Quasiclassical approximation for the Dirac equation

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Quasiclassical expressions are obtained for the energies and phases of a Dirac particle in a static centrally-symmetric field, and formulas are also obtained for the scattering cross sections at small and large angles.

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The quasiclassical approximation for the four-dimensional Dirac equation is well known (see [1,2]). In the case of a static centrally-symmetric potential one can, however, proceed much farther; the goal of the present article is to give a simple derivation of the pertinent formulas.

1. As is well known, the wave function of a Dirac particle with a given angular momentum j in a static central field V(r) is represented in the form (the notation is the same as in [3])

$$\Psi=\frac{1}{r}\begin{pmatrix} f(r)\Omega_{jlm} \\ (-1)^{(1+l-l')/2}\Omega_{jl'm}g(r)\end{pmatrix}, \tag{1}$$

where f and g satisfy the system of equations

$$\frac{df}{dr}+\frac{\varkappa}{r}f-\mu g=0,\qquad \frac{dg}{dr}-\frac{\varkappa}{r}g+(\mu-2m)f=0, \tag{2}$$

where $\mu = E + m - V$. In principle this system might be reduced to the Schrödinger equation; however, in this connection an extremely complicated effective potential is obtained. The reduction of the system (2) to the Riccati equation, proposed in [4], is a more convenient method for the transition to the quasiclassical approximation. Namely, it is shown in this article that if the substitution

$$g=\Phi f, \tag{3}$$

is made in Eqs. (2), then

$$f=r^{-\varkappa}\exp\left[\int\limits_a^r \mu\Phi\,dr\right], \tag{4}$$

and Φ obeys the equation

$$\frac{d\Phi}{dr}-\frac{2\varkappa}{r}\Phi+\mu\Phi^2+\mu-2m=0. \tag{5}$$

This equation is convenient for the transition to the quasiclassical approximation; denoting the distance over which the potential changes significantly by a and introducing the notation

$$n=\left[1-\frac{2EV-V^2}{k^2}-\frac{\varkappa^2}{x^2(ka)^2}\right]^{1/2},\quad k^2=E^2-m^2,\quad x=\frac{r}{a}, \tag{6}$$

let us solve Eq. (5) with respect to Φ:

$$\Phi=\frac{1}{\mu a}\left(\frac{\varkappa}{x}\pm ikan\left[1+\frac{1}{ka}\frac{\mu}{k}\frac{1}{n^2}\frac{d\Phi}{dx}\right]^{1/2}\right). \tag{7}$$

The formal expansion parameter associated with the transition to the quasiclassical approximation is $\lambda = (ka)^{-1} \ll 1$; in this connection one must be careful that all of the functions appearing in connection with higher powers of this parameter are not large. In addition, it is necessary to take into consideration that values $\kappa \sim ka$ are important, as follows from the known connection between the angular momentum and the impact parameter.

Solving Eq. (7) according to perturbation theory, we obtain

$$\Phi=\frac{1}{\mu a}\frac{\varkappa}{x}\pm i\frac{k}{\mu}n\pm\frac{i}{2ka}\frac{\Phi'}{n}\mp\frac{i}{8(ka)^2}\left(\frac{\Phi'}{n}\right)^2+\ldots, \tag{8}$$

where the prime denotes the derivative with respect to x. The first and second terms in Eq. (8) are the zeroth approximation. The following conditions must be satisfied in order for the expansion to be valid: 1) n doesn't vanish anywhere, i.e., x does not lie near the turning points; 2) none of the derivatives of n tend to infinity, i.e., the potential is a smooth function of x. More precisely as follows from Eq. (7) it is necessary that

$$\frac{1}{kan^2}\frac{\mu}{k}\frac{d}{dx}\left(\frac{1}{\mu a}\frac{\varkappa}{x}\pm i\frac{k}{\mu}n\right)\ll 1. \tag{9}$$

Under these conditions, by using Eq. (4) the function f can be represented in the form

$$f_\pm=C_\pm\sqrt{\frac{\mu}{kn}}\exp\left\{\pm i\left[ka\int\limits_{r_0}^r\left(n+\frac{1}{2}\frac{\partial n}{\partial\varkappa}\right)dx+\frac{\varkappa}{2ka}\int\frac{dx}{\mu nx}\frac{dV}{dx}\right]+O\left(\frac{1}{ka}\right)\right\}.$$

Introducing the notation

$$S(r)=\int\limits_{r_0}^r p\,dr,\quad p=\left[k^2-2EV+V^2-\frac{\varkappa^2}{r^2}\right]^{1/2}, \tag{10}$$

where r_0 denotes the value of r corresponding to the zero of p, we obtain the quasiclassical wave function:

$$\Psi=\frac{c}{r}\sqrt{\frac{\mu}{p}}\begin{pmatrix}\Omega_{jlm}\sin(\varphi(r)+\delta) \\ (-1)^{(1+l-l')/2}\Omega_{jl'm}\left[\frac{p}{\mu}\cos(\varphi(r)+\delta)+\frac{\varkappa}{\mu r}\sin(\varphi(r)+\delta)\right]\end{pmatrix} \tag{11}$$

$$\varphi(r)=S+\frac{1}{2}\frac{\partial S}{\partial\varkappa}+\frac{1}{2}\Delta, \tag{12}$$

$$\Delta=\varkappa\int\limits_{r_0}^r\frac{dr}{\mu pr}\frac{dV}{dr}. \tag{13}$$

The phase δ is determined from a comparison of expression (11) with the asymptotic form of the wave function for free motion:

$$\Psi\approx\frac{1}{r}\left(\frac{E+m}{\pi E}\right)^{1/2}\begin{pmatrix}\Omega_{jlm}\sin\left(kr-\frac{l\pi}{2}\right) \\ -\left(\frac{E-m}{E+m}\right)^{1/2}\Omega_{jl'm}\sin\left(kr-\frac{l'\pi}{2}\right)\end{pmatrix}, \tag{14}$$

whence it follows that

$$\delta=\pi/4. \tag{15}$$

It also follows from expression (14) that, for unbounded motion associated with normalization by $\delta(k - k')$, we have

$$C=\sqrt{k/\pi E}. \tag{16}$$

The expression $S + \partial S/2\partial\kappa$, appearing in φ, can be considered as an expansion of the formula

$$S'=\int p'\,dr,\quad p'=[k^2-2EV+V^2-(\varkappa+1/2)^2/r^2]^{1/2}, \tag{17}$$

in powers of $1/ka$ (for $\kappa \sim ka$), which corresponds to the substitution $l(l+1) \to (l+1/2)^2$ in the nonrelativistic case. In connection with the transition to the nonrelativistic limit, the lower component of the bispinor in expression (11) and Δ tend to zero, and the only difference from the Schrödinger equation consists in the presence of Ω_{jlm} instead of Y_{lm}. In the relativistic situation all terms are of the same order. We note that the quantity Δ originates exclusively from the spin-orbit interaction.

2. The discrete spectrum will be examined in this section. Let two turning points exist, a and b, and let the motion take place in the domain $a < x < b$. To the right of the turning point a, the wave function is of the form (11) with $\delta = \pi/4$ and S and Δ determined in expressions (10) and (12), where $r_0 = a$. The wave function is attenuated to the right of the point b; in order to obtain it, one must make the substitutions $\pm in \to \pm|n|$, $\pm i/n \to \pm 1/|n|$ in expressions (8) and (9); then $\pm iS \to \pm|S|$ and $\pm i\Delta \to \pm|\Delta|$. Discarding the increasing exponential, we obtain:

$$\Psi(x>b)=\frac{C'}{r}\sqrt{\frac{\mu}{|p|}}\exp\left[-|S|-\frac{1}{2}\frac{\partial|S|}{\partial\varkappa}+\frac{\Delta}{2}\right]\times\begin{pmatrix}\Omega_{jlm}\\ \frac{1}{\mu}\left(\frac{\varkappa}{r}-|p|\right)(-1)^{(1+l-l')/2}\,\Omega_{jl'm}\end{pmatrix}. \quad (18)$$

In order to find Ψ to the left of the turning point it is necessary, as is well known, [5] to analytically continue (18) in the complex r-plane; in this connection we obtain the result that, to the left of b the wave function (18) corresponds to the function (11) but with $r_0 = b$. In order that both functions coincide for all $a < x < b$, it is necessary that

$$\int_a^b\left(p+\frac{1}{2}\frac{\partial p}{\partial\varkappa}+\frac{\varkappa}{2pr}\frac{1}{\mu}\frac{dV}{dr}\right)dr+\frac{\pi}{2}=\pi(n_r+1), \quad (19)$$

where n_r is equal to the number of nodes in the radial wave function, that is, we obtain a generalization of the Bohr-Sommerfeld quantization rule to the relativistic case. For a Coulomb field the quasiclassical approximation is valid, just as in the nonrelativistic case, for all values of κ if the Coulomb parameter $\nu = \alpha ZE/p$ is large, or for all energies if κ is large. Formula (19) gives the exact expression for the energy of a Dirac particle in a Coulomb field, as one can easily verify. If the substitution $p + (1/2)(\partial p/\partial\kappa) \to p'$ is used, where p' is given in (17), we obtain a formula valid to within $(n_r + \kappa)^{-1}$ (in contrast to the nonrelativistic approximation, where both formulas give the same expression for the energy).

The wave function of the discrete spectrum has the form (11) with a normalization constant which is determined in the same manner as in the nonrelativistic case (see [5]); it is easy to obtain the result

$$C^{-2}=\int_a^b dr\frac{E-V}{p}.$$

3. Let us consider the scattering of Dirac particles. Using the partial wave expansion of the amplitude and changing from a summation over l to an integration over the dimensionless impact parameter $b = l/ka$, we obtain the following result accurate to terms of order $(ka)^{-1}$

$$f=A-iB\mathbf{v}\sigma,$$

$$A=\frac{k^2a}{2i}\int_0^\infty P_{kab}(\cos\theta)\,b\,db\,[e^{2i\delta(b)}(1+e^{-2i\Delta(b)})-2],$$
$$B=\frac{k^2a}{2i}\int_0^\infty P^1_{kab}(\cos\theta)\,db\,e^{2i\delta(b)}(1-e^{-2i\Delta(b)}), \quad (20)$$

where Δ is given in Eq. (13), P_l and P_l^1 are Legendre polynomials,

$$\delta=\frac{\Delta}{2}-kr_0+\frac{\pi}{2}\left(l+\frac{1}{2}\right)+\int_{r_0}^\infty(p(r)-k)\,dr+\frac{1}{2}\frac{\partial}{\partial l}\int_{r_0}^\infty p(r)\,dr,$$

and p is given in (10) with the replacement of κ by l.

In the case of small scattering angles, replacing the Legendre polynomials by their asymptotic expressions in terms of Bessel functions, we find that for $\theta \ll (ka)^{-1/3}$ the impact parameter representation is valid for the amplitudes:

$$A=\frac{ka^2}{4\pi i}\int e^{i\mathbf{qb}}[e^{2i\delta}(1+e^{-2i\Delta})-2]\,d^2\mathbf{b},$$
$$B=\frac{ka^2}{4\pi i}\int e^{i\mathbf{qb}}\mathbf{q}_0\mathbf{b}_0e^{2i\delta}(1-e^{-2i\Delta})\,d^2\mathbf{b}, \quad (21)$$

where $\mathbf{q}$ is the dimensionless momentum transfer, and $\mathbf{q}_0$ and $\mathbf{b}_0$ are unit vectors in the directions $\mathbf{q}$ and $\mathbf{b}$. We note that in contrast to the eikonal formulas, in Eqs. (21) no restrictions are imposed on the magnitude of the potential. The eikonal approximation is obtained from (21) provided that $EV/k^2 \ll 1$; in this connection $V \ll E + m$, $\Delta \to 0$, and $B \to 0$, that is, at high energies the spin-flip scattering amplitude does not contribute to the diffraction peak. The asymptotic (in the limit $E \to \infty$) expressions for the phases and for the cross sections coincide with the corresponding formulas for the Klein-Gordon equation, for example, from (21) and the optical theorem:

$$\sigma_{tot}(E\to\infty)=8\pi a^2\int_0^\infty b\,db\sin^2\left(\int_0^\infty V\,dz\right),\quad z^2=r^2-(ba)^2.$$

By operating in the same way as in the nonrelativistic case [5], we obtain the following results for large scattering angles:

$$A=\frac{(ka)^{3/2}}{ik(2\pi\sin\theta)^{1/2}}\int_0^\infty\sqrt{b}\,db\,(e^{i\zeta_+}+e^{i\zeta_-})\cos\Delta,$$
$$B=\frac{(ka)^{3/2}}{ik(2\pi\sin\theta)^{1/2}}\int_0^\infty\sqrt{b}\,db\,(e^{i\zeta_+}-e^{i\zeta_-})\sin\Delta,$$

where

$$\zeta_\pm=2\delta-\Delta\pm\left[(l+{}^1/_2)\theta-\frac{\pi}{4}\right]$$
$$=ka\left[2\int_{x_0}^\infty(n-1)\,dx-2x_0+b(\pi\pm\theta)\right]+\frac{\partial}{\partial b}\int_{x_0}^\infty n\,dx+\frac{\pi\pm\theta}{2}\mp\frac{\pi}{4},$$
$$n(b)=\left(1-\frac{2EV-V^2}{k^2}-\frac{b^2}{x^2}\right)^{1/2}.$$

Since $ka \gg 1$, one can use the method of steepest descents; then

$$A=fe^{i\gamma}\cos\Delta_0,\quad B=\varepsilon fe^{i\gamma}\sin\Delta_0,$$

where f is the classical, relativistic, spinless scattering amplitude:

$$f=a\left(\frac{b_0}{\sin\theta}\frac{db_0}{d\theta}\right)^{1/2},$$

b_0 and $db_0/d\theta$ are determined from the usual condition

$$-\frac{\partial}{\partial b}\int_{x_0}^\infty n\,dx=\frac{\pi\pm\theta}{2}, \quad (22)$$

where the upper sign corresponds to an attractive potential, the lower sign corresponds to a repulsive potential, γ is a common phase factor which does not give a contribution to the cross section, ϵ is the sign function, $\epsilon = 1$ for the upper sign in Eq. (22), $\epsilon = -1$ for the lower sign, and $\Delta_0 = \Delta(b_0)$. If there are several b's which satisfy condition (22) for a given θ, it is necessary to write A and B in the form

$$A=\sum_k f_k \exp(i\gamma_k)\cos\Delta_k,\quad B=\sum_k \varepsilon_k f_k \exp(i\gamma_k)\sin\Delta_k. \qquad (23)$$

Since the phases γ are very large (of order ka), interference between different terms in (23) is practically unobservable, and the cross section is equal to the sum of the contributions from the terms with identical γ_k. Therefore

$$\frac{d\sigma}{d\Omega}=\frac{a^2}{\sin\theta}\sum_k \left| b_k \frac{db_k}{d\theta}\right| \{1+2\mathbf{s}_2\sin\Delta_k[\boldsymbol{\nu}(\mathbf{s}_1\boldsymbol{\nu})\sin\Delta_k+\varepsilon[\boldsymbol{\nu}\mathbf{s}_1]\cos\Delta_k\}.$$

Here $\mathbf{s}_1$ and $\mathbf{s}_2$ are the initial and final polarizations, and $\boldsymbol{\nu}$ is a unit vector perpendicular to the plane of the scattering.

For an unpolarized incident beam, polarization of the scattered beam is absent; if the incident beam is polarized along the direction of motion, the scattered beam is polarized in the scattering plane perpendicular to the direction of the incident beam.

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