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## A model simplification of dielectric responses and metal surface electrodynamics

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**Résumé.** — Nous proposons d'abord un modèle simplifié pour la réponse diélectrique en volume d'un métal d'électrons libres incluant à la fois les modes d'excitation individuel et collectif (plasmon) qui sont regroupés en un seul mode électron-trou d'intensité spectrale appropriée. Nous modélisons ensuite l'excitation locale de paires électron-trou en surface par l'addition d'un terme phénoménologique d'amplitude ajustable. Ceci fournit une fonction réponse en surface approchée. Le premier modèle donne de bons résultats pour l'effet photoélectrique interne. Au second modèle nous ajoutons une barrière de surface (une marche carrée, le jellium étant supprimé pour assurer la conservation de la charge) et une fonction d'onde électronique correspondante. Ceci donne d'assez bons résultats pour le rendement photonique total, compte tenu de la nature simplifiée du modèle.

**Abstract.** — First the dielectric response of a bulk free electron metal is simplified so that it contains both collective mode (plasmon) and single particle mode structure, taken up by one single effective electron-hole pair mode of appropriate spectral strength. Then the enhanced local excitation of electron hole pairs in the surface region is modelled by addition of a phenomenological term with empirically adjustable amplitude. This provides an approximate surface response function. The first model yields very good results for the internal photoyield. The second is supplemented with a simplified surface barrier (a square step with the jellium edge withdrawn to ensure charge conservation) and corresponding electronic wavefunctions. This yields fairly good results for the total photoyield, while providing a very substantial simplification.

### 1. Introduction.

The model one uses to describe the bulk medium is of paramount importance for the study of surface electrodynamics. The simplest example is the unphysical (singular) charge accumulation at the surface when one uses local dielectric functions. Thus, while many standard optical properties may in practice be well described in terms of a nondispersive dielectric function,  $\varepsilon(\omega)$ , for any situation in which the details of the electromagnetic field near the surface do matter a local model is ruled out. Then nonlocality, or spatial dispersion, becomes necessary. Of the vast literature on nonlocal surface electrodynamics it suffices to mention the three recent reviews of references [1, 2 and 3].

For the physically more interesting case of P-mode incident electromagnetic field it is mainly the structure of the longitudinal dielectric function  $\varepsilon_L(k, \omega)$  that matters. This structure describes the spectrum of the

normal modes which can be excited in the response of the medium to the field. Existing calculations basically fall in two classes, namely, (a) those in which  $\varepsilon_L(k, \omega)$  contains the collective model (plasmons) and also the full spectrum of single particle, or electron-hole pair, incoherent modes and (b) those in which there is no electron-hole pair structure. In the hydrodynamic approximation, for example, one bare single particle mode becomes just one collective (dressed) plasmon, while the transverse dielectric function,  $\varepsilon_T(\omega)$ , is local. An improvement upon this is the plasmon-pole approximation [4], in which the spectral structure is qualitatively as in the hydrodynamic model, but  $\varepsilon_L(k, \omega)$  contains a more elaborate  $k$ -dependence which ensures correct behaviour for large  $k$ .

Now, while these approximations prove useful for some problems in surface electrodynamics, there is in principle a second major question arising with dispersive dielectric functions. When the response is

nonlocal, one needs some model for the reflection of the conduction electron at the *inner* face of the surface [5]. Most calculations assume a specular reflection model, in which case all hinges on the structure of  $\epsilon_L(k, \omega)$ , while  $\epsilon_T(\omega)$  can be local. However, if the model is assumed to be nonspecular, then one needs also a dispersive  $\epsilon_T(k, \omega)$ . For example, nonspecular surface scattering is mainly responsible for the decay of surface plasmons and here one must go beyond approximations of the hydrodynamic or plasmon-pole type. A phenomenological model for diffuse scattering at (inner) metal surfaces, together with a method for solving this type of model was introduced by Flores and García-Moliner [6] and has been used to study several problems. This model proves also useful in some cases [7], but it shares with the hydrodynamic and plasmon-pole approximations the limitation of not having electron-hole pair structure in  $\epsilon_L$ . Consider, for example, the theory of internal photoyield [8]. This is rather more sensitive to details than other properties like, e.g., absorptance [8-10]. The model of Flores and García-Moliner [6] proves useful to demonstrate the enhancement of photoyield due to diffuse surface scattering and, even for a specular model [11], to study quantitatively the internal photoyield for  $\omega > \omega_p$ . However, it fails to produce the structure due to electron-hole pair excitations for  $\omega < \omega_p$ . Likewise it could not produce the peak structure which is found for  $\omega < \omega_p$  in the study of the absorptance in thin films with an elaborate dielectric function which includes electron-hole pair structure [9, 10].

Having framed the rôle of nonspecular surface scattering, the discussion henceforth will assume a specular reflection model and concentrate on the structure of  $\epsilon_L(k, \omega)$  and on other facts to be mentioned presently.

Everything discussed so far is based on a semiclassical infinite barrier (SCIB) model. In fact, there is a third consideration of major importance for surface electrodynamics. The surface barrier is not infinite and abrupt, but finite and smooth (although the change with distance can be very rapid) and the electronic charge density has, correspondingly, a strong but smooth inhomogeneity which does not correspond to the step function implied in semiclassical models. The associated self-consistency problem, is already non trivial for the static surface profile and then this system must respond to the electromagnetic field. The question of selfconsistency arises again in a dynamical sense and all these facts finally determine the minute details of the field in the surface region, i.e., in the range of the static inhomogeneity and beyond, until the field settles down to its bulk value. Part of this selfconsistency problem is of course the response function itself. Mukhopadhyay and Lundqvist [12] have discussed the problem of constructing the electromagnetic field near the surface. Their analysis reproduces the results of the

SCIB model, and also connects with the elaborate calculations of Feibelman [13] for long wavelengths. This work shows that the details of the field near the surface, for  $\omega < \omega_p$ , are essentially determined by the excitation of electron-hole pairs, which originates strong oscillations of vanishing amplitude away from the surface. For  $\omega > \omega_p$  the field dependence on  $z$  is smoother [13] and plasmon excitation is dominant, with the result that nondecaying oscillations penetrate into the bulk, a fact previously noted by others [8, 14].

Some interesting attempts at describing the field near the surface have been made by Barberán and Inglesfield [15] and by Apell [16]. These will be discussed later.

Focusing now on the model used to describe the longitudinal dielectric response, the position could be stated as follows : take a completely noninteracting electron gas with  $N$  bare single particle modes with given  $k$ . Switch on the electron-electron interactions. The  $N$  bare incoherent normal modes then become *one* collective plasma mode and  $N - 1$  dressed single particle (or electron-hole pair) modes with the same  $k$ . Hydrodynamic and similar approximations wipe out all of the  $N - 1$  electron-hole pairs. One saves a great of computation but some significant physics is lost, which is more or less important depending on the problem under study. More elaborate dielectric functions contain all the single particle structure to different degrees of approximation (e.g. Boltzmann-type, or Lindhard-type, perhaps with lifetime effects as in Mermin's  $\epsilon_L$ ). The price is usually a numerical *tour de force*.

The purpose of this paper is to suggest an intermediate type of approximation in which the physics associated with electron-hole pair excitations is in some way present but the structure of the incoherent part of the spectrum is drastically simplified so as to alleviate considerably the numerical task. The problem will be discussed first in connection with the SCIB model (§ 2) and then for finite surface barriers (the photoyield is sensitive to details of the EM field near the surface and then for finite surface barriers). The photoyield is sensitive to details of the EM field near the surface and will be taken as the problem of physical interest for which the model will be tested.

## 2. Model dielectric function for a semiclassical infinite surface barrier.

We start by discussing the semiclassical infinite surface barrier. Although it is well-known that this model is not good for obtaining the surface photoyield, it has been taken in this paper as a case where testing the approximation we introduce for the bulk dielectric function. To this end, we shall compare the internal photoyield as obtained in the semiclassical infinite surface barrier, by using both the RPA [8] and our model for the dielectric function.

The idea is to replace all of the  $(N - 1)$  incoherent modes, for given  $k$ , by just *one* effective electron-hole pair, adjusted so as to take up all the spectral strength which does not correspond to the plasmon. This amounts to an extension of the plasmon-pole approximation to the RPA, in which one puts for  $\varepsilon_L$  :

$$\varepsilon_L(k, \omega) = \frac{[ak^4 + \beta_L^2 k^2 + \omega_p^2 - \omega^2 - i\omega\tau^{-1}][ak^4 + \beta_{ch}^2 k^2 - \omega^2 - i\omega\gamma]}{[ak^4 + \beta_1^2 k^2 - \omega^2 - i\omega\tau^{-1}][ak^4 + \beta_2^2 k^2 - \omega^2 - i\omega\gamma]} \quad (2.1)$$

Here  $\tau$  is a kind of conduction electron relaxation time, as one would have for example in a Boltzmann equation model, while  $\gamma$  is intended to represent phenomenologically a different kind of lifetime effect, of the Landau type, associated with electron-electron interactions. Apart from lifetime effects, the four parameters in this formula are :  $\beta_1$  and  $\beta_2$ , associated with the two starting bare normal modes (poles of  $\varepsilon_L$ );  $\beta_L$ , associated with the plasmon (a zero of  $\varepsilon_L$ ) and  $\beta_{ch}$ , associated with the dressed electron-hole pair (another zero of  $\varepsilon_L$ ).

The four conditions which one can use to obtain these four parameters (with  $\tau^{-1} = \gamma = 0$ ) are : (i) to reproduce the low  $k$  part of the plasmon dispersion relation as obtained in the RPA. This yields  $\beta_L^2 = V_F^2 3/5$ , as in the hydrodynamic and plasmon-pole approximations. (ii) To adjust the low  $k$  edge of the electron-hole pair spectrum as obtained in the RPA. This yields  $\beta_{ch}^2 = V_F^2$  [12]. (iii) The two modes together must saturate the sum rule

$$\int_0^\infty \omega \operatorname{Im} \{ \varepsilon_L(k, \omega) \} d\omega = \omega_p^2 \pi/2. \quad (2.2)$$

This yields

$$\beta_L^2 + \beta_{ch}^2 = \beta_1^2 + \beta_2^2. \quad (2.3)$$

(iv) Consider the loss function, associated with the power loss of an external charge  $Ze$  moving with velocity  $V$  through an electron gas. The plasmon strength in this loss function is the residue

$$8 \pi^2 Z^2 e^2 \omega(k) \delta(\omega - k.v)/k^2 \left| \frac{\partial \varepsilon_L(k, \omega)}{\partial \omega} \right|_{\omega(k)} \quad (2.4)$$

evaluated at  $\omega(k) = \omega$  (plasmon). The fourth condition is that (2.4) must give the same result with (2.1) as it does with  $\varepsilon_{L,RPA}$  in the low  $k$  limit. This yields

$$(\beta_L^2 - \beta_1^2)(\beta_{ch}^2 - \beta_2^2) = -6^2 V_F^4/7 \times 5^2. \quad (2.5)$$

From (2.3) and (2.5) one has  $\beta_1^2 = 1.296 V_F^2$  and  $\beta_2^2 = 0.304 V_F^2$ .

For the damping parameter one must proceed empirically. In our approach, we have taken  $\tau^{-1} = \gamma$  as the standard relaxation time for each given metal. The main point to be noted about this approximation

$$\varepsilon_{pp}(k, \omega) = \frac{\omega^2 - \omega_p^2 - \beta^2 k^2 - ak^4}{\omega^2 - \beta^2 k^2 - ak^4}; \quad a = \hbar^2/4 m^2.$$

The term  $ak^4$  is chosen to ensure the right behaviour for high  $k$ . In line with this approximation we now try the somewhat more complete dielectric function

is that the results obtained in this paper are practically independent of the small values taken below for  $\tau^{-1}$  and  $\gamma$ . The reason is that the main contribution to the energy dissipated in the metal comes from the zeros of  $\varepsilon_L$  : the electron-hole pairs ( $\omega < \omega_p$ ) or plasmon modes ( $\omega > \omega_p$ ) [6]. For a dielectric function with no electron-hole pair structure,  $\tau^{-1}$  would be responsible for the energy dissipated at  $\omega < \omega_p$ .

Having decided on  $\varepsilon_L$ , the first task is to construct the EM inside the medium which, in the SCIB model, will be assumed to fill up the half space  $z > 0$ . This can be done by proceeding as in the study of thin films [7].

Consider P-polarized incident radiation with wave-vector component parallel to the surface  $k_x = \kappa, \mathbf{k} = (\kappa, 0, \lambda)$ . Then (2.1) can be conveniently cast in the form

$$\varepsilon_L(\kappa, \lambda) = \sum_{i=1}^4 (\lambda^2 + L_i^2)/(\lambda^2 + l_i^2), \quad (2.6)$$

where

$$\begin{aligned} L_{1,2} &= \{ \kappa^2 + (\beta_L^2/2 a) \times \\ &\quad \times [1 \mp (1 - 4 a(\omega_p^2 - \omega^2 - i\omega\tau^{-1})/\beta_L^4)^{1/2}] \}^{1/2}; \\ L_{3,4} &= \{ \kappa^2 + (\beta_{ch}^2/2 a) \times \\ &\quad \times [1 \mp (1 + 4 a(\omega^2 + i\omega\gamma)/\beta_{ch}^4)^{1/2}] \}^{1/2}. \end{aligned} \quad (2.7)$$

Likewise, for a nondispersive  $\varepsilon_T(\omega)$ ,

$$k^2 - \varepsilon_T \omega^2/c^2 = \lambda^2 + R^2; \quad R = [\kappa^2 - \varepsilon_T \omega^2/c^2]^{1/2}. \quad (2.8)$$

The explicit form of the  $l_i$ 's will be given later. With the present sign conventions, in all square roots the branch to be taken is the one having a positive real part.

The field inside the medium is then a combination of longitudinal and transverse modes of the form

$$\begin{aligned} E_x &= \sum_{i=1}^4 E_i \exp(-L_i z) + E_R \exp(-Rz); \\ E_z &= \sum_{i=1}^4 iL_i \kappa^{-1} \exp(-L_i z) + i\kappa R^{-1} E_R \exp(-Rz); \\ H_y &= -i\kappa(\kappa^2 - R^2) \omega^{-1} R^{-1} E_R \exp(-Rz), \end{aligned} \quad (2.9)$$

and  $E_i$  ( $i = 1, 2, 3, 4$ ),  $E_R$  are the five amplitudes to be determined.

It is worth commenting at this point that, although equation (2.9) gives four longitudinal modes, only two of them ( $i = 1, 3$ ) can be interpreted as a normal electron-hole pair ( $i = 1$ ) or a plasmon mode ( $i = 3$ ), the reason being that for  $i = 2, 4$  the imaginary part of  $L$  is very great. The formal solution given in this

paper, however, must be built up with all the modes satisfying the equation  $\varepsilon_L(k, \omega) = 0$ .

Now, the field equation

$$\nabla \wedge (\nabla \wedge \mathbf{E}) - \omega^2 \mathbf{E}/c^2 = 4 \pi \omega^2 \mathbf{P}/c^2. \quad (2.10)$$

must hold everywhere for  $z > 0$ . The polarization  $\mathbf{P}$ , for the specular reflection model, is given by

$$\mathbf{P}(z) = \int_0^\infty \{ [\varepsilon(z - z') - \delta(z - z') \mathbf{I}] + [\varepsilon(z + z') - \delta(z + z') \mathbf{I} \cdot \boldsymbol{\alpha}] \} \cdot \mathbf{E}(z') dz' \quad (2.11)$$

where

$$\boldsymbol{\alpha} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (2.12)$$

is a matrix used to describe mirror image symmetry. The space dependence of  $\varepsilon$  is obtained by Fourier transforming (2.6).

This yields

$$\begin{aligned} \varepsilon_{xx}(z) &= \varepsilon_T \delta(z) + \frac{1}{2} \kappa^2 \sum_{i=1}^4 A_i l_i^{-1} \exp(-l_i |z|); \\ \varepsilon_{xz}(z) &= \frac{1}{2} i \kappa \operatorname{sgn} z \sum_{i=1}^4 A_i \exp(-l_i |z|); \\ \varepsilon_{zz}(z) &= \delta(z) - \frac{1}{2} \sum_{i=1}^4 A_i l_i \exp(-l_i |z|), \end{aligned} \quad (2.13)$$

where

$$\begin{aligned} l_{1,2} &= \{ \kappa^2 + (\beta_1^2/2a) [1 \mp (1 + 4a(\omega^2 + i\omega\tau^{-1})/\beta_1^4)^{1/2}] \}^{1/2}; \\ l_{3,4} &= \{ \kappa^2 + (\beta_2^2/2a) [1 \mp (1 + 4a(\omega^2 + i\omega\gamma)/\beta_2^4)^{1/2}] \}^{1/2}, \end{aligned} \quad (2.14)$$

and

$$A_i = \prod_{j \neq i} \{ (L_j^2 - l_i^2)/(l_j^2 - l_i^2) \} \frac{L_i^2 - l_i^2}{\kappa^2 - l_i^2}. \quad (2.15)$$

These results are used to evaluate  $\mathbf{P}(z)$ , which is then inserted in (2.10). On doing this one finds that  $\mathbf{P}$  contains: (a) the same exponentials as appear in (2.9). The equality between the coefficients of these exponentials on both sides of (2.10) merely leads to identities, as must be the case if the field is correctly constructed so that it satisfies the field equation. And (b) one finds also in  $\mathbf{P}$  terms in  $\exp(-l_i z)$  which are not present on the l.h.s. of (2.10). The vanishing of the corresponding coefficients yields the four equations

$$\sum_{j=1}^4 \{ E_j L_j (l_i^2 - \kappa^2)/(l_i^2 - L_j^2) \} + E_R \kappa^2/R = 0, \quad (i = 1, 2, 3, 4). \quad (2.16)$$

There are six unknowns (the five amplitudes  $E_i$ ,  $E_R$  and the amplitude of the field outside) and six equations (the four conditions (2.16) and the two matching conditions, i.e., continuity of  $E_x$  and  $H_y$  at the surface). The problem is determined and one can construct the EM field inside the medium.

Having found the field one can find the current and then evaluate the internal photoyield [8]

$$Y = \frac{4 \pi}{c \cos \theta} \int_0^\infty \exp(-z/\zeta) \operatorname{Re} [\mathbf{E}(z) \cdot \mathbf{J}^*(z)] dz, \quad (2.17)$$

where  $\theta$  is the angle of incidence and  $\zeta$  is taken to be a representative value of the escape length. In a more accurate calculation this should of course depend on the energy of the excited electrons, but (2.17) suffices for the present purpose. As it stands (2.17) cannot

be directly compared with experimental data. One might argue that the ratio of  $Y$  for  $P$  and  $S$  polarizations might be very insensitive to the probability of crossing the surface barrier and that this quantity ( $Y_p/Y_s$ ) might be compared with experiment (apart

from the approximations involved in taking one single value of  $\zeta$ ). Nevertheless the main purpose of this paper is not to give a physical theory of photoemission but to see whether (2.1) can provide a reasonable approximation to an elaborate  $\epsilon_L$ . For this it suffices to evaluate (2.17) for  $P$  polarization and to compare with the results of Kliewer [8], who performed accurate numerical calculations using Mermin's dielectric function, i.e., the full electron-hole pair structure in  $\epsilon_L(k, \omega)$ .

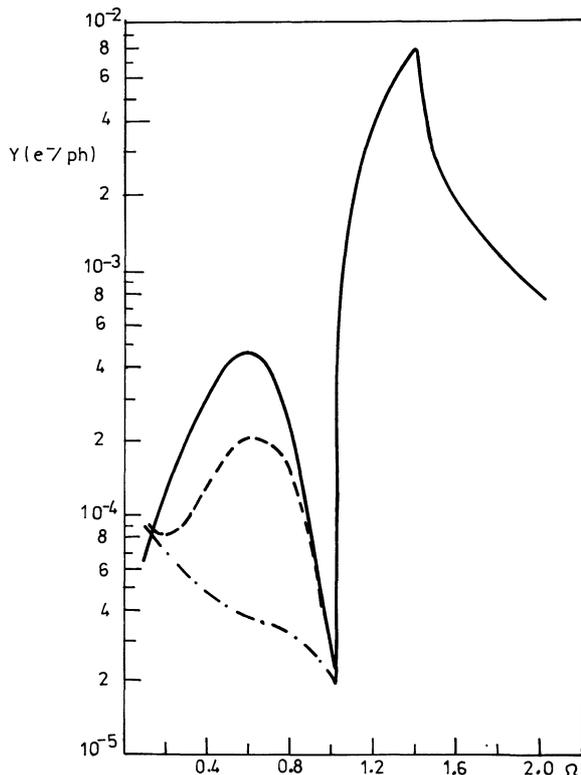


Fig. 1. — Internal photoyield for Na vs.  $\Omega = \omega/\omega_p$ . Full line : Ref. [8]. Dash-dots : Ref. [11]. Dashed line : present work including electron-hole pair excitations. Angle of incidence  $45^\circ$ . Specular scattering model throughout.

The results are shown in figure 1. Three levels of an approximation are compared. One involves all the single particle structure [8]. The second one [11] involves a dielectric function  $\epsilon_L$  with no single particle modes. The third one is the result of the present calculation based on (2.1) and taking  $\tau^{-1} = \gamma = 10^{-3}$ . (In fact, the results are rather insensitive to changes in  $\gamma$  and  $\tau^{-1}$ .) For  $\omega > \omega_p$  all calculations give nearly the same result, as the situation is determined by plasmon excitation. The significant feature is the remarkable improvement for  $\omega < \omega_p$  due to the inclusion of just one effective single particle.

### 3. A model dielectric response with finite surface barriers.

Petersen and Hagström [17] have attempted to set up an experiment designed to measure directly the *surface*

*photoeffect* in Al. While the interpretation of these experiments is not completely obvious, it is nevertheless very useful to draw attention to the details associated with the selfconsistency problem just in the region of the surface layer. Apell [16] has attempted to study the above results by introducing a *local plasmon* [18] in which  $\omega_p^2$  varies with the inhomogeneous charge density  $n(z)$ . Although this analysis is limited to low frequencies ( $\omega < \omega_p$ ), it is also useful in demonstrating the importance of the selfconsistent profiles of charge density and potential barrier for the surface photoeffect.

The clearest case so far appears to be that of Al (100), for which the total photoyield for electrons excited from the Fermi level and from the surface state has been measured and calculated for normal emission [19, 20]. Barberán and Inglesfield [15] have attempted to produce a simplified interpretation in terms of a hydrodynamic dielectric function and an abrupt (but finite) potential step such as a surface barrier. These authors find that in order to obtain a fair approximation to the experimental ratio between the heights of the two peaks observed above and below  $\omega_p$ , one must withdraw the jellium edge by a distance  $d$  from the surface barrier. In their calculation  $d = a_0/4$ , where  $a_0$  is the lattice constant. This is an interesting qualitative observation. The main defect of the semiclassical model is that it violates charge neutrality and the way to make up for this is to withdraw the jellium edge [5]. One can see, for example, that this alone yields the main quantum correction for the long wave phase velocity of the surface plasmon [21]. However, the hydrodynamic model has the inherent limitation already discussed, so that one cannot expect it to give a good description for  $\omega < \omega_p$ , where single particle excitations ought to dominate. For example, for emission from the Fermi level the experimental peak appearing at  $\hbar\omega = 12$  eV is obtained by Barberán and Inglesfield [15] at  $\hbar\omega = 8$  eV. Moreover, even if one introduced some electron-hole pair structure in the manner of (2.1), one could not expect great quantitative improvement for the total photoyield which is very sensitive to the details of the surface inhomogeneity, as discussed in various forms by Petersen and Hagström [17], Apell [16] and Levinson *et al.* [19].

The most complete calculation so far appears to be that of Feibelman [13] which involves a selfconsistent evaluation of electronic wavefunctions, response and EM field. This amounts to taking into account both the details of the surface inhomogeneity and the detailed structure of the excitation spectrum through extensive numerical computation. These produce excellent results for the photo-yield for emission from the Fermi level in Al [20] and will be taken here as a term of reference. What one learns from these calculations is that the surface inhomogeneity enhances the local excitation of electron-hole pairs, in line with Apell's observation [16]. However, as indicated above, simple approximations to the dielectric response are

unable to describe well the situation for  $\omega < \omega_p$ , and an attempt at a more complete approximation for the response of the bounded electron gas will be proposed here. The idea is to proceed in the spirit of (2.1) but

to add the extra possibility of local excitations at  $z = 0$  as the key feature which condenses the physics of the surface inhomogeneity. This suggests the following phenomenological form

$$\begin{aligned} \varepsilon_{xx}(z, z') = \varepsilon_T \delta(z - z') + \frac{1}{2} \kappa^2 \sum_{i=1}^4 A_i l_i^{-1} \exp(-l_i |z - z'|) + \frac{1}{2} \kappa^2 C [l_1^{-1} \exp(-l_1 |z|) + \\ + l_2^{-1} \exp(-l_2 |z|) - l_3^{-1} \exp(-l_3 |z|) - l_4^{-1} \exp(-l_4 |z|)] \delta(z') \end{aligned} \quad (3.1a)$$

$$\begin{aligned} \varepsilon_{xz}(z, z') = \frac{1}{2} i \kappa \operatorname{sgn}(z - z') \sum_{i=1}^4 A_i \exp(-l_i |z - z'|) + \frac{1}{2} i \kappa C [\exp(-l_1 |z|) + \\ + \exp(-l_2 |z|) - \exp(-l_3 |z|) - \exp(-l_4 |z|)] \delta(z') \end{aligned} \quad (3.1b)$$

$$\begin{aligned} \varepsilon_{zz}(z, z') = \delta(z - z') - \frac{1}{2} \sum_{i=1}^4 A_i l_i \exp(-l_i |z - z'|) - \frac{1}{2} C [l_1 \exp(-l_1 |z|) + \\ + l_2 \exp(-l_2 |z|) - l_3 \exp(-l_3 |z|) - l_4 \exp(-l_4 |z|)] \delta(z'). \end{aligned} \quad (3.1c)$$

Compare with (2.13). The terms describing the response of the bulk are identical, the  $l_i$ 's describing the normal mode excitations which go into the making of (2.6). The terms in  $\delta(z')$  force the same type of excitations to take place at the surface. The amplitudes  $A_i$  are formally different, but in actual fact take similar value in the frequency range of physical interest. Moreover, the terms associated with  $l_2$  and  $l_4$  have in practice very little weight, due to their fast decay. Thus there is no point in taking a more general model with different amplitudes. The only factor which needs care is the sign of the different exponentials. These signs are those needed to satisfy the condition

$$\lim_{\omega \rightarrow \infty} \varepsilon(z, z') = (1 - \omega_p^2/\omega^2) \delta(z - z') \mathbf{I}. \quad (3.2)$$

The bulk part of (3.1) satisfies this by itself. On the other hand one finds from (2.14)

$$\lim_{\omega \rightarrow \infty} l_1^2 = \lim_{\omega \rightarrow \infty} l_3^2 = - \lim_{\omega \rightarrow \infty} l_2^2 = - \lim_{\omega \rightarrow \infty} l_4^2 = - \omega a^{-1/2} \quad (3.3)$$

thus the terms in  $\delta(z')$  in (3.1) cancel out and (3.2) is satisfied.

Note that the surface excitation gives essentially, for  $\omega < \omega_p$ , an electron-hole pair mode since all the other modes ( $i = 2, 3, 4$ ) have at these frequencies a much too great damping.

The surface excitations introduced by equations (3.1) represent different outgoing modes, moving away from the surface : this guarantees that the surface excitation verifies causality. On the other hand, equation (3.2) is the basic limit behaviour related to many other different sum rules : note that equation (3.2) means that, in our approximation, we are working inside the semi-classical infinite barrier (*corrected* by the surface modes given in Eq. (3.1)), for which  $n(z) = n_0$  if  $z > 0$ .

The next question is how to determine  $C$ , in general

a complex number, which measures the relative amplitude of the surface excitations, and is dependent on the surface inhomogeneity. At this point, we are guided by the work of Apell [16] and Feibelman [13]. According to Apell's work, we expect the electron-hole pairs excited at the surface below  $\omega_p$ , to be roughly related to the excitation of a local plasmon created at a point  $z_1$ , for which

$$1 - \frac{4 \pi n_0(z_1) e^2}{m \omega^2} = 0,$$

where  $n_0(z)$  is the surface electronic profile. This suggests taking  $C$  proportional to  $\frac{d}{dz} n_0(z_1)$  and  $\exp\{ik_F(z_1 - z_0)\}$ , where  $z_0$  is the jellium edge;  $\frac{d}{dz} [n_0(z_1)]$  tells us that the strength of the surface excitation increases with a more abrupt electronic profile, while  $\exp\{ik_F(z_1 - z_0)\}$  measures the phase-shift associated to the fact that the surface electron-hole pair is created at the point  $z_1$ . On the other hand, we take advantage of Feibelman's work, where it is shown that the imaginary part of the induced surface charge is not only proportional to the derivative of the density surface profile, but to the frequency as well (this is a general behaviour for any response function at  $\omega \ll \omega_F$ ). All these results suggest that  $C$  can be written as follows :

$$C = C_0 \omega \frac{d}{dz} [n_0(z_1)] \exp\{ik_F(z_1 - z_0)\}, \quad (3.4)$$

where  $C_0$  is a constant which has been taken as  $3.25 \times \omega_p$  in order to obtain the best agreement with photoemission results (see below). In all the calculations given below, we have used for  $n_0(z)$  the charge density given by the calculations of Lang and Kohn [22].

Having decided on the form of the model *surface dielectric function*, one must consider the method to obtain the EM field. Now, it is not possible to proceed as in [2] because charge conservation is not automatically guaranteed as in the specular SCIB model. A simple way of solving this problem, which arises already with all nonspecular semi-classical models has been discussed in general terms elsewhere [5]. The idea is to introduce a surface dipole of amplitude  $\mathcal{D}(\kappa, \omega)$ , which creates an electric field  $4\pi\mathcal{D}\delta(z)\hat{z}$  perpendicular to the surface. This throws some charge current into the bulk and the strength  $\mathcal{D}$  is determined by the condition that total charge must be conserved.

The equations equivalent to (2.16) are now ( $i = 1, 2, 3, 4$ )

$$\begin{aligned} & \sum_{j=1}^4 \{ E_j A_j L_j (l_i^2 - \kappa^2) / (l_i^2 - L_j^2) \} + \\ & + \frac{1}{2} C \sum_{j=1}^4 E_j (\kappa^2 - l_i L_j) + \\ & + E_R \kappa^2 R^{-1} \left[ A_j + \frac{1}{2} C (R - l_i) \right] + 4\pi i \kappa \mathcal{D} A_i l_i = 0. \end{aligned} \quad (3.5)$$

The equation resulting from charge conservation, conveniently simplified by using (3.5), is

$$\sum_{j=1}^4 E_j L_j \kappa^{-1} + E_R \kappa R^{-1} [1 - \epsilon_T(\omega)] = 0. \quad (3.6)$$

With these and the standard EM matching equations, the field is again determined.

Having written down a model for the response function and constructed accordingly the EM field, it remains to be seen how one could base a reasonable calculation of the photoyield on such model. This involves the further question of the surface barrier and the electronic wavefunctions. This has also been simplified by taking a finite *step* barrier of height  $V = \Phi + E_F$  ( $\Phi$  is the work function, 4.41 eV for Al). In the light of the above discussion, the jellium was withdrawn through a distance  $d$  inwards, away from the barrier, in order to have charge neutrality. The photoyield was calculated by using the EM field as described above, and the wavefunction corresponding to this simplified surface barrier and the reverse time prescription given by Pendry [23] (see [2] and [13] as well). As stressed by Barberán and Inglesfield, interference effects associated to the barrier position may introduce important changes in the photoyield. Figure 2 shows the result for Al with ( $C_0 \neq 0$ ) and without ( $C_0 = 0$ ) surface excitation of electron-hole pairs compared with experimental data [20]. The curve for  $C_0 \neq 0$  was normalized to fit the same maximum height as obtained by Levinson and Plummer [20].

Although the low frequency peak appears at a lower frequency than the experimental one, the improvement upon the case  $C_0 = 0$  is remarkable. Also, the calculated photoionization cross section turns out to be

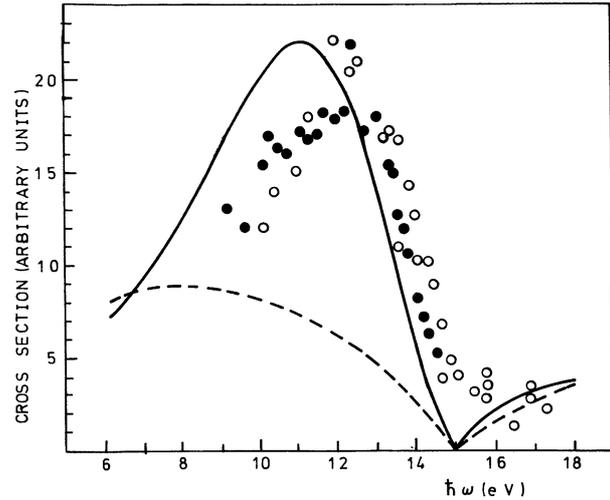


Fig. 2. — Photoionization cross section from Al (100) Fermi level at normal emission, calculated with and without surface electron-hole pair excitation. Full line : with surface electron-hole pairs. Dashed line : without surface electron-hole pairs. The dots are the experimental points [20].

in good agreement with the experimental or the calculated selfconsistent results. At  $\hbar\omega = 12$  eV (1 eV above the maximum) the present approximation yields  $8 \times 10^{-4}$  electrons/photon eV sr., while at  $\hbar\omega = 13$  eV (1 eV above the maximum in both the experimental data and the selfconsistent calculation) the results are, in the same units,  $7 \times 10^{-4}$  and  $10 \times 10^{-4}$  respectively.

#### 4. Conclusion.

The physics of the response of a surface system (assumed to be *externally* flat) to an external EM field involves basically three problems, namely : (i) The specularity or not of the reflection of conduction electrons at the inner surface. (ii) The spectral structure included in the dielectric function used to describe the bulk. (iii) The details of the surface barrier and their consequences.

Problem (i) can be treated fairly satisfactorily with a simple phenomenological model. Problems (ii) and (iii) would seem to be harder. The single particle structure plays an important rôle, especially in the surface region itself, where local excitation of electron-hole pairs dominates the details of the EM field for  $\omega < \omega_p$ . This paper presents a possible simplification which permits the construction of a very simple model capable of producing rather reasonable approximations. The spectral strength can be distributed between one plasmon (collective) mode and *one* effective single particle mode in a model dielectric function (2.1) for the bulk. This describes rather well the rôle of incoherent excitations in the *internal* photoyield (Fig. 1). The same idea can be incorporated in an approximate, inhomogeneous dielectric function (3.1) which is a sort of model *surface dielectric function*. The main

surface effect is embodied in a local excitation of electron-hole pairs at  $z = 0$ . With this one can obtain good approximations to the field in and near the surface region.

The total photoyield is sensitive to the details of this field and, furthermore, for an accurate theory one needs also the self-consistent electronic wavefunctions. A great deal of computation can be saved by using a simple square (step) potential barrier while withdrawing the jellium edge as required by charge neutrality. With this, one can obtain a fair approximation for the total photoyield, surface effects included, although it should be stressed that the total photoyield for  $\omega < \omega_p$  is very weakly sensitive to the barrier shift as required by charge neutrality. The small loss in accuracy is out of proportion with the large simplifi-

cation effected and the amount of computation one saves. The term describing phenomenologically the surface excitation of electron-hole pairs, in particular, plays a significant rôle.

The model is thus constructed in a way which bears out the physics involved in the various aspects of surface electrodynamics while it can be used for quantitative calculations capable of yielding fair results for different problems, the total photoyield being among the most sensitive to details. This also opens the way to combining the phenomenological model for questions (ii) and (iii) with a phenomenological model for question (i), which would provide an overview of different aspects of surface electrodynamics hitherto studied piecewise. Work on this is currently in progress.

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