Exact solution for the reflection and diffraction of atomic de Broglie waves by a travelling evanescent laser wave

N S Witte
Research Centre for High Energy Physics, School of Physics, University of Melbourne, Parkville, Victoria 3052, Australia
and
Institute of Mathematical Sciences, CIT Campus, Taramani Chennai 600113, India

Received 27 May 1997, in final form 29 September 1997

Abstract. The exact solution to the problem of reflection and diffraction of atomic de Broglie waves by a travelling evanescent wave is found starting with a bare-state formulation. The solution for the wavefunctions, the tunnelling losses and the non-adiabatic losses are given exactly in terms of hyper-Bessel functions, and are valid for all detuning and Rabi frequencies, thus generalizing previous approximate methods. Furthermore, we give the limiting cases of the amplitudes in the uniform semiclassical limit, which is valid in all regions including near the classical turning points, and in the large and weak coupling cases. Exact results for the zero detuning case are obtained in terms of Bessel functions. We find our uniform semiclassical limit to be closer to the exact result over the full range of parameter values than the previously reported calculations.

1. Introduction

Several theoretical analyses of the reflection and diffraction of atomic de Broglie waves by laser radiation have been made by Cook and Hill (1982), Hajnal and Opat (1989), Deutschmann et al (1993a, b) and Wallis (1995) following the interest in forming atomic mirrors and gratings from laser waves. In the model considered here a laser beam propagating inside a quartz block is totally internally reflected at the quartz-vacuum interface, thus producing a travelling evanescent wave on the vacuum side of the interface. Incident on the interface from the vacuum side is a beam of atoms, which is taken to be a two-level atom whose level spacing is near the laser frequency. See figure 1 of Hajnal and Opat (1989) for the geometry of the problem and the conventions for coordinates. In this case there will be a single-reflected and a single-diffracted beam. Another more commonly explored configuration is where the laser beam, after total internal reflection, is retro-reflected, and so one has two counter-propagating beams. In this case the evanescent wave is a standing wave and an infinite number of higher-order diffracted atomic beams arise. We do not consider this more complicated case here. In the bare-state picture (see Hajnal and Opat 1989) a Green function formulation was approximately solved numerically using a perturbative Born series approach, even though the dimensionless coupling parameter in practical cases is very large (~10^4). In the dressed-state picture Deutschmann et al (1993a, b) employed a semiclassical WKB solution, without any reliable or controllable error estimates, although in some physical situations these results may have relevance. We present the exact solution to this problem and also seek to reconcile all these different treatments by investigating
the physically significant limiting cases to the exact solution that have been the basis of
the approximate schemes employed above. We do not, however, discuss the limitations
of this model, in particular the assumptions made in deriving it, such as the two-state
approximation, or the absence of spontaneous decay, etc.

The differential equations describing this model have also arisen in other fields where
their exact solutions have been found. Because the models are physically different and
consequently the boundary conditions are different, these results cannot be translated into
ours. Also the approach taken here is quite different and is intended to be as complete
as possible. The earliest application arose in the investigation of the lateral vibrations
of bars whose cross section is a function of the distance from one end. In this context
asymptotic expressions for these solutions when the argument becomes large were first
detailed in Wrinch (1921a,b). Another early application was found in the oblique reflection
of long wavelength radio waves from a reflecting region of the ionosphere where the earth’s
magnetic field was vertical and the wave frequency was much less than the gyro-frequency.

The exact solution of the differential equations under these circumstances was found
to be the generalized hypergeometric function, or specifically the hyper-Bessel function
$\,_{0}F_{3}(\rho; z)$, and leading-order asymptotic forms as $z \to \infty$ were found using the Mellin–
Barnes integral representations of these functions. These were identical to those found
earlier by Wrinch (1921a). More recently this type of differential equation has arisen in a
wide range of problems ranging from charge transfer in atomic collisions to vibrational
transitions in molecular scattering, in particular the Demkov–Rosen–Zener models. In
Osherov and Voronin (1994) and Zhu (1996) coupled Schrödinger equations with model
potentials resulting from separating out angular variables and truncating the basis were
solved by comparing the differential equations with the defining differential equations of
the Meijer $G$-function, which in these cases reduces to that of the hyper-Bessel function.
From the known asymptotic (see Luke 1975) forms as $z \to 0, \infty$ the non-adiabatic transition
matrices for 1, 2 or 3 open channel cases could be found exactly in terms of the gamma and
elementary functions. The interest in an exact expression is that it provides a description of
collision processes where the energy transfer is small and which occur at large separations,
whereas the traditional treatment elaborated in the works of Landau, Zener and Stueckelberg
only describes non-adiabatic transitions near avoided crossings and where the energy transfer
is large.

Our results require some considerable technical work, of a purely mathematical nature,
and in order to make the essential physical answers accessible we have divided the paper into
two parts. The first part contains the physical results, without any derivation, and the second
part, the majority of the paper, provides the mathematical justification and explanation. In
the first part, section 2 describes the mathematical formulation of the problem and relates
our parameters to the key physical quantities. In section 3 we give the exact solution to
this model in terms of a class of generalized hypergeometric functions, the hyper-Bessel
functions. Here we give expressions for the wavefields, tunnelling losses and non-adiabatic
losses for arbitrary parameters. Immediately following that, in section 4, we give the simple
limiting forms in the cases of weak coupling, strong coupling and zero detuning. We also
give the uniform semiclassical approximation which is valid in the region of the classical
turning point, or regardless of the proximity of this point to any boundary. We sometimes
only offer one expression as an example of how one might obtain the others, and all the
expressions are available in Witte (1996). In the second part of the paper, we begin by
deriving the solution in section 5. In section 6 we report a number of old results which
are required in order to prove some identities arising in the physical model and also to
facilitate computation of these functions. In the final section, section 7, we derive the
Reflection and diffraction of atomic de Broglie waves

uniform semiclassical approximation for the particular type of hyper-Bessel function that arises in this work. A preliminary report of some of the results given here has already appeared in Feng et al (1996).

2. Formulation of the model

According to Hajnal and Opat (1989), the Schrödinger equation for the wavefunctions of the different diffraction orders leads to the pair of coupled second-order homogeneous differential equations defined on the half-interval \( y \geq 0 \)

\[
\left( \frac{d^2}{dy^2} + k_0^2 \right) \phi_0(y) = -\Omega_e^2 e^{-qy} \phi_1(y)
\]

\[
\left( \frac{d^2}{dy^2} + k_1^2 \right) \phi_1(y) = -\Omega_e^2 e^{-qy} \phi_0(y)
\]

where \( \phi_0 \) is the reflected or ground state (channel 0) and \( \phi_1 \) the diffracted or excited state (channel 1) atomic wavefunctions. In addition, the following parameters appear,

\[
k_0^2 = k_y^2 \quad k_1^2 = k_y^2 - 2k_x Q_x - Q_x^2 + \frac{2m}{\hbar} (\omega - \omega_a) \quad \Omega_e^2 = \frac{2m \mu E_0}{\hbar^2}
\]

where \( \hbar (k_x, -k_x) \) are the atomic momentum components, \( m \) is the atomic mass, \( \mu \) is the static electric dipole moment of the atom, \( \omega_a \) is the atomic level spacing, \( \omega \) is the laser frequency, \( q \) is the inverse decay length of the evanescent wave, \( Q_x \) is the x-component of the laser wavenumber, and \( E_0 \) is the electric field amplitude of the laser beam. In all that follows we take \( k_0, k_1, q \) and \( \Omega_e^2 \) to be real and positive.

Before proceeding any further we scale our system variables to physically dimensionless ones by forming ratios with evanescent scale length, and this will also simplify the mathematical analysis,

\[
x \equiv 2qy \quad \alpha_0 \equiv k_0/2q \quad \alpha_1 \equiv k_1/2q \quad \beta \equiv \Omega_e/2q \quad \psi(x) \equiv \frac{1}{2q} \phi(y)
\]

Thus it will be assumed that \( q \) is non-zero, as the situation with a zero scale length is trivial. Our new quantities are simply related to the dimensionless parameters defined in Deutschmann et al (1993a) by the following

\[
8\beta^2 = \frac{\Omega_R}{\Delta_q} \quad 4(\alpha_1^2 - \alpha_0^2) = \Delta = \frac{\Delta_{\text{eff}}}{\Delta_q} \quad 4\alpha_0^2 = \frac{T_{\infty, y}}{\hbar \Delta_q}
\]

which are the dimensionless Rabi frequency, the dimensionless detuning parameter and the dimensionless perpendicular kinetic energy respectively, referred to \( \hbar \Delta_q \equiv \hbar^2 q^2/2m \). With these definitions the defining equations (1) become

\[
\left( \frac{d^2}{dx^2} + \alpha_0^2 \right) \psi_0(x) = -\beta^2 e^{-\frac{i}{2}x} \psi_1(x)
\]

\[
\left( \frac{d^2}{dx^2} + \alpha_1^2 \right) \psi_1(x) = -\beta^2 e^{-\frac{i}{2}x} \psi_0(x)
\]

and the boundary conditions (8) are

\[
\psi'_0(0) + i\alpha_0 \psi_0(0) = 0 \quad \psi'_1(0) + i\alpha_1 \psi_1(0) = 0.
\]

Conventionally, we take an incoming or left-moving wave to be of the form \( e^{-i\omega t - iky} \) and an outgoing or right-moving wave \( e^{-i\omega t + iky} \), so that incoming and outgoing directions
are referred to the origin. The boundary conditions at infinite distance from the interface are
\[ \psi_0(x) \rightarrow 1 \cdot e^{-i\omega_0 x} + R_0 e^{+i\omega_0 x} \quad \psi_1(x) \rightarrow 0 \cdot e^{-i\omega_1 x} + R_1 e^{+i\omega_1 x} \] (7)
which represent a unit incoming atomic wave in channel 0 and its outgoing reflection with amplitude \( R_0 \), and an outgoing wave in channel 1 with amplitude \( R_1 \). The amplitude \( R_1 \) represents the non-adiabatic losses from the atomic beam. At the interface, as \( x \rightarrow 0^- \), the boundary conditions are
\[ \psi_0(0^-) \rightarrow T_0 e^{-i\omega_0 x} + 0 \cdot e^{+i\omega_0 x} \quad \psi_1(0^-) \rightarrow T_1 e^{-i\omega_1 x} + 0 \cdot e^{+i\omega_1 x} \] (8)
which represent transmitted left-moving waves with amplitudes \( T_0 \) and \( T_1 \). In other words, once an atom crosses the interface it is assumed to enter a non-interaction region and can never be reflected back across the interface, to be lost from the system. Both the amplitudes \( T_0 \) and \( T_1 \) represent tunnelling losses across the interface.

Utilizing the boundary conditions (6) one can express the solution for the wavefields in terms of the field values at the origin \( \psi_0(0) \equiv \psi_0, \psi_1(0) \equiv \psi_1 \). If we write the asymptotic behaviour in the following way
\[ \psi_0(x) \rightarrow e^{+i\omega_0 x} (\psi_0 S_{00}^+ + \psi_1 S_{10}^+) + e^{-i\omega_0 x} (\psi_0 S_{00}^- + \psi_1 S_{10}^-) \]
\[ \psi_1(x) \rightarrow e^{+i\omega_1 x} (\psi_0 S_{10}^+ + \psi_1 S_{11}^+) + e^{-i\omega_1 x} (\psi_0 S_{10}^- + \psi_1 S_{11}^-) \] (9)
in terms of dimensionless amplitudes \( S \). We can then completely solve our system by specifying the boundary conditions at infinity
\[ \psi_0 S_{00}^+ + \psi_1 S_{10}^+ = R_0 \quad \psi_0 S_{10}^+ + \psi_1 S_{11}^+ = R_1 \]
\[ \psi_0 S_{00}^- + \psi_1 S_{01}^- = 1 \quad \psi_0 S_{10}^- + \psi_1 S_{11}^- = 0 \] (10)
where we have after solving for \( \psi_0 \) and \( \psi_1 \)
\[ R_0 = \frac{S_{00}^+ S_{11}^- - S_{01}^+ S_{10}^-}{S_{00}^+ S_{11}^- - S_{01}^+ S_{10}^-} \quad R_1 = \frac{S_{10}^+ S_{11}^- - S_{11}^+ S_{10}^-}{S_{00}^+ S_{11}^- - S_{01}^+ S_{10}^-} \]
\[ T_0 = \frac{S_{00}^- S_{11}^- - S_{01}^- S_{10}^-}{S_{00}^+ S_{11}^- - S_{01}^+ S_{10}^-} \quad T_1 = \frac{-S_{10}^-}{S_{00}^+ S_{11}^- - S_{01}^+ S_{10}^-}. \] (11)

While the above boundary conditions are appropriate in realistic situations it is advantageous to generalize them in a symmetrical way, by including arbitrary weights into the incoming channels. We let, as \( x \rightarrow \infty \)
\[ \psi_0(x) \rightarrow a_0 e^{+i\omega_0 x} + b_0 e^{-i\omega_0 x} \quad \psi_1(x) \rightarrow a_1 e^{+i\omega_1 x} + b_1 e^{-i\omega_1 x} \] (12)
and as \( x \rightarrow 0^- \)
\[ \psi_0(x) \rightarrow T_0 e^{-i\omega_0 x} \quad \psi_1(x) \rightarrow T_1 e^{-i\omega_1 x} \] (13)
and define two transition matrices, a non-adiabatic transition matrix, \( \mathbf{UL}^{-1} \), and a tunnelling loss matrix \( \mathbf{L}^{-1} \) via
\[ \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \mathbf{U} \cdot \mathbf{L}^{-1} \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} \quad \begin{pmatrix} T_0 \\ T_1 \end{pmatrix} = \mathbf{L}^{-1} \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} \] (14)
where the \( \mathbf{U}, \mathbf{L} \) matrices are then
\[ \mathbf{U}, \mathbf{L} = \begin{pmatrix} S_{00}^\pm & S_{01}^\pm \\
S_{10}^\pm & S_{11}^\pm \end{pmatrix}. \] (15)
Reflection and diffraction of atomic de Broglie waves

In this way we can find a normalization condition and this is done by noting that the following flux is a constant
\[
J = \frac{d\psi_0}{dx} \psi_0^* - \psi_0 \frac{d\psi_0^*}{dx} + \frac{d\psi_1}{dx} \psi_1^* - \psi_1 \frac{d\psi_1^*}{dx}
\]  
(16)
and that by equating the limiting forms of this as \( x \to \infty \) and \( x \to 0^- \) we find the condition
\[
\alpha_0(|a_0|^2 + |b_0|^2) + \alpha_1(|a_1|^2 + |b_1|^2) = \alpha_0|b_0|^2 + \alpha_1|b_1|^2.
\]  
(17)
This in turn implies a condition on the \( S \)-functions given that all outgoing amplitudes are solved in terms of arbitrary incoming ones
\[
\alpha_0 = \alpha_0(|S_{00}^-|^2 - |S_{00}^+|^2) + \alpha_1(|S_{10}^-|^2 - |S_{10}^+|^2)
\]
\[
\alpha_1 = \alpha_1(|S_{11}^-|^2 - |S_{11}^+|^2) + \alpha_0(|S_{01}^-|^2 - |S_{01}^+|^2)
\]
\[
0 = \alpha_0(S_{00}^- S_{01}^+ - S_{00}^+ S_{01}^-) + \alpha_1(S_{11}^- S_{10}^+ - S_{11}^+ S_{10}^-).
\]  
(18)
Normally we will only exhibit \( R_0, R_1 \) and \( T_0, T_1 \), the only non-zero elements of the non-adiabatic and tunnelling loss matrices appropriate to the usual boundary conditions, and as the other elements can be easily found using the same techniques described below.

The above description constitutes one based on the bare-state or diabatic picture, and one can also use the dressed-state or adiabatic picture as discussed in Compagno et al (1982) and Deutschmann et al (1993a, b) although in our case it yields no attendant simplification.

The two quasipotentials are then
\[
W_\pm(x) = \mp \frac{1}{2} |a_0^2 + a_1^2| \pm [(a_1^2 - a_0^2)^2 + 4\beta^4 e^{-\gamma}]^{1/2}
\]  
(19)
and the classical turning points \( x_0 \) defined by \( W_\pm(x_0) = 0 \) are given by \( \alpha_0^2 \alpha_1^2 = \beta^4 e^{-\gamma} \).
Their definitions \( W_- \) and \( W_+ \) are the upper and lower branches respectively. By defining the dressed states \( \psi_0, \psi_1 \) corresponding to the quasipotentials \( W_- \), \( W_+ \) respectively we have the following transformation relating the two pictures
\[
\begin{pmatrix}
\psi_0 \\
\psi_1
\end{pmatrix} = \begin{pmatrix}
\cos(\Theta) & \sin(\Theta) \\
-\sin(\Theta) & \cos(\Theta)
\end{pmatrix} \begin{pmatrix}
\psi_0 \\
\psi_1
\end{pmatrix}
\]  
(20)
and where the rotation angle is given by
\[
\Theta = \frac{1}{2} \tan^{-1} \left( \frac{2\beta^2 e^{-\gamma/2}}{a_1^2 - a_0^2} \right) \quad \Delta > 0
\]
\[
\Theta = \frac{\pi}{2} - \frac{1}{2} \tan^{-1} \left( \frac{2\beta^2 e^{-\gamma/2}}{a_0^2 - a_1^2} \right) \quad \Delta < 0
\]  
(21)
so that when \( \Delta > 0 \) then \( \Theta \to 0 \) as \( x \to \infty \), i.e. the upper branch approaches the ground state, and the lower branch the excited state, while in the opposite case \( \Delta < 0 \) then \( \Theta \to \pi/2 \), and the associations are reversed compared with the previous case. As \( \Delta \to 0 \) then \( \Theta \to \pi/4 \).

3. Exact solution

We give the exact solution for the wavefields here, and the derivation from first principles can be found in section 5. For the wavefield \( \psi_0(x) \) we have
\[
ir^{-3} \cosh \pi \delta \cosh \pi \sigma \psi_0(x) = \frac{e^{-i\delta x_0}}{\sinh 2\pi \alpha_0} 0 f_3(1 + 2i\alpha_0, \frac{1}{2} + i\delta, \frac{1}{2} + i\sigma; \beta^4 e^{-\gamma})
\]
\[
x + \beta^2 \psi_1 \cdot 0 f_3(1 - 2i\alpha_0, \frac{3}{2} - i\delta, \frac{1}{2} - i\sigma; \beta^4)
\]
where \( \delta \equiv \alpha_0 - \alpha_1, \sigma \equiv \alpha_0 + \alpha_1 \) and \( \psi_0, \psi_1 \) are the field values at the origin. The corresponding solution for \( \psi_1(x) \) is simply given by the equation above with the interchange \( 0 \leftrightarrow 1 \). Here the generalized hypergeometric \( {}_0f_3 \) or hyper-Bessel function is defined by the series definition, or its relation to the Meijer-G function by

\[
0f_3(a, b, c; z) = \frac{1}{\Gamma[a, b, c]} {}_0F_3(a, b, c; z) = G^{10}_{04}(ze^{-iz}|0, 1 - a, 1 - b, 1 - c)
\]

(23)

where the gamma function products are defined by equation (53).

As \( x \to \infty \) the wavefunctions, as given in equation (22), evolve to purely undamped travelling wavesolutions as they must. From the above solution the \( S \)-amplitudes are given by

\[
S^+(0, \alpha_0, \alpha_1, \beta) = \beta^4 \Gamma[+2i\alpha_0, \frac{1}{2} + i\sigma, \frac{1}{2} + i\sigma] {}_0f_3(2 + 2i\alpha_0, \frac{3}{2} + i\sigma, \frac{3}{2} + i\sigma; \beta^4)
\]

\[
S^+(0, \alpha_0, \alpha_1, \beta) = -\beta^4 \Gamma[+2i\alpha_0, \frac{1}{2} + i\sigma, \frac{1}{2} + i\sigma] {}_0f_3(1 + 2i\alpha_0, \frac{3}{2} + i\sigma, \frac{3}{2} + i\sigma; \beta^4)
\]

\[
S^-(0, \alpha_0, \alpha_1, \beta) = \Gamma[-2i\alpha_0, \frac{1}{2} - i\sigma, \frac{1}{2} - i\sigma] {}_0f_3(-2i\alpha_0, \frac{1}{2} - i\sigma, \frac{1}{2} - i\sigma; \beta^4)
\]

\[
S^+(0, \alpha_0, \alpha_1, \beta) = -\beta^4 \Gamma[-2i\alpha_0, \frac{1}{2} - i\sigma, \frac{1}{2} - i\sigma] {}_0f_3(1 - 2i\alpha_0, \frac{3}{2} - i\sigma, \frac{3}{2} - i\sigma; \beta^4)
\]

(24)

As a check the previous sections analysis was repeated for the time reversed case, that is to say \( e^{-i\omega t} \to e^{+i\omega t} \) so that incoming and outgoing beams are interchanged, and the final results for these \( ^\dagger S \)-amplitudes was

\[
^\dagger S^+(0, \alpha_0, \alpha_1, \beta) = S^-(0, \alpha_0, \alpha_1, \beta)
\]

\[
^\dagger S^0(0, \alpha_0, \alpha_1, \beta) = S^-(0, \alpha_0, \alpha_1, \beta)
\]

(25)
as would be expected. Finally we should note that the normalization conditions, given in equations (17) and (18), imply a number of identities for our particular combination of hyper-Bessel functions.

4. Special cases

There are a number of limiting cases that can be found from our exact solution, which lead to simpler expressions and which would make contact with the results using approximate methods that are appropriate to the particular regime. These cases are weak and strong coupling, the zero detuning and the semiclassical regimes.

4.1. Weak coupling

When the laser field is weak, as reflected in a small value of the parameter $\beta$ then one can simply take the series representation of the hyper-Bessel functions (see equation (23)) and truncate it at some order. Here we display the results for the lowest few non-trivial orders,

\[
R_0 = \frac{2}{(+2i\alpha_0)(+2i\alpha_1)(1 + 2i\alpha_0)(\frac{1}{2} + i\delta)} \beta^4 + O(\beta^8)
\]

\[
R_1 = -\frac{1}{(+2i\alpha_1)(\frac{1}{2} + i\sigma)} \beta^2 + O(\beta^6)
\]

\[
T_0 = 1 + \frac{(+2i\alpha_1)(\frac{1}{2} + i\delta) + \frac{1}{2} - i\sigma}{(+2i\alpha_0)(+2i\alpha_1)(\frac{1}{4} + \delta^2)(\frac{1}{2} - i\sigma)} \beta^4 + O(\beta^8)
\]

\[
T_1 = -\frac{1}{(+2i\alpha_1)(\frac{1}{2} + i\delta)} \beta^2 + O(\beta^6).
\]

These expressions also satisfy the normalization conditions, namely equation (17), to order $O(\beta^8)$. From these results it is clear that in the case of no coupling the atomic beam is completely transmitted, that in the next lowest order of weak coupling a diffracted ($R_1$) and transmitted beam ($T_1$) emerges (order $\beta^2$), and at the following order one gets a reflected beam ($R_0$) and a reduction in the transmission ($T_0$) of the incident beam (order $\beta^4$). Also it can be observed that the coefficients behave as expected with respect to the detuning $\Delta$, for example $|T_0|$ increases to unity as $\Delta$ increases from zero.

4.2. Large coupling

At the other extreme from the preceding section, we now look at large coupling $\beta \gg 1$ while all other parameters $\alpha_0, \alpha_1$ remain $O(1)$, and in order to do this we appeal to the asymptotic properties of the hyper-Bessel function. The series definition of the hyper-Bessel function has an infinite radius of convergence, and so is valid for large coupling, but it is completely impractical and even misleading to evaluate it in this regime using the series form. The nature of the asymptotic behaviour of the $0f_3$ for a large real positive argument is discussed in some depth in section 6, and the leading-order consists of a sum of an exponential growth term and a subdominant oscillatory component, equation (65),

\[
0f_3(; a, b, c; z) \sim \frac{e^{\theta/4}}{2(2\pi)^{3/2}} \left[ e^{z^{1/4}} + 2\cos \left( \frac{z^{1/4}}{2} + \frac{\pi}{2} \theta \right) \right]
\]

where $\theta \equiv \frac{1}{2} - a - b - c$. There is a fourth component, not displayed here, which is exponentially small. One very important consequence of the form of our reflection and
transmission coefficients and the exact properties of the hyper-Bessel function is that all products of two dominant exponential terms occurring in the numerators and denominators of \( R_0 \) and \( R_1 \) (and the denominators of \( T_0 \) and \( T_1 \) too) given in equation (11) cancel. Thus, we require the full subdominant oscillatory components of the asymptotic expansion. This cancellation is be proven using the results in section 6, namely using equations (61)–(64). Furthermore the resulting leading-order term in the numerator or denominator of a coefficient is a product of a dominant exponential and a subdominant oscillatory factor and this common exponential factor disappears when the ratio is taken.

Taken to the lowest order we have, after much cancellation and simplification for the main beam

\[
R_0 \sim \beta^{-8i\alpha_0} \Gamma \left[ +2i\alpha_0 \right] \left[ \frac{\frac{1}{2} + i\delta}{\frac{1}{2} - i\sigma} \right] \left[ \frac{1 + i\tan(4\beta + \pi/4) \tanh \pi \sigma}{1 - i\tan(4\beta + \pi/4) \tanh \pi \sigma} \right] \tag{28}
\]

and using the reflection properties of the gamma function the modulus of this is

\[
|R_0| \sim \left\{ \frac{1 + \tan^2(4\beta + \pi/4) \tanh^2 \pi \sigma}{1 + \tan^2(4\beta + \pi/4) \tanh^2 \pi \sigma} \right\}^{1/2} \tag{29}
\]

In a similar manner we have for the diffracted beam

\[
R_1 \sim \beta^{-4i4\alpha_0} \Gamma \left[ +2i4\alpha_1 \right] \left[ \frac{\frac{1}{2} + i\sigma}{\frac{1}{2} - i\delta} \right] \left[ \frac{i\tan(4\beta + \pi/4) (\tanh \pi \sigma - \tanh \pi \delta)}{1 - i\tan(4\beta + \pi/4) \tanh \pi \sigma} \right] \tag{30}
\]

and the modulus of this is

\[
|R_1| \sim \left( \frac{\alpha_0}{\alpha_1} \right)^{1/2} \left| \tan(4\beta + \pi/4) \right| \left\{ \frac{\tanh^2 \pi \sigma - \tanh^2 \pi \delta}{1 + \tan^2(4\beta + \pi/4) \tanh^2 \pi \sigma} \right\}^{1/2} \tag{31}
\]

For the transmission amplitudes we have

\[
T_0 \sim \frac{(2\pi)^{3/2} \beta^{-7/2} (-4i\alpha_0) \sech \pi \delta}{4\Gamma[-2i\alpha_0, \frac{1}{2} - i\delta, \frac{1}{2} - i\sigma] \cos(4\beta + \pi/4) \cosh \pi \sigma - i \sin(4\beta + \pi/4) \sinh \pi \sigma} \tag{32}
\]

with \( T_1 \sim T_0 \) so that the magnitude for both is

\[
|T_0| = |T_1| \sim \left( \frac{\alpha_0}{\beta} \sinh 2\pi \alpha_0 \cos \pi \sigma \cos \pi \delta \right)^{1/2} \{\cos^2(4\beta + \pi/4) + \sinh^2 \pi \sigma \}^{-1/2}. \tag{33}
\]

The normalization conditions (17) are satisfied by these expansions of the coefficients to order \( O(\beta^{-1}) \). If one notes the variation of, say, \( |T_0| \) in this regime as \( \Delta \) increases from zero then this coefficient decreases exponentially which seems contrary to what one would expect. However, the results of this regime can only be applied when \( \Delta \ll \beta^2 \), and the exact transmission coefficient for all detuning parameters actually shows that it decreases initially with \( \Delta \), then reverses and rises to approach unity as the detuning continues to grow. Another point of observation, is that all the coefficients have a degree of oscillatory behaviour with respect to the coupling \( \beta \), to the extent that the reflection coefficient of the excited state beam can vanish when \( 4\beta + \pi/4 = n\pi \). To understand this, one can take the zero detuning case in addition, as the effect arises most simply there, and one finds the two dressed states then decouple into two Schrödinger equations with position-dependent wavenumbers

\[
k_0^2(x) = \beta^2(e^{-x_0/2} + e^{-x/2}), \quad 0 \leq x < \infty \tag{34}
\]

\[
k_1^2(x) = \beta^2(e^{-x_0/2} - e^{-x/2}), \quad x_0 \leq x < \infty.
\]
The relative phase shift of the outgoing dressed states, given that the incoming ones are in phase with our choice of boundary conditions, is then given by the phase integrals

\[ \int_0^\infty k_0 \, dx - \int_0^\infty k_1 \, dx + \frac{\pi}{4} \beta \xrightarrow{\beta \to \infty} 4\beta + \frac{\pi}{4}. \] (35)

4.3. Zero detuning

The particular case of zero detuning, in which \( \alpha_1 \to \alpha_0 \equiv \alpha \) or \( \Delta = 0 \), is particularly interesting even though it lacks physical significance due to the maximal state mixing by spontaneous emission in this regime. In the dressed state picture the two quasipotentials are separated by \( \hbar \Delta_{\text{eff}} \) and so the situation with a positive value is physically distinct from that in which it is negative. The parameter \( \alpha_0 \) or \( \alpha \) now represents the \( y \)-component of the incoming atomic beam.

Mathematically the simplification which arises in this case, taking the series representation, is that one of the hypergeometric parameters becomes degenerate \( \frac{1}{2} \pm i(\alpha_0 - \alpha_1) \to \frac{1}{2} \), and the four factorial factors coalesce into two by using the duplication formulae for the gamma function. In this way the \( f_3 \) reduces to \( f_1 \), that is to say the standard Bessel functions. It is found that the wavefunction becomes

\[
\psi_0(x) = \psi_0[-I_{4\alpha}(4\beta e^{-x/\alpha})L_{1-4\alpha}(4\beta) - J_{4\alpha}(4\beta e^{-x/\alpha})J_{1-4\alpha}(4\beta)]
\]

\[+I_{-4\alpha}(4\beta e^{-x/\alpha})I_{1+4\alpha}(4\beta) - J_{-4\alpha}(4\beta e^{-x/\alpha})J_{1+4\alpha}(4\beta)]
\]

\[+\psi_1[I_{4\alpha}(4\beta e^{-x/\alpha})L_{1-4\alpha}(4\beta) - J_{4\alpha}(4\beta e^{-x/\alpha})J_{1-4\alpha}(4\beta)]
\]

\[+I_{-4\alpha}(4\beta e^{-x/\alpha})I_{1+4\alpha}(4\beta) - J_{-4\alpha}(4\beta e^{-x/\alpha})J_{1+4\alpha}(4\beta)] \] (36)

and the \( S \)-amplitudes are

\[
S_{00}^+ = S_{11}^+ = (2\beta)^{1-4\alpha} \Gamma(4\alpha) \frac{1}{2} [I_{1+4\alpha}(4\beta) - J_{1+4\alpha}(4\beta)]
\]

\[
S_{00}^- = S_{11}^- = (2\beta)^{1+4\alpha} \Gamma(-4\alpha) \frac{1}{2} [-I_{1+4\alpha}(4\beta) - J_{1+4\alpha}(4\beta)]
\]

As remarked above for the asymptotic expansion in large couplings, an exact cancellation of the exponentially dominant terms occurs in the cross products of the \( S \)-functions, and this occurs here in the exact expressions. All the products of the modified Bessel functions and of the products of the \( I \) and \( J \) Bessel functions cancel exactly leaving products of \( I \) and \( J \) Bessel functions. The reflection and transmission amplitudes are given by

\[ R_0 = (2\beta)^{-8\alpha} \Gamma \begin{bmatrix}
4\alpha \\
-4\alpha
\end{bmatrix} \begin{bmatrix}
\frac{1}{2} & \{ I_{1+4\alpha}(4\beta) \} \\
\{ I_{1-4\alpha}(4\beta) \} & \{ J_{1+4\alpha}(4\beta) \}
\end{bmatrix}
\]

\[ R_1 = -(2\beta)^{-8\alpha} \Gamma \begin{bmatrix}
4\alpha \\
-4\alpha
\end{bmatrix} \begin{bmatrix}
\frac{1}{2} & \{ I_{1+4\alpha}(4\beta) \} \\
\{ I_{1-4\alpha}(4\beta) \} & \{ J_{1+4\alpha}(4\beta) \}
\end{bmatrix}
\]

\[ T_0 = (2\beta)^{-1-4\alpha} \Gamma \begin{bmatrix}
1 \\
\frac{1}{2}
\end{bmatrix} \begin{bmatrix}
1 & \{ I_{1-4\alpha}(4\beta) \} \\
\{ J_{1-4\alpha}(4\beta) \}
\end{bmatrix}
\]

\[ T_1 = (2\beta)^{-1+4\alpha} \Gamma \begin{bmatrix}
1 \\
\frac{1}{2}
\end{bmatrix} \begin{bmatrix}
1 & \{ J_{1-4\alpha}(4\beta) \} \\
\{ J_{1-4\alpha}(4\beta) \}
\end{bmatrix} \] (38)

Several cross-checks of this result can be made with our earlier expressions. First the small coupling limit \( \beta \to 0 \) of equations (38) can be shown to lead to the same result as the
zero detuning limit of the small coupling case, as in section 4.1, equation (26). A similar
correlation of the large coupling limit of the above expressions with the zero detuning limit
of the large coupling case of section 4.2, equations (28), (30) and (32) also yield identical
results. Furthermore, the above coefficients can be shown to satisfy the normalization
condition (17) exactly by using the Wronskian and recurrence relations for the \( I, J \) Bessel
functions. Again oscillatory dependence of the coefficients on the coupling \( \beta \) is evident
here as well, as can be seen from the occurrence of the \( J \) Bessel functions.

We will need to consider some other limiting cases of the above expressions, so that
we can make connection with other approximate forms of the exact case. Specifically we
use the recent expansions for the Bessel functions given by Dunster (1990) and Temme
(1994) for a large real argument and large imaginary order. For the \( J \) Bessel function the
full expansion is

\[
J_{-iv}(vz) \sim \left( \frac{2}{\pi v} \right)^{1/2} (1 + z^2)^{-1/4} \left\{ \cos \left( v\xi - \pi/4 + \frac{1}{2} \pi iv \right) \sum_{s=0}^{\infty} (-)^s \frac{U_{2s}(\xi)}{\pi^{2s+1}} + \sin \left( v\xi - \pi/4 + \frac{1}{2} \pi iv \right) \sum_{s=0}^{\infty} (-)^s \frac{U_{2s+1}(\xi)}{\pi^{2s+2}} \right\}
\]

(39)

with \( p = (1 + z^2)^{-1/2} \) and

\[
\xi = \ln \left( \frac{z}{1 + \sqrt{1 + z^2}} \right) + \sqrt{1 + z^2}
\]

(40)

and which is valid when \( |\arg(z)| < \pi/2 \), real \( v > 0 \). While the modified \( I \) Bessel function
has the expansion

\[
I_{-iv}(vz) \sim \frac{e^{\pi v/2}}{2^{1/3} v^{1/3}} \left\{ \sum_{s=0}^{\infty} (-)^s \frac{A_s(\xi)}{v^{2s+1}} + \sum_{s=0}^{\infty} (-)^s \frac{B_s(\xi)}{v^{2s+4/3}} \right\}
\]

(41)

with

\[
2 s^{3/2} = \ln \left( \frac{1 + \sqrt{1 - z^2}}{z} \right) - \sqrt{1 - z^2}
\]

(42)

and the standard Airy functions \( A_i, B_i \) (the above is a corrected version of the result in
Dunster (1990)). This is valid when \( |\arg(z)| < \pi \) and \( v > 0 \). The coefficients \( U_{2s}, U_{2s+1},
A_s, B_s \) are given in the above references but we require only the first members, which are
tall enough. With these expressions it is easy to show that the Bessel functions appearing
in our coefficients have leading-order terms of the form, starting with the modified Bessel
function

\[
(2\pi \beta)^{1/2} I_{-4\alpha}(4\beta) \sim e^{2\pi \alpha - \pi i/4} \pi^{1/2} [\sin \epsilon]^{-1/2} \times [e^{-\pi i/12} \cos \epsilon \beta \text{Im} (h)]^{1/6} A_i(e^{2\pi i/3} |\beta\text{Im} (h)|^{2/3}) - e^{\pi i/12} \sin \epsilon \beta \text{Im} (h)]^{1/6} A_i(e^{2\pi i/3} |\beta\text{Im} (h)|^{2/3})
\]

(43)

with the definitions \( \cos \epsilon = \hat{\alpha} \equiv \alpha / \beta \) and \( \beta \text{Im} (h) = 6\alpha \tan \epsilon - 6\alpha \epsilon \). The corresponding
case for the \( J \) Bessel function is

\[
(2\pi \beta)^{1/2} J_{-4\alpha}(4\beta) \sim (\hat{\alpha}^2 + 1)^{-1/4} \cosh(iX - U - 2\pi \alpha)
\]

(44)

with \( iX - U = 4\beta \sqrt{\hat{\alpha}^2 + 1} - (1 + 4i\alpha) \ln(\sqrt{\hat{\alpha}^2 + 1} + \hat{\alpha}) + \pi i/4 \). The apparent arbitrariness
in our choice of notation in both these cases will be made clear when we come to discuss
the uniform semiclassical approximation in sections 4.4 and 7.
4.4. Uniform semiclassical approximation

If one fixes the kinetic energy of the ground- and excited-state beams and the Rabi frequency, while letting \( \hbar \) tend to zero we enter the semiclassical regime where in terms of our dimensionless variables \( \alpha_0^2, \alpha_1^2, \beta^2 \to \infty \). In sections 6 and 7 we have developed such an expansion for the \( \alpha_0^2, \alpha_1^2 \) functions whereby the ratios \( \hat{\alpha}_0 \equiv \alpha_0/\beta, \hat{\alpha}_1 \equiv \alpha_1/\beta \) are fixed that is valid for all parameters regimes including in the region of the classical turning points. We also use the ratios \( \delta \equiv \delta/\beta, \hat{\alpha}_0 \equiv \hat{\alpha}_0/\beta, \hat{\alpha}_1 \equiv \hat{\alpha}_1/\beta \) as parameters, any two of which are independent. The intermediate result for the uniform semiclassical approximation of one of the transmission coefficients, the tunnelling loss \( |T_0| \), is given in equations (102) and (103). Again we refer the reader to Witte (1996) for results on the other coefficients. These formulae need to be used in conjunction with the explicit roots to a quartic and all the derived quantities that are described in the discussion following these equations. Using all of the analysis presented in section 7 to carry out the process of assembling these pieces and making all possible simplification we arrive at our final expression for \( |T_0| \). We give the most general result for this coefficient, but with the only restriction that \( \alpha_0^2 \alpha_1^2 < \beta^2 \), so that we have a classical turning point. The result is

\[
|T_0|^2 \sim 2M\hat{\alpha}_0^4 + \sin^4 \chi \sinh 2\pi \omega_0 \cosh \pi \sigma \cosh \pi \delta 
\times \left[ e^{-\pi i/2} [B^{(+)} e^{W+i\pi-2i\gamma} + B^{(-)} e^{-W-i\pi+2i\gamma}] + 2\alpha_0 M^{-1/2} e^{-\pi \sigma} \cosh(iX - V - 2i\alpha_1)^2 \right. 
\left. \div e^{-\pi i/2} [B^{(+)} e^{W-2i\gamma \alpha_1+iX-1/2iU+1/2U-i\pi + i\pi}] + B^{(-)} e^{-W+2i\gamma \alpha_1-iX+1/2iU+1/2U+i\pi - i\pi}] \right] 
\times \cosh(1/2 V - 1/2 U + 1/2iY) \cosh(\pi \delta - 1/2iY) 
\times \left[ B^{(+)} e^{W-2i\gamma \alpha_1-iX+1/2iU+1/2iY+i\pi + i\pi}] + B^{(-)} e^{W+2i\gamma \alpha_1+iX-1/2iU-1/2iU-i\pi - i\pi}] \right] 
- \hat{\alpha}_0 M^{-1/2} e^{-\pi \sigma} \sinh(V - U) \sinh(2\pi \delta)^2
\]

where in addition to \( \chi \) defined by equation (87) the auxiliary variables take the following definitions

\[
M \equiv \sqrt{\hat{\alpha}_0^2 + \sin^2 \chi} \quad e^{2U} \equiv \frac{M + \hat{\alpha}_0^2}{M - \hat{\alpha}_0^2} \quad e^{2V} \equiv \frac{M + \hat{\alpha}_0 \hat{\alpha}_1}{M - \hat{\alpha}_0 \hat{\alpha}_1}
\]

\[
X \equiv 4BM/\hat{\alpha}_0 + \pi/4 - 2U\alpha_0 - 2V\alpha_1 \quad \sin \gamma \equiv \hat{\alpha}_0 \hat{\alpha}_1 \tan \epsilon 
\]

\[
W \equiv i\epsilon + 4\alpha_0 \tan \epsilon - 2\sigma \epsilon - 1/4i.
\]

In addition the Airy function phase terms, \( B^{(+)}(\cdot), B^{(-)}(\cdot) \) arising from the classical turning points have the forms

\[
B^{(+)} = \pi^{1/2} e^{-\pi/2}[\beta] \left[ e^{-\pi i/3} [\beta] [\text{Im}(h)^3]^{1/6} \text{Ai}(e^{\pi i/3} [\beta] [\text{Im}(h)^3]^{1/6}) \right] 
+ e^{\pi i/3} [\beta] [\text{Im}(h)^3]^{1/6} \text{Ai}'(e^{\pi i/3} [\beta] [\text{Im}(h)^3]^{1/6})
\]

\[
B^{(-)} = \pi^{1/2} e^{\pi i/2}[\beta] \left[ e^{\pi i/6} [\beta] [\text{Im}(h)^3]^{1/6} \text{Ai}(e^{\pi i/3} [\beta] [\text{Im}(h)^3]^{1/6}) \right] 
+ e^{-\pi i/6} [\beta] [\text{Im}(h)^3]^{1/6} \text{Ai}'(e^{\pi i/3} [\beta] [\text{Im}(h)^3]^{1/6})
\]

where \( \text{Im}(h) \) is given by equation (101).

If one takes the limit \( \hat{\alpha}_0, \hat{\alpha}_1 \to 0 \) of the above approximation to the transmission coefficient then one recovers the large coupling expression given in equation (33). Using equation (47) for the phase functions it is possible to show that the combinations of these
functions appearing in the transmission coefficient approaches a weakly varying function (of $|\text{Im} \,(h)|$) for large arguments as the individual phase functions approach unity (see following equation (78)), while for small arguments they go over to constant values as the divergent individual terms combine to cancel exactly. To see this it is necessary to note that $\beta |\text{Im} \,(h)| \sim \alpha_0 M^2 \epsilon^3 \alpha_0^2 \alpha_1^2 \alpha_1 \rightarrow 1$ or $\epsilon \rightarrow 0$. There is another limit which yields a check on our general result and that is the zero detuning case. It is possible to show that this limit of equation (45) is identical to the limit $\alpha, \beta \rightarrow \infty$ of the zero detuning case, namely equations (38), using the uniform asymptotic expansions of the Bessel functions as given in equations (43) and (44).

The case where a classical turning point exists is also the only one treated in any detail by Deutschmann et al (1993a) and their estimate of the tunnelling loss, when expressed in our notation, is

$$|T_0|^2 \sim e^{-2\tau}$$

where the tunnelling depth is $\tau = \frac{2}{3} \beta \text{Im} \,(h)$, using equation (101). This is just the WKB expression for tunnelling through the adiabatic potential barrier and is not appropriate for small detuning parameters or large couplings. Such factors are clearly present in our uniform semiclassical result (see the phase factors in equation (47)), but the full result is clearly more complex than this, and our result remains closer to the exact result over all parameter ranges than equation (48), as one can see from figure 1. The oscillatory behaviour with coupling, found in the large coupling and zero detuning cases, can also be found here, in its most general form, through the phase angle $X$ in equation (46). We do not exhibit the results for the other amplitudes $T_1, R_0, R_1$ but similar results for these could be easily found from the analysis of section 7.

5. Solution method

There are many ways to proceed from the formulation of the model, as given in equations (5) and (6), towards the exact solutions. One way applied many times before is to recast the two coupled second-order differential equations into a single fourth-order one, transform the independent variable $z \equiv e^{-x \beta} \frac{d}{dx}$ and arrive at the following

$$[D + i\alpha_0][D - i\alpha_0][D - \frac{1}{2} + i\alpha_1][D - \frac{1}{2} - i\alpha_1] \psi_0 - z \psi_0 = 0$$

(49)

where $D \equiv z d/dz = -d/dx$. One can then immediately identify the solution with the hypergeometric or Meijer $G$-functions and apply the boundary conditions. However, we pursue a different approach of deriving the solution from first principles, which has significant advantages that will become apparent later.

Given that our system is a homogeneous, the linear differential equation system defined on the half-interval it is an obvious candidate for application of the Laplace transformation, $\Phi_{0,1}(t) \equiv \int_0^\infty e^{-st} \psi_{0,1}(x) \, dx$ (50) valid for Re $< 0$. Eliminating, say $\Psi_1$, from the coupled difference equations results in the following first-order inhomogeneous difference equation

$$[(t + \frac{1}{2})^2 + \alpha_1^2] \psi_0(t) - \beta^4 \psi_0(t + 1)$$

$$\equiv [(t + \frac{1}{2})^2 + \alpha_1^2] \psi_0(t) + t \psi_0(t) - \beta^2 \psi_1(t)$$

(51)

defined on the complex $t$ half-plane.
Reflection and diffraction of atomic de Broglie waves

Figure 1. A comparison of the uniform semiclassical approximation (USCA) to the transmission coefficient $T_0$ (see equation (45)) with the Deutschmann et al (1993a) WKB approximation (DEW) (see equation (48)), versus the detuning parameter $\Delta$. Both coefficients are normalized with respect to the exact coefficient and the dimensionless parameter values are $\alpha_0 = 2$, $\beta = 4$.

Because this difference equation is only first order and has coefficients which are polynomial in $t$ it is immediately soluble. The homogeneous term in the solution must be zero because of two considerations—first, the inversion integral must be convergent and the homogeneous term contains a factor which is periodic in $t$ with real period 1, and secondly because the inhomogeneous term is the only term which is a linear combination of the four boundary values of the wavefunctions $\psi_0, \psi_0', \psi_1,$ and $\psi_1'$. So the solution for the inversion integrand is

$$\Psi_0(t) = \sum_{m=0}^{\infty} \left( -\beta^{4m+2} [\psi_1'(0) + (t + m + \frac{1}{2})\psi_1(0)] \right)$$

$$\times \Gamma \begin{bmatrix} t + i\alpha_0 & t - i\alpha_0 & t + \frac{1}{2} + i\alpha_1 & t + \frac{1}{2} - i\alpha_1 \\ t + m + 1 + i\alpha_0 & t + m + 1 - i\alpha_0 & t + m + \frac{3}{2} + i\alpha_1 & t + m + \frac{3}{2} - i\alpha_1 \end{bmatrix}$$
\[ + \beta_{2m} \left[ \psi_0(0) + (t + m) \psi_0(0) \right] \times \Gamma \left[ \begin{array}{cccc}
t + i \alpha_0 & t - i \alpha_0 & t + \frac{1}{2} + i \alpha_1 & t + \frac{1}{2} - i \alpha_1 \\
t + m + 1 + i \alpha_0 & t + m + 1 - i \alpha_0 & t + m + \frac{1}{2} + i \alpha_1 & t + m + \frac{1}{2} - i \alpha_1 \
\end{array} \right] \] (52)

where \( \Gamma \) is the symbolic notation for the products of gamma functions.

\[ \Gamma \left[ \begin{array}{cccc}a_1 \ldots a_n \\ b_1 \ldots b_m \end{array} \right] = \prod_{n=1}^{a_n} \Gamma(a_n) / \prod_{n=1}^{b_n} \Gamma(b_n) \] (53)

The \( m \)th term of the integrand has the following finite sequences of simple poles to the left of the contour \( t = -l + i \alpha_0 \) for \( l = 0 \ldots m \) and \( t = -l - \frac{1}{2} + i \alpha_1 \) for \( l = 0 \ldots m \), and one can simplify the integral by deforming the contour to enclose these poles. If in addition one employs the boundary conditions equations (6) one arrives at the following series representation for the solution

\[ \psi_0(x) = \sum_{m=0}^{\infty} \sum_{l=0}^{m} \beta_{4m} \frac{(-)^l}{l!(m-l)!} \times \left\{ e^{-tx - i\alpha_x} \left[ \begin{array}{c} -\beta^2 \psi_1 \\
(\psi_0)
\end{array} \right] \right. \\
+ e^{-tx + i\alpha_x} \left( \begin{array}{c} (\psi_0) \\
(-l - 2i\alpha_0)_m (-l + \frac{1}{2} + i\delta)_m (-l + \frac{1}{2} - i\sigma)_m \\
\end{array} \right) \\
+ e^{(t+\frac{1}{2})x - i\alpha_{1x}} \left( \begin{array}{c} (\psi_0) \\
(-l - 2i\alpha_1)_m (-l - \frac{1}{2} + i\delta)_m (-l - \frac{1}{2} - i\sigma)_m \\
\end{array} \right) \\
+ e^{(t+\frac{1}{2})x + i\alpha_{1x}} \left( \begin{array}{c} (\psi_0) \\
(-l + 2i\alpha_1)_m (l - \frac{1}{2} - i\delta)_m (l - \frac{1}{2} + i\sigma)_m \\
\end{array} \right) \\
+ e^{(t+\frac{1}{2})x + i\alpha_{1x}} \left( \begin{array}{c} (\psi_0) \\
(-l + 2i\alpha_1)_m (l - \frac{1}{2} - i\delta)_m (l - \frac{1}{2} + i\sigma)_m \\
\end{array} \right) \left\{ \right. \] (54)

where \((a)_n = \Gamma(a + n) / \Gamma(a)\) is the standard Pochhammer symbol. So one can see that the advantage of solving this model with a Laplace transform approach is that we have incorporated the boundary condition (6) easily and also effected considerable simplification. It is possible to further simplify this result and re-express it in terms of a generalized hypergeometric function by explicitly performing the \( m \) and \( l \) summations. By reversing the order of the \( m-l \) summations, into two infinite summations over \( q = m-l \) and \( l \), a clean factorization of the summand gamma functions into a \( q \)-dependence and a \( l \)-dependence occurs, thus allowing both summations to be done. This yields the final result given in equation (22). From our analysis it is clear why this class of functions should arise in the travelling wave or two beam problem—on the one hand we have a pair of quadratic
coefficients in the first-order difference equation (51), and equivalently in real-space we have a fourth-order ordinary differential equation—both leading to the hyper-Bessel function $0_f^3$.

6. The $0_f^3$ hyper-Bessel functions

In this half of our work we discuss the more mathematical properties of the hyper-Bessel functions that are motivated by the physical applications just discussed, and in addition we describe some of a general nature by way of a background to these functions as they are not so commonly used or widely known. They have been discussed for some time, since the times of Barnes, as a special case of generalized hypergeometric functions or their generalization to the Meijer $G$-functions, but it is only since the work of Delerue have the specific incarnations been investigated in the form we have employed. In a series of papers Delerue (1949, 1950a, b, 1953a, b) investigated the natural generalizations of the Bessel functions $J_\nu(x), I_\nu(x)$ etc to the functions $0_f^n$ for arbitrary integer $n$. In these works many properties are derived—the generating functions, the addition formulae, recurrence relations, the ordinary differential equations, Poisson-type integral representations, Sonine-type integral representations, and Weber integrals. The succeeding work has been performed by the Bulgarian School around Dimovski and Kiryakova where these functions have been approached using fractional calculus. For instance results for Poisson representations of hyper-Bessel functions have been found using fractional integrals. The work of many papers (see Dimovski and Kiryakova 1986, 1987 and Kiryakova 1987a, b) has been summarized in the recent monograph Kiryakova (1994). To simplify notational matters we consider the function

$$0_f^3(\rho_1, \rho_2, \rho_3; z) \equiv 0_f^3(a, b, c; z) \quad (55)$$

and will use the two forms interchangeably throughout the paper.

6.1. Connection relations

This function satisfies a fourth-order ordinary differential equation

$$D \prod_{i=1}^3 (D + \rho_i - 1)U - zU = 0 \quad (56)$$

where $D \equiv zd/dz$, which has a regular singular point at $z = 0$ and an irregular singular point at $z = \infty$. The fundamental system of four linearly independent solutions in the neighbourhood of $z = 0$ including the one given above are the following

$$U_1(a, b, c; z) = 0_f^3(a, b, c; z)$$
$$U_2(a, b, c; z) = z^{1-a}0_f^3(2 - a, 1 + b - a, 1 + c - a; z)$$
$$U_3(a, b, c; z) = z^{1-b}0_f^3(2 - b, 1 + a - b, 1 + c - b; z)$$
$$U_4(a, b, c; z) = z^{1-c}0_f^3(2 - c, 1 + a - c, 1 + b - c; z). \quad (57)$$

The Wronskian for this fundamental set is

$$W[U_1, U_2, U_3, U_4] = \frac{\prod_{i=1}^3 \sin \pi \rho_i \prod_{1 \leq i < j \leq 3} \sin \pi (\rho_i - \rho_j)}{\pi h_2^3 + \sum \rho_i}. \quad (58)$$

For our purposes this set of four will always be linearly independent, because our parameters do not lead to degeneracy, and so we do not have to consider logarithmic solutions. There are also four linearly independent solutions of the fundamental system in
the neighbourhood of \( z = \infty \) and we define these according to their asymptotic behaviour in the following way

\[
E(a, b, c; z) \sim 2^{-5/2} \pi^{-3/4} z^{3/4} e^{-i \pi} z^{3/4} \varepsilon^{1/4}
\]

\[
D(a, b, c; z) \sim 2^{-5/2} \pi^{-3/4} z^{3/4} e^{-i \pi} \varepsilon^{1/4} z^{3/4}
\]

\[
C(a, b, c; z) \sim 2^{-5/2} \pi^{-3/4} z^{3/4} \cos \left( 4 \pi z^{1/4} + \frac{\pi}{2} \theta \right)
\]

\[
S(a, b, c; z) \sim 2^{-5/2} \pi^{-3/4} z^{3/4} \sin \left( 4 \pi z^{1/4} + \frac{\pi}{2} \theta \right)
\]

(59)

The \( \mp \) sign in the phase of \( D \) is the manifestation of the Stokes phenomena across the positive real axis, which is the ray along which the solution \( D \) has maximal subdominance. One notes that all four of this fundamental set have an essential singularity at \( z = \infty \). Then the exact connection equations between the two sets of solutions are the following

\[
U_1 = E + 2C + D
\]

\[
U_2 = E + 2 \cos(2\pi a)C - 2 \sin(2\pi a)S + e^{\mp i\pi} \varepsilon^4 D
\]

\[
U_3 = E + 2 \cos(2\pi b)C - 2 \sin(2\pi b)S + e^{\mp i\pi} \varepsilon^4 D
\]

\[
U_4 = E + 2 \cos(2\pi c)C - 2 \sin(2\pi c)S + e^{\mp i\pi} \varepsilon^4 D
\]

(60)

The eight \( S \)-amplitudes of the exact solution, equation (37), can be divided into two sets when viewed as solutions of the defining differential equation of the hyper-Bessel function. From the first set \( \{ S_{00}^+, S_{00}^-, S_{10}^+ S_{10}^- \} \) a fundamental system of solutions to the ordinary differential equation (ODE) with \( a = 2 + 2i\alpha_0, b = \frac{3}{2} + i\delta, c = \frac{3}{2} + i\sigma \) can be constructed

\[
S_{00}^+ \rightarrow s_{01} \equiv f_3(2 + 2i\alpha_0, \frac{3}{2} + i\delta, \frac{3}{2} + i\sigma; \beta^4)
\]

\[
S_{00}^- \rightarrow s_{02} \equiv \beta^{-4i\alpha_0} f_3(-2i\alpha_0, \frac{1}{2} - i\delta, \frac{1}{2} - i\sigma; \beta^4)
\]

\[
S_{10}^+ \rightarrow s_{03} \equiv \beta^{-2i\alpha_1} f_3(1 + 2i\alpha_1, \frac{1}{2} - i\delta, \frac{3}{2} + i\sigma; \beta^4)
\]

\[
S_{10}^- \rightarrow s_{04} \equiv \beta^{-2i\alpha_1} f_3(1 - 2i\alpha_1, \frac{3}{2} + i\delta, \frac{1}{2} - i\sigma; \beta^4).
\]

(61)

From the second set \( \{ S_{11}^+, S_{11}^-, S_{01}^+, S_{01}^- \} \) a fundamental system of solutions to the ODE with \( a = 2 + 2i\alpha_1, b = \frac{3}{2} - i\delta, c = \frac{3}{2} + i\sigma \) can be constructed

\[
S_{11}^+ \rightarrow s_{11} \equiv f_3(2 + 2i\alpha_1, \frac{3}{2} - i\delta, \frac{3}{2} + i\sigma; \beta^4)
\]

\[
S_{11}^- \rightarrow s_{12} \equiv \beta^{-4i\alpha_1} f_3(-2i\alpha_1, \frac{1}{2} + i\delta, \frac{1}{2} - i\sigma; \beta^4)
\]

\[
S_{01}^+ \rightarrow s_{13} \equiv \beta^{-2i\alpha_0} f_3(1 + 2i\alpha_0, \frac{3}{2} + i\delta, \frac{3}{2} + i\sigma; \beta^4)
\]

\[
S_{01}^- \rightarrow s_{14} \equiv \beta^{-2i\alpha_1} f_3(1 - 2i\alpha_0, \frac{3}{2} - i\delta, \frac{1}{2} - i\sigma; \beta^4).
\]

(62)

Then the connection with the fundamental system having asymptotic growth \( E_0 \), evanescent decay \( D_0 \), and cosine \( C_0 \) and sine \( S_0 \) oscillatory behaviours is, in the case of the first set,

\[
s_{01} = E_0 + 2C_0 + D_0
\]

\[
s_{02} = E_0 + 2 \cosh(4\pi \alpha_0)C_0 - 2i \sinh(4\pi \alpha_0)S_0 + e^{\pm 8i \alpha_0} D_0
\]

\[
s_{03} = E_0 - 2 \cosh(2\pi \delta)C_0 + 2i \sinh(2\pi \delta)S_0 + e^{\pm 4i \delta} D_0
\]

\[
s_{04} = E_0 - 2 \cosh(2\pi \sigma)C_0 + 2i \sinh(2\pi \sigma)S_0 + e^{\pm 4i \sigma} D_0
\]

(63)
and in the case of the second set,
\[ s_{11} = E_1 + 2C_1 + D_1 \]
\[ s_{12} = E_1 + 2 \cosh(4\pi\alpha_1)C_1 - 2i \sinh(4\pi\alpha_1)S_1 + e^{4\pi\alpha_1}D_1 \]
\[ s_{13} = E_1 - 2 \cosh(2\pi\delta)C_1 - 2i \sinh(2\pi\delta)S_1 + e^{2\pi\delta}D_1 \]
\[ s_{14} = E_1 - 2 \cosh(2\pi\sigma)C_1 + 2i \sinh(2\pi\sigma)S_1 + e^{2\pi\sigma}D_1. \]

Using equations (63) and (64) it is then straightforward to show that all products of the form \( E_0 E_1 \) in the numerators and denominators of a reflection or transmission coefficient combine to cancel exactly.

6.2. Asymptotic regime

In the large coupling regime one might require accurate evaluation of the hyper-Bessel functions beyond just the lowest order and recursive procedures have been found to generate higher-order terms. The leading-order terms were first found by Wrinch (1921a, b) and later in Wright (1935, 1940), Braaksma (1963) for the specific hyper-Bessel function \( n = 3 \) and the general case \( 0 f_n \), and the specific results were rederived in Heading and Whipple (1952). The extension to higher-order terms had been completed by Wrinch (1923), Riney (1956, 1958), and Wright (1958), and is laid out in the works by Luke (1969) and Paris and Wood (1986). The full asymptotic expansion is (after dropping the exponentially damped terms)

\[ 0 f_3(a, b, c; z) \sim \frac{e^{a/4}}{2(2\pi)^{3/2}} \left\{ e^{b/4} \sum_{j=0}^{\infty} z^{-j/4} N_j \right\} \]

where \( \theta \equiv \frac{3}{2} - a - b - c \) and the coefficients \( N_j \) are functions of \( a, b, \) and \( c \). The lowest order has \( N_0 = 1 \) while the next two orders can be found in Witte (1996).

7. Uniform semiclassical approximation

Motivated by interest in semiclassical approximations to the exact solution we derive here the asymptotic expression for the hyper-Bessel function for large parameters and arguments. We require as our starting point an integral representation for the hyper-Bessel function, but neither the Poisson–Dimovski transformation equation nor the generalized Poisson-type integral representation quoted in Kryakova (1994) are suitable. A simple multidimensional representation for the hyper-Bessel function can be found by utilizing the Laplace formula for the gamma function

\[ \frac{1}{\Gamma(z)} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} du \ e^{a+iu}(a+iu)^{-z} \]

which is valid for any real positive \( a \) and \( \text{Re}(z) > 0. \) By expressing the denominator gamma functions in the series definition in this way, and interchanging the order of summation and integrations the sum can be performed, yielding

\[ 0 f_3(\rho; z) = \frac{1}{(2\pi)^{3/2}} \int_{R^3} \int_{R^3} \int_{R^3} du_1 du_2 du_3 \]

\[ \times \exp \left\{ \sum_{j=1}^{3} (a_j + iu_j - \rho_j \ln(a_j + iu_j)) + z \prod_{j=1}^{3} (a_j + iu_j)^{-1} \right\}. \]
The significance of this representation is that it is explicitly symmetrical in the parameter arguments \( \rho_j \).

We choose to express the hyper-Bessel function in terms of new scaled variables, that is we take \( z = \beta^4 \) and scale the variables with a large real positive number \( \lambda \), thus

\[
\beta = \lambda b \quad \rho_j = \lambda \rho_j + r_j \quad a_j = \lambda c_j \quad u_j = \lambda v_j
\]

with \( b, p_j, r_j, c_j \) all of order \( O(1) \). Applying this to the integral representation (67) we arrive at a three-dimensional stationary-phase integral

\[
0 f_3(\beta; \rho^4) = (2\pi)^{-3/2} \int_{R^3} d^3 v g(v) e^{i \lambda f(v)}
\]

with \( f(v) = \sum_{j=1}^3 [X_j + i p_j \ln(X_j)] + b^4 \prod_{j=1}^3 X_j^{-1} \quad g(v) = \prod_{j=1}^3 X_j^{-r_j} \quad X_j = v_j - i c_j \).

To ensure convergence we have to require \( \text{Re} (p_j) > 0 \), whereas in our final application these parameters will be completely imaginary. We will proceed making all the necessary assumptions in order to apply certain theorems, and will appeal to analytic continuation arguments to make our specific applications. Using the standard theory to leading order of the saddle-point method, see Wong (1989) and Connor (1973a). The contribution from one critical point is

\[
\int_{R^n} d^n v g(v) e^{i \lambda f(v)} \sim \left( \frac{2\pi i}{\lambda} \right)^{n/2} (\det A_0)^{-1/2} g(v_0) e^{i \lambda f(v_0)}
\]

where \( v_0 \) is the critical point and \( A_0 \) is the Hessian matrix of \( f \) at the critical point. We have chosen this particular manifestation of the saddle-point method because our critical point, and the Hessian elements will in general be complex, and not real. This expression only applies for isolated critical points, and we will have need to consider a generalization of this later. The critical points, \( t_0 \), are given by the solutions to the following quartic

\[
q(t) = t^4 - \prod_{j=1}^3 (1 + R_j t)
\]

where \( p_j/b = i R_j \) and the \( R_j \) are purely real, and where \( X_j^0 = b R_j + b/t_0 \). The Hessian matrix is given by

\[
A_{ij} = \left( \frac{\partial^2 f}{\partial X_i \partial X_j} \right)_0 = b^{-1} I_n \delta_{ij} d_j^{-1} + d_i^{-1} d_j^{-1}
\]

where \( d_j \equiv 1 + R_j t \). It is easy to establish that the determinant of this is

\[
|A_0| = b^{-3} t_0^{-1} \left[ 1 + \sum_{j=1}^3 d_j^{-1} \right]_0 = b^{-3} t_0^{-4} \frac{dq}{dt} \biggr|_0.
\]

What is clear from these expressions is that the Hessian can become degenerate when \( 1 + \sum_j d_j^{-1} = 0 \), and the occurrence of this is directly related to that of multiple roots to the quartic, i.e. that some critical points can coalesce.

While the roots of the quartic are distinct the leading-order term for the expansion is

\[
0 f_3(\beta; \rho^4) \sim \sum_{j=1}^3 (2\pi)^{-3/2} \left( \frac{\beta}{t} \right)^{3/2} \prod_{j=1}^3 d_j^{1/2 - \rho_j} \left[ 1 + \sum_{j=1}^3 d_j^{-1} \right]^{-1/2} \exp \left\{ 4i \beta/t + i \beta \sum_{j=1}^3 R_j \right\}
\]

(75)
Reflection and diffraction of atomic de Broglie waves

with the sum over all critical points. Care has to be exercised when using this equation and its generalization with regard to the branches chosen because of the algebraic branch points. The arguments of \( t, d_j, 1 + \sum d_j^{-1} \) are decided by restricting \( 0 \leq \arg(t) < 2\pi, \) i.e. we cut the \( t \)-plane along the positive real axis.

However, because two critical points can coalesce the above asymptotic expansion will fail in the region of the classical turning points. There exist uniform asymptotic expansions to cover precisely this case and which are valid everywhere in the \( \hat{\sigma} - \hat{\delta} \) plane (Wong 1989, Connor 1973a). In this generalization the contributions due to the two coalescing critical points at \( v_+ , v_- \rightarrow v_0 \) becomes

\[
\int_{R^n} dx v g(v) e^{i\phi(v)} \sim \left( \frac{2\pi i}{\lambda} \right)^{n/2} \left\{ B^{(+)}(-\lambda^{2/3} \zeta) \frac{g(v_+)}{(\det A_+)^{1/2}} e^{i\phi(v_+)} \\
+ B^{(-)}(-\lambda^{2/3} \zeta) \frac{g(v_-)}{(\det A_-)^{1/2}} e^{i\phi(v_-)} \right\}
\]

(76)

where now

\[
\frac{4}{3} \xi^{3/2} \equiv f(v_-) - f(v_+)
\]

(77)

and

\[
B^{(\pm)}(-z) \equiv \pi^{1/2} e^{\mp i(\pm^{3/2} - \frac{1}{4})} \left\{ z^{1/4} Ai(-z) \pm iz^{-1/4} A'(-z) \right\}
\]

(78)

with \( Ai(z) \) the standard Airy function. It should be noted that we label the coalescing roots \( \mp \) in the sense that when \( \zeta \) is real then it is also positive. The above form goes over smoothly to the well separated critical point case as

\[
(1) \quad B^{(+)}(-z) \rightarrow 1 \text{ as } z \rightarrow +\infty,
\]

\[
(2) \quad B^{(-)}(-z) \rightarrow 1 \text{ as } -z \rightarrow e^{-\pi i} \infty, \text{ and}
\]

\[
(3) \quad B^{(\pm)}(-z) \rightarrow 1 \text{ as } -z \rightarrow e^{\pm\pi i} \infty.
\]

These cases cover all the eventualities, because when the two roots are real then \(-\lambda^{2/3} \zeta\) is real and negative, and when the roots are a complex conjugate pair then with a suitable choice of branch this argument is real and positive,

\[
-\lambda^{2/3} \zeta = +\left(\frac{2}{3} \lambda |\text{Im}(f(v_-))|^{2/3}. \right.
\]

(79)

When the points coalesce \( \xi \rightarrow 0 \) the two terms combine to give a convergent result even though separately they diverge. The leading-order approximation of the hyper-Bessel function with coalescing critical points has the same form as equation (75), except there are additional factors of \( B^{(\pm)} \) attached for each pair of coalescing points.

To further investigate the possibility of degeneracy in the saddle-point method we specialize to the particular form of the hyper-Bessel functions arising in our application and parametrize the coefficients \( R_j \) in the following way

\[
R_1 = \hat{\delta} = \frac{\beta}{\beta} \quad R_2 = \hat{\sigma} = \frac{\sigma}{\beta} \quad R_3 = R_1 + R_2.
\]

(80)

After forming the discriminant of the reducing cubic to the quartic (72) following Cajori (1943)

\[
D = \frac{1}{256} (\hat{\sigma}^2 - \hat{\delta}^2 - 4)(\hat{\delta}^2 - \hat{\hat{\delta}}^2 + 4)(\hat{\delta}^2 \hat{\delta}^2 + 4)^2
\]

(81)

it is possible to show that there are only three possible configurations of the roots:

\[
(1) D > 0 \quad \text{and there are two pairs of distinct real roots in a region of } \hat{\sigma} - \hat{\delta} \text{ space outside of the four hyperbolae } \hat{\delta}^2 - \hat{\hat{\delta}}^2 = \pm 4 \text{ and therefore applies when the effective coupling vanishes, as say at large distances } x,
\]
(2) \( D < 0 \) and there are two real distinct roots and a complex conjugate pair in a region in \( \hat{\sigma} - \hat{\delta} \) space inside of the four hyperbolae \( \hat{\sigma}^2 - \hat{\delta}^2 = \pm 4 \).

(3) \( D = 0 \) and one pair of the roots are equal, the others are distinct.

When degeneracy occurs at \( D = 0 \) it is clear that this is precisely the condition for a classical turning point \( \alpha_0 \alpha_1 = \beta^2 \). Here the \( \beta \) parameter can be the position-dependent quantity \( \beta e^{-x/4} \).

We see that the roots are grouped in pairs and we will denote a pair by \( t, \bar{t} \). While there exists a number of paths to the explicit solution of a general quartic, via a reducing cubic equation, we shall see that our particular quartic has symmetries which yield simple explicit solutions and avoids the construction of a cubic equation. To begin with we will require the solutions of four related quartics

\[ A: \text{where } \hat{\delta}, \hat{\sigma} \text{ have the generic sign;} \]

\[ B: \text{where } \hat{\delta} \text{ has the generic sign and } \hat{\sigma} \rightarrow -\hat{\sigma}; \]

\[ C: \text{where } \hat{\delta} \rightarrow -\hat{\delta} \text{ and } \hat{\sigma} \text{ has the generic sign;} \]

\[ D: \text{where both } \hat{\delta} \rightarrow -\hat{\delta} \text{ and } \hat{\sigma} \rightarrow -\hat{\sigma}. \]

First there are the obvious symmetries \( tC = -tB, \ bar{t}C = -\bar{t}B, \ tD = -tA, \ bar{t}D = -\bar{t}A \), \( \forall j \).

In addition, there are homographic transformations which we state without proof

\[ tA = \frac{tC}{1 - \hat{\delta}tC}, \quad tB = \frac{tD}{1 - \hat{\delta}tD}, \quad tA = \frac{tB}{1 - \hat{\sigma}tB}, \quad tC = \frac{tB}{1 + (\hat{\delta} - \hat{\sigma})tB}. \quad (82) \]

and if one combines the sign symmetry with the appropriate homographic transformation then one gets a relation between the pair of roots to the same quartic, namely

\[ \bar{t}A = \frac{-tA}{1 + (\hat{\delta} + \hat{\sigma})tA}, \quad \bar{t}B = \frac{-tB}{1 + (\hat{\delta} - \hat{\sigma})tB}, \quad \bar{t}C = \frac{-tC}{1 + (-\hat{\delta} + \hat{\sigma})tC}, \quad \bar{t}D = \frac{-tD}{1 + (-\hat{\delta} - \hat{\sigma})tD}. \quad (83) \]

We will need to label specific roots like \( t_v \) and its pair \( \bar{t}_v \) in order to keep track of a given root and where we sometimes use a superscript \( Q = A, B, C, D \) to indicate which quartic we are referring to. In addition we can form useful combinations which have nice transformational properties, such as

\[ \frac{dQ_{2v}}{(tQ_v)^2} \frac{dQ_{3v}}{(tQ_v)^2} = 1, \quad \frac{dQ_{1v}}{(tQ_v)^2} \frac{dQ_{4v}}{(tQ_v)^2} = 1, \quad \frac{dQ_{2v}}{(tQ_v)^2} = \frac{dQ_{2v}}{(tQ_v)^2}. \quad (84) \]

Finally we relate all the derived quantities of a pair of roots for quartic case \( A \)

\[ \bar{t}A = -\frac{tA}{dA}, \quad \bar{d}A = \frac{dA}{dA}, \quad \bar{d}A = \frac{dA}{dA}, \quad \bar{d}A = \frac{dA}{dA}. \quad (85) \]

So in summary we relate any quantity for quartics \( B, C, D \) to that of quartic \( A \) and any quantity of one member of a pair of roots to quartic \( A \) to the other member.

There are further consequences of the above transformations which will ultimately lead to explicit solutions, but to start with we need to motivate the forms of our solutions. All discussion now refers to quartic \( A \). We take the \( D < 0 \) case first. If the pair of roots \( t, \bar{t} \)
are complex conjugate then from equation (85) \(|d_3| = |\bar{d}_3| = 1\), so \(d_3\) is purely a phase factor. From this \(|d_1| = |d_2| = |t|^2\). So we can set \(d_3 = e^{i\chi}\) and thus solve for \(t\)

\[
t = i \frac{\sin \chi}{\hat{a}_0} e^{i\chi}
\]

and \(\bar{t}\) is given by \(\chi \rightarrow -\chi\). Using \(d_1 + d_2 = d_3 + 1\) and \(d_1 = d_2^* d_3\) one can solve for \(d_1, d_2\) in terms of \(\chi\) and \(\hat{a}_0\). All of these combined identically satisfy the quartic so in order to solve for \(\chi\) we introduce a relation involving \(\hat{a}_1\). This yields

\[
\sin \chi = \hat{a}_0 \left[ i \sqrt{4 + \hat{\sigma}^2 \hat{\delta}^2 - \frac{1}{2} \hat{\delta} \hat{\delta}} \right]^{1/2}.
\]

The positive sign for \(\chi\) gives \(t\), while the negative sign \(\bar{t}\), so we restrict \(0 \leq \chi \leq \pi/2\). This gives the simple expressions for \(d_1, d_2\)

\[
d_1 = \frac{e^{i\chi}}{\hat{a}_0} [\hat{a}_0 \cos \chi - i \hat{a}_1 \sin \chi] = \frac{\hat{\sigma} + \hat{\delta} e^{2i\chi}}{\hat{\delta} + \hat{\sigma}}
\]

\[
d_2 = \frac{e^{i\chi}}{\hat{a}_0} [\hat{a}_0 \cos \chi + i \hat{a}_1 \sin \chi] = \frac{\hat{\sigma} + \hat{\delta} e^{2i\chi}}{\hat{\delta} + \hat{\sigma}}.
\]

and

\[
1 + \sum_j d_j^{-1} = 2 e^{-i\chi} \frac{\cos \chi}{\sin^2 \chi} [\hat{a}_0^4 + \sin^4 \chi].
\]

The conjugate pair merge at \(D = 0\) when \(\chi = \pi/2\). Having found the conjugate roots of a quartic the remaining real pair \(t_1, t_2\) are given by

\[
t_1, t_2 = \frac{\hat{a}_0}{\sin^2 \chi} [\hat{a}_0^2 \pm \sqrt{\hat{\alpha}_0^4 + \sin^2 \chi}] \tag{90}
\]

So that \(t_1 > 0\) and \(t_2 < 0\) (\(\text{arg}(t) = +\pi\)). For \(t_1\)

\[
d_3 = \left\{ \frac{\hat{\alpha}_0^2 + \sqrt{\hat{\alpha}_0^4 + \sin^2 \chi}}{\sin \chi} \right\}^2 > 0
\]

\[
d_1 = \frac{\hat{\alpha}_0 \hat{a}_0 \hat{a}_1 + \sqrt{\hat{\alpha}_0^4 + \sin^2 \chi}}{\sin^2 \chi} \left[ \hat{\alpha}_0^2 + \sqrt{\hat{\alpha}_0^4 + \sin^2 \chi} \right]
\]

\[
d_2 = \frac{\hat{\alpha}_0 \hat{a}_0 \hat{a}_1 + \sqrt{\hat{\alpha}_0^4 + \sin^2 \chi}}{\sin^2 \chi} \left[ \hat{\alpha}_0^2 + \sqrt{\hat{\alpha}_0^4 + \sin^2 \chi} \right]
\]

and for \(t_2\) one uses the above equations with the sign of the square root radical reversed. It should be noted that \(d_j, 1 + \sum_j d_j^{-1}\) for the real pair \(t_1, t_2\), are always positive in this region.

Now we seek to extend the above analysis to the region \(D > 0\). Let us denote the four roots \(t, \bar{t}, t_1, t_2\) where we demand continuity with their namesakes across \(D = 0\). Now the product of all roots is \(-1\) so either one or three roots are negative. If we consider the case
of only one negative root then both members of the other pair must be positive, but this
contradicts the first equation in equation (85). So three of the roots must be negative and
it will turn out that both \( t \), \( \bar{t} \) are negative. In the other pair \( t_1 \), \( t_2 \) we can take \( t_1 \) as positive
and \( t_2 \) negative. It is easy to see that for this root all \( d_j \) are positive, and consequently all
the \( d_j \) for its partner are positive. So whatever sign \( D \) takes the \( d_j \) for this pair are positive.
So for the root \( t_1 \) we can set
\[
    d_3 = e^{2\chi} \quad \text{(we use the same symbol } \chi \text{ again, in this context)}
\]
and again solve for \( t_1 \)
\[
    t_1 = \frac{\sinh \chi}{\hat{a}_0} e^\chi \quad \text{(92)}
\]
and parallel to the analysis of the previous paragraph we have
\[
    \sinh \chi = \hat{a}_0 \left( \frac{1}{2} \sqrt{4 + \hat{\alpha}_0^2 \hat{\delta}^2 + \frac{1}{2} \hat{\delta}^2} \right)^{1/2} \quad \text{(93)}
\]
The positive sign for \( \chi \) gives \( t_1 \), while the negative sign \( t_2 \), so we restrict \( 0 \leq \chi < \infty \). This
gives the similar expressions for \( d_1, d_2 \)
\[
    d_1 = \frac{e^\chi}{\hat{a}_0} [\hat{a}_0 \cosh \chi - \hat{\alpha}_1 \sinh \chi] = \frac{\hat{\sigma} + \hat{\delta} e^{2\chi}}{\hat{\sigma} + \hat{\delta}} \quad \text{(94)}
\]
\[
    d_2 = \frac{e^\chi}{\hat{a}_0} [\hat{a}_0 \cosh \chi + \hat{\alpha}_1 \sinh \chi] = \frac{\hat{\delta} + \hat{\sigma} e^{2\chi}}{\hat{\delta} + \hat{\sigma}}
\]
and
\[
    1 + \sum_j d_j^{-1} = 2e^{-\chi} \frac{\cosh \chi}{\sinh^4 \chi} [\hat{\alpha}_0^4 + \sinh^4 \chi] \quad \text{(95)}
\]
For this pair of roots \( d_j \), \( 1 + \sum_j d_j^{-1} \) are always positive in this region. Having found the
above pair of roots the remaining real pair \( t, \bar{t} \) are given by
\[
    t, \bar{t} = \frac{\hat{a}_0}{\sin^2 \chi} \left[ -\hat{\alpha}_0^2 \pm \sqrt{\hat{\alpha}_0^4 - \sinh^2 \chi} \right] \quad \text{(96)}
\]
For \( t \)
\[
    d_3 = - \left\{ \frac{-\hat{\alpha}_0^2 - \sqrt{\hat{\alpha}_0^4 - \sinh^2 \chi}}{\sinh \chi} \right\}^2 < 0
\]
\[
    d_1 = \frac{\hat{a}_0 \hat{\alpha}_1 + \sqrt{\hat{\alpha}_0^4 - \sinh^2 \chi}}{\sinh^2 \chi} \left[ -\hat{\alpha}_0^2 - \sqrt{\hat{\alpha}_0^4 - \sinh^2 \chi} \right]
\]
\[
    d_2 = \frac{\hat{a}_0 \hat{\alpha}_1 + \sqrt{\hat{\alpha}_0^4 - \sinh^2 \chi}}{\sinh^2 \chi} \left[ -\hat{\alpha}_0^2 - \sqrt{\hat{\alpha}_0^4 - \sinh^2 \chi} \right]
\]
(97)
\[
    1 + \sum_j d_j^{-1} = \frac{2(\hat{\alpha}_0^4 + \sinh^4 \chi) \sqrt{\hat{\alpha}_0^4 - \sinh^2 \chi}}{\hat{\alpha}_0^4 \left[ \hat{\alpha}_0^2 + \sqrt{\hat{\alpha}_0^4 - \sinh^2 \chi} \right]}
\]
and for \( \bar{t} \), again one uses the above expressions with the sign of the square root radical
reversed. The conjugate pair merge at \( D = 0 \) when \( \sinh \chi = \hat{\alpha}_0^2 \).
Finally in the degenerate case \( D = 0 \) the quartic roots simplify to

\[
t, \tilde{t} = -\frac{1}{\hat{\alpha}_0} \\
t_{1,2} = \hat{\alpha}_0 \left[ \hat{\alpha}_0^2 \pm \sqrt{\hat{\alpha}_0^4 + 1} \right].
\]

(98)

Having found explicit forms for the critical points and all the derived parameters appearing in the semiclassical approximation for distinct critical points, equation (75), we need to find equivalent results for the coalescing critical point situation. Expressing the argument of the Airy functions, equation (79), in terms of the quartic roots we have

\[-\chi^{2/3} \zeta = \begin{cases} 
-\beta h(t, \tilde{t})^{2/3} & \text{real roots} \\
+\beta |\text{Im}(h(t, \tilde{t}))|^{2/3} & \text{complex conjugate roots}
\end{cases}
\]

(99)

where the explicit form for the function \( h \) is

\[
h = \frac{3}{2} \left\{ -4 \sqrt{\hat{\alpha}_0^4 - \sinh^2 \chi} \hat{\alpha}_0 + \hat{\alpha}_0 \ln \left( \frac{\hat{\alpha}_0^2 + \sqrt{\hat{\alpha}_0^4 - \sinh^2 \chi}}{\hat{\alpha}_0^2 - \sqrt{\hat{\alpha}_0^4 - \sinh^2 \chi}} \right) \right. \\
+ \hat{\alpha}_1 \ln \left( \frac{\hat{\alpha}_0 \hat{\alpha}_1 + \sqrt{\hat{\alpha}_0^4 - \sinh^2 \chi}}{\hat{\alpha}_0 \hat{\alpha}_1 - \sqrt{\hat{\alpha}_0^4 - \sinh^2 \chi}} \right) \right\}
\]

(100)

in the case of real roots and

\[
\text{Im} (h) = \left\{ 2 \hat{\alpha}_0 \cot \chi + \hat{\alpha}_0 (\chi - \pi/2) - \hat{\alpha}_1 \tan^{-1} \left( \frac{\hat{\alpha}_0}{\hat{\alpha}_1} \cot \chi \right) \right\}
\]

(101)

for complex conjugate roots. It fulfills the following symmetries \( h = h_A = h_B, h_C = -h_B, h_D = -h_A \).

Collecting the uniform semiclassical expressions for all the component hyper-Bessel functions together into the transmission coefficient \( T_0 \) (for the others see Witte (1996)) one has the following intermediate result, after much simplification

\[
T_0 \sim \frac{(2\pi)^{1/2} \beta^{-1/2-4\text{Im} e^{-4\text{Im}}}}{\Gamma(-2\text{Im} \alpha_0, \frac{1}{2} - i\delta, \frac{1}{2} - i\sigma)} \sum_{\mu} B^{(\mu)} e^{\text{Ai}(\mu)} \left[ 1 + \sum_{j} d_{j\mu}^{-1} \right]^{-1/2} Z_0(\mu) \\
+ \left[ \sum_{\mu, \mu'} B^{(\mu)} B^{(\mu')} e^{\text{Ai}(\mu') + 1/2} \right] \left[ 1 + \sum_{j} d_{j\mu'}^{-1} \right]^{-1/2} \left[ 1 + \sum_{j} d_{j\mu}^{-1} \right]^{-1/2} X_d(\mu, \mu')
\]

(102)

where the important phase functions are defined

\[
Y_d = \left( \frac{i}{t_{\mu}} \right)^{1/2} \left( \frac{i}{t_{\mu'}} \right)^{1/2} \left( \frac{d_{j\mu}}{d_{j\mu'}} \right)^{1/2} \left[ \left( \frac{i}{t_{\mu}} \right)^2 d_{2\mu} \left( \frac{i}{t_{\mu'}} \right)^2 \frac{1}{d_{1\mu} d_{3\mu'}} \right]^{\text{id}} \\
\times \left[ \left( \frac{i}{t_{\mu}} \right)^2 d_{1\mu} \left( \frac{i}{t_{\mu'}} \right)^2 d_{1\mu'} \right]^{\text{ig}}
\]

(103)

\[
Z_0 = \left( \frac{i}{t_{\mu}} \right)^{1/2} \left( \frac{i}{d_{2\mu}} \right)^{1/2} \left[ \left( \frac{i}{t_{\mu}} \right)^2 \frac{1}{d_{1\mu} d_{3\mu}} \right]^{\text{id}} \left[ \left( \frac{i}{t_{\mu}} \right)^2 d_{1\mu} \right]^{\text{ig}}.
\]
The \( B(\mu) \) functions are a shorthand for \( B(\mu)(-\beta h)^{3/2} \) which is defined by equation (78) and its argument \( h \) by equations (100) and (101). The \( t_{\mu} \) are the roots of the quartic (72) with parameters \( R_j \), equation (80), and \( \mu \) labelling the different ones. By convention we take \( \mu = +, - \) to indicate the roots which are complex conjugates in the classically forbidden region, while \( \mu = 1, 2 \) denote the roots which are real for all parameters. By definition \( B(1,2) = 1 \) as these roots do not coalesce. Explicit expressions for the roots can be found from equations (86), (87) and (90) or equations (92), (93) and (96). The derived functions \( d_{j\mu} \) of the root \( t_{\mu} \) are defined following equation (73) again with equation (80) and their final explicit forms are given in equations (91) and (97). We wish to emphasize here that the argument of the complex roots \( t_{\mu} \) and consequently the \( d_j \) must be correctly chosen to yield the true result and certain algebraic relations which confuse the arguments of the different roots should not be used. Several observations can be made of the above expressions. First those terms in the sum over the roots with \( \mu = \mu' \) vanish which means that the product of two exponentially dominant terms (\( \text{Re} \,(t_{\mu}) > 0 \)) is absent. So the exponentially large factors cancel out of the resulting amplitudes as in the large coupling case. The above amplitudes reduce to the large coupling case, namely equations (28), (30) and (32) when \( \hat{\delta}, \hat{\sigma} \to 0 \).

In the final step of the analysis this intermediate expression for the transmission coefficient \( |T_0| \) is further reduced and simplified by introducing the explicit quartic solutions and this final result is displayed as equation (45) in section 4.4.

8. Conclusions

In this work we have derived an exact solution to the reflection and diffraction of atomic de Broglie waves by a travelling evanescent laser wave, the ‘two-beam’ case. We have found that the wavefields and the elements of the non-adiabatic transition matrix and the tunnelling loss matrix are given exactly by a specific case of a hyper-Bessel function, \( f_3 \), which are natural generalizations of the traditional modified Bessel function. We have given a number of exact representations of these hyper-Bessel functions, some already known and others that are new, that enable a practical or numerical analysis to be employed. Furthermore, we have investigated in detail all of the asymptotic and limiting regimes whereby these functions reduce to simpler and well known special functions, using again some known results and establishing some new ones concerning the uniform asymptotic approximation for large parameters and arguments. In particular we have found expressions for the regimes of:

- weak and strong coupling between the atoms and laser fields but the detuning and kinetic energy are moderate;
- the detuning is exactly zero, and other parameters are arbitrary; and
- strong coupling between the atoms and laser fields and large detuning and kinetic energy, where the semiclassical approximation is approached, and which is uniform with respect to the location of any classical turning points.

In real experimental situations the semiclassical is usually quite accurate and would be employed because of the relative simplicity of the results, namely the use of elementary and Airy functions, rather than the exact expressions.

The comparison of the exact solution and the uniform semiclassical approximation with approximation schemes employing adiabatic assumptions and treating these with a WKB method reveals the weakness of this commonly used approach, especially for small detunings or large couplings. Similarly perturbation expansions in the couplings are revealed to be quite unsuitable and extremely inefficient in the light of our analysis. This model has little to say about the Landau–Zener theory as there are no level crossings in the two-beam case.
Acknowledgments

The author is indebted to John Murphy for bringing this problem to his attention and for many subsequent discussions on this subject, to Professor V G Minogin for his advice on the physical models, and to Andy Rawlins for his assistance in preparing the numerical computations and graphical displays. The final version of this work has also benefited from many insightful criticisms and numerous corrections made by the two anonymous referees. This work was supported by the Australian Research Council.

References

Braaksma B L J 1963 Asymptotic expansions and analytic continuations for a class of Barnes-integrals *Compositio Math.* 15 239–341
Cajori F 1943 *Introduction to the Modern Theory of Equations* (New York: MacMillan)
Delerue P 1949 Note sur une formule opératoire nouvelle en calcul symbolique *C. R. Acad. Sci., Paris* 229 1197–9
——1950a Sur l’utilisation des fonctions hyperbesséliennes à la résolution d’une équation différentielle et au calcul symbolique à n variables *C. R. Acad. Sci., Paris* 230 912–14
——1987 Generalized Poisson representations of $\rho F_q p < q$ using fractional integrals *Mathematics and Mathematical Education* ed G Gerov (Sofia: Bulgarian Academy Science) pp 205–12
Heading J and Whipple R T P 1952 The oblique reflexion of long wireless waves from the ionosphere at places where the Earth’s magnetic field is regarded as vertical *Phil. Trans. R. Soc. A* 244 469–503
——1987b Generalized fractional derivative representations of $\rho F_q p < q$. *Mathematics and Mathematical Education* ed G Gerov (Sofia: Bulgarian Academy Science) pp 228–35
——1994 Generalized fractional calculus and applications *Pitman Research Notes in Mathematics Series* vol 301 (New York: Longman)
Temme N M 1994 Steepest descent paths for integrals defining the modified Bessel functions of imaginary order *Meth. Appl. Anal.* 1 14–24
Witte N S 1996 Exact solution for the reflection and diffraction of atomic de Broglie waves by a travelling evanescent laser wave. UMP-96/82
Wong R 1989 *Asymptotic Expansions of Integrals* (San Diego, CA: Academic)
Winch D 1921a An asymptotic formula for the hypergeometric function 0F4(z) *Phil. Mag.* 41 161–73
—— 1921b A generalized hypergeometric function with n parameters *Phil. Mag.* 41 174–86
—— 1923 Some approximations to hypergeometric functions *Phil. Mag.* 45 818–27