

Construction of the Dirac Equation Central Potential from Phase Shifts and Bound States*

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The connection between phase shifts, bound-state energies, and the potential is studied for a Dirac particle in a spherically symmetric potential. An explicit method is developed for the construction of the potential from the scattering and bound-state data for a single angular momentum and parity. The technique used in this relativistic problem is an extension, appropriately generalized to matrices, of the methods used by Jost and Kohn for the nonrelativistic case. For potentials with $\int_0^\infty r^n |V(r)| dr$ finite for $n=0, 1$, and 2 , it is shown that a spectral function can be constructed from the phase shifts, the bound-state energies, and the norm of the bound-state wave functions. A generalization of the Gel'fand and Levitan method is developed for the determination of the potential from the spectral function. First, eigenvectors associated with two different potentials are related; from the operator that connects the two systems of eigenfunctions,

a modified kernel is defined which satisfies an integral equation determined by the spectral function and eigenfunctions corresponding to a "comparison potential" and the spectral function associated with the "unknown potential." Second, the potential difference is obtained by the differentiation of a certain combination of the elements of the modified kernel.

These properties lead to the following method for the construction of the potential: (1) the spectral function is determined from the data for both positive and negative energies; (2) with the spectral function for the unknown potential and the spectral function and eigenfunctions of a convenient comparison potential, the integral equation for the modified kernel is constructed; (3) from the solution of the integral equation the difference between the unknown and the comparison potentials is determined.

I. INTRODUCTION

IN this article a method will be developed for the construction of a spherically symmetric potential in the Dirac equation from scattering and bound-state data. This problem is of general theoretical interest, since a central problem of physics is to determine the structure of interactions from directly measurable data. The problem treated is admittedly too simplified to describe general particle interactions, but it represents an extension to the relativistic domain of previous work on nonrelativistic systems, and thus is a step toward the goal of determination of relativistic interactions from observation of elementary particle reactions.

The general problem of constructing a spherically symmetric potential or potentials that will give a determined set of phase shifts and bound-state energy eigenvalues has been definitely discussed in the case of the nonrelativistic Schrödinger equation by Jost and Kohn¹ and by Levinson,² by combining the results of Jost's³ analysis of the properties of the solution of the radial wave equation with the elegant techniques used by Gel'fand and Levitan⁴ in their solution of the inverse Sturm-Liouville problem.

The method can also be generalized to deal with

more complicated potentials than the central potential, such as that of the tensor force with spin-orbit coupling. The first step in this direction was taken by Newton and Jost⁵ who extended the techniques to the case of systems of differential equations formally similar to the Schrödinger equation. This extended technique was used by Fulton and Newton⁶ for constructing examples of spin-orbit and tensor potentials for which the solutions of the Schrödinger equation can be given explicitly. The Gel'fand and Levitan theory has also been stated in a different form by Kay and Moses,⁷ using the theory of operators in a vector space. In most of this work, the data for only a single angular momentum but all energies are used. Wheeler⁸ has shown how it is also possible to consider determination of the potential by knowledge of the phase shift for all angular momenta at a single fixed energy.

All the above-mentioned contributions to the problem of the connection between phase shifts and potential have been restricted to the nonrelativistic domain. It is natural to examine the problem when the particle has to be described by a relativistic equation and see whether the method found for the Schrödinger-type particle can be extended. The first attempt in this direction is due to Corinaldesi⁹ who considered the case of the Klein-Gordon particle in a central potential for $l=0$ (S waves). In this paper¹⁰ we show how a procedure analogous to that of Jost and Kohn can be

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¹ R. Jost and W. Kohn, *Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd.* **27**, No. 9 (1953). See for introductory discussion and other references R. Jost and W. Kohn, *Phys. Rev.* **87**, 977 (1952).

² N. Levinson, *Phys. Rev.* **89**, 753 (1953).

³ R. Jost, *Helv. Phys. Acta* **20**, 256 (1947).

⁴ I. M. Gel'fand and B. M. Levitan, *Izvest. Akad. Nauk. U.S.S.R. Ser. Mat.* **15**, 309 (1951) [translation: *Am. Math. Soc. Trans.* **1**, 253 (1953)].

⁵ R. G. Newton and R. Jost, *Nuovo cimento* **1**, 590 (1955).

⁶ T. Fulton and R. G. Newton, *Nuovo cimento* **3**, 276 (1956).

⁷ I. Kay and H. E. Moses, *Nuovo cimento*, **3**, 276 (1956), where reference to previous papers by the same authors can be found.

⁸ J. A. Wheeler, *Phys. Rev.* **99**, 630 (A), (1955).

⁹ E. Corinaldesi, *Nuovo cimento* **11**, 468 (1954).

¹⁰ This work was previously reported in *Bull. Am. Phys. Soc. Ser. II*, **3**, 36 (1958). For a more detailed discussion of many of the items in this paper, see Ph.D. dissertation of Francisco Prats, University of Maryland, 1958 (unpublished).

established for the Dirac equation. Similar results have been obtained by Verde,¹¹ who has applied them to a discussion of the high-energy limit of potential scattering. The relativistic case differs from the Schrödinger case in two main respects: first, we have to deal with a system of differential equations instead of with an ordinary equation, and, second, the relativistic energy as a function of momentum is a double-valued function. These features lead to the somewhat greater complexity of the methods necessary for the relativistic case.

An analysis of the properties of the Dirac eigenfunctions for central potentials similar to that of Jost³ for the Schrödinger equation has been carried out by Carter.¹² In Sec. II, we use Carter's results to discuss the properties of expansions of arbitrary functions in terms of the Dirac eigenfunctions. The orthogonality and closure properties are established. All these properties are conveniently expressed by the introduction of the spectral function. In Sec. III we derive expressions for the relation between eigenfunctions associated to two different potentials, and some properties of the kernel that appear in the relation between eigenfunctions are also obtained. In Sec. IV it is shown how these results provide a method for the construction of the potential when the phase shifts for both positive and negative energies and the bound-state energies for a given value of angular momentum are given.

II. PROPERTIES OF THE SOLUTIONS OF THE DIRAC RADIAL WAVE EQUATION

1. Definitions and Properties; $f(k)$

The radial-dependent parts $F(r)/r$, $G(r)/r$ of the Dirac wave function for a particle in a central potential $V(r)$ satisfy the system of differential equations¹³

$$\begin{aligned} [E+m-V(r)]F &= dG/dr + (\lambda/r)G, \\ [E-m-V(r)]G &= -dF/dr + (\lambda/r)F, \end{aligned} \quad (1)$$

where the units are chosen so that $\hbar=c=1$, $\lambda = \pm(j+\frac{1}{2})$, j is the total angular momentum eigenvalue ($j = \frac{1}{2}, \frac{3}{2}, \dots$), and $|F(r)|$ and $|G(r)|$ are uniformly bounded.

We introduce the spin vector notation,

$$\varphi = \begin{pmatrix} F \\ G \end{pmatrix} = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix},$$

and the matrices

$$\omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

¹¹ M. Verde (private communication). Some of the results appear in *Nuovo cimento* 4, 560 (1958). We thank Professor Verde for the communication of his result prior to publication.

¹² D. S. Carter, Ph.D. thesis, Princeton University, 1952 (unpublished).

¹³ See, for instance, P. A. M. Dirac, *The Principles of Quantum Mechanics* (Clarendon Press, Oxford, 1947), third edition, p. 266, or L. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), pp. 314 and 322.

Then Eq. (1) reads:

$$\omega d\varphi/dr + \sigma_1(\lambda/r)\varphi - \sigma_3 m\varphi + V(r)\varphi = E\varphi. \quad (2)$$

For potentials $V(r)$ such that

$$\int_0^\infty r^n |V(r)| dr \text{ is finite for } n=0, 1, \text{ and } 2, \quad (3)$$

Carter¹² has shown that for a given E with $|E| > m$ there is a unique solution, $f_\lambda(k, r)$, of Eq. (2) such that

$$f_\lambda(k, r) \underset{r \rightarrow \infty}{\sim} (ik)^\lambda \begin{pmatrix} -i(E-m)/k \\ 1 \end{pmatrix} e^{-ikr}, \quad (4)$$

with $k = (E^2 - m^2)^{\frac{1}{2}}$. In other words, $f_\lambda(k, r)$ is the solution of Eq. (2) that is asymptotic to an incoming spherical wave of momentum k . $f_\lambda(-k, r) = f_\lambda^*(k, r)$ is also a solution of Eq. (2), which is asymptotic to an outgoing spherical wave. The pair of solutions $f_\lambda(k, r)$, $f_\lambda(-k, r)$ form a fundamental system of solutions of Eq. (2), and therefore the physically admissible solution can be expressed as a linear combination of them. The physically admissible solution is denoted by $\varphi(E, r)$. It is defined by the boundary condition at $r=0$,

$$\left. \frac{\varphi_\lambda(E, r)}{r^\lambda} \right|_{r=0} = \begin{pmatrix} 1/\gamma_{\lambda-1} \\ 0 \end{pmatrix}, \quad (5)$$

where we use $\gamma_\lambda = 1 \times 3 \times 5 \times \dots \times (2\lambda + 1)$. From Carter's result¹² it is easy to show that, in terms of the solutions asymptotic to spherical waves, we have

$$\varphi_\lambda(E, r) = \frac{1}{\Delta_\lambda(k)} \{ f_\lambda(-k) f_\lambda(k, r) - f_\lambda(k) f_\lambda(-k, r) \}, \quad (6)$$

where we have introduced

$$\Delta_\lambda(k) = \det \{ f_\lambda(k, r), f_\lambda(-k, r) \} = -2ik^{2\lambda-1}(E-m), \quad (7)$$

and

$$f_\lambda(k) = \frac{r^\lambda f_{\lambda 2}(k, r)|_{r=0}}{\gamma_{\lambda-1}}. \quad (8)$$

[$f_{\lambda 2}(k, r)$ is, according to the notation introduced in Eq. (2), the second component of the vector $f_\lambda(k, r)$.] From the asymptotic behavior of $f_\lambda(k, r)$ and $f_\lambda(-k, r)$ [of Eq. (4)] it follows that

$$\begin{aligned} \varphi_\lambda(E, r) \underset{r \rightarrow \infty}{\sim} & \frac{|f_\lambda(k)|}{k^\lambda} \\ & \times \begin{pmatrix} \cos[kr - \frac{1}{2}\pi\lambda + \eta_\lambda(k)] \\ [k/(E-m)] \sin[kr - \frac{1}{2}\pi\lambda + \eta_\lambda(k)] \end{pmatrix}. \end{aligned} \quad (9)$$

$\eta_\lambda(k)$, the λ th phase shift, is equal (mod 2π) to $\arg\{f_\lambda(k)\}$. It is also clear from Eq. (6) that the λ th

eigenvalue of the S matrix, $S_\lambda(k)$, is given by

$$S_\lambda(k) = f_\lambda(k)/f_\lambda(-k). \tag{10}$$

In all the above properties we have been referring to solutions of Eq. (2) for $E > +m$ or $E < -m$, which correspond physically to scattering states. For these, k was a real number, $k = \pm(E^2 - m^2)^{1/2}$.

If we now consider $f_\lambda(k, r)$ as a function of the parameter k , then since $E = \pm(k^2 + m^2)^{1/2}$, $f_\lambda(k, r)$ is a double-valued function of k . Carter has shown that this $f_\lambda(k, r)$ can be extended into a double-valued function of the complex variable k , which has branch points at $k = \pm im$. The two Riemann sheets can be conveniently separated by introducing cuts extending along the imaginary k axis from $+im$ to $+i\infty$ and from $-im$ to $-i\infty$; on each sheet in this cut k plane, the sign of $\text{Re}\{E\}$ is fixed, so we designate the two sheets of $f_\lambda(k, r)$ by $f_\lambda^\sigma(k, r)$ with $\sigma = +$ or $-$, where $\sigma = \text{sign}[\text{Re}\{E\}]$. Carter has also shown¹² that, with the assumptions (3), $f_\lambda(k, r)$ is a solution of Eq. (2) which satisfies the asymptotic condition (4) and is an analytic function of k in $\text{Im}\{k\} \leq 0$ in the cut k plane. Further, for $|k| \rightarrow \infty$ in $\text{Im}\{k\} \leq 0$,

$$f_\lambda^\sigma(k, r) \sim f_\lambda^{0\sigma}(k, r) \exp\left[-i\epsilon_\sigma \int_r^\infty V(t) dt\right], \tag{11}$$

where $f_\lambda^{0\sigma}(k, r)$ is the free solution [$V(r) = 0$] of Eq. (2) with the asymptotic behavior (4) and

$$\epsilon_\sigma = \lim_{|k| \rightarrow \infty} \frac{k}{E_\sigma(k)}. \tag{12}$$

The zeros of $f_\lambda^\sigma(k)$, $k_{l\sigma}$, in $\text{Im}\{k\} \leq 0$ all lie on the imaginary axis, between 0 and $-im$ ($k_{l\sigma} = -ik_{l\sigma}$, $0 \leq \kappa_{l\sigma} \leq m$). Except for the case $\lambda = 1$ when $f_1^-(0)$ may be zero and there is not a bound state at $E = -m$ (see reference 12), there is a one-to-one correspondence between the zeros of $f_\lambda^\sigma(k)$ on the lower imaginary axis and the energy levels. The level corresponding to the zero $k_{l\sigma} = -ik_{l\sigma}$ has the energy value

$$E_{l\sigma} = \sigma(m^2 - \kappa_{l\sigma}^2)^{1/2}. \tag{13}$$

The eigenfunction corresponding to $E_{l\sigma}$ is proportional to $f_\lambda^\sigma(-ik_{l\sigma}, r)$, which is real and for $r \rightarrow \infty$

$$f_\lambda^\sigma(-ik_{l\sigma}, r) \sim (\kappa_{l\sigma} r)^\lambda \left(\frac{E_{l\sigma} - m}{\kappa_{l\sigma}} \right) \frac{1}{1} \exp(-\kappa_{l\sigma} r). \tag{14}$$

Also $\varphi_\lambda(E_\sigma(k), r)$ is a solution of Eq. (2) with the boundary condition (5) for any k with $|k|$ finite in the cut k plane and, considered as a function of k , it is analytic there. It is simple to show, by use of some of Carter's results, that

$$\varphi_\lambda(E_\sigma(k), r) \sim \frac{1}{k^\lambda} \left(\frac{\cos[kr - \frac{1}{2}\pi\lambda - \epsilon_\sigma\mu(r)]}{\epsilon_\sigma \sin[kr - \frac{1}{2}\pi\lambda - \epsilon_\sigma\mu(r)]} \right), \tag{15}$$

where

$$\mu(r) = \int_0^r V(r') dr'. \tag{16}$$

2. Construction of $f(k)$

It is apparent from the properties of $f_\lambda^\sigma(k)$ stated above that phase shifts and bound-state energies are determined from $f_\lambda^\sigma(k)$. The converse is also true: phase shifts (for both positive and negative energies) and bound-state energies determine $f_\lambda^\sigma(k)$. The procedure for construction of $f_\lambda^\sigma(k)$ depends on a repeated application of a theorem due to Titchmarsh¹⁴ and is a slight modification of the procedure used in the non-relativistic case.¹ This modification is to introduce¹⁵ the functions $F(k)$ and $G(k)$ given by

$$F(k) = \ln[f^+(k)f^-(k)], \tag{17}$$

$$G(k) = \frac{k}{E_+(k)} \ln\left[\frac{f^+(k)}{f^-(k)}\right] + 2i\mu(\infty), \tag{18}$$

where

$$\mu(\infty) = \int_0^\infty V(r) dr$$

according to Eq. (16). First consider the case when no bound states exist; then $F(k)$ and $G(k)$ are analytic and bounded functions in the lower half of the complex k -plane. Furthermore

$$\int_{-\infty}^{+\infty} |\text{Im}F(k)|^2 dk \quad \text{and} \quad \int_{-\infty}^{+\infty} |\text{Im}G(k)|^2 dk$$

can be shown to be finite by use of the following property¹⁶ of the phase shifts:

$$\eta^\sigma(k) \underset{k \rightarrow \infty}{\sim} -\frac{E_\sigma(k)}{k} \mu(\infty) + O(1/k).$$

From this it follows¹⁴ that

$$\text{Re}F(k) = -\frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Im}F(k') dk'}{k' - k}, \quad (k \text{ real}) \tag{19}$$

$$\text{Re}G(k) = -\frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Im}G(k') dk'}{k' - k}, \quad (k \text{ real}) \tag{20}$$

where, from Eqs. (17) and (18), for k real, we have

$$\text{Im}F(k) = \eta^+(k) + \eta^-(k), \tag{21}$$

$$\text{Im}G(k) = (k/E_+(k))[\eta^+(k) - \eta^-(k)] + 2\mu(\infty). \tag{22}$$

¹⁴ E. C. Titchmarsh, *Theory of Fourier Integrals* (Clarendon Press, Oxford, 1948), p. 128.

¹⁵ This procedure is used by Corinaldesi in his discussion of the Klein-Gordon equation, reference 9.

¹⁶ This property was proved by G. Parzen, *Phys. Rev.* **80**, 261 (1950) and was further discussed by Carter, reference 12.

It is therefore possible to obtain, by means of expressions (19) and (20), $f^+(k)$ and $f^-(k)$ when $\eta^+(k)$ and $\eta^-(k)$ are given.

So far we have assumed that no bound states were present in order that $F(k)$ and $G(k)$ satisfy the condition of boundedness in the lower half of the k plane. If bound states are present, $f^\sigma(k)$ is equal to zero at those points which correspond to bound states. Those zeros are simple and all lie in the k imaginary axis: $k_l = -i\kappa_l$ with $0 < \kappa_l < +m$. We then define a modified $\tilde{f}^\sigma(k)$ and $\tilde{\eta}^\sigma(k)$ according to

$$\tilde{f}^\sigma(k) = f^\sigma(k) \prod_{l\sigma} \frac{k - i\kappa_{l\sigma}}{k + i\kappa_{l\sigma}}, \tag{23}$$

$$\tilde{\eta}^\sigma(k) = \eta^\sigma(k) - 2 \sum_{l\sigma} \arctan \frac{\kappa_{l\sigma}}{k}, \tag{24}$$

where the product and summation are extended to all the bound states associated to the same branch σ of E .

Then, since $\tilde{\eta}^\sigma(k) = \text{Im}\{\ln \tilde{f}^\sigma(k)\}$ and $\tilde{f}^\sigma(k)$ is nonzero in the lower half k -plane, Eqs. (19) and (20) will hold for $F(k)$ and $G(k)$, where by F and G we mean the expressions obtained by substituting f, η by $\tilde{f}, \tilde{\eta}$ in Eqs. (17), (18) and (21), (22). Thus, for a given λ , if the phase shifts for both positive and negative energies $\eta^\sigma(k)$ ($\sigma = +, -$) and all the binding energies $E_{l\sigma}$ are known, then $f^\sigma(k)$ is easily constructed.

3. Orthogonality of Eigenfunctions

Assume λ fixed. (The subscript λ will be omitted hereafter except when needed for clarity.)

From the results reviewed in the previous paragraphs it appears that there are solutions $\varphi(E, r)$ of Eq. (2) [with $V(r)$ satisfying the conditions (3)] together with the boundary condition (5) for any E such that $+m \leq E < \infty$ or $-\infty < E \leq -m$, and perhaps also for a certain finite number of isolated points E_l such that $-m < E_l < +m$. All these values of E , associated with solutions $\varphi(E, r)$ constitute the eigenvalue spectrum. The eigenfunctions $\varphi(E, r)$ possess orthogonality properties when their scalar product is appropriately defined and this property allows one to make generalized Fourier expansions in terms of the $\varphi(E, r)$.

Consider two eigenfunctions $\varphi(E, r), \varphi(E', r)$ corresponding to different eigenvalues E, E' of the energy. They satisfy the differential equation (2), and the boundary condition (5), which implies that $\varphi(E, 0) = 0$. With the notation $\tilde{\varphi} = \text{transposed of } \varphi$, that is, if

$$\varphi = \begin{pmatrix} F \\ G \end{pmatrix}, \quad \tilde{\varphi} = (FG),$$

and the properties

$$\tilde{\omega} = -\omega, \quad \tilde{\sigma}_1 = \sigma_1, \quad \tilde{\sigma}_3 = \sigma_3,$$

multiplication of Eq. (2) by $\tilde{\varphi}(E', r)$ on the left and of

the differential equation for $\tilde{\varphi}(E', r)$ by $\varphi(E, r)$ on the right, and subtraction, yields

$$\frac{d}{dr} [\tilde{\varphi}(E', r) \omega \varphi(E, r)] = (E - E') \tilde{\varphi}(E', r) \varphi(E, r),$$

from which, by integration between 0 and r and use of the boundary condition at $r=0$, one obtains

$$\int_0^r \tilde{\varphi}(E', r) \varphi(E, r') dr' = \frac{\det\{\varphi(E', r), \varphi(E, r)\}}{E - E'}. \tag{25}$$

If we let $r \rightarrow \infty$ in Eq. (25) and call

$$\int_0^\infty \tilde{\varphi}(E', r) \varphi(E, r') dr' = (\varphi(E', r), \varphi(E, r)), \tag{26}$$

the scalar product of $\varphi(E', r)$ and $\varphi(E, r)$, then the scalar product of two eigenfunctions is determined by the asymptotic behavior of the eigenfunctions according to Eq. (25). By use of Eq. (6) for $\varphi(E, r)$ in terms of $f(k, r)$ and $f(-k, r)$ in the right-hand side of Eq. (25), it can be shown that

$$\begin{aligned} \int_0^\infty \tilde{\varphi}(E_l, r) \varphi(E_l, r) dr &= \frac{1}{C_l} \delta_{l'l}, \\ \int_0^\infty \tilde{\varphi}(E, r) \varphi(E', r) dr &= g(E) \delta(E - E'), \\ \int_0^\infty \tilde{\varphi}(E_l, r) \varphi(E', r) dr &= 0, \end{aligned} \tag{27}$$

where $E_l, E_{l'}$ are discrete eigenvalues, E, E' continuous ones, and $C_l, g(E)$ are given in terms of $f(k)$ by

$$\begin{aligned} \frac{1}{C_l} &= \frac{1}{2} \frac{E_l}{E_l - m} f(-k_l) \left(\frac{df(k)}{idk} \Big|_{k=k_l} \right) / k_l^{2\lambda}, \\ g(E) &= \frac{\pi |f(k)|^2}{k^{2\lambda-1}(E-m)}. \end{aligned} \tag{28}$$

4. Expansions in Eigenfunctions

The orthogonality properties of the radial eigenfunctions for a fixed value of λ suggest the possibility of expanding arbitrary vectors $F(r)$ in terms of them. By an arbitrary vector $F(r)$ we mean a one-column two-component matrix, the components of which are arbitrary functions of r , integrable square in the range $(0, \infty)$:

$$F(r) = \begin{pmatrix} F_1(r) \\ F_2(r) \end{pmatrix}.$$

As in the case of expansion of an arbitrary function in terms of a Sturm-Liouville problem eigenfunctions,

the expansion formula is most concisely written when a so-called spectral function $\rho(E)$ is introduced.

We define $\rho(E)$ by

$$d\rho/dE = 1/g(E) \text{ for } E \geq +m \text{ or } E \leq -m, \quad (29)$$

$$= \sum_l C_l \delta(E - E_l) \text{ for } -m < E < +m,$$

where $g(E)$, C_l are the same quantities that appear in the orthogonality relations (27), and the sum \sum_l extends over all bound states.

With the spectral function as defined above, we can write the expansion of $F(r)$ in terms of the eigenvectors $\varphi(E, r)$ in the form

$$F(r) = \int d\rho(E) a(E) \varphi(E, r). \quad (30)$$

For such an $F(r)$ the expansion coefficient $a(E)$ is determined by $F(r)$ and $\varphi(E, r)$ according to

$$a(E) = \int_0^\infty \tilde{\varphi}(E, r) F(r) dr, \quad (31)$$

as can be seen by multiplying Eq. (30) by $\tilde{\varphi}(E, r)$, integrating over r , and making use of the orthogonality properties of the eigenvectors given by Eq. (27).

That Eq. (30), with $\rho(E)$ and $a(E)$ given by Eqs. (29) and (31), is actually true for an arbitrary function $F(r)$ is a consequence of the "closure" property of the eigenvectors $\varphi(E, r)$ which will be proved in the next section. We remark also that a property similar to Parseval's theorem holds for the expansion (30). This is seen by introducing in the expression for the norm of $F(r)$ the expansion (30). It is found that

$$\int_0^\infty \tilde{F}(r) F(r) dr = \int d\rho(E') [a(E')]^2, \quad (32)$$

where we have made use of Eqs. (27) and (29).

5. Closure Property

The eigenvectors $\varphi(E, r)$ possess the property

$$\int d\rho(E) \varphi(E, r) \varphi(E, t) = 1\delta(r - t), \quad (33)$$

(1 = unit 2×2 matrix) which shall be called "closure." We shall prove Eq. (33) utilizing the analytic properties of the eigenvectors in the complex k plane.

Before entering into the proof of the closure property some remarks about the spectral function are necessary. We want $\rho(E)$ to be a monotonic increasing function, a consequence of the relation between the derivative of the spectral function and normalization integrals given by Eqs. (27) and (29). On the other hand, expressions (28) for $g(E)$ and C_l and the definition (29) imply that

$$\frac{d\rho}{dE} = \frac{1}{\pi} \frac{k^{2\lambda-1}(E-m)}{|f(k)|^2} \text{ for } E \geq +m \text{ or } E \leq -m, \quad (34)$$

$$= \sum_l C_l \delta(E - E_l) \text{ for } -m < E < +m.$$

Therefore we have to establish k as a function of E so that $d\rho/dE \geq 0$ for all E 's. This is done by taking for $k(E)$ in the spectral function the function

$$k = +(E^2 - m^2)^{1/2} \text{ for } E \geq +m, \quad (35)$$

$$= -(E^2 - m^2)^{1/2} \text{ for } E \leq -m.$$

To prove Eq. (33) we evaluate the matrix integral P :

$$P(r, t) = \int d\rho(E) \varphi(E, r) \varphi(E, t).$$

Use of Eq. (34) with definition (35) gives

$$P = Q + \sum_\sigma \sum_{l\sigma} C_{l\sigma} \varphi(E_{l\sigma}, r) \tilde{\varphi}(E_{l\sigma}, t), \quad (36)$$

where

$$Q = \int_{-\infty}^{-m} + \int_{+m}^{+\infty} \left\{ \frac{d\rho}{dE} \varphi(E, r) \tilde{\varphi}(E, t) \right\} dE.$$

Change of the integration variable from E to k and use of the properties of the integrand under the change $k \rightarrow -k$ and of the expression (6) for $\varphi(E, r)$ gives

$$Q = -\frac{1}{2\pi i} \int_{\infty}^{+\infty} dk \sum_{\sigma} \frac{k}{E_{\sigma}(k)} \frac{1}{f_{\sigma}(k)} f_{\sigma}(k, r) \tilde{\varphi}(E_{\sigma}(k), t).$$

The integrand in this expression is a meromorphic function in $\text{Im}\{k\} < 0$ in the cut k -plane, because the only singularities correspond to the zeros of $f_{\sigma}(k)$ which are simple zeros, and $f_{\sigma}(k, r)$ and $\tilde{\varphi}(E_{\sigma}(k), t)$ are analytic functions of k . Also the integrand is continuous for $\text{Im}\{k\} \leq 0$.

Therefore we can deform the path of integration into the lower half plane as shown in Fig. 1. The integrations over the contour Γ are to be understood in the limit as $K \rightarrow \infty$. There are contributions from the residues at $k = k_{l\sigma}$ and from Γ . Since $f_{\sigma}(k)$ is analytic we can evaluate the residues immediately:

$$\text{Res.}[k = k_{l\sigma}] = -\frac{1}{2\pi i} \frac{k_{l\sigma}}{E_{l\sigma}} \frac{f_{\sigma}(k_{l\sigma}, r)}{[df_{\sigma}(k)/dk]_{k=k_{l\sigma}}} \tilde{\varphi}(E_{l\sigma}, t)$$

$$= (1/2\pi i) C_{l\sigma} \varphi(E_{l\sigma}, r) \tilde{\varphi}(E_{l\sigma}, t),$$

where the expression for $C_{l\sigma}$ given in (28) has been used. The contribution from Γ comes only from the two-quarter circles because the integrals along the sides of the cut cancel each other and the contribution from the circle around the branch point $-im$ goes to zero in the limit of vanishing radius. The contribution from the two-quarter circles is evaluated using the asymptotic expressions ($|k| \rightarrow \infty$) for $f(k, r)$ and $\varphi(E, t)$. One finds

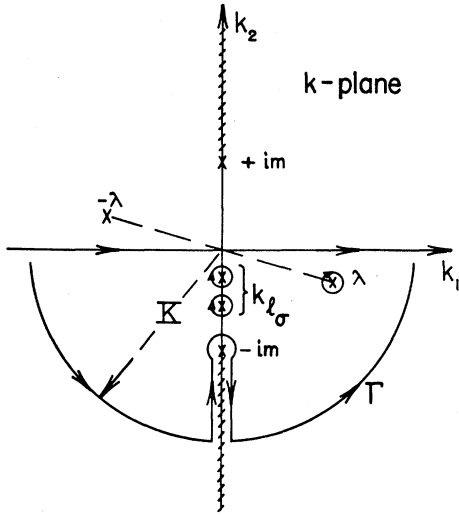


FIG. 1. Contour for the proof of Eq. (33) and the evaluation of expressions I and J .

then that

$$Q = -\sum_{\sigma} \sum_{l\sigma} C_{l\sigma} \varphi(E_{l\sigma}, r) \tilde{\varphi}(E_{l\sigma}, t) + 1\delta(r-t),$$

which, introduced in Eq. (36), gives $P = 1\delta(r-t)$, thus proving Eq. (33).

III. RELATION BETWEEN EIGENFUNCTIONS OF DIFFERENT POTENTIALS

1. Derivation of Relation

We shall show now that there exists a relation between the eigenfunctions $\varphi(E, r)$, $\varphi_1(E, r)$ associated, respectively, to potentials $V(r)$, $V_1(r)$. We shall assume that both potentials satisfy the conditions (3). A fixed value of λ will be assumed and both systems of eigenfunctions correspond to this same value of λ .

Following a procedure similar to that used by Jost and Kohn¹ in the case of the Schrödinger equation, we consider the two expressions

$$I = \int d\rho(E') \varphi(E', r) \int_0^r \tilde{\varphi}_1(E', s) \varphi_1(E, s) ds,$$

$$J = \int d\rho_1(E') \varphi(E', r) \int_0^r \tilde{\varphi}_1(E', s) \varphi_1(E, s) ds.$$

The integration over E' can be carried out by utilizing the properties of the eigenfunctions in the k plane and it is found that I and J are simply related to the eigenfunctions φ and φ_1 . Then, the relation between φ and φ_1 results by subtraction of I and J .

Calculation of I .—The integration over E' is changed to an integration over k as in the proof of the closure property

$$I = -\frac{1}{2\pi i} \int_{-\infty}^{+\infty} dk \sum_{\sigma} \frac{k}{E_{\sigma}(k)} \frac{1}{f_{\sigma}(k)} f_{\sigma}(k, r) \times \int_0^r \tilde{\varphi}_1(E_{\sigma}(k), s) \varphi_1(E, s) ds + \sum_{\sigma} \sum_{l\sigma} C_{l\sigma} \varphi(E_{l\sigma}, r) \times \int_0^r \tilde{\varphi}_1(E_{l\sigma}, s) \varphi_1(E, s) ds. \quad (37)$$

The path of integration can be deformed into the lower cut half k plane as shown in Fig. 1. We get contributions from the zeros of $f_{\sigma}(k)$ and from the two halves of the semicircle $|k| \rightarrow \infty$. Contributions from both sides of the cut cancel. The sum of residues cancels the summation on the right-hand side of Eq. (37) when one makes use of Eq. (28). Then I is equal to the sum of the contributions from the two halves of the semicircle as $|k| \rightarrow \infty$. These contributions are calculated making use of the asymptotic expressions $f_{\sigma}(k, r)$ and $\varphi_1(E_{\sigma}(k), s)$ for $|k| \rightarrow \infty$, $\text{Im}\{k\} < 0$, Eqs. (11) and (15). One obtains

$$I = \frac{1}{2} M(r) \varphi_1(E, r), \quad (38)$$

introducing

$$M(r) = 1 \cos[\mu(r) - \mu_1(r)] + \omega \sin[\mu(r) - \mu_1(r)]. \quad (39)$$

Calculation of J .—By use of Eq. (25), J can be written:

$$J = \int d\rho_1(E') \varphi(E', r) \frac{1}{E - E'} \tilde{\varphi}_1(E', r) \omega \varphi_1(E, r).$$

To avoid the singularity of the integrand at $E' = E$, consider instead $J(\epsilon)$ obtained by putting ϵ instead of E in J , where ϵ is complex and $\epsilon = E + i\eta$ with $\eta > 0$. We obtain by the same transformations used repeatedly before that

$$J(\epsilon) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{dk}{k - \lambda} \sum_{\sigma} \frac{k}{E_{\sigma}(k)} \frac{\epsilon + E_{\sigma}(k)}{\lambda + k} \frac{1}{f_{1\sigma}(k)} \times \varphi(E_{\sigma}(k), r) \tilde{f}_{1\sigma}(k, r) \omega \varphi_1(\epsilon, r) + \sum_{\sigma} \sum_{l\sigma} C_{l\sigma'} \varphi(E_{l\sigma'}, r) \times \frac{1}{\epsilon - E_{l\sigma'}} \tilde{\varphi}_1(E_{l\sigma'}, r) \omega \varphi_1(\epsilon, r), \quad (40)$$

where λ has been chosen to be that root of $\epsilon^2 - m^2$ that lies in the lower half k plane. We can now calculate this integral by deforming the path of integration into the lower cut half k plane. As in previous cases the contribution from the integrals along the sides of the cut is zero. There are contributions from the poles due to zeros of $f_1(k)$ and the pole at λ , and from the two halves of the semicircle as $|k| \rightarrow \infty$. The residue from $k = \lambda$ contributes $\varphi(\epsilon, r)$. The remaining residues cancel the sum in Eq. (40) when $\eta \rightarrow 0$. The integrals over the two halves of the semicircle $|k| \rightarrow \infty$, $\text{Im}\{k\} < 0$ can be

evaluated as in the calculation of I by use of the asymptotic expressions for f and φ . Collecting these results, one obtains that

$$J = \varphi(E, r) - \frac{1}{2}M(r)\varphi_1(E, r).$$

Hence

$$J - I = \varphi(E, r) - M(r)\varphi_1(E, r) = \int_0^r K(r, s)\varphi_1(E, s)ds, \quad (41)$$

where

$$\int d[\rho_1(E') - \rho(E')] \varphi(E', r)\tilde{\varphi}_1(E', s) = K(r, s). \quad (42)$$

Equation (41) gives the relation between the eigenfunctions φ , φ_1 . Notice that $K(r, s)$ is a matrix independent of E .

Except for the matrix $M(r)$, defined in (39), that multiplies φ_1 , Eq. (41) is formally similar to the one that appears in the nonrelativistic case.

2. Integral Relation for the Kernel

As has just been shown in the previous section, the eigenfunctions φ , φ_1 are related by Eq. (41) with $K(r, s)$ and $M(r)$, respectively, defined according to Eqs. (42) and (39).

Multiplying Eq. (41) by $\varphi_1(E, t)$ on the right and integrating with weight $d[\rho_1(E) - \rho(E)]$ we obtain, using Eq. (42), that

$$K(r, t) = M(r)G(r, t) + \int_0^r K(r, s)G(s, t)ds, \quad (43)$$

where

$$G(r, t) = \int d[\rho_1(E) - \rho(E)] \varphi_1(E, r)\tilde{\varphi}_1(E, t). \quad (44)$$

Equation (43) is an integral equation of the Fredholm type for the kernel $K(r, t)$. Notice that the matrix $G(r, t)$, that is the kernel in this integral equation and appears in the inhomogeneity term, is constructed from both spectral functions $\rho_1(E)$ and $\rho(E)$ and from the eigenfunctions associated only with the potential $V_1(r)$. It is convenient to transform this equation so as to eliminate the explicit appearance of the orthogonal matrix $M(r)$. To do this, we define a transformed kernel according to

$$\tilde{M}(r)K(r, t) = F(r, t). \quad (45)$$

From Eq. (43) the matrix $F(r, t)$ is shown to satisfy the following integral equation, formally similar to the Gel'fand-Levitan integral equation:

$$F(r, t) = G(r, t) + \int_0^r F(r, s)G(s, t)ds. \quad (46)$$

If we introduce $\varphi(E, r)$ as given by Eq. (41) into the Dirac radial wave equation (2) and use the corre-

sponding equation for $\varphi_1(E, r)$, we obtain the condition for the kernel:

$$\omega K(r, r) - K(r, r)\omega + (\tilde{M} - M)(\sigma_1\lambda/r - \sigma_3m) = 0.$$

This condition on $K(r, r)$ can be easily transformed into the following condition on $F(r, r)$:

$$\omega F(r, r) - F(r, r)\omega + (\tilde{M}\tilde{M} - 1)(\sigma_1\lambda/r - \sigma_3m) = 0. \quad (47)$$

This equation for the matrix elements $F_{ij}(r, r)$ yields only two independent conditions, which are conveniently written as

$$\begin{aligned} F_{12}(r, r) + F_{21}(r, r) &= S(r) = 2 \sin\Delta\mu [\lambda/r \cos\Delta\mu \\ &\quad - m \sin\Delta\mu], \\ F_{22}(r, r) - F_{11}(r, r) &= D(r) = 2 \sin\Delta\mu [m \cos\Delta\mu \\ &\quad + (\lambda/r) \sin\Delta\mu], \end{aligned} \quad (48)$$

where $\Delta\mu = \mu(r) - \mu_1(r)$. By simple algebra and differentiation, we obtain:

$$V(r) - V_1(r) = \frac{d}{dr} \left[\arctan \frac{D(r)}{S(r)} \right] - \frac{d}{dr} \left(\arctan \frac{mr}{\lambda} \right). \quad (49)$$

In addition to Eq. (49), the elements of $F(r, r)$ satisfy a second condition which can be combined with Eq. (49) to give other equivalent formulas for the potential $V(r)$. This connection between the elements can be given as:

$$[(\lambda/r) - D]^2 + (m + S)^2 = (\lambda/r)^2 + m^2, \quad (50)$$

which is readily obtained from Eq. (48).

IV. METHOD FOR CONSTRUCTING THE POTENTIAL

From the properties relating the eigenfunctions corresponding to the two potentials $V(r)$ and $V_1(r)$ a procedure can be established to construct $V(r)$ when the phase shifts $\eta_\sigma(k)$ and the bound-state energies $E_{l\sigma}$ ($l=1, 2, \dots, m_\sigma$), $\sigma=+, -$ are given for both positive and negative energies for fixed angular momentum, that is for a fixed λ . The steps in this procedure are as follows:

1. First $f_\sigma(k)$ ($\sigma=+, -$) can be constructed from $\eta_\sigma(k)$ and $E_{l\sigma}$ by the Hilbert transform type of relations [Eqs. (19) and (20)].

2. From $f_\sigma(k)$ we obtain $d\rho/dE$ by means of Eq. (34). Since $\eta(k)$, E_l do not determine the constants $C_{l\sigma}$, these can be chosen *arbitrarily* as long as they are positive, in accordance with their definition (27). Once these constants are chosen the spectral function derivative is known.

3. If a comparison potential $V_1(r)$ is taken for which everything (i.e., spectral function and eigenfunctions) is known, we can construct the matrix $G(r, t)$ according to Eq. (44). Then we have the kernel and inhomogeneity of the generalized Gel'fand-Levitan integral equation (46).

4. The solution of the generalized Gel'fand-Levitan integral equation for $r \geq t$ yields $F(r,t)$; the difference of the unknown potential $V(r)$ and the comparison potential $V_1(r)$ is given by Eq. (49), and we can construct the matrix $M(r)$ defined by Eq. (39) and then the kernel $K(r,t)$ from Eq. (45). Once $K(r,t)$ is known, the eigenfunctions $\varphi(E,r)$ are given from the $\varphi_1(E,r)$ by Eq. (41).

V. DISCUSSION

The procedure derived above for the construction of the potential in the Dirac equation is similar in most respects to the previously known method^{1,2} for the nonrelativistic Schrödinger equation. In fact, each step in the procedure can be shown to reduce in the limit of small velocities to the corresponding step in the nonrelativistic case.¹⁷ In this nonrelativistic limit, the phase shifts for the same angular momentum and opposite parities become equal; the positive- and negative-energy regions are no longer interdependent but split into separate problems; in each the phase shifts and bound-state data (e.g., for positive energies only) will be sufficient to determine the potential.

The procedure for construction of the potential that has been presented is mathematically straightforward but there are three reasons for the lack of practical usefulness in the direct analysis of experimental values:

1. The interaction was restricted to a spherically symmetric static potential; all actual physical interactions are more complicated. Furthermore, in most cases when relativistic effects are important ($E - mc^2 \approx mc^2$) the possibilities of recoil or of inelastic effects, or even of particle creation, are significant. The present method could probably be generalized to include some of these complications, but this is not of great importance because of the other limitations of applicability.

2. The method for construction of the potential requires *exact* knowledge of the phase shifts for all energies. Since experimental values have limited accuracy and are available only for a finite range of

¹⁷ For details, see Chap. VI of the dissertation of reference 10.

energy, an application of the method to experimental values should be accompanied by a discussion of the effect of an error in the data on the predicted potential. This problem is especially difficult and has not been thoroughly analyzed even in the simpler nonrelativistic case.¹⁸

3. The method presented is necessarily quite cumbersome. The procedure for the nonrelativistic case was already so complicated as to preclude many practical applications, and the present relativistic treatment is necessarily much more involved.

In the nonrelativistic case, Bargmann described¹⁹ interesting families of potentials for which the solutions $f(k,r)$ of the Schrödinger equation were rational functions of k . These examples were especially instructive, because the phase shifts, wave functions, and potentials were given in convenient closed form. We have investigated to see if similar families of solutions can be found for the Dirac equation. However, it is easy to show that the $f(k,r)$ cannot be rational functions even in the two variables E and k , because such a nontrivial rational form is inconsistent with the asymptotic behavior in the complex k plane [see Eq. (11)]; no simple transformation has been found which can meet this difficulty.

The procedure of Sec. IV exhibits the one-to-one correspondence between potentials satisfying the integrability conditions (3) and "allowable" sets of scattering data (including phase shifts and bound-state energies and norms). However, it remains to find convenient characterizations of the class of phase shifts that can be obtained from a Dirac equation potential.

VI. ACKNOWLEDGMENTS

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¹⁸ For a discussion of some effects of such variations, see R. G. Newton, *Phys. Rev.* **101**, 1588 (1956).

¹⁹ V. Bargmann, *Revs. Modern Phys.* **21**, 488 (1949).