PHYSICAL REVIEW VOLUME 186, NUMBER 1 5 OCTOBER 1969

Asymptotic Behavior of the Generalized Width and Shift Functions in the Electron-Impact Broadening Theory of Neutral Spectral Lines in Plasmas

C. Deutsch and L. Herman
Département de Recherches Physiques, Faculté des Sciences, Tour 22, 9 Quai Saint-Bernard, Paris 5ème, France

and

H. W. Drawin
Association Euratom-CEA,
Département de la Physique du Plasma et de la Fusion Contrôlée, Centre d'Etudes Nucléaires
Boite Postale n° 6–92 Fontenay-aux-Roses (France)
(Received 25 February 1969)

Explicit asymptotic formulas are derived for the generalized functions $A(z_1, z_2)$ and $B(z_1, z_2)$, which define the matrix elements of the electron-collision operator, in the impact broadening theory of Griem, Baranger, Kolb, and Oertel, recently extended in order to take into account any degree of degeneracy of the overlapping lines in plasmas. The results are shown graphically and confirm a complementary behavior previously predicted. The shift function remains greater than the width function in the whole asymptotic domain.

I. INTRODUCTION

Recently, a unified treatment of the electron-impact broadening of neutral lines[1] has been obtained, with the evaluation of the off-diagonal matrix elements of the electron-collision operator, defined in the generalized impact broadening theory of Griem, Baranger, Kolb, and Oertel.[2] The new functions $A(z_1, z_2)$ and $B(z_1, z_2)$ graphed in Ref. 1 were for values of adiabaticity parameters z_1 and z_2 from -2 to 2.

However, for the complete calculation of the electron broadening of partially degenerate lines,[3] there is need for values of the width and shift functions for values of $|z_1|$ and $|z_2|$ greater than three. The explicit representation of the B function given previously[1] is not well adapted for providing these asymptotic values. So, we are led to establish directly the asymptotic expansion of the shift function. It is the purpose of this paper to calculate and discuss $A(z_1, z_2)$ and $B(z_1, z_2)$ for $|z_1|$ values greater than three.

II. GENERAL EXPRESSIONS

Our starting point will be the expression for the angular average, taken over the electronic perturber trajectories $\vec{r}=\vec{\rho}+\vec{v}u$, of the impact broadening for the sublevels (n,i), (n,l'), and (n,l) constituting the upper state n of a given line, i.e.,

$$\{\langle ni|S_n(0)-I|nl\rangle\}_{\text{angular average}} = -\frac{1}{3}\left(\frac{e^2}{\hbar\rho v}\right)^2 \sum_{\sigma,l'} \langle ni|r_\sigma|nl'\rangle\langle nl'|r_\sigma|nl\rangle$$

$$\times \int_{-\infty}^{+\infty} dx_1 \int_{-\infty}^{x_1} dx_2 \left[(1+x_1x_2)\, e^{i(z_1x_1-z_2x_2)}/(1+x_1^2)^{3/2}(1+x_2^2)^{3/2}\right], \tag{1}$$

considered in the monopole-dipole approximation, and expressed with the aid of the dimensionless quantities $z_1=\omega_{il'}\rho/v$, $z_2=\omega_{ll'}\rho/v$, and $x=vu/\rho$. Here, $\omega_{il'}$ and $\omega_{ll'}$ represent the angular frequencies corresponding to transitions between the given sublevels in presence of a static Stark effect. $S_n(0)$ is the one-electron collision matrix at time $u=0$, I is the unit matrix, and r_σ denotes a component of the optical electron position vector $\vec{r}$. The main result of Ref. 1 was a rigorous evaluation of the integral

$$\tfrac{1}{2}\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{x_1} dx_2\, e^{i(z_1x_1-z_2x_2)} \frac{(1+x_1x_2)}{(1+x_1^2)^{3/2}(1+x_2^2)^{3/2}} = A(z_1,z_2)+iB(z_1,z_2). \tag{2}$$

Unfortunately, because of the double integrals therein, the expression then obtained for $B(z_1, z_2)$ is not at all suited to provide asymptotic values. Therefore, if one desires an asymptotic expression for B, the best thing to do is to derive it directly for Eq. (2), with the aid of an integration by parts. This procedure, outlined in Appendix A, allows us to write first

$$A(z_1, z_2) = |z_1| \; |z_2| K_1(|z_1|) K_1(|z_2|) + z_1 z_2 K_0(|z_1|) K_0(|z_2|) \;, \tag{3}$$

an expression already given in Ref. 1 and valid for all z_1, z_2 values. The asymptotic values of B will be computed using the relation

$$\begin{aligned} B(z_1, z_2) & |z_1| K_1(|z_1|) z_2 \left[{}_1F_2\left(1; \tfrac{1}{2}, \tfrac{3}{2}; \frac{z_2^2}{4}\right) - \frac{\pi}{4} |z_2| \; {}_1F_2\left(\tfrac{3}{2}; 2, \tfrac{3}{2}; \frac{z_2^2}{4}\right)\right] \\ & - z_1 K_0(|z_1|) \left[{}_1F_2\left(1; \tfrac{1}{2}, \tfrac{1}{2}; \frac{z_2^2}{4}\right) - \frac{\pi}{2} |z_2| \; {}_1F_2\left(\tfrac{3}{2}; 1, \tfrac{3}{2}; \frac{z_2^2}{4}\right)\right] + \frac{1}{z_2} \left[- |z_1| K_1(|z_1|) + \frac{\pi}{8} \right. \\ & \left. \times e^{-|z_2 - z_1|} \sum_{k=0}^{1} \frac{(2-k)!}{k!} \frac{(2|z_2 - z_1|)^k}{(1-k)!} \right] + \frac{1}{z_2^2} \left[\frac{\pi}{8} (z_2 - z_1)(1 + |z_2 - z_1|) e^{-|z_2 - z_1|} - z_1 K_0(|z_1|) \right] \\ & - \frac{3}{z_2^3} \left[|z_1| K_1(|z_1|) - \frac{\pi e^{-|z_2 - z_1|}}{2^8} \left(\sum_{k=0}^{3} \frac{(6-k)!(2|z_2 - z_1|)^k}{k!(3-k)!} - 8 \sum_{k=0}^{2} \frac{(4-k)!(2|z_2 - z_1|)^k}{k!(2-k)!} \right) \right] \\ & + \frac{1}{z_2^4} \left[\frac{\pi}{4} (z_2 - z_1) e^{-|z_2 - z_1|} \left(\frac{5}{2^7} \sum_{k=0}^{3} \frac{(6-k)!(2|z_2 - z_1|)^k}{k!(3-k)!} - (3 + 3|z_2 - z_1| + |z_2 - z_1|^2) \right) - 9 z_1 K_0(|z_1|) \right] \\ & + \epsilon_4 / z_2^5 \;, \quad \text{as} \quad z_2 \to \infty \;. \end{aligned} \tag{4}$$

In Eqs. (3) and (4), $K_n(x)$ represents a modified Bessel function of the second kind, and ${}_1F_2(a; b, c; \frac{1}{4} z^2)$ is a hypergeometric function.

The symmetry properties[1]

$$A(z_1, z_2) = A(z_2, z_1) = A(-z_1, -z_2), \qquad B(z_1, z_2) = B(z_2, z_1) = -B(-z_1, -z_2) \tag{5}$$

and the relation

$$B(z_1, z_2) = 0, \quad \text{if} \quad z_1 z_2 \leq 0 \tag{6}$$

show clearly that Eq. (4) exhibits the asymptotic behavior of $B(z_1, z_2)$, whatever z_1 and z_2 may be. So, in the remaining part of this work, the B values will be discussed only for positive (z_1, z_2) values.

A. Asymptotic Expressions for $A(z_1, z_2)$

Values of $A(z_1, z_2)$ for large values of z_1 and z_2 are immediately obtained by inserting the asymptotic expansion (see, for instance, Ref. 5, p. 963)

$$K_n(|z|) \sim \left(\frac{\pi}{2|z|}\right)^{1/2} e^{-|z|} \; {}_2F_0\left(\tfrac{1}{2} + n, \tfrac{1}{2} - n; -\frac{1}{2|z|}\right), \quad \text{as} \quad |z| \to \infty, \tag{7}$$

in Eq. (3). If ones keeps the atomic ratio $a = z_2/z_1$ fixed, one gets first

$$A(z, az) \sim \frac{\pi}{2|a|^{1/2}} |z| (|a| + a) e^{-|z| - |az|}, \quad \text{as} \quad |z| \to \infty, \tag{8}$$

and the isolated-line result, previously given by Seaton[4] and Griem *et al.*,[2]

$$A(z, z) \sim \pi |z| e^{-2|z|} \left(1 + \frac{1}{4|z|} + \frac{1}{32z^2} + \cdots\right), \quad \text{as} \quad |z| \to \infty,$$

is recovered for $a = 1$.

When z_1 remains fixed and $|a|$ unbounded, the off-diagonal matrix elements of the electron-collision operator may exhibit another asymptotic expansion

$$A(z, az) \sim \left(\frac{\pi}{2|a|}\right)^{1/2} |z|^{3/2} e^{-|az|} [|a| K_1(|z_1|) + a K_0(|z|)], \quad \text{as} \quad |a| \to \infty, \tag{9}$$

which reduces to Eq. (8) with $|z| \to \infty$.

As a first result, Eqs. (8) and (9) show that the inelastic collisions with $a \leq 0$ give a negligible asymptotic contribution to the width.

B. Asymptotic Expressions for $B(z_1, z_2)$

Now we have to extract the corresponding expansions for $B(z_1, z_2)$ from Eq. (4). This will be done if one expands the hypergeometric functions explicitly. However, the divergent asymptotic behavior[5] of ${}_1F_2(a; b, c; \frac{1}{4}z^2)$ does not allow a straightforward approach, and it is much more interesting to start from the relations established in Appendix B:

$$\begin{aligned} &{}_1F_2\left(1; \tfrac{1}{2}, \tfrac{3}{2}; \frac{z^2}{4}\right) - \frac{\pi}{4}|z|\, {}_1F_2\left(\tfrac{3}{2}; 2, \tfrac{3}{2}; \frac{z^2}{4}\right) = S_{-1,-1}(|z|), \\ &{}_1F_2\left(1; \tfrac{1}{2}, \tfrac{1}{2}; \frac{z^2}{4}\right) - \frac{\pi}{2}|z|\, {}_1F_2\left(\tfrac{3}{2}; 1, \tfrac{3}{2}; \frac{z^2}{4}\right) = 1 - |z| S_{0,0}(|z|), \end{aligned} \tag{10}$$

where $S_{\mu,\nu}(|z|)$ denotes the Lommel function.[5]

Then the asymptotic series[5]

$$\begin{aligned} &S_{0,0}(z) \sim z^{-1}\left[1 - \frac{1}{z^2} + \frac{9}{z^4} + \cdots\right], \qquad \text{as} \quad z \to \infty, \\ &S_{-1,-1}(z) \sim z^{-2}\left[1 - \frac{3}{z^2} + \frac{45}{z^4} + \cdots\right], \qquad \text{as} \quad z \to \infty, \end{aligned} \tag{11}$$

introduced in Eq. (4) give immediately

$$\begin{aligned} B(z_1, az_1) \sim{}& \pi(8az_1)^{-1} e^{-z_1|a-1|} \sum_{k=0}^{1} \frac{(2-k)!\,(2z_1|a-1|)^k}{k!\,(1-k)!} + (a^2 z_1)^{-1} \\ &\times\left[-2K_0(|z_1|) + \frac{\pi(a-1)}{8}(1 + z_1|a-1|)\, e^{-z_1|a-1|}\right] - 3(a^3 z_1^3)^{-1}\left[2z_1 K_1(|z_1|) - \frac{\pi e^{-z_1|a-1|}}{2^8}\right. \\ &\times\left.\left(\sum_{k=0}^{3} \frac{(6-k)!\,(2z_1|a-1|)^k}{k!\,(3-k)!} - 8\sum_{k=0}^{2} \frac{(4-k)!\,(2z_1|a-1|)^k}{k!\,(2-k)!}\right)\right] + (a^4 z_1^3)^{-1}\left[\frac{\pi(a-1)}{4} e^{-z_1|a-1|}\right. \\ &\times\left.\left(\frac{5}{2^7}\sum_{k=0}^{3} \frac{(6-k)!\,(2z_1|a-1|)^k}{k!\,(3-k)!} - [3 + 3z_1|a-1| + z_1^2(a-1)^2]\right)\right] + \epsilon_5(az_1)^{-5}, \quad \text{as} \quad a \to \infty, \end{aligned} \tag{12}$$

for finite values of $z_1 \geq 2$. If we let z_1 reach arbitrary high values, Eq. (12) becomes

$$B(z_1, az_1) \sim \frac{\pi}{4az_1} e^{-z_1(a-1)}\left(1 + \frac{|a-1|}{2a}\right)(1 + z_1|a-1|) + O[(az_1)^{-3}], \quad \text{as} \quad z_1 \to \infty \tag{13}$$

in a second-order expansion.

Moreover, the isolated-line result

$$B(z, z) \sim \frac{\pi}{4z} + \frac{9}{32}\frac{\pi}{z^3} + O(z^{-5}), \quad \text{as} \quad z \to \infty, \tag{4'}$$

is derived in a straightforward manner from the Eq. (4). The first term in the right-hand side of Eq. (4′) has already been obtained by Griem *et al.*[2]

III. RESULTS AND DISCUSSION

In Figs. 1 and 2, respectively, formulas (8) and (9) for $A(z_1, z_2)$ and formulas (12) and (13) for $B(z_1, z_2)$ completed with the exact expressions of Ref. 1, are plotted versus the variable z_1 in the range $3 \leq z_1 \leq 9$, the atomic ratio a in $z_2 = az_1$ being considered as a parameter. The essential features of these curves can be summarized in Sec. III A.

A. Positive Atomic Ratio ($a > 0$)

In contrast with the case of small z_1 values,[1] the shift function $B(z_1, z_2)$ always remains greater than the width function $A(z_1, z_2)$ in the asymptotic domain and decreases much more slowly.

The complementary relations[1]

$$A(z, az) \geq A(z, z), \quad B(z, az) \leq B(z, z), \tag{14}$$

with $0 \leq a \leq 1$, and also for $z = a'z$ with $a' = a^{-1}$ when

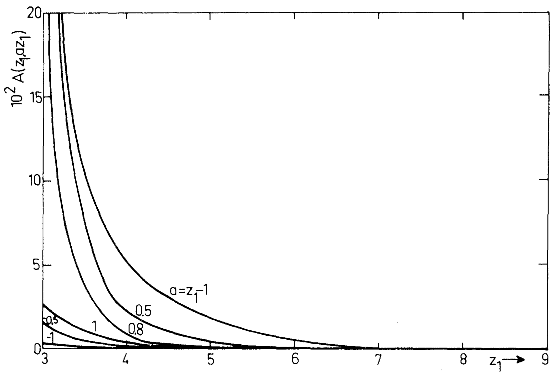

FIG. 1. Graphs of $A(z_1, az_1)$ as a function of z_1 for different values a taken as a parameter.

$a > 1$, are clearly verified in the asymptotic domain. The corresponding graphs define, respectively, upper and lower bounds for the A and B values. It is also of interest to note that Eq. (9) gives A values systematically greater than those shown by Eq. (8). On the other hand, B values calculated with Eq. (12) exhibit a reversed trend for $z_1 \geqslant 3$, when they are compared with the results of Eq. (13). More generally, the B values are widespread over the whole range of the ordinate, while the A values show a strong tendency to merge into a unique curve. It is then possible to summarize the foregoing discussion with the following argument: $A(z_1, z_2)$ is mainly dependent on the z_1 values, while $B(z_1, z_2)$ is mostly influenced by the z_2 variations.

Physically, this amounts to saying that the width is essentially given by the first step of the second-order atomic transition $i \to l' \to l$, and the shift by the second one.

B. Negative Atomic Ratio ($a \leqslant 0$)

In view of Eqs. (5) and (6), we have only to discuss the $A(z_1, z_2)$ values for positive z_1 and z_2 values. They reproduce a behavior already seen for $a > 0$ and fulfill the condition

$$A(z_1, -z_2) < A(z_1, z_2) \tag{15}$$

for all positive values of z_1 and z_2. Finally, we have to note that the isolated-line results tabulated by Griem[6] for the functions $A(z, z)$ and $B(z, z)$ are in good agreement with ours when $z \geqslant 3$.

IV. CONCLUSION

The results derived in this work will allow the electronic contribution to the complete Stark profile of neutral lines (and also of hydrogenic ionized lines at high electron temperature[7]) to be calculated for any degree of partial degeneracy. Furthermore, the shift and width functions exhibit strong complementary features.

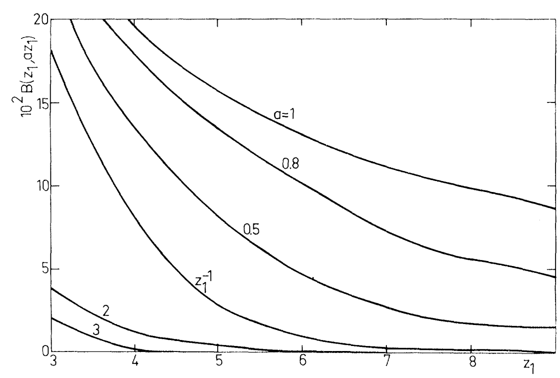

FIG. 2. Graphs of $B(z_1, az_1)$ as a function of z_1 for different values a taken as a parameter.

APPENDIX A

We now present the derivation of Eqs. (3) and (4). Starting from Eq. (2),

$$I(z_1, z_2) \equiv A(z_1, z_2) + iB(z_1, z_2) = \frac{1}{2}\int_{-\infty}^{+\infty} dx_1 \int_{-\infty}^{x_1} \frac{e^{i(z_1x_1 - z_2x_2)}(1 + x_1x_2)}{(1 + x_1^2)^{3/2}(1 + x_2^2)^{3/2}}\, dx_2 , \tag{A1}$$

it appears of interest to take (A1) in the form

$$\int_0^{\infty} dx_1 \int_0^{\infty} dx_2 \pm \int_0^{\infty} dx_1 \int_{x_1}^{\infty} dx_2 \ .$$

Expressing the definite integrals in terms of special functions, we obtain

$$I = I_1 + I_2 , \tag{A2}$$

where
$$\tfrac{1}{2} I_1 = A(z_1, z_2) + i\Big\{ |z_1| K_1(|z_1|) z_2 \Big[{}_1F_2\Big(1; \tfrac{1}{2}, \tfrac{3}{2}; \frac{z_2^2}{4}\Big) - \frac{\pi}{4}|z_2|\, {}_1F_2\Big(\tfrac{3}{2}; 2, \tfrac{3}{2}; \frac{z_2^2}{4}\Big)\Big]$$
$$- z_1 K_0(|z_1|) \Big[{}_1F_2\Big(1; \tfrac{1}{2}, \tfrac{1}{2}; \frac{z_2^2}{4}\Big) - \frac{\pi}{2}|z_2|\, {}_1F_2\Big(\tfrac{3}{2}; 1, \tfrac{3}{2}; \frac{z_2^2}{4}\Big)\Big]\Big\} ,$$

and $$I_2 = I_{21}(z_1, z_2) + I_{22}(z_1, z_2) - I_{21}(-z_1, z_2) - I_{22}(-z_1, z_2), \tag{A3}$$

with
$$I_{21}(z_1, z_2) = -\int_0^\infty \frac{dx_1\, e^{-iz_1x_1}}{(1+x_1^2)^{3/2}} \int_0^{x_1} \frac{dx_2\, e^{iz_2x_2}}{(1+x_2^2)^{3/2}},$$
$$I_{22}(z_1, z_2) = -\int_0^\infty \frac{dx_1 x_1\, e^{-iz_1x_1}}{(1+x_1^2)^{3/2}} \int_0^\infty \frac{dx_2 x_2\, e^{iz_2x_2}}{(1+x_2^2)^{3/2}}. \tag{A4}$$

Equation (4) will be evaluated with the aid of the incomplete Fourier integral

$$J(z_2) = \int_0^{x_1} dx_2\, e^{iz_2x_2}\, \Phi(x_2), \tag{A5}$$

$\Phi(x_2)$ being a continuous and differentiable function for x_2 values ranging from 0 to x_1. Furthermore, if $\Phi^{(p)}(x_2)$ represents a derivative of order p, we can write

$$\lim_{x_2 \to \infty} \Phi^{(p)}(x_2) = 0. \tag{A6}$$

Integrating $J(z_2)$ by parts, it is then possible to get a series expansion with respect to z_1^{-1}, which will define the asymptotic expansion of I_2.

Thus, we are led to write[8]

$$J(z_2) = B_N(z_2) - A_N(z_2) + O(z_2^{-N}), \quad (z_2 \to \infty)$$

with
$$A_N(z_2) = \sum_{n=0}^{N-1} i^{n-1}\, \Phi^{(n)}(0)\, z_2^{-(n+1)},$$
$$B_N(z_2) = \sum_{n=0}^{N-1} i^{n-1}\, \Phi^{(n)}(x_1) z_2^{-(n+1)}\, e^{iz_2x_2}, \tag{A7}$$

N being an arbitrary integer. The remainder term $O(z_2^{-N})$ is proportional to

$$\int_0^{x_1} dx_2\, \Phi^{(N)}(x_2)\, e^{iz_2x_2},$$

a quantity vanishing with $z_2 \to \infty$, as is shown by Riemann's lemma. Finally, the asymptotic expansion of I_2 will be obtained with the integration of $J(\pm z_2)/(1+x_1^2)^{3/2}$ with respect to x_1, term by term. Such a procedure is permissible here because the final series is convergent. Restricting the development of $J(z_2)$ to $N=4$, which is largely sufficient in practice, the integration of the successive derivatives of $\Phi(x)$ will give

$$\frac{1}{2i} I_2 = \frac{1}{z_2}\left[-\int_0^\infty \frac{dx_1 \cos z_1x_1}{(1+x_1^2)^{3/2}} + \int_0^\infty \frac{dx_1 \cos(z_2 - z_1)x_1}{(1+x_1^2)}\right]$$
$$+ \frac{2}{z_2^2}\left[2\int_0^\infty \frac{dx_1\, x_1 \sin(z_2 - z_1)x_1}{(1+x_1^2)^3} - \int_0^\infty \frac{dx_1\, x_1 \sin z_1x_1}{(1+x_1^2)^{3/2}}\right]$$
$$- \frac{3}{z_2^2}\left[2\int_0^\infty \frac{dx_1 \cos z_1x_1}{(1+x_1^2)^{3/2}} - 3\int_0^\infty \frac{dx_1 \cos(z_2 - z_1)x_1}{(1+x_1^2)^4} + 2\int_0^\infty \frac{dx_1 \cos(z_2 - z_1)x_1}{(1+x_1^2)^3}\right]$$
$$+ \frac{1}{z_2^4}\left[60\int_0^\infty \frac{dx_1\, x_1 \sin(z_2 - z_1)x_1}{(1+x_1^2)^5} - 24\int_0^\infty \frac{dx_1\, x_1 \sin(z_2 - z_1)x_1}{(1+x_1^2)^4} - 9z_1K_0(|z_1|)\right] + \epsilon_5/z_2^5, \tag{A8}$$

an expression easily expanded with the aid of (see Ref. 5, p. 429)

$$\int_0^\infty \frac{\cos[(z_2-z_1)x]\,dx}{(1+x^2)^n} = \frac{\pi e^{-|z_2-z_1|}}{2^{2n-1}(n-1)!}\sum_{k=0}^{n-1}\frac{(2n-k-2)!\,(2|z_2-z_1|)^k}{k!\,(n-k-1)!}\,,$$

$$\int_0^\infty \frac{x\sin[(z_2-z_1)x]\,dx}{(1+x^2)^{n+1}} = \frac{\pi(z_2-z_1)e^{-|z_2-z_1|}}{2^{2n}n!}\sum_{k=0}^{n-1}\frac{(2n-k-2)!\,(2|z_2-z_1|)^k}{k!\,(n-k-1)!}\,.$$

Finally, with Eqs. (A2), (A3), and (A8), we obtain Eqs. (3) and (8).

APPENDIX B

Here, we establish the relations (10). First, we use (see Ref. 5, p. 687) the integral representations

$$\begin{aligned} {}_1F_2(1;\tfrac{1}{2},\tfrac{3}{2};\tfrac{1}{4}z_2^2)-\frac{\pi}{4}|z_2|\,{}_1F_2(\tfrac{3}{2};2,\tfrac{3}{2};\tfrac{1}{4}z_2^2) &= \int_0^\infty \frac{dt\,t\,J_1(t)}{t^2+z_2^2}\,,\\ {}_1F_2(1;\tfrac{1}{2},\tfrac{1}{2};\tfrac{1}{4}z_2^2)-\frac{\pi}{2}|z_2|\,{}_1F_2(\tfrac{3}{2};1,\tfrac{3}{2};\tfrac{1}{4}z_2^2) &= \int_0^\infty \frac{dt\,t^2J_0(t)}{t^2+z_2^2}\,. \end{aligned} \tag{B1}$$

Next, let us consider the decompositions

$$\begin{aligned} \int_0^\infty \frac{tJ_1(t)dt}{t^2+z^2} &= 2z^2\int_0^\infty \frac{J_0(t)dt}{(t^2+z^2)^2} - \int_0^\infty \frac{J_0(t)dt}{t^2+z^2}\,,\\ \int_0^\infty \frac{t^2J_0(t)dt}{t^2+z^2} &= 1-z^2\int_0^\infty \frac{J_0(t)dt}{t^2+z^2}\,, \end{aligned} \tag{B2}$$

of which the first has been obtained by using the differential relation $J_1(t)=-J_0'(t)$ and an integration by parts. Then we can write

$$\int_0^\infty \frac{J_0(t)dt}{t^2+z^2} = \frac{1}{|z|}S_{0,0}(|z|)\,,\qquad \int_0^\infty \frac{J_0(t)dt}{(t^2+z^2)^2} = \frac{1}{2z^2}\left[\frac{1}{|z|}S_{0,0}(|z|)+S_{-1,-1}(|z|)\right]\,. \tag{B3}$$

The second relation of (B3) is established with a differentiation of the first one with respect to z^2, and the relation $S_{0,0}'(|z|)=-S_{-1,-1}(|z|)$.

Collecting together Eqs. (B1)–(B3), we obtain Eq. (10).

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