J. Phys. B: At. Mol. Opt. Phys. **33** (2000) 2847–2857. Printed in the UK PII: S0953-4075(00)50312-5

A classical interpretation of the off-shell Coulomb transition matrix

J Fiol† and R O Barrachina‡

Centro Atómico Bariloche and Instituto Balseiro§, 8400 SC de Bariloche, Río Negro, Argentina

E-mail: `fiol@cab.cnea.gov.ar`

Received 10 March 2000, in final form 23 May 2000

Abstract. We analyse the transition matrix for the two-body Coulomb scattering problem out of the energy shell. This quantity appears in high-order perturbation treatments of multichannel processes and plays a central role in the generalization of the scattering theory to include long-range interactions. In particular, its branch-point singularities on the initial and final half of the energy shell are known to produce sizeable effects in multiple-scattering amplitudes for rearrangement and ionization collisions. In this paper we present a classical description of the off-shell collision process which helps to clarify its essential concepts.

1. Introduction

Due to the infinite range of the Coulomb potential, the formal scattering theory is not strictly applicable to the collision of charged particles. The asymptotic condition, one of the basic postulates of standard scattering theory, is not fulfilled in the presence of Coulomb interactions (Hack 1958, Dollard 1964). This represents a rather puzzling situation: the collision of two particles interacting via a pure Coulomb potential is one of the few quantum-mechanical systems where the scattering amplitude can be evaluated analytically by solving the Schrödinger equation. However, this same amplitude cannot be obtained from the scattering theory in its usual form.

Since the pioneering and influential papers by Dollard in the late 1960s (1964, 1968, see also 1971), much work has been done to modify and extend the standard scattering theory in order to cover the Coulomb case. In a time-dependent theory of potential scattering, the isometric Møller operator has to be multiplied by a 'renormalization' term $D(t)$ with a logarithmic diverging phase which compensates the long-range effects of the Coulomb interaction (Dollard 1964). These diverging phases can be readily eliminated in a wavepacket description of the collision process (Dettmann 1971), by evaluating the transition probability 'before' taking the limit of infinite time. The translation of these ideas to a time-independent description is a more subtle and cumbersome subject. Different approaches were proposed during the 1970s, which can be roughly sorted into two broad groups. One idea (Mulherin and Zinnes 1970) is to develop a time-independent Lippmann–Schwinger formalism by means of distorted asymptotic states of the eikonal form. A completely different approach was

† Author to whom correspondence should be addressed.

‡ Also a member of the Consejo Nacional de Investigaciones Científicas y Técnicas, Argentina.

§ Comisión Nacional de Energía Atómica and Universidad Nacional de Cuyo, Argentina.

0953-4075/00/152847+11$30.00

proposed by van Haeringen in 1976. He also introduced modified Coulomb asymptotic states, but did so in a way that avoided the use of any distorting potential (see also Prugovečki 1971, 1973a, b, Prugovečki and Zorbas 1973a, b, Zorbas 1974a, b, 1976, 1977). This idea was further developed to obtain the Coulomb T-matrix as a well defined on-shell limit of an adequately regularized off-shell T-matrix (Roberts 1985, 1997). However, it is important to mention that, at least for the simplest case of Rutherford scattering of two charged particles, both approaches can be rigorously derived from Dollard's formalism, and shown to be equivalent (Barrachina and Macek 1989). In fact, Mulherin and Zinnes' theory represents a conventional distorted-wave description of van Haeringen's more fundamental approach.

In principle, the idea that the Coulomb scattering amplitude can be obtained as the on-shell limit of an adequately regularized off-shell transition matrix is not new. In fact, many different authors (Schwinger 1964, Okubu and Feldman 1960, Mapleton 1961, Hostler 1964a, b) had already noticed that, when the standard short-range theory is applied to the long-range Coulomb scattering, expressions are obtained which, however, are defined only off the energy shells. The on-shell limit of the T-matrix can only be correctly evaluated when certain additional branch-point singularities on the initial and final half of the energy shell are removed. Therefore, the novelty of van Haeringen's approach is not in the idea of this regularization, but in that it shows how to do this in a consistent way, leading to the formulation of a Lippmann–Schwinger theory of Coulomb scattering processes.

As in the case of short-range interactions, the off-shell T-matrix provides all the necessary information about the reacting system. Its simple poles correspond to the bound states (and their residues are related to the corresponding wavefunctions), while the continuous positive energy spectrum manifests itself as a branch-point singularity with a cut along the positive energy axis. Furthermore, as we have already mentioned, the off-shell T-matrix represents the cornerstone of the generalization of the time-independent scattering theory. Two-body off-shell T-matrices also constitute the basic building blocks for many-body problems (Watson and Nutall 1967). In fact, these problems can be reduced to the solution of a set of coupled equations whose kernel is composed of two-body off-shell T-matrices. Besides, the branch-point singularities of these matrices on the initial and final half of the energy shell have very important effects when any multiple-scattering expansion is applied to a system with Coulomb interactions. For instance, different higher-order perturbation descriptions of multichannel scattering processes incorporate 'intermediate' T-matrices or wavefunctions off the energy shell. This is the case, for instance, of the so-called channel-distorted strong-potential Born (DSPB) approximation for charge-exchange processes in highly asymmetric collisions (Taulbjerg *et al* 1990). In these models, the difference δE between the energy of the electron in the intermediate and final states is small. However, due to the on-shell singularity of the off-shell wavefunction, it produces a sizeable effect on the rearrangement cross section. In addition, it has been shown that the position of the binary-encounter peak in ionization collisions is affected by off-shell effects in the quasi-free scattering of the target electron in the field of the incident projectile (Madsen and Taulbjerg 1994). More generally, it has been claimed that the Coulomb branch-point singularities on the initial and final half of the energy shell produce a leading contribution to the multiple-scattering amplitudes for both rearrangement and scattering collisions in the high-energy limit (Chen and Kramers 1972).

We see that the off-shell two-body Coulomb T-matrix is a central quantity not only for the formulation of a Lippmann–Schwinger theory of scattering processes, but also in multichannel problems. Thus, it is clear that further progress on the description of collision processes in the presence of long-range Coulomb interactions depends critically on a better understanding of this basic quantity.

Despite the difficulties associated with the long-range nature of the Coulomb potential, mathematically well defined representations of the off-shell two-body Coulomb T-matrix can be expressed in closed form (Chen and Chen 1972). Therefore, the primary source of difficulties with the manipulation of these quantities does not arise from their calculation but from their anomalous on-shell behaviour. In particular, a clear understanding of the origin of these Coulomb branch-point singularities is still lacking. In order to gain a clearer insight into this basic issue, different authors have analysed the long-range limit of T-matrices for screened Coulomb potentials (Dalitz 1951, Ford 1964, 1966, Kolsrud 1978). Basically, it has been observed that their absolute values converge to the results of standard short-range theory when the momenta are fixed before the limiting process (Kolsrud 1978). In the present paper we take a different route, by presenting a classical calculation of the square modulus of the *off-shell* Coulomb T-matrix. This classical description can help in the understanding of the essential concepts underlying the definition of this quantity.

It is well known that the classical and quantum expressions for the square modulus of the *on-shell* Coulomb T-matrix, being proportional to the Rutherford scattering cross sections, are identical. Moreover, the semiclassical cross section for scattering of identical particles—which includes the quantum-mechanical phase—is exact (Rost and Heller 1994). Surprisingly enough, the same seems to be valid off the energy shell, and our classical expression for the square modulus of the *off-shell* T-matrix is almost identical to the quantum-mechanical result. A comparison of both expressions enables us to single out the different terms in the off-shell Coulomb T-matrix, providing a clearcut interpretation of their origin.

2. Classical definition of the off-shell Coulomb continuum state

Under single-collision conditions, the dispersion of a beam of particles by a target assembly amounts only to repeating the elementary scattering of one reduced particle by a force centre, many times with similar initial conditions (Fiol *et al* 1997). In this sense, and due to the lack of information on its microscopic details, the scattering process can be analysed by means of a stationary state describing the steady flow of an *ensemble*. The density of particles $n(\boldsymbol{r})$ in each point of space can easily be evaluated by studying the deformation of a control volume due to the motion of each particle in the potential field $U(r)$ of the target (Samengo *et al* 1999).

In order to describe an off-shell scattering state, we have to imagine a situation where the initial kinetic energy E_k of the particle is not equal to its total energy E. This initial condition is immediately achieved if each particle impinges upon the force centre not from infinity but from a finite distance R, as shown in figure 1. In this case, the total and initial energies differ by $\delta E = U(R)$.

We assume that the starting points of the trajectories in the ensemble are uniformly distributed over the surface of a sphere of radius R around the force centre. Thus, the number of projectiles of mass m and initial impulse $\boldsymbol{k}$ (energy $E_k = k^2/2m$) inside a control volume $\delta V_0 = (k/m)\delta t\, \rho\, \delta\rho\, \delta\varphi$ located on the sphere at a distance $\rho = R\sin\phi$ from the symmetry axis is given by $\delta N = (\xi_0/R\cos\phi)\,\delta V_0$, where ξ_0 is an arbitrary normalization constant and ϕ is the azimuth angle on the sphere. At later times t, the control volume δV occupied by this particle changes as shown in figure 2, giving rise to a spatial dependence of the particle density $n(\boldsymbol{r}) = \delta N/\delta V$ in the ensemble. After a little algebra, it is possible to eliminate all explicit dependences on the time variable t (Fiol *et al* 1997, Samengo *et al* 1999),

$$n(\boldsymbol{r}) = \frac{\delta N/\delta V_0}{\sin\theta}\left|\left(\frac{\partial r}{\partial \rho}\right)_\theta\right|^{-1} = \frac{\xi_0\, R}{\sin\theta}\left|\left(\frac{\partial r}{\partial \phi}\right)_\theta\right|^{-1}.$$

We see that the spatial density of particles in the ensemble can readily be evaluated, provided

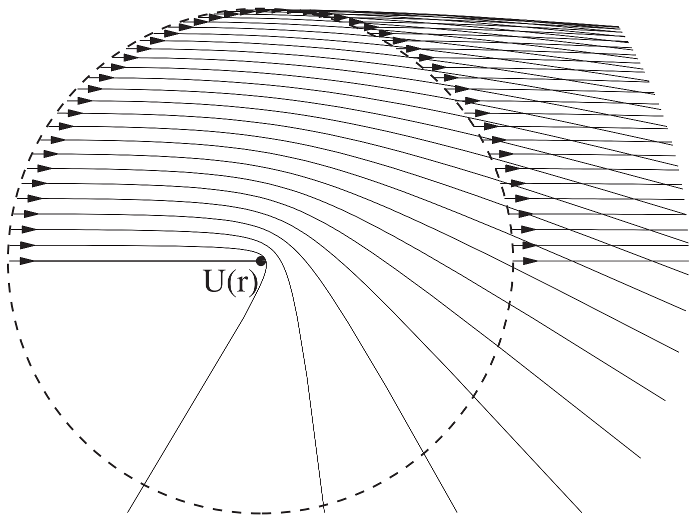

Figure 1. Classical description of an off-shell collision process. Each projectile starts its trajectory from a point on the surface of a sphere of radius R around the force centre.

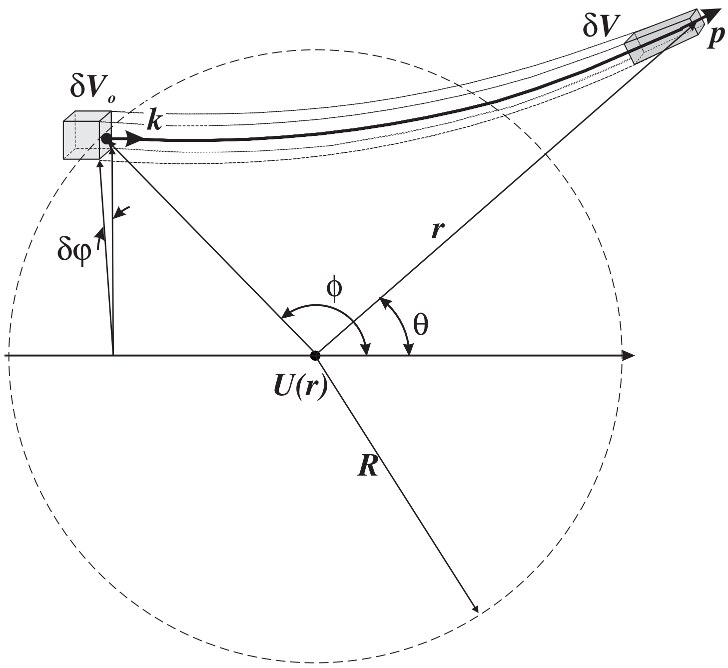

Figure 2. An initial control volume δV_0, occupied by a fixed number of particles, changes to δV as time goes by due to the different trajectories followed by these particles in the field of the potential $U(r)$. The coordinates r and θ give the position in the collision plane of the particle of impulse $\boldsymbol{p}$.

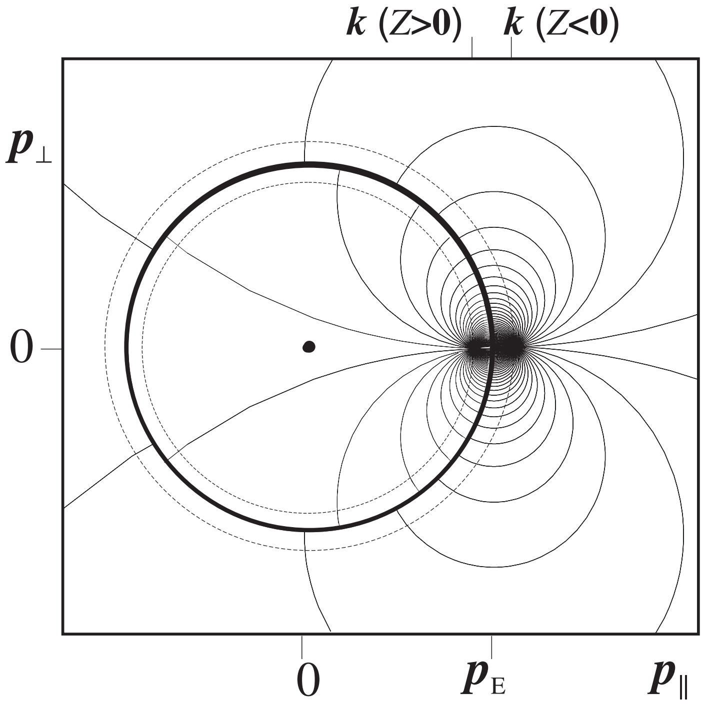

Figure 3. Trajectories in the space of momentum. Those trajectories corresponding to an attractive ($Z < 0$) and a repulsive ($Z > 0$) Coulomb interaction are restricted to move outside or inside the sphere of radius $p_E = \sqrt{2\,mE}$, respectively.

that the orbit $\boldsymbol{r} = \boldsymbol{r}(\theta, \phi)$ is already known. This is actually the case for the Coulomb potential $U(r) = Z/r$, where the orbits are given by

$$\frac{R\sin\phi}{r} = -\frac{\delta E/E_k}{\sin\phi}\,(1 + \cos\phi\cos\theta) + \left(1 + \frac{\delta E}{2E_k}\right)\sin\theta. \tag{1}$$

However, the corresponding quantum density, related to the position representation of the off-shell Coulomb scattering state

$$|\boldsymbol{k}, \delta E\rangle = (1 + G(E_k + \delta E)V)\,|\boldsymbol{k}\rangle$$

cannot be given in closed form, and the analysis of its anomalous on-shell behaviour is extremely complicated. These states have been studied by Macek and Alston (1982) in relation to the appearance of off-shell effects in asymmetric electron capture collisions and their Sturmian expansion was obtained by Dubé and Broad (1990), deriving basis set representation, of the off-shell and half-shell T-matrices. On the other hand, the density of particles in momentum space is trivially related to any of the mathematically well defined expressions for the off-shell transition matrix. Thus, any comparison of the quantum-mechanical and classical off-shell quantities can be performed more simply in momentum space.

Since the classical ensemble describes a situation where each point $\boldsymbol{r}$ in the coordinate space is associated with a well defined impulse $\boldsymbol{p}$, the density of particles $n(\boldsymbol{p})$ in momentum space can be readily evaluated by means of the transformation

$$n(\boldsymbol{p}) = n(\boldsymbol{r})\left|\frac{\partial(\boldsymbol{r})}{\partial(\boldsymbol{p})}\right|.$$

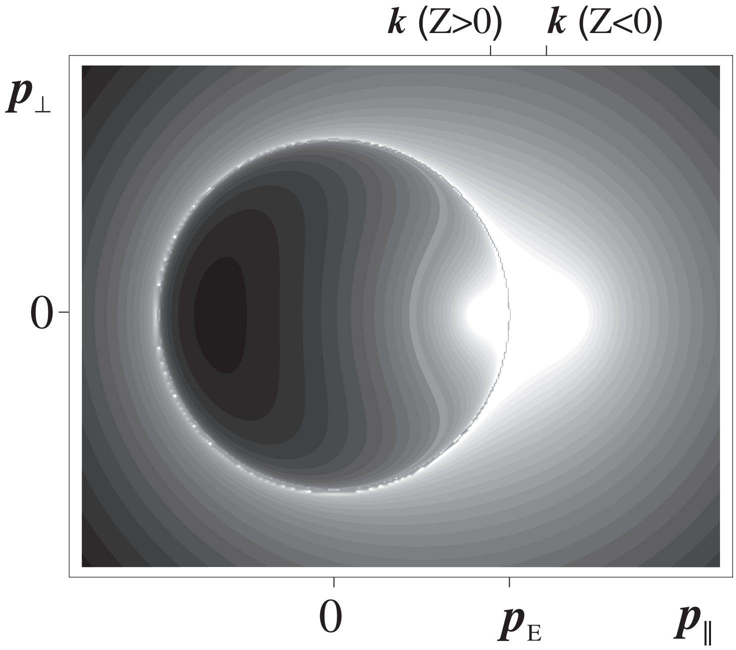

Figure 4. Classical off-shell particle density in the space of momentum for the Coulomb potential. The region inside the sphere of radius p_E corresponds to an attractive interaction, while outside corresponds to the repulsive case. Lighter shades indicate a higher density.

Up to now, we have been assuming that only one trajectory passes through any given point $\boldsymbol{r}$, and that the relation $\boldsymbol{r} \leftrightarrow \boldsymbol{p}$ is one-to-one. Nevertheless, these assumptions are generally untrue and all possible contributions have to be added (Samengo *et al* 1999).

In the momentum representation, the trajectories (1) are transformed into arcs of circumference of ratio

$$\frac{k}{\sin\phi}\left|\frac{\delta E}{2E_k}\right|$$

and centred at the point

$$-\frac{\delta E}{2E_k}\,\frac{k}{\tan\phi}\hat{\rho}+\left(1+\frac{\delta E}{2E_k}\right)\boldsymbol{k}$$

as shown in figure 3. Here $\hat{\rho}$ is a unit vector on the scattering plane and normal to the initial impulse $\boldsymbol{k}$.

Now, the classical density of particles in momentum space can be readily evaluated. With a convenient definition of the arbitrary constant ξ_0 we obtain

$$n(\boldsymbol{p}) = \frac{1}{(E_k-E_p+\delta E)^2}\,\frac{1}{|\boldsymbol{k}-\boldsymbol{p}|^2}\,\frac{1}{|(1+\delta E/E_k)\boldsymbol{k}-\boldsymbol{p}|^2} \times\Theta\left(Z(E_k-E_p+\delta E)\right)\Theta\left(Z\delta E\right)) \qquad (2)$$

where $\Theta(x)$ is Heaviside's step function, i.e. $\Theta(x)=1$ for $x\geqslant 0$ and $\Theta(x)=0$ for $x<0$. The location of the different divergent structures of this classical density and of its on-shell limit

$$n_{\mathrm{on}}(\boldsymbol{p}) = \frac{1}{(E_k-E_p)^2}\,\frac{1}{|\boldsymbol{k}-\boldsymbol{p}|^4}\,\Theta\left(Z(E_k-E_p)\right)$$

are shown in figure 4. We have depicted in this figure the classical density for both the repulsive and attractive potentials, in the interior and exterior of the sphere where it does not vanish, respectively.

3. Off-shell Coulomb transition matrix

The classical density (2) has to be compared with the quantum-mechanical one as given by the square modulus of the off-shell momentum wavefunction, normalized to the initial condition of our classical model,

$$n_{\mathrm{QM}}(\boldsymbol{p}) = |\langle \boldsymbol{p}|\boldsymbol{k}, \delta E\rangle|^2 . \qquad (3)$$

Excluding the forward direction, that is for $\boldsymbol{p} \neq \boldsymbol{k}$, this result can be easily related to the off-shell Coulomb transition matrix,

$$n_{\mathrm{QM}}(\boldsymbol{p}) = \left| \frac{1}{E_k + \delta E - E_p + \mathrm{i}\eta} \langle \boldsymbol{p}|T(E_k + \delta E + \mathrm{i}\eta)|\boldsymbol{k}\rangle \right|^2 .$$

For most quantum-mechanical systems, the off-shell T-matrix cannot be given in closed form. In this sense, the case of two particles that interact via a Coulomb potential is exceptional, since mathematically well defined expressions of the off-shell two-body Coulomb T-matrix can be obtained. One of its possible representations reads (Chen and Chen 1972)

$$\langle \boldsymbol{p}|T\ (E + \mathrm{i}\eta)\ |\boldsymbol{k}\rangle = \frac{\sqrt{E_k/E}}{2\pi\nu} \frac{1}{|\boldsymbol{k} - \boldsymbol{p}|^2} \{1 + \tau_a + \tau_b\} \qquad (4)$$

where

$$\tau_a = \frac{1}{\sqrt{1+\varepsilon}} \left[1 - 2 \sum_{n=0}^{\infty} \frac{\nu^2}{n^2 + \nu^2} \left(\frac{\sqrt{1+\varepsilon} - 1}{\sqrt{1+\varepsilon} + 1} \right)^n \right]$$

and

$$\tau_b = \frac{1}{\sqrt{1+\varepsilon}} \frac{2\pi\nu}{1 - \mathrm{e}^{-2\pi\nu}} \left(\frac{\sqrt{1+\varepsilon} - 1}{\sqrt{1+\varepsilon} + 1} \right)^{\mathrm{i}\nu} .$$

Here ν is Sommerfeld's parameter, $\nu = mZ/\hbar\sqrt{2\,mE}$, and the variable

$$\varepsilon = \frac{(E + \mathrm{i}\eta - E_k)(E + \mathrm{i}\eta - E_p)}{(E + \mathrm{i}\eta)\ |\boldsymbol{k} - \boldsymbol{p}|^2/2m}$$

is related to the hyperbolic angle β on the Minkowski sphere in a stereographic projection of momentum space, $\cosh\beta = 1 + 1/\varepsilon$ (Bander and Itzykson 1966, Norcliffe and Percival 1968a, b).

We see that the term in τ_a includes all the poles at $\nu = \mathrm{i}n$ of the discrete energy spectrum. In the half-energy-shell limit ($E_p \to E$ or $E_k \to E$) and on the energy shell $E_p, E_k \to E$, τ_a goes to -1 and exactly cancels the first-order Born approximation represented by the first term in equation (4). Thus, the anomalous behaviour of the on-shell limit of the off-shell Coulomb transition matrix is completely dominated by the term in τ_b, which in the limit $\eta \to 0$ behaves in the form,

$$\tau_b = |\tau_b| \times \begin{cases} 1 & \text{for} \quad E > E_p, E_k \\ \mathrm{e}^{-\pi\nu} & \text{for} \quad E_p < E < E_k \quad \text{or} \quad E_k < E < E_p \\ \mathrm{e}^{-2\pi\nu} & \text{for} \quad E < E_p, E_k. \end{cases}$$

Furthermore, it is interesting to note that in the limit $|\nu| \to \infty$, the series in τ_a converges to 1 (see equation (147) of Chen and Chen (1972)). Therefore, the term $(1 + \tau_a)/2\pi\nu$ in equation (4) vanishes and the classical limit is also determined by τ_b. In fact, this term can be expressed as a sum over classical paths of exponential actions (Norcliffe *et al* 1969a, b, Norcliffe 1975). This simple result demonstrates quite directly that the anomalous on-shell behaviour of the off-shell Coulomb transition matrix is a purely semiclassical effect, dominated by the term τ_b.

After some algebra, the previous expression for the off-shell Coulomb transition matrix can be written as

$$\langle \boldsymbol{p}|T\,(E+\mathrm{i}\eta)\,|\boldsymbol{k}\rangle = \frac{1}{|\boldsymbol{k}-\boldsymbol{p}|}\,\frac{1}{|(E/E_k)\boldsymbol{k}-\boldsymbol{p}|}\,\mathrm{e}^{\mathrm{i}S_{\mathrm{cl}}/\hbar}\,\mathcal{S}(E,E_p,E_k).$$

Here, the function $\mathcal{S}$ reads

$$\mathcal{S}(E,E_p,E_k) = \frac{1}{2\pi\nu}\left\{\left(\frac{\sqrt{1+\varepsilon}-1}{\sqrt{1+\varepsilon}+1}\right)^{-\mathrm{i}\nu}\sqrt{1+\varepsilon} + \frac{2\pi\nu}{1-\mathrm{e}^{-2\pi\nu}} - \left[\sum_{n=-\infty}^{\infty}\frac{\nu^2}{n^2+\nu^2}\left(\frac{\sqrt{1+\varepsilon}-1}{\sqrt{1+\varepsilon}+1}\right)^{n-\mathrm{i}\nu}\right]\right\}.$$

The phase

$$S_{\mathrm{cl}} = \frac{mZ}{\sqrt{2\,mE}}\ln\left(\frac{\sqrt{(1+\varepsilon)}-1}{\sqrt{(1+\varepsilon)}+1}\right)$$

is the classical action from $\boldsymbol{k}$ to $\boldsymbol{p}$ along the trajectory of fixed energy E in momentum space (Gutzwiller 1990). It is due to this that the Mott cross section for identical particles can be evaluated semiclassically (Rost and Heller 1994). This action even includes part of the anomalous behaviour at the on-shell limit. In fact, it can be shown that

$$\lim_{E_p,E_k\to E} S_{\mathrm{cl}} = 2\left(\sigma_0 - \frac{mZ}{\sqrt{2mE}}\ln\sin\theta/2\right)$$

where θ is the scattering angle and σ_0 is the divergent factor

$$\sigma_0 = \frac{mZ}{\sqrt{2mE}}\ln\left(\frac{(E-E_k)(E-E_p)}{4E}\right).$$

Since this divergence is restricted to a phase factor that does not depend on the scattering angle θ, it does not affect either the elastic or the Mott cross sections (Rost and Heller 1994).

It can be shown that in the classical limit

$$\lim_{|\nu|\to\infty}\left|\mathcal{S}(E,E_p,E_k)\right|^2 = \Theta\left(Z\,(E-E_k)\right)\Theta\left(Z\,(E-E_p)\right).$$

Thus the quantum-mechanical density (3) converges, as expected, to the classical expression (2). In addition, the momentum representation of the off-shell *wavefunction* approaches the semiclassical result.

4. Comparison of the classical and quantum-mechanical results

We are now in a position to provide a clearcut interpretation of the different terms in the off-shell Coulomb transition matrix by comparing the quantum-mechanical and classical momentum densities. Let us consider, for instance, the divergence in $(E_k - E_p + \delta E)$. In the quantum-mechanical approach, this is the matrix element of the free Green operator and represents the asymptotic free evolution of the projectile. Here, due to the long-range nature of the Coulomb interaction, the projectile does not converge to a free orbit, but its kinetic energy approaches a well defined limit given by $E_p = E_k + \delta E$ for infinite time.

We also observe two other terms, proportional to $|\boldsymbol{k} - \boldsymbol{p}|$ and $|(1 + \delta E/E_k)\boldsymbol{k} - \boldsymbol{p}|$, which can produce a divergence of the off-shell density $n(\boldsymbol{p})$. At this point, it is interesting to note that the $|\boldsymbol{k} - \boldsymbol{p}|^{-2}$ divergence of Rutherford's elastic transition matrix

$$t_{\text{on}}(\boldsymbol{p}, \boldsymbol{k}) = \frac{\Gamma(1 + \mathrm{i}\nu)}{\Gamma(1 - \mathrm{i}\nu)} \frac{1}{|\boldsymbol{k} - \boldsymbol{p}|^2} \left(\frac{4k^2}{|\boldsymbol{p} - \boldsymbol{k}|^2} \right)^{\mathrm{i}\nu}$$

originates from the on-shell limit of these two different contributions. The first one is due to the initial condition of the scattering process. The second one, on the other hand, does not lead to a real divergence in the classical approach, since it is located at a point of momentum space that is forbidden by energy conservation. Therefore, this contribution does not diverge except in the on-shell limit $\delta E \to 0$. In our classical model, this limit is equivalent to pushing the initial condition towards infinity, i.e. $R \to \infty$. Thus, the divergence originates in those trajectories with arbitrarily large impact parameters ρ, for which the impulse $\boldsymbol{p}$ is always close to the initial value $\boldsymbol{k}$. In the off-shell case, this situation is allowed in the quantum-mechanical approach, but not in the classical limit where the impact parameter is bounded by the condition $\rho \leqslant R$.

We also observe that the classical density is multiplied by Heaviside's functions, which are related to the conservation of energy. In momentum space, the orbits are restricted to remaining outside or inside a sphere of radius $p_E = \sqrt{2\,mE}$, depending on whether the Coulomb potential is attractive ($Z < 0$) or repulsive ($Z > 0$), respectively. As we have already seen, this effect is reproduced in the quantum-mechanical approach by the distortion factor $\mathcal{S}$ in the limit $|\nu| \to \infty$. Furthermore, in the half-energy-shell limit ($E_p \to E$ or $E_k \to E$) the function $\mathcal{S}$ is dominated by the singular 'Gamow' factor

$$g_{\pm}(E, \delta E) = \Gamma(1 \mp \mathrm{i}\nu)\, \mathrm{e}^{-\pi\nu/2} \left(\frac{\delta E}{4E} \right)^{\pm \mathrm{i}\nu}$$

as expected from the well known limit of the off-shell Coulomb T-matrix (Schwinger 1964, Roberts 1985)

$$\lim_{E_p, E_k \to E} \langle \boldsymbol{p} | T\,(E + \mathrm{i}\eta)\, | \boldsymbol{k} \rangle \approx g_{+}(E_p, E - E_p) t_{\text{on}}(\boldsymbol{p}, \boldsymbol{k}) g_{+}(E_k, E - E_k).$$

Thus, it can be shown that in the classical limit both Heaviside's functions $\Theta(Z\delta E)$ are approximated by $|g_{+}(E, \delta E)|^2/2\pi|\nu|$.

5. Conclusions

The present classical description of the off-shell Coulomb transition matrix clearly indicates that a shift δE off the energy shell is equivalent to considering an initial condition set at a finite time. In connection with this result, it is important to note that, except for a gamma function, the anomalous on-shell behaviour of the Coulomb transition matrix is described by the same distortion factor $D_{\pm}(E,t) = \exp[\mp i\nu \log(4E|t|/\hbar)]$ of Dollard's time-dependent theory, evaluated at $t = \hbar/\delta E$, namely

$$g_{\pm}(E, \delta E) = \Gamma(1 \mp i\nu) D_{\pm}(E, t = \hbar/\delta E).$$

In this sense, the off-shell regularization technique is the time-independent counterpart of Dettmann's early proposal of postponing the limit of infinite time in the time-dependent formalism (Dettmann 1971).

We have shown that the different structures of the off-shell transition matrix originate from particular regions of the projectile's orbit. In particular, the on-shell anomaly (represented by the distortion factor $g(E, \delta E)$) is related in the classical limit to the constraints on the impulse p due to the conservation of energy. Moreover, the classical action gives the correct quantum-mechanical phase off the energy shell, which diverges in the on-shell limit. These facts show that the singular behaviour of the Coulomb T-matrix is a purely semiclassical effect arising from the long range of the interaction.

Further progress on multichannel Coulomb collision processes depends critically on a better understanding of the off-shell two-body Coulomb transition matrix. In this sense, it is clear that classical and semiclassical descriptions, such as that presented in this paper, can help to clarify our understanding of this basic quantity.

Acknowledgment

This work has been supported by the Agencia Nacional de Promoción Científica y Tecnológica (Contrato de Préstamo BID 802 OC-AR, grant no 03-04021).

References

Bander M and Itzykson C 1966 *Rev. Mod. Phys.* **38** 330
Barrachina R O and Macek J H 1989 *J. Math. Phys.* **30** 2581
Chen J C Y and Chen A C 1972 *Adv. At. Mol. Phys.* **8** 71
Chen J C Y and Kramers P C 1972 *Phys. Rev.* A **5** 1207
Dalitz R H 1951 *Proc. R. Soc.* A **206** 509
Dettmann K 1971 *Z. Phys.* **244** 86
Dollard J D 1964 *J. Math. Phys.* **5** 729
——1968 *J. Math. Phys.* **9** 620
——1971 *Rocky Mountain J. Math.* **1** 5
Dubé L J and Broad J T 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** 1711
Fiol J, Pregliasco R G, Samengo I and Barrachina R O 1997 *Am. J. Phys.* **65** 433
Ford W F 1964 *Phys. Rev.* B **133** 1616
——1966 *J. Math. Phys.* **7** 626
Gutzwiller M C 1990 *Chaos in Classical and Quantum Mechanics* (New York: Springer)
Hack M N 1958 *Nuovo Cimento* **9** 731
Hostler L 1964a *J. Math. Phys.* **5** 591
——1964b *J. Math. Phys.* **5** 1235
Kolsrud M 1978 *J. Phys. A: Math. Gen.* **11** 1271
Macek J and Alston S 1982 *Phys. Rev.* A **26** 250
Madsen J N and Taulbjerg K 1994 *J. Phys. B: At. Mol. Opt. Phys.* **27** L165
Mapleton R A 1961 *J. Math. Phys.* **2** 482
Mulherin D and Zinnes I I 1970 *J. Math. Phys.* **11** 1402
Norcliffe A 1975 *Case Studies in Atomic Physics* vol IV, ed E W McDaniel and M R C McDowell (Amsterdam: North-Holland) p 4
Norcliffe A and Percival I C 1968a *J. Phys. B: At. Mol. Phys.* **1** 774
——1968b *J. Phys. B: At. Mol. Phys.* **1** 784

Norcliffe A, Percival I C and Roberts M J 1969a *J. Phys. B: At. Mol. Phys.* **2** 578
——1969b *J. Phys. B: At. Mol. Phys.* **2** 590
Okubu S and Feldman D 1960 *Phys. Rev.* **117** 292
Prugovečki E 1971 *Nuovo Cimento* B **4** 105
——1973a *J. Math. Phys.* **14** 957
——1973b *J. Math. Phys.* **14** 1410
Prugovečki E and Zorbas J 1973a *J. Math. Phys.* **14** 1398
——1973b *Nucl. Phys.* A **213** 541
Roberts M J 1985 *J. Phys. B: At. Mol. Phys.* **18** L707
——1997 *J. Phys. B: At. Mol. Opt. Phys.* **30** L175
Rost J M and Heller E J 1994 *J. Phys. B: At. Mol. Opt. Phys.* **27** 1387
Samengo I, Pregliasco R G and Barrachina R O 1999 *J. Phys. B: At. Mol. Opt. Phys.* **32** 1971
Schwinger J 1964 *J. Math. Phys.* **5** 1606
Taulbjerg K, Barrachina R O and Macek J 1990 *Phys. Rev.* A **41** 207
van Haeringen H 1976 *J. Math. Phys.* **17** 995
Watson K M and Nutall J 1967 *Topics in Several Particle Dynamics* (San Francisco, CA: Holden-Day)
Zorbas J 1974a *Lett. Nuovo Cimento* **10** 121
——1974b *J. Phys. A: Math. Gen.* **7** 1557
——1976 *Rep. Math. Phys.* **9** 309
——1977 *J. Math. Phys.* **18** 1112