States of the Dirac Equation in Confining Potentials

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We study the Dirac equation in confining potentials with pure vector coupling, proving the existence of metastable states with longer and longer lifetimes as the nonrelativistic limit is approached and eventually merging with continuity into the Schrödinger bound states. The existence of these states could concern high energy models and possible resonant scattering effects in systems like graphene. We present numerical results for the linear and the harmonic cases and we show that the density of the states of the continuous spectrum is well described by a sum of Breit-Wigner lines. The width of the line with lowest positive energy well reproduces the Schwinger pair production rate for a linear potential: this gives an explanation of the Klein paradox for bound states and a new concrete way to get information on pair production in unbounded, nonuniform electric fields, where very little is known.

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The absence of bound states for the Dirac equation in confining potentials poses a delicate question of physical interpretation. It was in fact shown in [1] that the asymptotically oscillating behavior of the solutions of the Dirac equation with vector coupling and a potential given by a positive power of the modulus of the position variable implies a purely continuous spectrum. The result has been subsequently confirmed and generalized by proving that even any self-adjoint extension of the boundary value problem has only a purely continuous spectrum [2]. This situation is contrary to physical intuition and makes it hard to justify a perturbative approach to the relativistic corrections, since no definite perturbed eigenvalues exist. Most later investigations have therefore tried different ways to introduce confining potentials into the Dirac equation, e.g., by scalar coupling or by projection onto the large component (see [3] for a review); in doing so, however, we do not find an appropriate description of physically relevant systems such as charged particles in strong electric fields. A possible way out of this difficulty was given in the mathematical paper [4], where a so called "weak quantization" was introduced to treat the $(1 + 1)$-dimensional Dirac equation with a linear potential. The analysis is developed in the complex plane of the energy; when the Schrödinger limit is approached it is shown that the real part of the energy converges to the nonrelativistic spectrum and the imaginary part becomes exponentially vanishing. For a linear potential, analytical solutions are available in terms of special functions and in [4] the spectral quantities were estimated by perturbative expansions, having thus a very limited range of validity, out of which no general picture can emerge. Moreover a coherent physical interpretation was clearly outside the mathematical purpose of the author. To our knowledge no further development along these lines is found in literature since.

From a physical point of view, the presence of an unbounded increasing potential brings to bear upon the problem arguments similar to those of the Klein paradox, widely studied both in first and in second quantization [5–7]. Recently, a field-theoretical interpretation using numerical methods based on spatial and temporal resolution was given in [8], where it is found that the pair production by the potential is suppressed when the spatial density of the incoming electron overlaps with the potential region and that the transmitted portion of the wave packet, in a single particle description, corresponds to the amount by which the electron reduces the positron's spatial density. Although in this Letter we strictly remain in a first quantized framework and we are dealing with the stationary problem defined by the Dirac equation rather than with a scattering picture, still we shall see that the pair production rate is recovered in a natural way. Our treatment follows the classical methods of the spectral analysis [9,10], and, in particular, it deals with an accurate evaluation of the density of the states of the continuous spectrum. It can be compared with the phenomenological approach in terms of Gamow vectors [11], mainly used to describe resonances in composite systems of solid state and nuclear physics. The investigation is necessarily numerical; thus it does not suffer the limitations of the perturbative expansion and it can easily be extended to more general potentials for which analytical solutions do not exist. We will present in detail the results of the linear and quadratic potentials. The general situation can be summarized as follows. In nonrelativistic quantum mechanics the spectrum is discrete, the eigenvalues correspond to the real zeroes and poles λ_i of a spectral function introduced by Weyl (traditionally denoted by $m(\lambda)$, [9]) and the density of the states reduces to a sum of δ functions, one for each bound state. In the Dirac equation the λ_i move off the real axis, the spectrum becomes purely continuous and the density of the states, $\rho(\lambda) = -\mathrm{Im}(m(\lambda)) + \mathrm{Im}(1/m(\lambda))$ for real λ, appears now as a sum of Breit-Wigner (BW) lines whose central values, determined by $\mathrm{Re}(\lambda_i)$, are closer and closer to the nonrelativistic eigenvalues and whose widths, determined by $\mathrm{Im}(\lambda_i)$, are more and more narrow for decreasing values of the ratio of the interaction to the mass energy.

The physical interpretation suggested by these facts is that the broadening of the δ lines is due to transitions between positive and negative energy sectors induced by the supercritical field; thus, although in the relativistic context the nature of the spectrum is completely changed, still narrow BW lines signify the presence of metastable states, giving rise to resonances in the scattering cross section around the line energies. On the one hand, therefore, the continuity to the nonrelativistic states is recovered. On the other, contrary to what occurs for the Schrödinger ground state, in the relativistic regime also the lowest positive energy state decays. The second quantized counterpart of this fact is that the Fock vacuum will not remain such forever, but, according to the usual theory of the effective action [6,12], it will decay with the exponential law $|\langle 0(t)|0(t+T)\rangle|^2 = \exp(-VTw^f)$, where w^f is the pair production rate for unit volume and unit time. We thus expect similar behaviors of the line width of the lowest positive energy state and of the pair production vs the interaction strength. This circumstance appears very well verified for the pair production rate in a constant electric field, as obtained by Schwinger [13,14], so that we are led to assume that the width of the first resonance can provide a quantum mechanical way of estimating the pair production for general situations where little is known from QED, as in the case of unlimited growing potentials (see [15,16] for recent developments). We then present new data for a quadratic potential, corresponding to an electron in a uniformly growing electric field, finding a pair production behavior very similar to the Schwinger's one. We finally believe that our results can be relevant not only in model building of quark systems [17,18], but also in investigations of Klein paradox in strong crystalline fields [19] as well as in the very recent and expanding subject of the graphene physics, where the influence of impurities is described by the Dirac equation with vector coupling [20]: the metastable states may prove essential for understanding possible effects of resonant scattering.

Consider the $(1+1)$-dim Dirac equation in a unit system with $\hbar = 1$,

$$\psi'(x) - [(1/c)\{E - U(x)\}i\sigma_y + mc\sigma_x]\psi(x) = 0 \quad (1)$$

where $\psi(x) = {}^t(\psi_1(x), \psi_2(x))$ and σ_i are the Pauli matrices. For the family of even potentials $U(x) = a|x|^n$ the Eq. (1) can be studied in $[0, \infty)$, having infinity as the unique singularity in the limit point case [9]. Therefore, from the Weyl general theory of singular boundary value problems [9,10], for $\mathrm{Im}(E) > 0$ there exists only one normalizable solution $\tilde\psi(x)$ of the equation, up to a constant factor. If $\{\psi^{(i)}(x,E)\}_{i=1,2} \equiv \{{}^t(\psi_1^{(i)}(x,E), \psi_2^{(i)}(x,E))\}_{i=1,2}$ is a fundamental system of spinor solutions of (1) corresponding to the initial conditions $\psi_j^{(i)}(0,E) = \delta_j^i$, $i, j = 1, 2$, the Weyl function $m(E)$ is defined by the expansion $\tilde\psi(x,E) = \psi^{(1)}(x,E) + m(E)\psi^{(2)}(x,E)$. Thus, because of the normalizability of $\tilde\psi(x)$, $m(E) = -\lim_{x\to\infty}\psi_i^{(1)}(x,E)/\psi_i^{(2)}(x,E)$ for both spinor components $i = 1$ and 2. From the conditions in zero we also have

$$m(E) = \tilde\psi_2(0,E)/\tilde\psi_1(0,E). \quad (2)$$

Finally the density of the states for real E_0 reads [10],

$$\rho(E_0) = \lim_{\nu\to 0+}(-\mathrm{Im}\{m(E_0 + i\nu)\} + \mathrm{Im}\{1/m(E_0 + i\nu)\}). \quad (3)$$

For calculation reasons, we find it convenient to define

$$\phi(x) = {}^t(\phi_1(x), \phi_2(x)) = 2^{-(1/2)}i(\sigma_y + \sigma_z)\psi(x) \quad (4)$$

obtaining for $\phi(x)$ the following equation:

$$\phi'(x) - [(i/c)\{E - U(x)\}\sigma_z - mc\sigma_x]\phi(x) = 0. \quad (5)$$

As previously we denote by $\{\phi^{(i)}(x,E)\}_{i=1,2}$ the fundamental spinor solutions of (5) with initial conditions $\phi_j^{(i)}(0,E) = \delta_j^i$. Hence, if $\tilde\phi(x,E)$ is the normalizable solution of (5) corresponding to $\tilde\psi(x,E)$ and we expand $\tilde\phi(x,E) = \phi^{(1)}(x,E) + \kappa(E)\phi^{(2)}(x,E)$, we have again the finite limit

$$\kappa(E) = -\lim_{x\to\infty}\phi_i^{(1)}(x,E)/\phi_i^{(2)}(x,E), \qquad i = 1, 2, \quad (6)$$

or the equivalent expression $\kappa(E) = \tilde\phi_2(0,E)/\tilde\phi_1(0,E)$. The relation between $m(E)$ and $\kappa(E)$ is thus found to be

$$m(E) = i[\kappa(E) + i][\kappa(E) - i]^{-1}. \quad (7)$$

Finally, introducing the "nonrelativistic energy" E_{NR} by $E = E_{\mathrm{NR}} + mc^2$, the elimination of $\phi_2(x)$ yields the second order equation for $\phi_1(x)$

$$\phi_1''(x) + [2m\{E_{\mathrm{NR}} - U(x)\} + c^{-2}R(x)]\phi_1(x) = 0 \quad (8)$$

where $R(x) = icU'(x) + \{E_{\mathrm{NR}} - U(x)\}^2$. The nonrelativistic limit for $c \to \infty$ is then evident.

Let us now consider the specific cases of the potentials $U(x) = \mathcal{E}|x|$ and $U(x) = (1/2)m\omega^2x^2$. For the linear potential we introduce

$$y = (2m\mathcal{E})^{1/3}x, \quad \lambda = \left(\frac{2m}{\mathcal{E}^2}\right)^{1/3}E_{\mathrm{NR}}, \quad \Omega = \frac{1}{4c^2}\left(\frac{2\mathcal{E}}{m^2}\right)^{2/3} \quad (9)$$

and for the quadratic potential we let

$$y = (m\omega)^{1/2}x \qquad \lambda = (2/\omega)E_{\mathrm{NR}}, \qquad \Omega = \omega/(4mc^2), \quad (10)$$

so that in both cases the nonrelativistic limit is obtained for $\Omega \to 0$. Equations (1), (5), and (8), then, specify to

$$\psi'(y) - \Omega^{1/2}[\Lambda_n(y) i\sigma_y + (2\Omega)^{-1}\sigma_x]\psi(y) = 0 \quad (11)$$

$$\phi'(y) - i\Omega^{1/2}[\Lambda_n(y)\sigma_z + i(2\Omega)^{-1}\sigma_x]\phi(y) = 0 \quad (12)$$

$$\phi_1''(y) + [\Omega\Lambda_n^2(y) + i\Omega^{1/2} n y^{n-1} - (4\Omega)^{-1}]\phi_1(y) = 0 \quad (13)$$

with $n = 1, 2$ and $\Lambda_n(y) = \lambda + 1/(2\Omega) - y^n$. When $n = 1$ the normalizable solutions of (13) with complex spectral parameter are known [4], and they are all proportional to the cylinder function $D_{i\tau}(-z)$, with $\tau = (2\Omega^{1/2})^{-3}$ and $z = (-4\Omega)^{1/4}\Lambda_1(y)$. Carrying out the calculations previously described, it is straightforward to arrive at the expression for the density of the states for Eq. (11). The general properties of $\rho(\lambda, \Omega)$, as in (3), can be appreciated by looking at the complete numerical results. First we see the convergence to the Schrödinger levels when $\Omega \to 0$. For instance, the peaks of the first resonances for $\Omega = 0.01$ are located at 1.0197, 2.3274, 3.2284, 4.0555, 4.7756: these should be compared with the first zeroes of the derivative of the Airy function and of the function itself (even and odd solutions, respectively), 1.0190, 2.3384, 3.2482, 4.0884, 4.8201. Secondly, in comparison with the nonrelativistic case, the spacing of corresponding resonances decreases for increasing values of the energy and of the interaction strength. In Fig. 1 we present the plot of $\rho(\lambda, \Omega)$ for $n = 1$, $\Omega = 0.3$ and 1. The fit of the density of the states by a sum $\sum_{i=1}^{N} c_i \lambda_{0i}^2 \gamma_i [(\lambda^2 - \lambda_{0i}^2)^2 + \lambda_{0i}^2\gamma_i^2]^{-1}$ of BW curves with the appropriate parameters λ_{0i}, γ_i and coefficients c_i, gives a perfect superposition with $\rho(\lambda, \Omega)$.

In the left part of Fig. 4 we compare the width γ of the first resonance with the pair production per unit length and time in a uniform electric field [13], that in the variables (9) reads

$$w^f(\Omega) = -\pi^{-1}\ln[1 - \exp(-\pi/(4\Omega^{3/2}))]. \quad (14)$$

As stated above, the excellent agreement, without any free parameter to be adjusted, proves that pair production and line broadening are two different descriptions of a same physical situation. The minor differences, mainly for increasing Ω, can be partly assigned to the description of the spectrum in terms of BW lines and partly to the fact that the Schwinger pair production is an effective one-loop calculation, possibly under-estimating the actual production rate [15]: one could make these small differences vanishing not by exponential but only by power law corrections in Ω.

Similar considerations also apply to the quadratic potential [$n = 2$ in (11)–(13)], although the computational technique is now different. Actually, solutions of (13) exist in terms of triconfluent Heun functions H_T, [21], $\phi_1(y) = Ae^f H_T(p, -3, q, z) + Be^{-f} H_T(p, 3, q, -z)$, where $f = -i\Omega^{1/2}[\lambda + (2\Omega)^{-1} - y^2/3]y$, $p = (3(4\Omega)^{-2})^{2/3}$, $q = (12\Omega)^{1/3}[\lambda + (2\Omega)^{-1}]$ and $z = -i(2\Omega^{1/2}/3)^{1/3}y$. Unfortunately no sufficient information on the asymptotic behavior of H_T is available, to our knowledge, to determine the normalizable solutions for complex λ. Hence we use a completely numerical scheme that extends to any potential $U(x) = a|x|^n$, for which analytical solutions do not exist when $n \geq 3$.

The calculations are straightforward and follow step by step the theory we have previously summarized. First we find, by numerical integration, a fundamental system of solutions of (12), from which we determine $\kappa(\lambda)$ according to (6). Some care must be used in taking the limit, that is approached not in a monotonic but in an oscillating way, as is evident by looking at the asymptotic leading terms of (13): the convergence is increased by constructing the sequence of the average points of pairs of nearby maxima and minima, whose limit is searched with sufficiently high absolute and relative precision. We then find the Weyl function $m(\lambda)$ from (7) and eventually, from (3), we deduce the density of the states, see Fig. 2. The maxima of the first four BW lines are displayed in Fig. 3. Starting from the odd integers, that correspond to the nonrelativistic values, we see that their spacing decreases both for increasing Ω and λ; the same effect has been observed for the relativistic Landau levels [20], and it loosely seems to propose, in

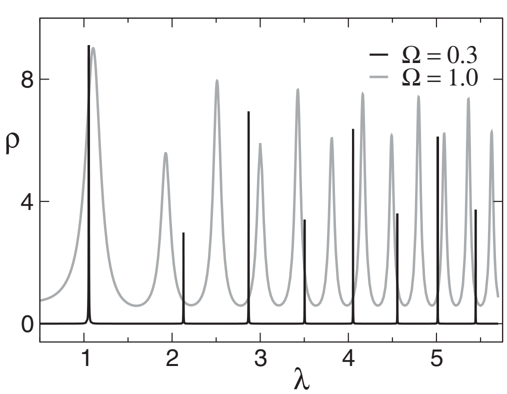

FIG. 1. The density of the states for the linear potential with $\Omega = 0.3$, 1. The scale for $\Omega = 0.3$ must be multiplied by 10^2.

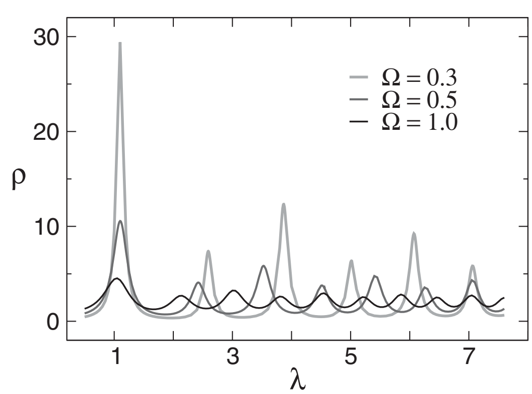

FIG. 2. $\rho(\lambda, \Omega)$ for the quadratic potential.

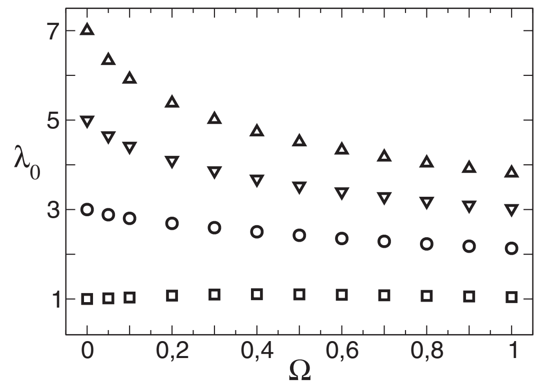

FIG. 3. The first BW maxima vs Ω for the quadratic potential. Nonrelativistic bound states correspond to odd integers.

relativistic quantum mechanics, the usual relationship between circular and harmonic motion. We can also remark that, as for the linear potential, the lowest resonance has a central value that always remains near the nonrelativistic value. The data of the higher resonances, instead, are well fitted by decreasing exponentials in Ω, they approach each other and their unequal spacing should be taken into account in the construction of quarkonium models. The right part of Fig. 4 reproduces the width of the first BW resonance vs Ω. According to what we said above, the plot can give an estimate of the pair production for this case, not treated by QED. Remark that the data are well approximated by a curve $w(\Omega)$ very similar to the production in a constant field.

In conclusion, by using the possibilities offered by quantum mechanics, we have proven the continuity from the nonrelativistic discrete spectrum to the continuous spectrum of the Dirac equation for an entire class of confining potentials. The study of the density of the states solves the apparent physical contradiction of the absence of bound states, by substituting them with BW resonances whose maxima give the relativistically correct metastable levels. It is thus clarified also the extent to which the notion of state can be used in model building. We have then shown that the width of the resonances vs the interaction strength reproduces very faithfully the pair production curve: this gives an explanation of the Klein paradox for bound states and it proposes a completely new and concrete way of estimating the pair production for nonhomogeneous fields where very little is known and active research is still in progress.

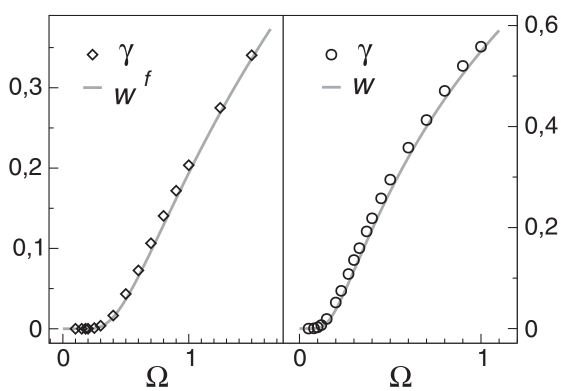

FIG. 4. Left plot: the width of the first resonance (diamonds) compared with the pair production curve $w^f(\Omega)$ (solid line). Right plot: the width of the first resonance (circles) for a quadratic potential. The solid line, giving a very good fit, is $w(\Omega) = -\pi^{-1}\ln[1 - \exp\{-\pi/(4^2\Omega^{3/2})\}]$, analogous to $w^f(\Omega)$.

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