ISSN 0015—3206
FZKAAA 23 (4) 375 (1991)

SCATTERING OF RELATIVISTIC WAVE PACKET

SLOBODAN D. BOSANAC

Ruđer Bošković Institute, POB 1016, Zagreb, The Republic of Croatia

Received 15 September 1991

Revised manuscript received 23 October 1991

UDC 530.145

Original scientific paper

Scattering of the relativistic wave packets is analyzed in three dimensions. An efficient method is described for evaluating the Fourier type integrals which appear in this analysis.

1. Introduction

The purpose of this paper is to describe a method for efficient evaluation of the Fourier type integrals which appear in the scattering analysis of the relativistic wave packets. There are several reasons why there is a need for developing such methods. For one, it is known that analysis of the scattering processes on the time scale may reveal new phenomena, which are not observed in a time independent picture[1]. As will be shown here, very often there is a qualitative difference between the two types of analysis. We shall put an emphasis on the relativistic wave packets since they have not been analyzed in great detail[2], with, perhaps the exception of the electromagnetic wave packets[3] (many useful references are found in Ref. 4). So far only the analysis of dynamics of the nonrelativistic wave packets have attracted great interest[5,6,7]. This is primarily because of the development of the experimental techniques with the ultra short laser pulses[8]. On the theoretical side it was also believed that the wave packet analysis is more appropriate if one is to study processes which require semiclassical approach[9,10], such as collisions of atoms and molecules.

As an example we shall consider the solutions of the Klein-Gordon equation. The method for propagating the wave packets is based on direct numerical integration of the Fourier type integral. The method is quite efficient and in a reasonable time the results for the three dimensional scattering can be obtained even on the smallest of the desktop computers. Therefore there was no need for implementing various other ideas for numerical solution of the time dependent wave equation[5,10]. In fact there are some drawbacks of these methods, and one is that they were primarily developed for solving the nonrelativistic wave equation. The other drawback is that by using these methods one is not able to analyze the solution in terms of some analytical approximations. Usually such approximations allow for deeper insight into the phenomena which underlie the scattering process.

2. *Scattering of wave packets*

Relativistic equation for a scalar particle is the Klein-Gordon (KG) equation

$$-\frac{\hbar^2}{c^2}\frac{\partial^2}{\partial t^2}\psi + \hbar^2 \Delta\psi = m^2c^2\psi. \tag{1}$$

It will be useful to redefine the variable t and the coordinates, by scaling them with respect to the Compton wavelength $l_0 = \hbar/(mc)$. From now on the time variable t represents tc/l_0 while the coordinates are normalized with respect to l_0. In these new variables Eq. (1) is

$$-\frac{\partial^2}{\partial t^2}\psi + \Delta\psi = \psi. \tag{2}$$

If at time $t = 0$ the wave packet has the form ψ_0 then at some later time the solution of (2) is given by

$$\psi = \int \mathrm{d}^3k\, \mathrm{e}^{-\mathrm{i}\omega t}\, A(\vec{k})\, \Phi(\vec{r}, \vec{k}) \tag{3}$$

where Φ is solution of the time independent KG equation

$$\Delta\Phi = (1 - w^2)\,\Phi \tag{4}$$

with the boundary condition for scattering

$$\Phi(\vec{r}, k) \underset{r\to\infty}{=} \mathrm{e}^{\mathrm{i}kz} + \frac{f(\vartheta, k)}{r}\,\mathrm{e}^{\mathrm{i}kr}. \tag{5}$$

In the solution (3) it is implicitly assumed that the interaction does not mixes two energy components. Extension of the method described here to a more general case is simple. As a consequence when the two energy components are included i. e. both $+w$ and $-w$ are considered, the wave packet splits into two components for $t > 0$, the two wave packets moving in the opposite directions.

The amplitude A is obtained from the initial condition by evaluating the

$$A(\vec{k}) = \frac{1}{(2\pi)^3} \int \mathrm{d}^3 r \, \psi_0 \, \mathrm{e}^{-\mathrm{i}\vec{k}\vec{r}} \tag{6}$$

which is obtained if one notices that ψ_0 is localized in the asymptotic region where the solution Φ has the form (5). There is a variety of initial conditions which might be considered but they are primarily determined by the experimental setup. In general, however, we shall assume that the extent of the wave packet perpendicular to the line of propagation is much more difficult to control than its wave front. In other words, we shall consider the wave packets which are limited along the direction of propagation, say along the z-axis, but they are unlimited perpendicular to this direction (in the x and y directions). Unlimited extent of the wave packet has relative meaning, but usually this means that it is much larger than the dimensions of the target.

Since the initial condition ψ_0 is a function of the z variable only then

$$A(\vec{k}) = \frac{\delta(k_x)\,\delta(k_y)}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}z \, \psi_0(z) \, \mathrm{e}^{-\mathrm{i}zk_z}. \tag{7}$$

A particularly simple case of the initial condition is the Gaussian function

$$\psi_0 = \exp\left(\mathrm{i}zk_0 - \frac{z^2}{2a^2}\right) \tag{8}$$

which gives for the amplitude $A(\vec{k})$

$$A(\vec{k}) = a(k_z)\,\delta(k_x)\,\delta(k_y) = \frac{a}{\sqrt{2\pi}} \exp\left[-\frac{a^2}{2}(k_z - k_0)^2\right]. \tag{9}$$

As an example we shall consider the Coulomb scattering (the Rutherford scattering) for which Eq. (4) is[11]

$$\left(-w + \frac{\varkappa}{r}\right)^2 \Phi + \Delta\Phi = \Phi \tag{10}$$

and at the short distances it is approximately

$$\Delta\Phi + \frac{\varkappa^2}{r^2}\Phi = -(w^2 - 1)\,\Phi. \tag{11}$$

In our model we shall assume interaction of the form

$$\Delta\Phi - U\Phi = -(w^2 - 1)\,\Phi \tag{12}$$

where

$$U = V_0 - \left(\frac{\lambda_0^2}{r^2} - \frac{\lambda_0^2}{r_0^2}\right) \qquad r < r_0$$
$$= 0 \qquad r \geq r_0 \tag{13}$$

where V_0 is constant and r_0 is the radius of interaction. Such a model potential assumes dominance of the psudeo-centrifugal term at short distances, modified by the interaction which have resemblance to the short range strong interaction (electrons do not show strong interaction, nevertheless we shall consider this as a model exercise). The pseudo centrifugal term causes any approaching particle to be absorbed, hence U can be used for modelling collisions which do not conserve probability

The usual way to obtain the solution is by writing expansion

$$\Phi(\vec{r}, k) = \frac{1}{r} \sum_{l=0}^{\infty} (2l + 1) P_l(\cos\vartheta) \Phi_l(r, k) \tag{14}$$

where $P_l(z)$ is Legendre polynomial and ϑ is the polar angle of $\vec{r}$. $\Phi_l(r, k)$ is the radial solution of the KG equation for the l-th partial wave, subjected to a particular boundary condition so that the asymptotic condition (5) is satisfied. However, if (14) is replaced in the integral (3) a serious difficulty is encountered in the application. Owing to the unscattered wave, the number of terms in the l expansion increases when r increases, i. e. in the far away scattering region, where the wave packet is monitored, the number of terms would be prohibitively large. Therefore, the sum (14) should be conveniently modified in order to avoid this problem.

It can be shown that $\Phi(\vec{r}, k)$ can be written as

$$\Phi(\vec{r}, k) = e^{ikz} + \sum_{l=0}^{\infty} i^l (2l + 1) P_l(\cos\vartheta) \left[\frac{i^{l+1} \Phi_l(r, k)}{2rk\, a_l(k)} - j_l(kr)\right] \tag{15}$$

which is solution of (12) for all r. $j_l(kr)$ is the regular spherical Bessel function, $\Phi_l(r, k)$ is the regular radial wave function and $a_l(k)$ are coefficients defined from the asymptotics of $\Phi_l(r, k)$

$$\Phi_l(r, k) \underset{r\to\infty}{=} e^{ikr} b_l(k) + e^{-ikr} a_l(k). \tag{16}$$

The advantage of this expression over (14) is that the number of terms l in the sum is independent of r, since the unscattered wave is explicitly taken outside the sum.

For our particular problem $\Phi_l(r, k)$ is

$$\Phi_l(r, k) = \sqrt{r}\, J_\nu(rk') \qquad r < r_0$$
$$= \sqrt{r}\,[A H_\lambda^{(1)}(kr) + B H_\lambda^{(2)}(kr)] \qquad r > r_0 \tag{17}$$

where $\lambda = l + 1/2$, $\nu = (\lambda^2 - \lambda_0^2)^{1/2}$ and $k' = [k^2 - V_0 - (\lambda_0/r_0)^2]^{1/2}$. When $\lambda_0 < \lambda$ the index ν is negative imaginary (it can be shown that positive imaginary ν does not lead to absorption). When k' is imaginary it has positive value. $H_\lambda^{(1)}(z)$ are the Hankel functions. The coefficients A and B are determined from the continuity of the wave function at $r = r_0$.

It is easily shown from the asymptotic value of Hankel functions that $a_l(k)$ is

$$a_l(k) = \frac{i^l}{2}\sqrt{\frac{\pi}{2k}}\,[kr_0\,H_{\lambda-1}^{(1)}(kr)\,J_\nu(r_0k') - r_0k'\,H_{\lambda_1}^{(1)}(kr_0)\,J_{\nu-1}(r_0k') + \\ + (\nu - \lambda)\,H_\lambda^{(2)}\,J_\nu(r_0k')]. \tag{18}$$

3. *Discussion and examples*

Few examples were calculated with the initial condition (8). In all cases considered we have taken $k_0 = 5$ (the relativistic case) and $a = 1$. In the first example, shown in Fig. 1, the parameters of the potential were: $V_0 = 5$ and $\lambda_0 = 3$, and

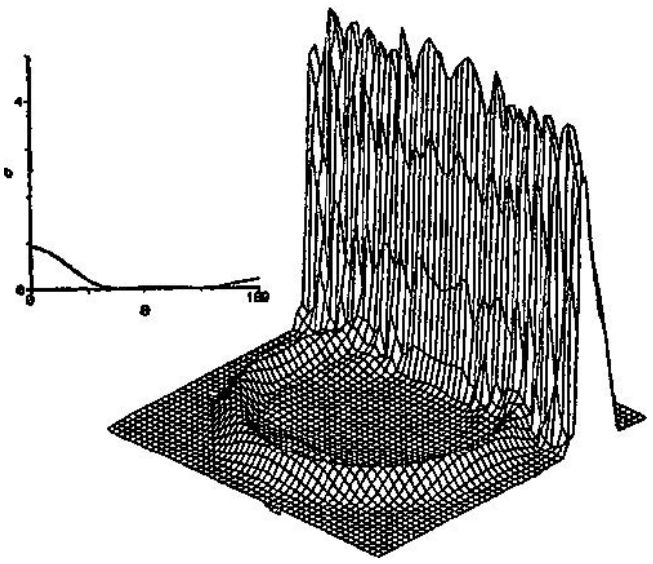

Fig. 1. Scattering of the Gaussian wave packet on the potential (13). The parameters are $V_0 = 5$ and $\lambda_0 = 3$ while $k_0 = 5$. The scattered wave packet is shown after $t = 15$ time units. The parameters are dimensionless because of the normalization discussed in (2).

the scattered wave packet was calculated after $t = 15$ units of time. The large «mountain« which doninates the figure, is the unscattered wave packet. The scattered wave packet is of much lower intensity and is radially going out of the scattering region. Two components of the scattered wave packet are noticed. The most out-

ward component corresponds to the scattering of the wave from the sharp edge of the potential[12]. The second component lags behind the first one and it is of lower intensity. The explanation is the following; part of the incoming wave packet is trapped inside the potential and comes out at some later time.

In the insert of the Fig. 1 the differential cross section is shown for stationary scattering, i. e. for the case of a plane incident wave (O^0 scattering angle in the cross section corresponds to the direction from the center of interaction towards the direction of propagation of the incident wave packet). The intensities of the cross section and the scattered wave packet do not match. The reason for this is that the differential cross section corresponds to an infinitely long wave packet so that the time component does not play any role. Therefore the intensities of the two scattered components in Fig. 1. interfere thus producing the pattern shown in the insert. This example points at a very important finding: scattering of plane waves is an idealization of the scattering problems, however, very often it works. When experiments with time resolution are considered this fact becomes important and no longer should be neglected

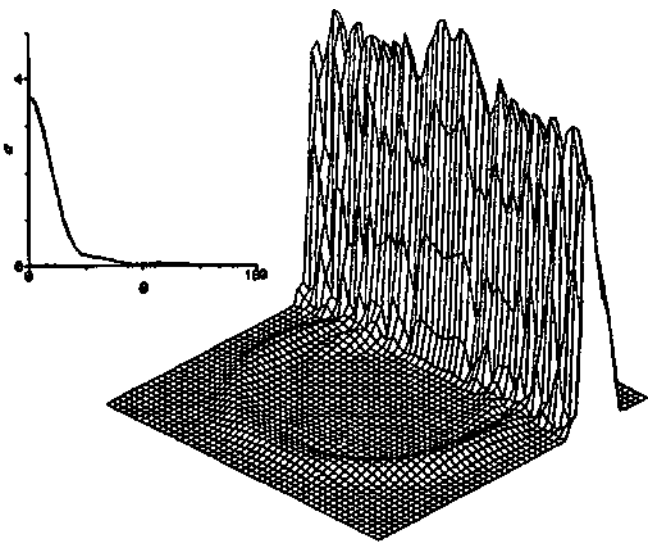

Fig. 2. Scattering of the wave packet as in Fig. 1 except $V_0 = 15$.

In another example shown in Fig. 2, the parameter V_0 was changed to $V_0 = 15$. The back-scattering is virtually zero, as can be seen from the differential cross section which is inserted in the figure. However, the scattered wave packet is not zero in the backward space, but again it has two components. Therefore, zero differential cross section does not necessarily imply zero intensity for the wave packets. The interference of the two components which appear in the wave packet produce in the plane wave small intensity.

If V_0 is negative one expects orbiting of the incident particle[12]. This effect produces a typical oscillatory pattern in the differential cross section. In Fig. 3. the potential well is $V_0 = -20$ while λ_0 is the same as in the previous figures.

The differential cross section is indeed oscillatory, with a peak in the backward direction, the backward glory, which is typical of orbiting. However, the scattered wave packet shows rather irregular structure, except the outward rim which is due to the scattering from the edge of the potential. The backward peak is also noticed, and lags behind the outward rim. This delay equals exactly the time the particle goes around the target, and then goes in the backward direction. Again the differential cross section and the intensity of the scattered wave packet do not match.

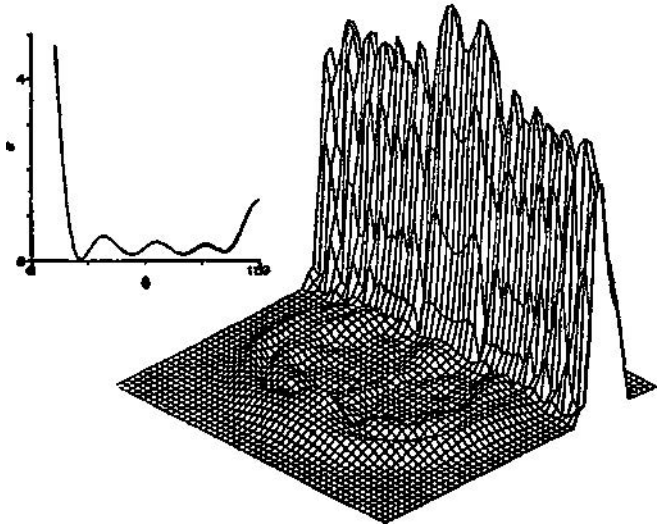

Fig. 3. Scattering of the wave packet as in Fig. 1 except $V_0 = -20$.

Another interesting case is shown in Fig. 4. which is calculated for $V_0 = -20$ and $\lambda_0 = 5$. For these parameters a resonance appears in the cross section, which is noted as a great enhancement of the backward glory, and the cross section looks symmetric with respect to 90°. The scattered wave packet is calculated for $t = 20$ units of time in order to show a beautiful manifestation of resonances. The backward glory is indeed very well pronounced, but in addition to this there are regular »stripes« of the scattered wave packet emanating from the center of interaction. These stripes are indication that a resonance is formed because, in a »popular« language, resonance is another way of saying that a standing wave is formed. The elongated look of these stripes is a consequence of the properties of resonances that they represent decaying states. At the moment of impact a resonance builds up and as soon as the incoming wave goes away, the accumulated probability in the interaction region leaks out and its intensity decays off exponentially[13,14]. All the stages of this process are very well observed in Fig. 4.

The last example is interesting for a different reason. It was calculated for $V_0 = 1$ and $\lambda_0 = 50$. The value of λ_0 implies large absorption of particles, however, as shown in Fig. 5, this is not the case. Closer inspection reveals that both the differential cross section (see the insert) and the scattered wave packet are almost identical to the case as if the potential V_0 is infinitely high, i. e. as if the collision

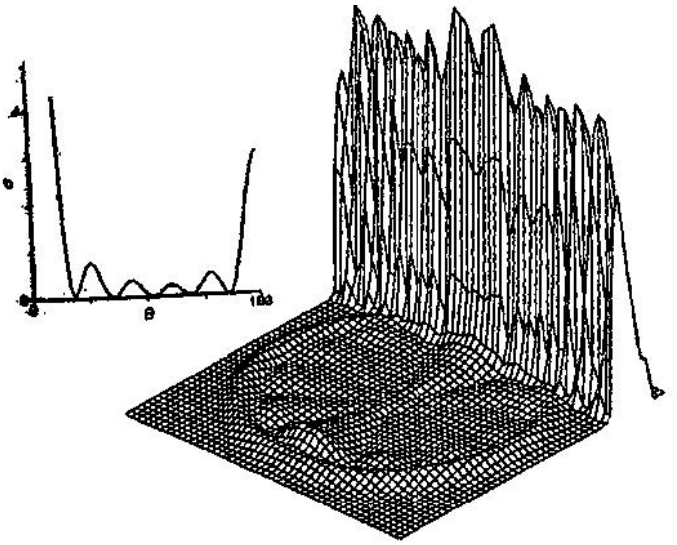

Fig. 4. Scattering of the wavepacket as in Fig. 1 except $V_0 = -20, \lambda_0 = 5$ and $t = 20$.

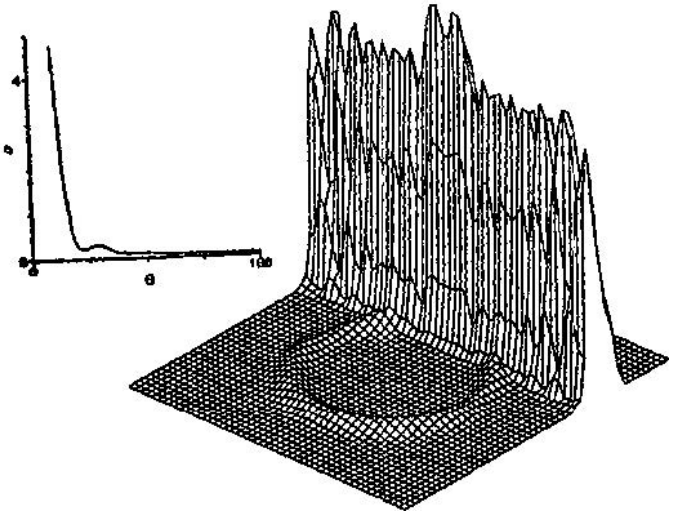

Fig. 5. Scattering of the wave packet as in Fig. 1 except $V_0 = 1$ and $\lambda_0 = 50$.

is for hard spheres. The reason for this is that owing to the large value of λ_0 the wave function oscillates very rapidly in the interaction region, which is on average zero. This is nothing but a boundary condition for hard spheres: in the potential the wave function must be zero.

In the preceding examples we have shown various cases of the scattering of the relativistic wave packets. A wave packet of the Gaussian shape was considered, which is not entirely realistic. It would be more appropriate to consider a semi-infinite initial wave packet. However, we wanted to present the beauty and the importance of the wave packet analysis. Analysis of more realistic wave packets would not alter the main conclusions, but would be more realistic for analysis of experiments.

References

1) S. D. Bosanac, *Rainbow effect in classical and quantum probability packets*, unpublished work;
2) J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics*, McGraw-Hill, New York, 1964, chapt. 3.3;
3) S. Bosanac, Phys. Rev. **A28** (1983) 577;
4) J. D. Jackson, *Classical Electrodynamics*, Wiley, New York, 1975, chapt. 17;
5) A. Goldberg, H. M. Chey and J. L. Schwartz, Am. J. Phys. **35** (1967) 177;
6) H. Guo and G. C. Schatz, J. Chem. Phys. **94** (1991) 379;
7) Go. Torres-Vega and J. H. Frederick, J. Chem. Phys. **93** (1990) 8862;
8) M. Dantus, M. J. Rosker and A. H. Zewail, J. Chem. Phys. **87** (1987) 2395;
9) E. J. Heller, J. Chem. Phys. **68** (1978) 2066;
10) D. Kosloff and R. Kosloff, J. Comp. Phys. **52** (1984) 35;
11) H. Bethe, *Intermediate Quantum Mechanics*, Benjamin, New York, 1964, chapt. 16;
12) J. N. Murrell and S. D. Bosanac, *Introduction to the Theory of Atomic and Molecular Collisions*, Wiley, Chichester, 1989;
13) S. D. Bosanac, *Long-Lived States in Collisions*, CRC Press, Boca Raton, 1988;
14) S. D. Bosanac, Z. Phys. **D15** (1990) 17.

RASPRŠENJE RELATIVISTIČKOG VALNOG PAKETA

SLOBODAN D. BOSANAC

Institut »R. Bošković«, Zagreb, Republika Hrvatska

UDK 530.145

Originalni znanstveni rad

Raspršenje relativističkog valnog paketa analizira se u tri dimenzije. Opisana je efikasna metoda za računanje Fourier tipa integrala koji se pojavljuje u tim analizama.