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A new amplitude-phase method for analyzing scattering solutions of the radial Dirac equation

Karl-Erik Thylwe

KTH-Mechanics, Royal Institute of Technology, S-100 44 Stockholm, Sweden

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Abstract

A novel amplitude-phase method for analyzing radial Dirac solutions is presented. This approach addresses the original *coupled* radial Dirac equations without first transforming them to *decoupled* second-order differential equations. As a reference test, the method is applied to the scattering problem of a Dirac particle (electron) in a long-range Coulomb 4-vector potential with zero space components. Numerical results for the partial-wave S-matrix are compared with those from an exact analytic S-matrix formula.

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Amplitude-phase decompositions of radial Schrödinger solutions have been introduced and discussed in several papers related to scattering states and bound states in atomic physics [1]. This classical, and well-established, approach is also applicable to the radial Dirac equations, once these equations have been transformed to decoupled *second-order* differential equations. However, as will be illustrated in this short presentation, it is also possible to construct an amplitude-phase decomposition of a similar 'classical' form that is directly applicable to the coupled first-order differential equations without any elaborate transformations (cf [2]).

The crucial idea with an amplitude-phase method is to find an 'almost constant' amplitude of a wave that is defined by some (typically) nonlinear, ordinary differential equation. This amplitude is then known to determine the phase of the wave by an auxiliary equation [1]. Nonlinear equations are known to possess differing types of solutions, depending on initial (or boundary) conditions. Hence, if the problem allows a single 'stationary' boundary condition, then a single well-behaved amplitude can be found that provides the physical solution. The computational advantages with a single amplitude approach are obvious, but sometimes high precision calculations require the use of several amplitude functions [3].

When the Dirac solutions for a particle of mass m and energy E have been factorized into an angular part and a radial part (see [4] or [5]), the first-order differential equations of the radial components are given by

$$\frac{\mathrm{d}F}{\mathrm{d}r} = -\frac{\kappa}{r}F + \frac{E - V(r) + mc^2}{\hbar c}G, \qquad \frac{\mathrm{d}G}{\mathrm{d}r} = -\frac{E - V(r) - mc^2}{\hbar c}F + \frac{\kappa}{r}G. \tag{1}$$

Here c is the speed of light, $\hbar = h/(2\pi)$ with Planck's constant h and $V(r)$ being the central (time-like) 4-vector potential function of the radial coordinate r. According to Berestetskii *et al* [4], the non-zero integer parameter κ appearing in (1) is given by $\kappa = -(\ell + 1) \leqslant -1$ for the angular momentum quantum numbers $\ell = 0, 1, 2 \ldots$ and $\kappa = \ell \geqslant 1$ for $\ell = 1, 2 \ldots$.

For scattering energies ($|E| > mc^2$) the so-called 'large component' of the regular Dirac solution, here represented by F, satisfies

$$F \sim \sin[kr + \eta \ln(2kr) - \pi\ell/2 + \delta_{\ell,\kappa}], \qquad r \to +\infty, \tag{2}$$

which completely defines the two sequences of partial wave phase shifts $\delta_{\ell,\kappa}$. The asymptotic behavior (2) contains a Coulomb (Sommerfeld) parameter

$$\eta = \frac{EZ\alpha}{k\hbar c}, \tag{3}$$

where $Z \geqslant 0$ is the (screened) nuclear charge number and the fine structure constant α is expressed in terms of the elementary charge unit e as

$$\alpha = \frac{e^2}{\hbar c}, \tag{4}$$

and k is the asymptotic wave number:

$$k = \left(\frac{E^2 - m^2c^4}{\hbar^2c^2}\right)^{1/2}. \tag{5}$$

The next step is to introduce a suitable amplitude-phase method for solving equation (1). Historically, an amplitude-phase method for second-order Schrödinger-type (or parametric oscillator) differential equations is based on an ansatz for solutions in their oscillatory (classically accessible) region of the radial variable. If there is only one relevant oscillatory region, then a single ansatz will automatically reproduce the solution also in the neighboring non-oscillatory region(s) (there are two such regions for a single-well bound-state problem). Since the radial Dirac equations (1) can be transformed to Schrödinger-type differential equations, both coupled (treated in [2]) and uncoupled ones (treated in [1] and recently in [3]), the relevant ansatz for equation (1) is assumed to be of the same form. Hence, each (single or multi-component) solution has formally an ansatz $u\exp(\mathrm{i}\phi)$, where u is the amplitude and ϕ is the phase. So far multi-component solutions have been defined with a common phase. The amplitude component solutions may still have different phases by allowing them to be complex valued. One may thus try the ansatz

$$\begin{pmatrix} F \\ G \end{pmatrix} \to \begin{pmatrix} u_F \\ u_G \end{pmatrix} \exp(\mathrm{i}\phi), \tag{6}$$

and consider (6) and its complex conjugate (or alternatively the real and imaginary parts of (6)) as two fundamental solutions of the real-valued Dirac equation (1).

It should be clear that an amplitude-phase method, even if it is an exact method as such, cannot claim that there exists a unique amplitude and a unique phase for an oscillatory solution. For example, one could as well, instead of (6), introduce an ansatz like

$$\begin{pmatrix} F \\ G \end{pmatrix} \to \begin{bmatrix} (E + mc^2 - V(r))^{1/2} u_F \\ (E - mc^2 - V(r))^{1/2} u_G \end{bmatrix} \exp(\mathrm{i}\phi),$$

where in this case u_F, u_G and ϕ are different functions compared with those in (6). The criteria for the amplitude-phase method are rather that the amplitude should be a sufficiently constant function and that the phase should vary sufficiently linear with the radial variable. Apart from the possibility of modifying the ansatz, the amplitude-phase method has other ways to 'optimize' the behaviors of the amplitude and the phase, as will be explained next.

For a single-component Schrödinger equation one introduces in the amplitude-phase approach two functions, the single amplitude u and the single phase ϕ, instead of the original solution. Thus, one has the freedom to define an auxiliary condition that actually *defines* the (non-unique) phase as a function of the amplitude. Historically, the choice $\mathrm{d}\phi/\mathrm{d}r = u^{-2}$ not only transformed the single-component Schrödinger equation to the nonlinear so-called Milne equation [1] for u, but also made the Wronskian of the two fundamental solutions, in this case $u\exp(\mathrm{i}\phi)$ and $u\exp(-\mathrm{i}\phi)$, constant; see [3]. Furthermore, for multi-component solutions of the Schrödinger type the phase has been defined in the same way, i.e. $\mathrm{d}\phi/\mathrm{d}r = u^{-2}$, but now u is generalized to be the (complex or real) norm of the multi-component amplitude [2]. Once this relation between the phase and amplitude has been introduced and the ansatz is substituted into the original differential equations, one obtains *nonlinear* differential equations for the amplitude components. Hence, the resulting solutions of amplitude components will depend on initial conditions. It is at this stage that one is interested in finding a point $r = r_0$, where the amplitude components are (almost) constants and where the very accurate numerical integration can be initialized.

When the two-component ansatz (6) is substituted into the Dirac equations (1), one obtains

$$\begin{aligned} \frac{\mathrm{d}u_F}{\mathrm{d}r} &= \left(-\mathrm{i}\phi' - \frac{\kappa}{r}\right) u_F + \frac{E - V(r) + mc^2}{\hbar c} u_G, \\ \frac{\mathrm{d}u_G}{\mathrm{d}r} &= -\frac{E - V(r) - mc^2}{\hbar c} u_F + \left(-\mathrm{i}\phi' + \frac{\kappa}{r}\right) u_G. \end{aligned} \tag{7}$$

Together with the auxiliary condition

$$\phi' = u^{-2}, \qquad \text{with} \quad u^2 = |u_F|^2 + |u_G|^2, \tag{8}$$

equations (7) constitute the nonlinear differential equations for the complex amplitude components. The four independent quantities to be calculated are the real and imaginary parts of u_F and u_G. With them and relation (8), the ansatz (6) and its complex conjugate define a set of fundamental solutions to the original *linear* differential equation (1) with *real* parameters.

The integration of (7) for scattering problems is initiated formally at $r = +\infty$, where the r-dependence of the coefficients in the original Dirac equation (1) vanishes. By requiring $\mathrm{d}u_{F,G}/\mathrm{d}r = 0$ in (7) with $r = +\infty$, one obtains an eigenvalue problem that results in

$$\phi'(+\infty) = k, \tag{9}$$

with k defined by (5), and

$$\begin{bmatrix} u_F(+\infty) \\ u_G(+\infty) \end{bmatrix} = N \begin{bmatrix} (E + mc^2)^{1/2} \\ \mathrm{i}(E - mc^2)^{1/2} \end{bmatrix}. \tag{10}$$

The normalization factor N is not determined by the solution of the eigenvalue problem itself, but can be determined from the auxiliary relation (8). One thus finds $N = (2Ek)^{-1/2}$ at $r = +\infty$. In practice one initiates the integration at a finite value $r = r_0$, where r_0 is chosen so that $|V(r_0)|$ and/or $|\kappa/r_0|$ are sufficiently small compared to $|E - mc^2|$. It is also possible to require $\mathrm{d}u_{F,G}/\mathrm{d}r = 0$ in (7) with $r = r_0$ and solve a modified eigenvalue problem as that mentioned above with $r = +\infty$. The solution of the modified eigenvalue problem can be seen as a first-order adiabatic solution of the two-component amplitude. Note, however, that the amplitude-phase solution (6) and its complex conjugate still provide a set of exact fundamental solutions.

To proceed, let the complex amplitude component $u_F(r)$ be written as

$$u_F(r) = |u_F(r)|\, \mathrm{e}^{\mathrm{i}\arg u_F(r)}, \tag{11}$$

Table 1. Selected values of the S-matrix for an electron scattered by a Coulombic 4-vector potential with zero space-like components and with $Z = 10$ (neon nucleus). (AP) denotes the amplitude-phase results and (Exact) denotes the result from the closed-form analytic S-matrix formula (16).

ℓ	κ	$S_{\ell,\kappa}$(AP)	$-\arg u_F(0)$	$S_{\ell,\kappa}$(Exact)
0	−1	0.826 3891 + 0.563 099i	0.339	0.826 390 5090 + 0.563 097 4390i
1	1	0.807 0921 − 0.590 426i	0.088	0.807 097 7945 − 0.590 417 7756i
1	−2	0.800 5618 − 0.599 250i	0.130	0.800 556 7332 − 0.599 256 9715i
10	10	−0.980 5816 + 0.196 112i	0.062	−0.980 581 4007 + 0.196 112 5073i
10	−11	−0.980 4249 + 0.196 894i	0.072	−0.980 424 6607 + 0.196 894 6002i
20	20	−0.411 4148 + 0.911 4482i	0.056	−0.411 413 9115 + 0.911 448 6237i
20	−21	−0.411 0614 + 0.911 6077i	0.065	−0.411 060 5650 + 0.911 608 0368i
30	30	0.139 6249 + 0.990 2045i	0.052	0.139 624 5888 + 0.990 204 5116i
30	−31	0.139 8757 + 0.990 1691i	0.062	0.139 878 0096 + 0.990 168 7446i
40	40	0.516 4830 + 0.856 2975i	0.050	0.516 483 2909 + 0.085 629 7268i
40	−41	0.516 6460 + 0.856 1992i	0.059	0.516 646 8108 + 0.856 198 6181i
50	50	0.755 2815 + 0.655 4005i	0.048	0.755 281 6466 + 0.655 400 3617i
50	−51	0.755 3813 + 0.655 2855i	0.057	0.755 381 4669 + 0.655 285 3112i
100	100	0.965 7478 − 0.259 4827i	0.042	0.965 748 7572 − 0.259 478 2650i
100	−101	0.965 7294 − 0.259 5510i	0.052	0.965729 3072 − 0.259 551 3547i

so that one can write the regular large Dirac component as

$$F(r) = A|u_F(r)|\sin[\phi(r) + \arg u_F(r) + \beta] \tag{12}$$

with A and β being constants and $\arg u_F(+\infty) = 0$ from the boundary condition (10). The constant A is unimportant here, but β has to make sure that the solution vanishes at the origin; see [6] for a general discussion on physically acceptable potentials that allow a unique vanishing solution at $r = 0$. The phase $\phi(r)$ in (12) is defined from (8) apart from a constant of integration that can be chosen so that the phase vanishes as $r \to 0$. The constant β in (12) is then uniquely determined from the requirement that the sine function vanishes. Hence, one has

$$\phi(0) = 0 \qquad \text{and} \qquad \beta = -\arg u_F(0). \tag{13}$$

The phase shift defined in (2) is thus obtained by the formula

$$\delta_{\ell,\kappa} = \lim_{r\to+\infty}[\phi(r) - kr - \eta\ln(2kr)] - \arg u_F(0) + \pi\ell/2. \tag{14}$$

A numerical test that allows comparisons with exact analytic results is provided by the Coulomb potential:

$$V(r) = -\frac{Ze^2}{r}. \tag{15}$$

Here, Z is the nuclear charge number and $e > 0$ is the Coulomb charge unit.

The amplitude phase computations are performed using MatLab's integration routine 'ode23' with a tolerance of 10^{-7}. Atomic units ($m = e = \hbar = 1$) with $c = 137$ are used. The scattering energy is chosen as $E = mc^2 + 10^2$ au. The integrations are initiated at $r = r_0 = 5 \times 10^3$ and terminated at $r = 10^{-10}$. A comparison is made with results from the closed-form Coulomb S-matrix given by (see [4])

$$S_{\ell,\kappa} \equiv \mathrm{e}^{2\mathrm{i}\delta_{\kappa,\ell}} = \frac{\kappa - \mathrm{i}\eta mc^2/E}{\Lambda - \mathrm{i}\eta}\frac{\Gamma(\Lambda + 1 - \mathrm{i}\eta)}{\Gamma(\Lambda + 1 + \mathrm{i}\eta)}\mathrm{e}^{\mathrm{i}\pi(\ell-\Lambda)}, \tag{16}$$

where

$$\Lambda = [\kappa^2 - (Z\alpha)^2]^{1/2} > 0. \tag{17}$$

Table 1 shows that the amplitude-phase equations can be effectively integrated using 'MatLab ode23' with minor deviations in the numerical accuracy for different values of the system parameters. The values of the local phase $-\arg u_F(0)$ appear to be rather sensitive to the initial (approximate) values of $u_F(r_0)$, but this sensitivity does not influence the final amplitude-phase result. Therefore, it is not relevant to show more than the first few decimals of $-\arg u_F(0)$ in the table.

This paper presents a new amplitude-phase approach for analyzing the radial Dirac equations. A more detailed account of the method and comparisons with the 'standard' amplitude-phase method (see [1]) and other methods will be presented elsewhere.

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