Computer Physics Communications 19 (1980) 299–303

COMPUTATIONAL METHODS FOR EIKONAL DIFFERENTIAL CROSS SECTIONS

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Received 19 February 1980

The present work deals with semianalytic methods for obtaining differential cross sections in the eikonal approximation. They are based on the development of the transition amplitudes in a polynomial basis and subsequent calculation of the eikonal integrals by complex Hankel transforms. A comparison between different methods in the case of high energy proton–hydrogen collision is given.

1. Introduction

An increasing interest in the study of differential cross sections has been observed in recent years, from thermal to high energy atomic (heavy particle) collisions [1–3]. Due to the large masses of the colliding particles with respect to the electron mass, semiclassical approximations have been considered [4]. They are based on a classical description of the heavy particles trajectory and a quantum treatment of the bounded electron dynamics. Particularly successful is the eikonal approximation which was first developed in the context of optics and nuclear physics [5–7]. This formalism has been extended to inelastic (electronic excitation or charge exchange) collisions [8–10]. A numerical procedure has been developed [11,12] in close analogy with the quantum mechanical (discrete) expression for the differential cross section, which was applied to the treatment of fundamental collision systems [13–17].

The aim of our work is to present new methods for evaluating the eikonal differential cross section.

In section 2 we show the eikonal formula and in section 3 we give methods for its evaluation. In section 4 we apply the results of section 3 to the study of proton–hydrogen collisions. In section 5 we obtain conclusions on the accuracy and speed of the proposed numerical methods.

Atomic units ($\hbar = m_e = e = 1$) are used except where otherwise stated.

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2. Eikonal differential cross section

In heavy particle collisions, even at low energies (i.e., relative velocity lower than the velocity of the active electron), many hundred or thousand partial waves contribute to the scattering for a given angle. Consequently, a semiclassical connection between the (discrete) angular momentum l and the continuum impact parameter ρ can be established as $\rho = (l + \frac{1}{2})/k$, where k is the relative momentum. Therefore, when the nuclear trajectories are assumed to be straight lines, the quantum mechanical expression for the differential cross section can be transformed into an integral called the "eikonal". Evidently, this approximation is valid for small scattering angles. This result has been first obtained for the case of potential scattering [5]. If the colliding system has internal degrees of freedom, it has been shown [8–10] that the differential cross section can be obtained in a similar way, by including in the eikonal integral the transition amplitudes

$$c(\rho, t = \infty) = \lim_{t \to \infty} \langle \Phi | \psi \rangle , \qquad (1)$$

where Φ is a wave function describing a particular final state and ψ is the total wave function. Then the eikonal differential cross section (in the centre of mass system) is

$$\mathrm{d}Q/\mathrm{d}\Omega(\theta, k) = k^2 |I(\theta, k)|^2 . \tag{2}$$

In (2), the eikonal integral is

$$I(\eta) = \int_0^\infty \rho c(\rho) J_M(\eta\rho)\, \mathrm{d}\rho , \tag{3}$$

where $\eta = 2k \sin(\theta/2)$, θ is the scattering angle and J_M a Bessel function of order $M = |M_i - M_f|$, M_i and M_f being the projections of the total electronic orbital angular momentum in the direction of the incident velocity, for initial i and final f states, respectively.

Since the Coulomb interaction is the same for all channels, it can be demonstrated that [8]

$$c(\rho) = a(\rho)\, \rho^{i\nu} , \tag{4}$$

where $\nu = 2ZZ'/v$. Here Z, Z' are the nuclear charges and v the relative velocity. The reduced transition amplitude $a(\rho)$ is obtained excluding the nucleus–nucleus interaction, which is taken into account in the $\rho^{i\nu}$ factor of eq. (4).

Introducing (4) in (3), we obtain

$$I(\eta) = \int_0^\infty \rho^{1+i\nu}\, a(\rho)\, J_M(\eta\rho)\, \mathrm{d}\rho . \tag{5}$$

A direct numerical evaluation of (5) requires the use of very small impact parameter intervals, since the first and third terms in the integrand are strongly oscillatory.

3. Calculation of the eikonal integral

3.1. McCarroll, Piacentini and Salin's (MPS) method

This method consists in returning, from the semiclassical (eikonal) differential cross section, to the quantum mechanical expression. In the latter, the transition amplitude (1) is considered instead of the scattering matrix [11].

In accordance with MPS's work [11], we introduce

$$W(\xi) = \frac{2ik}{\xi} \sum_{l=0}^{l_{mx}} (2l+1)\, c\left(\frac{2l+1}{\xi}\right) \times J_M\left(\frac{\eta}{\xi}(2l+1)\right) , \tag{6}$$

where $l_{mx} = (\xi\rho_{mx} - 1)/2$. Then, $W(\xi)$ can be related to the eikonal integral (3), by

$$I(\eta) = \lim_{\xi\to\infty} W(\xi) . \tag{7}$$

The usual choice for ξ is $\xi = 2k$, so the relation between l and ρ is given by the semiclassical expression $\rho = (l + \frac{1}{2})/k$.

3.2. Hankel transform – Laguerre expansion (HTLE) method

The eikonal integral (5) can be seen as the complex Hankel transform of the transition amplitudes. In cases when $a(\rho)$ is described by a simple function, the final result can be obtained easily from tables [18]. But these are very particular examples, where strong approximations have been made in order to arrive at an analytical expression. In the general case $a(\rho)$ is obtained numerically, after solving a system of integro–differential equations [19,20]. Then, one possibility is to expand $a(\rho)$ in Laguerre polynomials as follows

$$a(\rho) = \exp(-b\rho) \sum_{m=1}^{N} A_m L_m(b\rho) , \tag{8}$$

where $L_1(b\rho) = 1$, since we start the summation at $m = 1$ (we work with transformed suffixes for computational facility).

From the orthogonality of the Laguerre polynomials we obtain

$$A_m = b \int_0^\infty a(\rho)\, L_m(b\rho)\, \mathrm{d}\rho . \tag{9}$$

Since

$$L_m(x) = \sum_{j=1}^{m} \frac{(-1)^{j-1}(m-1)!}{(m-j)![(j-1)!]^2} x^{j-1} , \tag{10}$$

substituting (10) in (8) gives

$$a(\rho) = \exp(-b\rho) \sum_{j=1}^{N} G_j \rho^{j-1} , \tag{11}$$

where

$$G_j = (-b)^{j-1}[(j-1)!]^{-2} \times \sum_{m=1}^{N} A_m (m-1)!/(m-j)! . \tag{12}$$

We have derived in (11) a *simple* expansion in powers of the impact parameter, where the weights G_j are obtained easily from a direct evaluation of the N integrals A_m.

The integral (5) can be expressed as

$$I(\eta) = \sum_{j=1}^{N} G_j I_j(\eta) , \tag{13}$$

where

$$I_j = \int_0^{\infty} \rho^{j+i\nu} J_M(\eta\rho) \exp(-b\rho)\, d\rho \tag{14}$$

is the complex Hankel transform of $\exp(-b\rho)$, having the following expression

$$I_j = (\eta/2)^M b^{-\gamma_j} [\Gamma(\gamma_j)/\Gamma(i + M)] \times {}_2F_1(\gamma_j/2, (1+\gamma_j)/2, 1+M, -\eta^2/b^2) . \tag{15}$$

Here Γ is the Gamma function, $\gamma_j = 1 + M + j + i\nu$ and ${}_2F_1$ is a hypergeometric function.

The analytic integration of (14) implies that we take into account *exactly* the infinite number of oscillations of the phase factor $\rho^{i\nu}$ and the Bessel function J_M. In order to avoid arguments greater than unity, we use the analytic continuation of the hypergeometric function [21]

$$I_j = (\eta/2)^M (\cos(\phi)/b)^{\gamma j} [\Gamma(\gamma_j)/\Gamma(i + M)] \times {}_2F_1(\gamma_j/2, (1 + 2M - \gamma_j)/2, 1 + M, \sin^2\phi) \tag{16}$$

with $\cos\phi = b/(b^2+\eta^2)^{1/2}$ and $\sin\phi = \eta/(b^2+\eta^2)^{1/2}$. Finally, in (13) we arrive at

$$I(\eta) = \sum_{j=1}^{N} H_j (\cos\phi)^{\gamma j} \times {}_2F_1(\gamma_j/2, (1 + 2M - \gamma_j)/2, 1 + M, \sin^2\phi) , \tag{17}$$

where

$$H_j = (\eta/2)^M b^{-\gamma j} [\Gamma(\gamma_j)/\Gamma(1 + M)]\, G_j . \tag{18}$$

3.3. Legendre–Laguerre polynomial expansion (LLPE) method

Another possibility for obtaining I_j of (15), is to relate the hypergeometric function ${}_2F_1$ to the associated Legendre polynomials of complex index [22]

$${}_2F_1(\gamma_j/2, (1+\gamma_j)/2, 1+M, -\eta^2/b^2) = (2b/\eta)^M \Gamma(1+M)(b/(b^2+\eta^2)^{1/2})^{\gamma_j - M} \times P^{-M}_{\gamma_j - M - 1}(b/(b^2+\eta^2)^{1/2}) . \tag{19}$$

From the definition of ϕ, formula (19) becomes

$${}_2F_1(\gamma_j/2, (1+\gamma_j)/2, 1+M, -\eta^2/b^2) = (2b/\eta)^M \Gamma(1+M)(\cos\phi)^{\gamma_j - M} \times P^{-M}_{\gamma_j - M - 1}(\cos\phi) . \tag{20}$$

Here, $P^{-M}_{\gamma_j - M - 1}$ can be expanded in the usual Legendre polynomials of integral index as [21]

$$P^{-M}_{\gamma_j - M - 1}(\cos\phi) = \pi^{-1} \sin\delta_j \pi \times \sum_{n=1}^{\infty} (-1)^n D_{n,j} P_n^{-M}(\cos\phi) , \tag{21}$$

where $\delta_j = \gamma_j - M - 1 = j + i\nu$ and $D_{n,j} = 1/(\delta_j + n) - 1/(\delta_j - n + 1)$.

Finally, in (13) we have

$$I = \sum_{n=1}^{\infty} E_n P_n^{-M}(\cos\phi) \tag{22}$$

with

$$E_n = \frac{(-1)^n}{\pi} \sum_{j=1}^{\infty} G_j \Gamma(\gamma_j) \left(\frac{\cos\phi}{b}\right)^{\gamma_j - M} \sin\delta_j \pi . \tag{23}$$

Note that there is a similarity between the expression (22) and the expansion in partial waves of the scattering amplitude for a central potential, if the angle ϕ is considered in place of the usual scattering angle θ.

4. Application to high energy proton–hydrogen collisions

We apply the methods of section 3 to the fundamental resonance charge exchange collision

$$H^+ + H(1s) \rightarrow H(1s) + H^+ \qquad (24)$$

at different energies and scattering angles. In particular, we consider the Coulomb–Brinkman–Kramers (CBK) approximation developed by Belkić and Salin [3], where in (4)

$$a(\rho) = 2i\rho^2(v + v^3/4)^{-1}K_2(\rho(1 + v^2/4)^{1/2}) . \qquad (25)$$

The corresponding differential cross section in the eikonal approximation is

$$dQ/d\Omega = (2^{10}\mu^2/v^2\alpha^5)(1 + 1/v^2)|\Gamma(1 + i/v)|^4$$

$$\times |{}_2F_1(1 + i/v, 3 + i/v, 1, -\eta^2/\alpha)|^2 , \qquad (26)$$

where μ is the reduced mass, $\alpha = 1 + v^2/4$ and K_2 is the modified Bessel function of the second kind and of order two. This CBK approximation is particularly interesting since we have an *exact* result (formula 26) to test our calculations.

The methods of sections 3.2 and 3.3 require the previous numerical determination of the weights A_m, which do not depend on the scattering angle. The rest of the calculation involves only analytical expressions.

In most problems, a closed form of $a(\rho)$ is not available as was described in paragraph 3.2. In order to assess the efficiency of our method in such cases, we have evaluated the A_m coefficients in the following way: a set of representative values of $a(\rho)$ given by (25) has been interpolated using a spline algorithm. Then, a Simpson integration of (9) has been performed quite fast, using the recurrence relation of the Laguerre polynomials. The parameter b introduced in (8), is obtained by fitting the asymptotic form of $a(\rho)$ for large ρ.

All the calculation of the eikonal differential cross section (2) have been done on an IBM 360/44 computer. The HTLE method gives results several times faster than the LLPE one, for a set of different energies and scattering angles. In order to try to reduce computing time, the regularization factor method [23] was applied to expression [22], which has the property of accelerating the convergence of infinite series through successive iterations. It consists essentially in a rearrangement of the term series (22), using the recurrence law of the Laguerre polynomials, in order to obtain a new series which converges faster. However, no significant reduction in time has been observed when a single iteration is used. It is expected that with several iterations the total time of computation may be slightly decreased.

In order to compare the HTLE and the usual MPS methods, we must realize that there are two possibilities for organizing the latter: a) To interpolate the transition amplitudes $c(\rho)$ given in (4) for *all* angular momenta, up to l_{mx} and to store it. These values are then used in (6) for *all* desired scattering angles at a given energy. b) To interpolate $c(\rho)$ for *each* angle. Case a) requires a large memory size (hundreds of kilobits for the present cases). On the contrary, case b) needs a small memory size (several kilobits), but the computing time is directly proportional to the number of scattering angles. For twelve angles between zero and 0.2°, which define quite well a non-oscillatory differential cross section, and a collision energy of 100 keV, case b) requires 24.5 min. Case a) is about four times faster than the latter.

For the same problem, the HTLE method (which needs only a few kilobits), spends about 30 s for the weight calculations, with $N = 12$, and from 0.5 to 5 s for each angle (depending on the hypergeometric function argument), with a total time of 70 s.

All numerical results obtained through the different methods were compared with the exact results given by formula (26). A precision of three significant figures in all cases was obtained, since in practice the $a(\rho)$ is determined numerically with this precision.

In atomic collisions between heavy particles (even non-hydrogen atoms) when the collision energy decreases, $a(\rho)$ becomes more oscillatory. Thus, eq. (8) requires a large number of Laguerre polynomials and consequently of A_m. In general, N is directly proportional to the number of oscillations of $a(\rho)$. Therefore, for small collision energies, the MPS method would be more adequate than the HTLE one.

5. Conclusions

In the present work, we have developed methods for calculating the eikonal differential cross section, since it is increasingly used in high energy atomic

collisions, besides its current applications in other fields.

We have shown that the more efficient method is the Hankel transform–Laguerre expansion (HTLE) one. It is faster by one order of magnitude than the MPS, using even a smaller memory size. This makes the HTLE method tractable on small computers, spending only a few minutes to obtain complete information on angle and energy of the differential cross sections. It must be noted that an adaptation of this method could be used for evaluating other types of integral transforms (like the Fourier one) of complex high oscillating functions.

Acknowledgements

We would like to thank Drs. R. Garibotti, M. Jakas and A. Salin for fruitful discussions and Dr. V.H. Ponce for a critical reading of the manuscript. J.E. Miraglia and R.D. Piacentini acknowledge the kind hospitality extended to them at the Instituto de Astronomía y Físisca del Espacio (Buenos Aires), during their stay there.

References

[1] H. Pauly and J.P. Toennies, Advan. Atomic Mol. Phys. 1 (1965) 195.
[2] R. McCarroll, in: Atoms, molecules and lasers (IAEA, Vienna, 1974).
[3] Dž. Belkić and A. Salin, J. Phys. B9 (1976) L397.
[4] N.F. Mott and H.S.W. Massey, The theory of atomic collisions (Clarendon, Oxford, 1965).
[5] G. Moliere, Z. Naturforsch. 2 (1947) 133.
[6] L.I. Schiff, Phys. Rev. 103 (1956) 443.
[7] R.J. Glauber, in: Lectures in theoretical physics, Vol. 1, eds. Brittin and Dunham (Wiley, New York, 1959).
[8] R. McCarroll and A. Salin, J. Phys. B1 (1968) 163.
[9] L. Wilets and S.J. Wallace, Phys. Rev. 169 (1968) 84.
[10] J.C.Y. Chen and K.M. Watson, Phys. Rev. 174 (1968) 152.
[11] R. McCarroll, R.D. Piacentini and A. Salin, J. Phys. B3 (1970) 147.
[12] R.D. Piacentini and A. Salin, Comput. Phys. Commun. 13 (1977) 57.
[13] R. McCarroll and R.D. Piacentini, J. Phys. B3 (1970) 1336.
[14] R. McCarroll and R.D. Piacentini, J. Phys. B4 (1971) 1026.
[15] R. McCarroll and R.D. Piacentini, J. Phys. B5 (1972) 973.
[16] J.C.Y. Chen, T. Ishihara, V.H. Ponce and K.M. Watson, J. Phys. B5 (1972) L204.
[17] M.C. Chidichimo-Frank and R.D. Piacentini, J. Phys. B7 (1974) 548.
[18] A. Erdélyi, W. Magnus, F. Oberhettinger and F. Tricomi, Tables of integral transforms, vol. 2 (McGraw-Hill, New York, 1954).
[19] C. Gaussorgues, R.D. Piacentini and A. Salin, Comput. Phys. Commun. 10 (1975) 223.
[20] R.D. Piacentini and A. Salin, Comput. Phys. Commun. 12 (1976) 199.
[21] I.S. Gradshtein and I.M. Ryzhik, Tables of integrals, series and products (Academic Press, New York, 1965).
[22] M. Abramowitz and I.A. Stegun, Handbook of Mathematical functions (Dover Publications, New York, 1965).
[23] R. Garibotti, F. Grinstein and J.E. Miraglia, to be published.