ON THE THEORY OF TUNNEL TRANSITIONS IN CRYSTALS

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It is demonstrated that the method of calculating the well-known expression for the probability for transition of an electron from one band to another under the action of a stationary electric field, which is based on shifting the integration with respect to k_x to the complex region and taking into account only the contribution from that part of the contour which is in the immediate vicinity of the branching point of the function $\epsilon_n(\mathbf{k}) - \epsilon_{n'}(\mathbf{k})$, is incorrect. In weak fields the disregarded terms may be considerably greater than the "main" term. If this circumstance is taken into account, as well as relation (8), one finds that the traditional exponential dependence of the transition probability on the field strength F is valid only in very strong fields. The transition probability is much greater than is usually assumed, in a very broad range of field strengths and is a power function of the field strength, $P \sim \beta F^2$.

1. FUNDAMENTAL RELATIONS

WE consider a nonmetallic crystal having a symmetry center and containing an electric field **F**. If this field is directed along the negative x axis, then the probability of a transition from band 1 (valence) to band 2 (conduction) in a time t can be defined as the square of the modulus of the following expression[1,2]:

$$a(\mathbf{k}_0, t) = -\frac{eF}{\hbar}\int_0^t \alpha(\mathbf{k}')\exp\left\{\frac{i}{\hbar}\int_c^{t'}[\varepsilon_2(\mathbf{k}'') - \varepsilon_1(\mathbf{k}'')]\,dt''\right\}dt', \tag{1}$$

where

$$\alpha(\mathbf{k}) = \alpha_{21}(\mathbf{k}) = \int_{\Omega_0} U_{2\mathbf{k}}^* \frac{\partial U_{1\mathbf{k}}}{\partial k_x}\,d\tau. \tag{2}$$

The integration in (2) is over the volume of the unit cell,

$$\mathbf{k} = \mathbf{k}(t) = \mathbf{k}_0 - e\mathbf{F}t/\hbar, \quad F_x = -F, \quad F_y = F_z = 0,$$
$$\mathbf{k}' = \mathbf{k}(t'), \quad \mathbf{k}'' = \mathbf{k}(t''), \tag{3}$$

$U_{n\mathbf{k}}$ is the amplitude of the Bloch function in the n-th band, normalized to the unit cell, $\epsilon_n(\mathbf{k})$ the electron energy in the band n, and c is an arbitrary constant.

As is well known, formula (1) does not provide an exact solution of the problem of the tunnel transition in a crystal. It was derived without allowance for the scattering of electrons by the thermal lattice vibrations, which was considered by Keldysh[3]. In addition, expression (1) is only the first term of a series representing the exact solution of the problem in which scattering by phonons is disregarded[2].

Nonetheless, expressions such as (1) are widely used in the analysis of tunnel transitions in electric fields and in the theory of tunnel diodes (see, for example,[1,4-7]. The integration in (1) is carried out here by shifting the contour in the complex k_x plane. However, usually only the contribution from the part of the contour in the immediate vicinity of the branch point of the function $\epsilon_2 - \epsilon_1$ is taken rigorously into account[1)]. It will be shown below that the terms discarded in this case turn out to be much larger than the "main" term in a wide range of fields.

To compare with the previously obtained results and to estimate the contribution given by the more accurate calculation of the integral (1), we shall use the same expression for $\epsilon_n(\mathbf{k})$ as in[1,4,7], namely:

$$\varepsilon_1(\mathbf{k}) = \frac{\hbar^2k^2}{2m} + \frac{\varepsilon_G}{2} - \frac{\varepsilon_G}{2}\left[1 + \frac{\hbar^2}{m_r\varepsilon_G}k^2\right]^{1/2},$$
$$\varepsilon_2(\mathbf{k}) = \frac{\hbar^2k^2}{2m} + \frac{\varepsilon_G}{2} + \frac{\varepsilon_G}{2}\left[1 + \frac{\hbar^2}{m_r\varepsilon_G}k^2\right]^{1/2},$$
$$\frac{1}{m_r} = \frac{1}{|m_1^*|} + \frac{1}{m_2^*}, \tag{4}$$

where ϵ_G is the width of the forbidden band, m_1^* and m_2^* are the effective masses in the corresponding bands, and we consider the motion of the electron with $k_y = k_z = 0$ and $k_x \neq 0$, assuming the x axis to be directed along one of the principal crystallographic axes. Then, changing variables and putting $c = -\hbar k_{0x}/eF$, we write (1) in the form

$$a(k_{0x}, t) = -\int_{k_{0x}}^{k_x} \alpha(k_x')\exp\left\{i2\varkappa\int_0^{c_1k_x'}\sqrt{1+\eta^2}\,d\eta\right\}dk'_x, \tag{5}$$

where

$$\varkappa = \frac{\varepsilon_G}{2c_1eF}, \quad c_1 = \frac{\hbar}{\sqrt{m_r\varepsilon_G}}. \tag{5a}$$

Taking the integral in the exponential of (5), we get

$$a(k_{0x}, t) = -\int_{k_{0x}}^{k_x} \alpha(k_x')\exp\{i\varkappa\varphi(c_1k_x')\}\,dk_x', \tag{6}$$

where

$$\varphi(x) = x\sqrt{1+x^2} + \ln(x + \sqrt{1+x^2}). \tag{7}$$

For further calculation of (6), it is necessary to know the explicit form of $\alpha(\mathbf{k})$. We note first the following general relation, which is satisfied for real **k**:

$$\alpha_{nn'}(-\mathbf{k}) = -\int_{\Omega_0} U^*_{n,-\mathbf{k}}(\mathbf{r})\frac{\partial}{\partial k_x}U_{n',-\mathbf{k}}(\mathbf{r})\,d\tau$$
$$= -\int_{\Omega_0} U_{n\mathbf{k}}(\mathbf{r})\frac{\partial}{\partial k_x}U^*_{n'\mathbf{k}}(\mathbf{r})\,d\tau = -\alpha^*_{nn'}(\mathbf{k}). \tag{8}$$

1) The presence of a pole in the function $\alpha(\mathbf{k})$ was likewise not taken into account in [1], as pointed out by Keldysh[3].

We have used here the well known property of the functions $U_{nk}(\mathbf{r})$:

$$U_{n,-\mathbf{k}}(\mathbf{r}) = U_{n\mathbf{k}}^*(\mathbf{r}).$$

On the other hand, it is easy to verify that $\alpha_{nn'}$ is a real quantity when $n' \neq n$. This follows from the relation[8]

$$\alpha_{nn'}(\mathbf{k}) = -\hbar p_{nn'}^x / m[\varepsilon_n(\mathbf{k}) - \varepsilon_{n'}(\mathbf{k})], \tag{9}$$

where

$$p_{nn'}^x = -i\hbar \int_{\Omega_0} U_{n\mathbf{k}}^*(\mathbf{r}) \frac{\partial}{\partial x} U_{n'\mathbf{k}}(\mathbf{r})\, d\tau.$$

Since $p_{nn'}^x$ is a real quantity, as follows from the invariance of the integral

$$\int U_{n\mathbf{k}}^*(\mathbf{r}) \frac{\partial}{\partial x} U_{n'\mathbf{k}}(\mathbf{r})\, d\tau$$

against inversion, it follows from (9) that $\alpha(\mathbf{k})$ is real. Then we get from (8) that $\alpha(\mathbf{k})$ is an odd function of k. To find the form of this function, we shall use the well known relation (the f-sum rule) [8]

$$\frac{2}{m^2} \sum_{n' \neq n} \frac{(p_{nn'}^x)^2}{\varepsilon_{n'}(\mathbf{k}) - \varepsilon_n(\mathbf{k})} = \frac{1}{m} - \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon_n(\mathbf{k})}{\partial k_x^2}.$$

Hence, by virtue of (9), we get

$$\alpha^2(\mathbf{k}) = \frac{1}{4(\varepsilon_2 - \varepsilon_1)} \left[\frac{\partial^2 \varepsilon_2}{\partial k_x^2} - \frac{\partial^2 \varepsilon_1}{\partial k_x^2} \right]. \tag{10}$$

The obtained formula is general for the chosen two-band model.

Substituting here $\epsilon_n(\mathbf{k})$ from (4), we obtain for the "one-dimensional" case under consideration

$$\alpha^2(k_x) = \frac{c_1^2}{4(1 + c_1^2 k_x^2)^2}$$

or

$$\alpha(k_x) = \frac{1}{2} \frac{c_1}{1 + c_1^2 k_x^2} \operatorname{sign} k_x, \tag{11}$$

where the sign function ensures the odd character of $\alpha(k_x)$ for real k_x. The characteristic discontinuity of the function $\alpha(k_x)$ at the point $k_x = 0$ can be observed by calculating $\alpha(k_x)$ directly with the aid of the **kp** perturbation theory. A similar calculation was performed by Kane[7], but as a result of an erroneous differentiation with respect to $|\mathbf{k}|$ instead of k_x, this discontinuity is not taken into account in his formulas. In fact, the expression for $\alpha(\mathbf{k})$ in[7] should contain an additional factor $k_x/|\mathbf{k}|$, which leads to a discontinuity at the point $\mathbf{k} = 0$.

Taking (11) into account, we get from (6)

$$a(k_{0x}, t) = \frac{c_1}{2} \int_{k_{0x}}^{k_x} \frac{\operatorname{sign} k_x'}{1 + c_1^2 k_x'^2} \exp\{i\varkappa\varphi(c_1 k_x')\}\, dk_x'. \tag{12}$$

We now must answer the question of which integration limits must be taken in (12) in order to obtain the natural characteristic of the penetration from band to band. Usually this quantity is chosen to be the transition probability per period of electron oscillations in the band. The integration with respect to k_x' is then carried out in (12) from $-K/2$ to $K/2$, where K is the width of the Brillouin zone in the x direction. Since φ is an odd function of k_x', by virtue of the equation[9]

$$\ln(x + \sqrt{1 + x^2}) = -\ln(-x + \sqrt{1 + x^2}),$$

it follows that the contribution to the integral from the exponential yields only $\sin\{\kappa\varphi(c_1 k_x')\}$ when these integration limits are used. But then we find that $a \to 0$ as $F \to \infty$, i.e., when the distance between bands tends to zero.

This result can be attributed to the fact that in the indicated limiting case the electron will execute, under the influence of the field, oscillations that encompass both bands, and at the end of a complete period of the oscillations the electron will be in the initial state, i.e., in the first band. We see therefore that the characteristics of the penetration should be taken to be the probability of the transition within a time equal to half the period, when the electron moves in the direction towards the second band. The limits of k_x' will then be 0 and K/2. Introducing a new integration variable $\xi = c_1 k_x'$, we obtain for the amplitude of the transition probability for each "approach" to the barrier

$$a = \frac{1}{2} \int_0^{\xi_0} \frac{1}{1 + \xi^2} \exp\{i\varkappa\varphi(\xi)\}\, d\xi, \quad \xi_0 = c_1 \frac{K}{2}. \tag{13}$$

2. CALCULATION OF THE TRANSITION PROBABILITY AMPLITUDE

To calculate the integral (13) we shall assume that ξ is complex and go over from the ξ plane to the complex z plane with the aid of the substitution $\xi = -iz$. Then expression (7) goes over into

$$-iz\sqrt{1 - z^2} + \ln(-iz + \sqrt{1 - z^2});$$

writing $\sqrt{1 - z^2} = i\sqrt{z^2 - 1}$ and using the equality

$$\ln(iw) = \tfrac{1}{2}\pi i + \ln|w| + i \arg w,$$

we get

$$a = -\frac{i}{2} \exp\left\{-\frac{\pi\varkappa}{2}\right\} \int_0^{i\xi_0} f(z)\, dz, \tag{14}$$

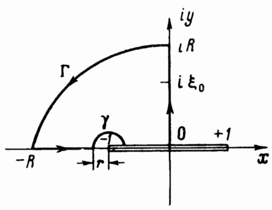
where

$$f(z) = \frac{1}{1 - z^2} \exp\{i\varkappa[z\sqrt{z^2 - 1} + \ln|\sqrt{z^2 - 1} - z| + i \arg(\sqrt{z^2 - 1} - z)]\}.$$

The exponential factor in front of the integral coincides with the expression obtained by Kane[10] (for $\mathbf{k}_\perp = 0$, $k_\perp^2 = k_y^2 + k_z^2$), and with the corresponding expressions in[1,11] and elsewhere. This factor is decisive in all the formulas for the transition probability in the cited papers, so that the transition probability turns out to be vanishingly small at fields weaker than $\sim 10^4$ V/cm. As will be shown below (see the Appendix), calculation of the integral in (14) gives rise to terms in which this exponential factor is cancelled out and by the same token the obtained transition probability in weak fields is much larger.

Let us consider the analytic properties of the integrand in (14). The factor preceding the exponential has simple poles at the points $z = \pm 1$, and the same points are also branch points of the function $\sqrt{z^2 - 1}$. There are no other singularities, and consequently the function is analytic in a plane with a cut from -1 to $+1$. The residue at the points $z = \pm 1$ of the function $-i/2(1 - z^2)$ is $\pm i/4$, which agrees with the results obtained by Keldysh[3].

In connection with the chosen substitution $\xi = -iz$, in order for the integral to coincide with the initial one on



the corresponding section of the contour, it is necessary to have

$$\operatorname{Im}\sqrt{z^2-1}<0 \text{ for } y>0, \quad z=x+iy.$$

This corresponds to a choice of the "second" sheet of the Riemann surface[12]. Further, f(z) decreases exponentially at infinity when

$$\operatorname{Im} z\sqrt{z^2-1}>0. \tag{15}$$

The latter inequality is satisfied in the second and fourth quadrants of the complex plane. This follows from the fact that if we put $\sqrt{z^2-1} = u + iv$, then $\operatorname{Im} z\sqrt{z^2-1} = xv + yu$, and the sign of the functions u and v on the second sheet of the Riemann surface are as follows:

$$\begin{aligned}
&\text{first quadrant: } u<0,\ v<0\\
&\text{second quadrant: } u>0,\ v<0,\\
&\text{third quadrant: } u>0,\ v>0,\\
&\text{fourth quadrant: } u<0,\ v>0.
\end{aligned} \tag{16}$$

Therefore the integration contour is chosen in the second quadrant of the complex plane with cut from -1 to $+1$ (see the figure)[2)].

Since f(z) has no singularities inside this contour, we can write

$$\int_0^{i\xi_0} f(z)\,dz = -\int_{i\xi_0}^{iR} f(z)\,dz - \int_\Gamma f(z)\,dz - \int_{-R}^{-1-r} f(z)\,dz - \int_\gamma f(z)\,dz - \int_{-1+r}^{0} f(z)\,dz.$$

In the limit as $R\to\infty$ and $r\to 0$, the integral along the contour Γ vanishes by virtue of the exponential decrease of f(z), and we get

$$\int_0^{i\xi_0} f(z)\,dz = -\int_\gamma f(z)\,dz - I_1 - I_2, \tag{17}$$

$$I_1=\lim_{r\to 0}\left(\int_{-\infty}^{-1-r} f(z)\,dz + \int_{-1+r}^{0} f(z)\,dz\right), \quad I_2=\int_{i\xi_0}^{i\infty} f(z)\,dz. \tag{17a}$$

The integral along the contour γ is calculated in elementary fashion:

$$\lim_{r\to 0}\int_\gamma f(z)\,dz = -\frac{\pi i}{2} \tag{18}$$

(the minus sign is due to the fact that the point $x = -1$ is circled clockwise). This integral is usually considered as the principal one, and the integrals over the remaining part of the contour are discarded, while in[7] the integration contour was chosen incorrectly, since it corresponds to an interval of integration with respect to ξ from $-\infty$ to $+\infty$.

We now consider the integrals I_1 and I_2. Unfortunately they cannot be calculated exactly. However, they can be estimated (see the Appendix). We then get from (14)

$$\begin{aligned}
\operatorname{Re} a &= \frac{1}{2}\exp\left\{-\frac{\pi}{2}\varkappa\right\}\left\{\frac{\pi}{2}-\operatorname{Im} I_1''-\operatorname{Im} I_2\right\}\\
\operatorname{Im} a &= \frac{1}{2}\exp\left\{-\frac{\pi}{2}\varkappa\right\}\{I_1'+\operatorname{Re} I_1''+\operatorname{Re} I_2\},
\end{aligned} \tag{19}$$

where the values of I_1', I_1'' and I_2 are given in (A.3), (A.4), (A.7), (A.8), (A.13), and (A.14).

We note that in the derivation of (19) from formula (1) no assumptions were made concerning the magnitude of the field. As shown by numerical estimates, the additional terms I_1 and I_2 are far from small compared with $\pi/2$ for arbitrary fields. In order to illustrate this, we shall carry out an analysis for the extreme cases of "small" and "large" fields, i.e., for the cases when $\kappa \gg 1$ and $\kappa \ll 1$ (κ is defined in (5a)).

For the case $\kappa \gg 1$, using the known asymptotic expansions of the functions S, C, and Ei, we obtain

$$\begin{aligned}
& I_1' \approx g\frac{1}{\varkappa}\exp\left\{\frac{\pi\varkappa}{2}\right\}, \quad \frac{1}{4}<g<\frac{2}{\pi},\\
& 0.9<\operatorname{Re} I_1''<\sqrt{\frac{\pi\varkappa}{2}}, \quad \frac{0.45}{\varkappa}<\operatorname{Im} I_1''<\sqrt{\frac{\pi\varkappa}{2}},\\
& \operatorname{Re} I_2 \approx -\frac{1}{2(\xi_0^2+1)^{3/2}}\exp\left\{\frac{\pi\varkappa}{2}\right\}\frac{1}{\varkappa}\cos[\varphi(\xi_0)\varkappa],\\
& \operatorname{Im} I_2 \approx -\frac{1}{2(\xi_0^2+1)^{3/2}}\exp\left\{\frac{\pi\varkappa}{2}\right\}\frac{1}{\varkappa}\sin[\varphi(\xi_0)\varkappa].
\end{aligned} \tag{20}$$

If we neglect the exponentially small terms, then we get from (19) and (20)

$$\begin{aligned}
\operatorname{Re} a &\approx \frac{1}{4(\xi_0^2+1)^{3/2}}\frac{F}{F_0}\sin\left[\frac{\varphi(\xi_0)F_0}{F}\right],\\
\operatorname{Im} a &\approx \frac{1}{2}\frac{F}{F_0}\left\{g-\frac{1}{2(\xi_0^2+1)^{3/2}}\cos\left[\frac{\varphi(\xi_0)F_0}{F}\right]\right\},
\end{aligned} \tag{21}$$

where

$$F_0 = m_r^{1/2}\varepsilon_G^{3/2}/2e\hbar, \quad \varkappa = F_0/F.$$

The probability of the tunnel transitions for one approach to the barrier is

$$P=|a|^2\approx\frac{1}{4}\left\{g^2+\frac{1}{4(\xi_0^2+1)^3}-\frac{g\cos[\varphi(\xi_0)F_0/F]}{(\xi_0^2+1)^{3/2}}\right\}\left(\frac{F}{F_0}\right)^2. \tag{22}$$

We now consider the case when $F_0/F = \kappa \ll 1$. Confining ourselves to the principal terms of the expansion, we get here

$$\begin{aligned}
& 0{,}45\,\varkappa < I_1' < \pi\varkappa/2,\\
& 0{,}9\sqrt{\pi\varkappa/2} < \operatorname{Re} I_1'' \approx \operatorname{Im} I_1'' < \sqrt{\pi\varkappa/2},\\
& \operatorname{Re} I_2 \approx -\frac{1}{\xi_0}\exp\left\{\frac{\pi\varkappa}{2}\right\}\sqrt{\frac{\pi\xi_0\varkappa}{2}},\\
& \operatorname{Im} I_2 \approx \frac{1}{\xi_0}\exp\left\{\frac{\pi\varkappa}{2}\right\}.
\end{aligned} \tag{23}$$

From this and from (19) we see that when $\kappa \ll 2\pi^{-1}\ln(\pi\xi_0/2)$ we get

$$\operatorname{Re} a \approx \frac{\pi}{4}\exp\left\{-\frac{\pi}{2}\frac{F_0}{F}\right\}, \tag{24}$$

and since the imaginary part is negligibly small under these conditions:

$$\lim_{\varkappa\to 0}\operatorname{Im} a \to 0, \tag{25}$$

we obtain Kane's expression for the transition probability[10].

2)In making the substitution $\xi = iz$ it is necessary to work, for the same reasons, in the first sheet in the fourth quadrant.

3. ESTIMATES AND DISCUSSION OF THE RESULTS

To obtain numerical estimates, we consider two examples of semiconductors with narrow and broad forbidden bands. The former is chosen to be InSb, which is considered also in[4] and in[10]. This crystal has no symmetry center and therefore it is not rigorously correct to apply our formulas to it, as well as the analogous formulas of Argyres and Kane. However, as noted by Kane, the resulting error is small. The second example is GaAs, which has the same structure as InSb, but a broad forbidden band. We must emphasize here that the main purpose of our estimates is not to obtain numerical results for the indicated concrete crystals, but to investigate the character of the dependence of the transmission coefficient on the width of the forbidden band and on the field intensity in the "weak" and "strong" field intervals.

We choose the InSb parameters as follows: $\epsilon_G = 0.18$ eV, $m_r = 6.5 \times 10^{-3}$m (reduced mass corresponding to electrons and light holes), d = 6.48 Å—lattice constant. At these values of the parameters we have $\xi_0 = 78$ and $F_0 = 1.1 \times 10^5$ V/cm.

For GaAs we choose $\epsilon_G = 1.4$ eV, $m_r = 6 \times 10^{-2}$m (electrons and heavy holes), and d = 5.63 Å. Accordingly, $\xi_0 = 11$ and $F_0 = 7.4 \times 10^6$ V/cm. (The width of the Brillouin zone in the x direction at $k_y = k_z = 0$ is $K = 4\pi/d$ in both cases.)

We consider first the case $\kappa = F_0/F \gg 1$. The expression (21) for Re a coincides, apart from a factor 2, with the asymptotic formula for a obtained by Argyres in a different manner ([4], formula (2.18)). However, the cited paper has no expression for Im a. The reason is that in the derivation used in[4], and incidentally also in other papers (see, for example[13]), no account was taken of the fact that $\alpha(\mathbf{k})$ is an odd function of k, and the integration was carried out from $-K/2$ to $K/2$ under the assumption that this is an even function. If we assume that (k) is even, then in integrating in (6) from $-K/2$ to $K/2$ we actually find, by virtue of the fact that φ is odd, that Im a vanishes, and the real part is twice the value obtained by us. It is very important that Im a in (21) is larger than Re a by two orders of magnitude in the case of InSb and by five orders of magnitude in the case of GaAs. Accordingly, the first term in the curly brackets of (22) is larger by several orders of magnitude than the remaining two. Consequently, we can write P in the form

$$P \approx \frac{g^2}{4}\left(\frac{F}{F_0}\right)^2. \tag{26}$$

Let us compare this expression with the corresponding formula obtained by Kane[10]

$$T = \frac{\pi^2}{9}\exp\left\{-\frac{\pi F_0}{F}\right\}. \tag{27}$$

If, for example, $\kappa = 10$, then it turns out that $P \sim 2 \times 10^{-4}$ and $T \sim 2 \times 10^{-14}$. In weaker fields, the difference is even larger.

Thus, the transition probability obtained from the power-law formula (26) is larger by many orders of magnitude than T in fields up to 10^4 V/cm in the case of InSb, and up to 7×10^5 V/cm in the case of GaAs, i.e., in a very wide interval of fields.

Let us analyze now the case of strong fields ($\kappa \ll 1$). In this case, the inequality leading to (24) is always satisfied and consequently the transition probability depends exponentially on the field intensity. The region where such a dependence takes place is determined by the requirements $F \gg 10^5$ V/cm in the case of InSb and $F \gg 7 \times 10^6$ V/cm in the case of GaAs. These conditions are approximately satisfied in tunnel diodes, where the internal field is of the order of 10^5—10^6 V/cm.

In conclusion we note that the fact that our analysis is confined to a simple two-band model, when the dispersion is given by formulas (4), is obviously not of fundamental significance. The quantities I_1 and I_2 which we took additionally into account, will definitely appear also under other conditions, for example, in the degenerate-band case considered in[14]; in any case, the analysis shows that Zener's traditional approach is incorrect. The so-called weak fields play a much more important role in interband transitions than is usually assumed, and more rigorous calculations lead apparently not only to quantitative but also to qualitative modifications in many problems.

The authors are grateful to A. A. Gol'dberg and V. P. Potapov for a discussion of the mathematical aspects of the paper.

APPENDIX

Let us consider the integral I_1 (formula (17a)). Taking (16) into account, we obtain in the interval $(-\infty, -1)$ [3)]

$$\sqrt{z^2-1} = \sqrt{x^2-1}, \quad \arg(\sqrt{z^2-1}-z) = 0,$$

and on the segment $(-1, 0)$

$$\sqrt{z^2-1} = -i\sqrt{1-x^2}, \quad \ln|\sqrt{z^2-1}-z| = 0,$$
$$\arg(\sqrt{z^2-1}-z) = -\operatorname{arctg}\frac{\sqrt{1-x^2}}{|x|} = -\arccos|x|.$$

Then, after changing the integration variable $x \to -x$, the expression for I_1 assumes in the limit as $r \to 0$ the form

$$I_1 = \int_0^1 \frac{1}{1-x^2}\exp\{\kappa\varphi_1'(x)\}\,dx + \int_1^\infty \frac{1}{1-x^2}\exp\{-i\kappa\varphi_1''(x)\}\,dx,$$

where

$$\varphi_1'(x) = \arccos x - x\sqrt{1-x^2},$$
$$\varphi_1''(x) = x\sqrt{x^2-1} - \ln(x+\sqrt{x^2-1}).$$

Both integrals diverge at the point x = 1, but their sum is finite. This can be directly verified by writing I_1 in the form

$$I_1 = \int_0^\infty \frac{dx}{1-x^2} + I_1' + I_1'', \tag{A.1}$$

where

$$I_1' = \int_0^1 \frac{1}{1-x^2}\{\exp[\kappa\varphi_1'(x)] - 1\}\,dx,$$
$$I_1'' = \int_1^\infty \frac{1}{1-x^2}\{1 - \exp[-i\kappa\varphi_1''(x)]\}\,dx.$$

The first integral in the right side of (A.1) exists in the sense of the principal value and vanishes, as can be readily verified. The integrand expressions in I_1' and I_1'' are finite at the point x = 1.

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3)The root of a positive quantity is henceforth taken with the plus sign.

We now estimate the integral I_1'. To find its upper limit we replace $\varphi_1'(x)$ and also the denominator of the integrand:

$$\varphi_1'(x)\to\frac{\pi}{2}(1-x),\quad 1-x^2\to 1-x. \tag{A.2}$$

Such a replacement increases I_1', since the numerator of the integrand increases and the denominator decreases in the entire interval (0, 1). Then, after elementary integration, we obtain

$$I_1'<\mathrm{Ei}\left(\frac{\pi\varkappa}{2}\right)-\ln\left(\frac{\pi\varkappa}{2}\right)-C\equiv\mathscr{F}_1', \tag{A.3}$$

where Ei(x) is the integral exponential function and C is Euler's constant[15].

On the other hand, from analogous considerations we have

$$I_1'>\frac{1}{2}\int_0^{\pi/4}\frac{1}{1-x}\left\{\exp\left[\frac{\pi\varkappa}{2}\left(1-\frac{4}{\pi}x\right)\right]-1\right\}dx.$$

Calculating this integral, we get

$$I_1'>\frac{1}{2}\left\{\exp\left[-\left(2-\frac{\pi}{2}\right)\varkappa\right]\left(\mathrm{Ei}(2\varkappa)-\mathrm{Ei}\left[\left(2-\frac{\pi}{2}\right)\varkappa\right]\right)+\ln\left(1-\frac{\pi}{4}\right)\right\}\equiv f_1'. \tag{A.4}$$

Numerical calculations show that f_1' and $\mathscr{F}_1'$ have the same order of magnitude in any field. Consequently, we can obtain from these estimates the correct order of magnitude of I_1'. Of course, the accuracy of these estimates can be easily improved if necessary.

The integral I_1'' is somewhat more difficult to estimate, since its integrand is an oscillating function. For these estimates we shall use the following theorem:

Assume that we have a converging integral

$$I=\int_{\xi_1}^{\infty}\psi(\xi)\sin\chi(\xi)\,d\xi,$$

where $\chi(\xi)$ is a function that increases monotonically to infinity and satisfies the condition $\chi(\xi_1) = 0$; $d\chi/d\xi$ is a non-decreasing function which is positive in the interval (ξ_1, ∞). Assume that we are also given a converging integral

$$\tilde{I}=\int_{\xi_1}^{\infty}\tilde{\psi}(\xi)\sin\chi(\xi)\,d\xi.$$

Then $\tilde{I} > 1$ if the difference $\tilde{\psi}(\xi)-\psi(\xi)$ is positive, and decreases monotonically and vanishes when $\xi\to\infty$.

To prove this statement, we make the change of integration variable $\chi(\xi) = \eta$, noting here that, by virtue of the monotonic increase of χ, the function $\xi(\eta)$ also increases monotonically. As a result we obtain

$$\Delta I=\tilde{I}-I=\int_0^{\infty}\mathscr{F}(\eta)\sin\eta\,d\eta,$$

where

$$\mathscr{F}(\eta)=(\tilde{\psi}[\xi(\eta)]-\psi[\xi(\eta)])\Big/\frac{d\chi[\xi(\eta)]}{d\xi}$$

is a function that decreases monotonically to zero.

Subdividing in the latter integral the integration region into intervals $[n\pi, (n+1)\pi]$, n = 0, 1, 2, ..., and applying to each interval the theorem of the mean, we get

$$\Delta I=2\sum_{n=0}(-1)^n\mathscr{F}(\bar{\eta}_n),$$

where

$$n\pi<\bar{\eta}_n<(n+1)\pi.$$

Since $\mathscr{F}(\bar{\eta}_n)$ tends monotonically to zero as $n\to\infty$, the series converges to a positive limit, $\Delta I > 0$, thus proving the theorem.

This theorem, as can be readily seen, is valid also for the case when the integrand contains $1-\cos\chi$ in lieu of $\sin\chi$. In order to use this theorem, we first make in I_1'' the following change of variables:

$$\varkappa\varphi_1''(x)=\varkappa(\xi-1)^2=\chi_1(\xi). \tag{A.5}$$

Then the factor preceding the oscillating term in the integrand will be

$$(\xi-1)/[x^2(\xi)-1]^{1/2}=\psi_1(\xi).$$

We now introduce the function $\tilde{\psi}_1(\xi) = 1/(\xi-1)^2$. The conditions of the theorem are then satisfied, as can be readily verified[4)], and since the integral $\tilde{I}_1''$ can be calculated exactly when ψ_1 is replaced by $\tilde{\psi}_1$, we get $I_1''<\tilde{I}_1''$.

Similarly, in order to obtain the lower bound, we make the substitution

$$\varkappa\varphi_1''(x)=\varkappa(\xi^2-1)=\chi_2(\xi); \tag{A.6}$$

which yields in front of the oscillating function the factor

$$\xi/[x^2(\xi)-1]^{1/2}=\tilde{\psi}_2(\xi).$$

Introducing further $\psi_2(\xi) = 1/G\xi^2$, we can show that the conditions of the theorem are satisfied if $G \geq 1.1$. The integral with $\psi_2(\xi)$ can also be calculated exactly. As a result we obtain the following estimates:

$$\mathrm{Re}\,I_1''<\sqrt{\pi\varkappa/2},$$
$$\mathrm{Re}\,I_1''>\frac{\sqrt{2\pi\varkappa}}{G}\left\{\cos\varkappa\left[\frac{1}{2}-S(\sqrt{\varkappa})\right]-\sin\varkappa\left[\frac{1}{2}-C(\sqrt{\varkappa})\right]\right\}\equiv f_{1r}'', \tag{A.7}$$

$$\mathrm{Im}\,I_1''>\frac{\sqrt{2\pi\varkappa}}{G}\left\{\cos\varkappa\left[\frac{1}{2}-C(\sqrt{\varkappa})\right]+\sin\varkappa\left[\frac{1}{2}-S(\sqrt{\varkappa})\right]\right\}\equiv f_{1i}'', \tag{A.8}$$

where S and C are the Fresnel sine and cosine integrals[15].

In the limiting case $\kappa\to 0$ $(F\to\infty)$, f_{1r}'' and f_{1i}'' turn out to be equal to $G^{-1}\sqrt{\pi\kappa/2}$, i.e., the upper and lower limits almost coincide in this case.

Let us consider further the integral I_2 defined in (17a). According to (16), we have on its integration contour z = iy

$$\sqrt{z^2-1}=-i\sqrt{y^2-1},\quad \ln|\sqrt{z^2-1}-z|=\ln(y+\sqrt{1+y^2}),$$
$$\arg(\sqrt{z^2-1}-z)=-\pi/2. \tag{A.9}$$

Then

$$I_2\equiv i\exp\left\{\frac{\pi}{2}\varkappa\right\}\int_{\xi_0}^{\infty}\frac{1}{1+y^2}\exp\{i\varkappa\varphi(y)\}\,dy, \tag{A.10}$$

where $\varphi(y)$ is defined in (7).

From (A.9), incidentally, we see directly that expression (14) transformed to complex integration variables actually coincides with the initial expression (13).

The method used to estimate I_1 cannot be used to estimate the integral in (A.10), since $\varphi(\xi_0)$, generally speaking, does not vanish. In this connection, we replace $\varphi(y)$ by a polynomial which coincides formally

4)To find $x(\xi)$ it is convenient to use a graphic method of solving the transcendental equation.

with the expansion of $\varphi(y)$ in a series in the vicinity of ξ_0, accurate to the quadratic term,

$$\varphi(y) \approx \varphi(\xi_0) - \frac{(\xi_0^2+1)^{3/2}}{\xi_0} + \frac{\xi_0}{\sqrt{\xi_0^2+1}}\left(y + \frac{1}{\xi_0}\right)^2, \tag{A.11}$$

and we replace $1 + y^2$ in the denominator by the expression

$$1 + y^2 \approx \frac{\xi_0^2}{\xi_0^2+1}\left(y + \frac{1}{\xi_0}\right)^2, \tag{A.12}$$

which coincides with $1 + y^2$ at $y = \xi_0$. We note that the difference between the right-hand and left-hand parts of these approximate equations does not exceed one-tenth of one per cent in the entire interval (ξ_0, ∞) of the variation of y with ξ_0 on the order of ten. With increasing ξ_0, the accuracy increases.

Using (A.11) and (A.12) we obtain in (A.10) integrals that can be readily calculated. The result is

$$\operatorname{Re} I_2 \approx \frac{1}{\xi_0}\exp\left\{\frac{\pi}{2}\varkappa\right\}\{-\sin[\varkappa\varphi(\xi_0)] + \sqrt{2\pi\zeta_0\varkappa}[\sin(\eta_0\varkappa)(1/2 - S(\sqrt{\zeta_0\varkappa})) - \cos(\eta_0\varkappa)(1/2 - C(\sqrt{\zeta_0\varkappa}))]\}, \tag{A.13}$$

$$\operatorname{Im} I_2 \approx \frac{1}{\xi_0}\exp\left\{\frac{\pi}{2}\varkappa\right\}\{\cos[\varkappa\varphi(\xi_0)] - \sqrt{2\pi\zeta_0\varkappa}[\cos(\eta_0\varkappa)(1/2 - S(\sqrt{\zeta_0\varkappa})) + \sin(\eta_0\varkappa)(1/2 - C(\sqrt{\zeta_0\varkappa}))]\}, \tag{A.14}$$

where

$$\zeta_0 = \frac{(\xi_0^2+1)^{3/2}}{\xi_0}, \qquad \eta_0 = \varphi(\xi_0) - \zeta_0.$$

It should be noted that the important exponential factor which cancels out a similar factor in (14) appears here perfectly rigorously (see (A.10)), and the approximation in the calculation of the integral affects only the expressions in the curly brackets of (A.13) and (A.14).

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