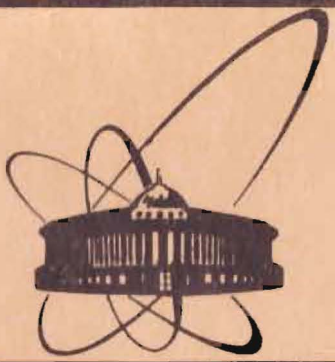

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GENERALIZED PRÜFER TRANSFORMATION AND THE EIGENVALUE PROBLEM FOR RADIAL DIRAC EQUATIONS

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The Prüfer transformation [1] provides an efficient tool for numerical computation of the eigenvalues for the radial Schrödinger equation (see, e.g., refs. [2-4] and references therein). The method consists in converting the original 2nd order linear differential equation into a nonlinear 1st order equation for a "phase function". The Prüfer phase function possesses a number of peculiar properties which greatly facilitate the calculation of the eigenvalues. Such a method can also be extended to coupled systems of radial Schrödinger equations [5,6].

It would be interesting to develop an analogous procedure also for the system of radial Dirac equations. Suitable transformations of the Dirac system were proposed independently in [4] and [7] *. The authors of ref. [7] dealt only with the particular case of an external magnetic monopole field and, correspondingly, the properties of the relevant phase function were discussed in a rather ad hoc manner. The class of external potentials considered for the numerical calculations in [4] is rather wide, but the properties of the phase function were not discussed there in detail.

The purpose of this note is to show that the phase function employed in ref. [4] possesses properties very similar to those encountered earlier in the well-studied case of the radial Schrödinger equation [2,3]. This is somewhat surprising, as now we are dealing with a 1st order linear system and a connection with the standard Prüfer transformation is far from obvious.

Let us begin with the formulation of the problem and some basic definitions. The system of radial Dirac equations can be written as (cf. [4])

$$u_1' - \frac{k}{x} u_1 = P(x,\epsilon) u_2 ,$$
$$u_2' + \frac{k}{x} u_2 = Q(x,\epsilon) u_1 , \qquad (1)$$

with

$$P(x,\epsilon) = -2m - \epsilon + v(x) , \quad Q(x,\epsilon) = \epsilon - v(x) , \qquad (2)$$

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* Let us remark that the transformation proposed for the 1st order linear differential systems by Atkinson (see [5], pp. 328-329) cannot be used for our purposes.

where m is the particle mass, $\epsilon = E - m$ (E being the relativistic total energy), $k = \pm(j + 1/2)$, $j = 1/2, 3/2, \ldots$, and $v(x)$ is a potential, $x \in (0,\infty)$. Throughout this paper we use dimensionless quantities. We shall assume for simplicity that $v(x)$ is bounded near the origin (the "regular potentials" of ref.[4]) although the relevant results could certainly be recovered also for potentials involving, e.g., the Coulomb singularity for $x \to 0$. Furthermore, we shall suppose that

$$\lim_{x \to \infty} x^2 v(x) = 0 . \tag{3}$$

The eigenvalue condition for the parameter ϵ reads

$$u_{1,2}(0,\epsilon) = 0 , \tag{4a}$$

$$u_{1,2}(\infty,\epsilon) = 0 . \tag{4b}$$

In what follows we restrict ourselves to $\epsilon \in (-m,0)$. The crucial object in the subsequent discussion will be the "phase function" defined by means of a generalized Prüfer transformation (cf. [4])

$$\mathrm{tg}\, z = \frac{u_2}{u_1} . \tag{5}$$

A trivial ambiguity of such a definition due to the periodicity of $\mathrm{tg}\, z$ can of course be removed by fixing the value of $z(0,\epsilon)$. From (1) and (5) one obtains the following nonlinear differential equation for z:

$$z' = Q \cos^2 z - \frac{2k}{x} \sin z \cos z - P \sin^2 z . \tag{6}$$

There is unique solution of eq. (6) corresponding to the regular solution (satisfying (4a)) of the original system (1). The appropriate initial conditions which determine this relevant solution fix the values of $z(0,\epsilon)$ and $z'(0,\epsilon)$; for example, for $k > 0$ one has

$$z(0,\epsilon) = 0 , \quad z'(0,\epsilon) = \frac{Q(0,\epsilon)}{2k+1} . \tag{7}$$

For more details, see ref.[4].

Let us now investigate the properties of the phase function z. First, we shall discuss the monotonicity of the $z(x,\epsilon)$ with respect to ϵ for a fixed value of x. To this end, it is useful to invoke the method of Atkinson [5]. In the spirit of [5], the definition (5) may be recast as

$$\mathrm{tg}\, z = \mathrm{tg}(\phi/2) ; \quad \exp(i\phi) = w \equiv (u_1 + iu_2)(u_1 - iu_2)^{-1} . \tag{8}$$

(Note that the relation (8) makes sense, as the u_1, u_2 cannot vanish simultaneously for $x > 0$; this follows immediately from a theorem on uniqueness of solutions of the system (1)). Then, without any reference to (1), the following identity holds (cf. the relation (10.2.24) in [5]):

$$w^* \frac{\partial w}{\partial \epsilon} = 2i\,(u_1^2 + u_2^2)^{-1} \left(u_1 \frac{\partial u_2}{\partial \epsilon} - u_2 \frac{\partial u_1}{\partial \epsilon}\right) . \tag{9}$$

Using equations (1) it is easy to obtain

$$\frac{\partial}{\partial x}\left(u_1 \frac{\partial u_2}{\partial \epsilon} - u_2 \frac{\partial u_1}{\partial \epsilon}\right) = u_1^2 + u_2^2 . \tag{10}$$

Integrating eq. (10) and observing that for regular solutions u_1, u_2 one has

$$\lim_{x \to 0} \left[u_1(x,\epsilon) \frac{\partial}{\partial \epsilon} u_2(x,\epsilon) - u_2(x,\epsilon) \frac{\partial}{\partial \epsilon} u_1(x,\epsilon)\right] = 0 , \tag{11}$$

we arrive at the relation

$$u_1 \frac{\partial u_2}{\partial \epsilon} - u_2 \frac{\partial u_1}{\partial \epsilon} = \int_0^x (u_1^2 + u_2^2)\, dt . \tag{12}$$

Equation (9) may be then rewritten as

$$\frac{\partial w}{\partial \epsilon} = i\omega w \tag{13}$$

with $\omega = 2(u_1^2 + u_2^2)^{-1} \int_0^x (u_1^2 + u_2^2)\, dt$.

Obviously, $\omega > 0$ for any $x > 0$; substituting $w = \exp(i\phi)$ into (13) and taking into account (8), one immediately gets the following important property of the z:

P1: $z(x,\epsilon)$ is an increasing function of ϵ for a fixed $x > 0$.

A closer look at the equation (6) reveals that in a region of sufficiently large x, the function z is also endowed with specific monotonicity properties with respect to the variable x, at special points where either $\sin z$ or $\cos z$ vanishes. Indeed, let ϵ be arbitrary but fixed. Let us choose x_P such that $v(x) - m < 0$ for $x > x_P$ and $x_Q(\epsilon)$ such that $\epsilon - v(x) < 0$ for $x > x_Q(\epsilon)$; obviously, x_P and $x_Q(\epsilon)$ exist, owing to (3). If we set

$$\bar{x}(\epsilon) = \max(x_P, x_Q(\epsilon)) . \tag{14}$$

it is clear (see (2)) that for $x > \bar{x}(\epsilon)$ both $P(x,\epsilon) < 0$ and $Q(x,\epsilon) < 0$. Now, if $x_0 > \bar{x}(\epsilon)$ is such that $z(x_0,\epsilon) = n\pi$ for an integer n, then eq. (6) implies $z'(x_0,\epsilon) < 0$, i.e., $z(x,\epsilon)$ is decreasing at $x = x_0$. Similarly, if for some $x_1 > \bar{x}(\epsilon)$ one has $z(x_1,\epsilon) = n\pi + \pi/2$, then $z(x,\epsilon)$ is increasing at $x = x_1$. This property of the z may be conveniently reformulated in the following way:

P2: Let $x_0 > \bar{x}(\epsilon)$, where $\bar{x}(\epsilon)$ is given by (14). If $z(x_0,\epsilon)$ lies between $n\pi - \pi/2$ and $n\pi$ for an integer n, then the trajectory $z(x,\epsilon)$ for $x > x_0$ remains trapped within the strip $n\pi - \pi/2 < z < n\pi$.

Next we shall discuss the limits of the phase function $z(x,\epsilon)$ for $x \to \infty$. For the rapidly decreasing potentials (3) it is not difficult to establish the asymptotic behaviour of the solutions of the system (1): For ϵ being an eigenvalue, the regular solution of eq. (1) behaves for $x \to \infty$ like

$$u_1(x,\epsilon) = Ae^{-\kappa x}(1 + o(1)), \qquad u_2(x,\epsilon) = Be^{-\kappa x}(1 + o(1)). \tag{15}$$

where

$$\frac{A}{B} = \left(\frac{2m - |\epsilon|}{|\epsilon|}\right)^{1/2}, \qquad \kappa = \left(|\epsilon|\,(2m - |\epsilon|)\right)^{1/2}, \tag{16}$$

while for ϵ which is not an eigenvalue, one has for $x \to \infty$

$$u_1(x,\epsilon) = Ce^{\kappa x}(1 + o(1)), \qquad u_2(x,\epsilon) = De^{\kappa x}(1 + o(1)), \tag{17}$$

with

$$\frac{C}{D} = -\left(\frac{2m - |\epsilon|}{|\epsilon|}\right)^{1/2}. \tag{18}$$

From the definition (5) and from (15) through (18) one readily gets the relevant limits for the z:

P3: ϵ is an eigenvalue for the original system (1) if and only if

$$\lim_{x \to \infty} \operatorname{tg} z(x,\epsilon) = \left(\frac{|\epsilon|}{2m - |\epsilon|}\right)^{1/2}. \tag{19}$$

ϵ is not an eigenvalue if and only if

$$\lim_{x \to \infty} \operatorname{tg} z(x,\epsilon) = -\left(\frac{|\epsilon|}{2m - |\epsilon|}\right)^{1/2}. \tag{20}$$

Thus, with minor modifications, the properties of the phase function corresponding to the transformation (5) are analogous to those encountered in the case of radial Schrödinger equation (cf. ref. /2/). Now we could formulate and prove a rigorous theorem on the eigenvalues pertaining to the system (1) in close analogy with the preceding papers /2,3/ (cf. Theorem 3.1 in ref. /2/ and Theorem 1 and 2 in /3/). Instead of doing this, we shall rather emphasize some practical aspects of actual numerical computation of the eigenvalues:

1. The presence of an eigenvalue is revealed as a discontinuity of the function $z(\infty,\epsilon) = \lim_{x \to \infty} z(x,\epsilon)$ with a step equal to π (see the properties P1 and P3).

2. In practice, one may usually only integrate eq. (6) numerically up to a "sufficiently distant" point x_∞ (in a sense specified below). Then changing ϵ by a very small amount yields a steep change of $z(x_\infty,\epsilon)$ (approximately by π) in the vicinity of an eigenvalue.

3. More precisely, if we want to determine the eigenvalues of ϵ lying in an interval $(-m, \epsilon_{max})$, $\epsilon_{max} < 0$, we estimate first the $\bar{x}(\epsilon_{max})$ according to (14). Further, the limits (19) and (20) indicate that for a given ϵ within the considered range, a sufficiently distant point $x_\infty \equiv x_\infty(\epsilon)$ satisfies the "trapping condition" $n\pi - \pi/2 < z(x_\infty,\epsilon) < n\pi$ for some integer n (see the property P2). The numerical integration of eq. (6) should be therefore carried out up to the values of x satisfying the above criteria.

4. Integrating numerically eq. (6), one may scan the whole range $\epsilon \subset (-m, \epsilon_{max})$ choosing an appropriate step $\Delta\epsilon$ for changing ϵ. We look for the neighbouring values ϵ_1, $\epsilon_2 = \epsilon_1 + \Delta\epsilon$ such that

$$\begin{aligned} &n\pi - \pi/2 < z(x_\infty,\epsilon_1) < n\pi, \\ &(n+1)\pi - \pi/2 < z(x_\infty,\epsilon_2) < (n+1)\pi, \end{aligned} \tag{21}$$

for some integer n. The fulfillment of (21) means that the interval (ϵ_1,ϵ_2) comprises just one eigenvalue. If $\Delta\epsilon$ happens to be inconveniently large, i.e., such that (21) cannot be achieved for some value of ϵ (indicating that there are several eigenvalues within $(\epsilon,\epsilon+\Delta\epsilon)$), it may be reduced, e.g., by successive halving, until (21) is attained for any "suspect" ϵ.

5. Once the eigenvalues are localized according to (21), the above-mentioned "halving procedure" may be applied systematically to refine the bounds on each eigenvalue in order to achieve the required accuracy (cf. also ref.[8]).

As an illustration of our method, we shall now present some results of an explicit numerical computation of the eigenvalues for the potential

$$v(x) = -5e^{-x}, \quad x \geq 0. \tag{22}$$

Table 1

ε	$z(x_\infty, \varepsilon)$
-2.10000	-0.79774
-1.85000	-0.73522
-1.75625	-0.71167
-1.73672	-0.70675
-1.73574	2.43509
-1.73281	2.43583
-1.72500	2.43780
-1.60000	2.46950

In the Table we give a set of the asymptotic values $z(x_\infty, \epsilon)$ ($x_\infty = 20$) in the vicinity of the lowest eigenvalue $\epsilon^{(0)}$ corresponding to the potential (22). The values of $z(x_\infty, \epsilon)$ are obtained by integrating eq.(6) for $k = 1$, using the initial conditions (7). Comparing the data in the Table with the conditions (21) one may observe that $\epsilon^{(0)}$ is approximately localized within the interval (-1.7367, -1.7357) (the required accuracy was 0.001). It is seen that an average slope of the curve corresponding to $z(x_\infty, \epsilon)$ changes drastically (by four orders) near the eigenvalue. In a similar way, one obtains for $k = 1$ two excited states with the eigenvalues $\epsilon^{(1)}$ and $\epsilon^{(2)}$ localized within the intervals (-0.5834, -0.5824) and (-0.0750, -0.0742) resp. Further examples of numerical results can be found in ref.[4].

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В Объединенном институте ядерных исследований начал выходить сборник *"Краткие сообщения ОИЯИ"*. В нем будут помещаться статьи, содержащие оригинальные научные, научно-технические, методические и прикладные результаты, требующие срочной публикации. Будучи частью "Сообщений ОИЯИ", статьи, вошедшие в сборник, имеют, как и другие издания ОИЯИ, статус официальных публикаций.

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Улегла И., Горжейши И. E2-85-695

Обобщенное преобразование Прюфера
и проблема собственных значений для радиальных уравнений Дирака

Рассматривается обобщенное преобразование Прюфера в связи с проблемой собственных значений энергии для системы радиальных уравнений Дирака. Для простоты мы ограничиваемся потенциалами регулярными в начале координат и быстро падающими на бесконечности. Показано, что соответствующая фазовая функция обладает свойствами, аналогичными тем, которые имеют место в случае радиального уравнения Шредингера. Собственные значения совпадают с точками разрыва фазовой функции по отношению к переменной энергии на пространственной бесконечности. Практически можно определить поведение фазовой функции в асимптотической области при помощи численной интеграции нелинейного дифференциального уравнения первого порядка и наблюдать резкие изменения соответствующего решения в окрестности собственного значения. Приведен пример численного расчета собственных значений в рамках указанной схемы.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Úlehla I., Hořejší J. E2-85-695

Generalized Prüfer Transformation
and the Eigenvalue Problem for Radial Dirac Equations

A generalized Prüfer transformation is introduced in connection with the eigenvalue problem for a system of radial Dirac equations. For simplicity we restrict ourselves to potentials bounded near the origin and decreasing rapidly in the infinity. It is shown that the corresponding phase function possesses properties closely similar to those encountered earlier in the case of the radial Schrödinger equation. The eigenvalues manifest themselves as points of discontinuity with respect to an energy variable of the phase function taken in the spatial infinity. In practice, one may determine the behaviour of the phase function in an asymptotic region by means of numerical integration of a nonlinear 1st order differential equation and observe abrupt changes of the corresponding solution in the vicinity of an eigenvalue. An example of numerical computation of the eigenvalues is briefly discussed.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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