10.1098/rspa.2001.0919

THE ROYAL SOCIETY

On the semiclassical approach to cold atomic collisions

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Received 23 May 2001; accepted 25 September 2001; published online 25 April 2002

We extend the semiclassical description of two-state atomic collisions to low energies for which the impact parameter treatment fails. The problem reduces to solving a system of first-order differential equations with coefficients whose semiclassical asymptotes experience the Stokes phenomenon in the complex coordinate plane. Primitive semiclassical and uniform Airy approximations are discussed.

Keywords: quantum scattering; cold atomic collisions; semiclassical approximation

1. Introduction

The theory of collisions between two atomic systems goes back to the early days of quantum mechanics (Mott 1931; Teller 1937; Landau & Teller 1936) and the basic 1930s models of state interaction are detailed in the recent review of Nikitin (1999). Typically, the colliding atoms undergo electronic transitions and one needs to solve a number (in the simplest case, two) of coupled radial Schrödinger equations. It has been noted since the early thirties that the relative motion of the heavy nuclei can be described classically (Mott 1931; Rosen & Zener 1932). Semiclassically, Stueckelberg (1932) first suggested the analytical continuation of the JWKB (Jeffreys–Wentzel–Kramers–Brillouin) wave functions into the complex plane of the internuclear separation and a proper handling of the Stokes phenomenon. His solution of the avoided crossing time-independent problem (Stueckelberg 1932) shows why a description of the interference in terms of adiabatic quasiclassical phases fails if the phase difference accumulated during the adiabatic motion of the two atoms between the centre of the coupling region and the turning points is small. The vexatious problem of the choice of branch cuts and the determination of Stokes constants via the comparison equation method, were largely resolved by Crothers (1971). Equally well, it was shown by Coveney *et al*. (1985) that the classically forbidden region is less amenable to generalized phase-integral analysis.

The classical approximation of the nuclear motion leads to the impact parameter treatment (Gaunt 1927; Landau 1932; Zener 1932). The impact parameter approximation (IPA) offers a simple physical picture in which fast electronic transitions occur as the slow nuclei follow a classical trajectory. By its nature, the IPA neglects

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the transitions induced in the classically forbidden region inaccessible to the classical motion. These, however, become more important at low collision energies when most of the coupling is concentrated under the centrifugal barrier. There exists a rich variety of literature aimed at improving the IPA (for reviews, see Bates & Holt 1966). In particular, Bates & Crothers (1970) considered the case when the classical trajectories are considerably different for the two states involved. To retain the attractive features of the IPA, they suggested modifying centrifugal potentials in both channels in order to force a common turning point for both states. In their approach they found it convenient to replace the two coupled radial equations by four exact first-order equations whose coefficients involved uncoupled wave functions satisfying at infinity purely ingoing and outgoing boundary conditions.

In this paper we use the Bates & Crothers equations as a basis for extending the semiclassical treatment to cold collisions for which the IPA fails. Mathematically, we study the problem of finding the semiclassical ($\hbar \to 0$) asymptote to the solution of a system of first-order differential equations whose coefficients themselves involve semiclassical wave functions (corresponding to the uncoupled system). As $\hbar \to 0$, their primitive semiclassical asymptotes become singular at their respective turning points and experience the Stokes phenomenon in the complex r-plane (where r is the internuclear separation). The paper is organized as follows. In § 2 we follow Bates & Crothers (1970) in deriving their equations and their reduction to the IPA method. In § 3 we analyse a simple non-crossing problem with exponential coupling and obtain the primitive semiclassical approximation for the S-matrix. We show that the use of the primitive asymptotes for the coefficients in the complex r-plane results in a loss of unitarity and to restore the latter we turn to the work of Berry (1989). In § 4 we consider the uniform Airy approximation for the coefficients and demonstrate a good agreement with the exact solution. Section 5 contains our conclusions.

2. Equations of Bates and Crothers. The impact parameter approximation

The atomic collision problem in the two-state approximation reduces to the solution of two coupled radial Schrödinger equations,

$$\left.\begin{aligned} \frac{\mathrm{d}^2 G_{0l}}{\mathrm{d}r^2} + \left(k_0^2 - \frac{l(l+1)}{r^2} - U_{00}(r)\right) G_{0l} = U_{01} G_{1l}, \\ \frac{\mathrm{d}^2 G_{1l}}{\mathrm{d}r^2} + \left(k_1^2 - \frac{l(l+1)}{r^2} - U_{11}(r)\right) G_{1l} = U_{10} G_{0l}, \end{aligned}\right\} \tag{2.1}$$

for each value of the total angular-momentum quantum number l. In (2.1), $U_{10} = U_{01}$ is the coupling matrix element and the wave vectors $k_j = k_j(\infty)$, $j = 0, 1$, are related to the relative velocity $v_j(\infty)$ of separated atoms in the state j as

$$k_j = \frac{M v_j(\infty)}{\hbar}, \tag{2.2}$$

where M is the reduced mass. The channel wave functions G_{jl} are regular at the origin,

$$G_{0l}(0) = G_{1l}(0) = 0, \tag{2.3}$$

and satisfy, as $r \to \infty$, the boundary conditions

$$\left.\begin{aligned} G_{0l}(r \to \infty) &= \mathrm{i}^l \sin(k_0(\infty)r - \tfrac{1}{2}l\pi) + \alpha_l \exp(\mathrm{i}k_0(\infty)r), \\ G_{1l}(r \to \infty) &= \beta_l \exp(\mathrm{i}k_1(\infty)r) \end{aligned}\right\} \tag{2.4}$$

if the colliding atoms are prepared in the state 0. The constant β_l is related to the S-matrix element $\mathcal{S}_{01}$ as

$$\mathcal{S}_{01} = \beta_l \exp(\tfrac{1}{2}\mathrm{i}\pi l)$$

and the (partial) transition probability P_l is given by

$$P_l = |\beta_l|^2 = |\mathcal{S}_{01}|^2. \tag{2.5}$$

The two coupled channel equations (2.1) can be transformed into four first-order ones (Bates & Crothers 1970) by introducing the uncoupled channel wave functions $S^{\pm}_{jl}$ (solutions of (2.1) without the right-hand side) containing at $r \to \infty$ only the outgoing and incoming waves, respectively,

$$S^{\pm}_{jl}(r) \approx k_j^{-1/2} \exp(\pm\mathrm{i}(k_j r - \tfrac{1}{2}l\pi)). \tag{2.6}$$

Expanding the solutions $G_{jl}(r)$ in the form

$$G_{jl}(r) = \alpha^{+}_{jl}(r)S^{+}_{jl}(r) + \alpha^{-}_{jl}(r)S^{-}_{jl}(r) \tag{2.7}$$

leads (cf. Bates & Crothers 1970) to the following exact equations for the coefficient functions $\alpha^{\pm}_{jl}$:

$$\left.\begin{aligned} \alpha^{+\prime}_{0l} &= -\tfrac{1}{2}\mathrm{i}U_{01}S^{-}_{0l}(\alpha^{+}_{1l}S^{+}_{1l} + \alpha^{-}_{1l}S^{-}_{1l}), \\ \alpha^{-\prime}_{0l} &= \tfrac{1}{2}\mathrm{i}U_{01}S^{+}_{0l}(\alpha^{+}_{1l}S^{+}_{1l} + \alpha^{-}_{1l}S^{-}_{1l}), \\ \alpha^{+\prime}_{1l} &= -\tfrac{1}{2}\mathrm{i}U_{10}S^{-}_{1l}(\alpha^{+}_{0l}S^{+}_{0l} + \alpha^{-}_{0l}S^{-}_{0l}), \\ \alpha^{-\prime}_{1l} &= \tfrac{1}{2}\mathrm{i}U_{10}S^{+}_{1l}(\alpha^{+}_{0l}S^{+}_{0l} + \alpha^{-}_{0l}S^{-}_{0l}). \end{aligned}\right\} \tag{2.8}$$

In terms of $\alpha^{\pm}_{jl}$, the boundary conditions (2.3), (2.4) may now be written as

$$\alpha^{-}_{0l}(\infty) = \tfrac{1}{2}k_0^{1/2}(\infty), \quad \alpha^{-}_{1l}(\infty) = 0, \quad \alpha^{+}_{jl}(0) + \alpha^{-}_{jl}(0) = 0, \quad j = 0, 1. \tag{2.9}$$

The advantage of representation (2.8) is that properties of the uncoupled system enter the equations through $S^{\pm}_{jl}(r)$. This makes (2.8) a convenient basis for semiclassical treatment, as one only needs to replace $S^{\pm}_{jl}(r)$ by their semiclassical asymptotes.

To simplify the treatment further, Bates & Crothers (1970) forced the common turning point, i.e. replaced the radial wave vectors by approximate expressions

$$\tilde{K}^2_{jl}(r) = k^2_j(r)\left[1 - \frac{(l + \frac{1}{2})^2}{r^2 k_0(r) k_1(r)}\right] \tag{2.10}$$

with

$$k^2_j(r) = k^2_j(\infty) - U_{jj}(r)$$

(we have included the Langer correction $l(l+1) \to (l + \frac{1}{2})^2$). Now both channel functions share the same turning point R_l, which is the greatest positive root of the expression in the square brackets in (2.10). Far away from R_l, in the classically allowed region, $S_{jl}^{\pm}(r)$ are given by

$$S_{jl}^{\pm}(r) = \tilde{K}_{jl}^{-1/2} \exp(\pm \mathrm{i} \tilde{\Phi}_{jl}), \tag{2.11}$$

where

$$\tilde{\Phi}_{jl} = \tfrac{1}{4}\pi + \int_{R_{jl}}^{r} K_{jl}(r)\,\mathrm{d}r. \tag{2.12}$$

Neglecting in (2.8) contributions from the classically forbidden region $r < R_l$, as well as highly oscillatory terms containing products $S_{0l}^{+}S_{1l}^{+}$ and $S_{0l}^{-}S_{1l}^{-}$ for $r > R_l$, results in the impact parameter equations (equations (20) and (21) of Bates & Crothers (1970)),

$$\left.\begin{aligned} \pm 2\mathrm{i}\tilde{K}_{0l}^{1/2}\tilde{K}_{1l}^{1/2}\alpha_{0l}^{\pm\prime} &= U_{01}\alpha_{1l}^{\pm}\exp[\mp\mathrm{i}(\tilde{\Phi}_{0l} - \tilde{\Phi}_{1l})], \\ \pm 2\mathrm{i}\tilde{K}_{0l}^{1/2}\tilde{K}_{1l}^{1/2}\alpha_{1l}^{\pm\prime} &= U_{10}\alpha_{0l}^{\pm}\exp[\pm\mathrm{i}(\tilde{\Phi}_{0l} - \tilde{\Phi}_{1l})]. \end{aligned}\right\} \tag{2.13}$$

These can be interpreted as describing the transitions between the two states involved as the nuclei follow a classical trajectory. The IPA has been detailed in Mott & Massey (1965) and fully considered in Bates & Holt (1966) as applied to the problem, so we shall not pursue it any further. In the next section we study the possibility of extending the semiclassical treatment of (2.8) beyond the impact parameter approximation (2.13).

3. Non-crossing model. Primitive semiclassical approximation

Let us consider a simple system with two parallel terms

$$U_{00} = U_{11} = 0$$

and an exponential coupling

$$U_{01} = U_{10} = U\exp(-\gamma r).$$

In (2.8) the coefficients $S_{jl}^{\pm}$ are now given by the spherical Hankel functions of the first $h_{\lambda}^{(1)}(k_j r)$ and second $h_{\lambda}^{(2)}(k_j r)$ kind,

$$\left.\begin{aligned} S_{jl}^{+} &= \mathrm{i}(kr)h_{\lambda}^{(1)}(k_j r) = \mathrm{i}(j_{\lambda}(k_j r) + \mathrm{i}y_{\lambda}(k_j r))kr, \\ S_{jl}^{-} &= -\mathrm{i}(kr)h_{\lambda}^{(2)}(k_j r) = -\mathrm{i}(j_{\lambda}(k_j r) - \mathrm{i}y_{\lambda}(k_j r))kr, \end{aligned}\right\} \tag{3.1}$$

where $\lambda = l + \frac{1}{2}$ and j_{λ} and y_{λ} are the spherical Bessel functions of the first and second kinds, respectively (Abramowitz & Stegun 1970).

Numerically, the S-matrix elements can be obtained by propagating two linearly independent vectors,

$$\alpha^0 \equiv (\alpha_i^0,\ i = 1,\ldots 4) = (1,-1,0,0) \quad \text{and} \quad \alpha^1 \equiv (\alpha_i^1,\ i = 1,\ldots 4) = (0,0,1,-1)$$

from the origin sufficiently far into the asymptotic region $r \to \infty$ and forming their linear combinations so as to cancel the coefficient multiplying one of the incoming waves of state.

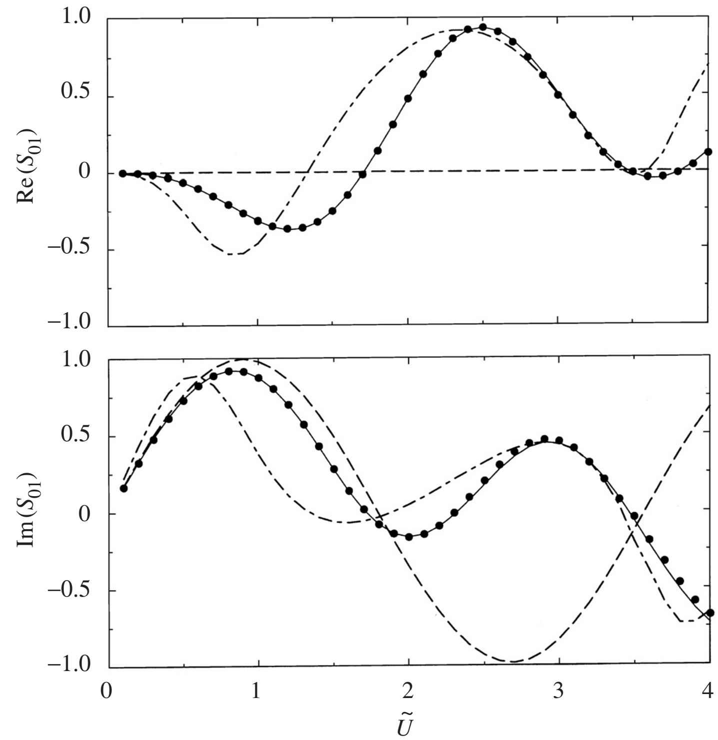

Figure 1. The off-diagonal S-matrix element $\mathcal{S}_{01}$ versus the coupling strength $\tilde{U}$ for $\tilde{k}_0^2 = 2.8$, $\Delta\tilde{\epsilon} = 0.55$ and $l = 3$: exact (solid line); impact parameter approximation (dashed line); primitive semiclassical approximation (3.2), (3.3) (dot-dashed line); and the uniform Airy approximation (filled circles).

Consider next the limits of validity of the impact parameter method. For a given angular-momentum quantum number l and the value of the energy splitting

$$\Delta\epsilon = k_1^2 - k_0^2,$$

there are three parameters left in the problem: the energy $E = k_0^2$, the coupling strength U and the size of the coupling region $r_0 = 1/\gamma$. In fact, if we introduce a new rescaled coordinate $\tilde{r} = r/r_0$, only two of them remain independent. Namely,

$$\tilde{E} = Er_0^2$$

($\tilde{k}_j^2 = k_j^2 r_0^2$, so that $\tilde{E} = k_0^2 r_0^2 = \tilde{k}_0^2/r_0^2 \cdot r_0^2 = \tilde{k}_0^2$), and in a similar way,

$$\tilde{U} = Ur_0^2.$$

Consider now the behaviour of the transition probability as a function of $\tilde{U}$ and $\tilde{E} = \tilde{k}_0^2$. If we increase the energy for a fixed coupling strength $\tilde{U}$, the turning points R_{0l} and R_{1l} in both channels will move towards the origin, until all the coupling is contained in the classically allowed region. There the transitions can be accurately described by the IPA (2.13). If, on the other hand, we increase the coupling strength for a fixed energy $\tilde{E}$, the transitions in the classically forbidden region will become

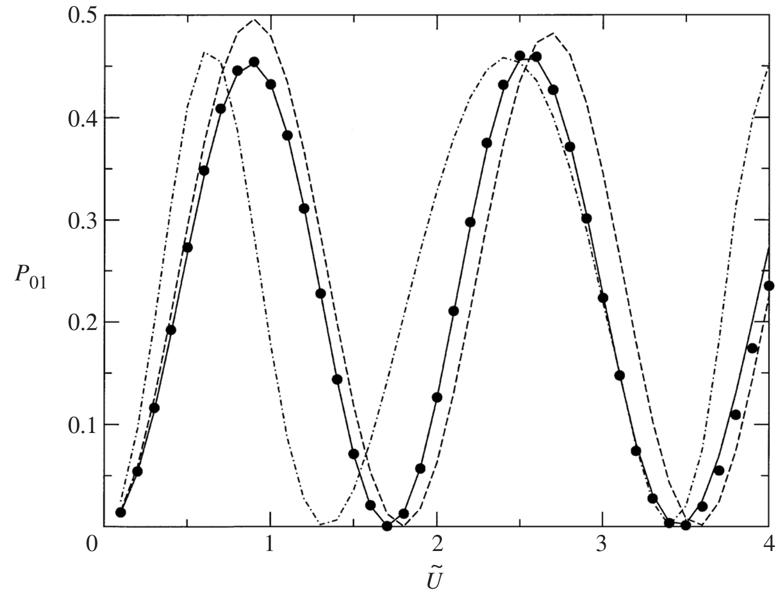

Figure 2. Transition probability P_{01} versus the coupling strength $\tilde{U}$: exact (solid line); impact parameter approximation (dashed line); primitive semiclassical approximation (3.2), (3.3) (dot-dashed line); and the uniform Airy approximation (filled circles). Other parameters are the same as in figure 1.

important and the IPA will break down, even though most of the coupling will be restricted to $r > R_{jl}$. Comparison between the IPA method (dashed line) and the exact numerical calculations (solid line) is shown in figure 1 for the S-matrix element and in figure 2 for the transition probability P_{01}. The following set of parameters was used: $l = 3$, $\tilde{E} = 2.8$, $\Delta\tilde{\epsilon} = 0.55$. Note that while the agreement between the transition probabilities P_{01} defined in (2.5) is reasonable, the phase of the S-matrix element is in error. Next we consider extension of the semiclassical treatment to large U.

We have four coupled first-order equations (2.8), whose coefficients $S_{jl}^{\pm}$ are the channel wave functions of the uncoupled ($U = 0$) problem. We start by attempting to obtain semiclassical solution of (2.8) by replacing $S_{jl}^{\pm}$ by their semiclassical asymptotes.

These are divergent at the turning points R_{jl} and it seems natural to deform the contour of integration of (2.8) away from the real axis so as to bypass R_{jl} sufficiently far in the complex r-plane. In the complex r-plane, each of the functions $S_{jl}^{\pm}$, defined by their behaviour at $r \to \infty$, has an asymptote that is analytic in the three sectors partitioned by the Stokes lines, as shown in figure 3. The new complex contour C consists of a segment of the real r-axis $[0, R_{\mathrm{a}}]$, a semicircle in the upper half-plane and the remainder of the real r-axis $[R_{\mathrm{b}}, \infty]$. The complex r-plane is dissected by the Stokes lines, implicitly defined by

$$\mathrm{Re}\left(\int_{R_{jl}}^{r} K_{jl}(r)\,\mathrm{d}r\right) = 0, \quad j = 0, 1,$$

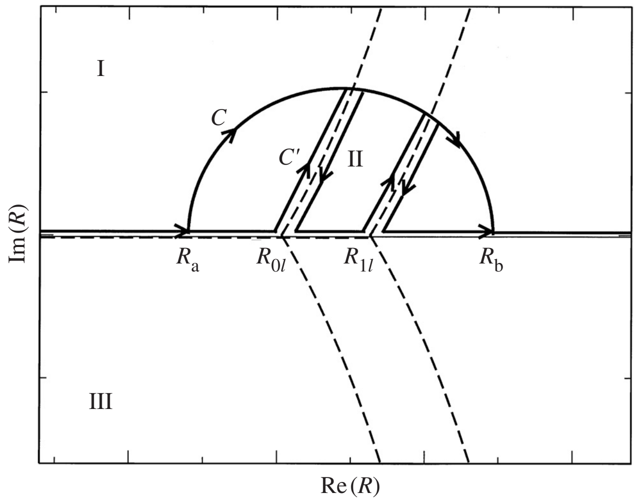

Figure 3. Schematic of the complex r-plane showing the behaviour of Stokes lines (dashed line) and the integration contours C and C'. Also shown are the turning points R_{0l} and R_{1l}.

$$K_{jl}^2(r) = k_0^2(\infty) - \frac{(l+\frac{1}{2})^2}{r^2},$$

and shown in figure 3. At the Stokes lines, the coefficient multiplying the subdominant (exponentially small) solution is discontinuous and (explicitly) we have, for instance, for the functions $S_{0l}^{\pm}$,

$$S_{0l}^{+} = K_{0l}(r)^{-1/2}\exp(\mathrm{i}\Phi_{0l})$$

in sectors I and II, but

$$S_{0l}^{-} = K_{0l}(r)^{-1/2}\exp(-\mathrm{i}\Phi_{0l}), \tag{3.2}$$

in sector I and

$$S_{0l}^{-} = K_{0l}(r)^{-1/2}\exp(-\mathrm{i}\Phi_{0l}) + K_{0l}(r)^{-1/2}\exp(\mathrm{i}\Phi_{0l})$$

in sector II, where (we do not force the common turning point, as has been done in (2.10))

$$\Phi_{0l} = \left(\tfrac{1}{4}\pi + \int_{R_{0l}}^{r} K_{0l}(r)\,\mathrm{d}r\right).$$

The functions $S_{1l}^{\pm}$ are given in a similar way, but in the sectors divided by the Stokes lines originating from the turning point R_{1l}. Inserting expressions (3.2) into (2.8) and integrating along the contour C in figure 3, we find that the S-matrix is no longer unitary, $P_{00} + P_{01} \neq 1$. This unsatisfactory result deserves further attention. Comparing the exact values of $S_{jl}^{\pm}$ with the asymptotes (3.2) along the arc of the semicircle (whose length we denote σ), we find the two in good agreement, as shown in figure 4*a*. Yet at the end of the arc, the approximate solutions of (2.8) differ significantly from those obtained with exact $S_{jl}^{\pm}$ (figure 4*b*). Clearly, this is because the small error in $S_{jl}^{\pm}$ accumulates along the arc. This, in turn, is a consequence of the

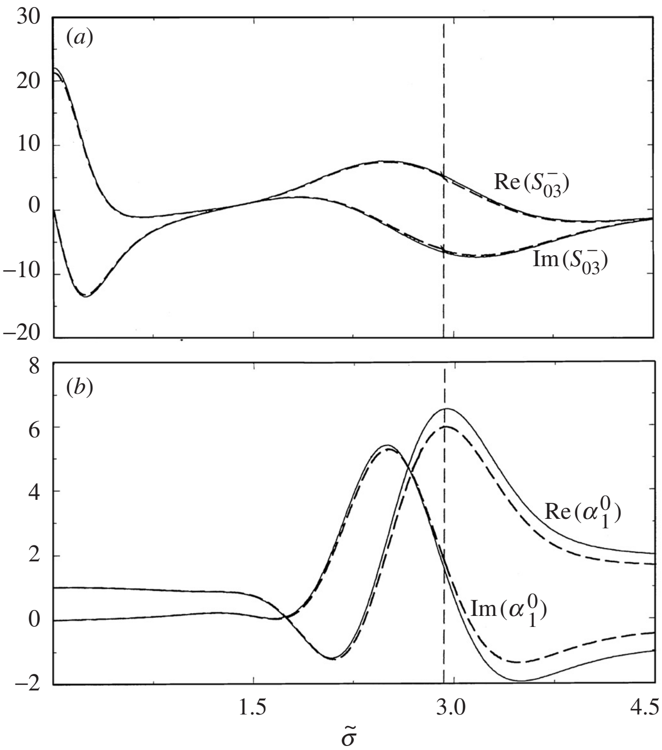

Figure 4. (a) The real and imaginary parts of $S_{03}^{-}(r)$ versus the arc length $\tilde{\sigma} \equiv \sigma/r_0$ along the integration contour C: exact (solid line) and semiclassical (dashed line). Intersection of the arc with the Stokes line is indicated by a vertical dashed line. (b) $\mathrm{Re}(\alpha_1^0)$ and $\mathrm{Im}(\alpha_1^0)$ versus $\tilde{\sigma}$ along the same contour: exact (solid line) and semiclassical (dashed line). Other parameters are $\tilde{k}_0^2 = 2.8$, $l = 3$ and $\tilde{U} = 11.1$.

fact that asymptotes (3.2) are not analytic in the whole of the complex r-plane. If we try to deform the contour C back to the real axis, we obtain additional contributions from the parts of the new contour C' that run up and down the Stokes lines in the upper half of the plane (figure 3). Thus our naive attempt to obtain an accurate semiclassical approximation by moving away from the singularities of $S_{jl}^{\pm}$ fails and we need to restore the unitarity.

To do so, we refer to Berry (1989), where it is shown that on the Stokes lines the semiclassical asymptotes of $S_{jl}^{\pm}$ change continuously and in such a manner that on a Stokes line the coefficient multiplying the subdominant solution equals half of the Stokes constant T. Since $S_{jl}^{\pm}$ are continuous across their respective Stokes lines in the upper half of the complex r-plane, we can neglect integrations along the corresponding sections of C'. The segment of the real axis $[0, R_{jl}]$ is also a Stokes line; there we replace $S_{jl}^{\pm}$ by

$$S_{jl}^{\pm} = K_{jl}(r)^{-1/2}(\exp(\mathrm{i}\Phi_{jl}) \pm \tfrac{1}{2}\mathrm{i}\exp(-\mathrm{i}\Phi_{jl})). \tag{3.3}$$

It is necessary to retain the subdominant solution in (2.8) in order to describe the transitions in the classically forbidden region $r < \min(R_{jl})$. It is readily seen that if

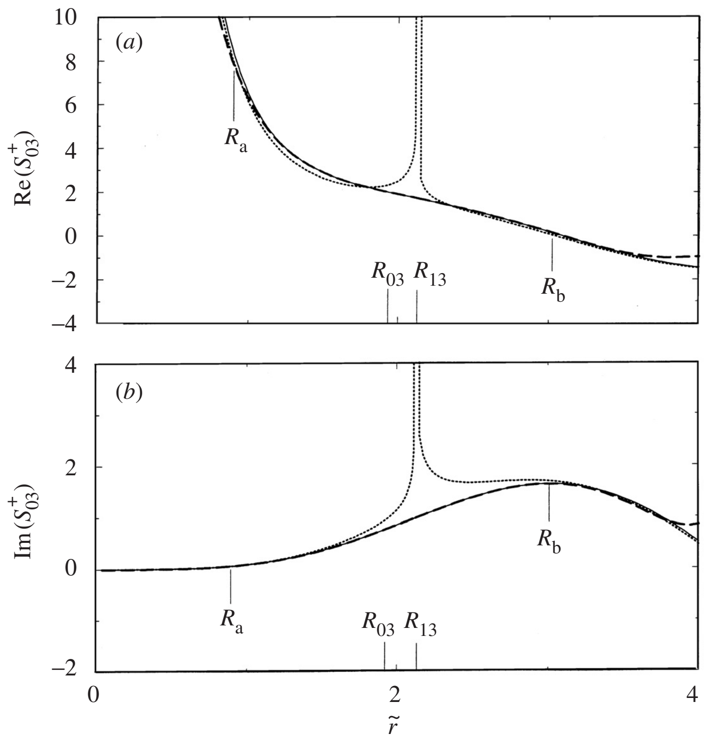

Figure 5. $\mathrm{Re}(S^+_{03})$ and $\mathrm{Im}(S^+_{03})$ versus $\tilde{r}$ along the real r-axis: exact (solid line), primitive semiclassical (dotted line) and uniform Airy (dashed line). Other parameters as in figure 4.

only the exponentially growing terms were kept, the right-hand side of (2.8) would vanish there identically.

Finally, we use the primitive semiclassical approximation of replacing $S^{\pm}_{jl}$ by (2.11). The semiclassical results are shown in figures 1 and 2 by a dot-dashed line. The unitarity is now restored, and the agreement has improved, but it is still far from perfect. In the next section we discuss the uniform Airy approximation.

4. The uniform Airy approximation

Since it is not possible, due to non-analyticity of the semiclassical asymptotes, to integrate (2.8) in the complex r-plane, we return to the real r-axis and replace $S^{\pm}_{jl}$ near their respective turning points by the appropriate Airy functions. This can be done as long as the potential near R_{jl} has a finite slope (Migdal 2000). In our case, the potential is a centrifugal barrier and the required uniform Airy approximation is just the transitional region expansions of the spherical Bessel functions (Abramowitz & Stegun 1970). More specifically, in (3.1) we use

$$(2k_j r/\pi)^{1/2} j_\lambda(kr) \sim \frac{2^{1/3}}{\lambda^{1/3}}\,\mathrm{Ai}(-2^{1/3}z)\left\{1+\sum_{k=1}^{\infty}\frac{f_k(z)}{\lambda^{2k/3}}\right\}+\frac{2^{2/3}}{\lambda}\,\mathrm{Ai}'(-2^{1/3}z)\sum_{k=0}^{\infty}\frac{g_k(z)}{\lambda^{2k/3}}, \qquad (4.1\,a)$$

$$(2k_j r/\pi)^{1/2} y_\lambda(kr)$$
$$\sim -\frac{2^{1/3}}{\lambda^{1/3}}\,\mathrm{Bi}(-2^{1/3}z)\left\{1+\sum_{k=1}^{\infty}\frac{f_k(z)}{\lambda^{2k/3}}\right\} - \frac{2^{2/3}}{\lambda}\,\mathrm{Bi}'(-2^{1/3}z)\sum_{k=0}^{\infty}\frac{g_k(z)}{\lambda^{2k/3}}, \quad (4.1\,b)$$

with

$$z \equiv \frac{k_j r - \lambda}{\lambda^{1/3}},$$

where $f_k(z)$ and $g_k(z)$ are the coefficients given in Abramowitz & Stegun (1970) and Ai, Bi and Ai$'$, Bi$'$ are the Airy functions and their derivatives, respectively. For each $S^{\pm}_{jl}$, asymptotes (4.1) are valid in a region $[R_\mathrm{a}, R_\mathrm{b}]$ containing the turning points R_{jl}. For a given l and k_j, the size of the transitional region is chosen so as to ensure that $[R_\mathrm{a}, R_\mathrm{b}]$ extends on both sides into the region where the primitive semiclassical asymptote holds (see figure 5, where the S^{+}_{03} is shown, as an example). For a given l, both R_a and R_b scale as k_j^{-1} as k_j increases. In general, we found it necessary to keep up to four terms in (4.1).

If the splitting $\Delta\epsilon$ is small, the two turning points $R_{0l} < R_{1l}$ are close to each other and the r-axis is divided into three distinct regions:

(a) $0 < r < R_{0l}$;

(b) $R_{0l} < r < R_{1l}$; and

(c) $r > R_{1l}$.

Region (a) lies deep in the classically forbidden region, where the coupling is large, but the bracketed terms on the right-hand side of (2.8) are small. We expect this region to become increasingly important as U becomes larger. In region (a) we approximate $S^{\pm}_{jl}$ by (3.3). Region (b) includes the vicinity of the classical turning points R_{jl}. Near the turning points the coupling may be smaller, but semiclassical wave functions are of order unity. There $S^{\pm}_{jl}$ are represented by their Airy approximations (4.1). Neither of these two regions is correctly described by the impact parameter approximation. Finally, region (c) lies in the classically allowed region, where the notion of a common classical trajectory holds, and therefore here we continue to use for $S^{\pm}_{jl}$ the primitive semiclassical approximation (2.11).

The results of numerical integration of (2.8) with coefficients defined as discussed above are shown in figure 1 by the filled circles. Both real and imaginary parts of the S-matrix element S_{01} agree with their exact values to numerical accuracy and strongly disagree with the prediction of the impact parameter method. In general, we find that all three regions contribute to the transition probability P_{01}.

5. Conclusions

To conclude, we have extended the semiclassical description to cold atomic collisions, which currently attract much interest in connection with the physics of Bose–Einstein condensation. At low energies, much of the coupling responsible for transition between atomic states is localized in the classically forbidden region or in the vicinity of the turning point of one or both channels. For this reason, the impact parameter method becomes inaccurate and needs to be extended. At the same time, the uncoupled channel wave functions can be described semiclassically and the required extension can be achieved by feeding semiclassical expressions for $S^{\pm}$ into the Bates–Crothers equations (2.8). We have shown that the use of the primitive semiclassical approximation for $S^{\pm}$ and integration of (2.8) in the complex r-plane along a contour avoiding the classical turning points yields an incorrect (and, in general, non-unitary) S-matrix. An improved primitive approximation can be obtained if an appropriate combination of the dominant and subdominant solutions is used in the classically forbidden region and integration is performed along the real axis. This permits the taking into account of transitions that occur in the classically forbidden region. Finally, a correct semiclassical description is obtained if uniform Airy approximations for $S^{\pm}$ (4.1) are used in the vicinities of the turning points.

E.B. gratefully acknowledges the support by The Royal Society, NATO and The Foreign and Commonwealth Office Chevening Fellowship during her stay in Belfast.

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