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BOUND STATES OF FERMIONS IN EXTERNAL AND
SELF-CONSISTENT FIELDS

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PREFACE

The properties of spin- $\frac{1}{2}$ fields in strong external potentials are investigated, motivated by the question 'What happens to the electron orbitals as the charge of the nucleus is increased without bounds?' Interest in this problem and in the related Klein paradox extends back nearly to the beginnings of relativistic quantum mechanics. However, the correct interpretation of the theory for overcritical potentials, where the parts of the complete set of single-particle solutions associated with particles and antiparticles are no longer distinct, was given only recently. The understanding of the spectrum of the Dirac equation is essential in order to obtain an appropriate physical description in the frame of quantum field theory. The strong binding by more than twice the rest mass of the particles in overcritical external potentials leads to spontaneous particle emission, accompanied by creation of a charged lowest energy state, i.e. a charged vacuum. In the limit of ever-increasing background (nuclear) charge, the charge of the vacuum can be described with the help of a relativistic Thomas-Fermi approximation. As a result, an average constant potential is found within the range of the background charge. This in turn permits the understanding and resolution of Klein's paradox. All these theoretical concepts can be tested by the observation of positron production from the decay of the neutral vacuum in heavy-ion collisions, such as uranium on uranium, in which overcritical potential strength is exceeded. This is an excellent experimental system, since as the distance between the ions changes, the overcritical potential is switched on and off.

A related problem is that of strongly interacting quantum fields. The investigations described here are motivated by the picture of quark bags, in which light quanta provide all the internal structure. It is assumed that a hadron is a bound state of a few (very) heavy particles (free quarks), which can be characterized by the properties of quasi-fermions (bound quarks) bound in an average gluon potential. From the point of view of the quasi-fermions this can be treated as an external potential problem -- but without an external source; the quasi-fermion amplitudes are the source of the average gluon field. These concepts lead to a c-number theory of interacting fields, amended by suitable boundary conditions.

The investigations of the region of validity of this approach to the description of strongly bound states (in three space dimensions) are as yet inconclusive. I believe that if the bound state has a significantly smaller mass than the free Fermi field masses the self-consistent method, described above, will be qualitatively correct.

The properties of the solutions of fermion fields interacting with meson fields are interesting in themselves, apart from the point of view presented above. Several general properties of such solutions are considered with the help of field

theory analogues of virial relations. A description of the algorithm used to generate examples of the self-consistent solutions in three space dimensions is also presented. Since it is difficult to associate the properties of strongly bound states with those of weakly interacting quasi-particles, several options for the candidates for the relevant interaction are considered. The present investigations deal only with Abelian fields; non-Abelian analogues of Abelian interactions may have quite new and surprising properties.

1. SOLUTIONS OF THE DIRAC EQUATION

In this section the recent work that deals with the solutions of the Dirac equation in strong external potentials is reviewed.

1.1 The Dirac equation

The Dirac equation for a particle of mass m moving in an (external) potential V takes the form¹⁾:

$$i \frac{\partial \Psi}{\partial t} = (\vec{\alpha} \cdot \vec{p} + \beta m + V) \Psi. \quad (1.1)$$

We take the matrices α and β in a special representation

$$\vec{\alpha} = \begin{bmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{bmatrix}, \quad \beta = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \quad (1.2)$$

The potential V in Eq. (1.1) transforms under Lorentz transformations as the time component of a four-vector. The solution of the Dirac equation may be written for a spherically symmetric potential $V(|\vec{r}|)$:

$$\Psi(\vec{r}) = \begin{bmatrix} g(r) \chi_{\kappa}^{\mu}(\hat{r}) \\ i f(r) \chi_{-\kappa}^{\mu}(\hat{r}) \end{bmatrix}. \quad (1.3)$$

where $\chi_{\kappa}^{\mu}(\hat{r})$ is an eigenfunction of the total angular momentum operator. It is a combination of spherical harmonics and Pauli spinors. Substituting Eq. (1.3) into the Dirac equation, and using the relations²⁾

$$\vec{\sigma} \cdot \vec{\ell} \chi_{\kappa}^{\mu} = -(\kappa + 1) \chi_{\kappa}^{\mu}, \quad (1.4)$$

$$\vec{\sigma} \cdot \vec{r} \chi_{\kappa}^{\mu} = -r \chi_{-\kappa}^{\mu}, \quad (1.5)$$

we find the coupled radial equations for the functions f and g

$$\left(\frac{d}{dr} - \frac{x-1}{r}\right) f(r) + (\varepsilon - V(r) - m) g(r) = 0, \quad (1.6a)$$

$$\left(\frac{d}{dr} + \frac{x+1}{r}\right) g(r) + (V(r) - m - \varepsilon) f(r) = 0. \quad (1.6b)$$

1.2 Bound states in a Coulomb potential

The solutions of the Dirac equation for a Coulomb potential V of a point nucleus

$$V_p = - \frac{Z\alpha}{r} \quad (1.7)$$

are well known. We recall here only that when $Z\alpha$ approaches the value one, all s states approach the eigenvalue $\varepsilon_{ns} = 0$ and the derivatives $\partial\varepsilon_{ns}/\partial Z$ become infinite. Beyond this point no usual s states can be found; the remainder of the usual spectrum is incomplete. Thus, in the case of a point nucleus, additional requirements are necessary to obtain a complete set of solutions of the Dirac equation³⁾. The physical choice is to consider a nucleus of finite size. Then, if one so desires, the limit of the point nucleus may be taken. However, since the actual nuclei have finite size, this is not a necessary step. The electrostatic Coulomb potential of a finite-size nucleus consisting of a uniformly charged sphere is:

$$V(r) = \begin{cases} -\frac{3}{2} \frac{Z\alpha}{R} \left(1 - \frac{1}{3} \frac{r^2}{R^2}\right), & 0 < r < R \\ -\frac{Z\alpha}{r}, & R < r < \infty. \end{cases} \quad (1.8)$$

Most of the recent calculations^{4,5)} have relied on numerical integration techniques both inside and outside the nucleus of Eq. (1.6), although in the special case (1.8) one can proceed further analytically. Results for the energy eigenvalues are shown in Fig. 1.1. The eigenvalues decrease monotonically as the charge increases. None of the eigenvalues or the wave functions exhibit any unusual behaviour at $Z\alpha = 1$. The points at which the levels join the lower continuum are well isolated. The critical value of $Z = Z^{cr}$ is ~ 170 , where the $1s$ level joins the lower continuum. The $2p_{1/2}$ level joins the lower continuum at about $Z = 183$. The exact location of Z^{cr} is an important question for the experimental verification of the theory. One has to consider in this context the effects of other atomic electrons (screening) as well as the effects of vacuum polarization⁵⁾.

1.3 Scalar potentials

The above bound state eigenvalues are based on electrostatic potentials. We consider next an example of a particle of mass m bound by a potential ϕ that transforms as a scalar under Lorentz transformations:

$$i \frac{\partial \psi}{\partial t} = (\vec{\alpha} \cdot \vec{p} + \beta (m + \phi)) \psi \quad (1.9)$$

Here it is possible to consider the potential as given by $\phi = -g/r$. Then one can find an analytic expression⁶⁾ for the energy eigenvalues

$$\epsilon_{\pm} = \pm m \left[1 - g^2 / (N + \sqrt{(k^2 + g^2)})^2 \right]^{1/2}, \quad (1.10)$$

where $N = 0, 1, 2, \dots$. The dependence of several of the lower eigenvalues on the strength of the potential g is shown in Fig. 1.2. In this figure and Eq. (1.10), the symmetry between positive and negative energies is apparent. From Eq. (1.10) it is clear that $\epsilon_{\pm} \rightarrow 0$ for all states as $g \rightarrow \infty$. After second quantization, the negative energy states are associated with antiparticles. Thus, unlike the case of strong electrostatic potentials, the parts of the spectrum associated with particles and antiparticles are always separated for finite g . This is the crucial difference between electrostatic potentials and scalar potentials.

1.4 Gravitational potential

Let us now consider the gravitational field as an external field. It is very much like any other external field. Any time-independent, spherically-symmetric mass distribution has a metric tensor g_{ik} of the particular form⁷⁾

$$g_{ik} = \begin{pmatrix} e^{\nu} & & & \\ & -e^{\lambda} & & \\ & & -r & \\ & & & -r^2 \sin^2 \theta \end{pmatrix} \quad (1.11)$$

where the two functions e^{ν} and e^{λ} are determined from solutions of Einstein's equations of motion. For the particular case of a Schwarzschild metric in empty space we have

$$e^{\nu} = e^{-\lambda} = 1 - \frac{2\tilde{M}}{r} \quad (1.12)$$

Here $\tilde{M} = (\kappa M/c^2)$ where κ is the gravitational constant ($\kappa = 6.67 \times 10^{-8}$ dyne cm²/g²) and M is the gravitating mass.

Given g_{ik} (to be understood as the external gravitational field), we can find the minimal coupling of the gravitational field to any other field by writing the Lagrangian in a general covariant form. We now consider the Dirac equation in the generally covariant form and replace the covariant derivative with the suitable connections Γ_{κ} ⁸⁾

$$[\gamma^{\kappa} (i (\partial_{\kappa} + \Gamma_{\kappa}) - e A_{\kappa}) - m] \psi = 0. \quad (1.13)$$

The connections Γ_{κ} for spinor differentiation are known in terms of the metric g_{ik} and the Dirac matrices γ_i that are determined with the aid of the g_{ik} :

$$\{\gamma_i, \gamma_k\} = 2g_{ik}. \quad (1.14)$$

The equations of motion become ⁸⁾

$$\begin{aligned} (e^{-\frac{\lambda}{2}} (\frac{d}{dr} + \frac{1}{r}) - \frac{\kappa}{r}) f(r) + (e^{-\frac{\nu}{2}} \epsilon - m) g(r) &= 0, \\ (e^{-\frac{\lambda}{2}} (\frac{d}{dr} + \frac{1}{r}) + \frac{\kappa}{r}) g(r) + (-e^{-\frac{\nu}{2}} \epsilon - m) f(r) &= 0, \end{aligned} \quad (1.15)$$

which should be compared with Eq. (1.6). Inclusion of the vector potential is straightforward, involving the replacement of ϵ by $\epsilon - V$.

Equation (1.15) is the Dirac equation in interaction with the external gravitational field. There are no discrete solutions of this equation of the Schwarzschild metric Eq. (1.12). It can be shown that the external field is of supercritical strength. Moreover, the singular behaviour is different from that encountered for point nuclei. In the case of gravitational interaction all bound states meet at $\epsilon = 0$ as the functions e^{ν} and e^{λ} approach the Schwarzschild values, in a suitable parametrization. The parametrization that has been employed can be associated with the metric of an incompressible fluid model for the constant mass density star, suitably augmented to avoid infinite pressure.

A typical spectrum of the Klein-Gordon equation in an external gravitational potential, which behaves as Eq. (1.15), is shown in Fig. 1.3 as a function of the mass radius R (which has been chosen unrealistically small only for numerical

convenience, $\tilde{M} = 1/\mu$, μ is the meson mass). We notice the collapse of the discrete solutions as the Schwarzschild metric solution is approached.

1.5 Continuum states of the square-well potential

Let us turn now to the discussion of the peculiarities of continuum solutions of the Dirac equation for $a(n)$ (electrostatic) square-well potential

$$V = -V_0 \Theta(R-r) . \quad (1.16)$$

Our main interest will be confined to the lower continuum. The central issue of this discussion is the appearance of a resonance in the lower continuum as the potential strength is increased beyond the critical value. This resonance is the analytic continuation of the bound state into the lower continuum. Requiring that the solutions inside and outside the (attractive) square-well potential are continuous at the surface $r = R$, the phase shift δ can be computed from the relation⁹⁾

$$\cot(pR + \delta) = \frac{(\epsilon + m)p'}{(\epsilon + m + V_0)p} \cot p'R + \frac{V_0}{pR(\epsilon + m + V_0)} . \quad (1.17)$$

Here $p' = \sqrt{(\epsilon + V_0)^2 - m^2}$, $p = \sqrt{\epsilon^2 - m^2}$. Phase shifts determined from this equation are shown for several values of the potential strength in Fig. 1.4. For $R = m^{-1}$ and $V_0 = 4.29 m$, a value slightly less than the critical value, the phase shift is negative and exhibits no sharp dependence on the energy. For the other value of V_0 , which are greater than V_0^{cr} , the phase shifts begin at zero and increase sharply through the point $\delta = \pi/2$, which is characteristic of a resonance. Thus, below the critical potential strength, the phase shift behaves like that for a repulsive potential and *above the critical potential strength the phase shift behaves like that for a strong, attractive potential*. In Fig. 1.5 the $\sin^2(\delta - \delta_0)$ is shown for several overcritical potential strengths. The quantity δ_0 is the phase shift computed at the same value of ϵ for $V_0 = 4.29 m$, an undercritical strength. Loosely speaking, the subtraction of the background phase serves to emphasize the new features associated with the appearance of the resonance in the lower continuum. The resonant peak, which appears only in the overcritical cases, moves further into the lower continuum and becomes broader as the potential strength is increased.

1.6 Perturbative treatment of the resonance in the continuum

Let us consider an overcritical potential, where the resonance is not so deeply immersed in the lower continuum as to have become too diffuse. We shall

show that one can obtain the properties of the resonance by expanding the eigenfunctions of the overcritical problem in terms of a reduced set of the basis functions of the critical potential¹⁰⁾. This reduced set includes only the bound state at $\varepsilon = -m$ and the lower continuum. We write the overcritical potential as the sum of the critical potential and a piece V' as follows:

$$V = V^{cr} + V', \quad (1.18)$$

and introduce the complete set of eigenfunctions associated with V^{cr} ;

$$\varepsilon \psi_{\varepsilon}^{cr} = (\vec{\alpha} \cdot \vec{p} + \beta m + V^{cr}) \psi_{\varepsilon}^{cr}, \quad (1.19)$$

which includes the bound state with the eigenvalue at $\varepsilon_0 = -m$.

We expand the overcritical functions with $\varepsilon < -m$ in the reduced basis involving the critical bound state at ε_0 and the lower continuum:

$$\psi_{\varepsilon} = a(\varepsilon) \psi_0^{cr} + \int_{-\infty}^{-m} d\varepsilon' h_{\varepsilon'}(\varepsilon) \psi_{\varepsilon'}^{cr}, \quad \varepsilon < -m. \quad (1.20)$$

To determine the expansion coefficients $a(\varepsilon)$, $h_{\varepsilon'}(\varepsilon)$, we recall that ψ_{ε} satisfies the Dirac equation with the potential V :

$$(\vec{\alpha} \cdot \vec{p} + \beta m + V^{cr} + V') \psi_{\varepsilon} = \varepsilon \psi_{\varepsilon}, \quad \varepsilon < -m. \quad (1.21)$$

Substituting the expansion of Eq. (1.20) into Eq. (1.21) and taking the scalar product of the result with ψ_0^{cr} and then with $\psi_{\varepsilon'}^{cr}$ leads to the equations

$$(\varepsilon - \bar{\varepsilon}) a(\varepsilon) = \int_{-\infty}^{-m} d\varepsilon' V_{\varepsilon'}^* h_{\varepsilon'}(\varepsilon), \quad (1.22)$$

$$(\varepsilon - \bar{\varepsilon}) h_{\varepsilon'}(\varepsilon) = V_{\varepsilon'} a(\varepsilon) + \int_{-\infty}^{-m} d\varepsilon'' U_{\varepsilon'\varepsilon''} h_{\varepsilon''}(\varepsilon), \quad (1.23)$$

where V_{ε} records the influence of the bound state on the continuum,

$$V_{\varepsilon} = \int d^3x \psi_{\varepsilon}^{cr\dagger}(\vec{x}) V'(\vec{x}) \psi_0^{cr}(\vec{x}), \quad (1.24)$$

and $U_{\varepsilon\varepsilon'}$ includes the effects of mixing among the continuum states,

$$U_{\epsilon\epsilon'} = \int d^3x \psi_{\epsilon}^{\dagger cr}(\vec{x}) V'(\vec{x}) \psi_{\epsilon'}^{cr}(\vec{x}). \quad (1.25)$$

The quantity $\bar{\epsilon}$ includes the diagonal shift in the energy of the former bound state, namely

$$\bar{\epsilon} = \epsilon_0 + \int d^3x \psi_0^{\dagger cr}(\vec{x}) V'(\vec{x}) \psi_0^{cr}(\vec{x}). \quad (1.26)$$

In solving for the coefficients $a(\epsilon)$ and $h_{\epsilon'}(\epsilon)$ we also require the relation

$$\delta(\epsilon - \epsilon') = a^*(\epsilon) a(\epsilon') + \int_{-\infty}^{-m} d\epsilon'' h_{\epsilon''}^*(\epsilon) h_{\epsilon''}(\epsilon'), \quad (1.27)$$

which arises from writing the normalization condition for ψ_{ϵ} in terms of the reduced basis.

The solution of Eqs. (1.22), (1.23), and (1.27) is straightforward. Ignoring the rearrangement of the continuum, Eq. (1.25), the results are

$$a(\epsilon) = V_{\epsilon}^* / (\epsilon - \bar{\epsilon} - F(\epsilon)), \quad (1.28)$$

$$h_{\epsilon'}(\epsilon) = \frac{V_{\epsilon'} a(\epsilon)}{\epsilon - \epsilon' + i\eta} + \delta(\epsilon - \epsilon'), \quad (1.29)$$

where η is a small positive number and $F(\epsilon)$ is given by

$$F(\epsilon) = \int_{-\infty}^{-m} d\epsilon' \frac{|V_{\epsilon'}|^2}{\epsilon - \epsilon' + i\eta}. \quad (1.30)$$

At the complex value ϵ_1 determined from the non-linear equation

$$\begin{aligned} \epsilon_1 &\equiv \epsilon_r + i\epsilon_i = \bar{\epsilon} + F(\epsilon_1) \\ &= \int_{-\infty}^{-m} d\epsilon' \frac{|V_{\epsilon'}|^2 (\epsilon_r - \epsilon')}{(\epsilon_r - \epsilon')^2 + \epsilon_i^2} - i \int_{-\infty}^{-m} d\epsilon' \frac{|V_{\epsilon'}|^2 \epsilon_i}{(\epsilon_r - \epsilon')^2 + \epsilon_i^2} \end{aligned} \quad (1.31)$$

the amplitude $a(\epsilon)$ has a pole. In the narrow resonance approximation we find

$$\epsilon_i \approx -\pi |V_{\epsilon_r}|^2 \quad (1.32)$$

and

$$\epsilon_r \approx \bar{\epsilon} + P \int_{-\infty}^{-m} d\epsilon' \frac{|V_{\epsilon'}|^2}{\epsilon_r - \epsilon'} \quad (1.33)$$

Here the quantity P denotes the Cauchy principal value.

1.7 Continuum solutions, Coulomb potential

As in the case of bound states, we can obtain the solutions numerically by integrating the Dirac equation at a given energy ϵ . Then from the well-known asymptotic behaviour of the continuum solutions a phase shift can be deduced. However, in the case of the long-range Coulomb potential the phase shift also includes spurious contributions that must be carefully eliminated. Further details will not be given here. All these points have been carefully considered elsewhere¹¹⁾, where the numerical calculations discussed here were also presented. The appearance of the resonance in the lower continuum for supercritical potentials can be well anticipated from the square-well solutions.

For the system $Z = 184$ ($_{92}\text{U} + _{92}\text{U}$) the resonance in the lower continuum is shown in Fig. 1.6. It is centred at $\epsilon_r = -926$ keV with $\Gamma = 4.8$ keV (the full width at half maximum).

The results for the positions of the $1s_{\frac{1}{2}}$ and $1p_{\frac{1}{2}}$ resonances as functions of the nuclear charge Z are shown in Fig. 1.7. The slopes of the curves near the upper continuum are the same as the slopes of the corresponding curves in Fig. 1.1 near the critical value of the potential. The position and width of the resonance can be parametrized as follows:

$$\epsilon_r \approx -(Z - Z^{\text{cr}}) \delta - (Z - Z^{\text{cr}})^2 \tau \quad (1.34)$$

$$\Gamma = 2|\epsilon_i| \approx (Z - Z^{\text{cr}})^2 \gamma, \quad (1.35)$$

provided that $(Z - Z^{\text{cr}})/Z < 1$. The second of these expressions is applicable only if $Z > Z^{\text{cr}} + 3$. For values of Z nearer Z^{cr} , it is necessary to include a damping factor which takes into consideration that the probability of finding low-energy positrons near the nucleus is small when $Z \approx Z^{\text{cr}}$. For the $1s_{\frac{1}{2}}$ state the following values for δ , τ , and γ have been found: $\delta \approx 29$ keV, $\tau \approx 0.33$ keV, $\gamma = 0.04$ keV. The motivation for writing the results in the form of Eqs. (1.34) and (1.35) was to make contact with the perturbative development of Section 1.6. The form of the expression (1.33) suggests strongly the functional form for ϵ_v , since V' is proportional to $Z - Z'$ and $|V_{\epsilon'}| \sim (Z - Z')^2$. Similarly, Eq. (1.32) suggests Eq. (1.35), provided that the matrix-element continuum bound state is Z -independent. This is the case when the above condition $Z > Z^{\text{cr}} + 3$ is fulfilled.

1.8 The two-centre Dirac equation

In order to find out about the motion of electrons in the vicinity of the (moving) heavy ions separated by the distance R , we have to consider the combined Coulomb potential of both nuclei. The problems involved in solving the associated two-centre Dirac equation^{12,13)} are probably an order of magnitude larger than those discussed above. This is because no operator has been found for the relativistic two-centre problem that plays the role of the square of the angular momentum J^2 , and which would then allow the separation of the eigenstate problem into radial-like and angular-like one-dimensional differential (or matrix) equations.

The two-centre Coulomb potential V in cylindrical coordinates ρ and z is given by

$$V(\rho, z) = V_1 + V_2 = -\frac{Z_1 \alpha}{[(z+R/2)^2 + \rho^2]^{1/2}} - \frac{Z_2 \alpha}{[(z-R/2)^2 + \rho^2]^{1/2}} \quad (1.36)$$

Suitable modifications for finite size and electron screening can be added when desired. The nuclei are located at $z = \pm R/2$, $y = 0$, $x = 0$.

A computer code has been developed¹³⁾ that for all intents and purposes is capable of solving the Dirac equation (1.1) exactly by a numerical integration. To avoid the great numerical effort associated with partial differential equations in two dimensions [the φ -dependence separates in view of the axial symmetry of Eq. (1.36)], an approach which discretizes one of the dimensions has been chosen. A solution ψ of Eq. (1.1) has been expanded in the spinor harmonics χ_κ [cf. Eqs. (1.4), (1.5)]

$$\psi(\vec{r}) = \sum_{\kappa, \bar{m}} \begin{pmatrix} f_\kappa^{\bar{m}}(|\vec{r}|) \chi_\kappa^{\bar{m}}(\hat{r}) \\ i g_\kappa^{\bar{m}}(|\vec{r}|) \chi_{-\kappa}^{\bar{m}}(\hat{r}) \end{pmatrix} \quad (1.37)$$

Similarly the potential V is considered as given by the multipole expansion. Then the Dirac equation becomes an infinite set of coupled differential equations for the radial functions $f_n^{\bar{m}}$ and $g_n^{\bar{m}}$. The coupling between different functions is a consequence of the multipole character of the potential V . A typical eigenvalue spectrum is shown in Fig. 1.8 for several collision systems as a function of the heavy ion separation R .

There is one particular aspect of the solutions of the two-centre problem which has the greatest impact on all calculations involving spontaneous positron production. The characteristic parameter is the critical distance R^{cr} between the heavy ions at which the binding of the electron exceeds twice its mass. The simplest method to estimate R^{cr} is to solve the Dirac equation with the monopole approximation for the two-centre potential V , that is with

$$V_0 = \begin{cases} -2Z\alpha/r & r > R/2 \\ -4Z\alpha/R & r < R/2, \end{cases} \quad (1.38)$$

which corresponds to a model in which the nuclear charge is distributed on a shell with the diameter corresponding to the distance between the nuclei. The critical distance in this approximation is a lower bound on the critical distance calculated with the full potential. The results of such monopole calculations are shown in Fig. 1.9 -- together with the exact solution obtained by the numerical integration of the Dirac equation.

In this section the surprising character of the continuum solutions of the Dirac equation has been described. We have found that a repulsive supercritical potential leads to resonant states (repulsive for 'negative frequency' positron states); this indicates that the relativistic equation of motion contains an attractive force irrespective of the sign of the potential. A related development has been reported for a Dirac particle with an anomalous magnetic moment coupled to the electromagnetic field¹⁴⁾.

2. QUANTUM FIELD THEORY OF SPIN- $\frac{1}{2}$ PARTICLES IN STRONG EXTERNAL FIELDS

The correct treatment of quantized Fermi fields in supercritical external potentials is presented in this section. In particular, it is demonstrated here that:

- a) In overcritical *external* fields, it is impossible to have a stable, neutral vacuum¹⁵⁾.
- b) The neutral vacuum decays by emitting positrons into a new ground state -- a charged vacuum¹⁵⁾.
- c) The charged vacuum is stable¹⁵⁾.
- d) In the *self-consistent* supercritical potential the neutral vacuum is stable¹⁶⁾.

We first consider the main physical distinction between the case of *undercritical* and *overcritical external* potentials. The minimal energy required to make a fermion pair is the energy difference between the lowest bound state and the lower continuum. As the strength of the external potential increases, it decreases. At the critical field strength, where the lowest bound level joins the lower continuum, this energy is zero. There the neutral vacuum, one-pair and two-pair states are all degenerate in energy. As the external field strength is *increased beyond the critical value, then the state containing two positrons has the lowest energy, and the neutral vacuum will spontaneously decay by the emission of two positrons.*

This change of the qualitative nature of the ground state as the potential increases through its critical strength is analogous to a phase transition, as is shown schematically in Fig. 2.1. There, the total energy, including that of the positron of zero kinetic energy, is plotted qualitatively as a function of the charge surrounding the nucleus. While in Fig. 2.1a the minimum is found for neutral vacuum, in the case of the supercritical potential strength it shifts in Fig. 2.1b to a finite value, chosen here to correspond to the supercritical $1s_{\frac{1}{2}}$ shell only.

In the remainder of this section we will make this picture more quantitative as well as prove the points (a) to (d) stated above.

2.1 The Green's function and its analytic structure

The quantized Fermi field describes both particles and antiparticles simultaneously. However, the distinction between the two is not as simple as it might appear.

For the free particles and the weak field case, the distinction is straightforward. All positive energy states may be identified as particle states, and all negative energy continuum states may be identified as antiparticle states. When

the potential becomes strong enough, so that some of the bound state eigenvalues become negative (as in Figs. 1.1 and 1.6), then one has to make a decision as to which category contains these states. The theory can be treated without further modifications by identifying localized negative energy eigenstates with either particles or antiparticles as long as the field strength is subcritical.

In order to treat the critical potential strength and beyond we must first recall the properties of the Feynman propagator.

Let us consider the case of a particle moving in a time-independent potential V_μ . A Green's function satisfies the equations

$$(i\gamma \frac{\partial}{\partial x} - \gamma \cdot V - m) G(x, x') = \delta^4(x - x'). \quad (2.1)$$

$$(-i \frac{\partial}{\partial x'} G(x, x')\gamma - G(x, x')(\gamma \cdot V + m)) = \delta^4(x - x'). \quad (2.2)$$

Because of the time independence of the potential, we may introduce a partial Fourier transformation

$$G_C(x, x') = \int_C \frac{d\omega}{2\pi} e^{-i\omega(t-t')} G(\vec{x}, \vec{x}'; \omega). \quad (2.3)$$

The choice of the contour C is related to boundary conditions satisfied by $G(x, x')$ as $t \rightarrow \pm\infty$. It plays the same role as the choice of the Fermi energy and makes the distinction between particles and antiparticles. The conventional choice of C , which leads to the Feynman boundary conditions, is shown in Fig. 2.2. There, the two branch cuts beginning at $\omega = \pm m$ as well as the poles associated with the bound states, are shown between particles and antiparticles. For undercritical fields, the choice of the Fermi energy is to some extent arbitrary. In weak fields, that is if all of the eigenstates are near the continuum, then one is free to choose the Fermi energy anywhere in the gap between the lowest bound state and the other continuum. The conventional choice is $\epsilon_F = 0$. Increasing the strength of the potential so that the lowest eigenvalue has the value zero poses no problem. One can simply lower the Fermi surface until $\epsilon_F = -m$.

The integrand of Eq. (2.3) may be represented as a sum over the entire spectrum of eigensolutions of the Dirac equation, namely,

$$G(\vec{x}, \vec{x}'; \omega) = \sum_{\epsilon} \frac{\psi_{\epsilon}(\vec{x}) \bar{\psi}_{\epsilon}(\vec{x}')}{\omega - \epsilon} \quad (2.4)$$

Substituting this expression into Eq. (2.3) and using the contour of Fig. 2.1 leads to the representation

$$S_F(x, x') = -i\theta(t-t') \sum_{\epsilon > \epsilon_F} \psi_\epsilon(\vec{x}) \bar{\psi}_\epsilon(\vec{x}') e^{-i\epsilon(t-t')} + i\theta(t-t') \sum_{\epsilon < \epsilon_F} \psi_\epsilon(\vec{x}) \bar{\psi}_\epsilon(\vec{x}') e^{-i\epsilon(t-t')} \quad (2.5)$$

for the Feynman propagator S_F .

In the discussion of the solutions of the Dirac equation we have learned that a bound state may become a resonance in supercritical potentials. The behaviour of $G(x, x'; \omega)$ in the complex ω plane reflects this property. As the potential strength is increased from an undercritical value to an overcritical value, the pole associated with the lowest bound state in Fig. 2.2 moves off the real axis and into the upper half of the complex plane as shown in Fig. 2.3. It is important to appreciate that this singularity is on the second sheet¹⁷⁾. The contour C can now either be deformed into the contour C' , so as to continue to embrace the pole, or the contour D is chosen, where the Fermi energy remains at $-m$. The path C' corresponds to the choice of the neutral vacuum as the reference state, while contour D is associated with a charged vacuum state (to be defined further below).

Substituting the first term of Eq. (1.20) into Eq. (2.4) for G , we find that

$$G_D(\vec{x}, \vec{x}'; \omega) \sim \int_{-\infty}^{\infty} d\epsilon \frac{|a(\epsilon)|^2}{\omega - \epsilon - i\eta} \psi_0^{cr}(\vec{x}) \bar{\psi}_0^{cr}(\vec{x}') + \dots, \quad (2.6)$$

where only the interesting part of G has been kept and η is negative when $\omega < -m$ and positive when $\omega > m$, as required by the choice of contour D . The modifications of Eq. (2.6), due to the continuum part of Eq. (1.20), are small. From Eq. (1.28) it is apparent that $a(\epsilon)$ carries the singularity associated with the resonance, that is the pole shown in the upper-half plane of Fig. 2.3. This pole, however, occurs on the second sheet and the only contribution to the integral of Eq. (2.6) arises from the pole at $\epsilon = \omega - i\eta$ (provided that $\omega < -m$). Thus the result of the integration is

$$G_D(\vec{x}, \vec{x}'; \omega) \sim i \frac{\Gamma \theta(-m - \omega)}{(\omega - \epsilon_r)^2 + \Gamma^2/4} \psi_0^{cr}(\vec{x}) \bar{\psi}_0^{cr}(\vec{x}') + \dots, \quad (2.7)$$

where we have treated the resonance approximately as discussed in Section 1.6. A very different result is obtained if we choose the contour C' . Then the pole at $\epsilon = \epsilon_{\text{res}} + i\Gamma/2$ makes a contribution of the form

$$G_{C'}(\vec{x}, \vec{x}'; \omega) \sim \frac{\psi_0^{cr}(\vec{x}) \bar{\psi}_0^{cr}(\vec{x}')}{\omega - \epsilon_r - i\Gamma/2} + \dots, \quad (2.8)$$

which is characteristic of a complex eigenvalue, a reflection of the lack of stability of the state of reference defined by the choice C' in the case of external fields. To summarize, every time a bound state descends into the negative energy continuum, we must redefine the Green's function so as to include only the remaining poles on the real axis. This is done by maintaining the fixed shape D of the contour. As described further below, this implies a change in the charge of the vacuum each time a pole crosses the fixed integration path D .

2.2 The reduced Hamiltonian and the instability of the neutral vacua in overcritical external fields

With the known analytical solutions for eigenstates of the Dirac equation even for the overcritical potentials, we can write the overcritical Hamiltonian in the reduced basis. We begin with the expansion of $\hat{\psi}$ in the complete set of basis functions of Eq. (1.19), which is separated into three categories for convenience,

$$\hat{\psi}(\vec{x}) = \sum_{p \neq 1s} \hat{b}_p^{cr} \psi_p^{cr}(\vec{x}) + \hat{b}_0^{cr} \psi_0^{cr}(\vec{x}) + \int_{-\infty}^{-m} d\epsilon \hat{d}_\epsilon^{cr\dagger} \psi_\epsilon^{cr}(\vec{x}). \quad (2.9)$$

Substituting this relation into the normal-ordered Hamiltonian yields

$$\begin{aligned} \hat{H} = & \sum_{p \neq 1s} \epsilon_p \hat{b}_p^{cr\dagger} \hat{b}_p^{cr} + \epsilon_0 \hat{b}_0^{cr\dagger} \hat{b}_0^{cr} - \int_{-\infty}^{-m} d\epsilon \epsilon \hat{d}_\epsilon^{cr\dagger} \hat{d}_\epsilon^{cr} \\ & + \int d^3x : \hat{\psi}^\dagger(\vec{x}) V'(\vec{x}) \hat{\psi}(\vec{x}) : \end{aligned} \quad (2.10)$$

where the last term arises because the basis functions are not eigenfunctions of the Dirac operator. If the resonance is not too deeply embedded in the lower continuum, then the essential features are contained in a reduced Hamiltonian,

$$\hat{H}_r = \hat{H}_0 + \hat{H}_I, \quad (2.11)$$

where

$$\hat{H}_0 = \bar{\epsilon} \hat{b}_0^{cr\dagger} \hat{b}_0^{cr} - \int_{-\infty}^{-m} d\epsilon \epsilon \hat{d}_\epsilon^{cr\dagger} \hat{d}_\epsilon^{cr}, \quad (2.12)$$

is the diagonal piece and

$$\hat{H}_I = \int_{-\infty}^{-m} d\epsilon (\hat{b}_0^{cr\dagger} \hat{d}_\epsilon^{cr\dagger} V_\epsilon^* + \text{h.c.}), \quad (2.13)$$

is the non-diagonal part. The first term of Eq. (2.12) includes the diagonal piece of the last term of Eq. (2.10), and the effects of the matrix elements $U_{\epsilon\epsilon'}$ have again been neglected. It is clear that H_I represents the effects of creating or destroying an electron and a positron.

The distinction between the neutral state in the presence of overcritical fields and the ordinary neutral state in undercritical potentials is subtle. In the undercritical region, one may obtain the neutral vacuum state from the state containing a single 1s electron with the following projection:

$$|\tilde{0}\rangle = \int d^3x \psi_{1s}^\dagger(\vec{x}) \hat{\psi}(\vec{x}) |1s\rangle, \quad (2.14)$$

where $\psi_{1s}(\vec{x})$ is the wave function for the 1s state. Both the 1s state and the vacuum are stable. In the overcritical case, the neutral state may be obtained from the state containing the electron charge as follows:

$$|0\rangle = \int_{-\infty}^{-m} d\epsilon a(\epsilon) \int d^3x \psi_\epsilon^\dagger(\vec{x}) \hat{\psi}(\vec{x}) |\tilde{q}\rangle, \quad (2.15)$$

where $\psi_\epsilon(\vec{x})$ is a(n) (overcritical) lower continuum eigenfunction and $a(\epsilon)$ is the amplitude (1.28) associated with the resonance. Only the charged vacuum state $|\tilde{q}\rangle$ in Eq. (2.15) is stable (disregarding the spin degeneracy). The state $|0\rangle$ is not an eigenstate of the Hamiltonian, since a superposition of solutions of the Dirac equation is involved in its description.

Let us consider a gedankenexperiment in which the neutral state (2.15) is prepared at time $t = 0$. Subsequently two positrons will be produced spontaneously and the charge of the region surrounding the nucleus will equal that of two

electrons in order to conserve charge. (One might be tempted to view this process as pair production, but we feel that characterizing it as *the spontaneous decay of the neutral vacuum* is more appropriate in view of the above discussion.) To describe this process, we make the following ansatz for its time dependence:

$$|t\rangle = y(t)|0\rangle + \int_{-\infty}^{-m} d\epsilon w_{\epsilon}(t) \hat{d}_{\epsilon}^{cr\dagger} \hat{b}_0^{cr} |0\rangle \quad (2.16)$$

where $|y(t)|^2$ represents the probability of finding the neutral vacuum and $|w_{\epsilon}(t)|^2$ gives the probability of finding a positron with energy ϵ . The inclusion of spin degeneracy is straightforward and will not be discussed here. The functions y and w_{ϵ} satisfy the initial conditions that we prescribe:

$$y(0) = 1, \quad w_{\epsilon}(0) = 0. \quad (2.17)$$

The time evolution of $|t\rangle$ is governed by the Schrödinger equation

$$(\hat{H}_0 + \hat{H}_I) |t\rangle = i \frac{\partial}{\partial t} |t\rangle. \quad (2.18)$$

Substituting the relations of Eqs. (2.12), (2.13), (2.16) into this expression and taking the scalar products with $\langle 0|$ and $\langle 0|b_0^{cr} d_{\epsilon}^{cr}$ yields the coupled differential equations,

$$i \frac{\partial}{\partial t} y(t) = - \int_{-\infty}^{-m} d\epsilon V_{\epsilon} w_{\epsilon}(t), \quad (2.19)$$

$$i \frac{\partial}{\partial t} w(t) = (\bar{\epsilon} - \epsilon) w_{\epsilon}(t) - V_{\epsilon}^* y(t). \quad (2.20)$$

The Fourier representations of y and w_{ϵ} take the form

$$y(t) = e^{-i\bar{\epsilon}t} \int_{-\infty}^{\infty} d\epsilon' e^{i\epsilon't} a(\epsilon') a^*(\epsilon'), \quad (2.21)$$

$$w(t) = e^{-i\bar{\epsilon}t} \int_{-\infty}^{\infty} d\epsilon' e^{i\epsilon't} a(\epsilon') h^*(\epsilon'), \quad (2.22)$$

in view of the conditions (2.17) and the relation of Eqs. (2.19) and (2.20) to Eqs. (1.22) and (1.23). The most straightforward method of evaluating these integrals is to use the methods of complex analysis. The solutions are:

$$y(t) = e^{-i\bar{\epsilon}t} [\theta(t) e^{i\epsilon_1^+ t} + \theta(-t) e^{i\bar{\epsilon}_1 t}], \quad (2.23)$$

$$w(t) = \frac{V_{\epsilon}^*}{\epsilon_1^+ - \epsilon} \theta(t) [e^{i(\epsilon_1^+ - \epsilon)t} - e^{i(\epsilon - \bar{\epsilon})t}] + \frac{V_{\epsilon}^*}{\bar{\epsilon}_1 - \epsilon} \theta(-t) [e^{i(\bar{\epsilon}_1 - \epsilon)t} - e^{i(\epsilon - \bar{\epsilon})t}], \quad \epsilon_1^{\pm} = \epsilon_r \pm i\epsilon_i \quad (2.24)$$

where we have written the equations in a form which shows that we have obtained solutions for which the origin of time is a centre of symmetry. It is apparent that the amplitude y decays according to the law

$$y(t) = e^{i(\epsilon_r - \bar{\epsilon})t} e^{-\Gamma|t|/2}, \quad (2.25)$$

and thus the probability of finding the neutral vacuum decays exponentially with time as $|y(t)|^2 = \exp(-\Gamma|t|)$. The spectrum of positrons is given by

$$|w_{\epsilon}(\pm\infty)|^2 = \frac{|V_{\epsilon}|^2}{(\epsilon - \epsilon_r)^2 + \Gamma^2/4} = |a(\epsilon)|^2, \quad (2.26)$$

which has usual Breit-Wigner form since the variation of $|V_{\epsilon}|^2$ near the resonance is unimportant. This establishes our claims that the neutral vacuum is unstable and spontaneously decays emitting positrons.

Let us now consider the charged state $|q\rangle = \hat{b}_0^{cr\dagger} |0\rangle$. Its time dependence is also determined by the Hamiltonian of Eqs. (2.12) and (2.13). However, in this case, the non-diagonal part of the Hamiltonian will not have any effect, all the relevant matrix elements being zero. Thus the time dependence of the charged state is

$$|q(t)\rangle = e^{-i\bar{\epsilon}t} |q\rangle. \quad (2.27)$$

Therefore no dramatic consequences ensue upon lowering a fully occupied state into the lower continuum. The total energy of the charged state is $\langle q | H_r | q \rangle = \bar{\epsilon}$, which is lower than the energy of the neutral vacuum $\langle 0 | H_r | 0 \rangle = 0$, and in fact exceeds it by more than the rest mass of the positron. This verifies our claim that the charged state is stable.

With this we have concluded our proof that, in order to have a stable reference state, we must choose the charged state and henceforth refer to it as *the charged vacuum*. This means that the Fermi surface must always be chosen just above the lower continuum.

2.3 Self-consistent potentials

From the preceding part of this section, we have learned about the unexpected properties of the supercritically bound states in external potentials. We now will consider the potential as not being prescribed externally. As the source of the *self-consistent* potential we choose the Dirac wave functions that are computed with such a potential. What we have in mind would conventionally be called Hartree approximation. It is important to realize that classical solutions of interacting field theories may have a meaning as approximation to quantum field theories even in régimes where the Hartree approximation should fail, for example in the limit of strong coupling and few bound particles (see also Section 4).

When fermions move in a *self-consistent* (shell) potential, then the total energy of the bound state is given by the sum of the Dirac eigenenergies and of the energy associated with the shell potential, sometimes also called "correlation energy". The condition for the transition to a state equivalent to the charged vacuum is now

$$\epsilon_0 + E_{\text{meson}} < 0 \quad (2.28)$$

and not

$$\epsilon_0 < 0 \quad (2.29)$$

as was the case when external fields were considered. It must be expected that the critical potential strength can be exceeded by the *self-consistent* potential and a resonance be embedded in the negative energy continuum of the Dirac equation. In view of Eq. (2.28) we recognize that even if the self-consistent field is supercritical, the neutral vacuum may remain stable. This last remark can only be appreciated after a thorough discussion of the case of an *external* potential.

For the sake of argument, let us assume now that we have found a theory such that Eq. (2.28) is satisfied. We then would find that a charged ground state has lower energy than the neutral state -- thus the latter state is the 'false vacuum'¹⁸⁾ which under certain circumstances could undergo a transition into the 'true vacuum'. The properties of such a macroscopic transition have been studied by Coleman in a model theory¹⁸⁾. Fortunately, we will find in Section 4.6 that it is hard to satisfy condition (2.28). It will be shown there in a model theory that the opposite of Eq. (2.28) is the case; that is, we find $\epsilon_0 + E_{\text{meson}} > 0$, although $\epsilon_0 < -m$, beyond a certain coupling strength. This means that despite the resonance of the Dirac equation we do not have a resonance of the complete Hamiltonian. However, as we shall see, the understanding of the resonant Dirac equation solution is a necessary prerequisite in order to obtain the correct description of the strongly interacting fields.

3. SUPERCHARGED VACUUM AND KLEIN'S PARADOX

We have seen that in the vicinity of a sufficiently large assembly of charged particles (held together in one place, for example, by the strong interaction) the electron-positron field becomes overcritical. Here the response of the overcritical electron field to an *ever-increasing* strength of the external potential¹⁹⁾ is described. In particular, we focus on two gedankenexperiments. In the first one, we consider a spherically symmetric external potential created by a large (nuclear) charge $Z > Z^{cr}$. Then we will turn to the discussion of Klein's paradox and its resolution in the theory of supercritical fields. In both cases we will employ the Thomas-Fermi approximation.

3.1 Relativistic Thomas-Fermi approximation

In the relativistic Thomas-Fermi approximation the density of electrons is related to the Fermi momentum $k_F(x)$ by

$$\varrho = \frac{e}{3\pi^2} k_F^3. \quad (3.1)$$

The effect of the spin degeneracy is included in Eq. (3.1). The relativistic relation between the Fermi energy E_F and Fermi momentum is

$$k_F^2 = [(E_F - V)^2 - m^2] \theta(E_F - V - m), \quad (3.2)$$

where V is the electrostatic potential. The step function ensures that k_F^2 is a positive quantity. E_F is the Fermi energy of the system considered.

From Eqs. (3.1) and (3.2) we now obtain for the charge density of the ground state characterized by a choice of the Fermi energy E_F :

$$\begin{aligned} \varrho &= \langle 0 | \hat{\varrho}(x) | 0 \rangle \\ &= (e/3\pi^2) [(E_F - V)^2 - m^2]^{3/2} \theta(E_F - V - m). \end{aligned} \quad (3.3)$$

Introducing the total charge density ρ_T , which is composed of the external "nuclear" part ρ_N and the electronic part,

$$\varrho_T = \varrho_N + \varrho, \quad (3.4)$$

and using Coulomb's law

$$\Delta V(\vec{r}) = -e \varrho_T(\vec{r}), \quad (3.5)$$

we find a self-consistent non-linear differential equation for the average potential V , that depends on the choice of the ground state $|0\rangle$ through the value of the parameter E_F

$$\Delta V(\vec{r}) = -e \varrho_N(\vec{r}) - (e^2/3\pi^2) [(E_F - V)^2 - m^2]^{3/2} \Theta(E_F - V - m), \quad (3.6)$$

As long as the nuclear system ρ_N is isolated from external sources of electrons the proper choice of E_F is $E_F = m$. If this condition is relaxed and an inexhaustible supply of electrons is available, we must account only for the kinetic energy of these electrons. Thus for neutral atomic systems one must take $E_F = m$, which gives the usual Thomas-Fermi model, in the limit $|-2mV| > |V^2|$. Equation (3.6) is very useful and may be applied to describe many interesting problems in atomic physics.

3.2 The charged vacuum in the Thomas-Fermi approximation

The point at which the 1s wave function joins the continuum solutions of negative frequency has been determined⁵⁾ to be about $Z = 172$, under "realistic" assumptions and extrapolations of the known properties of nuclear and electromagnetic interactions. Similarly, the next critical point, for which the $2p_{1/2}$ state is expected to join the continuum is about $Z = 183$. At this point the charge of the vacuum becomes four. Soon, as we increase the nuclear charge, higher angular momentum states will also join the lower continuum, and the charge of the vacuum will rise even faster. Thereafter, the self-interaction of the vacuum charge will become an important aspect. In particular, we can already foresee that the vacuum charge may screen a substantial part of the nuclear charge and prevent more states from joining the lower continuum, or, from another point of view, the repulsive interaction of an electron with the surrounding vacuum charge may become comparable with the attractive force of the nuclear charge.

It has been proposed¹⁹⁾ to treat that complex situation by use of the relativistic Thomas-Fermi approximation. The charge density of the vacuum is equal to the charge density carried by all of the states that have joined the lower continuum. In the Thomas-Fermi model, this sum over all of these states is represented by an integral over all the momentum states within the Fermi sphere of radius k_F as defined by Eq. (3.2) with the Fermi energy fixed at $E_F = -m$. This means that only the states accessible to spontaneous decay are filled. Inserting $E_F = -m$ into Eq. (3.6) yields

$$\Delta V(\vec{r}) = -e \varrho_N(\vec{r}) - (e^2/3\pi^2) (2mV + V^2)^{3/2} \Theta(-V - 2m). \quad (3.7)$$

We now proceed to discuss the solution of Eq. (3.7). Since the charge density of the vacuum must be confined to the vicinity of the external charge, we require a solution such that

$$V(r) = \lim_{r \rightarrow \infty} - \gamma \alpha / r, \quad (3.8)$$

(α is the fine structure constant). For every choice of Z , γ is determined by the boundary condition on the electrostatic potential at the origin

$$\left. \frac{\partial V}{\partial r} \right|_{r=0} = 0 \quad (3.9)$$

Equations (3.7) and (3.9) are therefore eigenvalue equations for γ , the unscreened part of the nuclear charge, and $Z - \gamma$ gives the charge of the vacuum.

Neglecting at first the inhomogeneity of the solution, we find that $V(0) = V_0$ is determined from the condition,

$$\varrho_T = \varrho + \varrho_N = 0, \quad (3.10)$$

in the limit of large Z , i.e. when the distribution of nuclear charge is large as compared with $1/m$, then

$$V_0 = \left\{ m - [m^2 + (3\pi^2 e \varrho_N / e^2)^{2/3}]^{1/2} \right\}. \quad (3.11)$$

Integration of Eq. (3.7) is straightforward¹⁹⁾. An equal number of protons and neutrons and normal nuclear density have been assumed for the nuclear-charge distribution. The results for γ are plotted in Fig. 3.1. From the figure, one can see that γ increases monotonically with Z and that γ/Z decreases as Z increases. In fact, from the requirement that V_0 remains constant with growing Z , at the surface of the nuclear charge distribution we find:

$$V_0 \sim - \frac{\gamma(Z)}{R(Z)}$$

and, since $R(Z) \sim Z^{1/3}$, we find

$$\gamma(Z) \sim Z^{1/3} \quad (3.12)$$

The single-particle results are denoted by crosses in Fig. 3.1 and agree reasonably well with an extrapolation of the Thomas-Fermi results into the realm of small values of $Z - \gamma$. We note here that the condition for the validity of the Thomas-Fermi approximation is $Z - \gamma \gg 1$. In Fig. 3.2 we consider the approach to infinite nuclear matter. As shown there, both the vacuum charge density and the potential approach a limit as Z increases from 10^4 to 10^5 . The radial total charge

density, calculated from the right-hand side of Eq. (3.7), is shown in Fig. 3.3. The results are scaled with γ so that each curve is normalized to unity. We see that the charge densities become more and more nearly those of a surface dipole with clearly defined regions of positive and negative charge.

In accordance with our expectations, the charge generated by successive levels joining the lower continuum is sufficient to screen most of the bare nuclear charge as it increases without bound. This property is evident in the fact that for $Z > 10^5$ the self-consistent potential does not change within the nuclear matter distribution.

3.3 Klein's paradox

Let us consider an electron of momentum p and energy $\varepsilon = \sqrt{p^2 + m^2}$ with spin up that is incident from the left on an electrostatic square-well barrier $V_0 > 0$. The discontinuous form of the potential requires that region I outside the potential well and region II inside the potential well be treated separately. In region I the solution of the Dirac equation is

$$\psi_I(z) = ae^{ipz} \begin{bmatrix} 1 \\ 0 \\ p/(\varepsilon+m) \\ 0 \end{bmatrix} + be^{-ipz} \begin{bmatrix} 1 \\ 0 \\ -p/(\varepsilon+m) \\ 0 \end{bmatrix}, \quad (3.13)$$

where the second part of the wave function describes the reflected wave. The form of the wave function in region II depends upon the magnitude of the potential strength. We first consider values of V_0 that are not too large. Then

$$\psi_{II}(z) = ce^{-\beta z} \begin{bmatrix} 1 \\ 0 \\ ip'(\varepsilon - V_0 + m) \\ 0 \end{bmatrix}, \quad (3.14)$$

where $p' = \sqrt{m^2 - (\varepsilon - V_0)^2}$. It is not necessary to add terms to Eqs. (3.13) and (3.14) that describe particles with spin down, since there is no probability of a spin flip. Requiring that the wave function be continuous at $z = 0$ leads to relations between the coefficients a , b and c . The ratios c/a and b/a take the form

$$c/a = 2/(1+i\Gamma), \quad (3.15a)$$

$$b/a = (1-i\Gamma)/(1+i\Gamma), \quad (3.15b)$$

where

$$\Gamma = [(\epsilon+m)(m-\epsilon+V_0)]^{1/2} \cdot [(\epsilon-m)(m+\epsilon-V_0)]^{-1/2} \quad (3.15c)$$

is real. The incident current may be calculated from $j_i = \psi_i^\dagger \alpha_3 \psi_i$, where the subscript i denotes only the first part of the wave function of Eq. (3.13). This current is equal to $2p|a|^2/(\epsilon+m)$. The ratio of the reflected current to the incident current is $|b|^2/|a|^2$, which is equal to one because of the form of Eq. (3.15b). The transmitted current is equal to zero. Thus all of the incident current is reflected, and the situation is analogous to non-relativistic quantum mechanics.

Let us now consider what happens as V_0 is increased beyond $\epsilon+m$. The wave function must be written as:

$$\psi_{II}(z) = d e^{ip''z} \begin{bmatrix} 1 \\ 0 \\ p''/(\epsilon+m-V_0) \\ 0 \end{bmatrix}, \quad \epsilon+m < V_0 \quad (3.16)$$

where $p'' = \sqrt{(V_0 - \epsilon)^2 - m^2}$. The continuity condition now leads to

$$d/a = 2/(1-\Gamma'), \quad (3.17a)$$

$$b/a = (1+\Gamma')/(1-\Gamma'), \quad (3.17b)$$

$$\Gamma' = [(\epsilon+m)(V_0-\epsilon+m)]^{1/2} [(\epsilon-m)(V_0-\epsilon-m)]^{-1/2}. \quad (3.17c)$$

The transmitted current is equal to $2p'|d|^2/(\epsilon+m-V_0)$, which is negative, and the magnitude of the reflected current is larger than that of the incident current. The transmission coefficient, which is the ratio of the transmitted current to the incident current, is given by

$$T = -4\Gamma' / (1 - \Gamma')^2. \quad (3.18)$$

In Fig. 3.4 the negative of the transmission coefficient is shown as a function of energy for $V_0 = 3m$ and for $V_0 = 10m$. We note that the transmitted current may be much larger than the incident current. This paradox was first noted by Klein²⁰⁾. Only in the context of a single-particle interpretation does this appear paradoxical. When one appreciates that electrons and positrons are inextricably connected in the Dirac theory, it is natural to identify the negative current in region II with the appearance of positrons. The increase of the reflected current over the incident current is necessary to conserve charge. The reflected current plus the transmitted current is always equal to the incident current.

The results we have obtained above would imply that the scattering of electrons of a repulsive, strong potential barrier induces pair production. As we have seen in the previous section, *one has to consider the spontaneous pair production beforehand*. Furthermore, as shown in Section 3.2, it is quite possible that a saturation in the pair production will occur.

In order to make a connection between our investigation of Klein's paradox and the supercritical potentials, we redefine the reference point of the energy: we consider the potential to be strongly attractive in region II ($V = -V_0 < 0$). Then we expect that within the range of this region (which may be infinite) all supercritical states are spontaneously filled with 'electrons', while the positrons are emitted to infinity. Now Klein's gedankenexperiment consists of scattering positrons of the (filled) attractive potential well. Since no final states are available for electrons within the well, we find that the transmission coefficient vanishes. Thus no matter can be transmitted into the region of the potential. This result must be, strictly speaking, supplemented by a proper quantum field theoretic formulation, which we will, however, not go into now. Here the non-linear system will be considered with a special emphasis on those aspects connected with the self-consistent treatment of the vacuum charge.

When the external charge is localized to the left of $z = 0$,

$$\varrho_N(\vec{x}) = \Theta(-z) \varrho_N^0(z), \quad (3.19)$$

then it is apparent that a solution for V must induce a vacuum charge confined also to the left. The requisite value of the Fermi energy is

$$\varepsilon_F = -m \quad (3.20)$$

Therefore all supercritical states satisfying

$$V + m < \epsilon < -m, \quad (3.21)$$

within the range of the potential well are occupied by electrons. The associated electron charge density, Eq. (3.3), becomes in this case:

$$e\varrho = -\Theta(-2) \frac{e^2}{3\pi^2} (2mV + V^2)^{3/2} \Theta(-V-2m) \quad (3.22)$$

The potential well can now be obtained solving Eq. (3.5). Since we want a potential step, all of the external charge must be screened, that is

$$\int (\varrho_N(\vec{x}) + \varrho(\vec{x})) d^3x = 0 \quad (3.23)$$

This can be achieved only with an oscillating electron charge, which in turn implies that the self-consistent potential must have an oscillating part. Thus a potential step with the deepness described as in Eq. (3.11), $V \approx -V_0$, can be only an approximate solution of the self-consistent Thomas-Fermi equation.

Before closing this section a comment can be made concerning the validity of our assertions for macroscopic charge distributions. In the microscopic charge distributions, like those associated with nuclei, an overcritical value of the total charge must be first exceeded in order for spontaneous positron production to begin. In infinite charge distributions any arbitrarily weak ρ_N is permissible, since over infinite volume sufficient strength for overcriticality will be attained. However, the barrier separating the particle and antiparticle states may become much too wide to allow the spontaneous decay of the neutral vacuum. The most common situation of this nature occurs with the Van de Graaff generator. There the potential step of several MeV is spread over macroscopic distances. As a consequence, the decay time of the neutral vacuum is so large that 'sparking' of the vacuum should never be observed in the vicinity of such generators.

4. STRONG FIELDS IN QUANTUM FIELD THEORY

In this section the case of a completely self-consistent potential as introduced in Section 2.3 is considered. Although the study of the self-consistent solutions of interacting classical field theory is an interesting topic in itself, a deeper motivation is provided by the possibility that, in the strong coupling limit ($g^2 \gg 1$), the classical solution contains relevant information about the interacting quantum system. The conventional perturbative treatment in quantum field theory proceeds via an expansion in the vicinity of non-interacting fields. It is argued below that the self-consistent solutions of c-number equations provide the natural basis for an expansion around a large coupling constant (as far as bound states are considered), provided that the c-number solutions satisfy

$$M \ll N m_q. \quad (4.1)$$

Here m_q is the mass of the single-particle states in the absence of an interaction, N is the number of bound particles and M is the bound state mass obtained from the self-consistent solution of c-number fields. Equation (4.1) thus presupposes that the interaction produces strongly bound states of N particles.

At this point we recognize the connection with the developments of previous sections, where the properties of strong binding in external potentials are investigated. This knowledge is now required in order to understand the properties of the self-consistent strongly bound solutions. In particular, we have learned that when the Dirac binding energy exceeds twice the rest mass, qualitatively new effects can occur.

4.1 Self-consistent 'quark bags'

As indicated in the above discussion we take the self-consistent solution of the coupled Dirac-meson fields to represent a bound state of strongly interacting fermions. This physical picture corresponds to the idea of a quark trapped in a self-consistent potential well²¹⁻²³). If taken seriously, this remark means that the solutions of the interacting fields contain information about experimentally measurable quantities. A preferred model then can emerge that has the 'best' phenomenological properties. I have found that such a 'pet' theory is that of interacting fermion-scalar gluon fields

$$\mathcal{L} = \bar{\Psi} (\gamma \cdot p - m) \Psi + g \Phi \bar{\Psi} \Psi + \partial_\mu \Phi \partial^\mu \Phi - (U(\Phi) - U(0)). \quad (4.2)$$

In the first part of this subsection we will make a connection between the classical theory and quantum field theory, using as an example the Lagrangian

(4.2), where we sometimes also write for the gluon potential U the simplest term

$$U(\Phi^2) \rightarrow \frac{1}{2} \mu^2 \Phi^2 \quad (4.3)$$

In order to treat the strongly interacting ($g^2 \gg 1$) limit of the quantum field theory, induced by the Lagrangian Eq. (4.2), let us now consider quasi-particles. These are entities carrying, typically, the same internal quantum numbers, for example spin, as the particles, but subject to a quite different interaction from the free modes. The advantage that is gained consists basically in the modification of the interaction; in particular, quasi-particles interact weakly and we may use the well-proved perturbative methods to treat the residual interaction. A quasi-fermion state with quantum numbers $|p\rangle$ can be obtained most readily from the quantum operator $\hat{\Psi}(\vec{x}, 0)$ by projecting with the associated amplitude $\psi_p(\vec{x})$ (a circumflex over a quantity indicates its q-number character)

$$|p\rangle = \int \hat{\Psi}^\dagger(\vec{x}, 0) \psi_p(\vec{x}) |0\rangle d^3x. \quad (4.4)$$

Here $|0\rangle$ denotes the ground state. The equations of motion for the amplitude ψ_p will be determined *a posteriori*. It is advantageous to introduce the quasi-particle and antiparticle operators in the usual manner:

$$\beta_p^\dagger = \int \hat{\Psi}^\dagger(\vec{x}, 0) \psi_p(\vec{x}) d^3x, \quad (4.5)$$

$$\gamma_n^\dagger = \int \psi_n^\dagger(\vec{x}) \hat{\Psi}(\vec{x}, 0) d^3x. \quad (4.6)$$

The completeness of the basis $\{\psi_p, \psi_n\}$ is reflected in

$$\delta^3(\vec{x} - \vec{x}') \delta_{\alpha\beta} = \sum_n \psi_n^\alpha(\vec{x}) \psi_n^{\beta\dagger}(\vec{x}') + \sum_p \psi_p^\alpha(\vec{x}) \psi_p^{\beta\dagger}(\vec{x}'). \quad (4.7)$$

Here (α, β) are the internal structure indices, for example spinor indices, while the sums also stand for possible integrals over continuous parts of the spectra. We now see that the internal structure of the quasi-particles is that of the particles and is a consequence of the (anti-)commutation relations of the fields $\hat{\Psi}$. Any quasi-particle state may be constructed from a product of the quasi-fermion operators acting on the ground state. Thus, for example, the three quasi-fermion baryon state B is

$$|B\rangle = \sum_{ijk} b_{ijk}^\dagger \hat{\beta}_i^\dagger \hat{\beta}_j^\dagger \hat{\beta}_k^\dagger e^{-i \int \hat{\Psi}^\dagger(\vec{x}, 0) \psi_c(\vec{x}) d^3x} |0\rangle \quad (4.8)$$

with suitable coefficients b_{ijk} that generate the symmetry properties of the state. The remaining factor in Eq. (4.8) will be explained in a moment.

The 'bag' field for the quarks is generated by the quasi-fermionic source

$$S = \langle B | \hat{\bar{\Psi}} \hat{\Psi} | B \rangle \quad (4.9)$$

The presence of a strong source, the strength being determined to a large extent by g^2 , generates an average gluon "shell" potential φ_c

$$\varphi_c = \langle B | \hat{\Phi} | B \rangle. \quad (4.10)$$

To achieve this property, we have introduced the exponential in Eq. (4.8), which makes $|B\rangle$ a coherent state for the meson field, where

$$\pi_\Phi = \frac{\delta \mathcal{L}}{\delta \Phi} \quad (4.11)$$

and

$$[\hat{\Phi}(\vec{x}, 0), \hat{\pi}_\Phi(\vec{x}', 0)] = i \delta^3(\vec{x} - \vec{x}') \quad (4.12)$$

Equipped with the trial state $|B\rangle$ (and similarly a meson state $|M\rangle$) we can minimize the invariant mass that is associated with them, as a function of the unknown functions φ_c and ψ_p . The Lorentz invariant momentum P_μ of our trial state $|B\rangle$ is given by

$$P_\mu = \int \langle B | \hat{T}_\mu^\nu(x) | B \rangle d^4 o_\nu, \quad (4.13)$$

where T_μ^ν is the energy momentum tensor following from the Lagrangian $\mathcal{L}$ under consideration. The hypersurface in the four-dimensional space is denoted by $d^4 o_\nu$. Note that we have chosen, in the above discussion,

$$d^4 o_\nu = n_\nu d^3 x, \quad (4.14)$$

with $n_\nu = (1, 0, 0, 0)$ associated with the laboratory frame of reference. We have written the fully covariant form of P_μ in Eq. (4.13) to show the Lorentz covariance of the bag approach. Furthermore, within the ansatz for $|B\rangle$ we have chosen, we search for solutions with vanishing momentum $\vec{P}$, i.e.

$$\int \langle B | \hat{T}_0^i | B \rangle d^3 x = 0 \quad (4.15)$$

If our solution satisfies condition (4.15), it is called a baryon in zero average momentum frame. By construction of our trial state we obtain the property

$$\langle B | \hat{\pi}_\phi(x) | B \rangle = 0, \quad (4.16)$$

which guarantees the vanishing of the average gluon momentum. Similarly, it is easy to show that the sum of quasi-fermion momenta vanishes. This is in agreement with a picture in which quarks follow closely the motion of the gluon bag and vice versa.

In the zero average momentum frame we therefore have

$$P_0 = M = \int d^3x \langle B | \hat{T}_0^0 | B \rangle = \int d^3x \mathcal{M}_B, \quad (4.17)$$

where for $\mathcal{L}_1$ defined by Eq. (4.2) we find, using the exact symmetry of all quarks in the bag:

$$\begin{aligned} \mathcal{M}_B = N \psi_i^\dagger (\vec{\alpha} \cdot \vec{p} + \beta(m_q - g\varphi_c)) \psi_i \\ + \frac{1}{2} |\vec{\nabla} \varphi_c|^2 + U(\varphi_c) - U_0, \end{aligned} \quad (4.18)$$

where $N = 3$ is the number of (valence) quarks.

A very similar results is also obtained for the mesons:

$$\begin{aligned} \mathcal{M}_M \equiv \langle M | \mathcal{H} | M \rangle = \psi_i^\dagger [\vec{\alpha} \cdot \vec{p} + \beta(m_q - g\varphi_c)] \psi_i \\ - (i \leftrightarrow j) + \frac{1}{2} |\vec{\nabla} \varphi_c|^2 + U(\varphi_c) - U_0, \end{aligned} \quad (4.19)$$

The usual $(-)$ sign for antiquasi-fermion amplitude ψ_j in (4.19) is necessary to change the sign of the negative frequency mode associated with the solution of its Dirac equation. For a scalar potential φ_c the spectrum of the Dirac equation is symmetric between particles and antiparticles, that is

$$E_p = -E_{ap} \quad (4.20)$$

and the wave functions transform like

$$\psi_p = \gamma_5 \gamma_0 \psi_{ap} \quad (4.21)$$

Therefore the invariant mass for all hadrons can be written as a function of the number of quarks in the bag only:

$$M_N = \int d^3x \mathcal{M}_N = \int d^3x [N \{ \psi_0^\dagger (\vec{\alpha} \cdot \vec{p} + \beta (m_q - g \varphi_c)) \psi_0 \} + \frac{1}{2} (\vec{\nabla} \varphi_c)^2 + (U(\varphi_c) - U_0)] = M_{N,f} + M_g. \quad (4.22)$$

The index '0' on the spinor wave function indicates that we must choose the lowest energy particle solution (which in the case of scalar interaction is the lowest positive energy eigenvalue solution of the Dirac equation) in order to obtain the smallest value of M_N . The equations of motion satisfied by ψ_0 and φ_c follow now from the variational condition:

$$\delta (M_N - \epsilon_0 N \int d^3x \psi_0^\dagger \psi_0) = 0, \quad (4.23)$$

where we have introduced the usual Lagrange multiplier in order to normalize the solutions:

$$\int \psi_0^\dagger \psi_0 d^3x = 1 \quad (4.24)$$

We find from Eq. (4.23) the self-consistent equations of motion

$$[\vec{\alpha} \cdot \vec{p} + \beta (m_q - g \varphi_c)] \psi_0 = \epsilon_0 \psi_0, \quad (4.25)$$

$$-\Delta g \varphi_c + \frac{\partial U}{\partial \varphi} = g^2 N \bar{\psi}_0 \psi_0. \quad (4.26)$$

N is equal to three for baryons and two for mesons. When solving the above equations, we consider all dimensional quantities in units of m_q . If we obtain the solutions as a function of g^2 , then it is possible to consider the case $N = 1$ only, and the relevant parameter is

$$g'^2 = g^2 N. \quad (4.27)$$

We note that M_N can be written as

$$M_N = N \left(\epsilon_0 [g'^2] + \frac{1}{g'^2} \int \left(\frac{1}{2} (\vec{\nabla} g \varphi_c)^2 + \frac{1}{2} \mu^2 (g \varphi_c)^2 \right) d^3x \right). \quad (4.28)$$

Thus M_N/N is only a function of g'^2 . We thus have seen that self-consistent solutions of classical interacting fields are closely related to the quark-bag solutions of N quarks. In the quark-bag approach the main approximation has been the following: only the diagonal part of the Hamiltonian matrix of the interacting fields in a trial state has been considered. The off-diagonal parts remain to be diagonalized and the renormalization program carried out.

An argument in favour of the bag approximation, applicable only in the limit of strong coupling, involves the large separation in energy between the mass of the trial state, M_N , and the free fermion mass, m . I believe that the second-order contributions to M from the off-diagonal matrix elements will be of the order of:

$$\begin{aligned} \delta M &\lesssim [\int \psi_i^\dagger g \varphi_c \psi_i d^3x]^2 / [Nm_q - M_N] \\ &\approx \left(\frac{M_N}{Nm_q} \right) M_N . \end{aligned}$$

If this is the case, then the ratio

$$\epsilon = M/m_q$$

is the small parameter that determines the validity of the bag approximation.

Above we have illustrated in some detail the properties of the bag with a scalar type of interaction. However, in spirit and with minor modifications our discussion applies to other interactions as well, in particular also to the vector interaction discussed in Section 4.6. A similar, but a more straightforward, derivation of the self-consistent equations is also given there.

Finally, I wish to make two points more explicit:

i) The expectation value (4.13) should include the zero-point energy of the Fermi field:

$$E_0 = \frac{1}{2} \left(\sum_p E_p [\varphi_c] - \sum_n E_n [\varphi_c] \right) ,$$

which is a (divergent) implicit function of φ_c . It is possible to include in the function $U(\varphi_c)$ the necessary counterterms -- the renormalized zero-point energy then is still a function of φ_c and should, in principle, be included in Eq. (4.19). However, such a contribution can be absorbed in the function $U(\varphi_c)$. Since we have, in principle, no idea about the form of U , we need not consider this point in further detail for the moment.

ii) It is instructive to notice that the choice of φ_c that is self-consistent in the sense of Eqs. (4.25) and (4.26) makes the remaining interaction purely off-diagonal. The full Hamiltonian of q-number fields is (up to the necessary symmetrization)

$$\hat{H} = \hat{H}_D + \hat{H}_\phi + \hat{H}_I$$

with

$$\hat{H}_D = \int d^3x \hat{\Psi}^\dagger (\vec{\alpha} \cdot \vec{p} + \beta m) \hat{\Psi}$$

$$\hat{H}_\phi = \int d^3x \frac{1}{2} (\hat{\pi}^2 + (\vec{\nabla} \hat{\phi})^2 + (U(\hat{\phi}) - U_0)^2)$$

$$\hat{H}_I = \int d^3x (-g \hat{\phi}) \hat{\Psi} \hat{\Psi}$$

Now let us add and subtract a term in $\hat{H}$

$$\hat{H} = (\hat{H}_D + \hat{H}_{ex}) + \hat{H}_\phi + (\hat{H}_I - \hat{H}_{ex}),$$

where

$$\hat{H}_{ex} = \int d^3x (-g \varphi_c) \hat{\Psi} \hat{\Psi}.$$

The approach presented above corresponds to such a choice of a trial state that the *diagonal* matrix elements of the new interaction

$$\hat{H}'_I = \hat{H}_I - \hat{H}_{ex}$$

vanish, while the Hamiltonian

$$\hat{H}_0 = (\hat{H}_D + \hat{H}_{ex}) + \hat{H}_\phi$$

is diagonal.

4.2 Numerical methods

Our aim in this section is to illustrate the numerical methods involved in minimization of the mass (or Hamiltonian) M_N , Eq. (4.28), as a function of the fields ψ_0 and φ_c , with the constraint that ψ_0 be the lowest frequency eigenmode of the quasi-fermion field.

Great care should be exercised in all numerical work, since the classical Dirac spectrum $\{\epsilon_i\}$ is not bounded below. Therefore M_N can be made arbitrary

negative by a choice of ψ_{trial} that includes large negative energy components. In practical calculations only eigenmodes of Eq. (4.25) for a given φ_c should be allowed. Let us go into this remark in more detail. Since the set of eigensolutions $\{\psi_k\}$ generated by φ_c is complete, a trial function ψ_t could be expanded as

$$\psi_t = \sum_k a_k^+ \psi_k. \quad (4.29)$$

Then we would find that the quantity we wish to minimize, Eq. (4.23), is

$$(H - \epsilon_t N) = N \sum_k |a_k^+|^2 (\epsilon_k - \epsilon_t) \quad (4.30)$$

With the unbound-below spectrum of the Dirac equation we thus find that a minimization with respect to parameters of the trial function could not be successful, since $\epsilon_0 - \epsilon_t$ can be smaller than zero.

From this consideration we recognize the need to constrain the number of allowed degrees of freedom of the Dirac field as arose naturally in the bag approximation. We must exclude from our considerations the possibility of a transition that a classical Dirac particle can undergo into a (classically) empty state of arbitrary large negative frequency. In a particular application this means that the Dirac equation must always be solved exactly for some prescribed potential, and an eigenstate ψ_0 obtained. We can thus consider the Hamiltonian to be given by

$$H_c^S = \epsilon_0[\varphi_c] + \int d^3x \left[\frac{1}{2} (\nabla \varphi_c)^2 + U(\varphi_c) - U_0 \right] \quad (4.31)$$

where ϵ_0 is given implicitly by the solution of Eq. (4.25) with the eigenvalue condition

$$\lim_{|\vec{x}| \rightarrow \infty} \psi_0(\vec{x}) = 0 \quad (4.32)$$

Any trial value of φ_c in Eq. (4.31) will give an upper limit for H^S .

But how do we actually obtain a self-consistent solution for φ_c with ψ_0 constrained as described above to the lowest particle solution? It is very inviting to proceed with an iterative algorithm in which, for a given spherical $\varphi_{c,n-1}$ and fixed g and μ/m , a solution ψ_0 of Eq. (4.25) is obtained as described for spherical potentials in Section 1. From Eq. (4.26) we then determine a new function $\varphi_{c,n}$. In practical calculations it turns out that the radius of convergence of such an iteration decreases rapidly as a function of g^2 , making it virtually impossible to obtain a solution for $g^2 \gtrsim 2$, a region in which we are mainly interested.

I have developed²⁴⁾ an algorithm that has so far shown an unrestricted radius of convergence when applied to equations of the type (4.23) to (4.26). Let us introduce for the purpose of clarity two additional functions

$$\phi = g\varphi_s \quad (4.33)$$

$$f = \varphi_s/g \quad (4.34)$$

Equations (4.25) and (4.26) can now be written in the generalized and self-explanatory fashion

$$D[\phi] \psi = 0, \quad (4.35)$$

$$Kf = g_s[\phi], \quad (4.36)$$

$$\phi = g^2 f. \quad (4.37)$$

Here D and K are linear operators, while the source ρ_s is $\bar{\psi}_0\psi_0$. Next we note that, using an arbitrary linear functional L , we can write Eq. (4.37) in the form

$$g^2 = L\phi / Lf. \quad (4.38)$$

We will return to the discussion of the actual form of L further below.

Our algorithm is: given a function ϕ_{n-1} the scalar density is found solving Eq. (4.35). Then we obtain from Eq. (4.36)

$$f_n = K^{-1} g_s[\phi_{n-1}] \quad (4.39)$$

and Eq. (4.38) gives us in turn

$$g_n^2 = L\phi_{n-1} / Lf_n. \quad (4.40)$$

The algorithm loop is closed by the use of Eq. (4.37)

$$\phi_n = g_n^2 f_n. \quad (4.41)$$

Note that we have iterated the coupling constant g^2 . For a given starting value ϕ_0 a convergent point

$$g^2 = \lim_{n \rightarrow \infty} g_n^2 \quad (4.42)$$

may be found that is dependent on the actual form of the initial function ϕ_0 . I have found empirically that there is a one-to-one correspondence between

$$\phi_c = \lim_{n \rightarrow \infty} \phi_n \quad (4.43)$$

and g^2 , Eq. (4.42), in the case of Eqs. (4.25), (4.26) and other similar theories discussed further below.

Now, as to the choice of the operator L , the difference between ϕ_{n-1} and $g_n^2 f_n = \phi_n$ needs to be small, in the sense that we are searching for the minimum of the integral

$$I_n = \int w(r) [\phi_{n-1} - g_n^2 f_n]^2 dr \quad (4.44)$$

as a function of g_n^2 . Here $w(r)$ is a weighting function that may be dependent on ϕ_{n-1} . This prescription gives us

$$L\phi = \int w(r) \phi dr. \quad (4.45)$$

The choice $w(r) = 1$ is usually sufficient to have a convergent algorithm. However, $w(r) = \rho_s[\phi_{n-1}]$ gives a quicker convergence in most cases. I would like to conjecture that the algorithm described above should be convergent in most similar cases of physical interest, provided that a suitable choice for the operator L has been made.

Finally, a few words concerning stability of the (radial) solutions φ_c . To prove the stability of the solutions it would be necessary to show that H^s , Eq. (4.31), is increased in second order by arbitrary variations of φ_c . The necessary constrained variational calculation requires a major computational effort and has not been carried out in that form. However, I have tried a large number of $\delta\varphi_s$ chosen at random. The change in M was positive in every case.

4.3 The virial approach to classical field equations

Before actually discussing the solutions of particular models, let us see how much we can learn about the general properties of self-consistent solutions from the equations of motion²⁵⁾. Basic to our considerations will be a (virial) relation describing the kinetic energy of the fermion field ψ in some prescribed potential $V(x)$, where V is a matrix in the spinor space and can, in principle,

consist of all possible couplings (S, V, P, A, T). Let H_D be the Dirac operator

$$H_D = \vec{\alpha} \cdot \vec{p} + \beta m + V \quad (4.46)$$

Then we have

$$[\vec{x} \cdot \vec{p}, H_D] = i \vec{\alpha} \cdot \vec{p} - i \vec{x} \cdot (\vec{\nabla} V). \quad (4.47)$$

Taking the expectation value of Eq. (4.46) between localized eigenfunctions ψ_i of H_D , we find the *virial* equation for the Dirac field:

$$\int d^3x [\psi_i^\dagger \vec{\alpha} \cdot \vec{p} \psi_i] = \int d^3x [\psi_i^\dagger \vec{x} \cdot (\vec{\nabla} V) \psi_i]. \quad (4.48)$$

This is a very useful relation which is valid only when ψ_i is an eigenfunction of H_D . We record that all of the ψ_i considered above are localized discrete eigenstates in configuration space. We now apply Eq. (4.48) to the Lagrangian field theory describing scalar, meson field in interaction with the Dirac field: the Lagrangian has been given in Eq. (4.2) and the equations of motion by Eqs. (4.25) and (4.26) with $N = 1$ and $\dot{\varphi}_c = 0$. Then Eq. (4.48) for the kinetic energy of the Dirac field becomes

$$\int d^3x [\psi_i^\dagger \vec{\alpha} \cdot \vec{p} \psi_i] = \int d^3x [(-\vec{x} \cdot \vec{\nabla} \varphi_c) g \bar{\psi}_i \psi_i]. \quad (4.49)$$

We find after some manipulations that

$$\int d^n x [\psi_i^\dagger \vec{\alpha} \cdot \vec{p} \psi_i] = \int d^n x \left[\frac{n-2}{2} |\vec{\nabla} \varphi_c|^2 + n(U - U_0) \right] + ST, \quad (4.50)$$

with a vanishing surface term for localized solutions, with

$$n \equiv \vec{\nabla} \cdot \vec{x} \quad (4.51)$$

as the dimensionality of the space. Normally $n = 3$, but to dramatize the uniqueness of the three-dimensional, physical space, let us consider the number of dimensions as a parameter.

The Hamiltonian associated with the Lagrangian (4.2) is, with a time-independent φ_c :

$$H^S = \int d^n x [\psi_0^\dagger (\vec{\alpha} \cdot \vec{p} + \beta m) \psi_0 - g \varphi_c \bar{\psi}_0 \psi_0 + \frac{1}{2} |\vec{\nabla} \varphi_c|^2 + U(\varphi_c) - U_0]. \quad (4.52)$$

We may use the above result, Eq. (4.50), together with the equations of motion (4.25) and (4.26) to obtain the following expression for the Hamiltonian:

$$E_{\text{eff}}^S = \int d^n x \left\{ \frac{n-3}{2} |\nabla \varphi_c|^2 + (n+1) [U(\varphi_c) - U_0] + (m_g - \varphi_c) \frac{\partial U}{\partial \varphi_c} \right\}. \quad (4.53)$$

As is well known, the above equation (4.53) cannot be used as a basis of a variational principle. For known φ_c , which minimizes Eq. (4.52) or better (4.31), it gives the proper value of H^S . Therefore we may view E_{eff}^S as an expression defining the total energy.

A striking feature of Eq. (4.53) is the fact that for $n < 3$ (n is the number of space dimensions) the effective kinetic energy of the scalar field becomes negative definite. It just vanishes for $n = 3$. Thus the energy content of E_{eff}^S in a normal number of space dimensions is only implicitly dependent on the derivatives of the field φ_c . The negative definite kinetic energy for $n < 3$ signals a possible instability of the Hamiltonian; the energy of the solution could be reduced by a small non-continuous variation of φ_c .

Another notable feature is that any φ_c^4 proportional term in U cancels out in three space dimensions (in n -dimensional space φ_c^{n+1} cancels). This is an important feature, since φ_c^4 is commonly held responsible for the stability of a theory with spontaneously broken symmetry^{22,26}). In the case of a one-dimensional world ($n = 1$), where the φ_c^2 contribution vanishes, this is obviously a necessary term to stabilize the theory. It would therefore seem that a φ^6 plays the role of the φ^4 term in three space dimensions, as compared with one-dimensional models.

A similar derivation can be carried out in the case of a Lorentz vector field A_μ of mass μ_v in interaction with the Dirac field. For the Lagrangian

$$\mathcal{L}_A = -\frac{1}{2} \partial_\mu A^\nu \partial^\mu A_\nu + \frac{1}{2} \mu_v^2 A_\mu A^\mu - g_v A_\mu \bar{\Psi} \gamma^\mu \Psi + \bar{\Psi} (\gamma \cdot p - m) \Psi \quad (4.54)$$

we find

$$E_{\text{eff}}^A = - \int d^n x \left[\frac{n-3}{2} (\nabla A_\mu)^2 + \frac{n-1}{2} \mu_v^2 A^2 - m \bar{\Psi}_0 \Psi_0 \right], \quad (4.55)$$

which is negative definite, considering the longitudinal component A_0 only. We note that the longitudinal part of the vector-type interaction is repulsive in the particle-particle channel and attractive in the particle-antiparticle channel.

The situation changes when the sign in the part of the Lagrangian corresponding to the free vector field is changed:

$$\mathcal{L}_A = \frac{1}{2} \partial_\mu A^\nu \partial^\mu A_\nu - \frac{1}{2} \mu_\nu^2 A^2 - g_\nu A_\mu \bar{\Psi} \gamma^\mu \Psi + \bar{\Psi} (\gamma \cdot p - m) \Psi. \quad (4.56)$$

We then find

$$E_{\text{eff}}^A = \int d^n x \left[\frac{n-3}{2} (\nabla A_\mu)^2 + \frac{(n-1)}{2} \mu_\nu^2 A^2 + m \bar{\Psi}_k \Psi_k \right], \quad (4.57)$$

which is positive definite, constrained to the longitudinal part of A_μ , provided that the scalar integral $\int d^n x \bar{\Psi}_0 \Psi_0 > 0$. The above-described change in sign accomplishes at the same time a change in the 'polarity' of the vector interaction -- the longitudinal part is now attractive in the particle-particle channel, while the particle-antiparticle channel becomes repulsive. The perturbative quantum field theory, if based on Eq. (4.56) would suffer from the well-known difficulties associated with the possible need for negative metric particles (ghosts) to guarantee a spectrum bounded below. Therefore, such modifications are usually not considered seriously. Such an example considered in the frame of classical field theory can serve as an educational example in order to gain experience with 'attractive' vector-type fields encountered in non-Abelian meson theories (quantum chromodynamics). Returning for a moment to Eq. (4.55), it should be mentioned that it is in principle possible to find a solution in which the space-vector part of A_μ dominates -- thus allowing a stable solution, even with the conventional choice for the sign of the vector field action.

We now consider the case of the self-interacting Dirac field, where H assumes the form, for scalar-type self-interaction²⁷⁾

$$H^P = \int d^n x \left[\Psi_0^\dagger (\vec{\alpha} \cdot \vec{p} + \beta m_q) \Psi_0 - \frac{G}{2} (\bar{\Psi}_0 \Psi_0)^2 \right] \quad (4.58)$$

In view of the equations of motion,

$$[\vec{\alpha} \cdot \vec{p} + \beta (m_q - G \bar{\Psi}_0 \Psi_0)] \Psi_0 = \epsilon_0 \Psi_0 \quad (4.59)$$

the virial relation reads as

$$T_0 = \int d^n x \Psi_0^\dagger \vec{\alpha} \cdot \vec{p} \Psi_0 = -\frac{G}{2} \int d^n x [(\vec{x} \cdot \vec{p}) (\bar{\Psi}_0 \Psi_0)^2]. \quad (4.60)$$

Upon partial integration of the right-hand side, we obtain, up to a vanishing surface term,

$$T_0 = -n V_0, \quad (4.61)$$

where

$$V_0 = - \int d^n x \frac{G}{2} (\bar{\psi}_0 \psi_0)^2. \quad (4.62)$$

The energy for the self-interacting Dirac field can be written now as

$$E_{\text{eff}}^P = (n-1) (-V_0) + m S_0. \quad (4.63)$$

S is the scalar integral

$$S_0 = \int d^n x (\bar{\psi}_0 \psi_0). \quad (4.64)$$

This result, Eq. (4.63), corrects a superficial impression that H^P , Eq. (4.58), is unbound, since it has the structure $x^2 - x^4$. This means that the kinetic energy of the Dirac field more than offsets the attractive self-interaction V_0 . Since $-V_0$ is always positive, we find that for all dimensions the positivity of the solution depends on the sign of the scalar integral. Further, we note that the eigenfrequency can be written as

$$\epsilon_0 = (n-2) (-V_0) + m S_0. \quad (4.65)$$

4.4 Properties of bound states of scalar self-consistent bags

Properties of bound states obtained within several models will be described here. In particular, we are interested in the geometric properties of the quasi-fermion amplitudes ψ_0 and mass densities $\mathcal{M}$. Furthermore, we consider also g^2 and μ/m systematics of the observable matrix elements of ψ_0 , such as the charge radius, the magnetic moment of the proton and axial coupling constant of the semi-leptonic charged current.

It is my feeling that although the average properties (involving matrix elements) of our variational solutions, belonging to some specific models, may be closer to reality than should be expected, a more detailed description is required for comparison of the theoretical and experimental form factors. In particular, we should recall that the amplitudes ψ_0 are, strictly speaking, transition matrix elements between N and $N \pm 1$ fermion states, and not probability amplitudes, as in the case of weakly interacting fields. Also, we have considered here only 'valence' quarks -- the sea quarks do also contribute significantly, in particular to the inelastic form factors.

In Fig. 4.1 we show some of the typical solutions associated with the Lagrangian (4.2) of the interacting fermion-scalar gluon fields²³⁾ for $U(\varphi^2) = \frac{1}{2}\mu^2 \varphi^2$ and $N = 3$. The self-consistent quasi-particle (bound quark) mass

$$m^* = m_q - g \varphi_c \quad (4.66)$$

is plotted for several values of the gluon mass μ/m_q and the coupling constant g^2 as a function of $r = |\vec{x}|$. For $\mu = 0.04m_q$ and $\mu = 0.02m_q$ we also show the vector

$$S_v = \psi_0^\dagger \psi_0 \quad (4.67)$$

and scalar

$$S_s = \bar{\psi}_0 \psi_0 \quad (4.68)$$

densities. We note that, in Fig. 4.1, ρ_s is enhanced by a factor of 10 in relation to ρ_v . For μ of the order of the bare quark mass m , $m^*(r)$ has a pronounced minimum. For coupling constants smaller than those considered here, i.e., for $g^2 \lesssim 10$, we have also found solutions *that were evenly distributed over the volume*. The transition from the volume to surface solution as a function of g^2 and μ/m is smooth. Qualitatively this behaviour can be easily understood in view of the particular nature of the scalar coupling. Disregarding the spin effects, the spectrum equivalent Schrödinger potential is given by

$$V_{\text{eff}} \sim \frac{(m - g\varphi_c)^2}{2m} \quad (4.69)$$

We notice that if $g\varphi_c(0) > m$, then a minimum of V_{eff} will occur at $m = g\varphi_c(R)$. Depending on the precise form of $g\varphi_c$, this minimum may be broad enough to support a wave function localized around R . Alternatively, only a minor perturbation of the volume solution may be found.

In Fig. 4.2 the mass density $\mathcal{M}$ is shown as a function of r , as defined by Eq. (4.19) for $N = 1$. We note, in particular, the existence of 'surface' solutions for which $\mathcal{M}$ peaks at a certain distance R for large values of the coupling constant, while there are also volume solutions for smaller coupling constants.

In Fig. 4.3 the masses²³⁾ of the bound states M_N are given as functions of g^2 for the gluon masses of 0.4, 0.1, 0.02 (m_q). We see that smaller gluon masses give considerably smaller bag masses. As g^2 rises we find a point g_c^2 such that

$$2M_2 < \mu, \quad g^2 > g_c^2 (\mu/m_q). \quad (4.70)$$

For $g^2 > g_c^2$ it can be argued that no free gluons can exist owing to their strong coupling to the hadronic states. As g^2 is increased with a fixed gluon mass μ , M_N decreases monotonically.

However, weakly bound exotic states are found as shown in Fig. 4.3. These states are conglomerates of the allowed hadronic states. This lack of saturation is particular for the scalar interaction. When other (repulsive) interactions are included, such states may easily become unbound.

There is an easy way of understanding the functional form of the curves shown in Fig. 4.3. The mass consists of two terms, cf. Eq. (4.22),

$$M_N = M_f + M_g, \quad (4.71)$$

where M_g is the energy contained in the gluon field φ_c . For large g^2 the eigenfrequency of the Dirac equation solution is

$$\epsilon_0 = R^{-1}, \quad (4.72)$$

where R is the radius of the bag. This relation is confirmed by results shown in Fig. 4.4, where the product $\epsilon_0 \cdot R$ is shown as a function of g^2 , for large values of g^2 . Let us assume that

$$M_g = \gamma g^2 R^\beta, \quad (4.73)$$

where β may be considered as a slowly varying function of R . The constants γ and β depend also upon μ/m . Thus we have

$$M_N = \frac{N}{R} + g^2 \gamma R^\beta = \frac{N}{R} (1 + g^2/N \gamma R^{\beta+1}). \quad (4.74)$$

Upon minimization at fixed g^2 and μ/m with respect to R

$$\frac{\partial M_N}{\partial R} = 0 = -\frac{N}{R^2} + g^2 \gamma \beta R^{\beta-1}. \quad (4.75)$$

We obtain

$$g^2/N \gamma R^{\beta+1} = \beta^{-1}, \quad (4.76)$$

and for Eq. (4.74)

$$M = M_f (1 + \beta^{-1}). \quad (4.77)$$

Defining

$$R_a = M_f / M_g, \quad (4.78)$$

we find

$$R_a = \beta \quad (4.79)$$

Thus the ratio of the fermionic to the gluonic part of the hadron mass has a geometrical meaning, since the value of β , Eq. (4.74), determines the nature of the solution. For $\beta = 3$ we have a volume bag with the glue distributed over the whole hadron. For $\beta = 2$ we have a surface solution, and $\beta = 1$ indicates a string-like solution. As shown in Fig. 4.5,

$$P = M_N R / N \simeq 1 + 1/R_a \quad (4.80)$$

tends to the value 1.5 for large g^2 , consistent with $R_a \lesssim 2$. We recall that for the SLAC bag²²⁾ $R_a = 2$ (surface bag) and for the MIT bag²⁷⁾ $R_a = 3$ (volume bag).

We can use relation (4.76) to eliminate R completely from Eq. (4.74). Then, with R_a as the second variable apart from g^2 we find

$$M_N \sim N^{R_a / (R_a + 1)} (g^2)^{-(R_a + 1)^{-1}}, \quad (4.81)$$

where the dependence on N follows from Eq. (4.28) which can also be written as

$$M_N(g^2) = N M_1(Ng^2). \quad (4.82)$$

In passing we note that the lack of saturation of the scalar interaction is apparent in Eq. (4.81). The energy per quark M_N/N is proportional to $N^{(R_a+1)^{-1}}$ and is therefore decreasing with an increasing number of quarks in the bag (of course, only colour singlets are allowed).

We consider the limit $g^2 \rightarrow \infty$, $m_q \rightarrow \infty$ in Eq. (4.81), while μ remains finite. If there is a relation between the values of m_q and g^2 such as

$$g^2 \sim \left(\frac{m_q}{\mu} \right)^{R_a + 1}, \quad (4.83)$$

then M_N stays constant in the limit $(m_q, g^2) \rightarrow \infty$ and we have permanent confinement in the sense that, though the free quark mass m_q is infinite, the mass of the bound state remains finite. It is apparent that the relation (4.83) between the parameters of the theory is rather arbitrary. The above remark is meant only to alert the reader to the fact that the ratio of the bound state mass M to the free quark mass m_q can be made arbitrarily small.

We now proceed to calculate other hadronic properties. We take wave functions with exact SU(6) symmetry of spin and flavour, and an extra internal quantum number, colour, in which the baryonic wave functions are antisymmetric, thus following the concepts set forth in the SLAC bag paper²²⁾. The baryon multiplet 56 has 56 states counting the spin states. Since the absolute value of the free quark mass m_q is not known, we choose to consider only quantities that are scale-independent. The simplest ones are the products of the r.m.s. radius of the baryons and mesons with their masses $N \cdot P$, Eq. (4.80), which are shown in Figs. 4.6a and 4.6b. The experimental number to compare with for baryons is, most likely, the product of the proton charge radius, 0.8 fm, with the average mass of the 56 multiplet, $M_{56} = 1280$ MeV, which is $5.2\hbar c$. We see that this lies well within values spanned by our calculations. We note that 5.2 implies for $N = 3$ and $\epsilon_0 \sim 1/R$ that $R_a \sim 1.7$. Thus it would seem that hadrons are surface-like, or $\epsilon_0 \neq 1/R$.

We can also calculate the absolute value of the magnetic moment of the proton, using as the basic unit $e\hbar/2M_{56}c$, that is the Bohr magneton *in units of the computed mass* (rather than the experimental value). Therefore the unknown quark mass m_q cancels out from our result. For comparison with the experiment we must scale up the experimental value of μ_p to account for the larger multiplet mass than that of the proton³⁾; we obtain for comparison with Fig. 4.6c a value $\mu_p^{\text{exp}} = 2.79 \times 1280/938 = 3.8$.

We see that the self-consistent bag results are of the right magnitude. We consider also the axial coupling constant g_A of the neutron decay process. The experimental value is $g_A^{\text{exp}} = 1.25$. The results shown in Fig. 4.6d are in the range $0.6 < g_A < 1$.

Finally, in Fig. 4.6e the ratio R_a as computed from the solutions is shown. We find $1 < R_a \leq 2$, indicating that the self-consistent quark bag is mostly surface-like. The small values of R_a for *small* g^2 cannot be as clearly associated with β , Eq. (4.74), since relation (4.72) is not satisfied in this range of g^2 , see Fig. 4.5.

As the final point on the subject, let us note that there is a simple relation between g_A , μ_p , and M_N , that can be derived using the Dirac equation (4.25) and which can be cast into the form

$$\begin{aligned} \mu_p &= (0.5 + 0.3g_A) \cdot N \cdot (1 + R_a^{-1}) \\ &= 2.625 (1 + R_a^{-1}) \end{aligned} \tag{4.84}$$

In the second line of Eq. (4.84) we have used $g_A = 1.25$, $N = 3$. Thus if we were able to find a $U(\varphi)$ such that μ_p would also have the desired value 3.8, R_a would

necessarily turn out to be 2.2. This means that in a 'perfect' scalar bag about 70% of the mass would be carried by the quarks. We further note that the bag could be volume-like. Since g_A must be 1.25, we know that a solution with $\epsilon_0 \langle r^2 \rangle^{\frac{1}{2}} > 1$ is needed. In this case the value $R_a = 2.23$ does not imply a surface-like solution. In view of the above remarks, it is quite possible that a theory based on scalar interaction with very good phenomenological properties could be found.

4.5 Properties of solutions of a self-coupled Dirac field

We have recognized that localized, stable solutions of classical field equations are the basic ingredients in the description of extended objects in quantum field theory. We now turn to the discussion of the self-coupled Dirac field $\bar{\psi}$ in *three* space dimensions governed by the action

$$L = \int d^4x [\bar{\psi} \gamma \cdot p \psi - m_q \bar{\psi} \psi + \frac{G}{2} (\bar{\psi} \psi)^2], \quad (4.85)$$

where m_q is the mass of the free ($G = 0$) fermion field. G , like the weak coupling constant, has the dimension of inverse mass squared.

The quantum field theory associated with Eq. (4.85) is known to lead to a non-renormalizable perturbation expansion in the vicinity of $G = 0$. I believe that the difficulties associated with the perturbation expansion do not provide a compelling argument for rejection of the Lagrangian (4.85). In particular it is quite possible that the properties of the theory change with increasing strength of the coupling G in a non-analytic fashion. I find²⁸⁾ that for $G > G_{\min} = 4.47/(4\pi m^2)$ localized solutions of the classical field equation arise.

Another way of seeing the self-interaction invokes the infinite gluon mass limit of a scalar meson field discussed in the last section. We have considered the properties of the Hamiltonian (4.58) associated with the self-coupled field already in Section 4.3. We therefore turn now to the discussion of the properties of the solutions obtained by the methods introduced in Section 4.2, with the modification that the equation defining a field ϕ in terms of $\bar{\psi}_0 \psi_0$ is very simple now and reads

$$\phi = G \bar{\psi}_0 \psi_0. \quad (4.86)$$

From this point on the iteration procedure can proceed as described previously. Use of numerical continuation of the solutions as a function of the coupling constant increased the convergence speed of the iteration. The solutions ψ_0 that will be discussed below are normalized to unity. We note a similar scale invariance as already noted with meson fields, Eq. (4.27); given an arbitrary norm

$$Q = \int d^3x \psi_0^\dagger \psi_0, \quad (4.87)$$

we can introduce

$$\psi'_0 = Q^{1/2} \psi_0. \quad (4.88)$$

Then ψ'_0 is a solution of the problem with the parameter

$$G' = G/Q, \quad (4.89)$$

that leads to the total energy

$$H'(G/Q) = H(G) * Q. \quad (4.90)$$

The dimensionless parameter of the model is

$$\beta = m^2 G/4\pi. \quad (4.91)$$

The lowest mass solution associated with lowest positive frequency solution has been computed. The energy (H/m) and the frequency (ϵ_0/m) are shown in Fig. 4.7a. We recognize that both functions fall monotonically with increasing β . We also find a minimum value of G for which the mass of the bound state is smaller than m . It is $G_{\min} = 4.47/(4\pi m^2)$, as mentioned previously. Interestingly enough, the qualitative behaviour of $H(Gm^2)$ changes when H is plotted in units of $G^{-1/2}$, as shown in Fig. 4.7b. We find

$$(H/G^{-1/2}) = (4\pi\beta)^{1/2} (H/m), \quad (4.92)$$

which monotonically rises. The lines in Fig. 4.7a may be understood also as obtained for fixed m with changing G , while in Fig. 4.7b, G is fixed and m varies.

In Fig. 4.8 the forms of the solutions for some representative values of $\beta = 22, 475, 2125$ are shown. The effective mass m^* as a function of r , is shown in Fig. 4.8a. With increasing coupling strength the size of the solution increases significantly, while the value of m^* at origin decreases. Notably, it remains always negative. In Figs. 4.8b, c, and d, the vector ρ_v and scalar ρ_s densities belonging to the same solutions are shown. As β increases, the vector density becomes more and more localized around the point where $m^* = 0$. The scalar density remains distributed over the whole volume of the solution. In that respect the self-interacting field solutions differ from the solutions involving a gluon field. There we have seen that the scalar density, like the vector density,

is localized at the surface of the solutions. The volume character of ρ_s in the present case is necessary to allow the relatively constant effective mass m^* over the space occupied by the solution.

In view of the results presented in Figs. 4.7 and 4.8, the self-interacting fermion field discussed here may also be taken as a prototype of a self-consistent quark bag *without gluons*. All we need to do in order to generate the bag solutions from the soliton solutions given above is to perform the transformation described in Eqs. (4.87) to (4.89) with $Q = N$. N is the number of quarks: $N = 3$ for baryons, $N = 2$ for mesons (the scalar self-coupling also does not distinguish between quarks and antiquarks). A self-interacting field provides a natural explanation of this phenomenon of quark confinement in that the free particle of mass m cannot be considered as a quantum of the fermion field for $G > G_{\min}$. Also, the absence of the gluons in the quark bag is satisfactory.

4.6 Supercritical fields in quantum field theory

In this section we shall consider the supercritical binding in the frame of the bag approach. Since some of the theoretical details concerning the bag approximation differ slightly from our previous considerations, we will briefly rederive the self-consistent c-number equations.

A simple and possibly relevant example of what I have in mind arises when considering strongly bound states in the (classical) field theory of (attractive) massive vector mesons interacting with fermion fields. The additional effects we expect have already been discussed qualitatively in Section 2.3.

We consider a fermion field coupled to a vector meson field with the Hamiltonian¹⁶⁾ (with $A \cdot A \equiv A^2 = A_0^2 - \vec{A} \cdot \vec{A}$)

$$H = \frac{1}{2} \left\{ \int d^3x \frac{1}{2} [\hat{\Psi}^\dagger (\vec{\alpha} \cdot \vec{p} + \beta m - g_v (\vec{\alpha} \cdot \vec{\hat{A}} - A^0)) \hat{\Psi}] - \frac{1}{2} \int d^3x [\hat{\pi}_\mu^2 + (\nabla \hat{A}_\mu)^2 + W(\hat{A} \cdot \hat{A}) - W(0)] + h.c. \right\}, \quad (4.93)$$

where $W(A^2)$ is an arbitrary potential energy of the vector field A_μ , which leads to the equations of motion

$$(\vec{\alpha} \cdot \vec{p} + \beta m - g_v (\vec{\alpha} \cdot \vec{\hat{A}} - \hat{A}_0)) \hat{\Psi} = i \frac{\partial \hat{\Psi}}{\partial t} \quad (4.94)$$

$$\hat{\pi}_\mu - \Delta \hat{A}_\mu + \hat{A}_\mu \frac{\partial W}{\partial A^2} = \frac{g_v}{2} [\hat{\Psi}, \gamma_\mu \hat{\Psi}]. \quad (4.95)$$

We also have the auxiliary condition

$$\langle ps | \partial_\mu \hat{A}^\mu | ps \rangle = 0 \quad (4.96)$$

for any physical state $|ps\rangle$.

For strong interactions it is most convenient to choose as the basis for the expansion of the Fermi field ψ the complete set of solutions of the Dirac equation with an average field A_c (p stands for both discrete and continuous indices):

$$(\vec{\alpha} \cdot (\vec{p} - g_v \vec{A}_c) + \beta m + g_v A_c^0) \psi_p = \epsilon_p \psi_p. \quad (4.97)$$

The field operator is expanded in the quasi-particle Fock space as

$$\psi(\vec{x}, 0) = \int_m^\infty b_\epsilon \psi_\epsilon(\vec{x}) d\epsilon + \sum_{m > \epsilon_p > -m} b_p \psi_p(\vec{x}) + \int_{-\infty}^{-m} d_\epsilon^\dagger \psi_\epsilon(\vec{x}) d\epsilon, \quad (4.98)$$

whenever the field A_c^μ is undercritical. A different expansion is appropriate, as discussed in Section 2.3, when a resonance of Eq. (4.97) is embedded in the negative energy continuum and the total energy remains positive. Then we have

$$\begin{aligned} \psi(\vec{x}, 0) = & \int_m^\infty b_\epsilon \psi_\epsilon d\epsilon + \sum_{m > \epsilon_p > m} b_p \psi_p + b_0 \int_{-\infty}^{-m} a(\epsilon) \psi_\epsilon d\epsilon \\ & + \int_{-\infty}^{-m} d_{\epsilon'}^\dagger \left[\int_{-\infty}^{-m} h_{\epsilon'}(\epsilon) \psi_\epsilon d\epsilon \right], \end{aligned} \quad (4.99)$$

where $a(\epsilon)$ and $h_{\epsilon'}(\epsilon)$ are suitable functions that describe the resonance in a negative energy continuum (see Section 2). If more than one resonance is embedded in the continuum, a generalization of Eq. (4.99) is in order.

It is important to stress again the difference between the self-consistent field problem and the case of an external field. The neutral vacuum, characterized by $b_n|0\rangle = d_n|0\rangle = 0$, may be a *stable*, zero-energy state even should supercritical binding described by (4.99) occur, since the total energy of the excited state $b_0^\dagger|0\rangle$ may be positive upon consideration of the meson energy included in Eq. (4.93), in contradistinction to the situation with *external* potentials.

Our choice of the mean field A_c^μ was directed by our desire to eliminate from the ground state most contributions from the virtual quasi-particle excitations. Therefore $A_c^\mu = \langle ps | A^\mu | ps \rangle$ and we obtain

$$-\Delta A_c^\mu + A_c^\mu \left(\frac{\partial W}{\partial A^2} \right)_{A_c^2} = g_v \langle ps | \frac{1}{2} [\hat{\bar{\Psi}}, \gamma^\mu \hat{\Psi}] | ps \rangle. \quad (4.100)$$

We consider the state $b_0^\dagger|0\rangle = |p\rangle$ as a trial state. Then Eq. (4.100) becomes (neglecting virtual vacuum polarization charge density):

$$-\Delta A_c^\mu + A_c^\mu \left(-\frac{\partial W}{\partial A^2}\right)_{A_c^2} = g_v \psi_0 \gamma^\mu \psi_0. \quad (4.101)$$

Here ψ_0 is the coefficient of b_0 in Eq. (4.99) or the lowest energy particle wave function in Eq. (4.98).

At this point, the interaction must be modified¹⁶⁾ to allow bound fermion states, bound only by 'electric' forces. That is to say the sign on the right-hand side of Eq. (4.10) has to be changed, as discussed in Section 4.3, Eq. (4.56):

$$-\Delta A_c^\mu + A_c^\mu \left(\frac{\partial W}{\partial A^2}\right)_{A_c^2} = -g_v \psi_0 \gamma^\mu \psi_0. \quad (4.102)$$

This change is motivated by the consideration of possible internal symmetry of the fields of interest -- the sign may be understood in analogy with the different possible signs of the z-component of the isospin. This change also means that the energy of the classical bound state becomes

$$E_v = E_{\text{Dirac}} + E_{\text{meson}} = \int d^3x \psi_0^\dagger (\vec{\alpha} \cdot \vec{p} + \beta m - g_v (\vec{\alpha} \cdot \vec{A} - A^0)) \psi_0 + \frac{1}{2} \int d^3x [(\nabla A_c^\mu)^2 + W(A_c \cdot A_c) - W(0)] = \int d^3x \mathcal{E}, \quad (4.103)$$

where we find

$$E_{\text{Dirac}} = \mathcal{E}_0 \quad (4.104)$$

In view of the arbitrary (but motivated) changes involved in writing (4.103), what follows should be understood only as illustrating a type of behaviour in a coupled field theory distinct from that found in the external field problem.

Let us devote the rest of our discussion to the special case

$$W = \mu^2 A^2 \quad (4.105)$$

where μ is the vector meson mass. We recall from Eq. (4.57) that the total energy is given by

$$E_{\text{eff}}^A = \int d^3x (\mu^2 A^2 + m \bar{\psi}_0 \psi_0). \quad (4.106)$$

The energy E_{eff}^A is positive definite if the scalar integral $\int d^3x \bar{\psi}_0 \psi_0$ is positive. No lower bound for the scalar integral is known when vector fields are present, but in all examples studied numerically it has been found to be positive definite and very small for large g_V^2 .

Equations (4.97) and (4.102) have been solved numerically with $W = \mu_V^2 A^2$ for the lowest energy particle state such that the Dirac wave functions (either eigenstates or resonances) are normalized to one. In Fig. 4.9 we show the energy of the bound fermion, E_{Dirac} [Eq. (4.97)], and the total energy E_V [Eq. (4.103)], as a function of the coupling constant g_V for vector meson masses $\mu = 0.2$ and $0.4m$. The energy is measured as usual in units of the bare fermion mass m . In this example, we see that the total energy is always positive for coupling constants $g_V^2/4\pi \gtrsim 4$, while the Dirac eigenvalues E_{Dirac} take large negative values. The scalar integral is a negligible contribution to E_V , Eq. (4.103), for strong coupling. Exact agreement of numerical results with those expected from the virial theorem [Eq. (4.106)] (as long as $E_{\text{Dirac}} > -m$) has been found. This is also a good check of the computer codes involved in solving the non-linear equations (4.97) and (4.102).

The main conclusion that can be drawn from this exercise is the recognition that in this simple model *the total energy of the strongly bound state lies above that of the neutral vacuum*, i.e. $E_V > 0$ even when the self-consistent potential is supercritical, i.e. $\epsilon_0 < -m$. Therefore the neutral vacuum is the stable ground state of the theory. Further we note that essential in obtaining a proper solution of Eqs. (4.97) and (4.102) is a proper treatment of resonant states in the antiparticle continuum when they occur. As described in Sections 1 and 2, the proper description of the system involves then the amplitude:

$$\psi_0 \approx \int_{-\infty}^{-m} \alpha(E) \psi_E dE. \quad (4.106)$$

Without the proper understanding of the supercritical spectrum a solution would seem discontinuous at the critical points, since we would take the lowest *discrete* state, for example a 2s state in place of the embedded 1s-state resonance.

Another way of seeing the difference between the presently considered case and the external field problem studied at the beginning of this paper involves the Green's function formulation considered in Section 2.1. There we learned that the pole associated with the critical state cannot drag the integration path off the real axis, as the *external potential* attains overcritical strength. Now, we have shown that the opposite is true for interacting fields studied in this subsection. The integration path C' of Fig. 2.3 should be taken to obtain the Green's function in the case of the interacting fields, instead of the previously

employed path D. A quite different result would follow if we had found that E_v in Eq. (4.103) is actually a negative quantity at certain values of g_v^2 . Then the path D would have to be taken again and we would expect that the vacuum state is really the charged vacuum. In contrast to the external field case we would then be faced with a microscopic phase transition. At every point in space the vacuum would be charged. Thus another procedure would be needed to determine the new ground state, since it is impossible to describe such a global change of the world by the single-mode approximation.

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Figure captions

- Fig. 1.1 : Z-dependence of the eigenvalues for electrons bound to a uniformly charged sphere. The dashed curves refer to results for a point nucleus.
- Fig. 1.2 : Energy eigenvalues based on a scalar potential with strength g .
- Fig. 1.3 : Solution of the Klein-Gordon equation with external gravitational field. The eigenstates collapse to $\epsilon = 0$ as the Schwarzschild metric is approached.
- Fig. 1.4 : Phase shifts for square-well potentials with strengths near the critical potential.
- Fig. 1.5 : The energy dependence of $\sin^2 (\delta - \delta_0)$ for several square wells with strengths near the critical potential.
- Fig. 1.6 : The energy dependence of $\sin^2 (\delta - \delta_0)$ in an overcritical electrostatic potential $Z = 184$.
- Fig. 1.7 : The positions of the $1s_{\frac{1}{2}}$ and $2p_{\frac{1}{2}}$ resonances as functions of the nuclear charge.
- Fig. 1.8 : Quasi-molecular correlation diagrams for several supercritical systems; both point- and finite-size nuclei are considered.
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- Fig. 2.1 : The relation between energy and charge for (a) undercritical and (b) overcritical potentials.
- Fig. 2.2 : The conventional choice of the contour in the complex ω plane. The contour C crosses the real axis at the Fermi energy ϵ_F .
- Fig. 2.3 : The contours in the overcritical case.
- Fig. 3.1 : The unscreened charge γ and the total charge of the vacuum ($Z - \gamma$) as a function of Z . The crosses denote points from single-particle calculations. The dashed line denotes the nuclear charge Z .
- Fig. 3.2 : The solutions of the relativistic Thomas-Fermi equation (3.7) for selected values of the nuclear charge as a function of r . Curve 1 -- $Z = 600$; curve 2 -- $Z = 1000$; curve 3 -- $Z = 2000$; curve 4 -- $Z = 5000$; curve 5 -- $Z = 10,000$; curve 6 -- $Z = 10^5$; curve 7 -- $Z = 10^6$. a) The self-consistent potential; b) the corresponding charge distribution of the vacuum.

- Fig. 3.3 : The total charge densities, scaled with γ . Same selected values of nuclear charge as in Fig. 3.2.
- Fig. 3.4 : Transmission coefficients as functions of energy.
- Fig. 4.1 : The effective quasi-particle mass $m^* = m_q - g\varphi_c$ (in units of m_q) as a function of r (in units of m_q^{-1}) for $\mu/m_q = 0.02, 0.1, 0.4$ and $g^2 = 2260, 1072, 642, 777$, correspondingly. The dashed curves are the vector and scalar densities for $\mu = 0.4m_q$, $g^2 = 642$ and $\mu = 0.02m_q$, $g^2 = 2260$. The vector density is normalized to one.
- Fig. 4.2 : The mass density of the soliton solution as a function of r ; several values of the characteristic parameters g^2 and μ in a double-logarithmic plot.
- Fig. 4.3 : The total mass M_N in units of the quark mass of several quark states; baryons ($N = 3$), mesons ($N = 2$) and exotic baryons ($N = 6$) as a function of the coupling constant g^2 for several values of the gluon mass $\mu/m_q = 0.02, 0.1, 0.4$.
- Fig. 4.4 : The product of the lowest positive Dirac eigenvalue with r.m.s. radius of the amplitude ψ_0 as a function of $\ln g^2$.
- Fig. 4.5 : The product of the mass of the quark bag with the r.m.s. radius as a function of $\ln g^2$.
- Fig. 4.6 : The structure constants of SU(6) hadrons as a function of the coupling constant g^2 for several values of the gluon mass, $\mu/m_q = 0.02, 0.1, 0.4$. a) The product of the mass of the baryon with its size. b) The same as in (a) for mesons. c) The magnetic moment of protons. d) The axial-coupling constant g_A . e) The ratio R_a of the energy (momentum) carried by the quarks to that carried by the neutral glue.
- Fig. 4.7 : The energy H and the eigenfrequency ϵ_0 as a function of the dimensionless coupling constant β : a) in units of m ; b) in units of $G^{-\frac{1}{2}}$.
- Fig. 4.8 : The soliton solutions of self-coupled Dirac fields for $\beta = 22, 475, 2125$. a) The effective mass m^* ; b), c), d) the scalar and vector densities.
- Fig. 4.9 : The Dirac eigenvalue and total energies of interacting Dirac-vector meson fields.

Fig. 1.1

Fig. 1.2

Fig. 1.3

Fig. 1.4

Fig. 1.5

Fig. 1.6

Fig. 1.7

Fig. 1.8

Fig. 1.9

Fig. 2.1

Fig. 2.2

Fig. 2.3

Fig. 3.1

Fig. 3.2

Fig. 3.3

Fig. 3.4

Fig. 4.1

Fig. 4.2

Fig. 4.3

Fig. 4.4

Fig. 4.5

Fig. 4.6

Fig. 4.7

Fig. 4.8

Fig. 4.9