THEORY OF INTERNAL PHOTOEMISSION IN SANDWICH STRUCTURES

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Abstract:

The internal photoemission in sandwich structures is treated as a multi-step process. The excitation functions for electrons in the electrodes are obtained as a result of a rigorous optical analysis of the light propagation and absorption. The electron–electron and electron–phonon interactions are described in terms of energy-dependent mean free paths. The calculation of the quantum yield and photocurrent includes the electrons which escape without scattering, after one scattering, and after two scattering processes. In calculating the probability for electrons to escape over the inner potential barrier within the structure account has been taken of both their being scattered within the barrier region and their quantum-mechanical character.

The present calculations can conveniently be used for theoretical investigations of the photoemission in its dependence on various parameters of the structure. The formulae also retain their validity for the photoemission of holes when the quantities due to electrons are correspondingly replaced. An adaptation of the theory to the vacuum photoemission from thick as well as very thin samples is possible without difficulties.

Contents:

1. Introduction

The internal photoemission is frequently used to investigate the electronic properties of metal–insulator–metal (MIM) or metal–insulator–semiconductor (MIS) sandwich structures [1, 2]. The most powerful tool of this method is probably the examination of the spectral dependence of the photocurrent flowing between the electrodes of the structure. Such measurements have also been performed with varying the other parameters of the structure, e.g. the insulator thickness, applied voltage, or thickness of the electrodes. The analysis of experimental results is almost exclusively based on the simple Fowler relation [1–4] $Y_F(\omega) \sim (\hbar\omega - \phi)^2$, ($Y_F(\omega)$ is the quantum yield per absorbed photon, $\hbar\omega$ is the photon energy, and ϕ is the photoelectric work function), obtained originally for the photoemission from metal into vacuum. Although in many cases this relation is very useful to describe the main features of the photoresponse above the threshold, it fails in explaining some detailed observations on sandwich structures, especially if the electrodes and/or the insulator are very thin [2, 4].

In the last years some attempts have been made to modify the Fowler relation in order to understand the particular observations. For example, Rouzeyre [5] has introduced some of the multiple reflections of the light in the sandwich into the calculation, Berglund and Powell [6] and Blossey [7] gave the treatment of the electron scattering in the barrier. Schuermeyer et al. [8] have applied the Monte Carlo method for calculation of the photocurrent. However, the internal photoemission in sandwich structures has never been described in all its aspects by a unified complex treatment. It is the purpose of this paper to outline such a theory which would be able to account for a variety of important effects influencing the photocurrent in sandwiches. At the same time in striving for a general treatment we also realize the disadvantage of such an approach: it cannot be used directly to analyze the experimental results. The complicated expressions can be effectively dealt with only by a computer. On the other hand, various functional dependences of parameters can be accounted for without involving strong simplifications. The question of the influence of a certain variable (e.g. electrode thickness) upon the photocurrent can be answered quite accurately. This is the way in which our theory can promote the understanding of internal photoemission in sandwich structures. Moreover, the calculation of electron scattering in the electrodes is believed to be of interest also in the theory of ultraviolet photoemission spectroscopy of metals and of secondary electron emission.

Some problems treated in this work arise only in the case of a thin-film sandwich structure and have no analogy in the vacuum photoemission from a semi-infinite solid. One of them is the presence of multiple reflections of light on the interfaces within the structure and their influence on the excitation of electrons. The exact analysis (within classical optics) of the propagation and absorption of the light wave is performed in section 2. Another special feature of sandwich structures is that the currents entering the barrier region from the two electrodes are in opposite directions; the net photocurrent is then calculated (in terms of quantum yields) as a difference of these currents (section 5). Transport of electrons through the electrode to the interface involving one-step and two-step scattering is calculated in section 3. The scattering probabilities are expressed in terms of energy-dependent mean free paths for electron–electron scattering l_e (inelastic processes) and for electron–phonon* scattering l_p (elastic or nearly elastic processes). The total mean free path l may be written as $l = l_e l_p/(l_e + l_p)$.

*By electron–phonon scattering we denote all lattice-related (defect, impurity, and phonon) scattering processes.

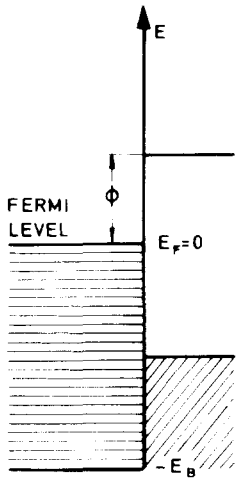


Fig. 1. Diagram of the energy scale at an interface (e.g. metal–insulator): the energy E is measured from the Fermi level.

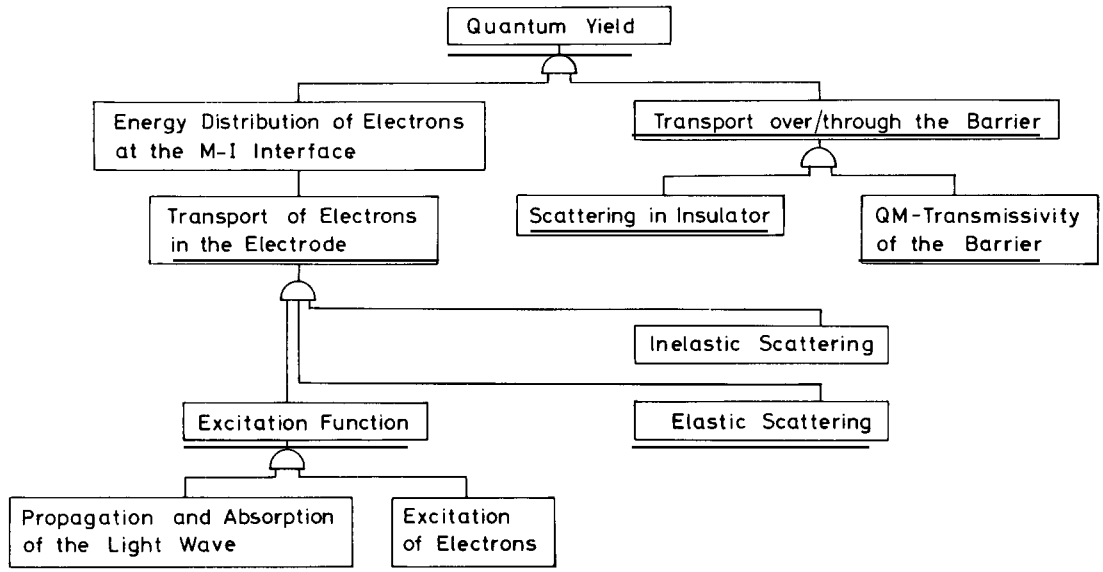
The energies are measured [9] with respect to the Fermi level ($E_F = 0$) of the electrode under consideration (see fig. 1). Using the parabolic-band approximation* *for the excited electrons* with energy $E \gtrsim \phi_m$, the magnitude of electron momentum is then $p = [2m(E + E_0)]^{1/2}$ and its x-directed component $p_x = [2m(\tilde{E}_x + E_0)]^{1/2}$ where ϕ_m is the maximum barrier height, m the effective electron mass, E the energy in excess of the Fermi level E_F and $\tilde{E}_x$ the part of energy above E_F associated with p_x. Then the kinetic energy E_x of an electron (within the electrode) associated with p_x is $\tilde{E}_x + E_0$. The value E_0 is given by the energy difference between the surface potential barrier (or inner potential barrier [10]) V_0 and the barrier height (or photoelectric work function) ϕ: $E_0 = V_0 - \phi$. [9] In the special case when the free-electron approximation remains valid down to the bottom of the conduction band, the energy E_0 is equal to the energy E_B which is the difference between the Fermi level and the bottom of the conduction band.

Concerning the escape of electrons from the electrode, we doubt the often expressed conviction that the quantum-mechanical character of electrons can be neglected in calculating the probability of escape over the barrier. The smearing of the quantum-mechanical transmission coefficient [11–13] over the energy in the vicinity of the barrier maximum ϕ_m (in comparison to the classical zero-or-one probability) can lead to a change of the functional dependence of the quantum yield on photon energy $\hbar\omega$ for $\hbar\omega \approx \phi_m$. Section 4 shows an approximate way to evaluate the escape probability which accounts for both the quantum-mechanical character of electrons and the possibility of their scattering in the barrier region.

We should mention that, although all the considerations are made for the emission of electrons into the conduction band of the insulator, the calculations in this paper are also directly applicable to the emission of holes into its valence band. As long as the parabolic-band approximation is valid for excited holes it is sufficient for the description of the hole emission to replace the quantities related to the electron emission (effective mass, energy E_0, density of filled states, mean free paths, potential barrier, and so on) by the corresponding quantities related to the hole emission.

*For non-parabolic bands see the comments in section 6.

Table I
Problems of the internal photoemission in (MIM) sandwich structures



A summary of the problems involved in the description of the internal photoemission in sandwich structures is presented in table I.

2. Optical analysis and excitation function

A rigorous optical treatment of the absorption in a sandwich structure will be given in this section. The analysis is based mainly on the work of Pepper [14]. Consider a plane-parallel sandwich structure (see fig. 2) consisting of three media M_1–M_2–M_3 (e.g. metal–insulator–metal). The structure is in optical contact on the left-hand side with a nonabsorbing medium M_0 and on the right-hand side with a medium M_4 (e.g. vacuum and glass substrate, respectively). Assuming, for simplicity, that all the media M_j are homogeneous and isotropic*, we can characterize them by a complex dielectric function $\epsilon_j(\omega)$ and a thickness d_j, where ω is the circular frequency of the light and the index j denotes the particular region. The dielectric function is related to the index of refraction $n_j(\omega)$ and the extinction coefficient $k_j(\omega)$ by $\epsilon_j(\omega) = [n_j(\omega) + ik_j(\omega)]^2$. The plane separating M_{j-1} from M_j is referred to as the interface j. According to the usual experimental conditions the analysis will be restricted to normal incidence** of the light from M_0 on the first interface, denoting this direction as the positively oriented x-axis with the origin ($x = 0$) at the first interface. If necessary, the real and imaginary parts of a complex quantity are denoted by primes and double primes, respectively.

*The treatment of uniaxially anisotropic media is indicated in Pepper's paper [14].
**The case of oblique incidence can be treated in a similar way distinguishing now between the two directions of polarization [14].

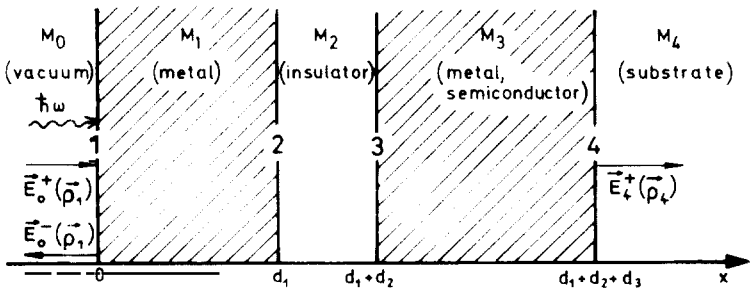


Fig. 2. Scheme of a plane-parallel sandwich structure: the interface 1 ($x = 0$) is illuminated from the medium M_0.

Assuming that absorption occurs via one-electron volume processes [9, 14], the excitation function $P_{\mathrm{exc},j}(E, \omega, x)$ in the medium M_j defined as the number of electrons (per unit energy, unit length in x-direction, and incident photon of energy $\hbar\omega$) excited to energy E at the position x is given by

$$P_{\mathrm{exc},j}(E, \omega, x) = P_{0j}(E, \omega) \cdot \eta_j(\omega, x) \qquad (E \geqslant 0). \tag{1}$$

Here $P_{0j}(E, \omega)$ is the normalized distribution function [9] for electrons excited to energy E, and the volumetric absorptance $\eta_j(\omega, x)$ is defined as the ratio of the number of photons absorbed per unit volume at the position x to the number of photons incident per unit area of the irradiated interface 1.

The distribution function $P_{0j}(E, \omega)$ involves the density of initial and final states and describes the kind of optical excitations (direct or nondirect transitions). It has been treated in detail elsewhere [9, 10, 15–19]. Our chief interest in this section will be devoted to the exact evaluation of the quantity $\eta_j(\omega, x)$ which gives the spatial distribution of the excited electrons along the x-axis.

Following Pepper [14] the volumetric absorptance $\eta_j(\omega, x)$ is given by the negative divergence of the Poynting vector $\boldsymbol{S}_j$ of the electromagnetic field in M_j divided by the incident flux S_{0x}^+:

$$\eta_j(\omega, x) = -\frac{\operatorname{div} \boldsymbol{S}_j}{S_{0x}^+} \,. \tag{2}$$

The Poynting vector is defined by

$$\boldsymbol{S}_j = \tfrac{1}{2} \operatorname{Re}\{\boldsymbol{E}_j^*(\boldsymbol{\rho}, t) \times \boldsymbol{H}_j(\boldsymbol{\rho}, t)\}, \tag{3}$$

where $\boldsymbol{E}_j(\boldsymbol{\rho}, t)$ and $\boldsymbol{H}_j(\boldsymbol{\rho}, t)$ are the electric and magnetic fields, respectively, and the star superscript means a complex conjugate; $\boldsymbol{\rho}$ is the position vector, t is time. The electric and magnetic components of the electromagnetic field may be taken as plane waves:

$$\begin{aligned} \boldsymbol{E}_j(\boldsymbol{\rho}, t) &= \boldsymbol{E}_j^+ \exp(\mathrm{i}\boldsymbol{k}_j^+ \boldsymbol{\rho} - \mathrm{i}\omega t) + \boldsymbol{E}_j^- \exp(\mathrm{i}\boldsymbol{k}_j^- \boldsymbol{\rho} - \mathrm{i}\omega t) \\ \boldsymbol{H}_j(\boldsymbol{\rho}, t) &= \boldsymbol{H}_j^+ \exp(\mathrm{i}\boldsymbol{k}_j^+ \boldsymbol{\rho} - \mathrm{i}\omega t) + \boldsymbol{H}_j^- \exp(\mathrm{i}\boldsymbol{k}_j^- \boldsymbol{\rho} - \mathrm{i}\omega t), \end{aligned} \tag{4}$$

where $\boldsymbol{E}_j$ and $\boldsymbol{H}_j$ are the complex amplitudes*, $\boldsymbol{k}_j$ is the propagation vector, and the superscript plus or minus denotes the quantities due to the wave propagating in the positive or negative x-direction, respectively. The amplitudes $\boldsymbol{E}_j$ and $\boldsymbol{H}_j$ of each wave are connected by Maxwell equations [14, 17]:

$$\boldsymbol{k}_j \times \boldsymbol{H}_j = -\omega\epsilon_v\epsilon_j\boldsymbol{E}_j, \qquad \boldsymbol{k}_j \times \boldsymbol{E}_j = \omega\mu_v\boldsymbol{H}_j, \tag{5}$$

where ϵ_v and μ_v are the permittivity and permeability of the vacuum (the media are assumed to be nonmagnetic). Using the proper boundary conditions [14, 17] for normal incidence, it follows that the tangential components of the propagation vector $\boldsymbol{k}_j$ in all the media are zero. Let us denote the x-component of $\boldsymbol{k}_j^+$ by ξ_j. Then from the law of reflection

$$k_{jx}^+ = -k_{jx}^- \equiv \xi_j = \frac{2\pi}{\lambda_v}\,\epsilon_j^{1/2}, \tag{6}$$

where λ_v is the vacuum wavelength of the incident light.

In order to calculate the Poynting vector in M_j it is convenient to express $\boldsymbol{E}_j^+$ and $\boldsymbol{E}_j^-$ in terms of $\boldsymbol{E}_0^+$:

$$\boldsymbol{E}_j^+ = T_j\boldsymbol{E}_0^+, \qquad \boldsymbol{E}_j^- = R_j\boldsymbol{E}_0^+. \tag{7}$$

The complex coefficients T_j and R_j can be found (see Appendix A) by solving the system of two linear equations

$$\begin{pmatrix}\boldsymbol{E}_j^+\\ \boldsymbol{E}_j^-\end{pmatrix} = \bar{\mathcal{M}}_j\bar{\mathcal{M}}_{j-1}\ldots\bar{\mathcal{M}}_2\bar{\mathcal{M}}_1\begin{pmatrix}\boldsymbol{E}_0^+\\ \boldsymbol{E}_0^-\end{pmatrix}, \tag{8}$$

where the square matrix $\bar{\mathcal{M}}_m$ connecting the amplitudes of the electric vector in the media M_{m-1} and M_m is determined by

$$\bar{\mathcal{M}}_m = \frac{1}{1-r_m}\,[-i(k_m^+ + k_m^- - k_{m-1}^+ - k_{m-1}^-)\rho_m]\begin{pmatrix}\exp[i(k_m^- - k_{m-1}^-)\rho_m] & -r_m\exp[i(k_m^- - k_{m-1}^+)\rho_m]\\ -r_m\exp[i(k_m^+ - k_{m-1}^-)\rho_m] & \exp[i(k_m^+ - k_{m-1}^+)\rho_m]\end{pmatrix}. \tag{9}$$

The amplitude reflection coefficient r_m at the interface m is given by $r_m = (\xi_{m-1} - \xi_m)/(\xi_{m-1} + \xi_m)$ (Fresnel reflection coefficient). The relation between $\boldsymbol{E}_0^-$ and $\boldsymbol{E}_0^+$ can be obtained from the condition that the wave in the final medium M_f propagates only in the positive x-direction, i.e. $\boldsymbol{E}_f^- \equiv 0$:

$$\begin{pmatrix}\boldsymbol{E}_f^+\\ 0\end{pmatrix} = \bar{\mathcal{M}}_f\bar{\mathcal{M}}_{f-1}\ldots\bar{\mathcal{M}}_2\bar{\mathcal{M}}_1\begin{pmatrix}\boldsymbol{E}_0^+\\ \boldsymbol{E}_0^-\end{pmatrix}. \tag{10}$$

In particular, $f = 4$ for our sandwich structure (we assume that M_4 is semi-infinite in the positive x-direction). With regard to the usual experimental situation we specialize the above results to a

*The complex amplitude in M_j is defined by the time-averaged field at the position $\boldsymbol{\rho} \equiv (0, 0, 0)$ (*not* by the field at the interface $j-1$).

structure where only the media M_1 and M_3 can absorb light (e.g. MIM or MIS). Consequently, we are interested in S_1 and S_3. First we calculate the complex coefficients T_j and R_j ($j = 1, 3$) using eqs. (7, 8, 9, 10). We obtain

$$T_1 = \frac{r_1 + 1}{R}\,[1 + r_3 r_4 \exp(2i\xi_3 d_3) + r_2 \exp(2i\xi_2 d_2)\{r_3 + r_4 \exp(2i\xi_3 d_3)\}],$$

$$R_1 = \frac{r_1 + 1}{R}\exp(2i\xi_1 d_1)[r_2\{1 + r_3 r_4 \exp(2i\xi_3 d_3)\} + \exp(2i\xi_2 d_2)\{r_3 + r_4 \exp(2i\xi_3 d_3)\}],$$

$$T_3 = \frac{r_1 + 1}{R}\,(r_2 + 1)(r_3 + 1)\exp[i(\xi_1 - \xi_3)d_1]\exp[i(\xi_2 - \xi_3)d_2], \tag{11}$$

$$R_3 = \frac{r_1 + 1}{R}\,(r_2 + 1)(r_3 + 1)r_4 \exp[i(\xi_1 + \xi_3)d_1]\exp[i(\xi_2 + \xi_3)d_2]\exp(2i\xi_3 d_3),$$

where

$$R = \{1 + r_1 r_2 \exp(2i\xi_1 d_1)\}\{1 + r_3 r_4 \exp(2i\xi_3 d_3)\} + \exp(2i\xi_2 d_2)\{r_2 + r_1 \exp(2i\xi_1 d_1)\}\{r_3 + r_4 \exp(2i\xi_3 d_3)\}.$$

Using the definition (3) and eqs. (4, 5, 6, 7) we obtain for the negative divergence of the Poynting vector in the medium M_j the expression

$$-\mathrm{div}\,\boldsymbol{S}_j = \frac{|\boldsymbol{E}_0^+|^2}{2\omega\mu_v}\,\alpha_j\xi_j'[|T_j|^2 \exp(-\alpha_j x) + |R_j|^2 \exp(+\alpha_j x) + 2\mathrm{Re}\{(T_j^* R_j)\exp(-2i\xi_j' x)\}], \tag{12}$$

where the absorption coefficient α_j is defined as $\alpha_j = 2\xi_j''$, and $\xi_j' = \mathrm{Re}\{\xi_j\}$, $\xi_j'' = \mathrm{Im}\{\xi_j\}$. Because the incident photon flux is

$$S_{0x}^+ = \frac{|\boldsymbol{E}_0^+|^2}{2\omega\mu_v}\,\xi_0 \qquad (\xi_0 \text{ is real}), \tag{13}$$

the volumetric absorptance is given by

$$\eta_j(\omega, x) = \alpha_j \frac{\xi_j'}{\xi_0}\,[|T_j|^2 \exp(-\alpha_j x) + |R_j|^2 \exp(+\alpha_j x) + 2\mathrm{Re}\{(T_j^* R_j)\exp(-2i\xi_j' x)\}] \tag{14}$$

and the excitation function by

$$P_{\mathrm{exc},j}(E, \omega, x) = P_{0j}(E, \omega)\alpha_j \frac{\xi_j'}{\xi_0}\,[|T_j|^2 \exp(-\alpha_j x) + |R_j|^2 \exp(+\alpha_j x) + 2\mathrm{Re}\{(T_j^* R_j)\exp(-2i\xi_j' x)\}]. \tag{15}$$

The three terms in the expression can physically be interpreted as the contributions due to the electromagnetic wave propagating in the positive x-direction, in the negative x-direction, and the interference field between these two waves, respectively. Let us denote these three terms of the excitation function successively by superscripts 1 (positively directed term), 2 (negatively directed term), and 3 (interference term).

Then

$$P_{\mathrm{exc},j}(E, \omega, x) = \sum_{k=1}^{3} P^{k}_{\mathrm{exc},j}(E, \omega, x). \tag{16}$$

We introduce further the formal absorption coefficients α_j^k:

$$\alpha_j^1 = \alpha_j \equiv 2\xi_j'', \qquad \alpha_j^2 = -\alpha_j \equiv -2\xi_j'', \qquad \alpha_j^3 \equiv 2\mathrm{i}\xi_j' \tag{17}$$

and the formal operators* $\hat{p}_j^k(\omega)$:

$$\begin{aligned}
&\hat{p}_j^1(\omega) \equiv |T_j|^2 \,\mathrm{Re}\{ && (\text{def.: } \hat{p}_j^1(\omega)X = |T_j|^2 \,\mathrm{Re}\{X\}),\\
&\hat{p}_j^2(\omega) \equiv |R_j|^2 \,\mathrm{Re}\{ && (\text{def.: } \hat{p}_j^2(\omega)X = |R_j|^2 \,\mathrm{Re}\{X\}),\\
&\hat{p}_j^3(\omega) \equiv 2\mathrm{Re}\{(T_j^* R_j) && (\text{def.: } \hat{p}_j^3(\omega)X = 2\mathrm{Re}\{(T_j^* R_j)X\}).
\end{aligned} \tag{18}$$

Then the k-term of the excitation function is

$$P^{k}_{\mathrm{exc},j}(E, \omega, x) = A_j(E, \omega)\hat{p}_j^k(\omega)\exp(-\alpha_j^k x) \qquad (k = 1, 2, 3) \tag{19}$$

and the excitation function

$$P_{\mathrm{exc},j}(E, \omega, x) = A_j(E, \omega) \sum_{k=1}^{3} \hat{p}_j^k(\omega)\exp(-\alpha_j^k x), \tag{20}$$

where we have denoted

$$A_j(E, \omega) = P_{0j}(E, \omega)\frac{\xi_j'}{\xi_0}\,\alpha_j. \tag{21}$$

The excitation function in the form (20) will be used for the calculation of the electron transport in the next section.

3. Electron transport in electrodes

In this section the transport of electrons excited at the position x in the medium M_j of thickness d_j to the interface will be calculated. The complicated transport problem is approached by describing the most important interactions between the excited electrons and the medium during their motion to the interface. It is assumed (see fig. 3) that an electron can (i) reach the interface without scattering, or (ii) suffer one elastic (electron–phonon: e–p) or one inelastic (electron–electron: e–e) scattering before reaching the interface, or (iii) suffer two scattering processes in one of the four possible combinations e–p/e–p, e–p/e–e, e–e/e–p, e–e/e–e before reaching the interface. The scattering processes of higher orders (three-step and more) are neglected because

*The definition of $\hat{p}_j^1(\omega)$ and $\hat{p}_j^2(\omega)$ including the operator of the real part Re{ is not obvious at the moment, but it simplifies the later formalism.

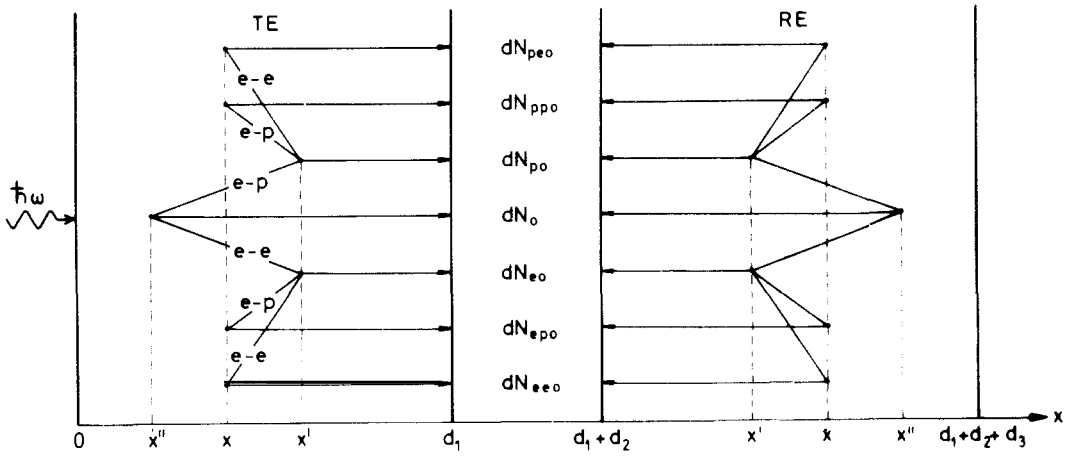


Fig. 3. Scheme of the scattering processes within the electrode.

the probability for contributing an electron with sufficient energy after suffering such many-step scattering is very small in most cases of practical interest. Likewise, with regard to the energy region of interest (not too far above the barrier maximum) the possibility of scattering by plasmons will not be considered. The calculation of items (i), (ii), and (iii) represents an extension of the results of Berglund and Spicer [18], first to the finite medium thickness, and second to the two-step scattering processes (e.g.: e–p/e–p). Furthermore, the calculation includes not only those electrons which escape from the illuminated surface of a (semi-infinite) solid (henceforth reflective photoemission, RE), but also the electrons escaping from the interface on the opposite side to the illuminated surface of a (relatively thin) emitting film (henceforth transmittive photoemission, TE). Contrary to the common practice [9, 18] we do not immediately evaluate the energy distribution of the escaped electrons, but rather first the differential energy distribution $dN_j(E, z, \omega)$ of electrons reaching the interface (before escaping) which depends on the electron energy E and the photon energy $\hbar\omega$, as well as on the direction (relative to the surface) of electron momentum $\boldsymbol{p}$. The distribution $dN_j(E, z, \omega)$ is defined as the number of electrons excited per unit energy by the incident photon $\hbar\omega$ which arrive at the interface with energy E and the x-component of $\boldsymbol{p}$ being p_x. The variable z in the distribution is equal to the cosine of the angle ϑ between $\boldsymbol{p}$ and the x-axis. The reason for this treatment is to preserve the explicit dependence of the distribution on the energy E_x associated with the electron motion in the x-direction, where $E_x = \tilde{E}_x + E_0 = p_x^2/2m$.

Similarly to previous work [9, 18], the following simplifying assumptions will be made:

1) The optically excited electrons are distributed isotropically in direction.

2) The probability of scattering processes may be described in terms of energy-dependent mean free paths.

3) Both elastic and inelastic scattering may be considered as isotropic.

4) The surface scattering is neglected.

As a supplement to the discussion [9, 18] of some of these assumptions we present the following remarks. Concerning 3), this assumption is the only one which allows a relatively simple analysis of the scattering. In the case of the inelastic scattering in the energy range under consideration, this assumption upon isotropy is based on the examination [20] of the solutions of the

Schroedinger equation for the scattering problem. The possible anisotropy of elastic events can roughly be taken into account by thinking of two scattering mechanism [21], an isotropic and a completely forward. Because the scattering is elastic (or nearly elastic), the forward component changes neither the energy nor the momentum. But such a process can at most influence the apparent cross section for the elastic scattering. Moreover, the photoemission experiments on sandwiches are normally performed with (evaporated) polycrystalline or amorphous electrodes at temperatures equal or above 77° K. Under such circumstances (especially at $T = 300°$ K) the possible anisotropy of the e–p scattering is practically washed out [22]. Isotropic elastic scattering has also been assumed in Ballantyne's calculation [19] of the phonon energy loss. Concerning 4), it has been shown [23] that the kind of surface scattering (specular or diffuse) does not change the number of electrons which are able to escape. The presence of surface scattering could, in principle, increase the number of these electrons [23] but it is not likely because of the very small escape cone for the electrons with energy just above the barrier height. On the other hand, electrons with energies several electronvolts above the barrier have a short mean free path for e–e scattering and the surface scattering increases the probability for the loss of the electron by a collision with another electron to the energy below the barrier height. Therefore we probably do not introduce a significant error by neglecting the surface scattering. In distinction to the previous work [3, 5, 6, 8, 9, 18] we *do not assume the classical (zero-or-one) escape probability* which is a gross approximation not only to the case of a thin insulator barrier, but also for the vacuum photoemission at high external fields if the electron energy is not far enough from the barrier height. This question has been investigated in detail elsewhere [11].

Under the assumptions 1) through 4) we formulate the probability of reaching the interface and the scattering probabilities in the medium M_j.

The probability for an electron with energy E and momentum $\boldsymbol{p}$ to reach the interface from a distance Δ without scattering (see fig. 4a) is [9, 18]

$$P_{\mathrm{surf},j}(E, z, x) = \tfrac{1}{2}\exp(-\Delta/l_j z), \tag{22}$$

where $l_j = l_j(E)$ is the total mean free path in M_j and $z = \cos\vartheta$.

The probability for an electron with energy E' and momentum $\boldsymbol{p}'$ to be scattered isotropically by another electron (e–e scattering) after moving a distance r' at an angle ϑ' (see fig. 4b) and produce a secondary electron with energy E and momentum $\boldsymbol{p}$ is*

$${}_{\mathrm{e}}P_{\mathrm{scat},j}(E', E, r', \vartheta') = \tfrac{1}{2}\sin\vartheta' S_{\mathrm{ee}j}(E', E)\,\frac{\exp(-r'/l'_j)}{l'_{ej}}, \tag{23}$$

where $l'_j = l_j(E')$ and $l'_{ej} = l_{ej}(E')$ are the total mean free path and the mean free path for e–e scattering of an electron with energy E', respectively. $S_{\mathrm{ee}j}(E', E)$ is the distribution function [9] for secondary electrons produced by e–e scattering of a primary electron with energy E'.

The probability for an electron with energy E' and momentum $\boldsymbol{p}'$ to be scattered isotropically by a phonon (e–p scattering) after moving a distance r' at an angle ϑ' and produce a secondary electron with energy E and momentum $\boldsymbol{p}$ is analogously

*The probability (23) is a generalization of expression (37) of ref. [9] which describes the e–e scattering probability in the case when no other scattering mechanism is allowed.

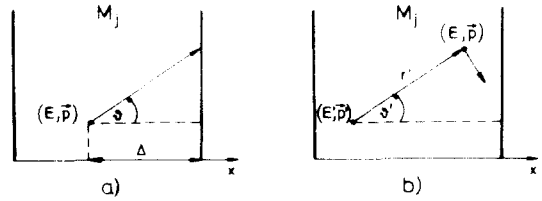


Fig. 4. Scheme of the geometry for the evaluation of the probability, a) of reaching the interface, and b) of scattering.

$$ {}_{\mathrm{p}}P_{\mathrm{scat},j}(E', E, r', \vartheta') = \tfrac{1}{2}\sin\vartheta' \, S_{\mathrm{ep}j}(E', E) \frac{\exp(-r'/l'_j)}{l'_{\mathrm{p}j}} , \tag{24} $$

where $l'_{\mathrm{p}j} = l_{\mathrm{p}j}(E')$ is the mean free path for e–p scattering. $S_{\mathrm{ep}j}(E', E)$ is the distribution function for secondary electrons produced by e–p scattering of a primary electron with energy E'. This distribution reduces to a δ-function at E' in the case of perfectly elastic scattering.

Corresponding to all possible electron interactions assumed in the excited medium M_j, the complete differential energy distribution $\mathrm{d}N_j(E, z, \omega)$ is given by

$$ \mathrm{d}N_j = \mathrm{d}N_{0j} + \mathrm{d}N_{\mathrm{p}0j} + \mathrm{d}N_{\mathrm{e}0j} + \mathrm{d}N_{\mathrm{pp}0j} + \mathrm{d}N_{\mathrm{pe}0j} + \mathrm{d}N_{\mathrm{ep}0j} + \mathrm{d}N_{\mathrm{ee}0j} \tag{25} $$

where the individual terms on the right are due to electrons which:
– reach the interface without scattering ($\mathrm{d}N_{0j}$)
– scatter once before reaching the interface ($\mathrm{d}N_{\mathrm{p}0j}$ and $\mathrm{d}N_{\mathrm{e}0j}$)
– scatter twice before reaching the interface ($\mathrm{d}N_{\mathrm{pp}0j}$, $\mathrm{d}N_{\mathrm{pe}0j}$, $\mathrm{d}N_{\mathrm{ep}0j}$ and $\mathrm{d}N_{\mathrm{ee}0j}$).

We now return to the case of a sandwich structure where only the media M_1 and M_3 absorb light and, consequently, can produce electrons. Our interest will be devoted to the electrons which are directed into the nonabsorbing medium M_2. In other words, we are interested in the differential energy distribution $\mathrm{d}N_1(E, z, \omega)$ due to the transmittive photoemission from M_1 through the interface 2, and $\mathrm{d}N_3(E, z, \omega)$ due to the reflective photoemission from M_3 through the interface 3. In the next parts of this section the terms of $\mathrm{d}N_1$ and $\mathrm{d}N_3$ will be calculated.

3.1. *Transmittive photoemission from* M_1 *through the interface 2; j = 1*

a) *no scattering:* $\mathrm{d}N_{01}$

The distribution is given by the product of the excitation function (20) and the probability (22) to reach the surface integrated over all possible positions of excitation x (fig. 5a):

$$ \mathrm{d}N_{01}(E, z, \omega) = \int_0^{d_1} \mathrm{d}x \, P_{\mathrm{exc},1}(E, \omega, x) \, P_{\mathrm{surf},1}(E, z, x). \tag{26} $$

Performing the integration we obtain

$$ \mathrm{d}N_{01}(E, z, \omega) = \tfrac{1}{2} A_1(E, \omega) \sum_{k=1}^{3} \tilde{T}^k_{01}(E, z, \omega), \tag{27} $$

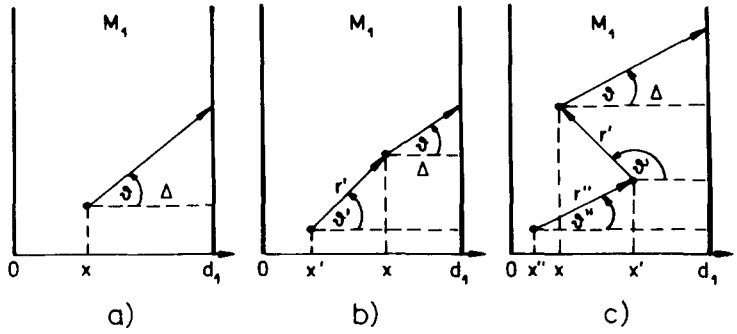


Fig. 5. Scheme of the geometry involved in the calculation for electrons which a) do not scatter, b) scatter once, c) scatter twice before reaching the interface.

where we defined

$$\tilde{T}^k_{01}(E, z, \omega) \equiv \hat{p}^k_1(\omega)\, T^k_{01}(E, z, \omega) \tag{28}$$

and

$$T^k_{01}(E, z, \omega) = \frac{l_1 z}{\alpha^k_1 l_1 z - 1}\left\{\exp\left(-\frac{d_1}{l_1 z}\right) - \exp(-\alpha^k_1 d_1)\right\}. \tag{29}$$

b) *e–p scattering*: $\mathrm{d}N_{p01}$

Consider an electron with energy E' at the position x'. It is scattered by a phonon after moving a distance r' at an angle ϑ' (see fig. 5b) with the probability ${}_pP_{\mathrm{scat},1}$ and reaches the surface with the probability $P_{\mathrm{surf},1}$. The distribution is then given by the product of the excitation function taken at energy E' at the position x' with these two probabilities integrated over all possible positions of excitation x', positions of scattering x, and over all primary energies E' contributing* to the final energy E. Introducing polar coordinates r' and ϑ' ($x = x' + r'\cos\vartheta'$) we have

$$\mathrm{d}N_{p01}(E, z, \omega) = \int_E^{\hbar\omega} \mathrm{d}E' \int_0^{d_1} \mathrm{d}x'\, P_{\mathrm{exc},1}(E', \omega, x')\left[\!\!\left[\int_0^{\pi/2} \mathrm{d}\vartheta' \int_0^{(d_1-x')/\cos\vartheta'} + \int_{\pi/2}^{\pi} \mathrm{d}\vartheta' \int_0^{-x'/\cos\vartheta'}\right]\!\!\right]$$

$$\times\, ({}_pP_{\mathrm{scat},1}(E', E, r', \vartheta')\, P_{\mathrm{surf},1}(E, z, r', \vartheta')), \tag{30}$$

where the expression in the double-brackets is to be applied as an integral operator on the function behind it. After some calculations (see Appendix B) we obtain:

$$\mathrm{d}N_{p01}(E, z, \omega) = \int_E^{\hbar\omega} \mathrm{d}E'\, A_1(E', \omega)\, S_{ep1}(E', E)\, \frac{1}{4l'_{p1}} \sum_{k=1}^{3} \tilde{T}^k_{p01}(E', E, z, \omega) \tag{31}$$

where we defined

*Strictly speaking, the lower limit in the integral over E' should read $E - \Delta E_p$ instead of E, because the electrons can, in principle, also gain the phonon energy ΔE_p. Since $\Delta E_p \ll E$ (e.g. $\Delta E_p \lesssim 10^{-2}$ eV in metals) one can write $E - \Delta E_p \approx E$.

$$\tilde{T}^k_{p01}(E', E, z, \omega) \equiv \hat{p}^k_1(\omega)\, T^k_{p01}(E', E, z, \omega) \tag{32}$$

and

$$T^k_{p01}(E', E, z, \omega) = -\frac{(l_1 z)^2}{\alpha^k_1 l_1 z - 1}\left\{\exp(-\alpha^k_1 d_1) Q_{11,1} + \exp\left(-\frac{d_1}{l_1 z}\right) Q_{12,1}\right\} \tag{33}$$

$$+\frac{l_1 z}{\alpha^k_1(\alpha^k_1 l_1 z - 1)}\left\{\exp(-\alpha^k_1 d_1) Q^k_{16,1} + \exp\left(-\frac{d_1}{l_1 z}\right) Q^k_{15,1}\right\} + \frac{l_1 z}{\alpha^k_1} E_1\left(\frac{d_1}{l'_1}\right)\left\{1 + \exp\left[-\left(\alpha^k_1 d_1 + \frac{d_1}{l_1 z}\right)\right]\right\}.$$

The expressions Q are defined later by eqs. (42), $E_1(\zeta)$ is the exponential integral of the first order (see Appendix B).

c) e–e *scattering*: dN_{e01}

Using the same consideration as in the calculation of dN_{p01} we obtain for dN_{e01} the following result:

$$dN_{e01}(E, z, \omega) = \int_E^{\hbar\omega} dE'\, A_1(E', \omega)\, S_{ee1}(E', E)\, \frac{1}{4 l'_{e1}} \sum_{k=1}^{3} \tilde{T}^k_{e01}(E', E, z, \omega), \tag{34}$$

where

$$\tilde{T}^k_{e01}(E', E, z, \omega) \equiv \tilde{T}^k_{p01}(E', E, z, \omega), \tag{35}$$

and $\tilde{T}^k_{p01}$ is determined by eqs. (32, 33, 42).

d) e–p/e–p *scattering*: dN_{pp01}

We proceed to the mathematically more complicated case of two-step scattering. An electron excited at the position x'' to energy E'' will be scattered by a phonon to energy E' after moving a distance r'' at an angle ϑ'' (see fig. 5c) with the probability ${}_pP_{scat,1}(E'', E', r'', \vartheta'')$. It travels on at a random angle ϑ' and will be scattered by a phonon for the second time to energy E after moving a distance r' with the probability ${}_pP_{scat,1}(E', E, r', \vartheta')$. Introducing polar coordinates r'', ϑ'' and r', ϑ' at the positions x'' and x', respectively ($x = x' + r'\cos\vartheta'$, $x' = x'' + r''\cos\vartheta''$) and integrating the product of the probabilities over all possible positions of excitation x'', positions of scattering x' and x, and over all energies E'' and E' contributing to the final energy E, we have

$$dN_{pp01}(E, z, \omega) = \int_E^{\hbar\omega} dE'' \int_E^{E''} dE' \int_0^{d_1} dx''\, P_{exc,1}(E'', \omega, x'')$$

$$\times \left[\left\{\int_0^{\pi/2} d\vartheta'' \int_0^{(d_1 - x'')/\cos\vartheta''} dr'' + \int_{\pi/2}^{\pi} d\vartheta'' \int_0^{-x''/\cos\vartheta''} dr''\right\}\left\{\int_0^{\pi/2} d\vartheta' \int_0^{(d_1 - x'' - r''\cos\vartheta'')/\cos\vartheta'} dr'\right.\right.$$

$$\left.\left. + \int_{\pi/2}^{\pi} d\vartheta' \int_0^{-(x'' + r''\cos\vartheta'')/\cos\vartheta'} dr'\right\}\right] \cdot ({}_pP_{scat,1}(E'', E', r'', \vartheta'')\, {}_pP_{scat,1}(E', E, r', \vartheta')\, P_{surf,1}(E, z, r', \vartheta')), \tag{36}$$

where the expression in the double-brackets is again an integral operator on the function behind it. The calculation of the multiple integral is too lengthy to be shown. Some essential steps are given in Appendix B. The result reads*:

$$dN_{pp01}(E, z, \omega) = \int_E^{h\omega} dE'' \int_E^{E''} dE' A_1(E'', \omega) S_{ep1}(E'', E') S_{ep1}(E', E)$$

$$\times \frac{1}{8 l''_{p1} l'_{p1}} \sum_{k=1}^{3} \tilde{T}^k_{pp01}(E'', E', E, z, \omega), \tag{37}$$

where we defined $$\tilde{T}^k_{pp01}(E'', E', E, z, \omega) \equiv \hat{p}^k_1(\omega) T^k_{pp01}(E'', E', E, z, \omega) \tag{38}$$

and

$$T^k_{pp01}(E'', E', E, z, \omega) \tag{39}$$

$$= -\frac{(l_1 z)^3}{\alpha_1^k l_1 z - 1}\left\{\exp(-\alpha_1^k d_1) Q_{1,1} - \exp\left(-\frac{d_1}{l_1 z}\right) Q_{2,1} - \exp\left[-\left(\alpha_1^k d_1 + \frac{d_1}{l_1 z}\right)\right] Q_{3,1} + Q_{4,1}\right\}$$

$$-\frac{l_1 z}{(\alpha_1^k)^2(\alpha_1^k l_1 z - 1)}\left\{\exp(-\alpha_1^k d_1) Q^k_{5,1} - \exp\left(-\frac{d_1}{l_1 z}\right) Q^k_{6,1} - \exp\left[-\left(\alpha_1^k d_1 + \frac{d_1}{l_1 z}\right)\right] Q^k_{7,1} + Q^k_{8,1}\right\}$$

$$-\frac{l_1 z d_1}{\alpha_1^k}\left\{\left[\exp(-\alpha_1^k d_1) + \exp\left(-\frac{d_1}{l_1 z}\right)\right] Q_{9,1} + \left[1 + \exp\left[-\left(\alpha_1^k d_1 + \frac{d_1}{l_1 z}\right)\right]\right] Q_{10,1}\right\}$$

$$-\frac{(l_1 z)^2}{\alpha_1^k(\alpha_1^k l_1 z - 1)}\left\{\exp\left(-\frac{d_1}{l_1 z}\right) Q_{12,1} Q^k_{17,1} - \exp(-\alpha_1^k d_1) Q_{11,1} Q^k_{18,1}\right\}$$

$$-\frac{(l_1 z)^2}{\alpha_1^k} E_1\left(\frac{d_1}{l''_1}\right)\left\{\exp\left[-\left(\alpha_1^k d_1 + \frac{d_1}{l_1 z}\right)\right] Q_{12,1} - Q_{11,1}\right\}$$

$$-\frac{l_1 z}{(\alpha_1^k)^2} E_1\left(\frac{d_1}{l'_1}\right)\left\{\left[\exp(-\alpha_1^k d_1) - \exp\left(-\frac{d_1}{l_1 z}\right)\right] E_1\left(\frac{d_1}{l''_1}\right) - Q^k_{17,1} + \exp\left[-\left(\alpha_1^k d_1 + \frac{d_1}{l_1 z}\right)\right] Q^k_{18,1}\right\}$$

$$-X^k_{T1}(E'', E', E, z, \omega).$$

The function X^k_{T1} is given by

$$X^k_{T1}(E'', E', E, z, \omega) = \int_1^{\infty} du\, \chi^k_{T1}(E'', E', E, z, \omega, u), \tag{40}$$

where χ^k_{T1} converges quickly to zero for higher u. For many cases of practical interest the function X^k_{T1} is negligible. If necessary, X^k_{T1} can be obtained by numerical integration of χ^k_{T1}, where

*Concerning the limits of the integrals over energy, see the footnote given in connection with (30).

$$\chi^k_{T1}(E'', E', E, z, \omega, u) =$$

$$= -\frac{(l_1 z)^3 d_1}{\alpha_1^k l_1 z - 1}\left\{\left[\exp(-\alpha_1^k d_1) L_2\left(\frac{l_1 z(l_1' u + l_1'')}{l_1''(l_1 z - l_1')}\right) - \exp\left(-\frac{d_1}{l_1 z}\right) L_2\left(\frac{l_1 z(l_1' u + l_1'')}{l_1''(l_1 z + l_1')}\right)\right]\frac{\exp[-(d_1/l_1' + d_1 u/l_1'')]}{l_1''}\right.$$

$$+\left[\exp\left[-\left(\alpha_1^k d_1 + \frac{d_1}{l_1 z}\right)\right] L_2\left(\frac{l_1''(l_1 z u + l_1')}{l_1'(l_1 z + l_1'')}\right) - L_2\left(\frac{l_1''(l_1 z u - l_1')}{l_1'(l_1 z - l_1'')}\right)\right]\frac{\exp(-d_1 u/l_1')}{l_1'}$$

$$\left.+\left[\exp\left[-\left(\alpha_1^k d_1 + \frac{d_1}{l_1 z}\right)\right] L_2\left(\frac{l_1'(l_1 z u + l_1'')}{l_1''(l_1 z + l_1')}\right) - L_2\left(\frac{l_1'(l_1 z u - l_1'')}{l_1''(l_1 z - l_1')}\right)\right]\frac{\exp(-d_1 u/l_1'')}{l_1''}\right\}$$

$$+\frac{l_1 z\, d_1}{(\alpha_1^k)^2(\alpha_1^k l_1 z - 1)}\left\{\left[\exp(-\alpha_1^k d_1) L_2\left(\frac{l_1' u + l_1''}{l_1''(1 - \alpha_1^k l_1')}\right) - \exp\left(-\frac{d_1}{l_1 z}\right) L_2\left(\frac{l_1' u + l_1''}{l_1''(1 + \alpha_1^k l_1')}\right)\right]\frac{\exp[-(d_1/l_1' + d_1 u/l_1'')]}{l_1''}\right.$$

$$+\left[\exp\left[-\left(\alpha_1^k d_1 + \frac{d_1}{l_1 z}\right)\right] L_2\left(\frac{l_1''(u + \alpha_1^k l_1')}{l_1'(1 + \alpha_1^k l_1'')}\right) - L_2\left(\frac{l_1''(u - \alpha_1^k l_1')}{l_1'(1 - \alpha_1^k l_1'')}\right)\right]\frac{\exp(-d_1 u/l_1')}{l_1'}$$

$$+\left[\exp\left[-\left(\alpha_1^k d_1 + \frac{d_1}{l_1 z}\right)\right] L_2\left(\frac{l_1'(u + \alpha_1^k l_1'')}{l_1''(1 + \alpha_1^k l_1')}\right) - L_2\left(\frac{l_1'(u - \alpha_1^k l_1'')}{l_1''(1 - \alpha_1^k l_1')}\right)\right]\frac{\exp(-d_1 u/l_1'')}{l_1''}\right\}$$

$$+\frac{l_1 z(\alpha_1^k l_1 z + 1) d_1}{(\alpha_1^k)^2}\left\{\left[\exp(-\alpha_1^k d_1) - \exp\left(-\frac{d_1}{l_1 z}\right)\right]\frac{\exp[-(d_1/l_1' + d_1 u/l_1'')]}{l_1''}\; L_2\left(1 + \frac{l_1'}{l_1''} u\right)\right.$$

$$\left.-\left[1 - \exp\left[-\left(\alpha_1^k d_1 + \frac{d_1}{l_1 z}\right)\right]\right]\left[\frac{\exp(-d_1 u/l_1')}{l_1'}\; L_2\left(\frac{l_1''}{l_1'} u\right) + \frac{\exp(-d_1 u/l_1'')}{l_1''}\; L_2\left(\frac{l_1'}{l_1''} u\right)\right]\right\}$$

$$+\frac{l_1 z d_1^2}{\alpha_1^k}\left[1 + \exp\left[-\left(\alpha_1^k d_1 + \frac{d_1}{l_1 z}\right)\right]\right]\left[\frac{\exp(-d_1 u/l_1)}{l_1'}\; L_2\left(\frac{l_1''}{l_1'} u\right) + \frac{\exp(-d_1 u/l_1'')}{l_1''}\; L_2\left(\frac{l_1'}{l_1''} u\right)\right]. \qquad (41)$$

The expressions Q are defined:

$$Q_{1,j} = +\ln\left(1 + \frac{l_j'}{l_j z}\right) Q_{13,j} - E_1\left(\frac{d_j}{l_j''} + \frac{d_j}{l_j z}\right) Q_{12,j} - \exp\left[-\left(\frac{d_j}{l_j'} + \frac{d_j}{l_j''}\right)\right]\left[L_2\left(1 + \frac{l_j'}{l_j''}\right) - L_2\left(\frac{l_j z(l_j' + l_j'')}{l_j''(l_j z - l_j')}\right)\right] \qquad (42)$$

$$+\ln\left(1 - \frac{l_j'}{l_j z}\right)\left[E_1\left(\frac{d_j}{l_j'} + \frac{d_j}{l_j''}\right) - \ln\left(1 - \frac{l_j''}{l_j z}\right)\right] - \ln\left(1 + \frac{l_j''}{l_j z}\right)\left[E_1\left(\frac{d_j}{l_j'} + \frac{d_j}{l_j''}\right) - E_1\left(\frac{d_j}{l_j'} + \frac{d_j}{l_j z}\right)\right]$$

$$-L_2\left(\frac{l_j z - l_j'}{l_j z + l_j''}\right) + L_2\left(\frac{l_j z}{l_j z + l_j''}\right) + L_2\left(\frac{l_j z - l_j'}{l_j z - l_j''}\right) - L_2\left(\frac{l_j z}{l_j z - l_j''}\right) + L_2\left(\frac{l_j z - l_j''}{l_j z - l_j'}\right) - L_2\left(\frac{l_j z}{l_j z - l_j'}\right) - L_2\left(\frac{l_j z - l_j''}{l_j z}\right) + \frac{\pi^2}{6},$$

$$Q_{2,j} = +\ln\left(1 - \frac{l_j'}{l_j z}\right) Q_{14,j} - E_1\left(\frac{d_j}{l_j''} - \frac{d_j}{l_j z}\right) Q_{11,j} - \exp\left[-\left(\frac{d_j}{l_j'} + \frac{d_j}{l_j''}\right)\right]\left[L_2\left(1 + \frac{l_j'}{l_j''}\right) - L_2\left(\frac{l_j z(l_j' + l_j'')}{l_j''(l_j z - l_j')}\right)\right]$$

$$+\ln\left(1 + \frac{l_j'}{l_j z}\right)\left[E_1\left(\frac{d_j}{l_j'} + \frac{d_j}{l_j''}\right) - \ln\left(1 + \frac{l_j''}{l_j z}\right)\right] - \ln\left(1 - \frac{l_j''}{l_j z}\right)\left[E_1\left(\frac{d_j}{l_j'} + \frac{d_j}{l_j''}\right) - E_1\left(\frac{d_j}{l_j'} - \frac{d_j}{l_j z}\right)\right]$$

$$-L_2\left(\frac{l_j z + l_j'}{l_j z - l_j''}\right) + L_2\left(\frac{l_j z}{l_j z - l_j''}\right) + L_2\left(\frac{l_j z + l_j'}{l_j z + l_j''}\right) - L_2\left(\frac{l_j z}{l_j z + l_j''}\right) + L_2\left(\frac{l_j z + l_j''}{l_j z + l_j'}\right) - L_2\left(\frac{l_j z}{l_j z + l_j'}\right) - L_2\left(\frac{l_j z + l_j''}{l_j z}\right) + \frac{\pi^2}{6},$$

$$Q_{3,j} = +\exp\left(-\frac{d_j}{l'_j}\right)\left[L_2\left(\frac{l''_j}{l'_j}\right) - L_2\left(\frac{l''_j(l_jz+l'_j)}{l'_j(l_jz+l''_j)}\right)\right] + \exp\left(-\frac{d_j}{l''_j}\right)\left[L_2\left(\frac{l'_j}{l''_j}\right) - L_2\left(\frac{l'_j(l_jz+l''_j)}{l''_j(l_jz+l'_j)}\right)\right], \quad \text{(42 cont.)}$$

$$Q_{4,j} = +\exp\left(-\frac{d_j}{l'_j}\right)\left[L_2\left(\frac{l''_j}{l'_j}\right) - L_2\left(\frac{l''_j(l_jz-l'_j)}{l'_j(l_jz-l''_j)}\right)\right] + \exp\left(-\frac{d_j}{l''_j}\right)\left[L_2\left(\frac{l'_j}{l''_j}\right) - L_2\left(\frac{l'_j(l_jz-l''_j)}{l''_j(l_jz-l'_j)}\right)\right],$$

$$Q^k_{5,j} = +\ln(1-\alpha_j^k l'_j)Q^k_{18,j} - \ln\left(\frac{1+\alpha_j^k l''_j}{1-\alpha_j^k l''_j}\right)Q^k_{16,j} + \exp\left[-\left(\frac{d_j}{l'_j}+\frac{d_j}{l''_j}\right)\right]\left[L_2\left(1+\frac{l'_j}{l''_j}\right) - L_2\left(\frac{l'_j+l''_j}{l''_j(1-\alpha_j^k l'_j)}\right)\right]$$
$$+\ln\left(\frac{1+\alpha_j^k l''_j}{1-\alpha_j^k l'_j}\right) E_1\left(\frac{d_j}{l'_j}+\frac{d_j}{l''_j}\right) + L_2\left(\frac{1-\alpha_j^k l'_j}{1+\alpha_j^k l''_j}\right) - L_2\left(\frac{1}{1+\alpha_j^k l''_j}\right) - L_2\left(\frac{1-\alpha_j^k l'_j}{1-\alpha_j^k l''_j}\right)$$
$$+L_2\left(\frac{1}{1-\alpha_j^k l''_j}\right) - L_2\left(\frac{1-\alpha_j^k l''_j}{1-\alpha_j^k l'_j}\right) + L_2\left(\frac{1}{1-\alpha_j^k l'_j}\right) + L_2(1-\alpha_j^k l''_j) - \frac{\pi^2}{6},$$

$$Q^k_{6,j} = +\ln(1+\alpha_j^k l'_j)Q^k_{17,j} - \ln\left(\frac{1-\alpha_j^k l''_j}{1+\alpha_j^k l''_j}\right)Q^k_{15,j} + \exp\left[-\left(\frac{d_j}{l'_j}+\frac{d_j}{l''_j}\right)\right]\left[L_2\left(1+\frac{l'_j}{l''_j}\right) - L_2\left(\frac{l'_j+l''_j}{l''_j(1+\alpha_j^k l'_j)}\right)\right]$$
$$+\ln\left(\frac{1-\alpha_j^k l''_j}{1+\alpha_j^k l'_j}\right) E_1\left(\frac{d_j}{l'_j}+\frac{d_j}{l''_j}\right) + L_2\left(\frac{1+\alpha_j^k l'_j}{1-\alpha_j^k l''_j}\right) - L_2\left(\frac{1}{1-\alpha_j^k l''_j}\right) - L_2\left(\frac{1+\alpha_j^k l'_j}{1+\alpha_j^k l''_j}\right)$$
$$+L_2\left(\frac{1}{1+\alpha_j^k l''_j}\right) - L_2\left(\frac{1+\alpha_j^k l''_j}{1+\alpha_j^k l'_j}\right) + L_2\left(\frac{1}{1+\alpha_j^k l'_j}\right) + L_2(1+\alpha_j^k l''_j) - \frac{\pi^2}{6},$$

$$Q^k_{7,j} = -\exp\left(-\frac{d_j}{l'_j}\right)\left[L_2\left(\frac{l''_j}{l'_j}\right) - L_2\left(\frac{l''_j(1+\alpha_j^k l'_j)}{l'_j(1+\alpha_j^k l''_j)}\right)\right] - \exp\left(-\frac{d_j}{l''_j}\right)\left[L_2\left(\frac{l'_j}{l''_j}\right) - L_2\left(\frac{l'_j(1+\alpha_j^k l''_j)}{l''_j(1+\alpha_j^k l'_j)}\right)\right],$$

$$Q^k_{8,j} = -\exp\left(-\frac{d_j}{l'_j}\right)\left[L_2\left(\frac{l''_j}{l'_j}\right) - L_2\left(\frac{l''_j(1-\alpha_j^k l'_j)}{l'_j(1-\alpha_j^k l''_j)}\right)\right] - \exp\left(-\frac{d_j}{l''_j}\right)\left[L_2\left(\frac{l'_j}{l''_j}\right) - L_2\left(\frac{l'_j(1-\alpha_j^k l''_j)}{l''_j(1-\alpha_j^k l'_j)}\right)\right],$$

$$Q_{9,j} = +\frac{l'_j}{d_j}\left[Q_{21,j} - \exp\left(-\frac{d_j}{l'_j}\right)E_1\left(\frac{d_j}{l''_j}\right)\right] + \frac{l''_j}{d_j}\left[Q_{19,j} - \exp\left(-\frac{d_j}{l''_j}\right)E_1\left(\frac{d_j}{l'_j}\right)\right] + E_1\left(\frac{d_j}{l'_j}\right)E_1\left(\frac{d_j}{l''_j}\right),$$

$$Q_{10,j} = +\frac{l'_j}{d_j}\left[\exp\left(-\frac{d_j}{l'_j}\right)Q_{22,j} - E_1\left(\frac{d_j}{l''_j}\right)\right] - \exp\left(-\frac{d_j}{l'_j}\right)L_2\left(\frac{l''_j}{l'_j}\right)$$
$$+\frac{l''_j}{d_j}\left[\exp\left(-\frac{d_j}{l''_j}\right)Q_{20,j} - E_1\left(\frac{d_j}{l'_j}\right)\right] - \exp\left(-\frac{d_j}{l''_j}\right)L_2\left(\frac{l'_j}{l''_j}\right),$$

$$Q_{11,j} = E_1\left(\frac{d_j}{l'_j}+\frac{d_j}{l_jz}\right) + \ln\left(1+\frac{l'_j}{l_jz}\right), \qquad Q_{12,j} = E_1\left(\frac{d_j}{l'_j}-\frac{d_j}{l_jz}\right) + \ln\left(1-\frac{l'_j}{l_jz}\right),$$

$$Q_{13,j} = E_1\left(\frac{d_j}{l_j''} + \frac{d_j}{l_j z}\right) + \ln\left(1 + \frac{l_j''}{l_j z}\right), \qquad Q_{14,j} = E_1\left(\frac{d_j}{l_j''} - \frac{d_j}{l_j z}\right) + \ln\left(1 - \frac{l_j''}{l_j z}\right), \qquad (42\text{ cont.})$$

$$Q^k_{15,j} = E_1\left(\frac{d_j}{l_j'} + \alpha_j^k d_j\right) + \ln(1 + \alpha_j^k l_j'), \qquad Q^k_{16,j} = E_1\left(\frac{d_j}{l_j'} - \alpha_j^k d_j\right) + \ln(1 - \alpha_j^k l_j'),$$

$$Q^k_{17,j} = E_1\left(\frac{d_j}{l_j''} + \alpha_j^k d_j\right) + \ln(1 + \alpha_j^k l_j''), \qquad Q^k_{18,j} = E_1\left(\frac{d_j}{l_j''} - \alpha_j^k d_j\right) + \ln(1 - \alpha_j^k l_j''),$$

$$Q_{19,j} = E_1\left(\frac{d_j}{l_j'} + \frac{d_j}{l_j''}\right) + \ln\left(1 + \frac{l_j'}{l_j''}\right), \qquad Q_{20,j} = E_1\left(\frac{d_j}{l_j'} - \frac{d_j}{l_j''}\right) + \ln\left(1 - \frac{l_j'}{l_j''}\right),$$

$$Q_{21,j} = E_1\left(\frac{d_j}{l_j''} + \frac{d_j}{l_j'}\right) + \ln\left(1 + \frac{l_j''}{l_j'}\right), \qquad Q_{22,j} = E_1\left(\frac{d_j}{l_j''} - \frac{d_j}{l_j'}\right) + \ln\left(1 - \frac{l_j''}{l_j'}\right),$$

where j is the index of the medium ($j = 1, 3$) and the superscript k corresponds to the three terms of the excitation function (20), $k = 1, 2, 3$. $E_1(\zeta)$ is the exponential integral of the first order, $L_2(\zeta)$ is the dilogarithm, and $\ln(\zeta)$ is the principal branch of the logarithmic function in the complex plane (cf. Appendix B).

e) e–p/e–e, e–e/e–p, *and* e–e/e–e *scattering, resp.:* dN_{pe01}, dN_{ep01}, *and* dN_{ee01}, *resp.*
In the same way as in the evaluation of dN_{pp01} we obtain

$$dN_{pe01}(E, z, \omega) = \int_E^{\hbar\omega} dE'' \int_E^{E''} dE'\, A_1(E'', \omega) S_{ep1}(E'', E') S_{ee1}(E', E)$$

$$\times \frac{1}{8 l_{p1}'' l_{e1}'} \sum_{k=1}^{3} \tilde{T}^k_{pe01}(E'', E', E, z, \omega), \qquad (43)$$

$$dN_{ep01}(E, z, \omega) = \int_E^{\hbar\omega} dE'' \int_E^{E''} dE'\, A_1(E'', \omega) S_{ee1}(E'', E') S_{ep1}(E', E)$$

$$\times \frac{1}{8 l_{e1}'' l_{p1}'} \sum_{k=1}^{3} \tilde{T}^k_{ep01}(E'', E', E, z, \omega), \qquad (44)$$

$$dN_{ee01}(E, z, \omega) = \int_E^{\hbar\omega} dE'' \int_E^{E''} dE'\, A_1(E'', \omega) S_{ee1}(E'', E') S_{ee1}(E', E)$$

$$\times \frac{1}{8 l_{e1}'' l_{e1}'} \sum_{k=1}^{3} \tilde{T}^k_{ee01}(E'', E', E, z, \omega). \qquad (45)$$

The calculation shows that

$$\tilde{T}^k_{\mathrm{pe}01}(E'', E', E, z, \omega) = \tilde{T}^k_{\mathrm{ep}01}(E'', E', E, z, \omega) = \tilde{T}^k_{\mathrm{ee}01}(E'', E', E, z, \omega) \equiv \tilde{T}^k_{\mathrm{pp}01}(E'', E', E, z, \omega), \tag{46}$$

where $\tilde{T}^k_{\mathrm{pp}01}$ is determined by eqs. (38–42).

3.2. *Reflective photoemission from* M_3 *through the interface;* $j = 3$

The terms of the differential energy distribution dN_3 are calculated below analogously to the evaluation of the terms in dN_1.

a) *no scattering:* dN_{03}

$$dN_{03}(E, z, \omega) = \int_{d_1+d_2}^{d_1+d_2+d_3} dx\, P_{\mathrm{exc},3}(E, \omega, x) P_{\mathrm{surf},3}(E, z, x) \tag{47}$$

because the possible positions of excitation are between $d_1 + d_2$ and $d_1 + d_2 + d_3$. Performing the integration we have

$$dN_{03}(E, z, \omega) = \tfrac{1}{2} A_3(E, \omega) \sum_{k=1}^{3} \tilde{R}^k_{03}(E, z, \omega), \tag{48}$$

where we defined

$$\tilde{R}^k_{03}(E, z, \omega) \equiv \hat{p}^k_3(\omega) R^k_{03}(E, z, \omega) \tag{49}$$

and

$$R^k_{03}(E, z, \omega) = \exp[-\alpha^k_3(d_1 + d_2)] \frac{l_3 z}{\alpha^k_3 l_3 z + 1} \left\{1 - \exp\left[-\left(\alpha^k_3 d_3 + \frac{d_3}{l_3 z}\right)\right]\right\}. \tag{50}$$

b) e–p *scattering:* $dN_{\mathrm{p}03}$

We write a parallel expression to (30):

$$dN_{\mathrm{p}03}(E, z, \omega) = \int_{E}^{\hbar\omega} dE' \int_{d_1+d_2}^{d_1+d_2+d_3} dx'\, P_{\mathrm{exc},3}(E', \omega, x') \tag{51}$$

$$\times \left[\int_0^{\pi/2} d\vartheta' \int_0^{(x'-d_1-d_2)/\cos\vartheta'} dr' + \int_{\pi/2}^{\pi} d\vartheta' \int_0^{(x'-d_1-d_2-d_3)/\cos\vartheta'} dr'\right] ({}_{\mathrm{p}}P_{\mathrm{scat},3}(E', E, r', \vartheta') P_{\mathrm{surf},3}(E, z, r', \vartheta')).$$

The calculation results

$$dN_{p03}(E, z, \omega) = \int_E^{\hbar\omega} dE' A_3(E', \omega) S_{ep3}(E', E) \frac{1}{4l'_{p3}} \sum_{k=1}^{3} \tilde{R}^k_{p03}(E', E, z, \omega) \tag{52}$$

where we defined

$$\tilde{R}^k_{p03}(E', E, z, \omega) \equiv \hat{p}^k_3(\omega) R^k_{p03}(E', E, z, \omega) \tag{53}$$

and

$$R^k_{p03}(E', E, z, \omega) = \exp[-\alpha^k_3(d_1 + d_2)] \left[+ \frac{(l_3 z)^2}{\alpha^k_3 l_3 z + 1} \left\{ Q_{11,3} + \exp\left[-\left(\alpha^k_3 d_3 + \frac{d_3}{l_3 z} \right) \right] Q_{12,3} \right\} \right. \tag{54}$$

$$\left. + \frac{l_3 z}{\alpha^k_3(\alpha^k_3 l_3 z + 1)} \left\{ Q^k_{15,3} + \exp\left[-\left(\alpha^k_3 d_3 + \frac{d_3}{l_3 z} \right) \right] Q^k_{16,3} \right\} - \frac{l_3 z}{\alpha^k_3} E_1\left(\frac{d_3}{l'_3} \right) \left\{ \exp(-\alpha^k_3 d_3) + \exp\left(-\frac{d_3}{l_3 z} \right) \right\} \right] .$$

c) e–e *scattering:* dN_{e03}

$$dN_{e03}(E, z, \omega) = \int_E^{\hbar\omega} dE' A_3(E', \omega) S_{ee3}(E', E) \frac{1}{4l'_{e3}} \sum_{k=1}^{3} \tilde{R}^k_{e03}(E', E, z, \omega) \tag{55}$$

where

$$\tilde{R}^k_{e03}(E', E, z, \omega) \equiv \tilde{R}^k_{p03}(E', E, z, \omega) \tag{56}$$

and $\tilde{R}^k_{p03}$ is determined by eqs. (53, 54, 42).

d) e–p/e–p *scattering:* dN_{pp03}

The parallel expression to (36) is:

$$dN_{pp03}(E, z, \omega) = \int_E^{\hbar\omega} dE'' \int_E^{E''} dE' \int_{d_1+d_2}^{d_1+d_2+d_3} dx'' P_{exc,3}(E'', \omega, x'')$$

$$\times \left[\left[\left\{ \int_0^{\pi/2} d\vartheta'' \int_0^{(x''-d_1-d_2)/\cos\vartheta''} dr'' + \int_{\pi/2}^{\pi} d\vartheta'' \int_0^{(x''-d_1-d_2-d_3)/\cos\vartheta''} dr'' \right\} \right. \right.$$

$$\left. \left. \times \left\{ \int_0^{\pi/2} d\vartheta' \int_0^{(x''-d_1-d_2-r''\cos\vartheta'')/\cos\vartheta'} dr' + \int_{\pi/2}^{\pi} d\vartheta' \int_0^{(x''-d_1-d_2-d_3-r''\cos\vartheta'')/\cos\vartheta'} dr' \right\} \right] \right]$$

$$\times ({}_pP_{scat,3}(E'', E', r'', \vartheta'')\, {}_pP_{scat,3}(E', E, r', \vartheta')\, P_{surf,3}(E, z, r', \vartheta')). \tag{57}$$

The calculation results

$$dN_{pp03}(E, z, \omega) =$$

$$= \int_E^{\hbar\omega} dE'' \int_E^{E''} dE' A_3(E'', \omega) S_{ep3}(E'', E') S_{ep3}(E', E) \frac{1}{8l''_{p3} l'_{p3}} \sum_{k=1}^{3} \tilde{R}^k_{pp03}(E'', E', E, z, \omega), \tag{58}$$

where we defined

$$\tilde{R}^k_{\mathrm{pp}03}(E'', E', E, z, \omega) \equiv \hat{p}^k_3(\omega) R^k_{\mathrm{pp}03}(E'', E', E, z, \omega) \tag{59}$$

and

$$\begin{aligned}
R^k_{\mathrm{pp}03}(E'', E', E, z, \omega) &= \exp[-\alpha^k_3(d_1+d_2)] \\
&\times \left[+ \frac{(l_3 z)^3}{\alpha^k_3 l_3 z + 1} \left\{ Q_{1,3} - \exp\left[-\left(\alpha^k_3 d_3 + \frac{d_3}{l_3 z}\right)\right] Q_{2,3} - \exp\left(-\frac{d_3}{l_3 z}\right) Q_{3,3} + \exp(-\alpha^k_3 d_3) Q_{4,3} \right\} \right. \\
&+ \frac{l_3 z}{(\alpha^k_3)^2(\alpha^k_3 l_3 z + 1)} \left\{ - \exp\left[-\left(\alpha^k_3 d_3 + \frac{d_3}{l_3 z}\right)\right] Q^k_{5,3} + Q^k_{6,3} + \exp(-\alpha^k_3 d_3) Q^k_{7,3} - \exp\left(-\frac{d_3}{l_3 z}\right) Q^k_{8,3} \right\} \\
&+ \frac{l_3 z d_3}{\alpha^k_3} \left\{ \left[1 + \exp\left[-\left(\alpha^k_3 d_3 + \frac{d_3}{l_3 z}\right)\right]\right] Q_{9,3} + \left[\exp(-\alpha^k_3 d_3) + \exp\left(-\frac{d_3}{l_3 z}\right)\right] Q_{10,3} \right\} \\
&+ \frac{(l_3 z)^2}{\alpha^k_3(\alpha^k_3 l_3 z + 1)} \left\{ Q_{11,3} Q^k_{17,3} - \exp\left[-\left(\alpha^k_3 d_3 + \frac{d_3}{l_3 z}\right)\right] Q_{12,3} Q^k_{18,3} \right\} \\
&+ \frac{(l_3 z)^2}{\alpha^k_3} E_1\left(\frac{d_3}{l''_3}\right) \left\{ \exp\left(-\frac{d_3}{l_3 z}\right) Q_{12,3} - \exp(-\alpha^k_3 d_3) Q_{11,3} \right\} \\
&+ \frac{l_3 z}{(\alpha^k_3)^2} E_1\left(\frac{d_3}{l'_3}\right) \left\{ - \left[1 - \exp\left[-\left(\alpha^k_3 d_3 + \frac{d_3}{l_3 z}\right)\right]\right] E_1\left(\frac{d_3}{l''_3}\right) - \exp\left(-\frac{d_3}{l_3 z}\right) Q^k_{17,3} + \exp(-\alpha^k_3 d_3) Q^k_{18,3} \right\} \\
&\left. + X^k_{\mathrm{R}3}(E'', E', E, z, \omega) \right].
\end{aligned} \tag{60}$$

The expressions Q are again defined by (42). The function $X^k_{\mathrm{R}3}$ is given by

$$X^k_{\mathrm{R}3}(E'', E', E, z, \omega) = \int_1^\infty \mathrm{d}u\, \chi^k_{\mathrm{R}3}(E'', E', E, z, \omega, u), \tag{61}$$

where

$$\begin{aligned}
&\chi^k_{\mathrm{R}3}(E'', E', E, z, \omega, u) = \\
&= -\frac{(l_3 z)^3 d_3}{\alpha^k_3 l_3 z + 1} \left\{ \left[L_2\left(\frac{l_3 z(l'_3 u + l''_3)}{l''_3(l_3 z - l'_3)}\right) - \exp\left[-\left(\alpha^k_3 d_3 + \frac{d_3}{l_3 z}\right)\right] L_2\left(\frac{l_3 z(l'_3 u + l''_3)}{l''_3(l_3 z + l'_3)}\right)\right] \frac{\exp[-(d_3/l'_3 + d_3 u/l''_3)]}{l''_3} \right. \\
&+ \left[\exp\left(-\frac{d_3}{l_3 z}\right) L_2\left(\frac{l'_3(l_3 z u + l'_3)}{l'_3(l_3 z + l''_3)}\right) - \exp(-\alpha^k_3 d_3) L_2\left(\frac{l'_3(l_3 z - l'_3)}{l'_3(l_3 z - l''_3)}\right)\right] \frac{\exp(-d_3 u/l'_3)}{l'_3} \\
&\left. + \left[\exp\left(-\frac{d_3}{l_3 z}\right) L_2\left(\frac{l'_3(l_3 z u + l'_3)}{l''_3(l_3 z + l'_3)}\right) - \exp(-\alpha^k_3 d_3) L_2\left(\frac{l'_3(l_3 z u - l''_3)}{l''_3(l_3 z - l'_3)}\right)\right] \frac{\exp(-d_3 u/l''_3)}{l''_3} \right\} \\
&+ \frac{l_3 z d_3}{(\alpha^k_3)^2(\alpha^k_3 l_3 z + 1)} \left\{ \left[L_2\left(\frac{l'_3 u + l''_3}{l''_3(1 + \alpha^k_3 l'_3)}\right) - \exp\left[-\left(\alpha^k_3 d_3 + \frac{d_3}{l_3 z}\right)\right] L_2\left(\frac{l'_3 u + l''_3}{l''_3(1 - \alpha^k_3 l'_3)}\right)\right] \frac{\exp[-(d_3/l'_3 + d_3 u/l''_3)]}{l''_3} \right.
\end{aligned}$$

$$+\left[\exp\left(-\frac{d_3}{l_3 z}\right)L_2\left(\frac{l_3''(u-\alpha_3^k l_3')}{l_3'(1-\alpha_3^k l_3'')}\right)-\exp(-\alpha_3^k d_3)L_2\left(\frac{l_3''(u+\alpha_3^k l_3')}{l_3'(1+\alpha_3^k l_3'')}\right)\right]\frac{\exp(-d_3 u/l_3')}{l_3'}$$

$$+\left[\exp\left(-\frac{d_3}{l_3 z}\right)L_2\left(\frac{l_3'(u-\alpha_3^k l_3'')}{l_3''(1-\alpha_3^k l_3')}\right)-\exp(-\alpha_3^k d_3)L_2\left(\frac{l_3'(u+\alpha_3^k l_3'')}{l_3''(1+\alpha_3^k l_3')}\right)\right]\frac{\exp(-d_3 u/l_3'')}{l_3''}\Bigg\}$$

$$+\frac{l_3 z(\alpha_3^k l_3 z-1)d_3}{(\alpha_3^k)^2}\left\{\left[1-\exp\left[-\left(\alpha_3^k d_3+\frac{d_3}{l_3 z}\right)\right]\right]\frac{\exp[-(d_3/l_3'+d_3 u/l_3'')]}{l_3''}L_2\left(1+\frac{l_3'}{l_3''}u\right)\right.$$

$$\left.-\left[\exp(-\alpha_3^k d_3)-\exp\left(-\frac{d_3}{l_3 z}\right)\right]\left[\frac{\exp(-d_3 u/l_3')}{l_3'}L_2\left(\frac{l_3''}{l_3'}u\right)+\frac{\exp(-d_3 u/l_3'')}{l_3''}L_2\left(\frac{l_3'}{l_3''}u\right)\right]\right\}$$

$$+\frac{l_3 z d_3^2}{\alpha_3^k}\left[\exp(-\alpha_3^k d_3)+\exp\left(-\frac{d_3}{l_3 z}\right)\right]\left[\frac{\exp(-d_3 u/l_3')}{l_3'}L_2\left(\frac{l_3''}{l_3'}u\right)+\frac{\exp(-d_3 u/l_3'')}{l_3''}L_2\left(\frac{l_3'}{l_3''}u\right)\right]. \quad (62)$$

The comments presented in connection with the function X_{T1}^k apply similarly for X_{R3}^k.

e) e–p/e–e, e–e/e–p, *and* e–e/e–e *scattering, resp.:* dN_{pe03}, dN_{ep03}, *and* dN_{ee03}, *resp.*
The expressions corresponding to (43), (44), and (45) are:

$$dN_{pe03}(E, z, \omega)=\int_E^{\hbar\omega'} dE''\int_E^{E''} dE' A_3(E'', \omega)S_{ep3}(E'', E')S_{ee3}(E', E)$$

$$\times\frac{1}{8l_{p3}''l_{e3}'}\sum_{k=1}^{3}\tilde{R}_{pe03}^k(E'', E', E, z, \omega), \quad (63)$$

$$dN_{ep03}(E, z, \omega)=\int_E^{\hbar\omega} dE''\int_E^{E''} dE' A_3(E'', \omega)S_{ee3}(E'', E')S_{ep3}(E', E)$$

$$\times\frac{1}{8l_{e3}''l_{p3}'}\sum_{k=1}^{3}\tilde{R}_{ep03}^k(E'', E', E, z, \omega), \quad (64)$$

$$dN_{ee03}(E, z, \omega)=\int_E^{\hbar\omega} dE''\int_E^{E''} dE' A_3(E'', \omega)S_{ee3}(E'', E')S_{ee3}(E', E)$$

$$\times\frac{1}{8l_{e3}''l_{e3}'}\sum_{k=1}^{3}\tilde{R}_{ee03}^k(E'', E', E, z, \omega). \quad (65)$$

The calculation shows that

$$\tilde{R}_{pe03}^k(E'', E', z, \omega)=\tilde{R}_{ep03}^k(E'', E', E, z, \omega)=\tilde{R}_{ee03}^k(E'', E', E, z, \omega)\equiv\tilde{R}_{pp03}^k(E'', E', E, z, \omega), \quad (66)$$

where $\tilde{R}_{pp03}^k$ is determined by eqs. (59–62, 42).

4. Escape of electrons

Consider a potential barrier (e.g. of an MIM structure) of the type indicated in fig. 6 with the maximum height ϕ_m at the distance x_m from one interface. We look for the probability that an electron coming to the barrier from this interface with energy E and the momentum direction determined by z (i.e. with a particular energy E_x) will surmount the barrier. Two effects will be accounted for: scattering of electrons in the barrier region, and their quantum-mechanical character.

The probability of arriving at the position x_m without scattering is given [6] by $\exp(-x_m/\lambda z)$, where λ is the (energy-dependent) mean free path of an electron for (electron–phonon) scattering in the barrier region. Assuming now that the propagation of electrons which *do not scatter before reaching the position of the barrier maximum* is described by the quantum-mechanical transmission coefficient $P_{qm}(E_x, V)$, the escape probability of an electron with energy E and momentum direction due to z is

$$P_{esc}(E, E_x, z, V) = P_{qm}(E_x, V) \exp(-x_m/\lambda z), \tag{67}$$

where V is the external voltage applied to the structure the sign of V being that of the electrode M_3. We note that $x_m = x_m(V)$ and $z = z(E, E_x)$.

In the above consideration two simplifying assumptions have been introduced. First, it was supposed that all the electrons reaching x_m without scattering are accelerated by the built-in field to the opposite electrode and so contribute to the current, and all the electrons which scatter before x_m are returned to the emitting interface and so do not contribute. In other words, the possibility of backscattering over the barrier maximum and/or of overcoming the maximum after a previous scattering before x_m have been neglected. Such an approach is based on the calculations [6, 24] showing that these processes can be described by a correction factor to P_{esc} changing slowly with x_m/λ compared to $\exp(-x_m/\lambda z)$. Moreover, this factor is for not too large x_m/λ in the

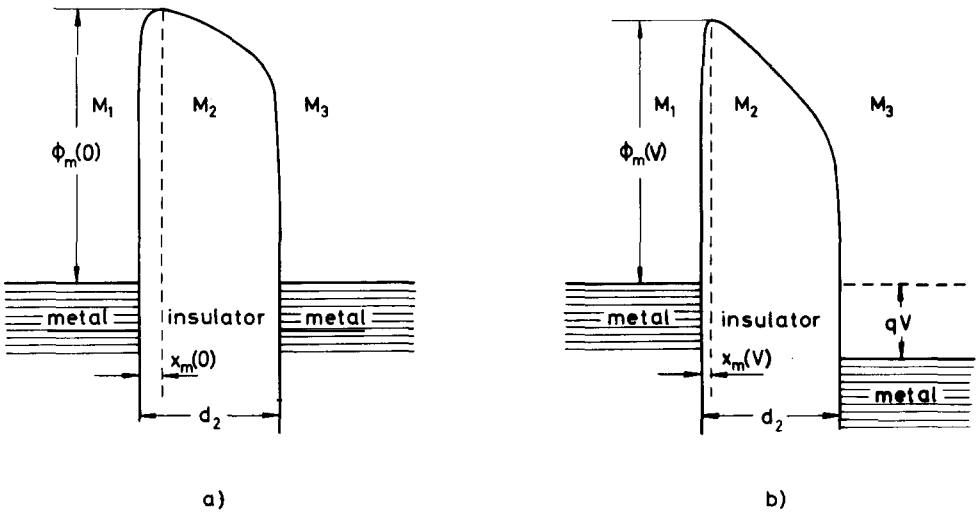


Fig. 6. Energy diagram of the potential barrier in a MIM sandwich structure: a) no voltage, b) voltage V applied.

order of unity. The second simplification regards the separation of the escape probability into the part describing the scattering and the part due to the quantum-mechanical character of an electron. These two parts are actually not independent of each other. For a more correct approach it would be necessary to evaluate the transmission coefficient into an intermediate scattering state within the barrier region. Instead, we have identified the transmission coefficient for the electrons which do not scatter before x_m with the coefficient $P_{qm}(E_x, V)$ calculated for $\lambda \to \infty$. Evaluating $P_{qm}(E_x, V)$, usual methods [12, 13, 25–28] of quantum mechanics can be used. The transmission coefficient $P_{qm}(E_x, V)$ is a function increasing from zero to one with increasing energy E_x. The functional dependence on E_x is influenced by the shape and height of the barrier and, consequently, also by the voltage V applied to the structure. A forthcoming paper [11] is devoted to the evaluation of $P_{qm}(E_x, V)$ for some barriers of practical interest and its influence on the photoemissive quantum yield.

We see that the escape probability (67) corresponds to that of Berglund and Powell [6] for electrons with $\tilde{E}_x > \phi_m$ when we assume a classical (zero-or-one) transmission coefficient. On the other hand, the escape probability is given by $P_{qm}(E_x, V)$ in absence of scattering ($\lambda \to \infty$).

We specialize our result to the sandwich structure in fig. 2 with a nonabsorbing medium M_2 of thickness d_2. Then the escape probability for electrons from M_1 which have the distribution $dN_1(E, z, \omega)$ is given directly by (67), where x_m is the distance between the interface 2 and the position of the barrier maximum ϕ_m. For electrons from M_3 with the distribution $dN_3(E, z, \omega)$ we replace x_m by $d_2 - x_m$ in the exponential function, and E_x by $E_x - qV$ in the transmission coefficient (because of the shift of Fermi level in M_3 by an amount qV, q is elementary charge) and obtain:

$$\overline{P}_{esc}(E, E_x, z, V) = P_{qm}(E_x - qV, V) \exp\left(-\frac{d_2 - x_m}{\lambda z}\right). \tag{68}$$

5. Quantum yield from M_1 and M_3: net quantum yield

The number of electrons with energy between E, $E + dE$ and the direction of momentum corresponding to values between z, $z + dz$ which flow from the medium M_1 into M_3 is given by

$$dN_1(E, z, \omega) P_{esc}(E, E_x, z, V)\, dE\, dz \tag{69}$$

(note that $E_x = E_x(E, z)$). We obtain the energy distribution $N_1(E, \omega)$ per unit energy and incident photon of electrons escaped from M_1 by integrating (69) over all momentum directions contributing to E (i.e. over an escape cone in a general sense). However, because of the explicit dependence on E_x in $P_{esc}(E, E_x, z, V)$ it is more convenient to split the composite variable z into the dependence on E and E_x and to integrate instead of over z over all $E_x \leqslant E_{01} + E$ contributing to a particular energy E. The constant E_{01} is equal to the value E_0 (see Introduction) taken in M_1. We substitute $z = [E_x/(E + E_{01})]^{1/2}$ into (69). Then

$$N_1(E, \omega) = \tfrac{1}{2}(E + E_{01})^{-1/2} \int_{E_{01} - qV}^{E_{01} + E} dE_x\, E_x^{-1/2}\, dN_1\left(E, \left[\frac{E_x}{E + E_{01}}\right]^{1/2}, \omega\right) P_{esc}\left(E, E_x, \left[\frac{E_x}{E + E_{01}}\right]^{1/2}, V\right) \tag{70}$$

and the quantum yield $Y_1(\omega)$ per incident photon

$$Y_1(\omega) = \int_0^{\hbar\omega} \mathrm{d}E\, N_1(E, \omega). \tag{71}$$

Correspondingly, for electrons escaping from M_3 into M_1 we obtain

$$N_3(E, \omega) = \tfrac{1}{2}(E + E_{03})^{-1/2} \int_{E_{03}+qV}^{E_{03}+E} \mathrm{d}E_x E_x^{-1/2}\, \mathrm{d}N_3\left(E, \left[\frac{E_x}{E + E_{03}}\right]^{1/2}, \omega\right) \bar{P}_{\mathrm{esc}}\left(E, E_x, \left[\frac{E_x}{E + E_{03}}\right]^{1/2}, V\right) \tag{72}$$

and

$$Y_3(\omega) = \int_0^{\hbar\omega} \mathrm{d}E\, N_3(E, \omega). \tag{73}$$

The net quantum yield $Y(\omega)$ per incident photon flowing between the electrodes is then

$$Y(\omega) = Y_1(\omega) - Y_3(\omega). \tag{74}$$

The lower limits $E_{01} - qV$ and $E_{03} + qV$ in the integrals in (70) and (72), respectively, originate from the fact that the electrons which have E_x below the Fermi level of the opposite electrode (cf. fig. 6) will find there practically no available states ($T = 0°\mathrm{K}$), and therefore their transition probability is identically zero. Our consideration makes no attempt to involve the tunnel currents which flow between the electron states situated energetically below the Fermi level of the negatively biased electrode. These currents are usually eliminated (e.g. by lock-in amplifier method) in photoemission experiments. In other words, eqs. (71) and (73) describe the "true" photocurrents which are due to photoexcitation. Furthermore, because the contribution to the photocurrent of electrons which are excited to energies far below the barrier maximum is small, the exact value of the lower limit in the integrals is not of relevance. The problems discussed in this paragraph vanish, of course, if $V = 0$.

6. Conclusion

Following the problems connected with the internal photoemission in sandwich structures and reviewed in table I we have successively evaluated the excitation function (20), the differential energy distribution $\mathrm{d}N_1(E, z, \omega)$ due to the transmittive photoemission from the top electrode M_1 (it equals the sum of the expressions (27), (31), (34), (37), (43), (44), and (45)), and the differential energy distribution $\mathrm{d}N_3(E, z, \omega)$ due to the reflective photoemission from the base electrode M_3 (it equals the sum of the expressions (48), (52), (55), (58), (63), (64), and (65)). Then accounting for both the scattering of electrons in the barrier region and their quantum-mechanical character, the escape probabilities (67) and (68) from M_1 and M_3, respectively, have been given. The net quantum yield $Y(\omega)$ (74) is calculated as a difference of the quantum yields $Y_1(\omega)$ (71) and $Y_3(\omega)$ (73) originating from M_1 and M_3, respectively. The net photocurrent which can be measured in an external circuit can be obtained by multiplying the net quantum yield $Y(\omega)$ by the elementary charge and by the photon flux incident per unit time.

Although the general expressions for calculation of the quantum yield are rather complicated, there can be found some conditions leading to considerable simplifications. So, for example, if the mean free path l_p for e–p scattering in the electrode for all electron energies under consideration is greater than the mean free path l_e for e–e scattering, then the contributions due to the twice-scattered electrons can be neglected.

In the Introduction we have for simplicity assumed a parabolic-band approximation for excited electrons. Then it was possible to separate simply the energy E_x which is connected with the motion in x-direction. We will briefly discuss whether our calculation can be used in the present form when the above assumption is not valid. It can clearly be seen that the formulations of sections 2 and 3 (optical analysis and electron transport in electrodes, respectively) are independent of the energy-momentum relation. However, exploiting the formulae of sections 4 and 5 (escape of electrons and calculation of the quantum yield) it is necessary to separate E_x. The sufficient condition to do this is that the partial derivative $\partial E/\partial p_x$ is independent* of the tangential components (p_y, p_z) of $\boldsymbol{p}$. This condition is, of course, fulfilled not only for the parabolic energy-momentum relation.

A more serious problem could, however, arise from the use of the generalized "escape cone"-concept (i.e. the introduction of the variable $z = p_x/p$ and its split into E and E_x). The original treatment [18] tacitly assumes that the energy E of an electron is unambiguously determined by the *magnitude* of its momentum, i.e. $E = E(p)$, but E does not depend on the electron direction. This is, for example, the case for free electrons. A simple consideration shows that the sufficient condition to introduce the generalized "escape cone"-concept is the rotational symmetry of energy-momentum relation with respect to the x-axis. In other words, the energy E_t connected with the motion in the tangential direction (to the surface) may depend only on the magnitude of the tangential momentum $p_t = (p_y^2 + p_z^2)^{1/2}$. So, strictly speaking, the utilization of the "escape cone"-concept means a restriction to special forms of the energy-momentum relation. On the other hand, if the range ΔE of excited energies above the barrier maximum ($\Delta E \approx \hbar\omega - \phi_m$) is not too large with respect to $E_B + E$ (E_B is the difference between the Fermi level and the bottom of the conduction band), the mean contribution to the photocurrent comes from the electrons reaching the interface with a small angle ϑ (see fig. 4a). But then the actual energy-momentum relation at these energies can be approached by a relation of required properties, e.g. by a fitted parabolic-band approximation. Moreover, in many cases of practical interest (metals) the actual Fermi surface [29] is not far from a sphere. So we believe that the use of the "escape cone"-concept presents no serious restriction on the above calculation of the photocurrent, especially not for photon energies in the vicinity of the barrier height ($\hbar\omega \approx \phi_m$).

So far we did not worry about the temperature at which the analysis is valid. And indeed, it was not necessary because all the temperature-dependent quantities (P_{0j}, S_{eej}, S_{epj}, l_j, l_{ej}, l_{pj}, λ, etc.) enter the resulting expressions in such a form that any kind of temperature dependence can be accounted for. In this sense the presented formulae can be used without regard to the temperature.

We have found [11] that the application of the quantum-mechanical transmission coefficient in the escape probabilities (67) and (68) is necessary in the investigation of the quantum yield in the vicinity of the threshold ($\hbar\omega \approx \phi_m$), especially when the barrier is very thin. The usefulness

*The author thanks K.H. Gundlach for this mathematically exact formulation.

of the optical analysis in section 2 has been confirmed by the numerical evaluation [30] of the excitation function (20) which shows some interesting features of the spatial distribution of excited electrons.

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Appendix A

Consider a system [31, 32] of optical media M_0, M_1, M_2, ... M_f separated by the interfaces 1, 2, ... f (see fig. A1). Denoting by

$$E_m^+(\rho) = E_m^+ \exp(ik_m^+ \rho) \tag{A1}$$

and

$$E_m^-(\rho) = E_m^- \exp(ik_m^- \rho) \tag{A2}$$

the time-averaged electric wave propagating in M_m in the positive and negative x-direction, respectively, solution of the equations of propagation leads to the following relations between the waves in M_m and M_{m-1}:

$$\begin{aligned} E_{m-1}^+(\rho_m) &= \frac{1}{r_m + 1}\,[E_m^+(\rho_m) + r_m E_m^-(\rho_m)] \\ E_{m-1}^-(\rho_m) &= \frac{1}{r_m + 1}\,[r_m E_m^+(\rho_m) + E_m^-(\rho_m)] \end{aligned} \tag{A3}$$

(r_m is the amplitude reflection coefficient defined in the main text, ρ_m is the position vector at the interface m). Substituting for $E^{\pm}(\rho_m)$ from (A1) and (A2), and writing in the matrix form we have

$$\begin{pmatrix} E_{m-1}^+ \\ E_{m-1}^- \end{pmatrix} = \mathcal{M}_m \begin{pmatrix} E_m^+ \\ E_m^- \end{pmatrix}, \tag{A4}$$

where

$$\mathcal{M}_m \equiv \frac{1}{r_m + 1} \begin{pmatrix} \exp[i(k_m^+ - k_{m-1}^+)\rho_m] & r_m \exp[i(k_m^- - k_{m-1}^+)\rho_m] \\ r_m \exp[i(k_m^+ - k_{m-1}^-)\rho_m] & \exp[i(k_m^- - k_{m-1}^-)\rho_m] \end{pmatrix}. \tag{A5}$$

For convenience, we multiply (A4) with the inverse matrix $\overline{\mathcal{M}}_m$ and obtain

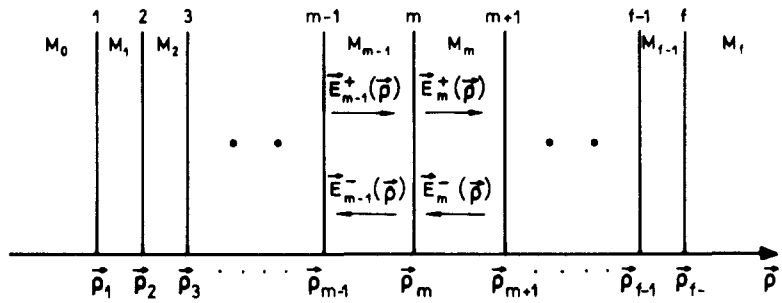

Fig. A1. Scheme of a plane-parallel system of optical media.

$$\begin{pmatrix} E_m^+ \\ E_m^- \end{pmatrix} = \bar{\mathcal{M}}_m \begin{pmatrix} E_{m-1}^+ \\ E_{m-1}^- \end{pmatrix}, \tag{A6}$$

where $\bar{\mathcal{M}}_m$ is given by eq. (9) in the main text. Using successively the recurrence formula (A6) the amplitudes of the electric vector in the medium M_j can be written in terms of the amplitudes in M_k ($k < j$) as:

$$\begin{pmatrix} E_j^+ \\ E_j^- \end{pmatrix} = \bar{\mathcal{M}}_j \bar{\mathcal{M}}_{j-1} \dots \bar{\mathcal{M}}_{k+2} \bar{\mathcal{M}}_{k+1} \begin{pmatrix} E_k^+ \\ E_k^- \end{pmatrix}. \tag{A7}$$

Appendix B

The evaluation of (30) and (36) can be done in the following way. Performing the elementary integration over r', x' and r', r'', x'', we obtain expressions which must be further integrated over the angles ϑ' and ϑ', ϑ''. The substitution $\cos\vartheta' = \pm t$ ($\cos\vartheta'' = \pm\tau$) converts the integrals into the type

$$\int_0^1 \mathrm{d}t \, \frac{Q(t)}{\Pi_{i=1}^q (a_i t + b_i)} f(t) \qquad (a_i \neq 0) \tag{B1}$$

where $Q(t)$ is a (generally complex) polynomial in t of order p ($p \leqslant q$) and $f(t)$ is one of the functions $\exp(-\gamma/t)$, $\ln(mt + n)$, $\ln(mt + n) \cdot \exp(-\gamma/t)$, or exponential integral $E_1(m/t + n)$. The solution of integral (B1) for real integrands has been published recently [33]. A generalization of the results for complex integrands must be used in the present calculation and the real part of the resulting formulae is taken to express the differential energy distribution (cf. (18) and the corresponding footnote). For convenience, we recall the general definitions of some complex functions occurring in the resulting formulae of this paper.

The exponential integral of the first order $E_1(\zeta)$ is defined for complex ζ by [34, 35]:

$$E_1(\zeta) = \int_\zeta^\infty \mathrm{d}y \, \frac{\exp(-y)}{y} \qquad (|\arg\zeta| < \pi). \tag{B2}$$

If $\zeta = t \mp \mathrm{i}0$ is real ($t > 0$) we have

$$E_1(-t \pm \mathrm{i}0) = -\mathrm{Ei}(t) \mp \mathrm{i}\pi,$$

where

$$\mathrm{Ei}(t) = \int_{-\infty}^t \mathrm{d}y \, \frac{\exp y}{y} \qquad (-\infty < t < \infty). \tag{B3}$$

The dilogarithm $L_2(\zeta)$ is defined by [36]:

$$L_2(\zeta) = -\int_0^{\zeta} dy \frac{\ln(1-y)}{y} \qquad (|\arg(1-y)| < \pi). \tag{B4}$$

The principal branch of the logarithmic function $\ln(\zeta)$ is defined by [35]:

$$\ln(\zeta) = \int_1^{\zeta} dy \frac{1}{y} \qquad (|\arg \zeta| < \pi). \tag{B5}$$

If $\zeta = t \mp i0$ is real ($t > 0$) we have

$$\ln(-t \pm i0) = \ln(t) \pm i\pi. \tag{B6}$$