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Quark condensation in quantum chromodynamics

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Working within a limited Fock-space approximation (LFSA), we argue that if the running coupling constant of quantum chromodynamics (QCD) exceeds a critical value of order 1 the vacuum becomes a condensate of quark-antiquark pairs. To evaluate the critical coupling constant we use a Mellin-transform technique which is first illustrated with a Schrödinger equation problem. We then apply it to scalar and spinor QED, as well as to QCD, using the LFSA.

I. INTRODUCTION

During the past few years, quantum chromodynamics (QCD) has emerged as the favored candidate for a theory of the strong interactions.[1] It is an asymptotically free field theory,[2] in which the interactions between quarks are logarithmically weaker than Coulomb interactions at short distances. This is compatible with the approximate scaling observed in deep-inelastic electron scattering.[3] QCD incorporates color, which "solved" the quark statistics problem: By making quarks triplets under color, and demanding that all physical states be color singlets, the lowest-lying baryons were able to have totally symmetrical spatial wave functions.

To be accepted as the dynamical theory of hadrons, QCD must solve the confinement problem. It must provide an explanation for the fact that all physical states are color singlets in which the number of quarks minus the number of antiquarks is a multiple of three. That QCD has this property is anything but obvious, since the most naive calculation of the force between quarks, single-gluon exchange, simply gives a Coulomb potential. If that were the whole situation, it would be hard to understand why free quarks would not be ionized out of hadrons at some finite excitation energy.

Of course, the true forces between quarks are not Coulombic. Perturbative corrections to single-gluon exchange indicate that at long distances the interaction between quarks is stronger than a Coulomb interaction.[4] This is the converse of asymptotic freedom: Forces get less weak at greater distances. Furthermore, there are perturbative contributions to the static potential between quarks that cannot be simply absorbed into the running coupling constant.

The conventional approach to the confinement problem relates this presumed aspect of QCD to nonperturbative properties of the gluon sector.[5] Thus it is generally argued that if pure QCD (i.e., gluon sector only) obeys the Wilson criterion,[6] the introduction of quarks will result in the formation of hadrons. In this paper we discuss an alternative to that picture.[7] We argue that confinement may occur even if Wilson's criterion is not obeyed. Confinement is then blamed on nonperturbative effects associated with quarks. We will argue that if the coupling constant in QCD, at long distances, exceeds a finite critical value of order 1, then the vacuum will contain a finite density of quark-antiquark pairs. If we picture this ground state in terms of excitations (quanta) on the naive vacuum, then we would describe the true ground state as being a plasma of $q\bar{q}$ pairs.

The forces between quarks, and the structure of quarks, would be strongly mofified by a $q\bar{q}$ condensate ground state. As is well known, such a condensate must violate chiral symmetry.[8] Furthermore, the condensate may have additional physical effects, and it is important to try to elucidate them, because they will surely affect the physical content of QCD. In this article, our calculations will be limited to arguing that the true ground state is in fact a $q\bar{q}$ pair condensate. We will discuss the physical effects of the condensate only qualitatively.

We should point out though, that if the analogy between the $q\bar{q}$ condensate and a plasma of charged objects is a valid one, then it suggests an explanation for the absence of colored states which is radically different from the conventional explanation based on a growing effective potential.

In a plasma, a charged particle such as an electron is screened by a cloud of charged particles in the plasma, Debye screening.[9] That is, the presence of an additional charged particle distorts the wave functions of the others in the plasma in such a way that, outside of a small finite region, the effective charge associated with the extra electron is seen to be zero. With an analogy between color and electrical forces, the plasma picture suggests that a process like Debye screening would lead to the neutralization of color. If the screening results in a color-singlet excitation of the vacuum involving effectively only a finite number of quarks and antiquarks, then this screened system will have integral electric charge and baryon number, because of the built-in correlation between fractional color and fractional flavor quantum numbers. Thus trying to explain the nonobservation of free quarks by asking how a growing effective potential could arise in QCD may be asking the wrong question. If the true vacuum is a colored plasma, then no colored object, quark or gluon, could be stable, because the condensate vacuum would respond to the presence of a colored object by neutralizing any local color imbalance.

To amplify this analogy, one should first show that the color analog of Debye shielding actually occurs in a $q\bar{q}$ condensate, and further, that if color shielding occurs, it is accompanied by the elimination of fractional flavor quantum numbers. Despite the fact that any system composed of a finite number of quarks, antiquarks, and gluons, which has zero total color will have only integral flavor quantum numbers (such as electric charge), it is possible for a system composed of an infinite number of quanta to have zero total color while at the same time having nonintegral electric charge.[10] We have no reason to expect that this preverse situation will actually occur. If the vacuum is a plasma of quark-antiquark pairs, then since Debye shielding occurs over a finite range, it is most natural to expect that there will be effectively only a finite number of quarks and antiquarks involved in shielding, and this presumably would lead to excitations with only integral flavor quantum numbers. The simplest way to analyze what actually happens is to examine the screening of an external (heavy) quark. This is the analog of Debye shielding of an external charge in a plasma. Such investigations are in progress. A more ambitious and physically relevant test would be to find the stable excitations of the condensate and examine whether they have fractional or integral charge.

A criterion for the ground state of QCD to contain a condensate of quark-antiquark pairs is that the coupling constant become large enough so that some $q\bar{q}$ state becomes degenerate with the no-particle state. Here we examine this criterion in the approximation of replacing the dressed vacuum and dressed $q\bar{q}$ states by bare states. However, having taken this lowest perturbative approximation to each state, we diagonalize the QCD Hamiltonian exactly on the space of bare $q\bar{q}$ states, and compare the lowest eigenvalue to its expected value in the bare vacuum. Since this approximation amounts to diagonalizing the Hamiltonian on a limited part of Fock space, we will call it the limited Fock-space approximation (LFSA).

We take the Hamiltonian to be normal ordered, so that its vacuum expected value remains zero. We diagonalize the Hamiltonian on the space of bare $q\bar{q}$ states by the variational principle, thus working to all orders in the coupling in this sector of Fock space. Within our LFSA α is a free parameter. When α exceeds a critical value α_c, we find that the lowest bound states in the particle-antiparticle sector develop negative energies. This then signals a phase transition causing the true vacuum to become a condensate of such pairs, in the same way as a Cooper pair with nonzero binding energy signals that a metal below a critical temperature is superconducting.

We argue that negative total energy $q\bar{q}$ states occur in QCD by the variational principle. Working in the radiation gauge,[11] we construct a physical quark-antiquark state by applying creation operators formed from the quark fields at a fixed time:

$$|\psi\rangle = \int d^3k\, \psi(k)\bar{q}^{(+)}(k)q^{(+)}(-k)|0\rangle .$$

(The notation is as follows: $q^{(+)}$ and $\bar{q}^{(+)}$ are the creation parts of the quark and antiquark fields, and ψ is the relative momentum wave function.) We then calculate the normalized expectation value of the QCD Hamiltonian in the state $|\psi\rangle$, and minimize it with respect to the wave function. This gives an effective wave equation for $\psi(k)$, and we solve it for its eigenvalues. We take the Hamiltonian to be normal ordered, so that the expected value of the energy in the no-particle state is zero, and then we are concerned with whether or not one of the eigenvalues of the wave equation for ψ is negative.

The wave equation for $\psi(k)$ is a singular integral equation in momentum space. We solve it by a technique based on the Mellin transform.[12] Because the equation is scale invariant, we are able to obtain an analytic solution. The equation for the Mellin transform of the momentum-space wave function is a first difference equation. The coefficients in the equation are rational functions of the Mellin transform variable, and so a solution

for the Mellin transform is a product of Γ functions. The resulting solution has singularities at locations in the Mellin-transform plane that are incompatible with the solution's being the Mellin transform of a normalizable wave function. We remove these unphysical singularities by multiplying by a periodic function which compensates for them. The result is a closed-form expression for the Mellin transform of the momentum-space wave function.

Within the framework of our technique for solving the wave equation, the question of whether or not negative-energy eigenvalues are allowed comes down to the question of whether or not a periodic function which eliminates all the unphysical singularities of the solution to the difference equation, including those at infinity, can be found. The locations of the singularities shift as a function of the coupling constant. For negative eigenvalues, an appropriate periodic function can only be found when the coupling constant exceeds a finite critical value.

The wave equations for ψ that emerge in the LFSA are exactly the same in QCD, in spinor electrodynamics, and in scalar electrodynamics. The only difference is that there is a numerical factor of $\frac{4}{3}$ due to SU(3) multiplying the coupling constant in the QCD equation, which is absent in either of the electrodynamics equations. The critical values of the coupling above which there are negative-energy bound states are $\alpha_c = \frac{3}{2}$ in QED and $\alpha_c = \frac{9}{8}$ in QCD.

There is, in addition, a simple physical explanation for the existence of a critical coupling constant. The physical system under consideration consists of two massless particles which interact by a Coulomb $1/r$ potential. Since both the relative kinetic and potential energies scale like $1/r$, if we consider a state whose characteristic size is R, then the kinetic energy of the system is roughly $1/R$, while the potential energy is roughly $-\alpha/R$. Thus, when α exceeds a value of order 1, the potential energy can exceed the kinetic and there will be bound states with total negative energy.

Our analysis using the LFSA is an approximation to a procedure which is well defined but very difficult to carry out. In an exact treatment the true vacuum and the two-particle sector of Fock space are mixtures of all the noninteracting sectors. The mixing could be evaluated in perturbation theory, though the calculation necessitates the introduction of a cutoff or a renormalization procedure. The LFSA is the lowest approximation to this procedure.

In QCD, the effective coupling varies with the distance scale and the range of its values is an intrinsic property of the theory. Therefore there is no free α parameter. Whether or not the interaction between quarks is large enough for the ground state to become a $q\bar{q}$ condensate is also an intrinsic property of the theory. In the LFSA that interaction is given by only a Coulomb term with α being an external parameter. We can try to take some features of the exact theory into account by letting α become a distance-dependent function as expected from renormalization-group analysis. This leads to the physical model discussed in Ref. 7.

Let us describe briefly the physical picture of quark condensation and confinement within the model based on the assumptions specified above. As a qualitative background for this description we compare in Fig. 1 a critical $-\alpha_c r^{-1}$ Coulomb potential with three curves all of which are logarithmically weaker at the origin, as expected of a QCD potential from asymptotic freedom.

Curve A corresponds to the common lore of an asymptotically rising potential leading to quark confinement. Curve B designates a situation where quark confinement does not exist. Curve C describes a situation where the phenomenon that we propose will take place: The vacuum will become a condensate of light $q\bar{q}$ pairs whose characteristic correlation length is of the order of the value of the point $r = R_0$ at which the curve C crosses $-\alpha_c/r$. Within this new vacuum, quarks may

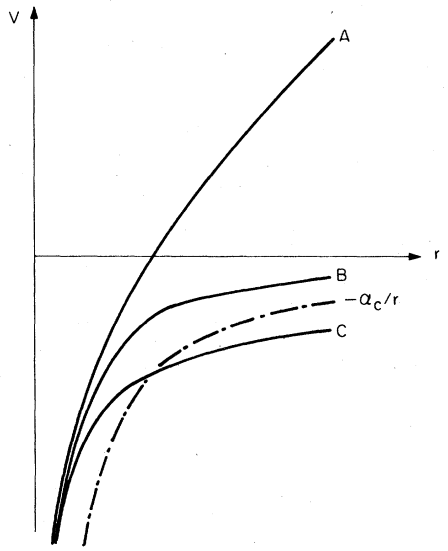


FIG. 1. The dashed curve is a $-\alpha_c/r$ potential, which is compared with three possibilities for the $q\bar{q}$ effective potential. Curve A is an asymptotically rising potential; curve B is weaker than $-\alpha_c/r$, and would not be expected to give confinement; curve C is stronger than $-\alpha_c/r$ at large distances, and would be expected to lead to pair condensation.

propagate freely for short distances, but the condensate will inhibit their long-distance propagation as free, stable particles.

Possible excitations of this condensate are collections of quarks and gluons which, together with all their associated fields, are confined to a region smaller than R_0. The primary example would be a compact $q\bar{q}$ system in a color-singlet state. Such a system would not set up a long-range color field, and so would not affect, nor in turn be affected by, the condensate. The $q\bar{q}$ state could be pictured as residing in the interstices of the condensate. It would have a finite, positive energy: finite, because it is a state of two massless quanta, confined to a finite-size region, attracting each other with a force weaker than a Coulomb interaction; positive, because at distances less than R_0 the negative potential energy from the attractive color interaction is less than the positive kinetic energy associated with their confinement to a region smaller than characteristic pair separation in the condensate. We would associate these excitations with physical mesons. Other small (relative to R_0) color-singlet systems, for example, qqq, $qq\bar{q}\bar{q}$, or $q\bar{q}$+gluons, would also be finite-energy excitations, corresponding to baryons or exotic mesons, respectively.

Finally, before turning to the technical problems to which this paper is devoted, let us address ourselves to the interesting question of whether a mechanism of the kind that we propose could also occur in QED and, if so, why it is not observed. The important difference between QED and QCD, as far as our mechanism is concerned, is that their effective couplings become large at opposite distance scales. Thus, whereas the weak potential regime of QCD is at short distances, the Coulomb force is the well-known manifestation of QED at large distances. Conventional expectations are that QED is part of a larger gauge theory[13] and therefore its running coupling constant will never increase too strongly. But even if this is not the case and its running coupling constant exceeds unity, this will happen at very short distances, of order $e^{-1/\alpha}/m_e$. In that case the vacuum would change its character only at distances which are much smaller than those which can be experimentally tested. In fact, gravitational effects should be expected to dominate even at a much larger distance scale.

The organization of this paper is as follows: In Sec. II we solve a simple model which illustrates both the dynamical ideas and the techniques of the QCD bound-state problem. The model is a massless particle moving in a $1/r$ potential. The Schrödinger equation for its bound states exhibits the same dimensionally homogeneous competition between the kinetic and potential energies as the QCD bound-state problem. In momentum space, it is an integral equation which we solve by our Mellin-transform technique. We solve the difference equation for the Mellin transform of the momentum-space wave function, and describe the locations of the singularities and zeros of the solution as a function of the coupling constant. We show explicitly how this leads to the possibility of negative eigenvalues only above a critical value of the coupling, and find the periodic function which eliminates unphysical singularities.

In Sec. III we derive the integral equations for the momentum-space bound-state wave functions of a particle-antiparticle pair in scalar and spinor QED and in QCD. Scalar electrodynamics is simplest because it lacks the complications due to spin, and so we discuss that case in the greatest detail. [Scalar QED, however, has a complication due to the $(\phi^*\phi)^2$ counterterm which is not present in the spinor bound-state equations.] Except for the numerical factor due to SU(3) in the QCD case, the integral equations are identical in all three theories. Because both massless QED and massless QCD are chirally invariant theories, the wave equations for pseudoscalar bound states in those theories are the same as the equations for the scalar bound states.

In Sec. IV we solve the bound-state equations using the Mellin-transform technique outlined above. The solutions are examined in great detail, and the value of the critical coupling above which there are negative-energy bound states is explicitly computed.

II. A SCHRÖDINGER EQUATION INSTABILITY MODEL

We will illustrate the formation of negative-total-energy bound states in an external potential model: a massless scalar particle moving in a Coulomb potential set up by an external charge of $-Z$ units. We will show that if $\alpha Z < \frac{1}{2}$, there are no bound states, while if $\alpha Z > \frac{1}{2}$, there are bound states. Since the mass of the scalar field is zero, bound states have negative total energy, and so represent configurations in which it is energetically favorable for a scalar electron to be produced and occupy a bound-state energy level.

We will describe this physical situation by means of a Schrödinger equation with Hamiltonian $H = H_0 + H_1$. The kinetic energy H_0 is $|\vec{p}|$ and the potential energy H_1 is $-\alpha Z/r$. The equation we will solve is the Schrödinger equation

$$\left(|\vec{p}| - \frac{\alpha Z}{|\vec{r}|}\right)|\psi\rangle = E|\psi\rangle . \tag{2.1}$$

We can deduce this same equation by applying a

variational approximation to massless scalar quantum electrodynamics. In the presence of an external charge, the Lagrangian is

$$\mathfrak{L} = -\tfrac{1}{4}F_{\mu\nu}F_{\mu\nu} + (\partial_\mu + ieA_\mu)\phi^*(\partial_\mu - ieA_\mu)\phi + eZ\,\delta^3(\vec{x})A_0(0,t)\ . \tag{2.2}$$

In the radiation gauge $\vec{\nabla}\cdot\vec{A}=0$, the Hamiltonian of this system takes the form

$$\mathcal{H} = \Pi^*\Pi + (\vec{\nabla} - ie\vec{A})\phi^*\cdot(\vec{\nabla} + ie\vec{A})\phi + \tfrac{1}{2}\vec{E}^2 + \tfrac{1}{2}\vec{B}^2 \tag{2.3}$$

and the longitudinal part of $\vec{E}$ is constrained by

$$\vec{\nabla}\cdot\vec{E} = -ie(\phi^*\Pi - \Pi^*\phi) + eZ\,\delta^3(\vec{x})\ . \tag{2.4}$$

The canonical momenta are defined by

$$\Pi^* = \frac{\delta\mathfrak{L}}{\delta\dot{\phi}}\ ,$$

$$\Pi = \frac{\delta\mathfrak{L}}{\delta\dot{\phi}^*}\ ,$$

so that starred fields have the opposite charge from unstarred fields. In the radiation gauge, the fields create only physical states and A_0 is a dependent field which can be expressed in terms of ϕ and Π. If we restrict this Hamiltonian to the subspace of states of one electron, we recover exactly the previous Schrödinger equation. To obtain this equation, consider the normalized expected value of the scalar electrodynamic Hamiltonian in the state of one electron:

$$\frac{\langle\psi|\int d^3x\mathcal{H}|\psi\rangle}{\langle\psi|\psi\rangle}\ , \tag{2.5}$$

where

$$|\psi\rangle = \int d^3k\psi(\vec{k})a^\dagger_{\vec{k}}|0\rangle = \int d^3k\psi(\vec{k})(\phi^\dagger_{\vec{k}} - i\Pi^\dagger_{\vec{k}})|0\rangle\ . \tag{2.6}$$

The requirement that this normalized expected value of H should be stationary with respect to variations of the wave function ψ,

$$\frac{\delta}{\delta\psi}\,\frac{\langle\psi|\int\mathcal{H}d^3x|\psi\rangle}{\langle\psi|\psi\rangle} = 0\ , \tag{2.7}$$

recovers the previous Schrödinger equation.

This physical situation has been previously analyzed in terms of a Klein-Gordon equation. The Klein-Gordon equation for a scalar particle in an external Coulomb potential arises in two ways. One is in considering the problem of the classical stability of the Coulomb potential of a point charge to small fluctuations in a charged scalar field. That problem is solved by considering the nonlinear equations of classical scalar electrodynamics and expanding the solution to those equations in an assumed small fluctuation about the Coulomb solution. The linearized equation for the fluctuation of the scalar field is exactly the Klein-Gordon equation for a massless scalar particle in the presence of a vectorially coupled Coulomb potential. This equation shows that the Coulomb potential is classically stable to small fluctuations so long as $\alpha Z < \frac{1}{2}$ but is unstable to infinitesimal fluctuations in the scalar field if $\alpha Z > \frac{1}{2}$.

This Klein-Gordon equation also is the relativistic wave equation for a scalar particle moving in a Coulomb potential.

It should be pointed out that in the case of a pure Coulomb potential arising from a point source, the mass of the electron cannot affect the critical value of αZ at which a transition from stability to instability occurs. The reason is that the electron mass is the only dimensional parameter in the problem of a scalar electron moving in a Coulomb potential. Since the critical coupling is a pure number, it cannot depend on any dimensional quantity. So, in particular, the critical coupling is the same for both massless and massive scalar electrodynamics. On the other hand, if instead of a pure Coulomb potential, one were to consider a Coulomb potential cut off at a radius r_0, then $m_e r_0$ is a pure number and could affect the critical coupling consistent. In fact, it is known from considerations of nuclei with large charge that the effect of a finite nuclear size is to increase the value of the critical coupling constant.

We will analyze the Schrödinger equation by a technique which generalizes to the other calculations that we will consider in this paper. We begin with the Schrödinger equation in momentum space:

$$|p|\psi(\vec{p}) - \frac{\alpha Z}{(2\pi)^2}\int\frac{d^3q}{(\vec{p}-\vec{q})^2}\,\psi(\vec{q}) = E\psi(\vec{p})\ . \tag{2.8}$$

We take the wave function to be spherically symmetrical, giving

$$p\psi(p) - \frac{\alpha Z}{\pi p}\int_0^\infty q\ln\left|\frac{p+q}{p-q}\right|\psi(q)dq = E\psi(p)\quad (p>0)\ . \tag{2.9}$$

This equation may be solved by Mellin transforming it to a soluble finite difference equation. If we define the Mellin transform of $\psi(p)$ by

$$\phi(\zeta) = \int_0^\infty p^{\zeta-1}\psi(p)\,dp \tag{2.10}$$

and transform the Schrödinger equation, then after interchanging orders of integration, we find the finite difference equation

$$D(\zeta)\phi(\zeta+1)=E\phi(\zeta)\ , \tag{2.11}$$

where

$$D(\zeta)=1+\frac{\alpha Z}{\zeta-1}\cot\frac{\pi\zeta}{2}\ . \tag{2.12}$$

The factor $\cot\frac{1}{2}\pi\zeta/(\zeta-1)$ is shown in Fig. 2. This is almost a simple equation, because except for the contangent, the relation between $\phi(\zeta)$ and $\phi(\zeta+1)$ is a rational function. If we iterate the equation once, to relate $\phi(\zeta)$ to $\phi(\zeta+2)$,

$$D(\zeta)D(\zeta+1)\phi(\zeta+2)=E^2\phi(\zeta)\ , \tag{2.13}$$

then in this iterated equation the cotangents are effectively constants. They have the same numerical value at each of the points related by the equation, since the cotangent has period π. It is very simple to write down one solution of a first-order difference equation with rational coefficients. If we are given the equation

$$X(\zeta+j)=c^j\,\frac{(\zeta-a_1)\cdots(\zeta-a_n)}{(\zeta-b_1)\cdots(\zeta-b_n)}\,X(\zeta), \tag{2.14}$$

then one solution to that equation is

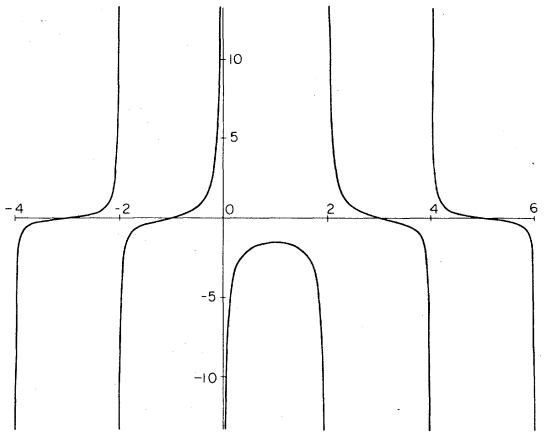


FIG. 2. The function $F(\zeta)=[1/(\zeta-1)]\cot\frac{1}{2}\pi\zeta$ which occurs in $D(\zeta)$. Each zero of $\overline{\phi}(\zeta)$ corresponds to a root of $F(\zeta+n)=-1/(\alpha Z)$, $n=0,1,2,\ldots$, Normalizable (bound-state) wave functions exist when the root of $F(\zeta)=-1/(\alpha Z)$ between 0 and 1 (ζ_0) occurs to the right of $\zeta=\frac{1}{2}$.

$$X(\zeta)=\frac{c^\zeta\Gamma((\zeta-a_1)/j)\cdots\Gamma((\zeta-a_n)/j)}{\Gamma((\zeta-b_1)/j)\cdots\Gamma((\zeta-b_n)/j)}\ . \tag{2.15}$$

Therefore we can write one solution to the Mellin-transform first-order difference equation:

$$\overline{\phi}(\zeta)=E^\zeta\,\frac{\Gamma(\frac{1}{2}(\zeta-1))\Gamma(\frac{1}{2}\zeta)}{\Gamma(\frac{1}{2}(\zeta-1+\alpha Z\cot\frac{1}{2}\pi\zeta))\Gamma(\frac{1}{2}[\zeta+\alpha Z\cot\frac{1}{2}\pi(\zeta+1)])} \tag{2.16}$$

Note that this satisfies the uniterated as well as the iterated equation. Note also that although it is a solution of the uniterated equation, it is hardly the most general solution since if $P(\zeta)$ is any periodic function with unit period, then

$$\phi(\zeta)=P(\zeta)\overline{\phi}(\zeta) \tag{2.17}$$

is also a solution to the difference equation.

There is only one physical choice of $P(\zeta)$. It is determined by the requirement that $\phi(\zeta)$ be the Mellin transform of a well-behaved wave function $\psi(p)$. If $\psi(p)$ is nonsingular at the origin in momentum space and normalizable, so that $\psi(p)$ falls off faster than $p^{-3/2}$ for large p, then its Mellin transform $\phi(\zeta)$ must be analytic in a strip in the complex plane where $0<\mathrm{Re}\zeta\leq\frac{3}{2}$. In fact, the analyticity strip may be wider than this, and we shall see that in general it extends to the right of $\frac{3}{2}$, but it cannot be narrower. In addition, since $\phi(\zeta)$ is a Mellin transform, it must be bounded by a polynomial as $|\zeta|$ goes to infinity in either direction inside the analyticity strip.

In fact, $\overline{\phi}(\zeta)$ is not analytic inside the required analyticity strip, for it has an essential singularity at $\zeta=1$. The second Γ function in the denominator behaves for ζ near 1 like

$$\Gamma(\tfrac{1}{2}[\zeta+\alpha\cot\tfrac{1}{2}\pi(\zeta+1)])\sim\Gamma\left(\frac{\alpha Z}{\pi(\zeta-1)}+\frac{1}{2}\right), \tag{2.18}$$

which shows that $\zeta=1$ is an accumulation point of zeros of $\overline{\phi}(\zeta)$; the zeros accumulate to the left of 1 on the real axis. Except for its singularities at integers, $\overline{\phi}(\zeta)$ is a smooth function of ζ whose magnitude goes to a constant as $|\zeta|\to\infty$ because $\cot(\pm i\infty)=\mp i$. If the energy E is less than 0, then $\overline{\phi}(\zeta)$ is not so well behaved, since the factor E^ζ diverges exponentially as $\mathrm{Im}\zeta$ goes to infinity in either the upper or the lower half plane.

In order to have a solution which represents the Mellin transform of a well-behaved wave function, $P(\zeta)$ must be chosen so that it removes the unphysical essential singularity of $\overline{\phi}(\zeta)$ at 1. Further-

more, in order to obtain a bound-state solution with $E<0$, $P(\zeta)$ must compensate for the unphysical exponential growth as $|\mathrm{Im}\zeta|\to\infty$.

We will construct the periodic function P as a product of three periodic functions,

$$P(\zeta)=P_1(\zeta)P_2(\zeta)P_3(\zeta)\ . \tag{2.19}$$

The function $P_1(\zeta)$ will be chosen to have the same essential singularity as the Γ function in the denominator, except for the fact that the locations of its poles will not be exactly the same as the locations of the zeros of the reciprocal Γ function. However, as ζ approaches 1 from any direction except the real axis below $\zeta=1$, $P_1(\zeta)$ will compensate for the essential singularity of the Γ function. The periodic function $P_2(\zeta)$ will be constructed as an infinite product which will have zeros at each of the poles of $P_1(\zeta)$ and poles at each of the poles of the denominator function. It will be free of other singularities, and will be chosen so that as ζ goes to 1 from any direction except the real axis below 1, it will approach a finite constant. Thus the product $P_1(\zeta)P_2(\zeta)$ will completely compensate for the essential singularities of $\overline{\phi}(\zeta)$. Finally, when we are interested in constructing bound-state wave function, $P_3(\zeta)$ will be chosen so as to overcompensate for the exponentially divergent growth of $\overline{\phi}(\zeta)$ as $|\mathrm{Im}\zeta|\to\infty$.

The function $P_1(\zeta)$ is easy to construct. A periodic function with exactly the same singularity as the argument of the denominator Γ function near $\zeta=1$ is

$$\alpha Z\cot\pi\zeta+\tfrac{1}{2}\ , \tag{2.20}$$

and so the choice

$$P_1(\zeta)=\Gamma(\alpha Z\cot\pi\zeta+\tfrac{1}{2}) \tag{2.21}$$

is a function which compensates for the essential singularity in $\overline{\phi}(\zeta)$ in the sense that

$$\lim_{\zeta\to 1}\frac{P_1(\zeta)}{(\Gamma\tfrac{1}{2}[\zeta+\alpha Z\cot\pi\tfrac{1}{2}(\zeta+1)])}=1, \tag{2.22}$$

so long as the limit is not taken along the real axis from below 1. Furthermore, as $|\zeta|\to\infty$ in the analyticity strip in either the lower or the upper half plane, $P_1(\zeta)$ approaches a finite constant. However, the poles of $P_1(\zeta)$ do not coincide with the zeros of $\overline{\phi}(\zeta)$. Poles of $P_1(\zeta)$ occur at

$$\alpha Z\cot\pi\zeta=-n-\tfrac{1}{2}, \tag{2.23}$$

while the zeros of $\overline{\phi}(\zeta)$ occur at values $\zeta^{(n)}$ which are the solutions of

$$\zeta^{(n)}+\alpha Z\cot\tfrac{1}{2}\pi(\zeta^{(n)}+1)=-2n\ . \tag{2.24}$$

The locations of these poles and zeros are shown in Fig. 3. We can construct by force a periodic function with exactly compensating poles and zeros as the infinite product

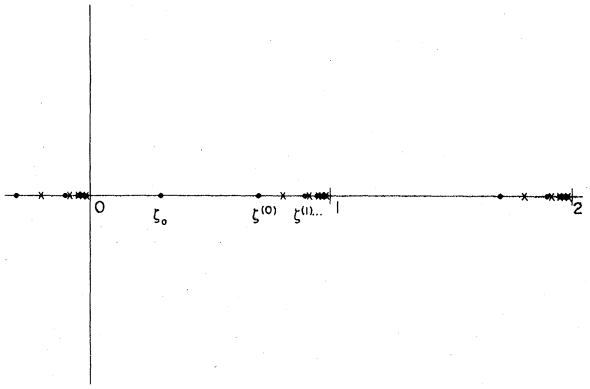


FIG. 3. The ζ plane for $P_1(\zeta)\overline{\phi}(\zeta)$, for αZ slightly greater than $\frac{1}{2}$. The dots are at the zeros of $\overline{\phi}(\zeta)$ and the crosses are at the poles of $P_1(\zeta)$. The locations of these poles and zeros are functions of the coupling αZ. As αZ increases, ζ_0 moves toward the right while all the other zeros and poles shown move toward the left. At $\alpha Z=2/\pi$, ζ_0 and $\zeta^{(0)}$ meet at $\zeta=1$, and for larger αZ they become a pair of conjugate zeros on the line $\mathrm{Re}\zeta=1$.

$$P_2(\zeta)=\prod_{n=0}^{\infty}\left[\frac{1+(\alpha Z\cot\pi\zeta)/(n+\frac{1}{2})}{1-\cot\pi\zeta/\cot\pi\zeta^{(n)}}\right]. \tag{2.25}$$

The solution $\phi(\zeta)=\overline{\phi}P_1P_2$ is the Mellin transform of a positive-energy wave function.

This Mellin transform is actually analytic in a somewhat larger analyticity strip than merely $0<\mathrm{Re}\zeta<\frac{3}{2}$. In fact, the right boundary of the analyticity strip occurs one unit above the zero ζ_1 of $D(\zeta)$ that lies between 1 and 2. This zero indicates that if $\phi(\zeta_1)$ is finite then $\phi(\zeta)$ will have a simple pole at ζ_1+1. This pole is on the boundary of the analyticity strip and determines the asymptotic behavior (as $p\to\infty$) of the wave function $\psi(p)$ of which $\phi(\zeta)$ is the Mellin transform. Note that this construction of the Mellin-transformed scattering wave function is unique. The reason is that any other solution would have to be obtained from $\phi(\zeta)$ by multiplying by an analytic periodic function which is bounded by a polynomial in ζ. Such a function must be an analytic function of $e^{2\pi i\zeta}$ and $e^{-2\pi i\zeta}$, which is to say, the sum of an analytic function of each. The requirement of polynomial boundedness in ζ, by Liouville's theorem, forces the function to be a constant.

For negative energies, the construction given so far fails to satisfy the boundary condition at $|\mathrm{Im}\zeta|\to\infty$. If for negative energies we conventionally choose the phase of E to be $e^{i\pi}$, then $E^{\zeta}=|E|^{\zeta}e^{i\pi\zeta}$ will diverge exponentially as $\mathrm{Im}\zeta\to-\infty$.

However, if we choose the third periodic function to be

$$P_3 = \frac{1}{e^{2\pi i\zeta} - e^{2\pi i\zeta_0}}, \tag{2.26}$$

then $\phi(\zeta) = \overline{\phi} P_1 P_2 P_3$ will be exponentially convergent as $|\zeta| \to \infty$ in either direction in the analyticity strip. However, we must choose ζ_0 to be the location of a zero of $\overline{\phi}_0(\zeta)$ which has not been removed by a pole of $P_2(\zeta)$. There is in fact always exactly one such zero. It occurs at the zero of $D(\zeta)$ between 0 and 1. However, it is not a periodic zero and so introducing the factor of $P_3(\zeta)$, while it will not introduce a pole in $\phi(\zeta)$ between 0 and 1, will introduce a pole one unit higher, between 1 and 2. Since $\phi(\zeta)$ must be analytic in a strip extending at least to $\mathrm{Re}\zeta = \frac{3}{2}$, in order that the bound-state wave functions be normalizable, ζ_0 must lie between $\frac{1}{2}$ and 1. As one can see from Fig. 1, this will be true if

$$D(\tfrac{1}{2}) < 0. \tag{2.27}$$

Since $D(\frac{1}{2}) = 1 - 2\alpha Z$, $\alpha Z = \frac{1}{2}$ is the critical value of the coupling constant above which one can construct normalizable bound-state wave functions and below which one cannot construct normalizable negative-energy bound-state wave functions. Note that at $\alpha Z = 2/\pi$, the zeros to both the left and right of $\zeta = 1$ coalesce and then move into the complex ζ plane. Both zeros then have unit real parts and equal and opposite imaginary parts. However, the number of zeros of $D(\zeta)$ does not change when these two zeros go into the complex plane, and furthermore, they remain to the right of $\zeta = \frac{1}{2}$, so that the construction of the bound-state wave functions for $\alpha Z > 2/\pi$ proceeds exactly the same as when $\frac{1}{2} < \alpha Z < 2/\pi$.

There is no further freedom in the determination of $\phi(\zeta)$, again as a consequence of Liouville's theorem. Any other solution would have to be obtainable from $\phi(\zeta)$ by multiplication by an analytic periodic function of ζ. Such a solution must be the sum of an analytic function of $e^{2\pi i\zeta}$ and one of $e^{-2\pi i\zeta}$. Thus, since it must be less singular than $e^{2\pi|\zeta|}$ as $|\mathrm{Im}\zeta| \to \infty$, it must be a constant.

The construction just given is valid not only for negative E, but for any phase of E. Thus, above the critical coupling, there are normalizable wave functions with all phases for their eigenvalues. These are, of course, not all orthogonal. The reason is simply that the integral operator in momentum space acting on bound-state wave functions is not uniformly convergent, and so is not a self-adjoint operator on the space of these functions.

The explicit construction of the wave function that we have given involves the factor $P_2(\zeta)$, which is a periodic function constructed as an infinite product, and is not any simple or well-known analytic function. However, the infinite product is rapidly convergent. For large n,

$$\alpha Z \cot\pi\zeta^{(n)} \sim -(n+\tfrac{1}{2}) + O\left(\frac{1}{n}\right), \tag{2.28}$$

so the infinite product converges like $\sum 1/n^3$. For the purpose of computing $P_2(\zeta)$ to high accuracy, it should be quite sufficient to merely take a few terms of the infinite product. In addition, for bound-state wave functions, the solution $\phi(\zeta)$ involving the factor of $P_3(\zeta)$ falls exponentially as $|\mathrm{Im}\zeta| \to \infty$. This means that if one wishes to reconstruct the momentum-space wave function ψ by taking the inverse Mellin transform of $\phi(\zeta)$, the inverse Mellin transform should be very rapidly convergent and so amenable to nonsingular numerical evaluation.

The eigenvalue E enters $\phi(\zeta)$ only through the factor E^{ζ}. This means that when $\psi(p)$ is reconstructed by computing the inverse transform, $|E|$ will set the scale for p but will not otherwise appear in $\psi(p)$.

III. THE BOUND-STATE EQUATIONS

In this section we will derive wave equations in the LSFA for the bound states of one electron and one positron in massless scalar electrodynamics (Sec. III A), in massless spinor QED (Sec. III B), and in QCD with massless quarks (Sec. III C). Except for a numerical factor of $\frac{4}{3}$ in QCD, which is essentially an SU(3) crossing-matrix element, the identical equation emerges in all three theories. Furthermore, the three derivations are very similar, so in the spinor cases we will make frequent reference to the details of the scalar derivation. The equation will be an integral equation for the relative momentum wave function of a bound state with zero total momentum. After having arrived at this integral equation we will convert it into a finite difference equation by means of a Mellin transform (Sec. III D). In Sec. IV we will analytically solve the resulting finite difference equation.

A. The LFSA scalar QED equation

Formally, the problem of deriving a wave equation for an electron-positron bound state may be thought of as the problem of diagonalizing the Hamiltonian for massless scalar electrodyanmics on a restricted subspace of states: those states that contain one physical electron, one physical positron, and no additional radiation. If the resulting equation is to be physically sensible, we must take care to include only physical states in the subspace on which we diagonalize the Hamiltonian. For

example, were we to carry out this calculation in the temporal gauge $A_0=0$, we would have to insure that Gauss's law $\vec{\nabla}\cdot\vec{E}=\rho$ was satisfied on each of the states we included in the subspace. In order to obviate the necessity for such a discussion, or equivalently, to insure that our two-particle states are actually gauge invariant and hence physical, we will carry out the calculation in the radiation gauge $\vec{\nabla}\cdot\vec{A}=0$. In the radiation gauge, the transverse components of the electromagnetic potential and the electric field create and annihilate physical photons, and the scalar field and its conjugate momentum create and annihilate the physical particle degrees of freedom along with their associated longitudinal electric fields.

We will make the perturbative identification of single-particle annihilation and creation operators. At a fixed time, we will associate the Fourier components of the scalar field and its conjugate momentum with creation and annihilation operators for scalar quanta. The normal-ordered Hamiltonian has zero expectation value in the state of no quanta and its expectation in the state of one physical electron or one physical positron is the absolute value of the momentum of the electron or positron, which shows that our identification of annihilation and creation operators for single-particle states is proper. Two-particle states, with one electron and one positron, will be taken to be those states obtained from the no-particle state by applying one electron and one positron creation operator.

The Lagrangian for massless scalar electrodynamics is

$$\mathcal{L}=(\partial_\mu+ieA_\mu)\phi^*(\partial_\mu-ieA_\mu)\phi-\tfrac{1}{4}F_{\mu\nu}F_{\mu\nu}\,. \quad (3.1)$$

This Lagrangian must be supplemented by a gauge condition, for which we take the radiation gauge,

$$\vec{\nabla}\cdot\vec{A}=0\,, \quad (3.2)$$

and by counterterms. In addition to counterterms with the same kinematic form as the terms of the Lagrangian, there is a mass counterterm for the scalar field and a counterterm proportional to $(\phi^*\phi)^2$, which, as is well known, is needed to make electron-electron and electron-positron scattering finite. The necessity for this last counterterm arises because diagrams in which two or more photons are exchanged between a pair of electrons or between an electron and a positron are logarithmically divergent in the ultraviolet. The counterterm, of course, preserves the gauge invariance of the Lagrangian. In order that the charge carried by starred fields and momenta be the same, and opposite to that of unstarred fields, we will denote the momentum operator conjugate to ϕ by Π^* and momentum conjugate to ϕ^* by Π.

The canonical momenta are

$$\Pi=\frac{\partial\mathcal{L}}{\partial\dot{\phi}^*}=(\partial_0-ieA_0)\phi\,,$$
$$\Pi^*=\frac{\partial\mathcal{L}}{\partial\dot{\phi}}=(\partial_0+ieA_0)\phi^*\,. \quad (3.3)$$

It is convenient to decompose the electric field into a transverse and a longitudinal part

$$\vec{E}=\vec{E}^T-\vec{\nabla}\chi\,, \quad (3.4)$$

where

$$\vec{\nabla}\cdot\vec{E}^T=0\,. \quad (3.5)$$

The momentum conjugate to the transverse electromagnetic potential is the transverse electric field

$$\frac{\partial\mathcal{L}}{\partial\dot{A}_i^T}=-F_{0i}^T=-E_i^T\,. \quad (3.6)$$

The canonical commutation relations of the fields and momenta are

$$[\Pi^*(\vec{x},0),\phi(\vec{y},0)]=[\Pi(\vec{x},0),\phi^*(\vec{y},0)]=-i\delta^3(\vec{x}-\vec{y})\,,$$
$$[E_i^T(\vec{x},0),A_j^T(\vec{y},0)]=i\delta_{ij}^T\delta^3(\vec{x}-\vec{y})\,. \quad (3.7)$$

Varying the Lagrangian with respect to the canonical fields, A_i^T, ϕ, and ϕ^* give the dynamical field equations for scalar electrodynamics;

$$(\partial_\mu-ieA_\mu)^2\phi=0\,,$$
$$(\partial_\mu+ieA_\mu)^2\phi^*=0\,,$$
$$\partial_\mu F_{\mu\nu}+ie[\phi^*\overleftrightarrow{\partial}_\nu\phi-2(eA_\nu\phi^*\phi)]=0\,. \quad (3.8)$$

Varying the Lagrangian with respect to A_0 gives the equation of constraint,

$$\vec{\nabla}\cdot\vec{E}+ie(\phi^*\Pi-\Pi^*\phi)=0\,. \quad (3.9)$$

The longitudinal part of the electric field, which alone enters the constraint equation, is equal to $-\vec{\nabla}A_0$ (i.e., $A_0=\chi$). From the constraint equation we identify the charge density carried by the scalar field as

$$\rho=-i(\phi^*\Pi-\Pi^*\phi)\,. \quad (3.10)$$

The total charge Q is the space integral of $\rho(x)$:

$$Q=\int d^3x\,\rho(x)\,. \quad (3.11)$$

From the canonical commutation relations it follows that ϕ and Π annihilate one unit of charge while ϕ^* and Π^* create one unit of charge:

$$[Q,\phi]=-\phi\,,$$
$$[Q,\phi^*]=+\phi^*\,,$$
$$[Q,\Pi]=-\Pi\,,$$
$$[Q,\Pi^*]=+\Pi^*\,. \quad (3.12)$$

Gauss's law, Eq. (3.9), the constraint equation of scalar electrodynamics, can be imposed as an operator constraint in the radiation gauge and, in fact, we will use the constraint as an operator equation to simplify the canonical Hamiltonian. All appearances of the longitudinal electric field or the scalar potential will be understood to be shorthand notations for appropriate expressions involving the scalar field and its conjugate momentum. The Hamiltonian scalar electrodynamics can be constructed by the canonical prescription

$$\mathcal{H}=\Pi^*\dot{\phi}+\Pi\dot{\phi}^*-\vec{E}^T\cdot\dot{\vec{A}}^T-\mathcal{L}\,. \tag{3.13}$$

By use of the constraint equation and the expressions for Π and Π^* in terms of the fields and their time derivatives the Hamiltonian can be put into the form

$$\mathcal{H}=\Pi^*\Pi+(\vec{\nabla}-ie\vec{A})\phi^*\cdot(\vec{\nabla}+ie\vec{A})\phi + \tfrac{1}{2}[(\vec{E}^T)^2+(\vec{B})^2+(\vec{\nabla}\chi)^2]\,, \tag{3.14}$$

where

$$\nabla^2\chi=-ie(\Pi^*\phi-\Pi\phi^*)\,. \tag{3.15}$$

The Hamiltonian should be understood as a normal-ordered product, and the counterterms, which are not displayed, are also to be understood as normal-ordered products. Normal ordering will be defined with respect to the Fourier components of the fields at time $t=0$.

Let us Fourier decompose the scalar field and conjugate momentum at $t=0$:

$$\phi(\vec{x})=\frac{1}{(2\pi)^{3/2}}\int\frac{d^3k}{(2|k|)^{1/2}}(e^{i\vec{k}\cdot\vec{x}}a_{\vec{k}}+e^{-i\vec{k}\cdot\vec{x}}b^\dagger_{\vec{k}})\,,$$

$$\phi^*(\vec{x})=\frac{1}{(2\pi)^{3/2}}\int\frac{d^3k}{(2|k|)^{1/2}}(e^{-i\vec{k}\cdot\vec{x}}a^\dagger_{\vec{k}}+e^{i\vec{k}\cdot\vec{y}}b_{\vec{k}})\,, \tag{3.16}$$

$$\Pi(\vec{x})=\frac{-i}{(2\pi)^{3/2}}\int\frac{d^3k}{\sqrt{2}}\sqrt{|k|}(e^{i\vec{k}\cdot\vec{x}}a_{\vec{k}}-e^{-i\vec{k}\cdot\vec{x}}b^\dagger_{\vec{k}})\,,$$

$$\Pi^*(\vec{x})=\frac{i}{(2\pi)^{3/2}}\int\frac{d^3k}{\sqrt{2}}\sqrt{|k|}(e^{-i\vec{k}\cdot\vec{x}}a^\dagger_{\vec{k}}-e^{i\vec{k}\cdot\vec{x}}b_{\vec{k}})\,.$$

The Fourier components are expressed in terms of the annihilation and creation operators a, $a^\dagger$, b, $b^\dagger$, and standard kinematic factors. Particle annihilation and creation operators have their usual commutation relations

$$[a_{\vec{k}},a^\dagger_{\vec{k}'}]=[b_{\vec{k}},b^\dagger_{\vec{k}'}]=\delta^3(\vec{k}-\vec{k}') \tag{3.17}$$

and these reproduce the canonical commutation relations of the fields. The a operators annihilate and create particles with charge +1 and the b operators annihilate and create their antiparticles, with charge −1.

We are interested in diagonalizing this Hamiltonian on the space of states consisting of one electron and one positron. The problem of diagonalizing the Hamiltonian on this space is equivalent to the problem of finding the local minima of the normalized expected value of the Hamiltonian in arbitrary states consisting of one positron and one electron. Since the states with which we are concerned contain no physical photons, we can neglect the transverse electromagnetic potential and the transverse electric field in computing the expected value of the Hamiltonian. For the computation of the expected value of the Hamiltonian in states without physical radiation, the Hamiltonian may be replaced by

$$\mathcal{H}_{\text{eff}}=\Pi^*\Pi+\vec{\nabla}\phi^*\cdot\vec{\nabla}\phi+\tfrac{1}{2}(\vec{\nabla}\chi)^2\,, \tag{3.18}$$

where χ is given by Eq. (3.15). The Hamiltonian thus consists of the quadratic kinematical part and the quartic nonlinear interaction. The interaction is simply the instantaneous Coulomb interaction between charged particles. Since the Hamiltonian is normal ordered, the trivial Coulomb self-energy of the single particle has been removed. Since the interaction is explicitly quartic, it does not effect the expected value of the Hamiltonian in states of zero or one particle.

The kinematic part of the Hamiltonian can be simply expressed in terms of the annihilation and creation operators a and b:

$$H_0=\int d^3x\,\mathcal{H}_0=\int d^3k\,|\vec{k}|(a^\dagger_{\vec{k}}a_{\vec{k}}+b^\dagger_{\vec{k}}b_{\vec{k}})\,. \tag{3.19}$$

The single-particle expected value of the Hamiltonian is given by the kinematic term alone, and so the expected value of the Hamiltonian in a single-particle state is the absolute value of its momentum. A two-particle state with zero total momentum is constructed from the ground state by applying $a^\dagger$ and $b^\dagger$:

$$|\vec{p},-\vec{p}\rangle=a^\dagger_{\vec{p}}b^\dagger_{-\vec{p}}|0\rangle\,. \tag{3.20}$$

The matrix element of the kinematic part of the Hamiltonian between two such states is

$$\langle\vec{q},-\vec{q}\,|H_0|\vec{p},-\vec{p}\rangle=2|\vec{p}\,|\delta^3(0)\delta^3(\vec{p}-\vec{q})\,. \tag{3.21}$$

Since these states have total momentum zero they are normalized to the total volume of space:

$$\langle\vec{q},-\vec{q}\,|\vec{p},-\vec{p}\rangle=\delta^3(0)\delta^3(\vec{p}-\vec{q})\,. \tag{3.22}$$

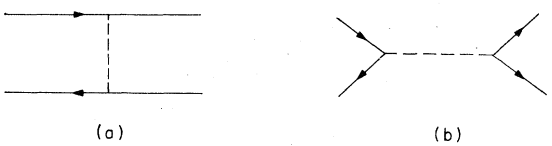


FIG. 4. (a) The coulomb photon exchange and (b) the Coulomb photon annihilation contributions to the electron-positron effective interaction Hamiltonian.

The nonlocal interaction part of the scalar field can be expressed as a multiple momentum integral

$$H_I = \int d^3x\, \mathcal{H}_I = + \frac{e^2}{8(2\pi)^3} \int d^3k\, d^3k'\, d^3k''\, \frac{1}{k^2}$$
$$:\left\{\left[\left(\frac{|\vec{k}'|}{|\vec{k}+\vec{k}|}\right)^{1/2} + \left(\frac{|\vec{k}+\vec{k}'|}{|\vec{k}'|}\right)^{1/2}\right](a^\dagger_{-\vec{k}'}\, a_{-\vec{k}-\vec{k}'} - b^\dagger_{\vec{k}+\vec{k}'}\, b_{\vec{k}'})\right.$$
$$\left. + \left[\left(\frac{|\vec{k}'|}{|\vec{k}+\vec{k}'|}\right)^{1/2} - \left(\frac{|\vec{k}+\vec{k}'|}{|\vec{k}'|}\right)^{1/2}\right](a^\dagger_{-\vec{k}'}\, b^\dagger_{\vec{k}+\vec{k}'} - a_{-\vec{k}-\vec{k}'}\, b_{\vec{k}'})\right\}$$
$$\times\left\{\left[\left(\frac{|\vec{k}''|}{|\vec{k}-\vec{k}''|}\right)^{1/2} + \left(\frac{|\vec{k}-\vec{k}''|}{|\vec{k}''|}\right)^{1/2}\right](a^\dagger_{-\vec{k}''}\, a_{\vec{k}-\vec{k}''} - b^\dagger_{-\vec{k}+\vec{k}''}\, b_{\vec{k}''})\right.$$
$$\left. + \left[\left(\frac{|\vec{k}''|}{|\vec{k}-\vec{k}''|}\right)^{1/2} - \left(\frac{|\vec{k}-\vec{k}''|}{|\vec{k}''|}\right)^{1/2}\right](a^\dagger_{-\vec{k}''}\, b^\dagger_{-\vec{k}+\vec{k}''} - a_{\vec{k}-\vec{k}''}\, b_{\vec{k}''})\right\}: . \tag{3.23}$$

Since we are interested in computing expecation values of the interaction between states consisting of one electron and one positron, the only terms of the interaction Hamiltonian of interest are those that contain one annihilation and one creation operator for a particle and an antiparticle. These terms are

$$H_{I\,\mathrm{eff}} = + \frac{e^2}{8(2\pi)^3} \int d^3k\, d^3k'\, d^3k''\, \frac{1}{k^2} \left\{\left[\left(\frac{|\vec{k}'|}{|\vec{k}+\vec{k}''|}\right)^{1/2} + \left(\frac{|\vec{k}+\vec{k}'|}{|\vec{k}'|}\right)^{1/2}\right]\left[\left(\frac{|\vec{k}''|}{|\vec{k}-\vec{k}''|}\right)^{1/2} + \left(\frac{|\vec{k}-\vec{k}''|}{|\vec{k}''|}\right)^{1/2}\right]\right.$$
$$\times(-1)(a^\dagger_{-\vec{k}}\, b^\dagger_{-\vec{k}+\vec{k}'}\, a_{-\vec{k}-\vec{k}'}\, b_{\vec{k}''} + a^\dagger_{-\vec{k}''}\, b^\dagger_{\vec{k}+\vec{k}''}\, a_{\vec{k}-\vec{k}''}\, b_{\vec{k}'})$$
$$+\left[\left(\frac{|\vec{k}'|}{|\vec{k}+\vec{k}'|}\right)^{1/2} - \left(\frac{|\vec{k}+\vec{k}'|}{|\vec{k}'|}\right)^{1/2}\right]\left[\left(\frac{|\vec{k}''|}{|\vec{k}-\vec{k}''|}\right)^{1/2} - \left(\frac{|\vec{k}-\vec{k}''|}{|\vec{k}''|}\right)^{1/2}\right]$$
$$\left.\times(-1)(a^\dagger_{-\vec{k}}\, b^\dagger_{\vec{k}+\vec{k}'}\, a_{\vec{k}-\vec{k}''}\, b_{\vec{k}''} + a^\dagger_{-\vec{k}''}\, b^\dagger_{-\vec{k}+\vec{k}''}\, a_{-\vec{k}-\vec{k}'}\, b_{\vec{k}'})\right\} . \tag{3.24}$$

The matrix elements of this part of the interaction between momentum eigenstates consisting of one electron and one positron are

$$\langle \vec{q}, -\vec{q}\,|H_I|\,\vec{p}, -\vec{p}\rangle$$
$$= -\frac{e^2\delta^3(0)}{4(2\pi)^3}\left(\frac{|\vec{q}|/|\vec{p}| + |\vec{p}|/|\vec{q}| + 2}{(\vec{p}-\vec{q})^2} - \frac{\vec{p}\cdot\vec{q}}{3p^2q^2}\right) . \tag{3.25}$$

Note that in computing the last term the integration variable k is kinematically constrained to be zero. The limit $k \to 0$ is singular, however, and we regularize the singularity by treating the $k \to 0$ as a spherically symmetrical limit, so that under the k integral $k_i k_j$ is replaced by $\frac{1}{3}k^2\delta_{ij}$.

The physical meaning of the terms in Eq. (3.25) is quite straightforward. The first terms, with denominator proportional to $(\vec{p}-\vec{q})^2$, come from single Coulomb photon exchange between the electron and the positron, and the last term comes from electron-positron annihilation into a Coulomb photon (see Fig. 4.). We are interested in diagonalizing the Hamiltonian on the full space of zero-total-momentum electron-positron states. A general state in that space is

$$|\psi\rangle = \int d^3p\, \psi(\vec{p}) a^\dagger_p b^\dagger_{-p}|0\rangle . \tag{3.26}$$

We diagonalize H by the variational principle. Varying the normalized expected value of the Hamiltonian in such a state and demanding that the variation be zero,

$$\delta\,\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = 0 , \tag{3.27}$$

gives a wave equation for the electron-positron states

$$\frac{\delta}{\delta\psi}\langle\psi|H|\psi\rangle = E\,\frac{\delta}{\delta\psi}\langle\psi|\psi\rangle , \tag{3.28}$$

with the eigenvalue E given by

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} . \tag{3.29}$$

The expected value of the Hamiltonian is given by

$$\langle\psi|H|\psi\rangle = \left[2\int d^3p\, |\psi(p)|^2|\vec{p}|\right.$$
$$\left. - \frac{e^2}{4(2\pi)^3}\int d^3q\, d^3p\, \psi^*(\vec{p})\psi(\vec{q})\right.$$
$$\left.\times\left(\frac{|\vec{q}|/|\vec{p}| + |\vec{p}|/|\vec{q}| + 2}{(\vec{p}-\vec{q})^2} - \frac{\vec{p}\cdot\vec{q}}{3p^2q^2}\right)\right]\delta^3(0) \tag{3.30}$$

and the normalization of states is

$$\langle\psi|\psi\rangle = \int d^3p\, |\psi(\vec{p})|^2\delta^3(0) , \tag{3.31}$$

so that the resulting wave equation is

$$(2|\vec{p}|-E)\psi(\vec{p})=+\frac{e^2}{4(2\pi)^3}\times\int d^3q\left(\frac{|\vec{q}|/|\vec{p}|+|\vec{p}|/|\vec{q}|+2}{(\vec{p}-\vec{q})^2}-\frac{\vec{p}\cdot\vec{q}}{3p^2q^2}\right)\psi(\vec{q})\,. \tag{3.32}$$

Note that the final term in the integral operator, corresponding to the annihilation diagram [Fig. 3(b)], contributes only to p-wave bound states or scattering states. We will look for s-wave solutions to the wave equation, and so this term will not contribute.

Note also that we have not explicitly mentioned the counterterms in the Hamiltonian. The mass counterterm would contribute to the energy of the single-particle states, and so in the approximation that we are discussing, namely, truncating the Hamiltonian to the spaces of zero, one, and two particles, such a counterterm is absent. However, the $(\phi^*\phi)^2$ counterterm, which makes no contribution to the energy of a single-particle state, can in fact be present. Such a counterterm would contribute only to s-wave states. As we shall show, such a counterterm is needed to regulate the high-momentum behavior of the wave equation.

To find the one-dimensional radial equation for s-wave bound or scattering states, we look for wave functions which depend only on the magnitude of the momentum $\vec{p}$. For such wave functions we can evaluate the angular integrals in the wave equation, and there exists an effective radial wave equation in momentum space

$$(2p-E)\psi(p)=\frac{e^2}{4(2\pi)^2p^2}\int_0^\infty dq(p+q)^2\times\ln\left|\frac{p+q}{p-q}\right|\psi(q)\,. \tag{3.33}$$

This wave equation is singular in the ultraviolet. There is, in fact, no consistent high-momentum behavior for the wave function $\psi(p)$. To see this, note that for very large momentum p, we can drop the eigenvalue of E from the left-hand side of the equation. The resulting equation will be dimensionally homogeneous, and so solutions to that equation would be $\psi\propto p^\nu$, where ν is some fixed power. However, with ψ proportional to any fixed power of p, the the integral in the wave equation diverges. If ν is less than -2, the integral diverges at the lower end, and if ν is greater than -2, it diverges at the upper end. If $\nu=-2$, the integral diverges at both ends.

The source of these high-momentum difficulties is easy to locate. Since in s-wave states the wave equation represents only Coulomb-photon exchange, the formal solution to the equation is the multi-Coulomb-photon exchange diagram shown in Fig. 5(a). This diagram contains, as internal parts, diagrams with two or more exchanged Coulomb photons, for example the diagram in Fig. 5(b). These diagrams are just those that lead to the necessity of a $(\phi^*\phi)^2$ counterterm in scalar electrodynamics, in order to make electron-electron and electron-positron scattering finite.

To cure the high-energy behavior of the wave equation, we will include, in the effective Hamiltonian, a counterterm

$$H_c=c\int[\phi^*(x)\phi(x)]^2d^3x\,. \tag{3.34}$$

The constant c will be determined to regularize the high-energy behavior of the wave equation. Since this counterterm is a point interaction, it contributes only to the s-wave electron-positron interaction.

We may analyze the effects of the counterterm Hamiltonian in a manner exactly parallel to the treatment of the instantaneous Coulomb interaction. The matrix elements of the Hamiltonian between states $|\psi\rangle$ are given by

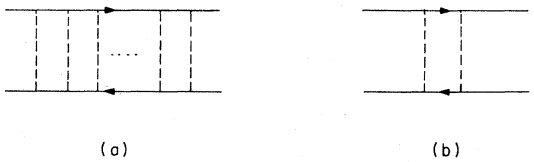
$$\langle\psi|H_c|\psi\rangle=\frac{c}{(2\pi)^3}\,\delta^3(0)\int d^3p\,d^3q\,\frac{\psi^*(\vec{p})\psi(\vec{q})}{|\vec{p}|\,|\vec{q}|}\,. \tag{3.35}$$

This additional contribution to the expectation value of the Hamiltonian adds an additional term to the three-dimensional form of the wave equation:

$$-\frac{c}{(2\pi)^3}\,\frac{1}{|\vec{p}|}\int d^3q\,\frac{\psi|\vec{q}|}{|\vec{q}|}\,. \tag{3.36}$$

If ψ is spherically symmetrical, then there results

$$-\frac{c}{2\pi^2p}\int_0^\infty dq\,q\psi(q) \tag{3.37}$$



(a) (b)

FIG. 5. (a) The formal diagrammatic solution to Eqs. (3.32) and (3.33). Each dashed line represents a Coulomb-photon exchange. An infinite number are exchanged, and there are no crossed exchanges. (b) An internal part of the diagram (a). It is logarithmically divergent and requires a $(\phi^*\phi)^2$ counterterm.

as an additional contribution to the wave equation (33). The value of c that eliminates the most singular term in the wave equation as q goes to infinity is

$$c = \tfrac{1}{4} e^2 . \tag{3.38}$$

Note that c is positive, so that Hamiltonian, including the counterterm, is positive definite.

The counterterm is also necessary to bound the Hamiltonian from below for small values of α. Without the counterterm, the expectation value of H in the state

$$|\psi_N\rangle = \int d^3p \sum_{i=1}^{N} \beta^{2i} e^{-\beta^i |\vec{p}|} a^\dagger_{\vec{p}} b^\dagger_{-\vec{p}} |0\rangle , \tag{3.39}$$

for $\beta > 6\pi/\alpha$, satisfies the inequality

$$\langle \psi_N | H | \psi_N \rangle \leq \frac{3N}{4} - \frac{3\alpha N}{2\pi} - \frac{\alpha}{2\pi}(N^2 - N) . \tag{3.40}$$

For sufficiently large N, $\langle \psi_N | \psi_N \rangle$ is negative. Scale invariance then implies that H is unbounded from below. The counterterm adds to $\langle \psi_N | H | \psi_N \rangle$ a term proportional to N^2. For $c \geq \frac{1}{4} e^2$ this changes the sign of the coefficient of N^2 in the inequality, vitiating the argument. A careful analysis of the domain of H shows that without the counterterm H is not self-adjoint on the two-particle zero-momentum subspace, and only the value $c = \frac{1}{4} e^2$ makes H self-adjoint for small α.

The nonsingular wave equation for s-wave bound states with the counterterm is

$$(2p - E)\psi(p) = \frac{e^2}{(4\pi)^2} \int_0^\infty dq \left(\frac{(p+q)^2}{p^2} \ln \left| \frac{p+q}{p-q} \right| - \frac{2q}{p} \right) \psi(q) . \tag{3.41}$$

This integral equation has simple dimensional scale properties and so its Mellin transform is a relatively simple finite difference equation. Both the term $2p$ and the integral operator have scale dimension m^1, while the eigenvalue has scale dimension m^0. That is, under a rescaling $p \to \alpha p$, the $2p$ term and the integral operator are multiplied by α while the eigenvalue stays unchanged.

B. The LFSA spinor QED equation

In this subsection we will derive the integral equation for electron-positron bound-state wave functions. The procedure will follow the derivation of the scalar QED bound-state wave equation, more precisely that part of Sec. III A between Eqs. (3.1) and (3.33).

The Lagrangian for spinor QED is

$$\mathcal{L} = \bar{\Psi}(1\not{\partial} - e\not{A})\Psi - \tfrac{1}{4} F_{\mu\nu} F_{\mu\nu} . \tag{3.42}$$

We will work in the radiation gauge so that the treatment of the electromagnetic field is exactly the same as that in Sec. III A. In particular, $\vec{A}$ is purely transverse, and $\vec{A}$ and the transverse part of $\vec{E}$ create and annihilate physical photons. The only difference between this and the scalar case is the spin of the charged field. The canonical momentum to the field Ψ is

$$\Pi_\Psi = \frac{\partial \mathcal{L}}{\partial \dot{\Psi}} = \Psi^\dagger = \bar{\Psi}\gamma_0 . \tag{3.43}$$

The fields Ψ and $\Psi^\dagger$ satisfy, at equal times, canonical anticommutation relations

$$\{\Psi_\alpha(\vec{x}, 0), \Psi^\dagger_\beta(\vec{y}, 0)\} = \delta_{\alpha\beta} \delta^3(\vec{x} - \vec{y}) . \tag{3.44}$$

The field Ψ can be decomposed into annihilation and creation operators

$$\Psi(\vec{x}, 0) = \frac{1}{(2\pi)^{3/2}} \sum_s \int \frac{d^3p}{(2|p|)^{1/2}} \left(b_{\vec{p},s} e^{i\vec{p}\cdot\vec{x}} u_{\vec{p},s} + d^\dagger_{\vec{p},s} e^{-i\vec{p}\cdot\vec{x}} v_{\vec{p},s} \right) . \tag{3.45}$$

The b operators create and annihilate electrons and the d operators create and annihilate positrons. They have the usual anticommutation relations, which reproduce the canonical anticommutation relations of Ψ and $\Psi^\dagger$:

$$\{b_{\vec{p}s}, b^\dagger_{\vec{p}',s'}\} = \{d_{\vec{p},s}, d^\dagger_{\vec{p}',s'}\} = \delta_{ss'} \delta^3(\vec{p} - \vec{p}') . \tag{3.46}$$

The longitudinal part of the electric field is not a dynamical degree of freedom. It is constrained by Gauss's law

$$\vec{\nabla} \cdot \vec{E} = e\rho , \tag{3.47}$$

where the charge density ρ is given by

$$\rho = \bar{\Psi}\gamma_0 \Psi . \tag{3.48}$$

With these preliminaries, we may write the Hamiltonian of QED in the radiation gauge as

$$\mathcal{H} = \bar{\Psi}\vec{\gamma} \cdot (-i\vec{\nabla} - e\vec{A})\Psi + \tfrac{1}{2}[(\vec{E}^T)^2 + (\vec{B})^2 + (\vec{\nabla}\chi)^2] . \tag{3.49}$$

The dependent field χ, whose negative gradient is the longitudinal part of the electric field, is given by

$$-\nabla^2 \chi = \rho = \bar{\Psi}\gamma_0 \Psi . \tag{3.50}$$

We have taken advantage of the fact that in the radiation gauge the constraint of Gauss's law may be imposed as an operator condition to simplify the Hamiltonian.

Since the operators b and d create physical electrons and positrons, along with the longitudinal electric fields required by Gauss's law, we can write the most general zero-momentum scalar electron-positron state as

$$|\psi\rangle=\sum_{ss'}\int\frac{d^3p}{2|p|}\,\psi(p)\bar{u}_{\vec{p}s}v_{-\vec{p},s'}\,b^{\dagger}_{\vec{p},s}d^{\dagger}_{-\vec{p},s'}|0\rangle. \tag{3.51}$$

The wave function ψ is a function of $|\vec{p}|$ only. In calculating the expectation value of the Hamiltonian, only those terms in the interaction with one annihilation operator and one creation operator for an electron and for a positron contribute. The expected value of the Hamiltonian in the state $|\psi\rangle$ is given by

$$\langle\psi|H|\psi\rangle=\left[16\pi\int_0^\infty p^3d^3p\,|\psi(p)|^2-\frac{e^2}{2\pi}\int_0^\infty dp\int_0^\infty dq\psi^*(p)\psi(q)\left((p+q)^2\ln\left|\frac{p+q}{p-q}\right|-2pq\right)\right]\delta^3(0) \tag{3.52}$$

and the state $|\psi\rangle$ is normalized to the total volume of space

$$\langle\psi|\psi\rangle=8\pi\int_0^\infty p^2dp\,|\psi(p)|^2\delta^3(0). \tag{3.53}$$

Demanding that the normalized expected value of the Hamiltonian be stationary,

$$\frac{\delta}{\delta\psi}\,\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}=0 \tag{3.54}$$

gives an effective wave equation for ψ:

$$(2p-E)\psi(p)=\frac{e^2}{16\pi^2}\int_0^\infty dq\left[\left(1+\frac{q}{p}\right)^2\times\ln\left|\frac{p+q}{p-q}\right|-2\frac{q}{p}\right]\psi(q). \tag{3.55}$$

This is exactly the same equation as that derived in Sec. III A for scalar electron-positron bound states.

Note that although spinor QED has no counterterm which is a counterpart of the $(\phi^*\phi)^2$ counterterm in scalar QED, the resulting wave equation is exactly the same as that obtained in scalar QED with the inclusion of this counterterm. Note also that massless QED is a chirally invariant theory, and so we would expect that the equation for pseudoscalar bound states would be the same as the scalar bound-state equation. In fact, if we were to take as a class of variational trial states the pseudoscalar states

$$|\psi_{ps}\rangle=\sum_{ss'}\int\frac{d^3p}{2|p|}\,\psi_{ps}(p)\bar{u}_{\vec{p},s}\gamma_5v_{-\vec{p},s'}\,b^{\dagger}_{\vec{p},s}d^{\dagger}_{-\vec{p}s'}|0\rangle, \tag{3.56}$$

where again ψ_{ps} is a function only of $|\vec{p}|$, then if we follow the same procedure as we did in deriving the scalar bound-state equation, we arrive at exactly the same wave equation for the pseudoscalar wave function as we did for the scalar wave function.

C. The LFSA QCD bound-state equation

In this subsection we will derive a wave equation for color-singlet bound states of a quark and an antiquark in QCD. The procedure identically parallels that of the previous two electrodynamic examples.

The QCD Lagrangian is

$$\mathcal{L}=\bar{q}\left(i\not{\partial}+g\sum_a\tfrac{1}{2}\lambda^a\not{A}^a\right)q-\tfrac{1}{4}\sum_a F^a_{\mu\nu}F^a_{\mu\nu}. \tag{3.57}$$

The gauge fields are expressed in terms of potentials by

$$F^a_{\mu\nu}=\partial_\mu A^a_\nu-\partial_\mu A^a_\nu+gf^{abc}A^b_\mu A^c_\nu. \tag{3.58}$$

The quark field q and its canonically conjugate momentum $\bar{q}\gamma_0$ can be decomposed into annihilation and creation operators for quarks and antiquarks (triplets Q and $\bar{Q}$):

$$q(\vec{x},0)=\frac{1}{(2\pi)^{3/2}}\sum_s\int\frac{d^3p}{(2|p|)^{1/2}}\left(Q_{p,s}e^{i\vec{p}\cdot\vec{x}}u_{\vec{p},s}+\bar{Q}^{\dagger}_{\vec{p},s}e^{-i\vec{p}\cdot\vec{x}}v_{\vec{p},s}\right). \tag{3.59}$$

In order to parallel our treatment of electrodynamics, we will work in the radiation gauge

$$\vec{\nabla}\cdot\vec{A}^a=0. \tag{3.60}$$

While it is known that under certain circumstances there are ambiguities in defining the gauge potentials in the radiation gauge, we will here be concerned only with states in which the expected value of the transverse electric field and transverse gauge potential are zero, so that these ambiguities are absent. As in electrodynamics, the Yang-Mills electric field is canonically conjugate to the Yang-Mills gauge potential:

$$[A^a_i(\vec{x},0),E^b_j(\vec{y},0)]=-i\delta^T_{ij}\delta^3(\vec{x}-\vec{y})\delta^{ab}. \tag{3.61}$$

Using Gauss's law,

$$\vec{\nabla}\cdot\vec{E}^a-gf^{abc}\vec{A}^b\cdot\vec{E}^c=-g\rho^a, \tag{3.62}$$

we may write the Hamiltonian of QCD as

$$\mathcal{H}=\bar{q}\vec{\gamma}\cdot\left(-i\vec{\nabla}+g\sum_a\tfrac{1}{2}\lambda^a\vec{A}^a\right)g+\tfrac{1}{2}\sum_a[(\vec{E}^{aT})^2+(\vec{B}^a)^2]-\tfrac{1}{2}\sum_a\rho^a\frac{1}{\nabla^2}\rho^a, \tag{3.63}$$

where the charge density receives contributions both from the quarks and from the Yang-Mills field itself:

$$\rho^a = \bar{q}\gamma_0 \tfrac{1}{2}\lambda^a q - f^{abc}\vec{A}^b\cdot\vec{E}^c . \tag{3.64}$$

In the radiation gauge, the quark field and its conjugate create and annihilate physical quarks and antiquarks, along with the gauge fields required by Gauss's law.

We will derive a wave equation for the bound states of one quark and one antiquark by calculating the expected value of the QCD Hamiltonian in a general quark-antiquark state, and then requiring that the normalized expected value of the Hamiltonian be stationary with respect to variations of the wave function of that state. We will concern ourselves exclusively with spatial-scalar color-singlet states. The effective potential between a quark and an antiquark in a color-octet state is repulsive, and will give rise to no bound states. The general color-singlet, scalar, zero-momentum state of one quark and one antiquark is given by

$$|\psi\rangle = \sum_{ss'} \int \frac{d^3p}{2|p|}\psi(p)\bar{u}_{\vec{p},s}v_{-\vec{p},s'}\bar{Q}^\dagger_{-\vec{p},s'}Q^\dagger_{\vec{p},s}|0\rangle , \tag{3.65}$$

where the wave function ψ depends only on the magnitude of the relative momentum of the quark and antiquark.

Except for the quark multiplicity due to color and the appearance of λ matrices (through) ρ^a in the Hamiltonian, the computation of the expected value of the QCD Hamiltonian is exactly the same as the computation the expected QED Hamiltonian performed in Sec. III B. The effect of there being three quarks is to introduce a factor of

$$\mathrm{Tr}I = 3 \tag{3.66}$$

into the kinetic energy term in the expected value of the Hamiltonian, and also into the normalization of the state $|\psi\rangle$. The effect of the color multiplicity of the quarks in the instantaneous interaction term is to introduce a factor of

$$\sum_{a=1}^{8} \mathrm{Tr}(\tfrac{1}{2}\lambda^a)^2 = 4 . \tag{3.67}$$

In computing the normalized expected value of the QCD Hamiltonian, the color effects on the kinetic energy and normalizations cancel out, and the only effect is to multiply the interaction term by the quotient of these factors $\frac{4}{3}$. Thus the normalized expected value of the Hamiltonian, and the wave equation for scalar bound states, is exactly the same as in spinor QED, but for the inclusion of the factor of $\frac{4}{3}$ by multiplying the coupling constant squared. The resulting wave equation is

$$(2p - E)\psi(p) = \frac{4}{3}\frac{g^2}{16\pi^2} \times \int_0^\infty dq\left[\left(1+\frac{q}{p}\right)^2 \ln\left|\frac{p+q}{p-q}\right| - 2\frac{q}{p}\right]\psi(q) . \tag{3.68}$$

If the color group were SU(N) instead of SU(3), the factor of $\frac{4}{3}$ would be replaced by $(N^2-1)/2N$.

As in spinor QED, we obtain the same wave equation for pseudoscalar quark-antiquark bound states as we do for scalar quark-antiquark bound states.

D. Conversion to a difference equation

We define the Mellin transform $\phi(\zeta)$ of the momentum-space radial wave function $\psi(p)$ by

$$\phi(\zeta) = \int_0^\infty p^{\zeta-1}\psi(p)dp . \tag{3.69}$$

The eigenvalue term of the integral equation gives, upon Mellin transformation, a result proportional to $\phi(\zeta)$. Since the other terms in the equation have dimension m^1, they will each give, upon Mellin transformation, terms shifted by one unit in ζ. That is, they will give terms proportional to $\phi(\zeta+1)$.

If we define

$$\lambda = \begin{cases} \dfrac{\alpha}{4} = \dfrac{e^2}{16\pi} , & \text{QED} \\ \dfrac{4}{3}\dfrac{\alpha}{4} = \dfrac{4}{3}\dfrac{g^2}{16\pi} , & \text{QCD} \end{cases} \tag{3.70}$$

then the Mellin transform of the s-wave equation is

$$E\phi(\zeta) = [2 - \lambda B(\zeta)]\phi(\zeta+1) , \tag{3.71}$$

where $B(\zeta)$ is given by

$$B(\zeta) = \frac{1}{\pi}\int_0^\infty dx\, x^{\zeta-1}\left[\left(1+\frac{1}{x}\right)^2 \ln\left|\frac{x+1}{x-1}\right| - \frac{2}{x}\right] . \tag{3.72}$$

Writing the Mellin transform of the integral part of the momentum-space wave equation in this form requires an interchange of integrals which is valid for $\zeta\in(0,2)$. For this derivation to be valid, there must be some part of that interval for which both $\phi(\zeta)$ and $\phi(\zeta+1)$ exist, as defined by the integral expression Eq. (3.69). As we shall see from the solution, this condition is met.

Some care is necessary in evaluating $B(\zeta)$ because the separate terms in the integral that defines it do not have Mellin transforms that exist on a common domain. Nonetheless, because the integral as a whole converges for $\mathrm{Re}\zeta\in(0,2)$, the Mellin transform is well defined and can be evaluated. The result is

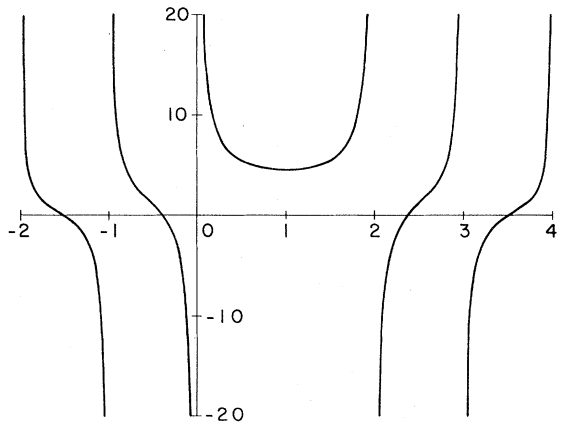


FIG. 6. The function $B(\zeta)$. Each zero of $\psi(\zeta)$ [Eq. (4.7)] corresponds to a root of $B(\zeta+n)=2/\lambda$, $n=0,1,2,\ldots$. Normalizable (bound-state) wave functions exist when the root of $B(\zeta)=2/\lambda$ between 0 and 1 occurs to the right of $\zeta=\frac{1}{2}$.

$$B(\zeta)=\left(\frac{1}{\zeta}+\frac{1}{\zeta-2}\right)\tan\frac{\pi\zeta}{2}-\frac{2}{\zeta-1}\cot\frac{\pi\zeta}{2}. \qquad (3.73)$$

Figure 6 shows a graph of $B(\zeta)$.

It should be stressed that the difference equation for $\phi(\zeta)$ is an analytic difference equation. Subject to the convergence of the integrals, ζ is an arbitrary complex variable. The difference equation is an analytic expression in the complex variable ζ, and so, although the equation has been derived only in a restricted domain of ζ, it has a unique analytic continuation to the entire ζ plane. Thus we should think of the difference equation (3.71) as an analytic relation, valid in the entire ζ plane, except perhaps for isolated singularities.

In addition to satisfying the difference equation, $\phi(\zeta)$ must obey several constraints because it is the Mellin transform of a wave function. It must be analytic inside a strip in the complex ζ plane parallel to the imaginary axis. The boundaries of the strip are determined by the asymptotic behavior as $p\to 0$ and $p\to\infty$ of $\psi(p)$. If

$$\psi(p)\sim p^{-\nu} \quad (p\to\infty) \qquad (3.74)$$

then $\phi(\zeta)$ will be singular at $\zeta=\nu$. This will mark the right boundary of the analyticity strip. Also if

$$\psi(p)\sim p^{-\mu} \quad (p\to 0) \qquad (3.75)$$

then $\phi(\zeta)$ will be singular at $\zeta=\mu$, and this will mark the left boundary of the analyticity strip.

In addition, as $|\zeta|\to\infty$, in either direction within the analyticity strip, $\phi(\zeta)$ must be polynominally bounded. The actual boundaries of the analyticity strip will be found by analyzing the difference equation.

We have expressed the problem of diagonalizing the electrodynamic and QCD Hamiltonians on the space of particle-antiparticle states as a difference equation whose solution must satisfy certain analytic constraints. The next section of this paper will be devoted to solving that equation, and in particular, to determining for what values of the coupling constant it is possible to find solutions with negative E.

IV. SOLUTION OF THE DIFFERENCE EQUATION

In the previous section, we reduced the relative momentum wave equation to the finite difference equation

$$[2-\lambda B(\zeta)]\phi(\zeta+1)=E\phi(\zeta), \qquad (4.1)$$

where

$$B(\zeta)=\frac{1}{\zeta}\tan\frac{\pi\zeta}{2}-\frac{2}{\zeta-1}\cot\frac{\pi\zeta}{2}+\frac{1}{\zeta-2}\tan\frac{\pi\zeta}{2}. \qquad (4.2)$$

In this section, we shall solve this difference equation by the same technique used on the difference equation obtained for a massless scalar particle in a Coulomb potential. We iterate Eq. (4.1) once to obtain

$$[2-\lambda B(\zeta+1)][2-\lambda B(\zeta)]\phi(\zeta+2)=E^2\phi(\zeta). \qquad (4.3)$$

If we denote $\tan\frac{1}{2}\pi\zeta$ by T, the factor $2-\lambda B(\zeta)$ can be written as the quotient of two cubics in ζ, with the coefficients being functions of T. In factored form

$$2-\lambda B(\zeta)=\frac{2[\zeta-r_1(T)][\zeta-r_2(T)][\zeta-r_3(T)]}{\zeta(\zeta-1)(\zeta-2)}, \qquad (4.4)$$

where $r_i(T)$ are the roots of the cubic polynomial

$$\tfrac{1}{2}\zeta(\zeta-1)(\zeta-2)[2-\lambda B(\zeta)].$$

Restoring the ζ dependence of T in Eq. (4.4) gives

$$2-\lambda B(\zeta)=\frac{2[\zeta-\zeta_1(\zeta)][\zeta-\zeta_2(\zeta)][\zeta-\zeta_3(\zeta)]}{\zeta(\zeta-1)(\zeta-2)}, \qquad (4.5)$$

where $\zeta_i(\zeta)\equiv r_i(\tan\frac{1}{2}\pi\zeta)$. With this form for $2-\lambda B(\zeta)$, the iterated difference equation (4.3) is effectively an equation with rational coefficients, since the ζ_i expressions have the same value at points related by the equation:

$$\left(\frac{2[\zeta-\zeta_1(\zeta)][\zeta-\zeta_2(\zeta)][\zeta-\zeta_3(\zeta)]}{\zeta(\zeta-1)(\zeta-2)}\right)\left(\frac{2[\zeta+1-\zeta_1(\zeta+1)][\zeta+1-\zeta_2(\zeta-1)][\zeta+1-\zeta_3(\zeta+1)]}{(\zeta+1)(\zeta)(\zeta-1)}\right)\phi(\zeta+2)=E^2\phi(\zeta). \qquad (4.6)$$

As indicated in Sec. II, this equation has a particular solution

$$\psi(\zeta)=(\tfrac{1}{2}E)^{\zeta}\prod_{i=1}^{3}\frac{\Gamma(\frac{1}{2}(\zeta+1-i))\,\Gamma(\frac{1}{2}(\zeta+2-i))}{\Gamma(\frac{1}{2}[\zeta-\zeta_i(\zeta)])\,\Gamma(\frac{1}{2}[\zeta+1-\zeta_i(\zeta+1)])}\,. \tag{4.7}$$

Equation (4.7) also gives a particular solution of Eq. (4.1), so that the general solution of Eq. (4.1) is

$$\phi(\zeta)=P(\zeta)\psi(\zeta)\,, \tag{4.8}$$

where $P(\zeta)$ is a periodic function of ζ with unit period.

$\phi(\zeta)$ is the Mellin transform of a wave function, so it must be analytic inside some strip $\mathrm{Re}\zeta\in(a,b)$ in the complex ζ plane containing $\zeta=\frac{3}{2}$. In addition, the analyticity strip must be at least one unit wide. There are two reasons for this. One is that since the wave operator is dimensionally homogeneous with dimension m^1, the interchange of orders of integration needed to show self-adjointness fails unless the analyticity strip is more than a unit wide. A related reason for demanding that the strip be wider than one unit is that otherwise the interchange of integration used to derive the difference equation would be invalid for all ζ.

The function $\psi(\zeta)$ has singularities that come from the poles and essential singularities of the $\Gamma(\frac{1}{2}[\zeta-\zeta_i(\zeta)])$ and $\Gamma(\frac{1}{2}(\zeta-i))$ factors. The Γ function $\Gamma(x)$ has poles at $x=0,-1,-2,\ldots$, and an essential singularity at $x=\infty$. Thus $\psi(\zeta)$ can have poles at $\zeta=2,1,0,-1,-2,\ldots$, which come from the Γ functions in the numerator, and essential singularities at the integers which come from the Γ functions in the denominator, since some $[\zeta-\zeta_i(\zeta)]\to\infty$ as $\zeta\to$ integer.

Near even integers, $\zeta=2N+\epsilon$, so that $T=\tan\frac{1}{2}\pi\epsilon$, and the three roots become

$$\zeta_1(2N+\epsilon)=2+O(\epsilon^2)\,, \tag{4.9a}$$

$$\zeta_2(2N+\epsilon)=0+O(\epsilon^2)\,, \tag{4.9b}$$

$$\zeta_3(2N+\epsilon)=-\frac{2\lambda}{\pi\epsilon}+1+O(\epsilon)\,. \tag{4.9c}$$

Near odd integers, $T=-\cot\frac{1}{2}\pi\epsilon$, so

$$\zeta_1(2N+1+\epsilon)=1+O(\epsilon)\,, \tag{4.10a}$$

$$\zeta_2(2N+1+\epsilon)=1+O(\epsilon)\,, \tag{4.10b}$$

$$\zeta_3(2N+1+\epsilon)=-\frac{2\lambda}{\pi\epsilon}+1+O(\epsilon)\,. \tag{4.10c}$$

The function $\psi(\zeta)$ has essential singularities at the integers since $\zeta_3(\zeta)$ diverges there. As $\mathrm{Im}\zeta\to\pm\infty$, $|\psi(\zeta)|\propto|\zeta|^{3/2}$. To see this, note that in these limits, $\tan\frac{1}{2}\pi\zeta\to\pm i$, so that ζ_i values have finite limits. Stirling's formula for the Γ function then gives

$$\psi(\zeta)\sim(\tfrac{1}{2}E)^{\zeta}\zeta^{-3/2+\sum_{i=1}^{3}\zeta_i}\,. \tag{4.11}$$

The sum of the ζ_i roots can be read off from the polynomial,

$$\sum_{i=1}^{3}\zeta_i=3\mp 2i\lambda\quad(\mathrm{Im}\zeta\to\pm\infty) \tag{4.12}$$

so

$$\psi(\zeta)|_{\zeta\to\pm i\infty}\propto(\tfrac{1}{2}E)^{\zeta}\zeta^{3/2\mp 2i\lambda}\,. \tag{4.13}$$

So long as E is real, ψ behaves asymptotically like a power in either direction along the analyticity strip.

For $\phi(\zeta)$ to be an acceptable solution, it must be analytic in a strip more than one unit wide and parallel to the imaginary axis and containing $\zeta=\frac{3}{2}$, and be polynomially bounded as $|\mathrm{Im}\zeta|\to\infty$. This requires that $P(\zeta)$ must be polynomially bounded and must cancel either the singularities of $\psi(\zeta)$ at $\zeta=1$ or at $\zeta=2$. Since $2-\lambda B(1)$ is finite, the singularity of $\psi(\zeta)$ at $\zeta=1$ is identical to its singularity at $\zeta=2$, so it is sufficient to choose $P(\zeta)$ to eliminate the singularity at $\zeta=1$.

The essential singularity of $\psi(\zeta)$ at $\zeta=1$ is due to two terms,

$$1/\Gamma(\tfrac{1}{2}[\zeta-\zeta_3(\zeta)]) \tag{4.14a}$$

and

$$1/\Gamma(\tfrac{1}{2}[\zeta+1-\zeta_3(\zeta+1)])\,. \tag{4.14b}$$

As $\zeta\to 1$,

$$\Gamma(\tfrac{1}{2}[\zeta-\zeta_3(\zeta)])\sim\Gamma\left(\frac{\lambda}{\pi(\zeta-1)}+O(\zeta-1)\right) \tag{4.15a}$$

and

$$\Gamma(\tfrac{1}{2}[\zeta+1-\zeta_3(\zeta+1)])\sim\Gamma\left(\frac{\lambda}{\pi(\zeta-1)}+\frac{1}{2}+O(\zeta-1)\right), \tag{4.15b}$$

which shows that $\zeta=1$ is an accumulation point of zeros. The strategy for removing the singularity of $\psi(\zeta)$ at $\zeta=1$ is to choose P to be the product of several periodic functions, each with unit period:

$$P(\zeta)=P_1(\zeta)P_2(\zeta)P_3(\zeta)P_4(\zeta)P_5(\zeta)\,. \tag{4.16}$$

$P_1(\zeta)P_2(\zeta)$ eliminates the singularity of Eq. (4.14a), $P_3(\zeta)P_4(\zeta)$ eliminates the singularity of Eq. (4.14b), and $P_5(\zeta)$ represents the remaining freedom in the choice of $P(\zeta)$. The function $P_1(\zeta)$ will be chosen to have same essential singularity as the Γ function in the denominator of Eq. (4.14a), except that its poles will not be in exactly the same locations as those of the Γ function. However, as $\zeta\to 1$ from any direction except the real

axis below $\zeta = 1$, $P(\zeta)$ will compensate for the essential singularity of Eq. (4.14a). $P_2(\zeta)$ will be constructed as a periodic infinite product that will have zeros at the poles of $P_1(\zeta)$ and poles at the zeros of Eq. (4.14a). $P_2(\zeta)$ will be free of other singularities and will approach a constant as $\zeta \to 1$ from any direction except the real axis from below. Thus $P_1(\zeta)P_2(\zeta)$ will completely compensate for the singularity of Eq. (4.14a) as $\zeta \to 1$. $P_3(\zeta)$ and $P_4(\zeta)$ will be the same as $P_1(\zeta)$ and $P_2(\zeta)$, except that they will be constructed to cancel the singularity of Eq. (4.14b).

To construct $P_1(\zeta)$, note that for ζ near 1

$$\Gamma(\tfrac{1}{2}[\zeta - \zeta_3(\zeta)]) = \Gamma\left(\frac{\lambda}{\pi\epsilon} + O(\epsilon)\right), \tag{4.17}$$

where $\epsilon = \zeta - 1$. Note also that

$$\Gamma(\lambda \cot\pi\zeta) = \Gamma\left(\frac{\lambda}{\pi\epsilon} + O(\epsilon)\right). \tag{4.18}$$

Thus, using Stirling's formula,

$$\lim_{\zeta \to 1} \frac{\Gamma(\lambda \cot\pi\zeta)}{\Gamma(\tfrac{1}{2}[\zeta - \zeta_3(\zeta)])} = 1, \quad |\arg\zeta - 1| < \pi. \tag{4.19}$$

We choose

$$P_1(\zeta) = \Gamma(\lambda \cot\pi\zeta). \tag{4.20}$$

The poles of $P_1(\zeta)$ occur at

$$\lambda \cot\pi\zeta = -N, \quad N = 0, 1, 2, \ldots. \tag{4.21}$$

The zeros of Eq. (4.14a) occur when

$$\tfrac{1}{2}[\zeta - \zeta_3(\zeta)] = -N, \quad N = 0, 1, 2, \ldots. \tag{4.22}$$

Denote the solutions of Eq. (4.22) by $\zeta_a^{(N)}$. To find $\zeta_a^{(N)}$ note that $\zeta_3(\zeta + 2N) = \zeta_3(\zeta)$, so $\zeta_a^{(N)}$ also satisfies

$$\zeta_a^{(N)} + 2N - \zeta_3(\zeta^{(N)} + 2N) = 0. \tag{4.23}$$

Since $\zeta_a^{(N)} + 2N - \zeta_3(\zeta_a^{(N)} + 2N)$ is a factor of $2 - \lambda B(\zeta_a^{(N)} + 2N)$, $\zeta_a^{(N)}$ satisfies

$$2 - \lambda B(\zeta_a^{(N)} + 2N) = 0. \tag{4.24}$$

The graph of $B(\zeta)$ for real ζ (Fig. 6) shows zeros of $2 - \lambda B(\zeta + 2N)$ near $\zeta = 1$ for $N = 1, 2, \ldots$, one for each value of N. The asymptotic formula for $\zeta_a^{(N)}$ is

$$\zeta_a^{(N)} = 1 - \frac{\lambda}{\pi N} + O\left(\frac{1}{N^3}\right), \quad N = 1, 2, 3, \ldots. \tag{4.25}$$

For λ sufficiently small, the graph of $B(\zeta)$ (Fig. 6) reveals an $N = 0$ zero of $2 - \lambda B(\zeta + 2N)$, $\zeta_a^{(0)}$. As ζ increases, this zero migrates to $\zeta = 1$ and then into the complex plane, on the line $\mathrm{Re}\zeta = 1$. As $\lambda \to 0$, $\zeta_a^{(0)} \to 0$, so its behavior for small λ is qualitatively different from the behavior of the $\zeta_a^{(N)}$'s which go to one as λ goes to zero.

There appear to be no other roots of Eq. (4.24). Such roots were sought by tracing the argument of $2 - \lambda B(\zeta)$ around loops in the rectangle bounded by $\mathrm{Re}\zeta = 0$, $\mathrm{Re}\zeta = 5$, $\mathrm{Im}\zeta = -10$, $\mathrm{Im}\zeta = 10$ for λ between 1 and 2. This search revealed no other zeros and presumably beyond this region the asymptotic analysis is complete.

We construct P_2 as the product

$$P_2(\zeta) = \prod_{N=1}^{\infty} \frac{(\lambda/1 + N)\cot\pi\zeta}{1 - \cot\pi\zeta/\cot\pi\zeta_a^{(N)}}. \tag{4.26}$$

Since $\cot\pi\zeta_a^{(N)} = -N/\lambda + O(1/N)$, for any finite ζ other than a pole or zero of $P_2(\zeta)$, the product converges like $\prod[1 + O(1/N^3)]$, that is, like $\sum 1/N^3$. For small ζ, $P_2(\zeta)$ converges like

$$\sum_{N=1}^{\infty} \left| \frac{1}{N \tan\pi\zeta + \lambda} \times O\left(\frac{1}{N^2}\right) \right|, \tag{4.27}$$

which is a uniformly convergent sum away from its poles. Therefore $P_2(\zeta)$ approaches a constant as $\zeta \to 1$ from any direction except on the real axis below 1.

Thus

$$P_1(\zeta)P_2(\zeta) \frac{1}{\Gamma(\tfrac{1}{2}[\zeta - \zeta_3(\zeta)])} \tag{4.28}$$

is analytic in a punctured disk around $\zeta = 1$, and has a finite limit as $\zeta \to 1$. The possibility of an isolated essential singularity may be eliminated by expanding Eq. (4.28) in a Laurent series about 1, and noting that since the expression has a uniform $\zeta \to 1$ finite limit (except perhaps from one isolated direction), all the coefficients of the singular terms must vanish. Thus Eq. (4.28) defines a function which is analytic at $\zeta = 1$.

Note that $P_2(\zeta)$ fails to cancel the poles of $P_1(\zeta)$ which occur at $\cot\pi\zeta = 0$, or the zero of Eq. (4.14a) that occurs at $\zeta_a^{(0)}$.

A parallel analysis eliminates the essential singularity of Eq. (4.14b). We take $P_3(\zeta)$ and $P_4(\zeta)$ to be

$$P_3(\zeta) = \Gamma(\lambda \cot\pi\zeta + \tfrac{1}{2}) \tag{4.29}$$

and

$$P_4(\zeta) = \prod_{N=0}^{\infty} \frac{1 + [\lambda/(N + \frac{1}{2})]\cos\pi\zeta}{1 - \cot\pi\zeta/\cot\pi\zeta_b^{(N)}}, \tag{4.30}$$

where $\zeta_b^{(N)}$ satisfies

$$\tfrac{1}{2}[\zeta + 1 - \zeta_3(\zeta + 1)] = -N, \quad N = 0, 1, 2, \ldots; \ \zeta \text{ near } 1. \tag{4.31}$$

For large N,

$$\zeta_b^{(N)} \sim 1 - \frac{\lambda}{\pi(N + \frac{1}{2})} + O\left(\frac{1}{(N + \frac{1}{2})^3}\right), \quad N = 0, 1, 2, 3, \ldots. \tag{4.32}$$

The product

$$P_3(\zeta)P_4(\zeta)\frac{1}{\Gamma(\frac{1}{2}[\zeta+1-\zeta_3(\zeta+1)])} \tag{4.33}$$

is analytic at 1. Note that $P_4(\zeta)$ cancels all the poles of $P_3(\zeta)$.

Thus

$$P_1(\zeta)P_2(\zeta)P_3(\zeta)P_4(\zeta)\psi(\zeta) \tag{4.34}$$

satisfies Eq. (4.1) and is analytic at $\zeta=1$ (and $\zeta=2$). However, it has simple poles at $\zeta=\frac{1}{2}$ and $\zeta=\frac{3}{2}$. These can be eliminated by multiplying by $\cot\pi\zeta$, which introduces poles at $\zeta=1$ and $\zeta=2$; however, Eq. (4.34) has zeros at $\zeta=1$ (and $\zeta=2$) so

$$\phi(\zeta)=\cot\pi\zeta P_1(\zeta)P_2(\zeta)P_3(\zeta)P_4(\zeta)\psi(\zeta) \tag{4.35}$$

is analytic for $\mathrm{Re}\zeta\in(0,2)$ and polynomially bounded for $E>0$. It is a valid solution for positive E and any λ. For $E<0$, however, it diverges exponentially as $\mathrm{Im}\zeta\to\infty$ in either the upper or the lower half plane. If for negative E we take the phase of E to be $e^{+i\pi}$, the $\mathrm{Im}\zeta$ dependence is controlled by $e^{i\pi\zeta}$. In this case we may consider a solution

$$\phi(\zeta)=\cot\pi\zeta P_1(\zeta)P_2(\zeta)P_3(\zeta)P_4(\zeta)P_5(\zeta)\psi(\zeta)\,, \tag{4.36}$$

where $P_5(\zeta)$ is chosen to cancel the exponential growth. $P_5(\zeta)$ must then have a periodic pole with period 1. Unless this pole is canceled by a zero of $\psi(\zeta)$, the analyticity strip of $\phi(\zeta)$ will not be more than one unit wide. The only remaining zero of $\psi(\zeta)$ is $\zeta_a^{(0)}$. For small λ, this zero is near $\zeta=0$, and as λ increases it migrates to $\zeta=1$, where it joins $\zeta_b^{(0)}$. At still higher λ, the two become complex-conjugate zeros at locations whose real parts are 1. Since the analyticity strip of $\phi(\zeta)$ must be more than one unit wide and must contain $\zeta=\frac{3}{2}$, there is no acceptable $P_5(\zeta)$ until $\zeta_a^{(0)}>\frac{1}{2}$. Then

$$P_5(\zeta)=\frac{1}{e^{2\pi i\zeta}-e^{2\pi i\zeta_a^{(0)}}} \tag{4.37}$$

allows $E<0$. Thus the critical value of λ at which negative energy pairs first appear is at

$$2-\lambda B(\tfrac{1}{2})=0\,. \tag{4.38}$$

This occurs at $\lambda=\frac{3}{8}$, which corresponds to

$$\alpha=\frac{e^2}{4\pi}=4\lambda=\tfrac{3}{2}\,,\quad \text{QED}$$
$$\alpha=\frac{g^2}{4\pi}=\tfrac{3}{4}4\lambda=\tfrac{9}{8}\,,\quad \text{QCD}\,. \tag{4.39}$$

Therefore the equation has negative-energy solutions for

$$\alpha>\alpha_c=\begin{cases}\frac{3}{2}\,, & \text{QED}\\ \frac{9}{8}\,, & \text{QCD}\,.\end{cases} \tag{4.40}$$

The bound-state wave functions we have constructed are also valid for complex E, which shows that for $\alpha>\alpha_c$ the Hamiltonian not only acquires negative eigenvalues, but in fact ceases to be self-adjoint on the space of normalizable pair states. While we omit all details here, we note that by appropriately modifying the domain of definition of the Hamiltonian, self-adjointness can be restored, and negative eigenvalues persist.

The critical value of α marks a transition to a regime in which the ground state should not be thought of as being dominantly free of quanta, with admixtures of pairs to be accounted for perturbatively. Above this value, the ground state will be filled with particle-antiparticle pairs.

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