On The Existence of Stationary States of the Mesotron Field

L. I. SCHIFF, H. SNYDER, AND J. WEINBERG
University of California, Berkeley, California
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For some electrostatic potentials, such as that represented by a sufficiently deep well, the Pauli-Weisskopf wave equation has complex frequencies. It is shown that when this happens the quantized field Hamiltonian can no longer be diagonalized. Some points of similarity and difference between this theory and the Dirac positron theory are discussed.

IT has been shown in the preceding paper[1] that the quantized field Hamiltonian of the Pauli-Weisskopf theory can be brought into diagonal form by a unitary transformation when

$$\epsilon_{kl} \equiv \int \psi_l^*(E_k + E_l^* - 2eV)\psi_k dv \qquad (1)$$

is diagonal. Here, the orthogonality relation between solutions ψ_k of the differential equation is $\epsilon_{kl}(E_k - E_l^*) = 0$. It is apparent that when any of the E_k become complex, ϵ_{kl} is no longer diagonal, $\epsilon_k = 0$, and the formalism of the preceding paper breaks down. In Section I of the present paper we show that complex frequencies actually can occur for a simple type of potential. In Section II it is shown that under these circumstances the Hamiltonian can no longer be diagonalized.

I.

The existence of complex frequencies of the Klein-Gordon differential equation is most readily demonstrated by solving the equation explicitly for a square well electrostatic potential. We take a potential that is attractive for a particle of charge e: $eV(r) = -V_0 < 0$ for $r < a$, and $eV(r) = 0$ for $r > a$; the character of the results obtained below for this potential do not depend on the discontinuity of $V(r)$ at $r = a$. The equation separates in spherical coordinates, and it is sufficient for our purposes to consider only the spherically symmetric part $\psi_0 \equiv u/r (l=0)$. The regular solution for a bound state of frequency E, which we shall assume for the moment to be real, corresponds to $E^2 < 1$, $(E+V_0)^2 > 1$, and is:

$$\begin{aligned} u &= A \sin(\xi r/a), \qquad r < a, \\ u &= A \sin \xi \cdot \exp[-\eta(r/a - 1)], \qquad r > a. \end{aligned} \qquad (2)$$

Here, $\xi \equiv a[(E+V_0)^2 - 1]^{\frac{1}{2}}$, $\eta \equiv a(1-E^2)^{\frac{1}{2}}$, and the boundary condition at $r = a$ gives:

$$\xi \cot \xi = -\eta. \qquad (3)$$

The solution of Eq. (3), giving E in terms of V_0, may be found by plotting $\xi \cot \xi$ and $-\eta$ against E for various values of V_0. It is found that there is no solution such that $E^2 < 1$ for small V_0; for $V_0 < 2$ but greater than a value V_1, there is just one root E_1 that decreases from $+1$ as V_0 increases. This state of affairs continues for V_0 somewhat greater than 2 but less than a value V_2, at which point a second root E_2 slightly greater than -1 appears. As V_0 increases further, E_1 continues to decrease while E_2 increases, until for a value V_3 of V_0 the two roots come together and the solutions become identical. For $V_0 > V_3$, the roots are complex and their solutions complex functions that are regular for all r. The pair of roots and the pair of solutions are then complex conjugates of each other. For sufficiently small a, V_1 can be greater than 2, while V_2 and V_3 are always greater than 2; all three decrease with increasing a.

We can readily evaluate ϵ from Eqs. (1) and (2):

$$\epsilon = 4\pi A^2 a[(E+V_0)(1 - \sin \xi \cos \xi/\xi) + E \sin^2 \xi/\eta],$$

from which it follows that

$$\epsilon = -(4\pi A^2 \sin^2 \xi/a)[(\partial/\partial E)(\xi \cot \xi) - (\partial/\partial E)(-\eta)].$$

By comparison with the slopes of the curves of

[1] H. Snyder and J. Weinberg, Phys. Rev., this issue; equations of this paper are referred to as I(34), for example. The units used in both papers are such that $c = \hbar = m_0 = 1$.

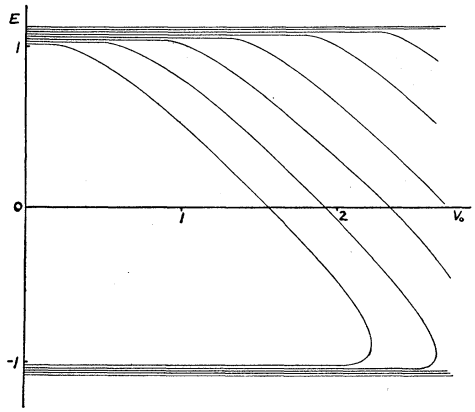

FIG. 1. The frequency E of the Klein-Gordon equation with a square well potential in a large box, as a function of the depth V_0 of the potential, for $l=0$.

$\xi \cot \xi$ and $-\eta$ against E, one sees that $\epsilon>0$ for the root E_1, $\epsilon<0$ for the root E_2, and $\epsilon=0$ for $E_1=E_2(V_0=V_3)$ since the two curves are tangent to each other at this point. This behavior of the lowest frequencies and their ϵ's is followed by the higher roots that arise from the other branches of the $\xi \cot \xi$ curve.

It is instructive to follow the behavior of the frequencies in the continuum as well as for $E^2<1$, in order to ascertain whether or not anything happens in the continuum to make up for the loss of pairs of real discrete eigenvalues. This can be accomplished by placing the potential well at the center of a spherical region of radius $R\gg a$, at which the current is made to vanish. The "continuum" ($E^2>1$) then consists of a set of closely spaced discrete states. The (unnormalized) regular solutions are properly joined pairs of the following:

$$\begin{aligned} u&=\sinh(\lambda r/a), \quad & r<a, \quad & (E+V_0)^2<1, \\ u&=\sin(\xi r/a), \quad & r<a, \quad & (E+V_0)^2>1; \end{aligned} \tag{4}$$

$$\begin{aligned} u&=\sinh[(\eta/a)(r-R)], \quad & r>a, \quad & E^2<1, \\ u&=\sin[(\mu/a)(r-R)], \quad & r>a, \quad & E^2>1; \end{aligned} \tag{5}$$

where $\lambda\equiv a[1-(E+V_0)^2]^{\frac{1}{2}}$, $\mu\equiv a(E^2-1)^{\frac{1}{2}}$. The positions of the roots are most readily found by plotting the logarithmic derivative of Eqs. (4) against $(E+V_0)$ and the logarithmic derivative of Eqs. (5) against E, superposing them on each other with the origin of the former curve shifted to the left by a variable amount V_0, and picking off the values of E for which intersections occur. The schematic curves of Fig. 1 were obtained in this way; they move to the left and crowd together as a increases. It is seen that the lowest level of the upper "continuum" ($E>1$) and the highest level of the lower "continuum" ($E<-1$) come together fist, then the second lowest of the upper and the second highest of the lower "continuum," etc. Thus the confluence of a pair of roots represents a genuine replacement of a pair of real frequencies by a conjugate complex pair of complex frequencies, accompanied by no other gain or loss of roots.

It must be remembered that the contribution of one of the real frequencies to the quantized field energy and charge is given by $NE\epsilon$ and $Ne\epsilon$, respectively, where N is the occupation number for the state in question. Thus the frequency E_1 represents (for $N=1$) a particle of charge e bound by an attractive potential, while the frequency E_2 represents a particle of charge $-e$ *bound by a repulsive potential* such that its energy is between 0 and 1. It should be remarked again that all of these results follow in qualitatively similar fashion for any sufficiently deep and broad potential well, and do not depend on the discontinuity of the above chosen $V(r)$ at $r=a$.

In view of the paradoxical result italicized above and the appearance of complex frequencies for sufficiently deep and broad potentials, it is of interest to see if similar results obtain in the case of a Dirac particle. Separating in spherical coordinates in the usual way[2] and considering only the pair of solutions of lowest angular momentum ($j=\frac{1}{2}$, $\kappa=\pm 1$), we obtain for the (unnormalized) solution corresponding to the first of Eqs. (5) and $\kappa=-1$:

$$\begin{aligned} rg&=\sinh[(\eta/a)(r-R)], \\ rf&=(1+E)^{-1}\{(\eta/a)\cosh[(\eta/a)(r-R)] \\ &\qquad -r^{-1}\sinh[(\eta/a)(r-R)]\}, \end{aligned}$$

with similar solutions for the other three cases. The same procedure for finding the frequencies may then be followed as in the Pauli-Weisskopf case, except that the boundary condition at $r=a$ is now that f/g be continuous.

The behavior of the roots is plotted schematically in Fig. 2; again the curves move to the left and crowd together as a increases. There is

[2] H. A. Bethe, *Handbuch der Physik* 24/1, p. 312.

no crossing or disappearance of real roots; they simply move successively from the bottom of the upper to the top of the lower "continuum." If the vacuum is defined as that state of the system in which the total charge is equal to just that of the filled negative energy "continuum" for $V_0=0$ and the energy is a minimum, then one sees that there are no bound positron states, and the paradoxical result obtained above for the Pauli-Weisskopf case does not occur here. For sufficiently large V_0, however, the vacuum is not the lowest possible energy state of the system, but differs from it by a charge and energy that are both finite for finite V_0. The states for $\kappa=+1$ are obtained from the above by interchanging f and g and changing the signs of E and V_0; they behave qualitatively the same as, and are separate from, the states for $\kappa=-1$.

II.

We have now to see whether it is possible to extend the methods of the preceding paper to this case that the Klein-Gordon frequencies may be complex. From the example given above it is clear that as the potential V is deepened, a pair of ϵ_k, one positive and one negative, vanish and that their respective frequencies E_k^+ and E_k^- become equal: $E_k^+=E_k^-=E$. As the potential is further deepened complex frequencies appear. It is easy to see that quite generally the ϵ_k must vanish in pairs, since the identities I (34, 35, 36) must hold uniformly as the potential is gradually altered.

For the special case that the potential is just deep enough to make a pair of ϵ_k vanish, energy and charge take the form

$$H=(N_+-N_-)E+\sum{}'N_kE_k\epsilon_k/|\epsilon_k|,$$
$$q=(N_+-N_-)e+e\sum{}'N_k\epsilon_k/|\epsilon_k|,$$

where the prime on the summation excludes states of vanishing ϵ_k. Since only (N_+-N_-) occurs in these forms, N_+ and N_- cannot be determined by charge and energy alone, and the system is degenerate: an arbitrary number of pairs may appear without contributing to the energy. For this state charge and current density will in general be infinite. This situation is the extreme limit for which stationary states of the field may be defined.

When complex frequencies E_k occur, $\epsilon_k=0$ also; and we must restate the essential conclusions of the preceding paper. Defining:

$$\epsilon_{kl}\equiv\int\psi_l^*(E_k+E_l^*-2eV)\psi_k dv,$$

and

$$\sum_l\zeta_{nl}\epsilon_{lk}\equiv\delta_{nk},$$

we get:

$$\epsilon_{kl}(E_k-E_l^*)=0$$

—orthogonality relation;

$$q=e\sum_{kl}\tfrac{1}{2}(a_ka_l^*+a_l^*a_k)\epsilon_{kl}$$

—total charge;

$$H=\sum_{kl}\tfrac{1}{2}(a_ka_l^*+a_l^*a_k)\epsilon_{kl}E_k$$

—total energy;

$$L(x,t';x',t')=i\sum_{kl}\zeta_{kl}\psi_k(x)\psi_l^*(x')=0$$

—Green's function;

$$[\psi(x),\psi^*(x')]=\sum_{kl}[a_k,a_l^*]\psi_k(x)\psi_l^*(x')=0$$

—commutation law.

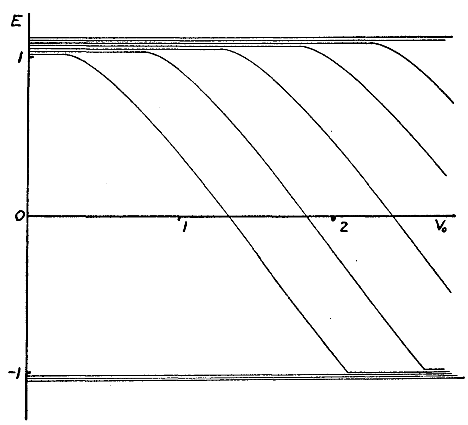

FIG. 2. The frequency E of the Dirac equation with potential as in Fig. 1, for $j=\frac{1}{2}$, $l=0$, $\kappa=-1$.

Either from the requirement $\dot{a}_k=-iEa_k=[a_k,H]$, or from the commutation laws I(8) taken together with the uniqueness theorem for the Green's function, we obtain the commutation rules:

$$[a_k,a_l^*]=\zeta_{kl},\qquad [a_l,a_k^*]=\zeta_{kl}^*,\tag{6}$$

with all other commutators zero.

If one state has the complex frequency $E=U+iW$ corresponding to a wave-function ψ

and quantized amplitude a, then ψ^* will also be a solution of I(14), with frequency $E^*=U-iW$, to which we may assign a quantized amplitude b^*. Since a, b, a^*, b^* commute with all other a_k, a_k^*, we may consider separately the terms q_0, H_0 in q, H, due to the former alone:

$$q_0/e=\tfrac{1}{2}(ab+ba)\epsilon+\tfrac{1}{2}(a^*b^*+b^*a^*)\epsilon^*,$$
$$H_0=\tfrac{1}{2}(ab+ba)\epsilon E+\tfrac{1}{2}(a^*b^*+b^*a^*)\epsilon^* E^*,$$

where the complex number ϵ is defined by:

$$\epsilon\equiv 2\int \psi^2(E-eV)dv,$$

and where

$$[a,b]=\epsilon^{-1}, \qquad [b^*,a^*]=\epsilon^{*-1}, \tag{7}$$

with all other commutators zero. We next define two Hermitian operators N, M:

$$N\equiv\tfrac{1}{2}(ab+ba)\epsilon+\tfrac{1}{2}(a^*b^*+b^*a^*)\epsilon^*,$$
$$M\equiv(1/2i)(ab+ba)\epsilon-(1/2i)(a^*b^*+b^*a^*)\epsilon^*,$$

which satisfy $[M,N]=0$. In terms of these,

$$q_0=Ne, \qquad H_0=NU-MW.$$

Simple application of (7) shows:

$$\begin{matrix}[a,N]=a, \\ [a,M]=-ia;\end{matrix} \quad \text{and} \quad \begin{matrix}[b,N]=-b, \\ [b,M]=ib.\end{matrix} \tag{8}$$

It can then be shown that if a has one finite matrix element in the representation in which M is diagonal, then M has at least one complex eigenvalue. But M was defined to be Hermitian and cannot have complex eigenvalues. Hence if there exists a diagonal representation of H_0 (and therefore of M) when complex values of E occur in I(14), the charge and current densities will be everywhere infinite. Since in this case there are no physically admissible solutions, we say that M cannot be diagonalized.

The preceding discussion may be applied equally well to scalar or vector mesotron fields, since the generalized relations (6) hold in either case.

In spite of the fact the M cannot be diagonalized, it is easy to find Hermitian matrices of infinite rank which satisfy (8). The off-diagonal elements of M in the rth row are of order r, and the roots of the rth-order secular determinant for the characteristic values of M approach no limit as $r\rightarrow\infty$. The physical origin of this divergence lies in the fact that the emission of pairs into these degenerate states stimulates, because of the Einstein-Bose quantization, the further emission into these same states.

The arguments given here show then that there are certain types of electrostatic potential for which it is not possible to find stationary states for the scalar field. A situation somewhat analogous to this occurs in the Dirac electron theory, with a Coulomb field and with $Z>137$, in the present scalar theory with $Z>\tfrac{1}{2}\cdot 137$, or even in nonrelativistic wave mechanics, for potentials a/r^2, for $a<-\tfrac{1}{4}$; in all these cases the S-state eigenfunctions become singular, and the set of functions satisfying the regularity conditions is not complete: wherever this is so, the field Hamiltonian cannot be brought to diagonal form. The case we have here considered, however, is unique in that the potentials V involved are nowhere infinite, and solutions of the Pauli-Weisskopf field equations free of singularities exist.

In all these cases where the energy cannot be brought to diagonal form, we must take into account either existing deviations from the assumed potential, such as the breakdown of the Coulomb law at small distances, or the reaction of the pair field itself on the external field. In the simple case discussed in Section I, it is clear that no finite work can maintain the potential indefinitely, and the power necessary to maintain it for a finite time can be calculated from time dependent solutions of the field equations.

It is a pleasure to thank Professor J. R. Oppenheimer for suggesting this problem and for many helpful discussions concerning its solution.