2}{3}\pi$ about an axis making equal direction cosines with the three rectangular axes. In other words, when operating on the coordinate axes, R causes a cyclic interchange of these axes. Thus, if (x,y,z) are the components of a vector,

$$\begin{aligned}&Rf(x,y,z)=f(z,x,y);\\\text{and}\qquad&\\&R^3=1,\quad\lambda_n=e^{\frac{2}{3}\pi in},\quad n=0,\,1,\,2.\end{aligned} \tag{55}$$

Further, suppose we choose the z axis along $\mathbf{k}$ and take $\mathbf{k}'$ to lie in the positive x half of the x-z plane, which in a rather complicated fashion specifies the orientation relative to $\mathbf{k}$ and $\mathbf{k}'$ of the axis of rotation of R. With $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$ as previously restricted, i.e., with $\psi_{\mathbf{k}}(\mathbf{x})$ independent of the azimuth of $\mathbf{x}$ about $\mathbf{k}$, it is intuitively obvious, and can be proved formally directly from Eqs. (5)–(7) using Eqs. (31), (41), and (47), that $B(\mathbf{k}\to\mathbf{k}')$, $B(-\mathbf{k}'\to-\mathbf{k})$, and $C(\mathbf{k}\to\mathbf{k}')$ are independent of the azimuth of $\mathbf{k}'$ about $\mathbf{k}$. Hence, insofar as rotations are concerned, these quantities can be written as $f(\mathbf{k},\mathbf{k}')\equiv f(\theta)$, with θ the scattering angle. Then for the

[13] One could arrive at the same result by inserting different even and odd interactions $u(x)$ in Eq. (44).

present choice of coordinate axes and of R, $R(\mathbf{k})f(\theta)=f(|\frac{1}{2}\pi-\theta|)$, $R^2(\mathbf{k})f(\theta)=f(\frac{1}{2}\pi)$, $P(\mathbf{k})f(\theta)=f(\pi-\theta)$, and we have

$$P_n=\tfrac{1}{3}\sum_{p=0}^{2}e^{-2\pi inp/3}R^p,$$
$$P_n(\mathbf{k})P_\pm(\mathbf{k})f(\theta)=\tfrac{1}{3}[f_\pm(\theta)+e^{-2\pi in/3}f_\pm(|\tfrac{1}{2}\pi-\theta|)+e^{2\pi in/3}f_\pm(\tfrac{1}{2}\pi)],\quad n=0,1,2 \tag{56}$$
$$f_\pm(\theta)=\tfrac{1}{2}[f(\theta)\pm f(\pi-\theta)].$$

Evidently, Eq. (56) combined with Eqs. (43), (49), and (50) generally does not yield the same result as Eq. (53).

IV. APPLICATION TO THE YUKAWA POTENTIAL

Procedure

We now describe the specific calculations we have performed. We have used the interaction

$$u(x)=u_0e^{-x}/x, \tag{57}$$

with $u_0=2.365$, which corresponds to the Yukawa well depth and range quoted in Sec. I. Scattering amplitudes have been computed at values of $k=0.6630$, 1.048, 1.406, 1.624, 1.816, corresponding to laboratory energies of 20, 50, 90, 120, 150 Mev. In the various variational formulations, the trial functions $\psi_\mathbf{k}$ and $\psi_{-\mathbf{k}'}$ are always

$$\psi_\mathbf{k}(\mathbf{x})=\exp(iK\mathbf{n}\cdot\mathbf{x}),\quad \psi_{-\mathbf{k}'}(\mathbf{x})=\exp(-iK\mathbf{n}'\cdot\mathbf{x}), \tag{58}$$

where $\mathbf{n}$ is the unit vector along the incident wave vector $\mathbf{k}$, and $\mathbf{n}'$ is the unit vector along the direction of the scattered wave $\mathbf{k}'$. Thus we use plane-wave trial functions, but do not necessarily equate the effective or average wave number K to the wave number k at infinity. This special choice of trial function is physically reasonable and permits evaluation in closed form of the integrals which occur. In fact, with Eqs. (57) and (58), Eqs. (5) and (6) readily yield

$$B(\mathbf{k}\to\mathbf{k}')=B(-\mathbf{k}'\to-\mathbf{k})=u_0g(K,k,\theta), \tag{59}$$

where

$$g(K,k,\theta)=1/(1+k^2+K^2-2kK\cos\theta), \tag{60}$$

with θ, the scattering angle, the angle between $\mathbf{n}$ and $\mathbf{n}'$. The only complicated integral is the one containing the Green's function in Eq. (7), which can be evaluated for arbitrary K by the same method as used by Jost and Pais[2] and by Dalitz[14] for the special case $K=k$, as well as by standard techniques, without introduction of auxiliary variables.[15] It is found that

$$C(\mathbf{k}\to\mathbf{k}')=u_0g(K,K,\theta)-u_0^2G(K,k,\theta), \tag{61}$$

where g is as in Eq. (60), and where

$$G(K,k,\theta)=\frac{1}{2K\sqrt{S}\sin(\theta/2)}\times\left\{\tan^{-1}\left(\frac{K(1+K^2-k^2)\sin(\theta/2)}{\sqrt{S}}\right)+\frac{i}{2}\log\frac{\sqrt{S}+2kK\sin(\theta/2)}{\sqrt{S}-2kK\sin(\theta/2)}\right\},$$
$$S\equiv(1+K^2+k^2)^2-4k^2K^2\cos^2(\theta/2). \tag{62}$$

In Eq. (62), $\sqrt{S}>0$ and the arctangent lies between $-\pi/2$ and $\pi/2$.

Perhaps the most consistent variational treatment would be to determine K variationally[16] at each scattering angle. However, this would require much additional numerical work, considerably more so than appears to be justifiable, see our remark at the end of Sec. II. Hence we have confined our calculations to the following three choices of the effective wave number K:

$$\text{(a)}\ K^2=k^2\equiv K_a^2,$$
$$\text{(b)}\ K^2=k^2+\tfrac{1}{8}u_0\equiv K_b^2, \tag{63}$$
$$\text{(c)}\ K^2=k^2+\tfrac{1}{2}u_0\equiv K_c^2.$$

The first is just the free-particle wave number, of course. The second is determined variationally from the requirement that the forward scattering cross section in the high-energy limit be stationary with respect to K. This is, at any rate, a high-energy variational determination of K, and is obtained without excessive manipulation. To be specific, we insert Eqs. (59)–(62) in Eq. (8) with $\theta=0$, let $K^2=k^2+\beta$, β finite, and equate to zero the derivative with respect to K in the limit that $k\to\infty$. The resultant Eq. (63b) is the same as would be found from the more complicated formulation Eq. (43), since in the high-energy limit the quantities B and C have sharp peaks in the forward direction, and are small at other angles. Consequently in $P_{N-n}(\mathbf{k})P_\pm(\mathbf{k})B(\mathbf{k}\to\mathbf{k}')$ for example, all terms in R and P are negligible compared to the term in R^0P^0, i.e., in this limit, at this angle, $P_{N-n}(\mathbf{k})P_\pm(\mathbf{k})$ is replaceable by $1/2N$, and Eq. (43) becomes identical with Eq. (8). Equation (63c) is determined from the condition

$$\int d\mathbf{x}u(x)e^{-i\mathbf{K}\cdot\mathbf{x}}[\nabla^2+k^2+u(x)]e^{i\mathbf{K}\cdot\mathbf{x}}=0. \tag{64}$$

Equation (64) is an expression of the requirement that the trial function $e^{i\mathbf{K}\cdot\mathbf{x}}$, which does not satisfy the

[14] R. H. Dalitz, Proc. Roy. Soc. (London) **A206**, 509 (1951).

[15] After transformation to momentum space, with $\mathbf{n}'$ as polar axis and the azimuth axis in the plane of $\mathbf{n}$, $\mathbf{n}'$, integration over azimuth and thence over the polar angle can be effected by successive use of formulas 300 and 195, of B. O. Peirce, *A Short Table of Integrals* (Ginn and Company, Boston, 1910). The resultant integral, though complicated in form, can be evaluated by closing the contour in the complex plane, taking care to avoid circling the branch points of the integrand.

[16] The scattering amplitude is complex and with a single variational parameter, as with K, in the present instance, it generally is not possible to cause the derivatives of the real and imaginary parts to vanish simultaneously. Thus it would be necessary to decide say that the magnitude of $A(\mathbf{k}\to\mathbf{k}')$ is to be made stationary, without regard to phase.

Schrödinger equation anywhere, at least satisfy the Schrödinger equation on an average weighted by the Yukawa potential, this weighted average favoring the region of space, where the integrands in B and C are significant.[17]

Three successively more complicated variational formulations have been employed, namely:

I. Equation (8), of course with the trial functions of Eq. (58).

II. Equation (43) in the form of Eqs. (53) and (54). This involves a decomposition into even and odd terms, and corresponds to using in Eq. (8) a trial function which is a linear combination of forward and backward traveling waves, with variationally determined amplitudes.

III. Equation (43) combined with the results of Eqs. (49), (50), and (56). This involves a further decomposition into the eigenfunctions of the rotation operator R of Eq. (55), and corresponds to using in Eq. (8) a trial function which is a linear combination of waves traveling in both directions along three mutually perpendicular axes including the forward and backward directions, with variationally determined amplitudes.

As with K, so in formulation III the orientation angles of the axis of rotation of R should presumably be regarded as variational parameters, to be determined for fixed N and K so as to make the scattering amplitude stationary at each scattering angle. Again the extra work required does not seem worth while, and we have fixed the orientation of the rotation axis mainly for reasons of convenience. Since according to Eq. (52) the results are independent of the orientation of the rotation axis when $\psi_{\mathbf{k}}$ and $\psi_{-\mathbf{k}'}$ are the true solutions, it is likely that the results will not depend strongly on the orientation of this axis provided the trial functions Eq. (58) are "reasonable." In any event this choice of rotation axis leads to good results, which only should be improved by a better founded choice of axis. It may seem that the cross sections using variational formulation III will be azimuth dependent, since we have specifically assumed $\mathbf{k}'$ lies in the $x-z$ plane in deriving Eq. (56), and in fact formulation III does correspond to the use of an azimuth dependent trial function in Eq. (8). The dependence on azimuth is only apparent however. We always keep $\mathbf{k}'$ in the positive x half of the $x-z$ plane, or in other words, we change the axis of rotation of R, Eq. (58), as the azimuth of $\mathbf{k}'$ changes, thereby retaining independence of the azimuth of $\mathbf{k}'$ relative to $\mathbf{k}$ in our final answer.

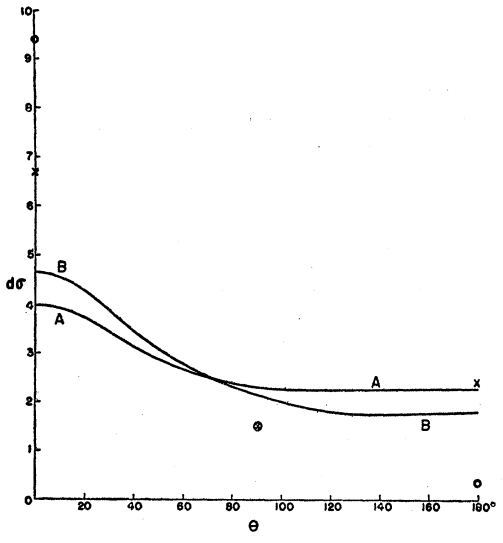

FIG. 1. Differential cross section at 20 Mev *vs* scattering angle. Curve A is the exact result, curve B the result according to variational formulation III, $K=K_b$. The circles and crosses are points computed respectively according to formulation I and II, $K=K_b$.

[17] Strictly speaking, Eqs. (63b) and (63c), which have been calculated on the assumption of ordinary forces, should be modified for exchange forces, but we shall not worry about this. They are merely reasonable guesses as to the best choice of K and, as will be seen, they do yield good estimates of the cross section when exchange forces are included.

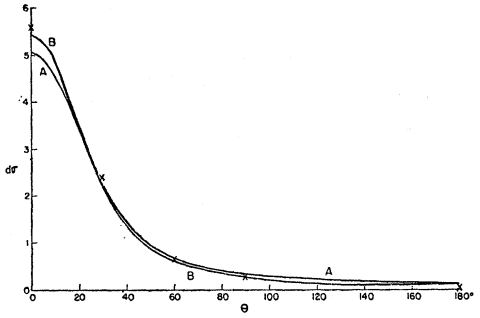

FIG. 2. Differential cross section at 90 Mev *vs* scattering angle. Curve A is the exact result, curve B the result according to variational formulation III, $K=K_b$. The crosses are points computed according to Born approximation.

Variational and Born Results

Our numerical results definitely show that the variational formulation III is superior to the simpler formulations I and II, and that formulation II is itself an improvement over the more customary formulation I. By and large, the choice $K=K_b$ is the best of the three we have tried, although at lower energies $K=K_a$ may be superior. In Figs. 1–3 we have plotted the differential cross sections $d\sigma$ computed according to formulation III, with $K=K_b$, at energies of 20 Mev, 90 Mev, and 150 Mev, including ordinary forces only, and, on the same graphs, display for comparison the exact differential cross sections[4] at the same energies. The differential cross sections, in these and subsequent figures, are given in the units a^2 per steradian, where a is the length introduced in Eqs. (1) and (57). In Fig. 1 we have plotted also the 0°, 90°, and 180° differential cross sections which are obtained from formulations I and II, with the same value of $K=K_b$. With the simple formulation I the variational values are much too high at 0° and much too low at 180°. Formulation II mixes

TABLE I. Differential cross sections *vs* energy and angle as calculated by different methods.

Energy (Mev)	Angle	Variational formulation I with effective wave number equal to K_a	K_b	K_c	Variational formulation II with effective wave number equal to K_a	K_b	K_c	Variational formulation III with effective wave number equal to K_a	K_b	K_c	Born	Exact
	0	8.61	9.36	3.73	6.12	6.70	3.79	4.93	4.64	3.13	5.60	3.99
20	$\pi/2$	1.51	1.49	1.36	1.51	1.49	1.36	1.89	2.14	2.26	1.58	2.28
	π	0.41	0.34	0.25	2.01	2.41	1.48	1.40	1.78	2.06	0.74	2.27
	0	6.81	7.19	4.38	6.05	6.39	4.13	5.09	5.08	3.25	5.60	4.58
50	$\pi/2$	0.345	0.353	0.372	0.345	0.353	0.372	0.561	0.659	0.757	0.546	0.752
	π	0.071	0.067	0.064	0.525	0.591	0.467	0.276	0.359	0.501	0.192	0.531
	0	6.27	6.50	4.74	5.99	6.21	4.59	5.34	5.42	3.95	5.60	5.07
90	$\pi/2$	0.121	0.125	0.137	0.121	0.125	0.137	0.248	0.283	0.333	0.227	0.309
	π	0.023	0.023	0.024	0.191	0.206	0.181	0.093	0.115	0.162	0.071	0.151
	0	6.10	6.28	4.90	5.94	6.11	4.80	5.44	5.54	4.31	5.60	5.25
120	$\pi/2$	0.072	0.074	0.081	0.072	0.074	0.081	0.163	0.183	0.214	0.142	0.190
	π	0.013	0.014	0.014	0.112	0.118	0.108	0.056	0.067	0.090	0.028	0.048
	0	6.00	6.14	5.01	5.90	6.04	4.93	5.50	5.60	4.56	5.60	5.31
150	$\pi/2$	0.048	0.049	0.054	0.048	0.049	0.054	0.117	0.129	0.149	0.097	0.127
	π	0.009	0.009	0.010	0.073	0.076	0.071	0.038	0.044	0.057	0.028	0.048

at 0° the 0° and 180° amplitudes of I, and similarly at 180°, with a consequent significant decrease in the variational estimate of $d\sigma$ at 0°, and a corresponding increase at 180°. The 90° point of formulation I is of course unaltered since the odd part of the scattering amplitude vanishes at 90°. By introducing the additional partial waves of formulation III we produce additional mixing at 90° and at other angles, and further improve the variational estimate of the angular distribution. In fact, in Fig. 1, the 90° value of formulation III is very nearly correct, but the variational estimate is still too high at low angles and too low at large angles. Presumably the introduction of more partial waves, with the more complicated mixing which would result, would produce further improvement in the differential cross section until finally we expand in the infinite set Y_L^m and attain the phase shift formulation of Eq. (11).

The relative merits of these three variational formulations are maintained at higher energies, but the differences between them become less marked in the forward peak, which makes the principal contribution to the total cross section. This is so because, just as explained in the discussion of Eq. (63b), at angles near 0° the large forward peak reduces the effectiveness of the mixing introduced by the projection operators. At wider angles the added partial waves of II and then III continue to improve the results. The correctness of these remarks and of the assertions in the preceding paragraph, can be gauged from Table I, which summarizes the 0°, 90°, and 180° results at the five energies for the three variational formulations and the three choices of K. Included also are the Born approximation results and the exact values.

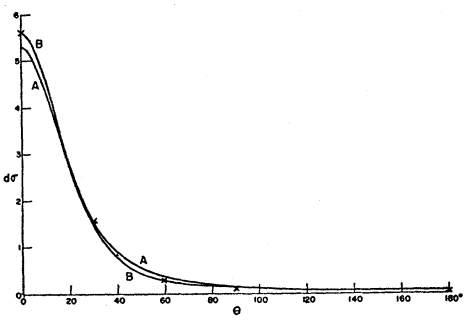

FIG. 3. Differential cross section at 150 Mev *vs* scattering angle. Curve A is the exact result, curve B the result according to variational formulation III, $K=K_b$. The crosses are points computed according to Born approximation.

It can be seen from Table I that Born approximation yields a fair estimate of the differential cross sections, especially at higher energies. This is illustrated in Figs. 2 and 3, in which we have plotted the 0°, 30°, 60°, 90°, and 180° Born approximation points. Variational formulation III with $K=K_b$ is superior to the Born approximation, but the difference is not marked. By 150 Mev there is not much to choose between Born approximation and formulation III with $K=K_a$ or $K=K_b$, while formulations I and II are inferior to Born approximation at all energies, for all three choices of K. This comparison of the Born approximation and the variational formulations is of particular interest in view of the considerably increased labor required to compute the differential cross sections for even the simplest variational formulation I.

Examination of the usual criteria for the validity of the Born approximation, which may be written as

$$u_0 \ll k^2, \quad u_0/k < 1, \tag{65}$$

in our notation,[18] shows that these are not satisfied even at 150 Mev where $k=1.816$, while $u_0=2.365$. Conse-

[18] The second of Eq. (65) expresses the requirement that across the scattering region the phase difference between the actual and free propagation be small. D. Bohm, *Quantum Theory* (Prentice-Hall, Inc., New York, 1951), pp. 553 ff.

quently, the good estimates of the differential cross sections yielded by the Born approximation seem rather accidental, and we anticipate that the phase of the complex scattering amplitude is not as happily estimated as is its magnitude.[19] This is demonstrated in Figs. 4 and 5 in which the computed scattering amplitudes are drawn in the complex plane. In each Argand diagram the circle is drawn with a radius equal to the exact scattering amplitude. The Born amplitude lies always on the real axis, as it must for any potential, while the variational and exact amplitudes are complex. The variational amplitudes in both figures are computed using formulation III, with $K=K_b$. In Fig. 4 we show the forward scattering amplitudes at 20, 90, and 150 Mev, and in Fig. 5 we plot the 90-Mev amplitudes at the angles $\pi/2$ and π. We observe that the phase of the exact scattering amplitude is in every case rather different from zero, and that this phase is much better estimated by the variational method than by the Born, although the magnitudes of the amplitudes are much the same, as we have already seen. We note also that the exact phase becomes smaller as the energy increases, and that the exact phase is larger at wide angles than at 0°. Similar figures at other energies share the same characteristics.

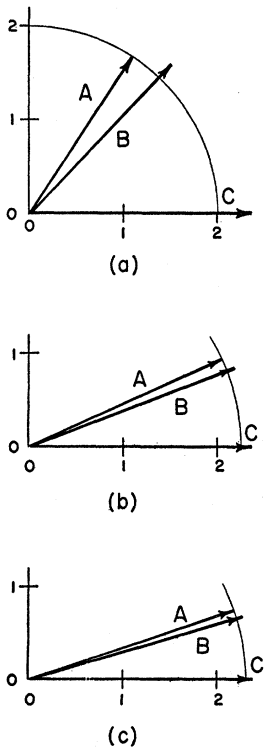

FIG. 4. Argand diagrams of the complex scattering amplitude in the forward direction for various energies: (a) 20 Mev, (b) 90 Mev, and (c) 150 Mev. In each case the vector A represents the exact amplitude, B the amplitude from variational formulation III, $K=K_b$, and C the Born amplitude. The arcs are drawn with radius equal to A.

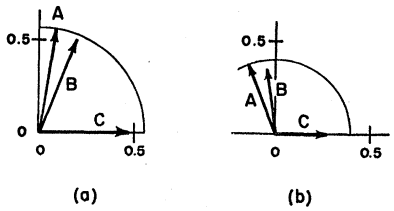

FIG. 5. Argand diagrams of the complex scattering amplitude at 90 Mev at scattering angles (a) $\theta=\pi/2$ and (b) $\theta=\pi$. In each case the vector A represents the exact amplitude, B the amplitude from variational formulation III, $K=K_b$, and C the Born amplitude. The arcs are drawn with radius equal to A.

At a scattering angle θ space exchange forces may be regarded as producing a mixture of the nonexchange amplitudes at θ and $\pi-\theta$. Since the Born amplitudes are always in phase, whereas the exact amplitudes have different phases at different scattering angles, it is apparent that it generally is not possible to have equally good results with the Born approximation for all combinations of ordinary and exchange forces. In the Yukawa case we have been discussing therefore, where Born approximation gives such good results for ordinary forces, we expect rather poorer results when exchange forces are introduced. In Figs. 6 and 7 we have plotted the exact and variational results at 90 and 150 Mev for two special combinations of ordinary and exchange forces, namely Serber forces in which the well is multiplied by P_+, and "anti-Serber" forces in which the well is multiplied by P_-. In the former case only the even waves contribute to the scattering, Eq. (51), while in the latter case we include correspondingly only the odd waves. We have used variational formulation III, with $K=K_b$, and have plotted also the Born results at 0°, 30°, 60°, and 90°. Figures 6 and 7 may be compared with the corresponding Figs. 2 and 3. Evidently, both the Serber and anti-Serber Born differential cross sections are relatively less accurate than were the Born estimates for ordinary forces, whereas the variational calculation remains about equally good for all three different types of forces. In fact for the odd scattering the variational calculation is practically indistinguishable from the exact at 90° and 150° Mev. Of course the variational calculation continues to give a good estimate of the phase as compared to the Born approximation, as is illustrated in Fig. 8 for the even forward scattering amplitude at 20 Mev. Figure 8 is constructed in the same fashion as Figs. 4 and 5, with the Born phase real, as always. We also use Fig. 8 to supplement Fig. 1 by showing how the phase as well as the amplitude is improved by adding more partial waves, and also compare the three different choices of effective wave number K. To avoid excessive complication of the figure, only formulations II and III are included in Fig. 8. We observe that both variational formulations and all choices of K give much better estimates of the phase than does Born approximation, even though the Born estimate of the magnitude of the amplitude is

[19] It is reasonable to attribute the good estimates of the Born approximation to the similarity of the Yukawa to the Coulomb potential. For the latter, the Born approximation happens to give the correct cross section but does not give the essentially infinite phase. The validity of Born approximation for a Yukawa well has been discussed by Jost and Pais and by Dalitz in the references cited. Dalitz also considers the transition to the Coulomb limit.

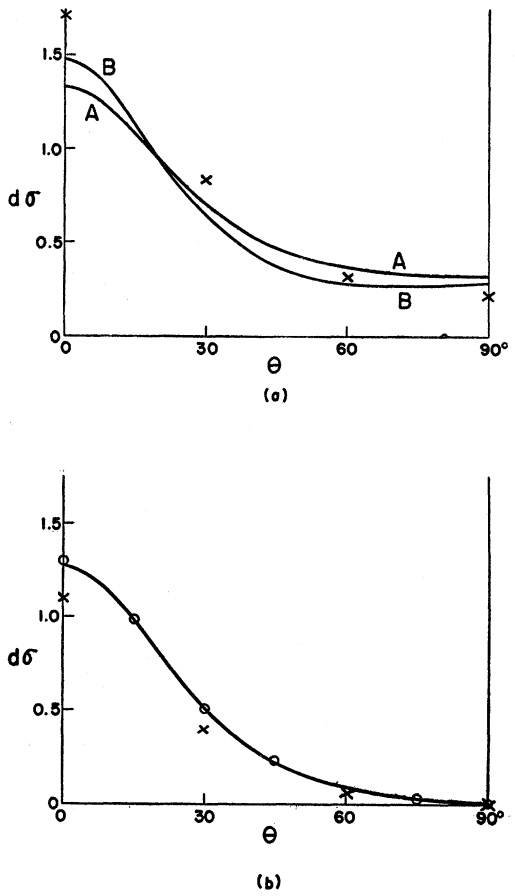

FIG. 6. (a) Even scattering cross section at 90 Mev *vs* scattering angle. Curve A is the exact result, curve B the result according to variational formulation III, $K=K_b$. The crosses are points computed according to Born approximation. (b) Odd scattering cross section at 90 Mev *vs* scattering angle. The curve represents the exact results, the circles are points computed according to variational formulation III, $K=K_b$, and the crosses are points computed according to Born approximation.

very good and certainly better than formulation II for $K=K_a$ and K_b. We see also that for the even scattering at 20 Mev, $K=K_c$ gives a better final estimate of the phase than does $K=K_b$. This is so for the even scattering at other energies as well, but the odd scattering phases definitely favor $K=K_b$, the differing behavior of the even and odd waves being especially marked at low energies. These effects can be understood. Especially at low energies the even scattering, which includes S wave scattering, arises from a region of space on the average closer to the origin than does the odd scattering, for which the wave function vanishes at the origin. Thus the effective wave number K for the even scattering is larger than for the odd scattering, especially at low energies. It is by considerations of this kind that a better choice of effective wave number can be made. For example, we have calculated the differential cross sections at 20 Mev, ordinary forces, formulation III for two modified choices of wave number, as follows. The even waves are calculated both times with $K=K_c$, but for the odd waves we calculate in one case with $K=K_a$, and in the other case with $K=K_b$. In Table II the results for these two modified choices are tabulated at 0°, 90°, and 180°, along with the exact values from Table I. The choice $K=K_b$ for the odd waves is seen to be superior, but both modifications are good. This use of different effective wave numbers for even and odd states does produce an over-all improvement, as may be seen by comparison of Table II with the 20-Mev variational formulation III section of Table I.

Utility of Variational Principle

We may infer correctly from Fig. 8, which is quite typical, that the variational method, even in its least sophisticated formulation I, with $K=K_a=k$, generally will give a better estimate of the phase of the scattering amplitude than does Born approximation. For example, at 20 Mev the correct phase angle, using ordinary forces, is 57°, while formulation I with $K=k$ is 45°. Thus in a very real sense for an arbitrary potential,

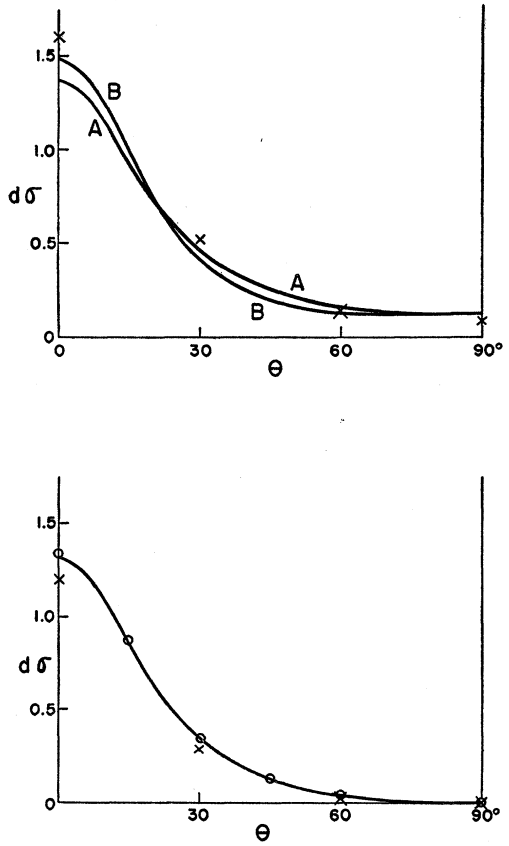

FIG. 7. (a) Even scattering cross section at 150 Mev *vs* scattering angle. Curve A is the exact result, curve B the result according to variational formulation III, $K=K_b$. The crosses are points computed according to Born approximation. (b) Odd scattering cross section at 150 Mev *vs* scattering angle. The curve represents the exact results, the circles are points computed according to variational formulation III, $K=K_b$, and the crosses are points computed according to Born approximation.

the variational method is an improvement on Born approximation, in that the variational method gives an estimate of both the real and imaginary parts of the scattering amplitude. The Born, on the other hand, estimates merely the magnitude of the amplitude, or perhaps its real part (it is not altogether clear which). It happens in the Yukawa case that the first Born approximation is very close to the correct magnitude while simultaneously the second Born correction term is large. Since for cross sections we are interested only in the magnitude of the scattering amplitude, and not in its phase, the present case evidently is especially favorable to the Born approximation.

At the same time, as we proceed to explain, it is unfavorable to the variational principle. Let us consider formulation I with $K=k$, i.e., with Born trial functions. Under these circumstances, by Eqs. (59) and (61),

$$B=u_0g(k,k,\theta), \quad C=u_0g(k,k,\theta)-u_0^2G(k,k,\theta), \quad (66)$$

where $u_0g(k,k,\theta)$ is precisely the Born approximation scattering amplitude. For the correct wave function B and C must be equal. Thus a measure of the closeness to the correct function of a given trial function is the difference between B and C. Now since $G(k,k,\theta)$ is

TABLE II. Differential cross sections at 20 Mev.

Angle	Differential cross sections: Variational formulation III, Even waves: $K=K_a$, Odd waves: K equal to K_a	K_b	Exact
0	4.45	4.28	3.99
$\pi/2$	2.26	2.26	2.28
π	1.92	1.95	2.27

complex whereas $g(k,k,\theta)$ is real, obviously B and C of Eq. (66) cannot be equal. In fact, as Jost and Pais[2] have shown, $u_0^2G(k,k,\theta)$, which is precisely the second Born approximation correction to the scattering amplitude, is comparable to $u_0g(k,k,\theta)$. Thus B and C in Eq. (66) are quite different, and the Born plane wave trial functions apparently are not close to the correct wave functions. To make B and C equal it is necessary to introduce a considerable modification of the trial function from the Born plane waves. On the other hand, such a modification in the direction of making B and C equal generally will change the magnitude of B, which in the present Yukawa case pulls the variational estimate of the differential cross section away from the very good Born value. To sum it up, when the magnitude of the second Born correction term is large, we may expect to have to use a considerably different trial function than the Born plane wave in order to get a reasonably good estimate of the differential cross section. Under such circumstances, it is difficult to get good results with the variational principle since Born plane waves so often provide, as in the calculations we

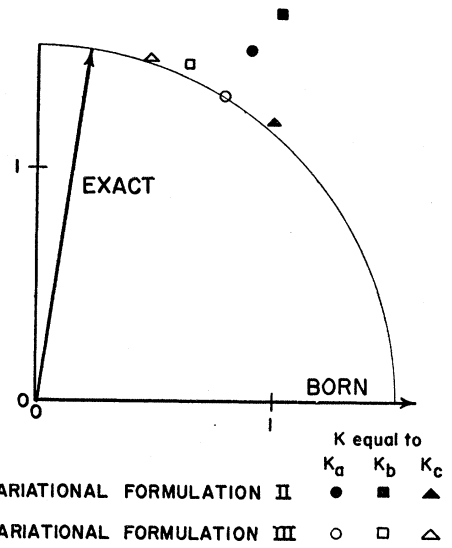

FIG. 8. Argand diagram for the even complex scattering amplitude at 20 Mev in the forward direction. The arc is drawn with radius equal to the magnitude of the exact amplitude.

are reporting, the only reasonable and tractable starting point.

If the imaginary part of C is small for Born trial functions, B and C may be made fairly close by introducing modifications to the trial function which keep B real. Moreover, since the differential cross section adds the real and imaginary parts in quadrature, it is clear that we can get a quite good variational estimate of the differential cross section in this way. When the imaginary part of C is appreciable however, we must somehow modify the trial function so that B is complex. In the Yukawa case we have been studying, the imaginary part of C which equals the imaginary part of $u_0^2G(k,k,\theta)$ actually is large. Thus we see one obvious reason why the modification provided by formulation II, which keeps B real whatever the choice of K, is inferior to the more general projection operator formulation III, in which the imaginary factors $e^{\pm 2\pi i/3}$ explicitly guarantee that B will be complex. As a matter of fact comparison of our numerical values in this formulation shows that the complex quantities B and C do turn out reasonably close to each other in formulation III. This suggests that for a potential for which exact differential cross sections are not available, the difference between B and C may prove useful as a measure of the rate of convergence of the variational method to the correct values.[20]

[20] Since B is proportional to the amplitude α of the trial function, and C is proportional to α^2, it is clear that $B-C$ or the relative difference $(B-C)/C$ may be made as large or small as desired merely by an appropriate choice of α. Thus, with a sequence of trial functions this measure of the rate of convergence is meaningful only if the amplitudes of the functions are maintained relatively constant, by fixing the value at the origin for example, or better perhaps by fixing $\int dx\psi^* u\psi$.

Second Born Approximation

As a further indication of the performance of the variational principle we compare second Born approximation with the variational results for the same trial function in Eq. (8), i.e., formulation I with $K=k$. We consider ordinary forces only so that the Born amplitude in this approximation is

$$A_B(\mathbf{k}\to\mathbf{k}')=u_0g(k,k,\theta)+u_0^2G(k,k,\theta), \tag{67}$$

while the variational estimate is

$$A_v(\mathbf{k}\to\mathbf{k}')=\frac{u_0g^2(k,k,\theta)}{g(k,k,\theta)-u_0G(k,k,\theta)}, \tag{68}$$

these expressions being essentially identical to terms of order $u_0^2G^2/g^2$ when the denominator is expanded in powers of u_0G/g. In Table III are given the differential

TABLE III. Differential cross sections in second Born approximations.

Energy (Mev)	Angle	Differential cross sections: Exact	Variational formulation I with $K=k$	Second Born approximation	Expansion parameter u_0G/g
20	0	3.99	8.61	13.2	$0.43+0.57i$
	$\pi/2$	2.28	1.51	6.1	$0.69+0.98i$
	π	2.27	0.41	4.03	$0.89+1.33i$
90	0	5.07	6.27	8.0	$0.13+0.37i$
	$\pi/2$	0.309	0.121	0.74	$0.34+1.20i$
	π	0.151	0.023	0.336	$0.42+1.66i$
150	0	5.31	6.00	7.1	$0.08+0.30i$
	$\pi/2$	0.127	0.048	0.30	$0.25+1.21i$
	π	0.048	0.009	0.125	$0.29+1.64i$

cross sections computed from Eqs. (67) and (68), at 20, 90, and 150 Mev, at angles of 0°, 90°, 180°, with again the exact values for comparison. The variational entries are of course identical with those in the $K=K_a$ variational formulation I column of Table I. We also tabulate the expansion parameter u_0G/g which, for Born trial functions, is the fractional difference between B and C and is therefore a reasonable measure of the accuracy of the variational method, as well as of the convergence of the Born expansion. Evidently the variational estimates are better than the second Born except at those energies and angles where the expansion parameter is so large that both the Born and variational estimates are extremely poor and their comparison is essentially meaningless. The variational phase angles are similarly closer to the exact phases than are the second Born approximation phases. With an arbitrary potential, where the first Born approximation generally is not close to the magnitude of the correct scattering amplitude, this comparison of the second Born approximation with the variational principle for the same trial function would be expected to be more indicative of the performance and utility of the variational method than comparison with first Born approximation, for moderate values of the expansion parameter. The results in Table III for the present Yukawa case suggest that with other potentials the variational method generally will indeed be an improvement on second Born approximation, and *a fortiori* on first Born approximation, even without improvement of the trial functions from first Born plane waves.

High-Energy Limit

In the foregoing discussion we have been thinking mainly of the intermediate energy region below those energies at which the usual criteria for the validity of the Born approximation are satisfied. For any presently reasonable potential purporting to describe neutron-proton scattering this region will be roughly the same 20–150 Mev region we have been considering. As the high-energy Born limit is approached with such a potential, we might expect the second Born correction term to become negligible.[21] Similarly the exact scattering phases ought to approach the Born value of zero, a behavior illustrated in Fig. 4. Simultaneously, according to the remarks in the preceding paragraph, the variational method even with Born trial functions, should generally be better than the Born and become more and more accurate, except that at high enough energies both the Born and the variational principle should yield results indistinguishable from the exact values.

For most potentials these expectations are fulfilled at zero scattering angle, as we can demonstrate. We employ the cross-section theorem,

$$\sigma=\frac{4\pi}{k}\,\mathrm{Im}A(\mathbf{k}\to\mathbf{k})=\frac{4\pi}{k}\,\mathrm{Im}A(0), \tag{69}$$

where σ is the total cross section, and $A(0)$ is the forward scattering amplitude. In the high-energy limit, $\sigma\simeq\pi\theta^2|A(0)|^2$, where $\theta\simeq 1/k$ is the width of the diffraction peak, with k in units of the range of the potential. Then from Eq. (69) we obtain

$$\frac{\mathrm{Im}A(0)}{|A(0)|}\simeq\frac{1}{4k}|A(0)|, \tag{70}$$

which approaches zero as $k\to\infty$, since $|A(0)|$ is quite generally bounded.

At angles for which the differential cross section is not a violently fluctuating function of angle, it is not difficult to prove, using an extension of the cross section theorem, that the phase still tends to zero.[22] If the

[21] In fact for our Yukawa case, examination of the high-energy limit of Eqs. (60) and (62) shows that Eq. (65) guarantees $u_0G/g\ll 1$, except that outside of the forward peak, $k\sin\theta/2\gg 1$, we require the somewhat stronger condition $(u_0/k)\log[4k^2\sin^2(\theta/2)]\ll 1$ to make the imaginary part of the ratio small. This extra condition probably is connected with the Coulomb-like nature of the scattering at wide angles or small impact parameters.

[22] For the Yukawa well this prediction seems to be borne out by our results.

cross section does fluctuate violently, however, it appears that large phase shifts may be expected. Thus we may draw a distinction between the high-energy limits at angles within the main diffraction peak, $k\sin(\theta/2)\ll 1$, and angles outside, $k\sin(\theta/2)\gg 1$. Within the peak, for most potentials, the cross section varies smoothly and the phase approaches zero in the Born limit. Outside the peak, even though the usual criteria for the validity of Born approximation may be satisfied, the phases in the high-energy limit generally are zero only for those potentials for which the true cross sections at those angles do not fluctuate markedly. Moreover, when such fluctuations occur, the first Born approximation cross sections can be expected to exhibit similar but certainly not coincident fluctuations, showing that the magnitude as well as the phase of the scattering amplitude has been poorly estimated. Correspondingly, we anticipate that at high energies the variational principle will be quite generally useful within the main diffraction peak, but that its utility outside the peak will depend on the potential. Where the cross sections fluctuate violently, the variational method probably will readily account for the qualitative wide angle behavior of the differential cross section, but will converge only slowly, i.e., will require trial functions very different from Born plane waves in order that further improvements in the trial functions change the results only slightly. Hence for such potentials it appears likely that at wide angles the variational method will be most useful and accurate at intermediate energies.

Total Cross Sections

We conclude by describing our results for the total cross sections. These have been computed by the variational method using Eq. (69), for the various energies, variational formulations, and choices of effective wave number K. The values so obtained are tabulated in Table IV, in units of πa^2, along with the exact and Born total cross sections. Naturally the Born total cross sections are computed by integrating the Born approximation differential cross sections, since for the Born amplitude Eq. (69) implies zero cross section. It is seen from Table IV that the variational formulations give fair estimates of the total cross section in almost all cases. These results are about as accurate as those reported earlier for the square well.[7] It is also seen from Table IV that, surprisingly enough, formulation II is usually superior to formulation III. We have no very good explanation of this unexpected result. As is apparent from inspection of the figures, however, total cross sections obtained by integration of the differential cross sections determined by variational principle III would give results in good agreement with the exact values at all energies and better than either formulation II or the Born total cross section.

TABLE IV. Total cross sections *vs* energy.

	Total cross section										
	Variational formulation I with effective wave number K equal to			Variational formulation II with effective wave number K equal to			Variational formulation III with effective wave number K equal to				
Energy (Mev)	K_a	K_b	K_c	K_a	K_b	K_c	K_a	K_b	K_c	Born	Exact
20	12.5	11.7	4.31	10.3	10.8	6.23	8.86	9.44	9.08	8.12	10.1
50	5.05	4.90	2.82	4.61	4.64	3.05	3.82	3.99	3.54	4.16	4.53
90	2.82	2.77	1.94	2.70	2.69	1.98	2.33	2.38	2.06	2.51	2.64
120	2.11	2.09	1.57	2.06	2.05	1.59	1.83	1.86	1.61	1.94	2.01
150	1.69	1.67	1.33	1.66	1.65	1.33	1.51	1.53	1.33	1.58	1.63

We should like to express our appreciation to Miss Patricia Childress of the National Bureau of Standards who performed most of the numerical computations reported above.