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A method of approximate solution of the Dirac equation for the case of particle scattering on analytical potentials

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В работе рассмотрено упругое рассеяния релятивистской частицы спина ½ в потенциальных полях. Предложен метод приближенного решения трехмерного уравнения Дирака на основе фазовых сдвигов. Эффективность алгоритма продемонстрирована на примере аналитического потенциала, допускающего наличие резонансных состояний. Исследовано резонансное поведение парциальных и полного сечений рассеяния и зависимость точности решения от параметров потенциала.
Ключевые слова: уравнение Дирака, фазовый сдвиг, сечение рассеяния, резонансные состояния.

In this paper we consider the elastic scattering of relativistic particles of spin ½ in potential fields. A method for approximate solution of the three-dimensional Dirac equation is developed on the basis of the phase shifts. The effectiveness of the algorithm is shown for an analytic potential example which allows existence of the resonant states. The resonant behavior of the partial and total cross sections and the dependence of the solutions accuracy on the potential parameters are investigated.
Keywords: three-dimensional Dirac equation, phase shift, scattering cross section, resonances.

Elementary particle scattering experiments are the most important source of information in the microphysics. The theoretical foundation for analysis of these experiments is quantum scattering theory, where the theory of elastic collisions is an essential part.

Resonance phenomena attract the greatest interest in non-relativistic quantum physics [1, p. 283]. At the same time the study of resonance effects in the relativistic theory has been carried out to a much less extent because calculations are more complicated. However, with the development of computational methods the study of resonant behavior of scattering amplitudes and scattering cross sections become more and more relevant on the basis of the relativistic equations, especially on the basis of the Dirac equation, describing particles of spin 1/2. In this paper, on the foundation of relativistic problems with prime square potentials (square well and square barrier) that have been discussed in the literature, a method is developed for approximate solution of the three-dimensional Dirac equation with analytic potentials.

Consider the three-dimensional stationary Dirac equation for a particle of mass *m* in an external field $V(\vec{x})$ [2, p. 71]. In the unit system $\hbar = c = 1$, the equation can be written in the form

$$\left\{ i\,\vec{\alpha}\,\vec{\nabla} + E - V(\vec{x}) - m\beta \right\} \psi(\vec{x}) = 0\,, \tag{1}$$

where $\vec{\alpha}$ and β are 4×4 matrices, which are obtained from Dirac γ-matrices. Since for a particle moving in a spherically symmetric field $(V(\vec{x}) = V(r))$ the total angular momentum and parity of the state are saved, the components of the wave function $\psi(\vec{x})$ can be written in terms of spherical spinors $\Omega_{j\ell m}(\theta,\phi)$ [3, p. 155]:

$$\psi(\vec{x}) = \begin{pmatrix} f(r)\,\Omega_{j\ell m}(\theta,\phi) \\ -i\,g(r)\,\Omega_{j\ell' m}(\theta,\phi) \end{pmatrix}. \tag{2}$$

Substituting (2) into (1), we obtain a system of ordinary differential equations for the radial wave functions $f(r)$ and $g(r)$ [2, p. 73]:

$$\begin{cases} g'(r) + \dfrac{1-\eta}{r}\,g(r) + \big(E - V(r) - m\big)\,f(r) = 0; \\ f'(r) + \dfrac{1-\eta}{r}\,f(r) - \big(E - V(r) + m\big)g(r) = 0, \end{cases} \tag{3}$$

where

$$\eta = \begin{cases} -(\ell+1), & j = \ell + 1/2; \\ \ell, & j = \ell - 1/2. \end{cases}$$

Let us consider the case when the potential tends to zero fast enough as $r \to \infty$. We divide the range of the variable r $(0 \le r < \infty)$ in two parts (figure 1): finite $0 \le r < r_{N-1}$, and semi-infinite $r_{N-1} \le r < \infty$. In the last part, we will suppose the potential to be small enough to be substituted by 0. We also divide the interval $0 \le r < r_{N-1}$ in $N-1$ parts: $0 \le r < r_1$; $r_1 \le r < r_{N-1}$; $\ldots r_{N-2} \le r < r_{N-1}$, in each of which the potential varies a little, so it can be substituted by a constant.

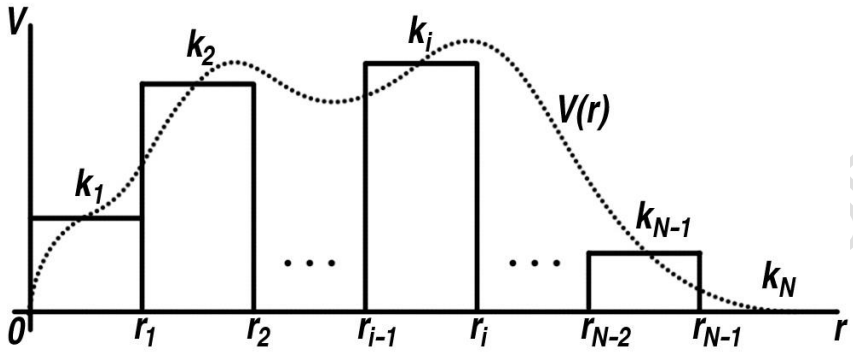

Figure 1 – Approximation of the potential.

These constants have to be some average value of the $V(r)-$ function on the intervals described. Then system (3) on each of the intervals can be solved analytically and the solutions are expressed in terms of the spherical Bessel and Neumann functions [2, p. 73]:

$$\begin{cases} f(r) = c\, j_{l_\eta}(k\,r) + d\, n_{l_\eta}(k\,r); \\ g(r) = \dfrac{k}{E - V + m}\left[c\, j_{l_{-\eta}}(k\,r) + d\, n_{l_{-\eta}}(k\,r) \right], \end{cases} \tag{4}$$

where k is the module of the particle momentum $(k^2 = (E-V)^2 - m^2)$, and the subscripts of spherical functions are

$$l_\eta = \begin{cases} \eta, & \eta > 0; \\ -\eta - 1, & \eta < 0, \end{cases} \qquad l_{-\eta} = \begin{cases} \eta + 1, & \eta > 0; \\ -\eta, & \eta < 0. \end{cases}$$

Thus, as a result we have a common solution for each specific region of the multi-step potential $(r_{i-1} \le r < r_i)$.

Let us consider particle scattering on such potential. In the semi-infinite region $r_{N-1} \le r < \infty$, where the potential is supposed to be zero, we represent the coefficients c and d via the phase shifts δ_η [4]. Then the radial functions $f(r)$ and $g(r)$ for the whole of range of the variable r will take the form

$$\begin{cases} f_i(r) = c_i\; j_{l_\eta}(k_i\,r) + d_i\, n_{l_\eta}(k_i\,r); \\ g_i(r) = \dfrac{k_i}{E - V_i + m}\left[c_i\; j_{l_{-\eta}}(k_i\,r) + d_i\, n_{l_{-\eta}}(k_i\,r) \right]; \end{cases} \qquad r \in [r_{i-1}; r_i);$$

. . . . . .

$$\begin{cases} f_N(r) = c_N \left[j_{l_\eta}(k_N\,r) - \dfrac{1}{\cot\delta_\eta}\, n_{l_\eta}(k_N\,r) \right]; \\ g_N(r) = \dfrac{k_N}{E - V_N + m}\, c_N \left[j_{l_{-\eta}}(k_N\,r) + \dfrac{1}{\cot\delta_\eta}\, n_{l_{-\eta}}(k_N\,r) \right]; \end{cases} \qquad r \in [r_{N-1}; \infty). \tag{5}$$

To find all the coefficients c and d, we have to use the conditions which smoothly connect functions $f_i(r)$, $g_i(r)$ and $f_{i+1}(r)$, $g_{i+1}(r)$ [5, p. 51]:

$$\left(\frac{g_i(r)}{f_i(r)}\right)_{r=r_i-0} = \left(\frac{g_{i+1}(r)}{f_{i+1}(r)}\right)_{r=r_i+0}. \qquad (6)$$

We obtained a few first coefficients c_i and d_i, on the basis of (5) and (6), then we defined the recurrence relations for c_i, d_i. As a result, we have obtained a compact expression for determining the phase shifts:

$$\cot\delta_\eta = \frac{K_N^1 - D_{N-1}K_N^2}{K_N^3 - D_{N-1}K_N^4}. \qquad (7)$$

Here

$$D_i = \frac{K_i^3 - D_{i-1}K_i^4}{K_i^1 - D_{i-1}K_i^2};$$

$$K_i^1 = \begin{pmatrix}\chi_i & \lambda_{i-1} & \chi_i'\end{pmatrix}\begin{pmatrix} j_{l_\eta}(\chi_i')\, n_{l_{-\eta}}(\chi_i) \\ -j_{l_{-\eta}}(\chi_i')\, n_{l_\eta}(\chi_i)\end{pmatrix}; \qquad K_i^2 = \begin{pmatrix}\chi_i & \lambda_{i-1} & \chi_i'\end{pmatrix}\begin{pmatrix} n_{l_\eta}(\chi_i')\, n_{l_{-\eta}}(\chi_i) \\ -n_{l_{-\eta}}(\chi_i')\, n_{l_\eta}(\chi_i)\end{pmatrix};$$

$$K_i^3 = \begin{pmatrix}\chi_i & \lambda_{i-1} & \chi_i'\end{pmatrix}\begin{pmatrix} j_{l_\eta}(\chi_i')\, j_{l_{-\eta}}(\chi_i) \\ -j_{l_{-\eta}}(\chi_i')\, j_{l_\eta}(\chi_i)\end{pmatrix}; \qquad K_i^4 = \begin{pmatrix}\chi_i & \lambda_{i-1} & \chi_i'\end{pmatrix}\begin{pmatrix} n_{l_\eta}(\chi_i')\, j_{l_{-\eta}}(\chi_i) \\ -n_{l_{-\eta}}(\chi_i')\, j_{l_\eta}(\chi_i)\end{pmatrix},$$

where $D_1 = 0$, $\chi_i = k_i r_{i-1}$, $\chi_i' = k_{i-1} r_{i-1}$, $\lambda_i = \dfrac{E - V_i + m}{E - V_{i+1} + m}$.

The matrix elements of the scattering operator can be expressed via the phase shifts δ_η. In turn the differential scattering cross section in the solid angle $d\Omega$ can be determined by means of the matrix elements. If the initial state is not polarized ($\vec{P} = 0$), then we have [3, p. 168]

$$\frac{d\sigma}{d\Omega} = |A|^2 + |B|^2, \qquad (8)$$

where

$$A = \frac{1}{2ik}\sum_{\ell=0}^{\infty}\left[(\ell+1)\left(e^{2i\delta_{-(\ell+1)}} - 1\right) + \ell\left(e^{2i\delta_\ell} - 1\right)\right]P_\ell(\cos\theta);$$

$$B = \frac{1}{2k}\sum_{\ell=1}^{\infty}\left[e^{2i\delta_{-(\ell+1)}} - e^{2i\delta_\ell}\right]P_\ell^1(\cos\theta).$$

and $P_\ell(\cos\theta)$, $P_\ell^1(\cos\theta)$ are the Legendre polynomials.

Integrating (8) over the whole solid angle $d\Omega$, we obtain the total scattering cross section which is represented as the sum of the partial cross sections. The next form of the result is convenient for subsequent calculations:

$$\sigma = \sum_{\ell=0}^{\infty}\sigma_\ell = \sum_{\ell=0}^{\infty}\frac{4\pi}{k^2}\left[\frac{\ell+1}{\cot^2\delta_{-(\ell+1)} + 1} + \frac{\ell}{\cot^2\delta_\ell + 1}\right]. \qquad (9)$$

Thus, substituting the parameters of multi-step potential into (7), and then producing the calculation of the partial cross sections (9), we obtain an approximate solution of the Dirac particles scattering problem on the smooth potential under consideration.

Let us consider the effectiveness of the algorithm using as an example the following potential:

$$V(r) = A\left[\frac{r}{u}\exp\left(1 - \frac{r}{u}\right)\right]^\nu. \qquad (10)$$

First, we approximate this smooth potential by a multi-step potential. The choice of the approximation method determines how quickly the numerical solution approaches the exact solution. We used several methods and identified how potential features define the best of them. Then we constructed the mesh of multi-step potential and the resulting array coordinates and momentum was used to calculate the phase shift (7). Then we found partial cross section (9).

Partial cross sections have the following feature: each of them has non-zero values only in an energy interval. In the $\ell = 0$ case the cross section has its maximum value at $E = m$, on the other hand for all other values of ℓ the partial cross sections tend to zero at $E = m$. It can be explained as follows: at low energies only central collision with $\ell = 0$ gives contribution to total cross section, at larger ℓ an low energies partial cross section decreases, because the particle goes far enough from the scattering center. It gives opportunity to construct the total cross section exactly following formula (9) for some energy interval.

The dependence of cross sections σ on particle energy E is shown in figure 2 for $v = 1,2,3$ and for various potential parameters: left – $u = 0{,}9\ \text{MeV}^{-1}$, $A = 3{,}8\ \text{MeV}$; right – $u = 1{,}3\ \text{MeV}^{-1}$, $A = 4{,}8\ \text{MeV}$. To obtain the correct total cross sections behavior in the energy interval $0{,}5 - 2{,}5\ \text{MeV}$ the following number of partial cross sections were summed: (a) – 19, (b) – 27, (c) – 13, (d) – 19, (e) – 11, (f) – 14. In calculations we used the number of steps N=50, as a result the relative discrepancy is not more then 1.3 %.

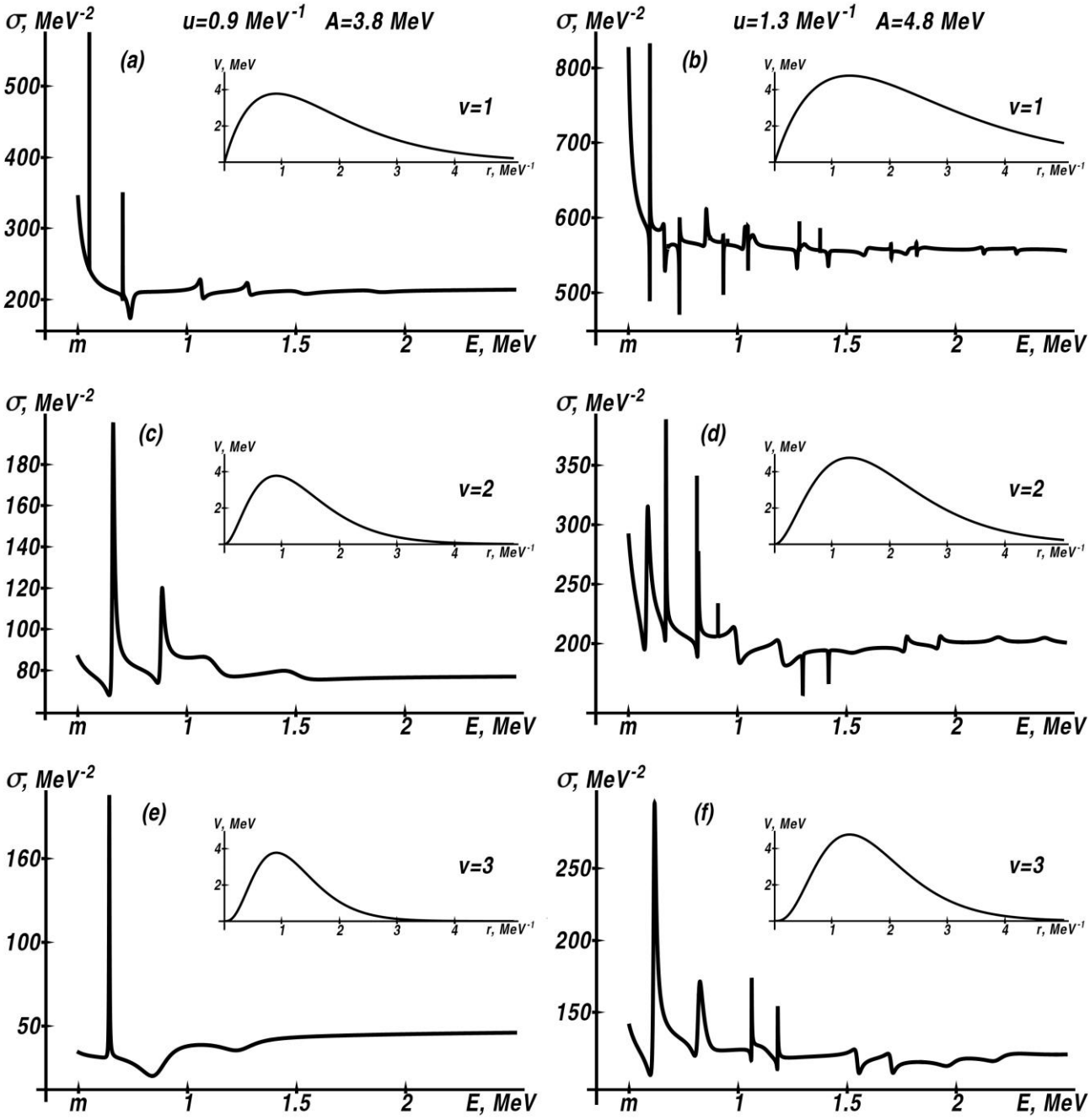

Figure 2 – The dependence of the total cross section σ on energy E for different values of potentials (m=0,5MeV).

The behavior of potentials (10) allows supposing the existence of resonant states and the solution results have confirmed their availability. The number of resonant states increases with the height of the barrier (with increasing parameter *A*). The width of the resonances decreases with increasing the width of the barrier (with increasing parameter *u*). The number of resonant states decreases with increasing the parameter *v*.

Figure 3 illustrates the dependence of the partial cross section σ_2 on energy *E* for different numbers of subdividing steps *N* on the corresponding form of the multi-step potential.

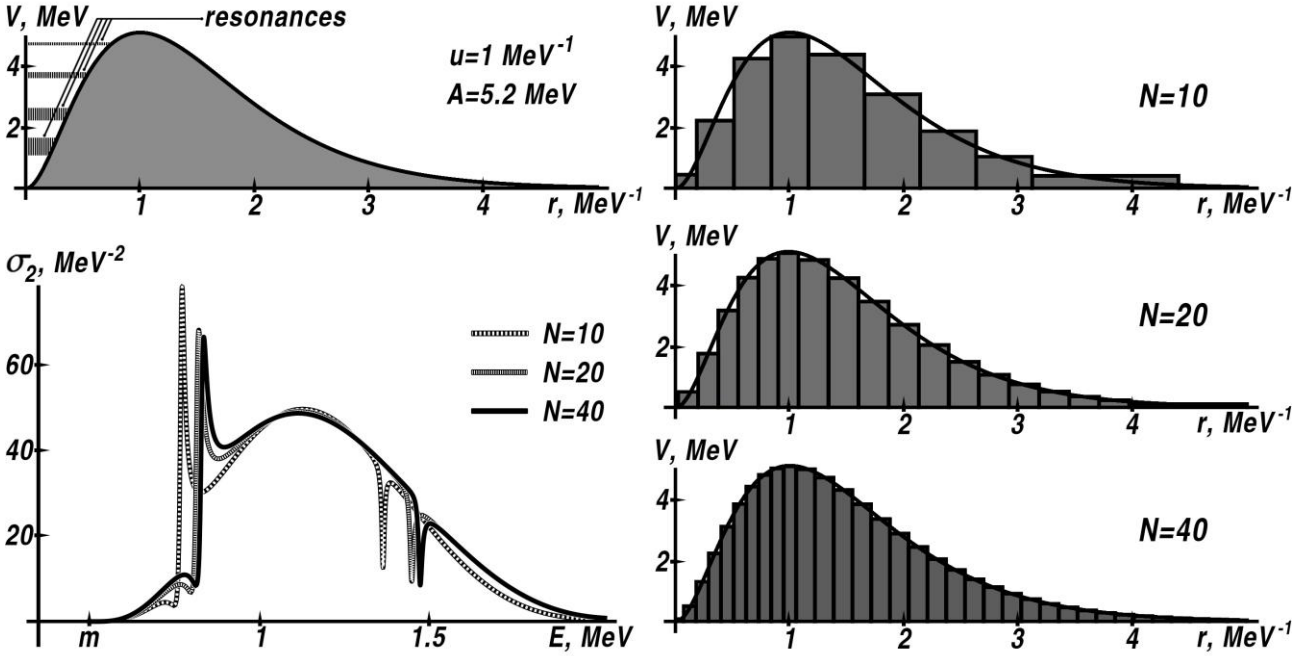

Figure 3 – The dependence of the partial cross σ_2 on energy *E* at $v = 2$ (m=0,5MeV).

It is seen in figure 3 that with increasing the number of steps the result converges quickly to the exact solution. With increasing the quantum number ℓ the accuracy of solution decreases, that can be compensated by enlarging the number of steps *N*. The error of the solution becomes bigger near the resonance energies.

Thus, the proposed method allows solving the Dirac equation with different potentials and observing physical effects that are contained in the exact solution, and calculating different characteristics of the relativistic particle scattering.

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