ON THE PROPERTIES OF THE DISCRETE AND CONTINUOUS SPECTRA OF THE RADIAL DIRAC EQUATION

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Abstract

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ON THE PROPERTIES OF THE DISCRETE AND CONTINUOUS SPECTRA OF THE RADIAL DIRAC EQUATION

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1. The radial Dirac equation ([1]) can be written in the form

$$\begin{gathered}\left(\frac{d}{dr}+\frac{k}{r}\right)\psi_1-[m+\lambda-V(r)]\psi_2=0,\\ \left(\frac{d}{dr}-\frac{k}{r}\right)\psi_2-[m-\lambda+V(r)]\psi_1=0,\\ 0\leqslant r<\infty,\qquad m>0.\end{gathered}\tag{1}$$

We shall assume that

$$V(r)=-\frac{A}{r}+q(r),\qquad \int_0^\infty |q(r)|\,dr<\infty,\qquad A>0.$$

For $q(r)\equiv 0$ we obtain the equation describing the hydrogen atom.
By $\psi(r,k,\lambda)=[\psi_1(r,k,\lambda),\psi_2(r,k,\lambda)]$ we denote a solution of equation (1) such that

$$\lim_{r\to 0}\psi(r,k,\lambda)r^{-\alpha}=[1,b_0],\qquad \alpha=\sqrt{k^2-A^2},\qquad \operatorname{Re}\alpha>0,\qquad b_0=(\alpha+k)A.$$

As $r\to\infty$ the representation

$$\psi(r,k,\lambda)=e^{\varepsilon r-A\lambda/\varepsilon}c(\varepsilon,k)[m+\lambda+o(1),\varepsilon+o(1)],\qquad \varepsilon=\sqrt{m^2-\lambda^2}.$$

is valid. Let $\operatorname{Re}\lambda\geqslant 0$; then the function $c(\varepsilon,k)$ is analytic in the variables ε and k in the domain $\operatorname{Re}\varepsilon>0$, $\varepsilon\in[m,+\infty)$, $k\in[-A,A]$.

In the present article the analytic properties of the function $c(\varepsilon, k)$ are studied in detail. Then the concepts of quantum defects of the continuous and discrete spectra of the Dirac equation (1) are introduced, the existence of quantum defects is proved, and formulas for their computation are derived.

The theory of quantum defects in the nonrelativistic case for the radial Schrödinger equation was considered earlier from semiempirical considerations (see ([2–4])) and was rigorously justified in ([5]).

2. We shall call the potential $q(r)$ regular if the following conditions are satisfied:

a) the function $q(r)$ is real for $r > 0$;

b) the function $q(r)$ is analytic in the domain $\operatorname{Re} r > 0$ and continuous for $\operatorname{Re} r \geqslant 0$, except, possibly, at $r = 0$;

c) the inequality holds

$$\int_0^\infty \hat{q}(t)\,dt < \infty,$$

where $\hat{q}(t) = \sup |q(te^{i\beta})|$, $-\pi/2 \leqslant \beta \leqslant \pi/2$.

In §§ 2–5 we shall assume that the listed conditions are fulfilled.

Theorem 1. *For regular potentials the function $c(\varepsilon, k)$ admits analytic continuation to the domain*

$$\varepsilon \in (-\infty, 0] \cup [m, +\infty), \qquad k \in [-A, A].$$

3. Let $k = \bar{k}$ and $|k| > A$. Then the discrete spectrum of the Dirac equation (1) is located, as is known, in the interval $(-m, m)$. If λ_n $(0 < \lambda_n < m)$ is a point of the discrete spectrum of equation (1), then

$$c(\varepsilon_n, k) = 0, \qquad \varepsilon_n = \sqrt{m^2 - \lambda_n^2}. \tag{2}$$

We denote, as usual,

$$c^{\pm}(\sigma, k) = \lim_{\tau \to \pm 0} c(\varepsilon, k), \qquad \varepsilon = \sigma + i\tau, \quad \sigma < 0.$$

Then the equality

$$\operatorname{Im} c^{\pm}(-i\varepsilon_n, k) = 0 \tag{3}$$

holds.

An analogous result is also valid in the case $\operatorname{Re}\lambda < 0$, with $\operatorname{Re}\sqrt{m^2 - \varepsilon^2} < 0$ everywhere. As in the nonrelativistic case ([5]), the behavior of the roots ε_n is sometimes better studied by using equality (3) than directly with the aid of equation (2).

In the case $q(r) \equiv 0$ the corresponding function $c_0(\varepsilon, k)$ has the form

$$c_0(\varepsilon, k) = \frac{A\varepsilon + (\alpha + k)(m + \lambda)}{2A\varepsilon} (2\varepsilon)^{-A\lambda/\varepsilon - \alpha} \frac{\Gamma(2\alpha + 1)}{\Gamma(-n' + 1)} \frac{1}{m + \lambda},$$

where $\lambda = \sqrt{m^2 - \varepsilon^2}$, $n' = A\lambda/\varepsilon - \alpha$.

4. The scattering amplitude is expressed, as is known ([3]), in terms of phase shifts

$$\eta_k(\varepsilon) = \arg c(\varepsilon, k) + \frac{A\lambda}{|v|} \ln 2|v|,$$

where k is an integer ($k \neq 0$), $\varepsilon = iv$ ($v < 0$).

We shall call the quantities

$$\delta(k, \pm m) = \frac{1}{\pi} \lim_{\lambda \to \pm m} \arg \frac{c(\varepsilon, k)}{c_0(\varepsilon, k)} \qquad (|\lambda| > m) \tag{4}$$

the quantum defects of the continuous spectrum.

We find sufficient conditions for the existence of the limits appearing on the right-hand side of (4). First we introduce the notation

$$g_2(r, k, m) = b_1 H_{2\alpha}^{(1)}(2\sqrt{2mAr}), \qquad g_1(r, k, -m) = b_2 H_{2\alpha}^{(1)}(2i\sqrt{2mAr}),$$

where $H_{2\alpha}^{(1)}(z)$ is the Hankel function,

$$b_1 = \frac{A^2 (2mA)^\alpha \pi}{i(\alpha + k)\Gamma(2\alpha + 1)}, \qquad b_2 = \frac{A\pi}{i\Gamma(2\alpha + 1)} (-2mA)^\alpha.$$

Let, moreover,

$$g_1(r, k, m) = -\frac{1}{A} \left(r\frac{d}{dr} - k \right) g_2(r, k, m),$$

$$g_2(r, k, -m) = \frac{1}{A} \left(r\frac{d}{dr} + k \right) g_1(r, k, -m), \tag{5}$$

$$S(k, \pm m) = 1 + \int_0^\infty \psi(r, k, \pm m) H_1(r) \begin{bmatrix} g_2(r, k, \pm m) \\ -g_1(r, k, \pm m) \end{bmatrix},$$

where

$$H_1(r) = \begin{bmatrix} 0 & q(r) \\ -q(r) & 0 \end{bmatrix}.$$

Theorem 2. Let the potential $q(r)$ be regular and, for any L, let the inequality

$$\int_0^\infty e^{L\sqrt{t}}\, \hat{q}(t)\, dt < \infty$$

hold.

Then for $\alpha > 1/2$ the limits exist

$$\lim_{\lambda \to \pm m} \frac{c(\varepsilon, k)}{c_0(\varepsilon, k)}, \qquad \lambda = \bar{\lambda}, \qquad |\lambda| > m,$$

and the equalities hold

$$\lim_{\lambda \to \pm m} \frac{c(\varepsilon, k)}{c_0(\varepsilon, k)} = S(k, \pm m).$$

Thus, the quantum defects are determined by the formulas

$$\delta(k, \pm m) = \frac{1}{\pi} \arg S(k, \pm m). \tag{6}$$

We note that formulas (4) and (6) determine the quantum defects up to an integer summand. For a unique determination let us consider the potential

$$V_\rho(r) = -A/r + \rho q(r), \qquad 0 \le \rho \le 1.$$

By $\arg \dfrac{c(\varepsilon, k)}{c_0(\varepsilon, k)}$ and $\arg S(k, \pm m)$ we shall mean the angle through which, about the origin, the vector representing respectively $c(\varepsilon, k, \rho)/c_0(\varepsilon, k, \rho)$ and $S(k, \pm m, \rho)$ turns, when ρ runs through the real values from 0 to 1. It is easy to see that equality (6) is preserved.

5. The discrete spectrum of the Dirac equation is located, as is known, inside the interval $(-m, m)$. If $A > 0$ and

$$\int_0^\infty |q(r)|\, dr < 0,$$

then the only accumulation point of the discrete spectrum is the point m. We give here a more detailed description of the discrete spectrum. Let us renumber its points λ_n in increasing order.

Theorem 3. *Let the potential $q(r)$ be regular and let, for any L, the inequality hold*

$$\int_0^\infty e^{L\sqrt{\ln t}}\,\hat{q}(t)\,dt < \infty.$$

Then, for $\alpha > 1/2$, the asymptotic equality holds

$$\lambda_n = \frac{m}{\sqrt{1 + A^2/[\alpha + n + \delta_k + \chi(n,k)]^2}}, \tag{7}$$

where $\chi(n,k) \to 0$ as $n \to \infty$, and δ_k does not depend on n.

In formula (7), $n = 1, 2, ...$ for $k > A$; $n = 0, 1, 2, ...$ for $k < -A$,

$$\delta_k = \frac{1}{\pi}\arg S(k,m). \tag{8}$$

The number δ_k will be called the quantum defect of the discrete spectrum. Recall that for $q(r) = 0$ the exact formula holds

$$\lambda_n^0 = \frac{m}{\sqrt{1 + A^2/(\alpha + n)^2}}.$$

It follows from Theorems 2 and 3 that the quantum defects of the discrete and continuous spectra are related by the equality:

$$\delta_k = \delta(k,m) = \frac{1}{\pi}\arg S(k,m).$$

We note that superpositions of potentials of the form

$$e^{-\beta r^\gamma} r^{-s} \qquad (\beta > 0,\ 1/2 < \gamma < 1,\ s < 1)$$

satisfy the conditions of Theorems 2 and 3.

6. The quantum defects $\delta(k, \pm\infty)$ of the continuous spectrum are defined by means of the equality

$$\delta(k, \pm\infty) = \frac{1}{\pi}\lim_{\lambda\to\pm\infty}\arg\frac{c(\varepsilon,k)}{c_0(\varepsilon,k)} \qquad (\varepsilon = \sqrt{m^2 - \lambda^2}).$$

We shall find the form of $\delta(k, \pm\infty)$, without assuming the potential $q(r)$ to be regular.

Theorem 4. Let $q(r) = \overline{q(r)}$, $\int_0^\infty |q(r)|\,dr < \infty$, $k = \bar{k}$, $|k| > A$.

Then the formula is valid

$$\lim_{\lambda\to\pm\infty} \frac{c(\varepsilon, k)}{c_0(\varepsilon, k)} = \exp\left[\pm i \int_0^\infty q(r)\,dr\right].$$

Corollary. If $\int_0^\infty |q(r)|\,dr < \infty$, then the quantum defects $\delta(k, \pm\infty)$ exist, do not depend on k, and have the form

$$\delta(\pm\infty) = \pm \int_0^\infty q(r)\,dr. \tag{9}$$

Thus, the equality holds:

$$\delta(+\infty) = -\delta(-\infty). \tag{10}$$

Let us recall that in the nonrelativistic case

$$\delta(\pm\infty) = 0.$$

From equality (10) and the form of $c_0(\varepsilon, k)$ it follows that

$$\lim_{\lambda\to\pm\infty} \eta_k(\varepsilon) = -\lim_{\lambda\to\mp\infty} \eta_k(\varepsilon) + \pi(\alpha + 1).$$

In conclusion, we note that the results concerning the continuous spectrum (items 2, 3, 4, 6) remain valid also for the case $A < 0$.

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Note: Figure translations are in progress. See original paper for figures.