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Coulomb propagator in the WKB approximation

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Abstract. Employing the WKB approximation, we derive an analytical expression for the two-body Coulomb propagator in terms of the asymptotic momentum $\boldsymbol{p}_{\mathrm{as}}$, coordinates $\boldsymbol{r}$ and $\boldsymbol{r}'$ and the difference of time τ. The momentum $\boldsymbol{p}_{\mathrm{as}}$ is a solution of the stationary phase equation. The problem of solving it is reduced to seeking the roots of some one-dimensional equation. The WKB Coulomb propagator is applied to calculate the continuum state of an atomic electron, subject to a sequence of δ-function impulses. The derived continuum state includes the effects of electron rescatterings into the continuum that may play an important role in various processes of atomic fragmentation.

1. Introduction

The time evolution of an atom subject to an external time-dependent field, $W_{\mathrm{ext}}(\boldsymbol{r}, t)$, is a fundamental problem of great importance in many branches of atomic, molecular and optical physics. The general solution of the time-dependent Schrödinger equation governing such a system is not known and therefore there is a need for simplifying a complicated system or process such that the simplified model Hamiltonian allows for an exact, i.e., analytical, solution. The kicked atom (see, e.g., Dhar *et al* (1983), Carnegie (1984), Grozdanov and Taylor (1987), Burgdörfer (1989), Hillermeier *et al* (1992), Casati *et al* (1994)) together with its counterpart, the kicked rotor (see, e.g., Schuster (1988)), represent the two fundamental prototype model systems for irregular classical dynamics in periodically perturbed Hamiltonian systems. The time evolution for kicked systems reduces to a sequence of discrete maps between adjacent kicks. This simplification permits detailed numerical studies of the long-term evolution using both classical and quantum dynamics, and hence, of the classical–quantum correspondence in microscopic systems that feature regular and chaotic dynamics.

Using the idea of the kicked atom, we can replace a continuous time-dependent field, $W_{\mathrm{ext}}(\boldsymbol{r}, t)$, by a series of non-periodic kicks of different intensity. This can be done in the following way. Suppose that W_{ext} can be written in the form $W_{\mathrm{ext}}(\boldsymbol{r}, t) = -\dot{\Phi}_{\mathrm{ext}}(\boldsymbol{r}, t)$, where $\Phi_{\mathrm{ext}}(\boldsymbol{r}, t) = -\int^t \mathrm{d}\tau\, W_{\mathrm{ext}}(\boldsymbol{r}, \tau)$ is a known function of time and electronic coordinates. Further, divide the time interval (t_0, t) into N subintervals (t_{i-1}, t_i), $i = 1, \ldots, N$ and assume that $\Phi_{\mathrm{ext}}(\boldsymbol{r}, t) \approx \Phi_{\mathrm{ext}}(\boldsymbol{r}, t_i)$ on the ith interval (t_{i-1}, t_i). Of course, this approximation is valid only if $\Phi_{\mathrm{ext}}(\boldsymbol{r}, t)$ does not change strongly on the interval (t_{i-1}, t_i) as a function of time. Then, we have a simplified model of an atom subject to a sequence of δ-function impulses. The corresponding Hamiltonian is

$$H = H_{\mathrm{at}} - \sum_{i=0}^{N-1} \Delta\Phi_{\mathrm{ext}}(\boldsymbol{r}, t_i)\delta(t - t_i) \tag{1}$$

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where $H_{\rm at}$ is the atomic Hamiltonian and

$$\Delta\Phi_{\rm ext}(\boldsymbol{r}, t_i) = \Phi_{\rm ext}(\boldsymbol{r}, t_{i+1}) - \Phi_{\rm ext}(\boldsymbol{r}, t_i) = -\int_{t_i}^{t_{i+1}} {\rm d}\tau\, W_{\rm ext}(\boldsymbol{r}, \tau).$$

For the N-kicked atom the time-evolution operator or propagator takes the form

$$\begin{aligned} K^{(N)}(t, t_0) &= K(t_N = t, t_{N-1}) \ldots K(t_1, t_0) \\ K(t_{i+1}, t_i) &= K_{\rm at}(t_{i+1}, t_i) \exp({\rm i}\Delta\Phi_{\rm ext}(\boldsymbol{r}, t_i)) \end{aligned} \tag{2}$$

where $K_{\rm at}(t_{i+1}, t_i) = \exp(-{\rm i}H_{\rm at}(t_{i+1} - t_i))$ is the atomic propagator that governs the system between two kicks and $\exp(\cdots)$ is a phase factor due to the kick at moment $t = t_i$. The general expansion (2) for the propagator may be useful in investigating nonlinear atomic dynamics in various time-dependent electric fields, in particular in studies of various processes taking place in ion–atom or ion–molecule interactions. Thus, expansions of the form (2) appear in the asymptotic expressions for continuum and bound states of an electron moving in the combined field of target and projectile ions (Kunikeev 1998, 1999a, b). Here, the phase function $\Phi_{\rm ext}$ near the target nucleus may be written as $\Phi_{\rm ext}(\boldsymbol{r}, t) = \boldsymbol{k}(t) \cdot \boldsymbol{r}$, where $\boldsymbol{k}(t)$ is an effective momentum of an electron modified by the projectile's field, and a number of approximate formulae for continuum and bound states may be derived.

The key element of the propagator (2) is seen to be the atomic propagator $K_{\rm at}$. In the Coulombic case, the well known expression for the energy-dependent, non-relativistic Green function has been obtained in closed form by Hostler and Pratt (1963) and Hostler (1964) in coordinate representation, while in momentum representation, an integral expression has been obtained by Schwinger (1964). Since then, significant progress has been made by many workers (see, e.g., the books by Rapoport *et al* (1978) and Zapryagaev *et al* (1985); for a recent review, see the paper by Maquet *et al* (1998) and references therein). Thus, Swianson and Drake (1991) have presented the energy-dependent Coulomb propagator for the relativistic and semi-relativistic problems, Hylton (1984) has calculated the radial reduced Dirac–Coulomb–Green function for all bound states, and Hill and Huxtable (1982) have evaluated radial matrix elements with the Coulomb–Green function.

Another situation emerges in the case of the time-dependent, non-relativistic Green function or propagator. It was Blinder (1991) who first obtained an analytic expression for the time-dependent, non-relativistic Coulomb propagator. Unfortunately, this expression is much more complicated than its energy-dependent counterpart and its direct use in calculating (2) ($3N$-dimensional integration) seems to be an intractable task, especially when a rapidly oscillating continuum state with an arbitrary initial function and phase function $\Delta\Phi_{\rm ext}$ should be evaluated numerically.

On the other side, there exists a general WKB expression for a propagator in terms of the classical two-point action function (see, e.g., the books by Maslov and Fedoriuk (1981) and Gutzwiller (1990)), but its rigorous calculation is not a trivial task, especially when the action is a multi-valued function. As is known, there is no explicit expression for the Coulombic action which is convenient to calculate. Here, one encounters a number of serious difficulties (Kay 1994), one of which is *the search problem.* For each pair of coordinates $\boldsymbol{r}$ and $\boldsymbol{r}'$ it is necessary to identify all classical trajectories that travel between these two points in time τ. Since trajectories are naturally specified by initial conditions $(\boldsymbol{r}', \boldsymbol{p}_i)$ and not boundary conditions $(\boldsymbol{r}', \boldsymbol{r})$, this procedure requires a search. Such a search is especially difficult for chaotic systems and long evolution times τ, since the number of trajectories connecting the two points becomes large and $\boldsymbol{r}$ becomes a very sensitive function of $\boldsymbol{p}_i$. The other is *the caustics problem.* The WKB propagator is not valid at caustics where it becomes infinite. At such points, the quasiclassical propagator should be replaced by more accurate (and more complicated) uniform expressions (Levit and Smilansky 1977, Levit *et al* 1978).

Therefore, in this paper we concentrate our efforts on deriving the corresponding WKB expressions for Coulomb propagators which are easy to calculate. Actually, we demonstrate that the task of *searching trajectories* can be reduced to seeking the roots of some elementary algebraic one-dimensional equation. The derived simple expressions are not valid at caustics.

The paper is organized as follows. In the next section, the WKB Coulomb propagator is developed. We then apply in section 3 the derived WKB formulae to the three-body continuum state, i.e. using the stationary phase approximation, we calculate expansions (2) as they appear in the three-body continuum states (Kunikeev 1999a, b). Finally, conclusions of our work are drawn in section 4. Atomic units are used throughout the paper.

2. The WKB Coulomb propagator

The propagator has the following spectral representation in terms of the complete set of eigenstates

$$K(\boldsymbol{r},\boldsymbol{r}',\tau=t-t')=\sum_{\alpha}\psi_\alpha(\boldsymbol{r})\psi^*_\alpha(\boldsymbol{r}')\exp(-\mathrm{i}\epsilon_\alpha\tau) \tag{3}$$

where summing is performed over discrete and continuum states ψ_α with eigenenergies ϵ_α. The bound-state contributions to the propagator can be easily included by direct calculation, while the continuum-state contribution requires special attention. In this case, one should perform an integration over intermediate continuum states

$$\psi(\boldsymbol{p},\boldsymbol{r})=\sum_{\alpha=\pm}\psi_\alpha(\boldsymbol{p},\boldsymbol{r})=\sum_{\alpha=\pm}a_\alpha(\boldsymbol{p},\boldsymbol{r})\exp(\mathrm{i}\boldsymbol{pr}+\mathrm{i}\Phi_\alpha(\boldsymbol{p},\boldsymbol{r})) \tag{4}$$

which represent a superposition of two waves; ψ_+ and ψ_- behave, respectively, as distorted plane and spherical waves as $r\to\infty$. According to this partition the continuum-state part of the propagator is

$$K_C(\boldsymbol{r},\boldsymbol{r}',\tau)=\sum_{\alpha,\beta=\pm}K_{\alpha\beta}(\boldsymbol{r},\boldsymbol{r}',\tau)=\sum_{\alpha,\beta}\int\frac{\mathrm{d}\boldsymbol{p}}{(2\pi)^3}a_\alpha(\boldsymbol{p},\boldsymbol{r})a_\beta(\boldsymbol{p},\boldsymbol{r}')\exp(\mathrm{i}S_{\alpha\beta}(\boldsymbol{p},\boldsymbol{r},\boldsymbol{r}',\tau)) \tag{5}$$

where the phase function is

$$\begin{aligned}S_{\alpha\beta}(\boldsymbol{p},\boldsymbol{r},\boldsymbol{r}',\tau)&=S_\alpha(\boldsymbol{p},\boldsymbol{r},t)-S_\beta(\boldsymbol{p},\boldsymbol{r}',t')\\ S_{\alpha=\pm}(\boldsymbol{p},\boldsymbol{r},t)&=-(p^2/2)t+\boldsymbol{pr}+\Phi_\pm(\boldsymbol{p},\boldsymbol{r}).\end{aligned} \tag{6}$$

In the WKB approximation S_α is the action function that satisfies the classical Hamilton–Jakobi equation

$$\frac{\partial S_\alpha}{\partial t}+\frac{1}{2}(\nabla_r S_\alpha)^2+V_c(r)=0. \tag{7}$$

For convenience we consider an electron in the Coulombic potential, $V_c(r)=-Z/r$, of the target nucleus of charge Z. The full integral of the Hamilton–Jakobi equation (7) containing three arbitrary constants, $\boldsymbol{p}$, components of the asymptotic momentum, has the form (Kunikeev and Senashenko 1996, Kunikeev 1999a)

$$\begin{aligned}&S_\alpha(\boldsymbol{p},\boldsymbol{r},t)=-\frac{p^2}{2}t+\boldsymbol{pr}+\nu\left(\frac{w_\alpha-1}{w_\alpha+1}+\ln\frac{w_\alpha-1}{w_\alpha+1}\right)+\varphi_\alpha(\nu)\\ &w_{\alpha=\pm}(\boldsymbol{p},\boldsymbol{r})=\pm(1-4\nu/\varsigma)^{1/2}\qquad \nu=-Z/p\qquad \zeta=pr+\boldsymbol{pr}\\ &\varphi_+(\nu)=-\nu\ln|\nu|\qquad \varphi_-(\nu)=\arg\nu-2\arg\Gamma(\mathrm{i}\nu)-\nu(2-\ln|\nu|).\end{aligned} \tag{8}$$

As is known, the quasiclassical approximation is applicable to a Coulomb field if $|\nu|\gg 1$ (Landau and Lifshitz 1974). Then, using the asymptotic formula for the gamma function,

$\Gamma(z)$, one obtains that $\varphi_-(\nu) = 2\arg\nu - \nu\ln|\nu|$, i.e. $\varphi_+(\nu) = \varphi_-(\nu)\ (\mathrm{mod}\ 2\pi)$. Considering that the functions (8) enter in the integral (5) as the difference (6), we can disregard the phases $\varphi_\pm(\nu)$ in (8).

The WKB amplitude a_α obeys the continuity equation

$$\nabla_r \cdot (a_\alpha^2(\boldsymbol{p}, \boldsymbol{r})\nabla_r S_\alpha(\boldsymbol{p}, \boldsymbol{r}, t)) = 0. \tag{9}$$

Within the asymptotic WKB approach, the integral (5) can be approximately evaluated by means of the stationary phase method (Fedoriuk 1987)

$$\begin{aligned}
K_C^{\mathrm{WKB}}(\boldsymbol{r}, \boldsymbol{r}', \tau) &= \sum_{\alpha,\beta} K_{\alpha\beta}^{\mathrm{WKB}}(\boldsymbol{r}, \boldsymbol{r}', \tau) \\
&= (-2\pi\mathrm{i})^{-3/2} \sum_{\alpha,\beta} a_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau) \exp\left(\mathrm{i}\tilde{S}_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau) - \mathrm{i}\frac{\pi}{2}\mu_{\alpha\beta}\right) \\
\tilde{S}_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau) &= S_{\alpha\beta}(\boldsymbol{p}_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau), \boldsymbol{r}, \boldsymbol{r}', \tau) \\
a_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau) &= a_\alpha(\boldsymbol{p}_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau), \boldsymbol{r}) a_\beta(\boldsymbol{p}_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau), \boldsymbol{r}') \\
&\quad \times \left|\det \frac{\partial^2}{\partial p^2} S_{\alpha\beta}(\boldsymbol{p}_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau), \boldsymbol{r}, \boldsymbol{r}', \tau)\right|^{-1/2}
\end{aligned} \tag{10}$$

where $\mu_{\alpha\beta} = \mathrm{inerdex}\frac{\partial^2}{\partial p^2} S_{\alpha\beta}(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r}, \boldsymbol{r}', \tau)$ denotes a negative inertia index of the matrix $\frac{\partial^2}{\partial p^2} S_{\alpha\beta}$ and $\boldsymbol{p} = \boldsymbol{p}_{\alpha\beta}$ is a solution of the stationary phase equation

$$\nabla_{\boldsymbol{p}} S_\alpha(\boldsymbol{p}, \boldsymbol{r}, t) = \nabla_{\boldsymbol{p}} S_\beta(\boldsymbol{p}, \boldsymbol{r}', t'). \tag{11}$$

It is assumed that $\det \frac{\partial^2}{\partial p^2} S_{\alpha\beta} \neq 0$. If equation (11) at given signs α and β has several or no solutions, then the corresponding contribution to (10) will consist of several terms or vanish. First let us consider solutions of equation (11).

2.1. The stationary phase equation

Substituting explicit expressions (8) for S_α and S_β in (11), we get

$$\begin{aligned}
-\boldsymbol{p}t + \boldsymbol{r} &+ \frac{w_\alpha - 1}{2}(\hat{\boldsymbol{p}}r + \boldsymbol{r}) + \frac{Z}{p^2}\hat{\boldsymbol{p}} \ln \frac{w_\alpha - 1}{w_\alpha + 1} \\
&= -\boldsymbol{p}t' + \boldsymbol{r}' + \frac{w'_\beta - 1}{2}(\hat{\boldsymbol{p}}r' + \boldsymbol{r}') + \frac{Z}{p^2}\hat{\boldsymbol{p}} \ln \frac{w'_\beta - 1}{w'_\beta + 1}
\end{aligned} \tag{12}$$

where

$$w_\alpha = w_\alpha(\boldsymbol{p}, \boldsymbol{r}) \qquad w'_\beta = w_\beta(\boldsymbol{p}, \boldsymbol{r}') \qquad \hat{\boldsymbol{p}} = \boldsymbol{p}/p.$$

The system of three equations (12) may be rewritten as a one equation derived from the projection of (12) on the direction of the momentum $\boldsymbol{p}$

$$\begin{aligned}
&p\tau + \frac{1}{2}(\eta - \eta') + \frac{1}{2}(w'_\beta \xi' - w_\alpha \xi) + \frac{Z}{p^2} \ln \frac{w'_\beta - 1}{w'_\beta + 1}\frac{w_\alpha + 1}{w_\alpha - 1} = 0 \\
&\xi = r(1 + \cos\theta) \qquad \eta = r(1 - \cos\theta) \qquad \cos\theta = \hat{\boldsymbol{p}} \cdot \hat{\boldsymbol{r}} \\
&\xi' = r'(1 + \cos\theta') \qquad \eta' = r'(1 - \cos\theta') \qquad \cos\theta' = \hat{\boldsymbol{p}} \cdot \hat{\boldsymbol{r}}'
\end{aligned} \tag{13}$$

and two equations from the transverse directions

$$(w_\alpha + 1) r \sin\theta \boldsymbol{n}_\varphi = (w'_\beta + 1) r' \sin\theta' \boldsymbol{n}_{\varphi'} \tag{14}$$

where $\boldsymbol{n}_\varphi$ and $\boldsymbol{n}_{\varphi'}$ are unit vectors in the direction of the vectors $\boldsymbol{r} - r\cos\theta\hat{\boldsymbol{p}}$ and $\boldsymbol{r}' - r'\cos\theta'\hat{\boldsymbol{p}}$, respectively. From equation (14) it follows that $\boldsymbol{n}_\varphi = \pm\boldsymbol{n}_{\varphi'}$, i.e. the vectors $\boldsymbol{p} = \boldsymbol{p}_{\alpha\beta}, \boldsymbol{r}, \boldsymbol{r}'$ lie in one plane. In the attractive potential ($Z > 0$), we have $|w_\alpha| > 1$ and, as a consequence,

$\boldsymbol{n}_\varphi = \boldsymbol{n}_{\varphi'}$ in the case of the ($\alpha = +, \beta = +$) and $(-, -)$ equations and $\boldsymbol{n}_\varphi = -\boldsymbol{n}_{\varphi'}$ in the case of the $(+, -)$ and $(-, +)$ equations. In the repulsive potential ($Z < 0$), one obtains $|w_\alpha| < 1$ and $\boldsymbol{n}_\varphi = \boldsymbol{n}_{\varphi'}$ for all equations. We confine our discussion to the case of attractive potentials (the repulsive potentials are considered in the same way).

Let us consider four cases. Case 1, the $(+, +)$ equation will be analysed in detail. For the other three cases, corresponding to different combinations of signs, only the final results will be written down. Denote by

$$a = \frac{4Z}{r(1+\cos\theta)} \qquad b = r\sin\theta$$
$$a' = \frac{4Z}{r'(1+\cos\theta')} \qquad b' = r'\sin\theta' \tag{15}$$

then the $(+, +)$ equation may be recast as

$$\left(\sqrt{p^2+a}+p\right)b = \left(\sqrt{p^2+a'}+p\right)b'. \tag{16}$$

Suppose $b > b'$ and transpose the term pb' from the right- to left-hand side of the equation, then squaring (16) one obtains

$$2b(b-b')p\sqrt{p^2+a} = b'^2a' - b^2a - 2b(b-b')p^2.$$

Again squaring the equation, we get the following expression for:

$$p^2 = \frac{(b'^2a' - b^2a)^2}{4bb'(b-b')(b'a'-ba)} \tag{17}$$

under the condition

$$b'^2a' - b^2a - 2b(b-b')p^2 > 0.$$

From (17) it follows that $b'a' > ba$. Substituting (17) into the inequality, we obtain

$$(b'^2a' - b^2a)(b'(b'a'-ba) + ba(b-b')) > 0.$$

Thus, we have that equation (17) is defined under the conditions

$$b > b' \qquad b'a' > ba \qquad b'^2a' > b^2a.$$

Similarly, we obtain

$$p^2 = \frac{(b'^2a' - b^2a)^2}{4bb'(b'-b)(ba-b'a')} \qquad \text{if} \quad b' > b \qquad ba > b'a' \qquad b^2a > b'^2a'. \tag{18}$$

Using explicit expressions (15), we get

$$b - b' = |\boldsymbol{r} - \boldsymbol{r}'|\sin(\theta \mp \gamma)$$
$$b'a' - ba = \pm\frac{4Z\sin(\delta/2)}{\cos(\theta/2)\cos((\theta\pm\delta)/2)} \tag{19}$$
$$b'^2a' - b^2a = 4Z|\boldsymbol{r} - \boldsymbol{r}'|(\cos\beta + \cos(\theta\mp\gamma))$$

where

$$\cos\beta = (r'-r)/|\boldsymbol{r} - \boldsymbol{r}'| \qquad \cos\gamma = (r - r'\cos\delta)/|\boldsymbol{r} - \boldsymbol{r}'|$$

and δ is the angle between the radius vectors $\boldsymbol{r}$ and $\boldsymbol{r}'$. Here, the upper sign corresponds to the conditions $0 < \theta < \pi - \delta$, $\delta < \theta' < \pi$, $\theta' = \theta + \delta$ ($\angle AOB'$, see figure 1) and the lower sign refers to $\delta < \theta < \pi$, $0 < \theta' < \pi - \delta$, $\theta' = \theta - \delta$ ($\angle A'OB$). Substituting the formulae (19) into (17) or (18) (that depends on what sings, upper or lower, are chosen in (19)), one obtains

$$p^2 = \pm\frac{Z|\boldsymbol{r} - \boldsymbol{r}'|}{4rr'\sin(\delta/2)}\frac{(\cos\beta + \cos(\theta\mp\gamma))^2}{\sin(\theta/2)\sin((\theta\pm\delta)/2)\sin(\theta\mp\gamma)} \tag{20}$$

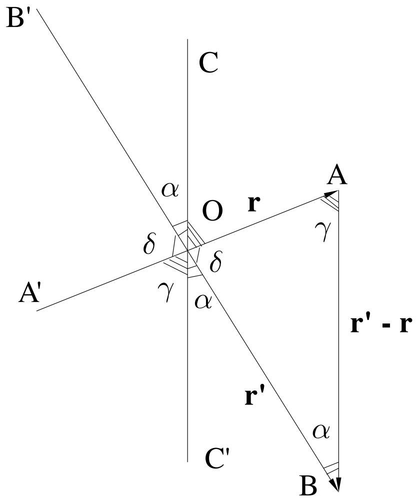

Figure 1. Angular sectors to which asymptotic momenta $\boldsymbol{p}_{\alpha\beta}$ ($\alpha, \beta = \pm$) may belong: $\boldsymbol{p}_{++}$ and $\boldsymbol{p}_{--}$ lie in $\angle B'OC$ or $\angle A'OC'$, while $\boldsymbol{p}_{+-}$ and $\boldsymbol{p}_{-+}$ in $\angle AOB$ or $\angle A'OB'$.

expressed as a function of θ. Further, one can see that the set of inequalities under which equation (17) is defined is equivalent to

$$\gamma < \theta < \min(\gamma+\alpha, \gamma+\pi-\beta) = \begin{cases} \gamma+\alpha & \text{if} \quad \cos\delta < 2r'/r - 1 \\ \gamma+\pi-\beta & \text{if} \quad \cos\delta > 2r'/r - 1 \end{cases} \tag{21}$$

where $\cos\alpha = (r' - r\cos\delta)/|\boldsymbol{r} - \boldsymbol{r}'|$; for inequalities in (18) one obtains

$$\delta+\alpha < \theta < \min(\pi, \pi+\beta-\gamma) = \begin{cases} \pi & \text{if} \quad \cos\delta < 2r/r' - 1 \\ \pi+\beta-\gamma & \text{if} \quad \cos\delta > 2r/r' - 1 \end{cases} \tag{22}$$

i.e. equation (20), with the upper and lower signs, are defined, respectively, in the angular sectors $\angle B'OC$ and $\angle A'OC'$ or in their parts if $\pi - \beta < \alpha$ in (21) and $\beta < \gamma$ in (22).

In case 2, the $(-,-)$ equation, we obtain the same expression (20) for the quadratic momentum but the regions (21) and (22), in which it is defined, should be replaced by

$$\begin{cases} \emptyset & \text{if} \quad \cos\delta < 2r'/r - 1 \\ \gamma+\pi-\beta < \theta < \gamma+\alpha & \text{if} \quad \cos\delta > 2r'/r - 1 \end{cases} \tag{23}$$

and

$$\begin{cases} \emptyset & \text{if} \quad \cos\delta < 2r/r' - 1 \\ \pi+\beta-\gamma < \theta < \pi & \text{if} \quad \cos\delta > 2r/r' - 1 \end{cases} \tag{24}$$

respectively. Note that the $(-,-)$ equation cannot have solutions if simultaneously $\cos\delta < 2r'/r - 1$ and $\cos\delta < 2r/r' - 1$. These conditions are fulfilled if, for example, $r = r'$.

For cases 3 and 4 corresponding to the (+, −) and (−, +) equations, we get the following general expression:

$$p^2 = \mp \frac{Z|\boldsymbol{r} - \boldsymbol{r}'|}{4rr'\sin(\delta/2)} \frac{(\cos\beta + \cos(\theta \pm \gamma))^2}{\sin(\theta/2)\sin((\theta \mp \delta)/2)\sin(\theta \pm \gamma)} \tag{25}$$

where the upper and lower signs correspond to $\angle AOB$: $0 < \theta < \delta, \theta' = \delta - \theta$ and $\angle A'OB'$: $\pi - \delta < \theta < \pi, \theta' = 2\pi - \theta - \delta$. In $\angle AOB$, the (+, −) and (−, +) equations are defined, respectively, in regions $0 < \theta < \delta + \alpha - \beta$ and $\delta + \alpha - \beta < \theta < \delta$, while in $\angle A'OB'$, the (+, −) and (−, +) equations are defined in regions

$$\begin{cases} \emptyset & \text{if} \quad \cos\delta > 2r'/r - 1 \\ \alpha + \gamma < \theta < \gamma + \pi - \beta & \text{if} \quad \cos\delta < \min(2r'/r - 1, 2r/r' - 1) \\ \alpha + \gamma < \theta < \pi & \text{if} \quad \cos\delta > 2r/r' - 1 \end{cases} \tag{26}$$

and

$$\begin{cases} \emptyset & \text{if} \quad \cos\delta > 2r/r' - 1 \\ \pi - \beta + \gamma < \theta < \pi & \text{if} \quad \cos\delta < \min(2r'/r - 1, 2r/r' - 1) \\ \alpha + \gamma < \theta < \pi & \text{if} \quad \cos\delta > 2r'/r - 1 \end{cases} \tag{27}$$

respectively. Thus, we can conclude that all the (α, β) equations for $p^2(\theta)$ are defined in different regions.

Substituting equation (20) or (25) into (13), we get a one-dimensional equation, defined in the given region, which should be solved for θ. Moreover, making use of (14) and the relationship

$$(w_\alpha^2 - 1)\xi = \frac{4Z}{p^2} = (w_\beta'^2 - 1)\xi' \tag{28}$$

we can simplify the logarithmic term such that equation (13) takes a simpler form

$$f_{\alpha\beta}(\theta) \equiv p\tau + \frac{1}{2}(\eta - \eta') + \frac{1}{2}(w_\beta'\xi' - w_\alpha\xi) + \frac{Z}{p^2}\ln\frac{\eta'}{\eta} = 0. \tag{29}$$

Let us stress that in passing from the (+, +) to (−, −) equation both the logarithmic terms in (13) and (29) reverse the sign. In (13), this property is seen straightforwardly, while the logarithmic term in (29) does not change its sign at first glance. A closer inspection of (29) shows that the property holds because of the fact that the (+, +) and (−, −) equations are defined in such different regions that if, for example, $\eta' > \eta$ in one region, then $\eta > \eta'$ in the other one. In particular, this property explains why the (+, +) and (−, −) equations cannot be defined in a common region.

In the limit $Z \to 0$, the Coulomb propagator tends to a free one and the phase equations (12) to a free counterpart. Since the amplitude $a_-(\boldsymbol{p}, \boldsymbol{r})$ is proportional to Z, only the (+, +) term survives in (10) as $Z \to 0$. However, not only the (+, +) equation but also the other ones make a sense as $Z \to 0$. As an example, consider the solution of the (+, +) and (+, −) equations (14) and (29) in the limiting case $Z \to 0$. From (14) it follows that $r\sin\theta = r'\sin\theta'$ for the (+, +) equation, i.e., we have the two solutions $\theta_1 = \gamma$, $\theta_1' = \gamma + \delta$ or $\theta_2' = \alpha$, $\theta_2 = \alpha + \delta$ (see figure 1). It means that the limiting momentum $\boldsymbol{p}_{++}^{Z=0}$ is parallel to the radius vector $\boldsymbol{r}' - \boldsymbol{r}$, i.e., $\hat{\boldsymbol{p}}_{++}^{Z=0} = \mp\widehat{(\boldsymbol{r}' - \boldsymbol{r})}$, where the upper and lower signs correspond to the solutions θ_1 and θ_2, respectively. As $Z \to 0$, equation (29) tends to

$$f_{++}^{Z=0}(\theta) \equiv p\tau + r'\cos\theta' - r\cos\theta = 0. \tag{30}$$

Substituting the above values for θ and θ' in (30), one obtains $p_{1,2}\tau = \pm|\boldsymbol{r} - \boldsymbol{r}'|$, where the upper and lower signs correspond to the alternative values $\theta_{1,2}$ and $\theta_{1,2}'$. Further, from the last equation we have $p_{++}^{Z=0} = p_1 = |\boldsymbol{r} - \boldsymbol{r}'|/\tau$ or $p_{++}^{Z=0} = p_2 = -|\boldsymbol{r} - \boldsymbol{r}'|/\tau$ if $\tau > 0$ or $\tau < 0$, respectively. Finally, we get that the (+, +) equation has a single solution $\boldsymbol{p}_{++}^{Z=0} = (\boldsymbol{r} - \boldsymbol{r}')/\tau$ for any signs of τ. Actually, this solution follows easily from the original vector equation (12) in the limit $Z \to 0$.

For the (+, −) equation, we get from (14) that $r\sin\theta = 0$ and $\theta_1 = 0$ or $\theta_2 = \pi$, i.e., $\hat{\boldsymbol{p}}_{+-}^{Z=0} = \pm\hat{\boldsymbol{r}}$. Instead of (30), we obtain

$$f_{+-}^{Z=0}(\theta) \equiv p\tau - r' - r\cos\theta = 0. \tag{31}$$

Substituting the values $\theta_{1,2} = 0, \pi$ in (31), we have $p_{1,2} = (r' \pm r)/\tau$. Thus, depending on the choices of r, r', and τ, equation (31) may have no solution, one or two solutions. If, for example, $r' > r$ and $\tau > 0$, then one obtains the two solutions: $(\boldsymbol{p}_{+-}^{Z=0})_{1,2} = (\boldsymbol{r} \pm r'\hat{\boldsymbol{r}})/\tau$.

Unfortunately, the general equation (29) does not allow an analytic solution and therefore we have to solve it numerically. As an example, we plot $f_{\alpha\beta}(\theta)$ at $r = 1, r' = 2, \delta = 60^\circ$ and $\tau = \pm 0.25, \pm 0.5$, and ± 1.0 in the case of an electron in the field of a proton, $Z = 1$, as a function of θ in all the angular sectors (figure 2). One can see that in $\angle COB'$: $90^\circ < \theta < 120^\circ$, $\theta' = \theta + 60^\circ$ only the (+, +) equation is defined and there is no root at $\tau = \pm 1, -0.25, -0.5$, while at $\tau = 0.5, 0.25$ we have a root $\theta_c(\tau) \to \gamma = 90^\circ$ as $\tau \to 0, \tau > 0$. Further, in $\angle A'OC'$: $90^\circ < \theta < 180^\circ, \theta' = \theta - 60^\circ$ both the (+, +) and (−, −) equations are defined: the (+, +) equation is defined in the interval $90^\circ < \theta < 180^\circ - \gamma + \beta \simeq 180^\circ - 90^\circ + 54.74^\circ = 144.74^\circ$ ($\cos\beta = \sqrt{3}/3$, $\beta \approx 54.74^\circ$); the (−, −) equation refers to $144.74^\circ < \theta < 180^\circ$. At the boundary angle $\theta_b \approx 144.74^\circ$, the quadratic momentum in (29) vanishes, $p^2(\theta_b) = 0$, and $\eta(\theta_b) = \eta'(\theta_b)$ since $p^2 \sim (\eta - \eta')^2$. The (+, +) equation is seen to have no root at $\tau > 0$ and there is a root $\theta_c(\tau) \to 180^\circ - \gamma = 90^\circ$ as $\tau \to 0, \tau < 0$, while the (−, −) equation has no solution in the interval $\theta_b < \theta < 180^\circ$. Besides, it can be easily checked that $f_{\alpha\beta}(\theta)|_{p(\theta)\to 0} \to 0$. Indeed, from (8) we get the following expansion:

$$\frac{w'_\beta - 1}{w'_\beta + 1}\frac{w_\alpha + 1}{w_\alpha - 1} = 1 + \frac{p}{\sqrt{Z}}(\alpha\sqrt{\xi} - \beta\sqrt{\xi'}) + \frac{p^2}{2Z}(\alpha\sqrt{\xi} - \beta\sqrt{\xi'})^2 + \mathrm{O}(p^3). \tag{32}$$

Using (32), we obtain

$$\frac{Z}{p^2}\ln\frac{w'_\beta - 1}{w'_\beta + 1}\frac{w_\alpha + 1}{w_\alpha - 1} = \frac{\sqrt{Z}}{p}(\alpha\sqrt{\xi} - \beta\sqrt{\xi'}) + \mathrm{O}(p). \tag{33}$$

Similarly,

$$\frac{1}{2}(w_\beta\xi' - w_\alpha\xi) = -\frac{\sqrt{Z}}{p}(\alpha\sqrt{\xi} - \beta\sqrt{\xi'}) + \mathrm{O}(p). \tag{34}$$

Finally, summing (33) and (34), we get

$$\frac{1}{2}(w_\beta\xi' - w_\alpha\xi) + \frac{Z}{p^2}\ln\frac{w'_\beta - 1}{w'_\beta + 1}\frac{w_\alpha + 1}{w_\alpha - 1} = \mathrm{O}(p). \tag{35}$$

This completes the proof. Thus, we have $f_{++}(\theta)|_{\theta\to\theta_b-0} \to 0$ and $f_{--}(\theta)|_{\theta\to\theta_b+0} \to 0$. In a similar way, we can readily verify that equation (14) is satisfied as $p \to 0$ and hence $\nabla_{\boldsymbol{p}} S_{\alpha\beta}(\boldsymbol{p}, \boldsymbol{r}, \boldsymbol{r}', \tau)|_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\theta\to\theta_b)} = 0$.

Furthermore, in $\angle AOB$: $0^\circ < \theta < \delta = 60^\circ$, $\theta' = \delta - \theta$, both the (+, −) and (−, +) functions are defined, respectively, in the intervals $0^\circ < \theta < \theta_b = \delta + \alpha - \beta \approx 35.26^\circ$ and $\theta_b < \theta < 60^\circ$. As above, we see that $f_{+-}(\theta)|_{\theta\to\theta_b-0} \to 0$ and $f_{-+}(\theta)|_{\theta\to\theta_b+0} \to 0$. Besides, one can see that the (+, −) equation has a root $\theta_c(\tau) \to 0^\circ$ as $\tau \to 0, \tau > 0$, while the (−, +) equation has a root $\theta_c(\tau) \to \delta = 60^\circ$ as $\tau \to 0, \tau < 0$. Finally, in $\angle A'OB'$: $180^\circ - \delta = 120^\circ < \theta < 180^\circ, \theta' = 360^\circ - \theta - \delta$ only the (+, −) function is defined and there is a root at $\tau = 1$ but no root at $\tau = \pm 0.25, \pm 0.5, -1.0$. Thus, we have that at the given parameters the stationary phase equations (12) have two solutions. The contributions from other roots at boundary angles $\theta = \theta_b$ cannot be considered within the standard stationary phase method because the momentum $p(\theta_b) = 0$ and we have the amplitude $a_\alpha(\boldsymbol{p}, \boldsymbol{r})|_{\theta\to\theta_b} \sim p^{-1/2} \to \infty$ and the determinant $|\det\frac{\partial^2}{\partial p^2}S_{\alpha\beta}|^{1/2}_{\theta\to\theta_b} \sim p^{-2} \to \infty$ (see section 2.3). We can, however, regularize the integral (5) by introducing the phase factor $\exp(\mathrm{i}p\epsilon)$. Then, equation (14) does not change its form and, therefore, $p(\theta)|_{\theta\to\theta_b} \to 0$, but equation (29) is replaced by

$$f^\epsilon_{\alpha\beta}(\theta) \equiv f_{\alpha\beta}(\theta) + \epsilon = 0.$$

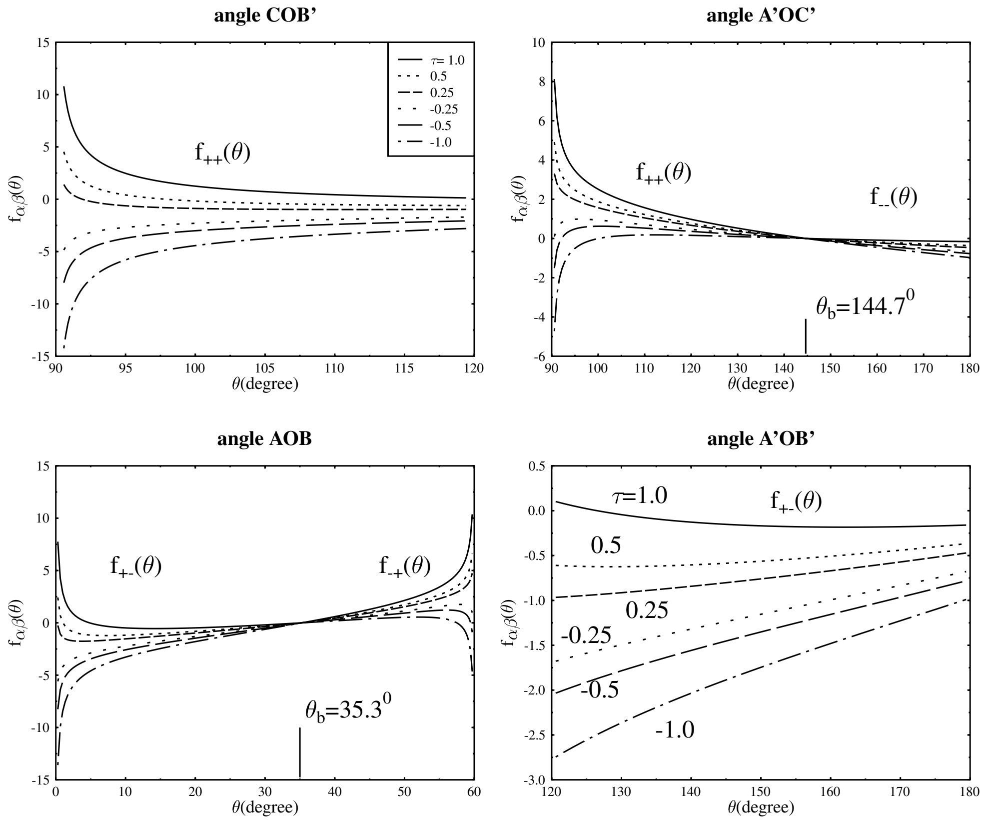

Figure 2. The function $f_{\alpha\beta}(\theta)$ defined by equation (29) in different angular sectors (see figure 1). The parameters are $r = 1$, $r' = 2$, $\delta = 60°$, and $\tau = \pm 0.25, \pm 0.5, \pm 1.0$.

Thus, the regularized function $f^{\epsilon}_{\alpha\beta}(\theta)$ is simply the function $f_{\alpha\beta}(\theta)$ shifted on ϵ, up or down, that depends on the sign of ϵ. The regularized equation has a root $\theta^{\epsilon}_b|_{\epsilon\to 0} \to \theta_b$ so that $p(\theta^{\epsilon}_b) \sim |\epsilon|$. Therefore, from (10) we get

$$a_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau)|_{\theta=\theta^{\epsilon}_b} \sim |\epsilon|$$

and the boundary points θ^{ϵ}_b does not contribute to (10) as $\epsilon \to 0$.

2.2. The two-point action function

Now we discuss how the derived stationary phase points are associated with the two-point action function. Denote by

$$\boldsymbol{q}_\alpha(\boldsymbol{p}, \boldsymbol{r}, t) = \nabla_{\boldsymbol{p}} S_\alpha(\boldsymbol{p}, \boldsymbol{r}, t) \tag{36}$$

the map: $\boldsymbol{r} \to \boldsymbol{q}_\alpha$; then the stationary phase equation tells us that $\boldsymbol{q}_\alpha(\boldsymbol{p}, \boldsymbol{r}, t) = \boldsymbol{q}_\beta(\boldsymbol{p}, \boldsymbol{r}', t')$ at $\boldsymbol{p} = \boldsymbol{p}_{\alpha\beta}$. According to implicit function theorem, this equation is solvable for $\boldsymbol{p}$ and defines the function $\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})$ that reduces the equation to an identity in the neighbourhood of $\boldsymbol{X} = (\boldsymbol{r}, t, \boldsymbol{r}', t')$ under the condition det $\frac{\partial^2 S_{\alpha\beta}}{\partial p^2}|_{\boldsymbol{p}_{\alpha\beta}, \boldsymbol{X}} \neq 0$. We can also reverse the map (36), namely, express $\boldsymbol{r}_\alpha = \boldsymbol{r}_\alpha(\boldsymbol{p}, \boldsymbol{q}, t)$ as a function of $\boldsymbol{p}, \boldsymbol{q}, t$ under the condition det $\frac{\partial^2 S_\alpha}{\partial \boldsymbol{p} \partial \boldsymbol{r}} \neq 0$. By the Jakobi theorem (Arnold 1978), $\boldsymbol{r}_\alpha(\boldsymbol{p}, \boldsymbol{q}, \tau)$ represents a set of classical trajectories depending on six constants $\boldsymbol{p}, \boldsymbol{q}$ such that $\boldsymbol{r}_\alpha(\boldsymbol{p}, \boldsymbol{q}, \tau = t) = \boldsymbol{r}$ and $\boldsymbol{r}_\beta(\boldsymbol{p}, \boldsymbol{q}, \tau = t') = \boldsymbol{r}'$ at $\boldsymbol{p} = \boldsymbol{p}_{\alpha\beta}$ and $\boldsymbol{q} = \boldsymbol{q}_\alpha = \boldsymbol{q}_\beta$. In the case $\alpha = \beta$, we have, therefore, a single trajectory $\boldsymbol{r}_\alpha(\boldsymbol{p}_{\alpha\alpha}, \boldsymbol{q}_\alpha, \tau)$ passing through the points $\boldsymbol{r}$ and $\boldsymbol{r}'$ at moments $\tau = t$ and t', respectively; while at $\alpha \neq \beta$ we obtain the two types of trajectories, the (+) and (−) trajectories: one trajectory $\boldsymbol{r}_\alpha(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{q}_\alpha, \tau)$ passes through $\boldsymbol{r}$ at $\tau = t$ and the other one, $\boldsymbol{r}_\beta(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{q}_\alpha = \boldsymbol{q}_\beta, \tau)$, passes through $\boldsymbol{r}'$ at $\tau = t'$.

Let us consider solving equation (36) for $\boldsymbol{r}$ at greater length. Substituting the explicit expression (8) for S_α into (36), we can rewrite the system of equations as

$$\begin{aligned} \boldsymbol{q}_\perp &= \frac{w_\alpha + 1}{2}(\boldsymbol{r} - (\hat{\boldsymbol{p}}\boldsymbol{r})\hat{\boldsymbol{p}}) \\ q_\parallel &= -pt + \frac{1}{2}(w_\alpha - 1)r + \frac{1}{2}(w_\alpha + 1)(\hat{\boldsymbol{p}}\boldsymbol{r}) + \frac{Z}{p^2}\ln\frac{w_\alpha - 1}{w_\alpha + 1} \end{aligned} \tag{37}$$

where $\boldsymbol{q} = q_\parallel\hat{\boldsymbol{p}} + \boldsymbol{q}_\perp = q_\parallel\hat{\boldsymbol{p}} + q_\perp\boldsymbol{n}_\perp$. From (37) we get that $\boldsymbol{r} - (\hat{\boldsymbol{p}}\boldsymbol{r})\hat{\boldsymbol{p}} = \pm r\sin\theta\boldsymbol{n}_\perp$ ($\cos\theta = (\hat{\boldsymbol{p}}\hat{\boldsymbol{r}})$, $Z > 0$) at $\alpha = \pm$, i.e., $\boldsymbol{r} = \boldsymbol{r}_{\alpha=\pm} = r_\alpha\cos\theta_\alpha\hat{\boldsymbol{p}} \pm r_\alpha\sin\theta_\alpha\boldsymbol{n}_\perp$ belongs to the plane that spans the vectors $\boldsymbol{p}$ and $\boldsymbol{q}$ and the first equation reduces to

$$q_\perp = \frac{1}{2}\left(\sqrt{1 + \frac{4Z}{p^2 r_\alpha(1 + \cos\theta_\alpha)}} \pm 1\right) r_\alpha\sin\theta_\alpha \qquad \text{at} \quad \alpha = \pm. \tag{38}$$

From (38) we can readily obtain $r_\alpha(\theta_\alpha)$ as a function of polar angle θ_α. The explicit expressions for the hyperbolic trajectories $r_\alpha(\theta_\alpha)$ are already written out, equations (28) and (31) in Kunikeev (1999a), but they were derived there in a different way, namely, by direct integration of the equations

$$\dot{\boldsymbol{r}}(t) = \nabla_{\boldsymbol{r}} S_\alpha(\boldsymbol{p}, \boldsymbol{r}, t) = \boldsymbol{p} + \frac{w_\alpha - 1}{2}p(\hat{\boldsymbol{p}} + \hat{\boldsymbol{r}}). \tag{39}$$

In passing, note that the right-hand side of (39) does not actually depend on t. Now establish a relationship between the constants of integration ρ_0 and θ_0, where ρ_0 is an impact parameter and θ_0 is an angle specifying the direction of the hyperbolic trajectory asymptote, in equations (28) and (31) by Kunikeev (1999a) and the parameter $q_\perp$ in (38). As $r_\alpha \to \infty$ in (38), we get $q_\perp = \rho_0$ at $\alpha = +$ and $q_\perp p^2/Z = \sin\theta_0/(1 + \cos\theta_0) = \tan(\theta_0/2)$ at $\alpha = -$. It follows that the parameters ρ_0 and θ_0 in the two types of trajectories, with $\alpha = \pm$, defined by (37) are not independent ones but related by equation

$$\rho_0 p^2/Z = \tan(\theta_0/2). \tag{40}$$

Finally, substituting the function $r_\alpha(\theta_\alpha)$ into the second equation of (37), we can solve it for θ_α, thus obtaining a function $\theta_\alpha(t)$.

Denote by $\Lambda^3_\alpha(\boldsymbol{r}) = (\boldsymbol{r}, \boldsymbol{p}_\alpha(\boldsymbol{p}, \boldsymbol{r}))$ the Lagrange manifolds defined at $\boldsymbol{r} \in \boldsymbol{R}^3 \backslash (D_\alpha \cup l_{c\alpha})$; here, D_α is the region where $\boldsymbol{p}_\alpha(\boldsymbol{p}, \boldsymbol{r})$ is not defined and $l_{c\alpha}$ is a set of the caustics points in which $\det\partial\boldsymbol{r}_\alpha/\partial\boldsymbol{q} = 0$. From (36) it follows that $\det\partial\boldsymbol{r}_\alpha/\partial\boldsymbol{q} = (\det\frac{\partial^2 S_\alpha}{\partial p\partial r})^{-1}$. Let us evaluate the last determinant. From (39) we get

$$\frac{\partial^2 S_\alpha}{\partial r_i\partial p_j} = \frac{w_\alpha + 1}{2}\delta_{ij} + \frac{w_\alpha - 1}{2}\frac{r_i}{r}\frac{p_j}{p} - \frac{Z}{w_\alpha p^2\xi^2}\left(\frac{r_i}{r} + \frac{p_i}{p}\right)\left(\frac{p_j}{p}(r + \xi) + r_j\right) \tag{41}$$

where indices $i, j = 1, 2, 3$ label projections of coordinates. Choose the system of coordinates such that $\boldsymbol{p} = (0, 0, p)$ and $\boldsymbol{r} = (r\sin\theta, 0, r\cos\theta)$; then the matrix (41) takes the form

$$\left(\frac{\partial^2 S_\alpha}{\partial r_i\partial p_j}\right) = \begin{pmatrix} \frac{w_\alpha+1}{4w_\alpha}(w_\alpha + 1 + (w_\alpha - 1)\cos\theta) & 0 & -\frac{w_\alpha-1}{2w_\alpha}\sin\theta \\ 0 & \frac{w_\alpha+1}{2} & 0 \\ -\frac{w_\alpha^2-1}{4w_\alpha}\sin\theta & 0 & \frac{1}{2w_\alpha}(w_\alpha + 1 - (w_\alpha - 1)\cos\theta) \end{pmatrix} \tag{42}$$

and

$$\det\left(\frac{\partial^2 S_\alpha}{\partial r_i \partial p_j}\right) = \frac{(w_\alpha + 1)^2}{4w_\alpha} \tag{43}$$

because coefficients of the characteristic polynomial $\det(A - \lambda E) = 0$ are independent of the choice of basis vectors.

One can see that the caustics points are defined by the conditions: $w_\alpha = 0, \pm\infty$. Recall that in the cases $Z > 0$ and $Z < 0$ we have $|w_\alpha| > 1$ and $|w_\alpha| < 1$, respectively. Hence, we obtain different sets of the caustics points: for attractive potential, $l_c^{Z>0} = \{\boldsymbol{r} : \xi = 0\}$ represents the negative semiaxes $(0 \leqslant r < \infty, \theta = \pi)$ and for repulsive potential, $l_c^{Z<0} = \{\boldsymbol{r} : \xi = \xi_c = 4|Z|/p^2\}$ is a two-dimensional surface (see figure 1 in Kunikeev (1999a)). In addition, we have $D_\alpha^{Z<0} = \{\boldsymbol{r} : \xi < \xi_c\}$ and $D_\alpha^{Z>0} = \emptyset$.

Consider the limiting behaviour of the momentum $\boldsymbol{p}_\alpha(\boldsymbol{p}, \boldsymbol{r})$ as $\boldsymbol{r}$ approaches to $l_c^{Z>0}$. We have

$$\boldsymbol{p}_{\alpha=\pm}(\boldsymbol{p}, \boldsymbol{r})|_{\theta\to\pi} = \boldsymbol{p} \pm \sqrt{\frac{2Z}{r}}(\boldsymbol{n}_r)_\perp \tag{44}$$

where $\boldsymbol{r} = r\cos\theta\hat{\boldsymbol{p}} + r\sin\theta\boldsymbol{n}_{r_\perp}$. One can see that (44) is not defined at $\boldsymbol{r} \in l_c^{Z>0}$ since the limit depends on the direction of the vector $\boldsymbol{n}_{r_\perp}$ or the plane in which the vectors $\boldsymbol{r}$ and $\hat{\boldsymbol{p}}$ lie when we approach the caustics point. This is because $l_c^{Z>0}$ is the set of points where infinitely many trajectories with different azimuthal angles are focused.

Note that the above trajectories $\boldsymbol{r}_\alpha(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{q}_\alpha, \tau)$ and $\boldsymbol{r}_\beta(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{q}_\alpha, \tau)$ cross in a focusing point. In fact, the (+) and (−) trajectories with impact parameter ρ_0 and angle θ_0 intersect $l_c^{Z>0}$ at the points $(r_{c+} = (p_{\alpha\beta}\rho_0)^2/(2Z), \theta = \pi)$ and $(r_{c-} = Z/(2p_{\alpha\beta}^2)\tan^2(\theta_0/2), \theta = \pi)$, respectively (Kunikeev 1999a). By (40), we have $r_{c+} = r_{c-}$ and, thus, these points coincide with each other. As follows from the second equation of (37), the trajectories intersect the caustics line at the one moment of time $\tau = t_c = -(q_\parallel + r_{c+})/p_{\alpha\beta}$. In addition, from (44) we get that the limiting momenta at the caustics point $\boldsymbol{r}_c$ are equal: $\boldsymbol{p}_\alpha(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r}_c) = \boldsymbol{p}_\beta(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r}_c)$. Therefore, we can define the single trajectory

$$\boldsymbol{r}_{\alpha\beta}(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{q}_\alpha, \tau) = \begin{cases} \boldsymbol{r}_\alpha(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{q}_\alpha, \tau) & \text{at} \quad t_c \leqslant \tau \leqslant t \\ \boldsymbol{r}_\beta(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{q}_\alpha, \tau) & \text{at} \quad t' \leqslant \tau \leqslant t_c \end{cases} \tag{45}$$

that smoothly connects the points $\boldsymbol{r}$ and $\boldsymbol{r}'$. In view of (39), the curve (45) also connects the corresponding points of the Lagrange manifolds Λ_α^3 and Λ_β^3; transition from Λ_β^3 to Λ_α^3 occurs at caustics point $\boldsymbol{r}_c$ at moment $\tau = t_c$.

By definition, the two-point action function is

$$\tilde{S}_{\alpha\beta}(\boldsymbol{r}, t, \boldsymbol{r}', t') = \int_{t'}^{t} \boldsymbol{p}\,\mathrm{d}\boldsymbol{r} - H_{\mathrm{at}}(\boldsymbol{p}, \boldsymbol{r})\,\mathrm{d}\tau = \left(\int_{t'}^{t_c} + \int_{t_c}^{t}\right)\boldsymbol{p}\,\mathrm{d}\boldsymbol{r} - H_{\mathrm{at}}(\boldsymbol{p}, \boldsymbol{r})\,\mathrm{d}\tau \tag{46}$$

where integration is performed along the path (45). On the path, the Hamilton function is a constant: $H_{\mathrm{at}}(\boldsymbol{p}, \boldsymbol{r}) = p_{\alpha\beta}^2/2$. In addition, we have $\boldsymbol{p} = \nabla_{\boldsymbol{r}} S_\beta(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r})$ and $\boldsymbol{p} = \nabla_{\boldsymbol{r}} S_\alpha(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r})$ on the time intervals (t', t_c) and (t_c, t), respectively. As is known, the integral $\int \boldsymbol{p}\,\mathrm{d}\boldsymbol{r}$ defined on the Lagrange manifolds Λ_β and Λ_α does not depend locally on a path, but it is a function of initial and final points of a path. Using these properties, we get

$$\begin{aligned} \tilde{S}_{\alpha\beta}(\boldsymbol{r}, t, \boldsymbol{r}', t') &= \boldsymbol{p}_{\alpha\beta}\boldsymbol{r} + \Phi_\alpha(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r}) - \boldsymbol{p}_{\alpha\beta}\boldsymbol{r}_c - \Phi_\alpha(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r}_c) \\ &\quad + \boldsymbol{p}_{\alpha\beta}\boldsymbol{r}_c + \Phi_\beta(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r}_c) - \boldsymbol{p}_{\alpha\beta}\boldsymbol{r}' - \Phi_\beta(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r}') - (p_{\alpha\beta}^2/2)(t - t') \\ &= S_\alpha(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r}, t) - S_\beta(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r}', t') = S_{\alpha\beta}(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r}, \boldsymbol{r}', \tau)|_{\boldsymbol{p}_{\alpha\beta} = \boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})} \end{aligned} \tag{47}$$

where we have used the relation: $\Phi_\alpha(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r}_c) = \Phi_\beta(\boldsymbol{p}_{\alpha\beta}, \boldsymbol{r}_c)$. An inspection of (10) and (47) shows that the phase function $\tilde{S}_{\alpha\beta}$ of the propagator is really the two-point action function (47).

A similar result is readily obtained in the case $\alpha = \beta$, where a path connecting two points does not intersect the caustics line.

Making use of (13), we can reduce (47) to the form

$$\tilde{S}_{\alpha\beta}(\boldsymbol{r}, t, \boldsymbol{r}', t') = -\tfrac{3}{2}p^2(t-t') + p(r'-r) + \boldsymbol{p}(\boldsymbol{r}-\boldsymbol{r}') + \zeta w_\alpha(\boldsymbol{p}, \boldsymbol{r}) - \zeta' w_\beta(\boldsymbol{p}, \boldsymbol{r}')|_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})}$$
$$\zeta = pr + \boldsymbol{pr} \qquad \zeta' = pr' + \boldsymbol{pr}'. \tag{48}$$

2.3. Maslov's determinant and the index $\mu_{\alpha\beta}$

Now let us prove that the amplitude $a_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau)$ in (10) is associated with the Maslov determinant by

$$a_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau) = \left|\det \frac{\partial^2 \tilde{S}_{\alpha\beta}(\boldsymbol{r}, t, \boldsymbol{r}', t')}{\partial \boldsymbol{r}\partial \boldsymbol{r}'}\right|^{1/2}. \tag{49}$$

Doubly differentiating equation (47) with respect to $\boldsymbol{r}$ and $\boldsymbol{r}'$, we obtain

$$\frac{\partial^2 \tilde{S}_{\alpha\beta}}{\partial \boldsymbol{r}\partial \boldsymbol{r}'} = \frac{\partial \boldsymbol{p}}{\partial \boldsymbol{r}}\frac{\partial^2 S_{\alpha\beta}}{\partial p^2}\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{r}'} + \frac{\partial^2 S_\alpha}{\partial \boldsymbol{r}\partial \boldsymbol{p}}\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{r}'} - \frac{\partial \boldsymbol{p}}{\partial \boldsymbol{r}}\frac{\partial^2 S_\beta}{\partial \boldsymbol{p}\partial \boldsymbol{r}'} + \frac{\partial S_{\alpha\beta}}{\partial \boldsymbol{p}}\frac{\partial^2 \boldsymbol{p}}{\partial \boldsymbol{r}\partial \boldsymbol{r}'}\bigg|_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})}. \tag{50}$$

In view of (11), the last term in (50) vanishes. As mentioned above, substitution of the function $\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})$ for $\boldsymbol{p}$ reduces (11) to an identity. First, differentiate this identity with respect to $\boldsymbol{r}$

$$\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{r}}\frac{\partial^2 S_{\alpha\beta}}{\partial p^2} + \frac{\partial^2 S_\alpha}{\partial \boldsymbol{r}\partial \boldsymbol{p}}\bigg|_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})} = 0 \tag{51}$$

and then, with respect to $\boldsymbol{r}'$,

$$\frac{\partial^2 S_{\alpha\beta}}{\partial p^2}\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{r}'} - \frac{\partial^2 S_\beta}{\partial \boldsymbol{p}\partial \boldsymbol{r}'}\bigg|_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})} = 0. \tag{52}$$

Using (51) and (52), we reduce (50) to

$$\frac{\partial^2 \tilde{S}_{\alpha\beta}}{\partial \boldsymbol{r}\partial \boldsymbol{r}'} = -\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{r}}\frac{\partial^2 S_{\alpha\beta}}{\partial p^2}\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{r}'}\bigg|_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})}. \tag{53}$$

In addition, from (51) and (52) we obtain

$$\frac{\partial \boldsymbol{p}_{\alpha\beta}}{\partial \boldsymbol{r}} = -\frac{\partial^2 S_\alpha}{\partial \boldsymbol{r}\partial \boldsymbol{p}}\left(\frac{\partial^2 S_{\alpha\beta}}{\partial p^2}\right)^{-1}\bigg|_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})} \qquad \frac{\partial \boldsymbol{p}_{\alpha\beta}}{\partial \boldsymbol{r}'} = \left(\frac{\partial^2 S_{\alpha\beta}}{\partial p^2}\right)^{-1}\frac{\partial^2 S_\beta}{\partial \boldsymbol{p}\partial \boldsymbol{r}'}\bigg|_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})}. \tag{54}$$

Substituting the derivatives (54) into (53), we get

$$\frac{\partial^2 \tilde{S}_{\alpha\beta}}{\partial \boldsymbol{r}\partial \boldsymbol{r}'} = \frac{\partial^2 S_\alpha}{\partial \boldsymbol{r}\partial \boldsymbol{p}}\left(\frac{\partial^2 S_{\alpha\beta}}{\partial p^2}\right)^{-1}\frac{\partial^2 S_\beta}{\partial \boldsymbol{p}\partial \boldsymbol{r}'}\bigg|_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})}. \tag{55}$$

Finally substituting (55) into the right-hand side of (49), we obtain

$$\left|\det \frac{\partial^2 \tilde{S}_{\alpha\beta}(\boldsymbol{r}, t, \boldsymbol{r}', t')}{\partial \boldsymbol{r}\partial \boldsymbol{r}'}\right|^{1/2} = \left|\det \frac{\partial^2 S_\alpha}{\partial \boldsymbol{r}\partial \boldsymbol{p}}\right|^{1/2}\left|\det \frac{\partial^2 S_{\alpha\beta}}{\partial p^2}\right|^{-1/2}\left|\det \frac{\partial^2 S_\beta}{\partial \boldsymbol{p}\partial \boldsymbol{r}'}\right|^{1/2}_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})}. \tag{56}$$

To conclude the proof, it remains to note that the Jakobian $\det \partial \boldsymbol{q}_\alpha/\partial \boldsymbol{r} = \det \frac{\partial^2 S_\alpha}{\partial \boldsymbol{p}\partial \boldsymbol{r}}$ satisfies the continuity equation (9) (lemma 5.1, part II in the book by Maslov (1988)) and therefore we have

$$a_\alpha(\boldsymbol{p}, \boldsymbol{r}) = \left|\det \frac{\partial^2 S_\alpha}{\partial \boldsymbol{p}\partial \boldsymbol{r}}\right|^{1/2}. \tag{57}$$

Thus, from (43) we get simple explicit expressions for the amplitudes (57). These expressions coincide with the results of direct integration of equation (9) (Kunikeev and Senashenko 1996). As $\xi \to \infty$, the amplitudes (57) have the following asymptotic behaviour: $a_+(\boldsymbol{p}, \boldsymbol{r}) \to 1$ and $a_-(\boldsymbol{p}, \boldsymbol{r}|Z|/(p\xi)$.

Equation (49) may by viewed as an abbreviated representation of the amplitude $a_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau)$, but equation (56) is its detailed form. In order to evaluate $a_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau)$ it remains to obtain an explicit expression for det $\frac{\partial^2 S_{\alpha\beta}}{\partial p^2}$. Again differentiating equation (12) with respect to $\boldsymbol{p}$, we get

$$\frac{\partial^2 S_{\alpha\beta}}{\partial p_i \partial p_j} = -\delta_{ij}\tau + \frac{1}{2p}\left(\delta_{ij} - \frac{p_i p_j}{p^2}\right)((w_\alpha - 1)r - (w'_\beta - 1)r') - \frac{Z}{p^3}\left(\frac{h_i h_j}{w_\alpha} - \frac{h'_i h'_j}{w'_\beta}\right)$$
$$+\frac{Z}{p^3}\left(\delta_{ij} - \frac{3p_i p_j}{p^2}\right)\ln\frac{w_\alpha - 1}{w_\alpha + 1}\frac{w'_\beta + 1}{w'_\beta - 1} \tag{58}$$

where

$$h_i = \left(\frac{p_i}{p}(2+\cos\theta) + \frac{r_i}{r}\right)\Big/ (1+\cos\theta) \; h'_i = \left(\frac{p_i}{p}(2+\cos\theta') + \frac{r'_i}{r'}\right)\Big/ (1+\cos\theta').$$

Expressing the logarithmic term from (13) and substituting it in (58), we obtain at the stationary phase point

$$\left.\frac{\partial^2 S_{\alpha\beta}}{\partial p_i \partial p_j}\right|_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})} = -\frac{3p_i p_j}{p^2}\tau + \left(\delta_{ij} - \frac{3p_i p_j}{p^2}\right)(r'\cos\theta' - r\cos\theta)/p$$
$$+\frac{w_\alpha - 1}{2p}r\left(-\delta_{ij}\cos\theta + \frac{p_i p_j}{p^2}(3\cos\theta + 2)\right) - \frac{w'_\beta - 1}{2p}r'$$
$$\times\left(-\delta_{ij}\cos\theta' + \frac{p_i p_j}{p^2}(3\cos\theta' + 2)\right)$$
$$+\left.\frac{Z}{p^3}\left(\frac{h'_i h'_j}{w'_\beta} - \frac{h_i h_j}{w_\alpha}\right)\right|_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})}. \tag{59}$$

Choose the system of coordinates such that $\boldsymbol{p}_{\alpha\beta} = (0, 0, p_{\alpha\beta})$ and $\boldsymbol{r} = (r\sin\theta, 0, r\cos\theta)$, $\boldsymbol{r}' = (\pm r'\sin\theta', 0, r'\cos\theta')$, where the upper sign corresponds to the (+, +) and (−, −) equations and the lower sign to the (+, −) and (−, +) equations (see section 2.1). In such a system of coordinates we have

$$\left(\frac{\partial^2 S_{\alpha\beta}}{\partial p_i \partial p_j}\right)_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})} = \begin{pmatrix} a_{11} & 0 & a_{13} \\ 0 & a_{22} & 0 \\ a_{13} & 0 & a_{33} \end{pmatrix}_{\boldsymbol{p}=\boldsymbol{p}_{\alpha\beta}(\boldsymbol{X})} \tag{60}$$

where

$$\begin{aligned}
a_{11} &= \frac{1}{2p}((w'_\beta + 1)r'\cos\theta' - (w_\alpha + 1)r\cos\theta) + \frac{Z}{p^3}\left(\frac{\tan^2(\theta'/2)}{w'_\beta} - \frac{\tan^2(\theta/2)}{w_\alpha}\right) \\
a_{22} &= \frac{1}{2p}((w'_\beta + 1)r'\cos\theta' - (w_\alpha + 1)r\cos\theta) \\
a_{33} &= -3\tau + (w_\alpha\xi - w'_\beta\xi' + \eta' - \eta)/p + \frac{4Z}{p^3}\left(\frac{1}{w'_\beta} - \frac{1}{w_\alpha}\right) \\
a_{13} &= \frac{2Z}{p^3}\left(\pm\frac{\tan(\theta'/2)}{w'_\beta} - \frac{\tan(\theta/2)}{w_\alpha}\right)
\end{aligned} \tag{61}$$

and

$$\det\left(\frac{\partial^2 S_{\alpha\beta}}{\partial p_i \partial p_j}\right)_{p=p_{\alpha\beta}(X)} = a_{22}(a_{11}a_{33} - a_{13}^2)|_{p=p_{\alpha\beta}(X)}. \tag{62}$$

From (60) the following eigenvalues of the matrix can be readily obtained:

$$\lambda_2 = a_{22} \qquad \lambda_{1,3} = \frac{a_{11} + a_{33} \pm \sqrt{(a_{11} - a_{33})^2 + 4a_{13}^2}}{2}. \tag{63}$$

The negative inertia index $\mu_{\alpha\beta}$ is a number of negative eigenvalues (63). Using (14) and (61), we can rewrite λ_2 in the form

$$\lambda_2 = \mp\frac{(w_\alpha + 1)r}{2p}\frac{\sin\delta}{\sin\theta'} \tag{64}$$

where the upper sign stands for solutions of the stationary phase equation lying in the angular sectors $\angle COB'$ and $\angle AOB$, while the lower sign is for $\angle AOB$ and $\angle A'OB'$ (figure 1). The sign of (64) is easily determined. Further, if the inequality $a_{11}a_{33} < a_{13}^2$ fulfils, then λ_1 and λ_3 have opposite signs. In the case $a_{11}a_{33} > a_{13}^2$, there are two possibilities: $\lambda_1 > 0$, $\lambda_3 > 0$, if $a_{11} + a_{33} > 0$ and $\lambda_1 < 0$, $\lambda_3 < 0$, if $a_{11} + a_{33} < 0$.

Thus, the WKB Coulomb propagator (10) is fully described. The algorithm of its calculation is as follows. First, one should seek all the stationary phase points in section 2.1. This task is essentially reduced to a numerical solution of the one-dimensional equation (29). Then, the action $\tilde{S}_{\alpha\beta}(\boldsymbol{r}, t, \boldsymbol{r}', t')$, the amplitude $a_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau)$, and the index $\mu_{\alpha\beta}$ are easily calculated with the help of equations (43), (48), (49), (56) and (61)–(64).

2.4. *The case* $\tau \to 0$

Let us demonstrate how the above equations work in the limiting case $\tau \to 0$. As $\tau \to 0$, a particle must move with greater velocities along a classical path in order to get from the point $\boldsymbol{r}'$ to $\boldsymbol{r}$ during the time τ. It is assumed that $\boldsymbol{r} \neq \boldsymbol{r}'$ are arbitrary but fixed points. Therefore, one should expect that the absolute value of the asymptotic momentum $|\boldsymbol{p}_{\alpha\beta}(\boldsymbol{r}, \boldsymbol{r}', \tau)| \to \infty$ as $\tau \to 0$. From (20) and (25) it follows that $p(\theta) \to \infty$ at $\theta \to \theta_1 = \gamma$ in $\angle B'OC$ or $\theta \to \theta_2 = \alpha + \delta$ in $\angle A'OC'$ for the (+, +) equation and at $\theta \to \theta_3 = 0$ or $\theta \to \theta_4 = \delta$ in $\angle AOB$ for the (+, −) or (−, +) equations, respectively. Note that the (−, −) equation is defined in such areas where $p(\theta)$ is finite and hence it does not give a contribution to the propagator as $\tau \to 0$.

We shall seek solutions to the stationary phase equation (29) in the neighbourhoods of points $\theta_1, \ldots, \theta_4$ where $p(\theta)$ takes large values. For example, from (20) near the point $\theta = \theta_1$ we get the following expansion for

$$p^2(\theta) \approx \frac{Z|\boldsymbol{r} - \boldsymbol{r}'|}{4rr'\sin(\delta/2)}\frac{(\cos\beta + 1)^2}{\sin(\gamma/2)\cos(\alpha/2)\sin\Delta\theta_1} \tag{65}$$

where $\theta = \theta_1 + \Delta\theta_1$, $\Delta\theta_1 \ll 1$. Neglecting the terms of order $O(p^{-2})$, equation (29) near the point $\theta = \theta_1$ can be reduced to

$$p(\theta)\tau - |\boldsymbol{r} - \boldsymbol{r}'| = 0. \tag{66}$$

Equation (66) has a solution if $\tau > 0$. Combining (65) and (66), we get

$$\Delta\theta_1 = \frac{Z\tau^2(|\boldsymbol{r} - \boldsymbol{r}'| + r' - r)^2}{4rr'|\boldsymbol{r} - \boldsymbol{r}'|^3\sin(\delta/2)\sin(\gamma/2)\cos(\alpha/2)} \qquad \tau > 0. \tag{67}$$

In the case $\tau < 0$, the $(+, +)$ equation has no solution near $\theta = \theta_1$. In contrast, we get a solution near the point θ_2 ($\theta = \theta_2 + \Delta\theta_2$):

$$\Delta\theta_2 = \frac{Z\tau^2(|\boldsymbol{r} - \boldsymbol{r}'| + r - r')^2}{4rr'|\boldsymbol{r} - \boldsymbol{r}'|^3 \sin(\delta/2)\sin(\alpha/2)\cos(\gamma/2)} \qquad \tau < 0. \tag{68}$$

Similarly, we have

$$\Delta\theta_3 = \left(\frac{\tau}{r + r'}\right)^2 \frac{Z\tan(\delta/2)}{r} \qquad \theta = \theta_3 + \Delta\theta_3 \qquad \tau > 0 \tag{69}$$

for the $(+, -)$ equation and

$$\Delta\theta_4 = \left(\frac{\tau}{r + r'}\right)^2 \frac{Z\tan(\delta/2)}{r'} \qquad \theta = \theta_4 - \Delta\theta_4 \qquad \tau < 0 \tag{70}$$

for the $(-, +)$ equation. Note that all the solutions (67)–(70) tends to zero as τ or $Z \to 0$. This asymptotic behaviour at $\tau \to 0$ is supported by numerical results presented in figure 2.

Substituting the above solutions into the matrix (60), one obtains

$$\left(\frac{\partial^2 S_{++}}{\partial p^2}\right)_{\tau\to 0} = \begin{pmatrix} -\tau & 0 & 0 \\ 0 & -\tau & 0 \\ 0 & 0 & -\tau \end{pmatrix} = -\tau E \tag{71}$$

$$\left(\frac{\partial^2 S_{+-}}{\partial p^2}\right)_{\substack{\tau\to 0\\ \tau>0}} = -\tau \begin{pmatrix} r/(r + r') & 0 & 0 \\ 0 & r/(r + r') & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{72}$$

$$\left(\frac{\partial^2 S_{-+}}{\partial p^2}\right)_{\substack{\tau\to 0\\ \tau<0}} = -\tau \begin{pmatrix} r'/(r + r') & 0 & 0 \\ 0 & r'/(r + r') & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{73}$$

From (71)–(73), we get

$$\begin{aligned} \mu_{++} &= \begin{cases} 3 & \text{if} \quad \tau > 0 \\ 0 & \text{if} \quad \tau < 0 \end{cases} \\ \mu_{+-} &= 3(\tau > 0) \qquad \mu_{-+} = 0(\tau < 0). \end{aligned} \tag{74}$$

Finally, substituting the above solutions into (10), we obtain in the limit $\tau \to 0$, $\tau > 0$ the well known expression for the free-particle propagator

$$K_{++}^{\mathrm{WKB}}(\boldsymbol{r}, \boldsymbol{r}', \tau)|_{\tau\to 0} = (2\pi \mathrm{i}\tau)^{-3/2} \exp\left(\mathrm{i}\frac{|\boldsymbol{r} - \boldsymbol{r}'|^2}{2\tau}\right) \tag{75}$$

and the term that corresponds to rescattering on the Coulombic centre

$$K_{+-}^{\mathrm{WKB}}(\boldsymbol{r}, \boldsymbol{r}', \tau)|_{\tau\to 0} = \frac{Z\tau^{1/2}}{(2\pi \mathrm{i})^{3/2} rr'(r + r')(1 + \cos\delta)} \exp\left(\mathrm{i}\frac{(r + r')^2}{2\tau}\right). \tag{76}$$

As is seen, the first term is leading and the rescattering term vanishes as $\tau \to 0$. In the case $\tau \to 0$, $\tau < 0$, we must evidently obtain the same two contributions, with the exception of the rescattering term K_{-+}^{WKB} that must appear instead of K_{+-}^{WKB}.

3. The three-body continuum state

Consider the system of three charged particles into continuum: the ejected electron (e) moving in the combined field of the scattered ion (p) and the recoil target ion (t). The three-body continuum state derived by Kunikeev (1999a, b) is

$$\begin{aligned} \Psi^- &= \Psi^-_{\alpha=+} + \Psi^-_{\alpha=-} \\ \Psi^-_\alpha &= \exp(\mathrm{i}\boldsymbol{k}_t\boldsymbol{r}_t + \mathrm{i}\boldsymbol{K}_p\boldsymbol{R}_p) F^-_{p\alpha}(\boldsymbol{k}_p, \boldsymbol{r}_p) F^-_N(\boldsymbol{R}(t)) F^-_\alpha(\boldsymbol{r}_t, \boldsymbol{R}(t)) \end{aligned} \tag{77}$$

where $\exp(\cdots)$ is a three-body plane wave, $F_{p\alpha}^{-}$ is the continuum distortion function due to electron–projectile interaction into the unscattered ($\alpha = +$) or scattered ($\alpha = -$) parts of the Coulomb wave satisfying incoming boundary conditions, and F_N^{-} denotes the phase factor due to internuclear interaction; $\boldsymbol{r}_t$, $\boldsymbol{r}_p$ are electronic coordinates with respect to target and projectile ions, $\boldsymbol{k}_t$, $\boldsymbol{k}_p$ are their corresponding momenta and $\boldsymbol{R}(t)$ is a time-dependent radius vector specifying the relative position of the ions. For the distortion function F_α^{-}, the following asymptotic expansion near the target nucleus ($r_t/R \ll 1$) is derived:

$$F_\alpha^{-}(\boldsymbol{r}_t, t) = \exp\left(- \mathrm{i}\boldsymbol{k}_\alpha(t)\boldsymbol{r}_t + \mathrm{i}\int_{t_0}^{t} \mathrm{d}\tau\, k_\alpha^2(\tau)/2\right) K^{(N)}(t, t_0)\psi^{-}(\boldsymbol{k}_\alpha(t_0), \boldsymbol{r}_t) \tag{78}$$

where the first factor $\exp(\cdots)$ represents the Volkov–Keldysh state (Keldysh 1965) which describes the motion of the unbound electron with definite value of momentum $-\boldsymbol{k}_t$ in the time-dependent field $\boldsymbol{E}_{p\alpha}(t) = \dot{\boldsymbol{k}}_{p\alpha}(t)$ produced by the projectile ion, while the second one, $K^{(N)}(t, t_0)\psi^{-}(\boldsymbol{k}_\alpha(t_0), \boldsymbol{r}_t)$, is due to virtual transitions of the ejected electron in the Coulomb field of the target ion induced by a series of δ-function impulses from an external time-dependent field of the projectile ion. Here, $K^{(N)}(t, t_0)$ is the propagator (2) that evolves the initial state, the Coulomb wave $\psi^{-}(\boldsymbol{k}_\alpha(t_0), \boldsymbol{r}_t)$, from an initial moment t_0 up to t. The phase function in (2) takes the form: $\Delta\Phi_{\mathrm{ext}}(\boldsymbol{r}_t, t_i) = (\boldsymbol{k}_\alpha(t_{i+1}) - \boldsymbol{k}_\alpha(t_i))\boldsymbol{r}_t = \Delta\boldsymbol{k}_\alpha(t_i)\boldsymbol{r}_t$, where $\boldsymbol{k}_\alpha(t) = \boldsymbol{k}_t + \boldsymbol{k}_{p\alpha}(t)$ is an effective electron momentum modified by the projectile's field.

Let us first examine the effect of one kick on the continuum state $\psi^{-}(\boldsymbol{k}_0, \boldsymbol{r})$. In the WKB approximation (10), we have

$$K^{(1)}(t_1, t_0)\psi^{-} = (-2\pi\mathrm{i})^{-3/2} \sum_{\alpha_1,\beta_1,\alpha_0} \int \mathrm{d}\boldsymbol{r}'\, a_{\alpha_1\beta_1}(\boldsymbol{r}, \boldsymbol{r}', \tau = t_1 - t_0) a_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}') \\ \times \exp\left(\mathrm{i}\tilde{S}_{\alpha_1\beta_1}(\boldsymbol{r}, \boldsymbol{r}', \tau) + \mathrm{i}\Delta\boldsymbol{k}\boldsymbol{r}' + \mathrm{i}S_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}') - \mathrm{i}\frac{\pi}{2}\mu_{\alpha_1\beta_1}\right) \tag{79}$$

where $\boldsymbol{k}_0 = \boldsymbol{k}_\alpha(t_0)$, $\Delta\boldsymbol{k} = \boldsymbol{k}_\alpha(t_1) - \boldsymbol{k}_\alpha(t_0)$ and the Coulomb wave is written as

$$\psi^{-}(\boldsymbol{k}_0, \boldsymbol{r}) = \sum_{\alpha_0=\pm} \psi_{\alpha_0}^{-}(\boldsymbol{k}_0, \boldsymbol{r}) = \sum_{\alpha_0=\pm} a_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}) \exp(\mathrm{i}S_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}')).$$

It is assumed that the indices α_1, β_1 in (79) take such values at which the WKB contributions to the Coulomb propagator are not negligible at the given parameters $\boldsymbol{r}$, $\boldsymbol{r}'$, τ. Using the stationary phase approximation, we can reduce the integral (79) to a sum over contributions from the stationary phase points

$$K^{(1)}(t_1, t_0)\psi^{-} = \sum_{\alpha_1,\beta_1,\alpha_0,k} A_{\alpha_1\beta_1\alpha_0}(\boldsymbol{r}, \boldsymbol{r}', \tau) \\ \times \exp\left(\mathrm{i}\tilde{S}_{\alpha_1\beta_1}(\boldsymbol{r}, \boldsymbol{r}', \tau) + \mathrm{i}\Delta\boldsymbol{k}\boldsymbol{r}' + \mathrm{i}S_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}') - \mathrm{i}\frac{\pi}{2}\mu_c\right)\bigg|_{\boldsymbol{r}'=\boldsymbol{r}_k'(\boldsymbol{r},\tau)}. \tag{80}$$

Here, the amplitude is

$$A_{\alpha_1\beta_1\alpha_0}(\boldsymbol{r}, \boldsymbol{r}', \tau) = a_{\alpha_1\beta_1}(\boldsymbol{r}, \boldsymbol{r}', \tau) a_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}') |\det D(\boldsymbol{r}, \boldsymbol{r}', \tau)|^{-1/2}$$

and the index $\mu_c = \mu_{\alpha_1\beta_1} + \mu_k + 1 (\mathrm{mod}\, 4)$, where $\mu_k = \mathrm{inerdex} D$ is a negative inertia index of the matrix

$$D(\boldsymbol{r}, \boldsymbol{r}', \tau)|_{\boldsymbol{r}'=\boldsymbol{r}_k'(\boldsymbol{r},\tau)} = \left.\frac{\partial^2(\tilde{S}_{\alpha_1\beta_1}(\boldsymbol{r}, \boldsymbol{r}', \tau) + S_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}'))}{\partial \boldsymbol{r}'^2}\right|_{\boldsymbol{r}'=\boldsymbol{r}_k'(\boldsymbol{r},\tau)}.$$

3.1. The stationary phase equation

The equation defining the stationary phase points $\boldsymbol{r}'_k(\boldsymbol{r}, \tau)$ is

$$\nabla_{\boldsymbol{r}'}(\tilde{S}_{\alpha_1\beta_1}(\boldsymbol{r}, \boldsymbol{r}', \tau) + S_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}')) + \Delta\boldsymbol{k} = 0. \tag{81}$$

In view of (11) and (47), we can rewrite (81) in the form

$$\nabla_{\boldsymbol{r}'} S_{\beta_1}(\boldsymbol{p}_{\alpha_1\beta_1}(\boldsymbol{r}, \boldsymbol{r}', \tau), \boldsymbol{r}') = \Delta\boldsymbol{k} + \nabla_{\boldsymbol{r}'} S_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}') \tag{82}$$

which represents the momentum conservation law. In fact, the right-hand side of (82) is an initial distribution of the electron momentum just after the kick at moment $t = t_0$. Between the kicks, the system evolves according to the WKB Coulomb propagator so that the electron moving along a hyperbolic path connecting the points $\boldsymbol{r}'$ and $\boldsymbol{r}$ has the initial momentum $\boldsymbol{p}_i(\boldsymbol{r}, \boldsymbol{r}', \tau) = \nabla_{\boldsymbol{r}'} S_{\beta_1}(\boldsymbol{p}_{\alpha_1\beta_1}(\boldsymbol{r}, \boldsymbol{r}', \tau), \boldsymbol{r}')$ at point $\boldsymbol{r}'$ at moment t_0 and the final momentum $\boldsymbol{p}_f(\boldsymbol{r}, \boldsymbol{r}', \tau) = \nabla_{\boldsymbol{r}} S_{\alpha_1}(\boldsymbol{p}_{\alpha_1\beta_1}(\boldsymbol{r}, \boldsymbol{r}', \tau), \boldsymbol{r})$ at point $\boldsymbol{r}$ at moment t_1. Thus, equation (82) tells us that one should seek the points $\boldsymbol{r}'$ at which the initial momentum $\boldsymbol{p}_i$ matches the momentum of the electron just after the kick at moment $t = t_0$.

On the other side, we can easily solve the reverse task, namely, find the reverse function $\boldsymbol{r}(\boldsymbol{r}', \tau)$. Indeed, let a particle have an initial momentum $\boldsymbol{p}_i$, the right-hand side of (82), at point $\boldsymbol{r}'$. Equation (39) defines a two-valued map of the asymptotic momentum $\boldsymbol{p} = \boldsymbol{p}_0$ into the momenta $\boldsymbol{p}_{\alpha=\pm}(\boldsymbol{p}_0, \boldsymbol{r})$ at each point $\boldsymbol{r}$. Our task is the reverse, that is, to determine $\boldsymbol{p}_0$ if the momentum $\boldsymbol{p} = \boldsymbol{p}_i$ is known at point $\boldsymbol{r} = \boldsymbol{r}'$. The absolute value of $\boldsymbol{p}_0$ is readily obtained from the energy conservation law

$$p_0/p = a(p, r) = \sqrt{1 - 2Z/(p^2 r)} \qquad 0 < a < 1. \tag{83}$$

From (39) we get

$$2x = a\left(-1 + x_0 \pm \sqrt{(1 + x_0)^2 + \frac{4Z}{p_0^2 r}(1 + x_0)}\right) \tag{84}$$

where $x_0 = \hat{\boldsymbol{p}}_0 \cdot \hat{\boldsymbol{r}}$, $x = \hat{\boldsymbol{p}} \cdot \hat{\boldsymbol{r}}$, $|x_0| \leqslant 1$, $|x| \leqslant 1$. Solving (84) for x_0, we obtain

$$x_0 = \frac{(x + a)^2 + x^2 - 1}{(x + a)^2 + 1 - x^2}. \tag{85}$$

It can be easily checked that (85) is a solution of the (+) or (−) equation (84) if $-a < x \leqslant 1$ or $-1 \leqslant x < -a$, respectively. At the boundary point $x = -a$, we obtain from (85) that $x_0 = -1$ and $\boldsymbol{r}$ locates at a caustics point. Thus, we have a single-valued map $\hat{p}_{\mathrm{as}}$: $\boldsymbol{p} \to \boldsymbol{p}_0$ that depends on the direction of $\boldsymbol{p}$ relative to $\boldsymbol{r}$ and the value a. This map enables us to construct a vector field $\boldsymbol{p}_\alpha(\boldsymbol{p}_0, \boldsymbol{r}) = \nabla_{\boldsymbol{r}} S_\alpha(\boldsymbol{p}_0, \boldsymbol{r}, t)$, where the sign $\alpha = \pm$ is uniquely defined by the condition $-a < x \leqslant 1$ or $-1 \leqslant x < -a$ in (85), so that $\boldsymbol{p}_\alpha(\boldsymbol{p}_0, \boldsymbol{r}') = \boldsymbol{p}_i$. Moreover, from the equation $\boldsymbol{q}_0 = \nabla_{\boldsymbol{p}} S_\alpha(\boldsymbol{p}_0, \boldsymbol{r}, t)$, where $\boldsymbol{q}_0 = \nabla_{\boldsymbol{p}} S_\alpha(\boldsymbol{p}_0, \boldsymbol{r}', t_0)$, we obtain the classical trajectory $\boldsymbol{r}_\alpha(\boldsymbol{q}_0, \boldsymbol{p}_0, t)$ (see section 2.2) such that $\boldsymbol{r}_\alpha(\boldsymbol{q}_0, \boldsymbol{p}_0, t_0) = \boldsymbol{r}'$, $\boldsymbol{r}_\alpha(\boldsymbol{q}_0, \boldsymbol{p}_0, t_1) = \boldsymbol{r}$ $(\tau = t_1 - t_0)$ and $\dot{\boldsymbol{r}}_\alpha(\boldsymbol{q}_0, \boldsymbol{p}_0, t_0) = \boldsymbol{p}_i$. It is obvious that for these points $\boldsymbol{r}'$ and $\boldsymbol{r}$ lying on the trajectory and for the difference of time τ the asymptotic momentum $\boldsymbol{p}_0$ obtained under the map $\hat{p}_{\mathrm{as}}$: $\boldsymbol{p}_i \to \boldsymbol{p}_0$ represents at the same time a solution of the stationary phase equation (12): $\boldsymbol{p}_{\alpha\beta}(\boldsymbol{r}(\boldsymbol{r}', \tau), \boldsymbol{r}', \tau) \equiv \boldsymbol{p}_0(\boldsymbol{r}')$. At small perturbations $\Delta\boldsymbol{k}$, we obtain the following expansion for

$$\boldsymbol{p}_0(\boldsymbol{r}') = \boldsymbol{k}_0 + \left(\frac{\partial^2 S_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}')}{\partial \boldsymbol{r}' \partial \boldsymbol{k}_0}\right)^{-1} \Delta\boldsymbol{k}. \tag{86}$$

We underscore the fact that the map $\hat{p}_{\mathrm{as}}$: $\boldsymbol{p}_i \to \boldsymbol{p}_0$ is well defined only if the kinetic energy $p_i^2/2$ is larger than the absolute value of the potential energy $V_c(\boldsymbol{r}')$. There exists a perturbation $\Delta\boldsymbol{k}$ at which

$$p_i^2/2 < |V_c(\boldsymbol{r}')|. \tag{87}$$

In this case, an electron makes a transition to a bound state under the influence of the momentum kick and its motion becomes finite. Let us determine the conditions imposed on $\Delta\boldsymbol{k}$ under which (87) is fulfilled. Substituting the right-hand side of (82) into (87), we obtain

$$\Delta k^2 + 2\Delta k k_0 \cos\theta_{\Delta\boldsymbol{k}} \sqrt{1 + \frac{|V_c(\boldsymbol{r}')|}{k_0^2/2}} + k_0^2 < 0 \tag{88}$$

where $\cos\theta_{\Delta\boldsymbol{k}} = \Delta\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{k}}_{\alpha_0}$ and $\boldsymbol{k}_{\alpha_0} = \nabla_{\boldsymbol{r}'} S_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}')$. The discriminant of the quadratic equation is

$$D = k_0^2 \left(\frac{\cos^2\theta_{\Delta\boldsymbol{k}}}{\cos^2\theta_c} - 1 \right)$$

where

$$\cos\theta_c = -\sqrt{\frac{k_0^2/2}{k_0^2/2 + |V_c(\boldsymbol{r}')|}}.$$

It follows that $D > 0$ if $\cos^2\theta_{\Delta\boldsymbol{k}} > \cos^2\theta_c$. The roots of the quadratic equation are

$$\Delta k_{1,2} = k_0 \left(\frac{\cos\theta_{\Delta\boldsymbol{k}}}{\cos\theta_c} \pm \sqrt{\frac{\cos^2\theta_{\Delta\boldsymbol{k}}}{\cos^2\theta_c} - 1} \right).$$

Thus we have $\Delta k_{1,2} > 0$ if $\cos\theta_{\Delta\boldsymbol{k}} < 0$ and (88) is fulfilled if

$$\Delta k_1 < \Delta k < \Delta k_2 \qquad \text{and} \qquad \theta_c < \theta_{\Delta\boldsymbol{k}} < \pi. \tag{89}$$

Note that at high energies $k_0^2/2 \gg |V_c(\boldsymbol{r}')|$ we have $\theta_c \to \pi$. In this case, it is highly unlikely that inequality (87) will be fulfilled.

Using this method, we can basically construct the function $\boldsymbol{r}(\boldsymbol{r}', \tau)$ defined at each point where (87) does not fulfil. Suppose that from this function we can also derive reverse function or functions $\boldsymbol{r}'_k(\boldsymbol{r}, \tau)$ in case where several points $\boldsymbol{r}'_k$ are related to the given point $\boldsymbol{r}$.

3.2. *The amplitude $A_{\alpha_1\beta_1\alpha_0}$*

Substituting the function $\boldsymbol{r}'_k(\boldsymbol{r}, \tau)$ into (81) reduces it to an identity. Differentiating this identity with respect to $\boldsymbol{r}$ gives

$$D(\boldsymbol{r}, \boldsymbol{r}'_k, \tau) \frac{\partial \boldsymbol{r}'_k}{\partial \boldsymbol{r}} = \frac{\partial^2 S_{\beta_1}}{\partial \boldsymbol{r}'_k \partial \boldsymbol{p}_{\alpha_1\beta_1}} \frac{\partial \boldsymbol{p}_{\alpha_1\beta_1}}{\partial \boldsymbol{r}}. \tag{90}$$

Combining (54) and (90), we get

$$\begin{aligned} D(\boldsymbol{r}, \boldsymbol{r}'_k, \tau) &= -\frac{\partial^2 S_{\beta_1}}{\partial \boldsymbol{r}' \partial \boldsymbol{p}} \left(\frac{\partial^2 S_{\alpha_1\beta_1}}{\partial p^2} \right)^{-1} \frac{\partial^2 S_{\alpha_1}}{\partial \boldsymbol{p} \partial \boldsymbol{r}} \left(\frac{\partial \boldsymbol{r}'}{\partial \boldsymbol{r}} \right)^{-1} \Bigg|_{\boldsymbol{p}=\boldsymbol{p}_{\alpha_1\beta_1}, \boldsymbol{r}'=\boldsymbol{r}'_k(\boldsymbol{r},\tau)} \\ &= -\frac{\partial^2 \tilde{S}_{\alpha_1\beta_1}}{\partial \boldsymbol{r}' \partial \boldsymbol{r}} \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{r}'} \Bigg|_{\boldsymbol{r}'=\boldsymbol{r}'_k(\boldsymbol{r},\tau)} \end{aligned} \tag{91}$$

where $\frac{\partial^2 \tilde{S}_{\alpha_1\beta_1}}{\partial \boldsymbol{r}' \partial \boldsymbol{r}}$ is a transpose of the matrix (55). Thus, from (49) and (91) we obtain

$$A_{\alpha_1\beta_1\alpha_0}(\boldsymbol{r}, \boldsymbol{r}'_k, \tau) = \left| \det \frac{\partial \boldsymbol{r}'_k}{\partial \boldsymbol{r}} \right|^{1/2} a_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}'_k). \tag{92}$$

Using the continuity equation (9) and the Gauss theorem, one can easily derive the relationship

$$\left| \det \frac{\partial \boldsymbol{r}'_k}{\partial \boldsymbol{r}} \right| = \frac{a_{\alpha_1}^2(\boldsymbol{p}_{\alpha_1\beta_1}, \boldsymbol{r})}{a_{\beta_1}^2(\boldsymbol{p}_{\alpha_1\beta_1}, \boldsymbol{r}'_k)} \tag{93}$$

which is also valid in the case where a path connecting the points $\boldsymbol{r}'_k$ and $\boldsymbol{r}$ intersects the caustics line. Therefore, equation (92) may be cast as

$$A_{\alpha_1\beta_1\alpha_0}(\boldsymbol{r}, \boldsymbol{r}'_k, \tau) = a_{\alpha_1}(\boldsymbol{p}_{\alpha_1\beta_1}, \boldsymbol{r}) \frac{a_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}'_k)}{a_{\beta_1}(\boldsymbol{p}_{\alpha_1\beta_1}, \boldsymbol{r}'_k)}. \tag{94}$$

3.3. The index μ_c

It remains to evaluate the index μ_c in (80). We can assume without loss of generality that the time interval τ is sufficiently small so that the initial and final points $\boldsymbol{r}'_k$ and $\boldsymbol{r}$ of a path are close to each other. Consider first the simpler case $\alpha_1 = \beta_1$, where a path does not contain caustics points. At small τ and $\Delta\boldsymbol{r} = \boldsymbol{r} - \boldsymbol{r}'_k$, we can develop the function $\frac{\partial^2 S_{\alpha\alpha}}{\partial p^2}$ as

$$\frac{\partial^2 S_{\alpha\alpha}}{\partial p^2} \approx \tau \left(-E + \left(\frac{\Delta \boldsymbol{r}}{\tau} \cdot \nabla_{r'} \right) \frac{\partial^2 S_\alpha(\boldsymbol{p}, \boldsymbol{r}')}{\partial p^2} \right). \tag{95}$$

Furthermore, putting $\Delta\boldsymbol{r}/\tau \approx \partial S_\alpha(\boldsymbol{p}, \boldsymbol{r}')/\partial \boldsymbol{r}'$, we rewrite (95) in the form

$$\frac{\partial^2 S_{\alpha\alpha}}{\partial p_i \partial p_j} = \tau \left(-\delta_{ij} + \frac{\partial}{\partial p_i} \left(\frac{\partial S_\alpha(\boldsymbol{p}, \boldsymbol{r}')}{\partial r'_k} \frac{\partial^2 S_\alpha(\boldsymbol{p}, \boldsymbol{r}')}{\partial r'_k \partial p_j} \right) - \frac{\partial^2 S_\alpha(\boldsymbol{p}, \boldsymbol{r}')}{\partial p_i \partial r'_k} \frac{\partial^2 S_\alpha(\boldsymbol{p}, \boldsymbol{r}')}{\partial r'_k \partial p_j} \right). \tag{96}$$

Differentiating the Hamilton–Jakobi equation (7) with respect to p_j, we obtain the relationship

$$\frac{\partial S_\alpha(\boldsymbol{p}, \boldsymbol{r}')}{\partial r'_k} \frac{\partial^2 S_\alpha(\boldsymbol{p}, \boldsymbol{r}')}{\partial r'_k \partial p_j} = p_j. \tag{97}$$

Substituting (97) into (96), we get

$$\frac{\partial^2 S_{\alpha\alpha}}{\partial p^2} = -\tau A^\top A \tag{98}$$

where

$$A = \frac{\partial^2 S_\alpha(\boldsymbol{p}, \boldsymbol{r}')}{\partial \boldsymbol{r}' \partial \boldsymbol{p}}$$

and $A^\top$ is a transpose of the matrix A. From (98) we easily get

$$\mu_{\alpha\alpha} = \begin{cases} 0 & \text{if} \quad \tau < 0 \\ 3 & \text{if} \quad \tau > 0 \end{cases} \tag{99}$$

since the quadratic form $(\boldsymbol{x}, A^\top A\boldsymbol{x}) = (A\boldsymbol{x}, A\boldsymbol{x})$ is positively defined. Substituting (98) into (91), we obtain

$$D = \frac{1}{\tau} \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{r}'} \tag{100}$$

where

$$\frac{\partial \boldsymbol{r}}{\partial \boldsymbol{r}'} \approx E + \tau \frac{\partial^2 S_\alpha(\boldsymbol{p}, \boldsymbol{r}')}{\partial \boldsymbol{r}'^2}. \tag{101}$$

The second term in (101) can be neglected at small τ since $\partial^2 S_\alpha/\partial \boldsymbol{r}'^2$ is a smooth matrix function in the case where a path does not contain caustics points. Then, from (100) and (101) we get

$$\mu_k = \begin{cases} 3 & \text{if} \quad \tau < 0 \\ 0 & \text{if} \quad \tau > 0 \end{cases} \tag{102}$$

and the index $\mu_c = 0 \pmod 4$.

Suppose now that a path contains a caustics point. Choosing the system of coordinates such that $\hat{\boldsymbol{p}} = (0, 0, 1)$, $\hat{\boldsymbol{r}} = (\alpha \sin\theta, 0, \cos\theta)$, and $\hat{\boldsymbol{r}}' = (\beta \sin\theta', 0, \cos\theta')$, we obtain near the caustics point (at $\theta = \pi - \Delta\theta$, $\theta' = \pi - \Delta\theta'$, $\Delta\theta, \Delta\theta' \ll 1$) the following expression:

$$\frac{\partial^2 S_{\alpha\beta}}{\partial p^2} = -\tau \begin{pmatrix} (a^2+1)/4 & 0 & -a/2 \\ 0 & -a^2/\Delta\theta\Delta\theta' & 0 \\ -a/2 & 0 & 1 \end{pmatrix} \tag{103}$$

where $a = (\sqrt{2Z/r})/p$ and $(\alpha, \beta) = (+1, -1)$ at $\tau > 0$ and $(\alpha, \beta) = (-1, +1)$ at $\tau < 0$. In deriving (103) the relations $r' - r = p\tau$ and $r\Delta\theta + r'\Delta\theta' = ap|\tau|$ following from equation (44) have been used. From (103) we readily obtain $\mu_{+-} = 2$ and $\mu_{-+} = 1$. Further, from (42) we get the following expressions for

$$\frac{\partial^2 S_+}{\partial \boldsymbol{p} \partial \boldsymbol{r}} = \begin{pmatrix} 1/2 & 0 & -a/2 \\ 0 & a/\Delta\theta & 0 \\ -\Delta\theta/2 & 0 & 1 \end{pmatrix} \tag{104}$$

and

$$\frac{\partial^2 S_-}{\partial \boldsymbol{r}' \partial \boldsymbol{p}} = \begin{pmatrix} 1/2 & 0 & \Delta\theta'/2 \\ 0 & -a/\Delta\theta' & 0 \\ -a/2 & 0 & 1 \end{pmatrix} \tag{105}$$

near the caustics point. Multiplying together all the matrices, we get

$$\frac{\partial^2 \tilde{S}_{+-}}{\partial \boldsymbol{r}' \partial \boldsymbol{r}} = \frac{\partial^2 S_-}{\partial \boldsymbol{r}' \partial \boldsymbol{p}} \left(\frac{\partial^2 S_{+-}}{\partial p^2} \right)^{-1} \frac{\partial^2 S_+}{\partial \boldsymbol{p} \partial \boldsymbol{r}} = -\frac{1}{\tau} E \qquad \tau > 0. \tag{106}$$

The same result is obtained in the $(-, +)$ case:

$$\frac{\partial^2 \tilde{S}_{-+}}{\partial \boldsymbol{r}' \partial \boldsymbol{r}} = -\frac{1}{\tau} E \qquad \tau < 0. \tag{107}$$

Thus, from (91), (106) and (107) we have

$$\mu_k = \begin{cases} \text{inerdex}(\partial \boldsymbol{r}/\partial \boldsymbol{r}') & \tau > 0 \\ 3 - \text{inerdex}(\partial \boldsymbol{r}/\partial \boldsymbol{r}') & \tau < 0. \end{cases} \tag{108}$$

The momenta $\boldsymbol{p}_\alpha(\boldsymbol{r})$ and $\boldsymbol{p}_\alpha(\boldsymbol{r} + \mathrm{d}\boldsymbol{r})$ given at close points $\boldsymbol{r}$ and $\boldsymbol{r} + \mathrm{d}\boldsymbol{r}$ are related by

$$\boldsymbol{p}_\alpha(\boldsymbol{r} + \mathrm{d}\boldsymbol{r}) - \boldsymbol{p}_\alpha(\boldsymbol{r}) = \frac{\partial^2 S_\alpha(\boldsymbol{p}, \boldsymbol{r})}{\partial \boldsymbol{r}^2} \, \mathrm{d}\boldsymbol{r}. \tag{109}$$

Divide both sides of (109) by the differential of time $\mathrm{d}t$. Then, the left-hand side of (109) will represent a force acting on a particle at point $\boldsymbol{r}$. Hence, we can write

$$\frac{\partial^2 S_\alpha(\boldsymbol{p}, \boldsymbol{r})}{\partial \boldsymbol{r}^2} \, \mathrm{d}\boldsymbol{r} = \frac{\partial^2 S_\beta(\boldsymbol{p}, \boldsymbol{r}')}{\partial \boldsymbol{r}'^2} \, \mathrm{d}\boldsymbol{r}' \tag{110}$$

since the force is assumed to be continuous near the caustics line. Making use of relation $\mathrm{d}\boldsymbol{r} = (\partial \boldsymbol{r}/\partial \boldsymbol{r}') \, \mathrm{d}\boldsymbol{r}'$, we obtain from (110) the following expression:

$$\frac{\partial \boldsymbol{r}}{\partial \boldsymbol{r}'} = \left(\frac{\partial^2 S_\alpha(\boldsymbol{p}, \boldsymbol{r})}{\partial \boldsymbol{r}^2} \right)^{-1} \frac{\partial^2 S_\beta(\boldsymbol{p}, \boldsymbol{r}')}{\partial \boldsymbol{r}'^2} \tag{111}$$

near the caustics line. Differentiating (39) with respect to $\boldsymbol{r}$, we get

$$\frac{\partial^2 S_\alpha}{\partial r_i \partial r_j} = -\frac{Z}{w_\alpha p \xi^2} \left(\frac{r_i}{r} + \frac{p_i}{p} \right) \left(\frac{r_j}{r} + \frac{p_j}{p} \right) + \frac{w_\alpha - 1}{2} \frac{p}{r} \left(\delta_{ij} - \frac{r_i r_j}{r^2} \right). \tag{112}$$

Choosing the system of coordinates such as in (103), we reduce the matrix (112) to

$$\frac{\partial^2 S_\alpha}{\partial r_i \partial r_j} = \begin{pmatrix} a_{11} & 0 & a_{13} \\ 0 & a_{22} & 0 \\ a_{13} & 0 & a_{33} \end{pmatrix} \tag{113}$$

where

$$a_{11} = -\frac{Z}{w_\alpha p r^2}\left(\frac{\sin\theta}{1+\cos\theta}\right)^2 + \frac{w_\alpha - 1}{2}\frac{p}{r}\cos^2\theta \qquad a_{22} = \frac{w_\alpha - 1}{2}\frac{p}{r}$$

$$a_{33} = -\frac{Z}{w_\alpha p r^2} + \frac{w_\alpha - 1}{2}\frac{p}{r}\sin^2\theta \qquad a_{13} = -\frac{\alpha Z}{w_\alpha p r^2}\frac{\sin\theta}{1+\cos\theta} - \alpha\frac{w_\alpha - 1}{2}\frac{p}{r}\sin\theta\cos\theta.$$

As above, we have near the caustics line

$$\frac{\partial^2 S_\alpha}{\partial r_i \partial r_j} = \frac{p}{r}\begin{pmatrix} -1/2 & 0 & a/2 \\ 0 & \alpha a/\Delta\theta & 0 \\ a/2 & 0 & 3\alpha a\Delta\theta/4 \end{pmatrix} \tag{114}$$

and

$$\frac{\partial^2 S_\beta}{\partial r'_i \partial r'_j} = \frac{p}{r'}\begin{pmatrix} -1/2 & 0 & a'/2 \\ 0 & \beta a'/\Delta\theta' & 0 \\ a'/2 & 0 & 3\beta a'\Delta\theta'/4 \end{pmatrix}. \tag{115}$$

Multiplying together the matrices, we get

$$\frac{\partial \boldsymbol{r}}{\partial \boldsymbol{r}'} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\Delta\theta/\Delta\theta' & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{116}$$

where we have set $r \to r'$ and $a = (\sqrt{2Z/r})/p \to a' = (\sqrt{2Z/r'})/p$ near the caustics line. Note that both equations (43) and (93), and equation (116), give the same result for $|\det(\partial\boldsymbol{r}/\partial\boldsymbol{r}')| = \Delta\theta/\Delta\theta'$ in the limit $\Delta\theta$, $\Delta\theta' \to 0$, $\Delta\theta/\Delta\theta' = \text{const}$. Further, from (108) and (116) we have

$$\mu_k = \begin{cases} 1 & \tau > 0 \\ 2 & \tau < 0 \end{cases} \tag{117}$$

and $\mu_c = 0\,(\mathrm{mod}\,4)$.

Summarizing, we can write equation (80) as

$$K^{(1)}(t_1, t_0)\psi^- = \sum_{\alpha_0, k}(\psi^-_{\alpha_1}(\boldsymbol{p}_0(\boldsymbol{r}'), \boldsymbol{r})/\psi^-_{\beta_1}(\boldsymbol{p}_0(\boldsymbol{r}'), \boldsymbol{r}'))\psi^-_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}')$$
$$\times \exp\left(-\mathrm{i}\frac{p_0^2(\boldsymbol{r}')}{2}\tau + \mathrm{i}\Delta\boldsymbol{k}\boldsymbol{r}'\right)\Bigg|_{\boldsymbol{r}'=\boldsymbol{r}'_k(\boldsymbol{r},\tau)}. \tag{118}$$

Here, $\boldsymbol{p}_0(\boldsymbol{r}') = \boldsymbol{p}_{\alpha_1\beta_1}(\boldsymbol{r}(\boldsymbol{r}', \tau), \boldsymbol{r}', \tau)$ is the asymptotic momentum defined by equations (83) and (85) under the map $\hat{p}_{\mathrm{as}}$: $\boldsymbol{p}_i(\boldsymbol{r}') \to \boldsymbol{p}_0(\boldsymbol{r}')$. The indices α_1 and β_1 are also determined by this map ($\beta_1 = \alpha_0$ at small $\Delta\boldsymbol{k}$); $\alpha_1 = \beta_1$ if the path connecting the points $\boldsymbol{r}$ and $\boldsymbol{r}'_k$ does not contain a caustics point and otherwise $\alpha_1 = -\beta_1$.

It is interesting to remark that equation (118) differs substantially from the corresponding one of the Maslov–Fedoriuk theory (1981) by a phase factor $\exp(-\mathrm{i}\pi\mu/2)$ where $\mu = \mathrm{inerdex}(\partial\boldsymbol{r}/\partial\boldsymbol{r}')$ is the Morse index of the path connecting the points $\boldsymbol{r}$ and $\boldsymbol{r}'$. This is because the propagator in Maslov's treatment (1988) is taken without the phase factor $\exp(-\mathrm{i}\pi\mu_{\alpha\beta}/2)$ at small τ. As is seen, the role of this factor appears to be essential since we obtain the index $\mu_c = 0\,(\mathrm{mod}\,4)$.

Let us consider the limiting behaviour of (118) as $\Delta\boldsymbol{k} \to 0$. In this limit, from (86) we obtain $\boldsymbol{p}_0(\boldsymbol{r}') = \boldsymbol{k}_0$ and $\beta_1 = \alpha_0$ and (118) reduces to

$$K^{(1)}(t_1, t_0)\psi^- = \sum_{\alpha_0, k}\psi^-_{\alpha_1}(\boldsymbol{k}_0, \boldsymbol{r})\exp\left(-\mathrm{i}\frac{k_0^2}{2}\tau\right). \tag{119}$$

By (44), near the caustics point ($r = r_c, \theta = \pi$) the perpendicular component of momentum $p_\perp$ is equal to $\sqrt{2Z/r_c}$. Denote by D_c the domain near the caustics line such that $D_c = \{\boldsymbol{r} = (r_\parallel, \boldsymbol{r}_\perp) : r_\parallel < 0, |\boldsymbol{r}_\perp| < r_{\max} = |\tau|\sqrt{2Z/|r_\parallel|}\}$, where $r_\parallel$ and $\boldsymbol{r}_\perp$ are components of the radius vector $\boldsymbol{r}$ parallel or perpendicular to $\boldsymbol{k}_0$ and the difference in time τ is assumed to be sufficiently small. If a path does not contain a caustics point, one should put in (119) $\alpha_1 = \alpha_0$ and $k = 1$, i.e., in this case the point $\boldsymbol{r} \notin D_c$ and the argument of the final function $\psi^-_{\alpha_1}(\boldsymbol{k}_0, \boldsymbol{r})$ is related to a single point $\boldsymbol{r}'_1$ of the initial function $\psi^-_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}'_1)$; we have the correspondences $\psi^-_+(\boldsymbol{k}_0, \boldsymbol{r}'_1) \to \psi^-_+(\boldsymbol{k}_0, \boldsymbol{r})$ and $\psi^-_-(\boldsymbol{k}_0, \boldsymbol{r}'_1) \to \psi^-_-(\boldsymbol{k}_0, \boldsymbol{r})$.

Suppose now that at some α_0, to be definite let $\alpha_0 = +1$, a path contains a caustics point. It is possible in the case $\boldsymbol{r} \in D_c$ and $\tau < 0$. Here, we have two classical trajectories coming to a point $\boldsymbol{r}$ from points $\boldsymbol{r}'_1$ and $\boldsymbol{r}'_2$ ($k = 2$) during the time τ. The difference between azimuthal angles of these radius vectors $\boldsymbol{r}'_1$ and $\boldsymbol{r}'_2$ appears to be π, i.e., $\boldsymbol{r}'_1$ and $\boldsymbol{r}'_2$ are located in different sides from the caustics line. These trajectories define, respectively, the functions $\boldsymbol{r}'_1(\boldsymbol{r}, \tau)$ and $\boldsymbol{r}'_2(\boldsymbol{r}, \tau)$ in (118). The initial function $\psi^-_+(\boldsymbol{k}_0, \boldsymbol{r}')$ generates the two terms: one term with $\alpha_1 = -1$, $\psi^-_+(\boldsymbol{k}_0, \boldsymbol{r}'_1) \to \psi^-_-(\boldsymbol{k}_0, \boldsymbol{r})$, corresponding to the path that passes through a caustics point and the other with $\alpha_1 = +1$, $\psi^-_+(\boldsymbol{k}_0, \boldsymbol{r}'_2) \to \psi^-_+(\boldsymbol{k}_0, \boldsymbol{r})$, that stems from a trajectory that does not intersect the caustics line. At the same time, the initial function $\psi^-_-(\boldsymbol{k}_0, \boldsymbol{r}')$ does not contribute to (119), i.e., for this component there is no point $\boldsymbol{r}'$ related to $\boldsymbol{r} \in D_c$ and we have $k = 0$. Thus, from (119) we get a WKB analogue

$$K^{(1)}(t_1, t_0)\psi^- = \sum_{\alpha_0} \psi^-_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}) \exp\left(-\mathrm{i}\frac{k_0^2}{2}\tau\right) = \psi^-(\boldsymbol{k}_0, \boldsymbol{r}) \exp\left(-\mathrm{i}\frac{k_0^2}{2}\tau\right) \tag{120}$$

of an exact result that gives an operation of Coulomb propagator on the Coulombic wave. In contrast, Maslov's formula gives a different result at $\boldsymbol{r} \in D_c$, namely, instead of $\psi^-(\boldsymbol{k}_0, \boldsymbol{r})$ we obtain

$$\psi^-(\boldsymbol{k}_0, \boldsymbol{r}) \to \psi^-_+(\boldsymbol{k}_0, \boldsymbol{r}) + \exp(-\mathrm{i}\pi/2)\psi^-_-(\boldsymbol{k}_0, \boldsymbol{r}) \tag{121}$$

where the first and second terms correspond to the paths that do not contain and contain a caustics point. As is seen, Maslov's formula does not work in D_c.

Further using the approximation (118) on the subsequent steps, we get straightforwardly

$$K^{(N)}(t, t_0)\psi^- = \sum_{k_0,\ldots,k_{N-1},\alpha_0} \prod_{i=0}^{N-1} (\psi^-_{\alpha_{i+1}}(\boldsymbol{p}_{0i}(\boldsymbol{r}_i), \boldsymbol{r}_{i+1})/\psi^-_{\beta_{i+1}}(\boldsymbol{p}_{0i}(\boldsymbol{r}_i), \boldsymbol{r}_i))\psi^-_{\alpha_0}(\boldsymbol{k}_0, \boldsymbol{r}_0)$$
$$\times \exp\left(- \mathrm{i} \sum_{i=0}^{N-1} \left(\frac{p_{0i}^2(\boldsymbol{r}_i)}{2}\tau_i - \Delta\boldsymbol{k}_i \boldsymbol{r}_i \right)\right)\Bigg|_{\boldsymbol{r}_i = \boldsymbol{r}_{k_i}(\boldsymbol{r}_{i+1}, \tau_i)}. \tag{122}$$

Here, the coordinates $\boldsymbol{r}_i$ ($i = 0, 1, \ldots, N-1$) are recursively related by

$$\nabla_{\boldsymbol{r}_i} S_{\beta_{i+1}}(\boldsymbol{p}_{\alpha_{i+1}\beta_{i+1}}, \boldsymbol{r}_i) = \Delta\boldsymbol{k}_i + \nabla_{\boldsymbol{r}_i} S_{\alpha_i}(\boldsymbol{p}_{\alpha_i\beta_i}, \boldsymbol{r}_i) \tag{123}$$

where the momentum $\boldsymbol{p}_{\alpha_{i+1}\beta_{i+1}}(\boldsymbol{r}_{i+1}(\boldsymbol{r}_i, \tau_i), \boldsymbol{r}_i, \tau_i) = \boldsymbol{p}_{0i}(\boldsymbol{r}_i)$ is obtained under the map $\hat{p}_{\mathrm{as}}$: $\boldsymbol{p}_i(\boldsymbol{r}_i) \equiv \Delta\boldsymbol{k}_i + \nabla_{\boldsymbol{r}_i} S_{\alpha_i}(\boldsymbol{p}_{\alpha_i\beta_i}, \boldsymbol{r}_i) \to \boldsymbol{p}_{0i}(\boldsymbol{r}_i)$. In addition, one should take into account that $\boldsymbol{p}_{\alpha_0\beta_0} = \boldsymbol{k}_0$, $\Delta\boldsymbol{k}_i = \Delta\boldsymbol{k}_\alpha(t_i)$, $\tau_i = t_{i+1} - t_i$ and $\boldsymbol{r}_N = \boldsymbol{r}$. Moreover, the index β_{i+1} is definitively determined by the map; $\alpha_{i+1} = \beta_{i+1}$ if path connecting the points $\boldsymbol{r}_{i+1}(\boldsymbol{r}_i, \tau_i)$ and $\boldsymbol{r}_i$ does not intersect the caustics line and otherwise $\alpha_{i+1} = -\beta_{i+1}$.

The continuum state (122) describes N rescatterings of an electron in the Coulomb field induced by N impulse kicks at moments $t = t_i$. It is clear that (122) satisfies the property (120) in the limit $\Delta\boldsymbol{k}_i \to 0$, $i = 0, 1, \ldots, N-1$. In this connection note that the continuum state, equation (46) obtained earlier in Kunikeev (1999a), does not fulfil this property. Thus, equation (122) improves the previous result considerably. We can further generalize equation (122) in different directions, for example, replace the WKB scattering waves $\psi^-_{\alpha=\pm 1}(\boldsymbol{p}, \boldsymbol{r})$ by their quantum mechanical counterparts (Kunikeev and Senashenko 1996) or assume as a perturbation the general function: $\Delta \boldsymbol{k}_i \rightarrow -\int_{t_i}^{t_{i+1}} \mathrm{d}\tau \, \nabla_{\boldsymbol{r}} W_{\mathrm{ext}}(\boldsymbol{r}_i, \tau)$, $\Delta \boldsymbol{k}_i \boldsymbol{r}_i \rightarrow \Delta \Phi_{\mathrm{ext}}(\boldsymbol{r}_i, t_i)$.

4. Summary and outlook

In this paper, we present a quasiclassical treatment convenient for detailed investigation of the complicated time-dependent dynamics of an atomic electron subject to a series of δ-function impulses. This description is developed to calculate the propagator (2) of a kicked atomic system. Let us review the main steps in solving this task. First, the two-body Coulomb propagator is derived in the WKB approximation. We obtained analytical expressions in terms of elementary functions for the Coulomb action equation (48), the amplitude defined by equations (43), (49), (56), (61) and (62) and the index $\mu_{\alpha\beta}$ derived from (63) and (64) as functions of the asymptotic momentum $\boldsymbol{p}_{\alpha\beta}$, the coordinates $\boldsymbol{r}$, $\boldsymbol{r}'$ and the difference in time τ. These expressions are fairly simple and may be useful in many applications. The asymptotic momentum $\boldsymbol{p}_{\alpha\beta}$ is a solution of the stationary phase equation (12). Solving this equation for $\boldsymbol{p}_{\alpha\beta}$ is reduced to a numerical solution of one-dimensional equation (29).

In the second step, we use the derived two-body WKB propagator to evaluate the action of (2) on the Coulombic wave. Such an expansion appears in constructing the three-body continuum state for the system of two heavy particles and a light particle (Kunikeev 1999 a, b). Equation (122) represents the result of this calculation. Unlike the results of Maslov and Fedoriuk (1981) and Maslov (1988), we obtained the index $\mu_c = 0 \pmod 4$. It is found that the zero value of μ_c provides a correct behaviour for the function (122) in the domain D_c near caustics points, while Maslov's quasiclassical formula with the phase factor $\exp(-\mathrm{i}\pi\mu/2)$ where μ is the Morse index of a trajectory does not work correctly in D_c. Moreover, we can assume that the equality $\mu_c = 0 \pmod 4$ must remain valid not only in the particular, Coulombic, case but, hypothetically, in a general case, for example, in a superposition of Coulombic and short-range potentials or in a Hartree–Fock atomic potential.

Note that a similar expansion can be readily developed, if one takes an arbitrary initial state $a_i(\boldsymbol{r}) \exp(\mathrm{i}S_i(\boldsymbol{r}))$ instead of a Coulombic wave. However, such one-centre expansions (near the target ion) may be inefficient when two-centre effects are important. If, for instance, the trajectory of electron starts or comes into the neighbourhood of a projectile ion, the projectile potential should be taken as an atomic potential V, while the target potential should be taken as a perturbation potential W_{ext}. If then, during the time evolution, the trajectory of an electron comes into the neighbourhood of a target ion, the choice of potentials V and W_{ext} should be reversed. In this way, using a choice of potentials V and W_{ext} corresponding to a particular situation, one can construct a two-centre continuum state with the aid of consecutive expansions of type (122). Further improvement could be achieved by using a split-operator technique (Feit and Fleck 1978, Fleck *et al* 1976) in equations (2). Since the atomic Hamiltonian H_{at} and the coupling to the external field W_{ext} do not in general commute, the error in the discretization of the time evolution may be reduced by splitting the 'atomic' propagation into two half steps before and after the kick by the field.

It is important to remark that the continuum state (122) incorporates intermediate rescatterings due to the stepped changes $\Delta \boldsymbol{k}_i$ ($i = 0, 1, \ldots, N-1$) of the momentum during the time evolution. As $\Delta \boldsymbol{k}_i \rightarrow 0$ and $N \rightarrow \infty$, it is expected that the stepped evolution will approach to a continuous one. Therefore, there is a great interest in studying effects of these intermediate rescatterings into continuum in various physical processes. For example, atomic ionization induced by ion impact or by short laser pulses are processes suitable to exhibit these effects in the spectra of ejected electrons. Further work is being carried out to compute transition matrices. Numerical results will be presented elsewhere when available.

Note added in proof. In calculating the initial phase $\varphi_-(\nu)$ at $|\nu| \gg 1$ in (8), the $\pi/2$ phase shift was lost. This means that the proper relation between the phases must be $\varphi_- = \pi/2 + \varphi_+$ and the phase function (6) at $\alpha \neq \beta$ acquires the additional phase shift $\pm\pi/2$ with respect to the action function (46). This phase shift arises during transition of a particle through a caustics point. Taking into account this phase shift, we actually obtain that the present results are fully compatible with Maslov's treatment. For more details, see a forthcoming paper by the author (Kunikeev 2000), in which the results are further generalized to the case of a general potential and, especially, the case of a Coulombic repulsive potential is considered.

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