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S-Matrix, Wave Functions, and Foundations of Quantum Mechanics

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The relation between the S-matrix approach and the conventional wave function method is discussed for bound-state problems. It is pointed out that the S-matrix method does not guarantee the proper boundary conditions for bound-state wave functions. It is pointed out further that the attempt to localize the probability distribution leads to an explicit construction of normalizable bound-state wave functions. Since the primary advantage of the S-matrix method is its ability to accommodate Lorentz covariance, the above conclusion forces us back to the difficult question of constructing relativistic bound-state wave functions. A covariant harmonic oscillator model in which wave functions carry a covariant probability interpretation is discussed.

I. INTRODUCTION

Wave functions are needed to represent the quantum superposition principle. Ever since the invention of quantum mechanics, persistent efforts have been made to incorporate the concept of relativistic spacetime into the quantum superposition principle. This is of course a difficult problem, and this difficulty is manifested by the notable absence of relativistic wave functions carrying a covariant probability interpretation.

This and other limitations of the wave function led Heisenberg[1] to reformulate non-relativistic quantum mechanics in terms of the S-matrix. A series of successful attempts have been made to Lorentz generalize quantum mechanics through the S-matrix formalism. The giant step in this direction was of course the formulation of covariant field theory by Feynman, Schwinger, and Tomonaga.[2]

During the course of this development, the role of wave functions became obscure. Frankly, the author does not know where the wave function stands in field theory. In order to prove this point, let us observe the following fact. In obtaining discrete energy levels of a bound state, we insist that the bound-state wave function should be normalizable and that this should correspond to a localized probability distribution. In the S-matrix approach, we construct Feynman amplitudes and calculate S-matrix elements. However, each external line of Feynman diagram represents a particle which is free either in the

remote past or in the remote future. Bound-state particles are not free. Therefore, a single Feynman diagram can never explain the bound state. Heisenberg foresaw this difficulty and suggested that the bound-state problem be handled by analytic continuation of the S-matrix to unphysical region.

In this paper, we discuss first a concrete example where the analytic continuation method leads to a violation of the localization concept. It is then pointed out that a method exists which will assure the proper boundary conditions of bound-state wave functions. However, this method is based on an explicit construction of the bound-state wave function. We are not aware of any other method which will guarantee the desired localization. While the primary advantage of the S-matrix approach is its ability to accommodate Lorentz covariance, our attempt to localize bound-state wave functions in the S-matrix framework leads to pre-Heisenberg wave functions. This forces us back to the difficult problem of constructing relativistic bound-state wave functions with appropriate probability interpretation. We discuss a possible model for studying this problem.

This paper is based on the results published by the author and his collaborators in their earlier papers on potential scattering[3] and covariant wave functions.[4] Therefore the present paper does not contain any new result on those subjects. The purpose of this paper is to reorganize those separately published results in order to make new preparations for attacking some of the difficult problems of quantum mechanics.

In Sec. II. we discuss within the framework of non-relativistic quantum mechanics how the violation of localization occurs in the S-matrix approach. In Sec. III, we present a possible method which will guarantee the desired localization. This method is based on the explicit construction of a bound-state wave function. Sec. IV deals with the problem of constructing a covariant harmonic oscillator model in which wave functions can carry a covariant probability interpretation. In Sec. V, we discuss possible applications of the oscillator model to high-energy particle physics.

Ⅱ. WAVE FUNCTIONS IN THE S-MATRIX

Since wave functions have well-defined meaning only in nonrelativistic quantum mechanics, we discuss the relation between the S-matrix and wave functions within the framework of non-relativistic potential scattering. We are interested in bound-state wave functions. Perhaps the best place to illustrate the use of bound-state wave functions is the first-order perturbation theory.[5] Let us consider the first-order energy shift in terms of the wave functions and a weak perturbing potential.

$$\delta E=(\phi,\ \delta V\ \phi) \qquad (1)$$

We now contemplate calculating the above quantity using only the S-matrix quantities which can be continued analytically to the unphysical region in the complex energy plane.

The S-matrix, in the physical region, contains both solutions of the Schrödinger equation satisfying the outgoing-wave [exp (ikr)] and the incoming-wave [exp$(-ikr)$] boundary conditions respectively. Let us now consider analytic continuation of the S-matrix to a bound state. The bound state is characterized in the S-matrix approach by an isolated pole in the complex plane. In order to reach this isolated point, we have to go through the complex unphysical region. During this process, the momentum becomes a purely imaginary quantity $i\kappa$ where κ is positive, and the outgoing wave becomes exp $(-\kappa r)$, while the

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incoming wave behaves like $\exp(\kappa r)$. We sketched these wave funtions in Fig. 1, and we call them "good" and "bad" wave functions respectively. When we reach the correct binding energy, the bad wave function is to be cut off by the law of dynamics. Since this localization condition is overlooked in many S-matrix approximations, it is easy to allow some bad wave functions to exist even at the exact binding energy.

Perhaps the best known work involving the above effect is the calculation of the n-p mass difference by the S-matrix perturbation method developed by Dashen and Frautschi[6] Let us review how this trouble occurs. Because their method fails to cut off all bad wave functions, their approximation leads in effect to

$$\delta E=(\phi^{good},\ \delta V\ \phi^{bad}) \qquad (2)$$

Now, for the electromagnetic perturbation,

$$\delta V=\frac{1}{r}\exp(-\lambda r), \qquad (3)$$

where $\lambda\to 0$, the integrand in normal circumstances (where only good wave functions are allowed) would have an exponential cutoff factor

$$\exp[-(2\kappa+\lambda)r], \qquad (4)$$

giving a comfortable cutoff factor even if $\lambda\to 0$. However, in the case of Eq. (2), the exponential cutoff factor is merely exp $(-\lambda r)$ which gives a logarithmic divergence for $\lambda\to 0$. It was shown that this indeed was the source of their spurious infrared divergence.[7]

It is widely believed that Dashen's calculation of the n-p mass difference is wrong and therefore does not deserve any further attention. We disagree. The Dashen-Frautschi case is indeed an excellent crossing point where both the S-matrix method and the conventional wave-function approach can be used for the same purpose. Recognizing the seriousness of the problem of boundary conditions, Kim and Vasavada [5,8] attempted to construct a method which will generate the desired localization in every step in the calculation. Let us review this method in the following section.

III. CONSTRUCTION OF BOUND-STATE WAVE FUNCTIONS FROM THE S-MATRIX

We have seen in the preceding section how "bad" wave functions can arise in the S-matrix approach. At present, the author is not aware of any S-matrix method which will guarantee the "good" behavior of the bound-state wave function. However, we are free to take the view that the physics remains unchanged whether we use the S-matrix, the wave function or a combination of both. With this in mind, we can now attempt to construct a "good" bound-state wave function from the S-matrix quantities.[5]

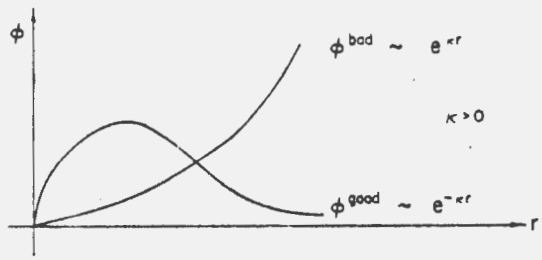

Fig. 1. "Good" and "bad" bound-state wave functions. The bad component comes from the failure to cut off the analytic continuation of the incoming wave component in the S-matrix.

Without loss of generality, we can consider the S-wave Schrödinger equation.

$$\left[\frac{d^2}{dr^2}+k^2-V(r)\right]\phi(k,r)=0 \qquad (5)$$

By solving this differential equation, we can obtain the wave function $\phi(k,r)$, and this procedure is well known. We can also convert this differential equation to an integral equation and obtain the S-matrix quantities by solving the integral equation. The most commonly

used S-matrix quantity is of course the Jost function. In terms of the Jost function $f(k)$, the S-matrix takes the form

$$S(k)=f(k)/f(-k). \tag{6}$$

It is well known that the Jost function can be calculated from the asymptotic form of the wave function $\phi(k,r)$. However, the point we like to stress here is that its inverse is also true. This mechanism is called the theorem of Gelfand and Levitan.[9] The mathematics of this theorem is somewhat lengthy. We shall therefore skip the full statement of the theorem and shall illustrate the use of the G-L formalism using the well-known completeness relation in quantum mechanics.

Let us state the completeness relation in the following way. Consider all regular solutions of the Schrödinger equation $\phi(k,r)$ normalized as

$$\lim_{r\to 0} \phi(k,r)=r. \tag{7}$$

Then the completeness relation becomes[10]

$$\frac{2}{\pi}\int_0^\infty k^2[f(k)\ f(-k)]^{-1}\phi^*\ (k,r)\phi(k,r')dk + \sum_b C_b\phi_b^*(k_b,r)\ \phi_b(k_b,r')=\delta(r-r') \tag{8}$$

where the summation b is overall bound states, and k_b is the imaginary momentum corresponding to the b-th binding energy. The constant C_b can be determined from the Jost function $f(k)$:

$$\frac{1}{C_b}=\frac{-1}{4ik^2}f(k)\frac{df(-k)}{dk}\bigg|_{k=k_b}. \tag{9}$$

We can now regard Eq. (8) as the equation in which the Jost $f(k)$ is an input and the wave function $\phi(k,r)$ is an output. It should be noted that this equation is only a completeness relation and does not allow us to obtain $\phi(k,r)$ uniquely from the S-matrix quantities. The Gelfand-Levitan theorem does not change the above input-output relation, but allows us to determine $\phi(k,r)$ uniquely from $f(k)$.

It is now possible to construct a bound-state wave function from the S-matrix quantities. It is not difficult to study the behavior of this wave function from its explicit expression. In fact, various approximation procedures exist in the literature.[3,5,9]

We are not concerned here with numerical accuracies of the above-mentioned approximations. What is important here is that the attempt to localize bound-state wave functions in the S-matrix approach brought us back to the wave function, whose explicit form we attempted to avoid because of the difficulty in Lorentz generalization.

The above cyclic process has been in exact pace with the development of strong-interaction physics during the past twenty years. Because of the practical difficulties in applying the present form of quantum field theory to strong interaction physics, it was felt twenty years ago that experimentally measurable relations could be obtained by analytic continuation of the S-matrix into the complex energy plane, while the analytic properties are to be determined from the well-defined physical principles.[11] However, the road

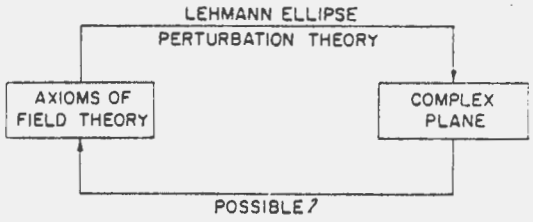

Figure 2. The realtion between the axioms of field theory and the complex plane. The local commutativity of the field theory operators leads to the analyticity needed to derive forward dispersion relations. However, we have not yet established the analyticity beyond the Lehmann ellipse from this causality axiom. Perturbation theory could give wider region of analyticity for more ambitious dynamical models.

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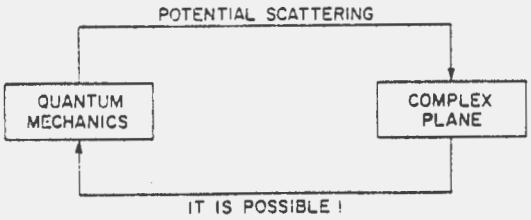

Figure 3. The relation between quantum mechanics and the complex plane. Here we study anlytic properties of the S-matrix constructed for potential scattering. Unlike the case of field theory, we can obtain the Schrödinger wave function from singularities in the complex plane.

to the complex plane did not turn out to be as smooth as was expected from the initial successes of dispersion relations. For this reason, less ambitious analyticity programs such as the use of perturbation theory or the use of potential scattering often served practical purposes. This trend is illustrated in Figs. 2 and 3.

This liberalization of analyticity made the connection between the physical principles and singularities in the complex plane relatively obscure, and led Chew[12] to question whether the physical principles, especially locality needed to describe bound states (or bootstrapped particles), can be formulated in the language of complex variables. This question is exactly the problem we discussed above in connection with the construction of normalizable bound-state wave functions from the S-matrix quantities.

We do not like wave functions because they cannot be Lorentz-generalized. Can we then completely avoid this quantity if we use the S-matrix? As far as we can see, the answer is "No". This means that we are forced back to pre-Heisenberg wave functions and to the difficult task of Lorentz generalizing the concept of wave function. In the following section, we shall discuss a simple theoretical model which is compatible both with the quantum superposition principle and with relativistic space-time.

IV. COVARIANT HARMONIC OSCILLATORS

The conclusion of the preceding section forces us to look into a possibility of constructing a model of covariant quantum mechanics based on relativistic wave functions. As we stressed in Sec. I, persistent efforts have been made for this purpose. Perhaps the most important steps were taken by Newton and Wigner,[13] and by Dirac.[14] Newton and Wigner were primarily interested in defining the position operator. Dirac's main interest was in representing the Poisson brackets in a covariant manner. The first attempt to construct a covariant standing wave was made by Yukawa in connection with Born's reciprocity relation.[15]

Yukawa started with the following Lorentz-invariant harmonic-oscillator differential equation.

$$\frac{1}{2}\left(\frac{\partial^2}{\partial x_\mu{}^2}-\omega^2 x_\mu{}^2\right)\psi(x,p)=\lambda\psi(x,p), \quad (10)$$

with the subsidiary condition

$$p^\mu\left(\omega x_\mu+\frac{\partial}{\partial x^\mu}\right)\psi(x,p)=0 \quad (11)$$

where x_μ is the relative space-time difference between the two point particles bound by a harmonic oscillator pontential, and p^μ is the total four momentum of the two-particle system.

Though the equation is simple and separable, it contains all the known "inconveniences" of the relativistic wave equation. It represents a noncompact group which will lead either to non-unitary representation or to infinite-component wave functions. This sometimes appears as negative norms or negative eigenvalues. These features prevented us, in the past, from attempting a probability interpretation.

The study of Eq. (10) in connection with a possible probability amplitude was revived by the form factor calculation of Fujimura

et al.[16] who related the asymptotic behavior of the nucleon form factor to the Lorentz contraction property of the ground-state solution of Eq. (10). This interest was further enhanced by Feynman *et al.*[17] who proposed the use of Eq. (10) and Eq. (11) for relativistic quark models. While their work does not provide significant innovations for treating covariant wave functions, it contains an important remark in relation to the conventional Feynman diagram approach to particle physics. Feynman *et al.* state that it would be difficult to expect dynamical regularities among resonances from the conventional field theory and that it is worth considering a new relativistic theory which is naive and obviously wrong in its simplicity, but which is definite and enables us to calculate as many things as possible. The model would be clearly "wrong" or incomplete if its wave functions did not carry a probability interpretation.

The relativistic wave functions which Feynman *et al.* used in their paper are not normalizable and do not give correct form factors. Lipes[8] attempted to reformulate their work using normalizable wave functions. However, his excited-state wave functions do not satisfy the harmonic oscillator wave equation except in the rest frame. Kim and Noz[4] observed this point and constructed ghost-free excited-state wave functions which are completely covariant and which satisfy the Lorentz invariant harmonic oscillator equation in all Lorentz frames.

The construction of Kim and Noz goes like this. The hyperbolic differential equation of Eq. (10) is separable in the x,y,z,t variables. It is also separable in their Lorentz transforms:

$$\begin{aligned} x' &= x \quad y' = y, \\ z' &= (1-\beta^2)^{-\frac{1}{2}}\ (z-\beta t), \\ t' &= (1-\beta^2)^{-\frac{1}{2}}\ (t-\beta z), \end{aligned} \tag{12}$$

where β is the velocity parameter of the four vector p. The normalizable solution then becomes

$$\psi(x,p) = H(x',y',z') \times \exp\left\{-\frac{\omega}{2}(x'^2+y'^2+z'^2+t'^2)\right\} \tag{13}$$

where $H(x',\ y',\ z')$ is a product of Hermite polynomials corresponding to excitations along the x', y' and z' directions. Eq. (11) suppresses time-like excitations along the t' direction.

We can now define the inner product of the two wave functions as

$$(\psi(x,p),\ \psi'(x,p')) = \int d^4x\ \psi^*(x,p)\ \psi'(x,p') \tag{14}$$

If the velocity parameters of p and p' are the same, then both wave functions are in the same Lorentz frame, and the inner product, after the time integral, becomes exactly that of non-relativistic quantum mechanics. If p and p' have different parameters, one wave function should see the Lorentz contraction effect of the other.

Let us ignore the trivial transverse excitations. It was shown by Ruiz[19] that these wave functions satisfy the orthogonality and Lorentz contraction properties which are summarized in Fig. 4. The orthogonality relation is preserved under Lorentz transformations. This means that the quantum number n has a Lorentz-invarianat meaning. Furthermore, the ground-state wave function with one half-wave with no node is contracted like a rigid rod. The n-th excited-state wave function with $(n+1)$ half waves and n nodes contains a polynomial of the n-th degree. For this reason, the wave function should be contracted like a multiplication of $(n+1)$ rigid rods. In fact, our excited-state wave functions behave exactly like that.

While it is still remote to attempt a completely covariant relativistic measurement theory,[20] the above-mentioned properties do not discourage us from attaching a covariant probability interpretation to our harmonic oscillator wave functions. In order to develop a measurement theory, we should look into the question of causality, the

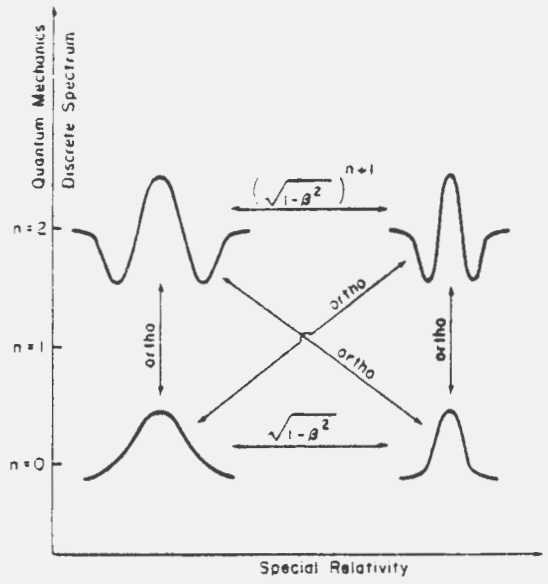

Fig. 4. Orthogonality relations and Lorentz contraction properties of the covariant harmonic oscillators. The vertical axis represents quantum mechanics where discrete energy levels come from the localization condition on bound-state wave functions. The horizontal axis describes Lorentz contractions in relativistic space-time.

role of probability in field theory and other important matters. One aspect which is at least as important as these fundamental questions is the ability of the above-mentioned probability to produce experimentally measurable numbers. In the following section we shall discuss possible applications of the above formalism to high-energy physics.

V. APPLICATION TO HIGH-ENERGY PHYSICS

One of the most important tasks in particle physics is to determine whether elementary particles are elementary. The most striking work in this regard was Hofstadter's observation that the nucleon is not a point particle and has a non-zero size.[21] Since this discovery, we have been constantly asking what the nucleon (and hadrons in general) is made of. The most successful answer to this question is of course the quark model.[22]

Although the quarks were originally introduced to explain SU (3) symmetry and its consequences, the immediate question was what forces are responsible for making quarks stay together in a localized region. Here again we have to use the language of quantum mechanics. We can consider quarks trapped in an attractive potential well. Then the most direct way to find out the nature of this binding force is to examine regularities in the mass spectrum. At present, the discrete particle-resonance spectra come from two distinct sources. One is the symmetry breaking interaction which removes degeneracies of the SU(6) symmetry, and the other is the Rydberg-like effect which is caused by the localization condition on spatial wave functions. Unlike the case of atomic physics, these two effects are of equal magnitude, and the study of one requires a careful examination of the other. We are of course interested in the spectra caused by the localization condition imposed on radial wave functions. The phenomenological study of this radial effect leads us to believe that the force between two quarks is indeed like that of a harmonic oscillator.[24]

Let us go to Fig. 4. We have just finished the argument that the vertical axis has relevance to particle physics. Let us next turn our attention to the horizontal axis. This axis describes the effect of Lorentz contraction. We know that hadrons are quantum mechanical bound states, and that they are subjected to Lorentz contraction when they move. Therefore Fig. 4 applies to *all* hadronic processes.

As far as the ground-state is concerned, the

form factor calculation of Fujimura *et al.*[17] demonstrates the existence of the Lorentz contraction effect. As for the excited states, Lipes made a careful analysis of the electromagnetic excitations of the nucleon resonances.[18]

Another place where the Lorentz contraction plays a role is the diffractive excitation where the Glauber model is applicable.[24]

Perhaps the physical process where the concept of probability could play a decisive role is the hadronic decay of resonances. This decay problem has been the central issue in the quark model calculations,[17] and the absence of covariant wave funcations used to be the serious weakness of those calculations. The above probability formulation removes this difficulty.

We can construct a hadronic decay amplitude simply by taking a probability overlap integral. This allows us to calculate the effect of internal motions of the quarks on the decay amplitude. This recoil effect can give observed polarization ratios in the hadronic decays of resonance excitations. In the case of meson decays, a preliminary calculation exists.[25] In the case of baryonic resonances, calculations are difficult and lengthy, but the experimental numbers are better established. Therefore, the baryon decay could be a decisive battleground for the relativistic quark model and for the concept of covariant probability which we discussed in Sec. IV.

CONCLUDING REMARKS

There are at present several different approaches to the reexamination of the quantum superposition principle. In most of these approaches, the primary interest is in logical consistencies of the probability interpretation, in the tradition of von Neumann.[26] In practice, one looks for possible logical deficiencies in the probability formalism based on the mathematics of Hilbert space. In this paper, we are also concerned with the concept of probability. We believe however that the most serious weakness of the probability interpretation is its lack of covariance. The present paper deals with a simple computable model for studying this problem.

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