Bound states of spinless particles with Coulomb interaction in the momentum representation

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Bound-state solutions of the Klein–Gordon Coulomb equation for vector and scalar potentials are investigated in the momentum representation. The collapse of the particle to the center for strong vector potentials is found. The corresponding wave function shows an anomalous oscillatory behaviour for large particle momentum. Particle collapse for strong scalar potentials does not exist.

L'on étudie les états liés à l'équation Klein–Gordon avec des potentiels coulombiens vectoriels et scalaires, dont les représentations d'impulsion. L'on y voit que la particule collapse vers le centre pour des potentiels forts. La fonction d'onde correspondante présente un comportement oscillatoire anormal pour de grandes valeurs de l'impulsion de la particule. Ce collapse ne se présente pas dans le cas de potentiels scalaires.

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1. Introduction

The Klein–Gordon equation (KGE) was the first relativistic quantum mechanical wave equation (1, 2). Nevertheless, the KGE was temporarily discarded, since the predicted spread of the fine structure of the H atom levels was much larger than was observed experimentally. The search for new relativistic equations culminated in the Dirac equation (3). At present, it is well known that the KGE describes a particle that has no spin, while the Dirac equation holds for spin 1/2 particles. In the last decade, the energy levels of spinless particles in the Coulomb field (for instance, pionic atoms) have been measured (4) and the KGE correctly predicts this spectrum. Hence, the original interest shown in this equation has been renewed.

The KGE for the Coulomb potential can be easily rewritten in the Schrödinger form (5), in the position representation, even in N-space dimensions (6). We shall see that the above statement also holds in the momentum representation. The momentum operators, in general curvilinear coordinates, have recently been discussed and reviewed by Zhang (7); in particular, the Hermiticity of these operators in spherical polar coordinates has been reexamined. In previous works, Lombardi (8, 9) has shown that for spherical polar coordinates the transform preserving the conjugate character of the variables is not of the Fourier type. The Fourier-transform space cannot be regarded as a true momentum space, since the variables, representing the total momentum and its polar coordinates, are not conjugate to any of the relevant spatial variables; in addition, these polar coordinates are not found to be Hermitian, so they do not represent physical magnitudes. Lombardi has solved the angular and the radial parts of the Schrödinger (8) and the Dirac (9) equations in a true momentum representation for particles in the electrostatic Coulomb potential. The radial wave function is solved with the aid of fractional-calculus techniques. In discussing his results, this author also pointed out that the momentum wave function for Dirac particles in a strong Coulomb field break down mathematically, as occurs in the position representation for such a potential.

One of the aims of this work is to extend previous treatments, including relativistic spinless particles, by solving the KGE directly in the momentum representation. In so doing, we shall be led to a second-order differential equation for the momentum wave function. Solutions of the radial equation are found by means of the usual techniques of differential equations, so we avoid the less common fractional calculus to clarify the solution of the problem. Provided that the bound-state solutions are square-integrable solutions, the energy levels of the particle are found in a straightforward manner. We also discuss the wave-function behaviour as the electrostatic potential becomes very strong; we shall come to the conclusion that single-particle wave equation can no longer describe spinless particles in a strong external Coulomb field (just as occurs for π mesons in superheavy nuclei). A relativistic field theory is indeed required to fully understand the phenomenon. Before concluding, however, a simple way to smear out the Coulomb singularity will be shown, if the single-particle treatment in the moment representation is to be retained.

2. Bound state solutions

As a generalization, we consider not only electrostatic potentials $V(r)$ (the time component of a four-vector) but also scalar $S(r)$ Coulomb potentials in the KGE. A scalar potential means that the particle mass is regarded as a function of the position. This kind of coupling can play an important role in describing spinless mesons like the σ meson, on which the well-known σ model of Gell–Mann and Lévy is based. The scalar Coulomb potential could originate from the exchange of massless scalar mesons between particles, in the same way as the electrostatic Coulomb field arises from the exchange of photons (10). To find the particle wave function for such a coupling, we replace m by $m+S(r)$ in the usual KGE, which is then written as ($\hbar = c = 1$)

$$[1] \quad \{p^2 + (m + S(r))^2 - (E - V(r))^2\}\,\psi(r) = 0$$

where $V(r) = -K_v/r$ and $S(r) = -K_s/r$. The angular part of the wave function in the momentum space becomes identical to the nonrelativistic results previously derived (8) and here we shall omit any detail. The radial part of the wave function is obtained from the following equation

$$[2] \quad \left\{-\left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{1}{r}\right)^2 + \frac{s(s+1)}{r^2} + m^2 - E^2 - 2(EK_v + mK_s)\frac{1}{r}\right\}\psi(r) = 0$$

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with $s(s+1) = l(l+1) + K_s^2 - K_v^2$. The possible values of the parameter s are

$$s_\pm = -1/2 \pm (1/2)[(2l+1)^2 + 4K_s^2 - 4K_v^2]^{1/2}$$

which satisfy $1 + s_\pm = -s_\mp$. For the moment, we consider only the real values of these parameters; in the next section we extend the discussions for including complex values of $s_\pm$.

To determine the equation governing the wave function $\psi(p)$ in the momentum representation, we would make the following operator replacements in [1]:

$$[3] \qquad -i\left(\frac{d}{dr}+\frac{1}{r}\right)\rightarrow p \qquad \frac{1}{r}\rightarrow -i\int^p dp'$$

where p is the Hermitian conjugate of r satisfying $[r,p] = i$. The lower limit of integration is chosen to ensure the condition $r^{-1}(r\psi(p)) = \psi(p)$. Transforming to momentum space we obtain

$$[4] \qquad (p^2 + m^2 - E^2)\psi(p) + 2i(EK_v + mK_s)\int^p dp'\,\psi(p') - s_\pm(s_\pm+1)\int^p dp'\int^{p'} dp''\,\psi(p'') = 0$$

Differentiating [4] twice with respect to p (this is equivalent to multiplying the KGE by a factor of r^2 in the position representation) we are led to a second-order differential equation. For the sake of simplicity we also introduce the dimensionless parameters

$$\eta = (m^2-E^2)^{1/2} \qquad \text{(real for bound states)}$$

$$\beta \equiv (EK_v+mK_s)/\eta$$

and the new variable

$$q = 2/[1+ip/\eta]$$

Finally, the following equation is obtained:

$$[5] \qquad \left\{(1-q)q^2\frac{d^2}{dq^2} + (\beta q-2)q\frac{d}{dq} + (2-s_\pm-s_\pm^2)\right\}\psi(q) = 0$$

which can be easily solved in terms of hypergeometric functions ${}_2F_1(a,b;c;z)$. The solution is as follows:

$$[6] \qquad \psi(q) = A\phi(1+s_\pm,\beta,q) + B\phi(-s_\pm,\beta,q)$$

with

$$\phi(z,\beta,q) = q^{z+1}\,{}_2F_1(z+1,\, z-\beta;\, 2z;\, q)$$

and A and B being two constants. Since $1+s_\pm = -s_\mp$ we can choose a unique value of the parameter s, so we shall take $s = s_+ \equiv s_l$ hereafter (the subscript indicates the dependence on l).

The asymptotic behaviour of solution [6] for high momenta is given by

$$\psi(p)\sim A(ip/2\eta)^{-s_l-2} + B(ip/2\eta)^{s_l-1}$$

Therefore, to obtain a finite expectation value for the operator

$$r^{-2}\rightarrow -\int dp\int dp'$$

appearing in the KGE, we reach the conclusion that B must vanish. The first term also diverges at low mometum values ($q\rightarrow 2$), unless the hypergeometric function is reduced to a polynomial expression. The quantum condition $\beta - s_l = n-l$ is then reached, $n = 1,2,\ldots$ being the principal quantum number (the usual inequality $n \geqslant l+1$ is deduced by taking into account $\beta - s_l$ must be a nonzero positive integer). This condition leads to the following equation for the allowed energy levels of the particle:

$$[7] \qquad +(m^2 - E_{nl}^2)^{1/2} = E_{nl}K_v/(n-l+s_l) \qquad E_{nl}K_v > 0$$

in a pure vector Coulomb field ($K_s = 0$), which is, of course, the same equation as that obtained by solving the KGE in the position representation. Note that this expression (and also the KGE) is invariant under the transformation $E\rightarrow -E$, $K_v\rightarrow -K_v$. This means that bound-state energies are positive for attractive potentials ($K_v > 0$), and that the binding or particles with negative energy for repulsive potentials ($K_v < 0$) exists.

For pure scalar Coulomb potential ($K_v = 0$), the energy levels are found through the relation

$$[8] \qquad +(m^2-E_{nl}^2)^{1/2} = mK_s/(n-l+s_l) \qquad K_s > 0$$

Pairs of energy levels appear in the case of attractive potentials $K_s > 0$ ([8] and the KGE remains unchanged by transforming $E\rightarrow -E$). This result agrees with the fact that a pure scalar potential can bind particles as well as antiparticles. There are no bound states for repulsive potentials $K_s < 0$.

From [6], the wave function in the momentum representation is found to be

$$[9] \qquad \psi_{nl}(p) = \sum_{t=0}^{n-l-1} 2^t\frac{(s_l+2)_t\,(1+l-n)_t}{t!\,(2s_l+2)_t}\left[\frac{1+ip}{(m^2-E_{nl}^2)^{1/2}}\right]^{-t-s_l-2}$$

where the normalization factor has been omitted. The Pochhammer symbol is defined in the usual form $(a)_0 = 1$ and $(a)_t = a\,(a+1)\ldots(a+t-1)$. In particular, the ground-state wave function is easily written as

$$[10] \qquad \psi_g(p) = 1 + ip/(m^2 - E_g^2)^{1/2-s_0-2}$$

where E_g denotes the ground-state energy.

As Lombardi pointed out (8), some advantages of using the momentum wave function are obtained as compared with the usual position solution (written in terms of generalized Laguerre polynomials) and to the standard Fourier-transform solution (given by Gegenbauer polynomials). As seen from [9], $\psi(p)$ is expressed as finite sums over imaginary poles; therefore, any matrix element is more easily calculated in the momentum representation than in the position representation if one invokes the tools of complex-plane calculus. Also, one should consider the momentum p as a complex variable (this fact cannot be deduced from the standard Fourier-transform solution); poles of $\psi(p)$ in the complex plane are related to ionisation potentials and dipole moments. This realization would be useful in relativistic treatments of multielectron atoms and molecules, where the KGE could provide a first insight into the problem. Obviously, these results could be subsequently improved by including the spin effects and the Darwin potential in a variational or perturbative way.

3. Effects of strong coupling

In the previous section, only real values of s_l have been considered; i.e., we have assumed that the condition $K_v^2 - K_s^2 < (l+1/2)^2$ was fulfilled. This inequality allows us to find normalizable wave functions, with the right behaviour for large

p values; the energy of the particle is always a real quantity and becomes quantized. Thus we are dealing with truly bound-state solutions. On the other hand, for $K_v^2 - K_s^2 > (l + 1/2)^2$ the parameter s_l becomes a complex number and it is then possible to write $s_l = -1/2 + i\gamma_l$, where

$$\gamma_l \equiv +[K_v^2 - K_s^2 - (l + 1/2)^2]^{1/2}$$

is a real parameter. Therefore, the wave function given in [6] rapidly oscillates

$$\psi(p) \sim p^{-3/2} \cos(\gamma_l \log p + \text{constant})$$

for large particle momenta, and hence it is found to be unnormalizable in the usual fashion. Moreover, in this case it is an easy matter to see that the square of the operators given in [3], which are related to the kinetic and potential energies of the particle, present infinite expectation values. Although the energy of the state satisfies the condition $|E|<m$, it never becomes a bound state. This anomalous behaviour, which does not depend on the attractive or repulsive nature of the potentials, should be regarded as a "collapse of the particle to the center." As far as we know, this problem has only been treated in the position representation before.

In the position representation, particle "falling" appears when the wave function $\psi(r)$ oscillates rapidly near the origin without reaching any limit (11, 12), presenting an essential singularity at that point. Moreover, the energy spectrum becomes continuous even if $|E| < m$, since no appropriate boundary conditions exist at $r=0$. Solutions of the KGE in the position representation show this particular behaviour for $K_v^2 - K_s^2 > (l+1/2)^2$ in the point-charge approximation for the nuclear size (in ref. 13 Popov has found that the falling of spin-0 particles occurs in electrostatic fields whenever $|K_v|>(l + 1/2)$). For the Dirac equation the collapse to the center occurs for $K_v^2 - K_s^2 > (j+1/2)^2$ (see ref. 14 for a detailed description of Dirac particles in overcritical electrostatic potentials). To get some insight into this problem, let us consider the radial KGE for small r values (for simplicity we also take $l = 0$):

$$[11] \quad \left\{-\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{1}{r}\right)^2 - \frac{K_v^2 - K_s^2}{r^2}\right\}\psi(r) = 0$$

which is a Schrödinger-like equation for the potential well $-(K_v^2 - K_s^2)/r^2$. It is well known that [11] has no square-integrable solutions for $K_v^2 - K_s^2 > 1/4$, in accordance with our previous suggestion that there are simply no bound states corresponding to large K_v.

To obtain further progress and substantiation on the behaviour of the particle wave function in strong electrostatic fields, we transform [11] to momentum space by using the prescriptions given in [3], and hence we obtain

$$[12] \quad p^2 \frac{\mathrm{d}^2\psi(p)}{\mathrm{d}p^2} + 4p\frac{\mathrm{d}\psi(p)}{\mathrm{d}p} + (2 + K_v^2 - K_s^2)\psi(p) = 0$$

whose solution is readily found to be $\psi(p) = p^{i\gamma_0 - 3/2}$, showing the anomalous oscillatory behaviour at large p values when $K_v^2 - K_s^2 > 1/4$, as seen above. We conclude that the occurrence of an essential singularity in the position wave function at the origin leads to the oscillations of the momentum wave function for large p values. This can be roughly understood by noting that the contribution of higher p values becomes important only near the origin (large kinetic energy), so there exists an obvious relation between $\psi(r)$ at the origin and $\psi(p)$ at high values of the particle momentum.

We should emphasize that the collapse of the particle has been discussed in terms (and within the limitations) of a single-particle wave equation. A many-particle approach is indeed necessary for a full description of strongly bound states (15). By using these kinds of theories, one notices that the vacuum becomes unstable against the creation of an indefinite number of virtual pairs, as the electrostatic coupling constant exceeds the overcritical value. To guarantee stable bound states, one must take into account the self-interaction of the boson field; i.e., we need a relativistic field theory (16). This description is beyond the scope of our single-particle treatment.

To extend the simple single-particle description of spinless particles to include strong electrostatic fields, one should assume some other physical considerations like the extended charge of the nucleus or the vacuum polarization. Allowance for the finite nuclear size avoids the collapse of the particle in position space because the singularity of the potential at the origin is removed. In addition, the vacuum polarization also results in the regularization of the Coulomb potential near the origin. Although the vacuum polarization is actually a many-particle effect, one can deal with it by considering an effective smooth potential at the origin in the single-particle wave equation. From the discussions above, one can observe that a "cut-off" P for large values of the particle momentum would also prevent particle falling. Therefore, the regularization of the Coulomb potential in the momentum space can be achieved by imposing a maximum particle momentum value P. The value of P may be roughly estimated to be $\sim R^{-1}$ because of the uncertainty relation, where R denotes here the cut-off for the Coulomb potential. For any arbitrarly large value of the electrostatic coupling constant, bound states could indeed appear by requring the boundary condition $\psi(P) = 0$ whenever the ground state does not dive into the continuum of negative energy. This condition also guarantees finite expectation values of the kinetic and potential energies of the particle. Unfortunately, it is also expected that the particle energy will strongly depend on the cut-off momentum P. The limit of the solutions as $P \to \infty$ will not be defined when the potential becomes overcritical.

Finally, note that this problem is absent for strong scalar potentials since s_l is always real in this case ($K_s^2 > K_v^2$), no matter how strong K_s is (also observe in [11] that the potential term r^{-2} behaves like a repulsive barrier rather than a well in this situation). The energy levels are compressed altogether and approach zero for strong coupling, as can be checked from [8]. The particle remains bounded in this limit. This regular behaviour could be easily explained if we note that the scalar potential couples the mass rather than the charge, and hence it cannot create charged virtual pairs, so the vacuum becomes stable even for strong potentials.

4. Conclusions

We have reached the following conclusions:

1. The Klein–Gordon Coulomb equation with both vector- and scalar-type potentials can be solved exactly in the momentum representation for all partial waves. The wave functions can be expressed as finite sums over poles lying on the imaginary axis for bound states.
2. Positive and negative bound-state levels occur for attractive and repulsive vector potentials, respectively, provided that

the coupling constant does not exceed the critical value $l + 1/2$. Pairs of bound-state levels appear ($\pm E$) for attractive scalar potentials. Nevertheless, there exists no binding of particles for repulsive scalar potentials.

3. Strong vector potentials (coupling constant exceeding $l + 1/2$) show the collapse of the particle to the center. The corresponding wave function oscillates rapidly for large particle momentum and becomes unnormalizable in the usual way. Therefore, there exists no binding of particles for such a electrostatic Coulomb potential. Nevertheless, one can overcome this difficulty by considering a maximum allowed value of the particle momentum, an equivalent procedure to regularize the Coulomb potential near the origin in the position representation. On the other hand, there is no particle falling for strong scalar potentials, which can support bound states.

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