PHYSICAL REVIEW B VOLUME 15, NUMBER 8 15 APRIL 1977

Photoemission from the Drude absorption

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(Received 22 November 1976)

A theory for the photoemission from an electron gas due to the Drude energy absorption is presented. The theory, for both p- and s-polarized incident light, is based upon the three-step photoemission model and exhibits significant effects of the second-order matrix elements involved. Photoyields, energy distributions, angular distributions, and energy-resolved angular distributions are obtained. The energy distributions are roughly triangular and there are striking asymmetries in the angular distributions. It is argued that there is a strong suppression of the p-polarized yield for frequencies such that the local dielectric function is slightly negative.

I. INTRODUCTION

Identification and characterization of the Drude absorption forms an important facet of optical studies of metals. Since this absorptance contribution is frequently an appreciable part of the total absorptance, even into the ultraviolet, we would anticipate significant photoemission associated with it. It is interesting, in view of the extent to which Drude effects have been emphasized in optical studies, that the associated photoemission has not been investigated. The reason for this, in part, is that the Drude absorptance is extremely easy to include in local optical theories; the phenomenological introduction of a finite electron lifetime is all that is needed. For photoemission, on the other hand, one must examine the physical processes leading to the finite electron lifetime in order to arrive at photoelectron distributions and the photoyield.

The distinction between local and nonlocal theories is important in the present context. In a local theory, the optical absorber (or photoemitter) is characterized by a dielectric constant $\epsilon(\omega)$, with the tacit assumption that the spatial variation of the electric field induced by the incident photon beam is sufficiently gentle on the scale of the parameters characterizing the electrons that it may be described by taking the $q\rightarrow 0$ limit of more general dielectric functions $\epsilon(q,\omega)$. Since q, the wave vector, is proportional to the momentum transfer, a statement frequently made to lend credence to the local approach is that the momentum of the photon is so small on the scale of electron momenta that it may be taken to be zero. While local theories dominate optical studies, they involve omissions which can be important. An example is the anomalous skin effect, the description of which requires a nonlocal theory with the spatial dependence of the field incorporated through dielectric functions $\epsilon(q,\omega)$ or in an alternative manner reflecting the equivalent physics.[1-17] In such a theory q can be large so the photons, with the intermediary the induced electric field, are capable of transferring large momenta.

As we noted above, the Drude absorption does occur in a local description, but represents, at the same time, processes involving large momentum transfer. The associated electronic transitions are nondirect with the momentum needed arising from scattering processes involving, for example, impurities or phonons. By introducing the electron lifetime τ, all of the large-momentum-transfer processes are incorporated, in some sense, into a single parameter which does not involve q explicitly and thus can legitimately be construed as a $q\sim 0$ entity appropriate to a local theory.

In a nonlocal theory for the surface photoeffect in the electron gas, developed by one of the present authors,[18-20] the surface effect was attributed to nondirect electronic excitations (q large) resulting from the surface-region electric field which is markedly different in character than the usual local field. By analyzing the momentum distribution of the absorbed energy, it was shown that the local, bulk effects, occurring for small q and representing the Drude absorption, were well separated from the large-q, nonlocal, surface effects. Thus their photoemission contributions could be studied separately and, in our previous work, we discussed in detail the nonlocal effects. The purpose of this paper is to extend the earlier work by investigating the photoemission role of the Drude absorption, including energy and angular distributions as well as the total yield, for the electron gas. In this case, the Drude absorption is the only "local" absorption process as there are no interband transitions. The basic procedure is presented in Sec. II, with the emphasis on the optical absorption. The photoemission theory is developed in Sec. III for s-polarized light and in Sec. IV for p polarization. Results are presented and discussed in Sec. V.

II. BASIC DRUDE THEORY

We take the photoemitter to be the half space $z>0$ with the light of angular frequency ω incident from the vacuum which fills $z<0$. When considering s-polarized light we take the plane of incidence to be the y-z plane with the electric field in the x direction. For p-polarized light the plane of incidence is the x-z plane. These various geometrical details are sketched in Fig. 1.

In a local description, the spatial distribution of the absorbed energy, dA_η/dz with $\eta=s$ or p, is given by[18-23]

$$\frac{dA_\eta}{dz}=\alpha A_\eta e^{-\alpha z}, \tag{2.1}$$

where A_η is the total absorptance and α is the absorption coefficient,

$$\alpha=(2\omega/c)\,\mathrm{Im}(\epsilon-\sin^2\theta_I^\eta)^{1/2}. \tag{2.2}$$

Here θ_I^η is the incident angle (see Fig. 1) and $\epsilon=\epsilon(\omega)$ is the local dielectric constant given by

$$\epsilon=1-[\Omega(\Omega+i\gamma)]^{-1} \tag{2.3}$$

for the electron gas. We have defined $\Omega=\omega/\omega_p$, with ω_p the plasma frequency, and used as a measure of damping $\gamma=(\omega_p\tau)^{-1}$, where τ is the mean electron lifetime. We emphasize that Eq. (2.1) results from simply including τ in the dielectric function and then using Maxwell's equations. If $\tau\rightarrow\infty$, $A_\eta\rightarrow 0$, so any absorptance is a consequence of a finite τ. This differs sharply from the situation in a nonlocal description where single-particle excitations and plasmons can give rise to absorptance even when $\tau\rightarrow\infty$. The theory to be developed now bears a formal resemblance to the customary local theory, but includes significant differences. In particular, the excited electron spectrum is treated microscopically.

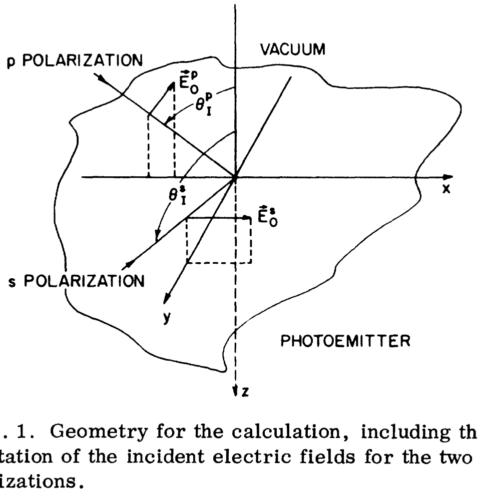

FIG. 1. Geometry for the calculation, including the orientation of the incident electric fields for the two polarizations.

The Drude absorptance is a second-order process involving photon absorption (with essentially no momentum transfer) and scattering (wherein large momentum transfer can occur), the two parts of the process occurring in either order. An expression for G', the net probability of absorbing a photon per unit time for the Drude process, has been given by Dumke,[24] and our treatment will be based on this expression. Dumke has assumed that the scattering process is essentially elastic[25] and his expression for G' includes the factor $W_{\vec{k}\vec{k}'}$, the probability per unit time for scattering between states characterized by wave vectors $\vec{k}$ and $\vec{k}'$. We will consider here isotropic scattering and take $W_{\vec{k}\vec{k}'}$ to be the constant W, independent of $\vec{k}$ and $\vec{k}'$. It is worthwhile noting that, while we will do the calculation for the electron gas, our results may have considerable generality since Dumke[24] has shown that effects associated with higher bands tend to cancel in the free-carrier absorption. It need hardly be added that there will be no energy gaps in our theory and consequently effects thereof will not appear herein.

We will now develop an expression for dA_η/dz, which includes G'. To do this, we think of a nonabsorbing medium of (real) dielectric function ϵ_1, which is rendered absorbing, in a perturbative sense, through the consequences of G'. We consider incident light of amplitude $\vec{E}_0^\eta$ ($\eta=s,p$; see Fig. 1) giving rise to an electric field $\vec{E}_\eta(z)$ within the photoemitter. The energy density we write then formally as $\epsilon_1|\vec{E}_\eta(z)|^2/4\pi$, even if $\epsilon_1<0$ as it would be for $\omega<\omega_p$. The number of photons absorbed per unit volume per unit time will then be $G'\epsilon_1|\vec{E}_\eta(z)|^2/4\pi\hbar\omega$. Now we note that G' contains a factor $1/\epsilon_1$, which is the only manifestation of the optics in the expression. Defining

$$G=\epsilon_1 G' \tag{2.4}$$

and writing the incident photon flux as $c|\vec{E}_0^\eta|^2\cos\theta_I^\eta/4\pi\hbar\omega$, we have

$$\frac{dA_\eta}{dz}=\frac{G|\vec{E}_\eta(z)|^2}{c\cos\theta_I^\eta|\vec{E}_0^\eta|^2}, \tag{2.5}$$

an expression appropriate for all frequencies.

To appreciate the role of G in this expression, we return to the standard local theory. In this case, the energy absorbed per unit area per unit time is $\mathrm{Re}(\vec{J}_\eta \cdot \vec{E}_\eta^*)$, where $\vec{J}_\eta(z)$ is the current density resulting from the field $\vec{E}_\eta(z)$. Since we are here proceeding locally, $\vec{J}_\eta = \sigma \vec{E}_\eta$, with the conductivity σ given by

$$\epsilon = 1 + 4\pi i \sigma/\omega .$$

The energy absorbed per unit volume per unit time is $(\mathrm{Re}\sigma)\,|\vec{E}_\eta(z)|^2$ and the incident energy flux is $c\,|\vec{E}_0^\eta|^2 \cos\theta_I^\eta/4\pi$ so $G = 4\pi\,\mathrm{Re}\sigma = \omega\epsilon_2$. We have written the complex dielectric function as $\epsilon = \epsilon_1 + i\epsilon_2$. The proportionality of G to ϵ_2 is the expected result since it is the real part of σ which represents photon absorption processes.

Before giving explicit expressions for dA_η/dz, we note a point of procedure. There are several ways to proceed, but the one which includes the highest degree of self-consistency is to consider henceforth the dielectric function for the electron gas to be

$$\epsilon = 1 - \Omega^{-2} + iG/\omega \tag{2.6}$$

and use this expression whenever ϵ appears. Thus we will, in calculating G, be obtaining an effective γ which we will denote γ_{eff}. One alternative procedure, necessary at very low frequencies, would be to view G as a means for calculating γ_{eff} which would then be used in Eq. (2.3). This would, however, require changes in the expression for G obtained by Dumke since he has not included line broadening, which means his expression is valid only if $\omega\tau_{\mathrm{eff}} \gg 1$ ($\tau_{\mathrm{eff}} = 1/\gamma_{\mathrm{eff}}\,\omega_p$). For the frequencies of interest in photoemission, this restriction is not of serious concern.

For s polarization, the local electric field in the photoemitter is

$$\vec{E}_s(z) = \frac{2\cos\theta_I^s\, e^{i\beta z} E_0^s}{\cos\theta_I^s + (\epsilon - \sin^2\theta_I^s)^{1/2}}\,\hat{x} \equiv \kappa_s e^{i\beta z} E_0^s \hat{x} , \tag{2.7}$$

where $\hat{x}$ is a unit vector in the x direction and

$$\beta = (\omega/c)(\epsilon - \sin^2\theta_I^\eta)^{1/2} . \tag{2.8}$$

So,

$$\frac{dA_s}{dz} = G\,|\kappa_s|^2 e^{-\alpha z}/c\cos\theta_I^s , \tag{2.9}$$

with α given by Eq. (2.2), but now ϵ is that of (2.6).

Proceeding within the three-step photoemission model, we introduce the escape length ξ which we take to depend only on ω, a point we will comment on further below. The yield of photoelectrons reaching the surface will then be

$$Y_s' = \frac{1}{2}\int_0^\infty \frac{dA_s}{dz} e^{-z/\xi}\, dz = \frac{G\,|\kappa_s|^2}{2c\cos\theta_I^s}\,\frac{\xi}{1+\alpha\xi} . \tag{2.10}$$

Conversion of this expression to an external photoyield will be made below.

Turning now to p polarization, the electric field in the photoemitter is

$$\begin{aligned}\vec{E}_p(z) &= \frac{2\cos\theta_I^p\, e^{i\beta z} E_0^p}{\epsilon\cos\theta_I^p + (\epsilon - \sin^2\theta_I^p)^{1/2}}\\ &\quad\times[(\epsilon - \sin^2\theta_I^p)^{1/2}\hat{x} - \sin\theta_I^p \hat{z}]\\ &\equiv E_0^p e^{i\beta z}(\kappa_{px}\hat{x} + \kappa_{pz}\hat{z}) ,\end{aligned} \tag{2.11}$$

with $\hat{z}$ a unit vector in the z direction. Thus,

$$\frac{dA_p}{dz} = \frac{Ge^{-\alpha z}}{c\cos\theta_I^p}(|\kappa_{px}|^2 + |\kappa_{pz}|^2) \tag{2.12}$$

and

$$Y_p' = \frac{G}{2c\cos\theta_I^p}(|\kappa_{px}|^2 + |\kappa_{pz}|^2)\,\frac{\xi}{1+\alpha\xi} . \tag{2.13}$$

There is a complication for p polarization, which will be addressed below.

III. PHOTOYIELD FOR s POLARIZATION

The expression for G, if we retain a specific polarization, is [see Eq. (20) of Ref. 24]

$$\begin{aligned}G = \frac{4\pi e^2 W}{\hbar\omega^3}\iint &[(\vec{v} - \vec{v}')\circ\hat{a}]^2 (f - f')\\ &\times\delta(E - E' + \hbar\omega)\frac{d^3k\, d^3k'}{(2\pi)^6} ,\end{aligned} \tag{3.1}$$

where W is the probability per unit time for elastic scattering (discussed above), $\hat{a}$ is a unit vector in the direction of the vector potential (or the electric field), and the states prior to photon absorption have velocity $\vec{v}$, energy E, Fermi function f, and wave vector $\vec{k}$. The primed quantities refer to the final states. We are interested in parabolic bands so we have $E = \hbar^2 k^2/2m$ and $d^3k = \frac{1}{2}(2m/\hbar^2)^{3/2}\sqrt{E}\, dE\, d\Omega$, where $d\Omega$ is the solid angle element specifying the direction of motion of the electrons in their initial states. With corresponding expressions for the final states, we have

$$\begin{aligned}G = \frac{4e^2 W}{\hbar\omega^3}\left(\frac{m}{\hbar^2}\right)^3 \frac{1}{(2\pi)^5}\\ \times\iint [(\vec{v} - \vec{v}')\cdot\hat{a}]^2 (f - f')\,\delta(E - E' + \hbar\omega)\\ \times\sqrt{E}\sqrt{E}'\, dE\, dE'\, d\Omega\, d\Omega' .\end{aligned} \tag{3.2}$$

Since the electric field here is directed in the x direction $[(\vec{v} - \vec{v}')\cdot\hat{a}]^2 = v_x^2 - 2v_x v_x' + v_x'^2$. Introducing a polar coordinate system with θ, the polar angle, measured from the outwardly directed normal to the surface and ϕ, the azimuthal angle, measured from the x axis (see Fig. 1), this can be written

$$v^2\sin^2\theta\cos^2\phi - 2vv'\sin\theta\sin\theta'\cos\phi\cos\phi' + v'^2\sin^2\theta'\cos^2\phi',$$

with primed (unprimed) angles referring to final (initial) states. We now do the integrals over the energy and the solid angle of the initial states, with the result that

$$G=\tfrac{4}{3}(e^2m^2W/\pi^3\omega^3\hbar^7)I \tag{3.3a}$$

and

$$I=\iint\left(\frac{E'-\hbar\omega}{4\pi}+\frac{3E'}{4\pi}\sin^2\theta'\cos^2\phi'\right)\times(E'-\hbar\omega)^{1/2}\sqrt{E'}\,dE'\,d\Omega'. \tag{3.3b}$$

We must keep in mind the Pauli-principle restrictions.

To get the lifetime into this expression, we introduce the usual expression for the relaxation time for momentum transfer,

$$\frac{1}{\tau_{E_2}}=\int W\delta(E_1-E_2)\left(1-\frac{\vec{v}_1\cdot\vec{v}_2}{v^2}\right)\frac{d^3k_1}{(2\pi)^3},$$

which can be immediately integrated to give

$$\frac{1}{\tau_{E_2}}=\frac{W\sqrt{E_2}}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}, \tag{3.4}$$

thereby providing a relation between τ_{E_2} and W. We will specialize this expression to τ at the Fermi energy τ_F,

$$\frac{1}{\tau_F}=\frac{W\sqrt{E_F}}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}, \tag{3.5}$$

with E_F the Fermi energy. Thus

$$G=\frac{8}{3}\frac{e^2}{\omega^3\hbar^4\pi}\left(\frac{m}{2}\right)^{1/2}\frac{1}{\tau_F\sqrt{E_F}}I. \tag{3.6}$$

We define

$$T=(1/E_F^2\hbar\omega)I \tag{3.7}$$

a dimensionless quantity, so

$$G=(\omega_p^2T/2\omega^2\tau_F), \tag{3.8}$$

with $\omega_p^2=4\pi ne^2/m$, n the electron density.

Let us now digress briefly from our photoemission direction and look at the optical absorption. To do so, we need only integrate T over all final states, recognizing that this is not the procedure which we will follow when we resume the photoemission discussion. Doing the solid angle integral gives

$$T=\frac{1}{E_F^2\hbar\omega}\int^{E_F+\hbar\omega}(2E'-\hbar\omega)(E'-\hbar\omega)^{1/2}\sqrt{E'}\,dE', \tag{3.9}$$

with the lower integration limit

$$E_F \text{ if } \hbar\omega<E_F,$$
$$\hbar\omega \text{ if } \hbar\omega>E_F.$$

Thus

$$T=\tfrac{2}{3}(E_F/\hbar\omega)\times\begin{cases}(1+\hbar\omega/E_F)^{3/2}, & \hbar\omega>E_F\\ (1+\hbar\omega/E_F)^{3/2}-(1-\hbar\omega/E_F)^{3/2}, & \hbar\omega<E_F.\end{cases} \tag{3.10}$$

In the ordinary local theory $\omega\epsilon_2=\omega_p^2/\omega^2\tau$ or $T_{\text{loc}}=2$, independent of frequency. For $\hbar\omega\ll E_F$, we find from (3.10) $T=2$. Thus the two results are in exact accord at low frequencies. However, T is not frequency independent, as we show in Fig. 2, where we have plotted T for a free-electron density of sodium so $E_F=3.26$ eV and $\hbar\omega_p=6.07$ eV. For $\Omega\sim1$, T is up to 13% less than 2 corresponding to an increase in the effective lifetime. The associated modification in the absorption is also illustrated in Fig. 2. We have calculated the absorptance from the present theory as follows. From Eq. (3.8) we see that

$$\gamma_{\text{eff}}=\tfrac{1}{2}\gamma T, \tag{3.11}$$

where we have taken τ as introduced in Eq. (2.3)

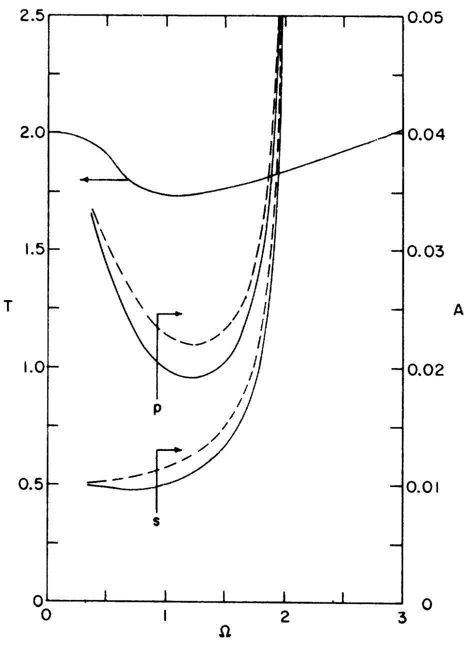

FIG. 2. T and the absorptance A as a function of frequency for an electron gas with $E_F=3.26$ eV. Absorptances have been calculated for both p and s polarizations with $\theta_I=60°$. Dashed absorptance curves were obtained from the standard local theory using ϵ of Eq. (2.3) with $\gamma=10^{-2}$. Full absorptance curves were obtained from the present theory with γ of (2.3) replaced by γ_{eff}, Eq. (3.11), and taking $\gamma=10^{-2}$.

to be τ_F. The calculations in Fig. 2 were made[26] with $\gamma = 10^{-2}$. We conclude this digression by emphasizing the disparity between the Drude theory as presented here and the "usual" Drude theory embodied in the free-electron dielectric function with damping.

We resume the photoemission discussion from Eqs. (2.10) and (3.8). The appearance of angular factors in T [see Eqs. (3.3)] means that the final-electron states are not distributed isotropically, a fact which has significant consequences. These anisotropies are a matrix element effect [that is, the factor $(\vec{v} - \vec{v}') \cdot \hat{a}$] and indicate that the number of final-state electrons moving in various directions differs. It is important to note that this does not indicate a correlation between E' and $d\Omega'$. Accordingly, we can use the standard specular escape condition, that is, an electron will escape if $E' \cos^2\theta' \geq E_F + \Phi$, where Φ is the work function. Thus our external photoyield Y_s is[27]

$$Y_s = \frac{|\kappa_s|^2}{c\cos\theta_I^s}\,\frac{\xi}{1+\alpha\xi}\,\frac{\omega_p^3\gamma}{2\omega^2}\,\frac{1}{E_F^2\hbar\omega} \times \int_\zeta^{E_F+\hbar\omega} dE' \int_0^{2\pi} d\phi' \int_0^{\cos^{-1}[(E_F+\Phi)/E']^{1/2}} \sin\theta'\, d\theta' \left(\frac{E'-\hbar\omega}{4\pi} + \frac{3E'}{4\pi}\sin^2\theta'\cos^2\phi'\right)(E'-\hbar\omega)^{1/2}\sqrt{E'}\,, \tag{3.12}$$

with the lower limit of the energy integration equal to

$$\zeta = \begin{cases} E_F + \hbar\omega, & \hbar\omega < \Phi \\ E_F + \Phi, & \Phi < \hbar\omega < E_F + \Phi \\ \hbar\omega, & \hbar\omega > E_F + \Phi\,. \end{cases} \tag{3.13}$$

Equation (3.12) is written in terms of the angles inside the photoemitter. If we are interested in energy-resolved angular distributions, it is necessary to rewrite Y_s in terms of the external polar angle θ_0. This can be readily accomplished with the result

$$Y_s = \frac{|\kappa_s|^2}{c\cos\theta_I^s}\,\frac{\xi}{1+\alpha\xi}\,\frac{\omega_p^3\gamma}{2\omega^2}\,\frac{1}{E_F^2\hbar\omega} \times \int_\zeta^{E_F+\hbar\omega} dE' \int_0^{2\pi} d\phi' \int_0^{\pi/2} d\theta_0 \left\{\frac{E'-(E_F+\Phi)}{E'}\sin\theta_0\cos\theta_0 \Big/ \left(1 - \frac{E'-(E_F+\Phi)}{E'}\sin^2\theta_0\right)^{1/2}\right\} \times \left(\frac{E'-\hbar\omega}{4\pi} + \frac{3}{4\pi}[E'-(E_F+\Phi)]\sin^2\theta_0\cos^2\phi'\right)(E'-\hbar\omega)^{1/2}\sqrt{E'}\,. \tag{3.14}$$

If we want only the energy distribution, it is simpler to obtain the result from (3.12):

$$Y_s = \frac{|\kappa_s|^2}{c\cos\theta_I^s}\,\frac{\xi}{1+\alpha\xi}\,\frac{\omega_p^3\gamma}{2\omega^2}\,\frac{1}{E_F^2\hbar\omega} \times \int_\zeta^{E_F+\hbar\omega} dE'\,(E'-\hbar\omega)^{1/2}\sqrt{E'}\left\{\frac{1}{2}\left[1 - \left(\frac{E_F+\Phi}{E'}\right)^{1/2}\right](E'-\hbar\omega) + \tfrac{3}{4}E'\left[\frac{2}{3} - \left(\frac{E_F+\Phi}{E'}\right)^{1/2} + \frac{1}{3}\left(\frac{E_F+\Phi}{E'}\right)^{3/2}\right]\right\}\,. \tag{3.15}$$

This expression can also be integrated to

$$Y_s = \frac{|\kappa_s|^2}{c\cos\theta_I^s}\,\frac{\xi}{1+\alpha\xi}\,\frac{\omega_p^3\gamma}{2\omega^2}\,\frac{1}{E_F^2\hbar\omega}\,I_s \tag{3.16}$$

with

$$I_s = \tfrac{1}{2}E_F^{3/2}\left[\tfrac{2}{3}(E_F+\hbar\omega)^{3/2} - (E_F+\Phi)^{1/2}(E_F+\hbar\omega) + \tfrac{1}{3}(E_F+\Phi)^{3/2}\right] \tag{3.17}$$

for $\hbar\omega > \Phi$.

Since dA_s/dz may be taken as a sum of a local and a nonlocal contribution,[28] the total s-polarized yield for the electron gas will be the sum of the two yields—the local as calculated here, and the nonlocal.[28] There is the possibility of interference and we will discuss this further below.

IV. PHOTOYIELD FOR p POLARIZATION

We must begin again with Eq. (3.2) recognizing that our velocity factor now is

$$|(\vec{v} - \vec{v}') \cdot \hat{a}|^2 = |(v_x - v_x')a_x + (v_z - v_z')a_z|^2\,, \tag{4.1}$$

with[29] [see Eq. (2.11)]

$$a_x = \frac{(\epsilon - \sin^2\theta_I)^{1/2}}{(|\epsilon - \sin^2\theta_I| + \sin^2\theta_I)^{1/2}} \tag{4.2}$$

and

$$a_z = \frac{-\sin\theta_I}{(|\epsilon - \sin^2\theta_I| + \sin^2\theta_I)^{1/2}}\,. \tag{4.3}$$

In expanding (4.1), we note that the next step will be an integral over the solid angle associated with the initial states. Hence, we only write those terms which will contribute following this integration and obtain

$$(v_x^2 + v_x'^2)|a_x|^2 + 2v_x'v_z' \operatorname{Re}(a_x a_z^*) + (v_z^2 + v_z'^2)|a_z|^2 \ . \tag{4.4}$$

Using the polar coordinates introduced in Sec. III, this becomes

$$\begin{aligned}(2/m)[&(E \sin^2\theta \cos^2\phi + E' \sin^2\theta' \cos^2\phi')b_x \\ &+ 2E' \cos\theta' \sin\theta' \cos\phi' b_c \\ &+ (E \cos^2\theta + E' \cos^2\theta')b_z] \ ,\end{aligned} \tag{4.5}$$

with

$$b_x = |a_x|^2 \ , \tag{4.6a}$$

$$b_z = |a_z|^2 \ , \tag{4.6b}$$

and

$$b_c = -\operatorname{Re}(a_x a_z^*) \ . \tag{4.6c}$$

We note the presence of the cross term (the one multiplying b_c), which will have important effects.

Since the procedure here is like that for s polarization, we will quote results. Defining M_p by

$$M_p = \frac{|\kappa_{px}|^2 + |\kappa_{pz}|^2}{c \cos\theta_I} \, \frac{\xi}{1 + \alpha\xi} \, \frac{\omega_p^3 \gamma}{2\omega^2} \, \frac{1}{E_F^2 \hbar\omega} \ , \tag{4.7}$$

the full energy-angular distribution in terms of the external polar angle is

$$\begin{aligned}Y_p = M_p \int_\zeta^{E_F + \hbar\omega} dE' \int_0^{2\pi} d\phi' \int_0^{\pi/2} d\theta_0 &\left\{ \frac{E' - (E_F + \Phi)}{E'} \sin\theta_0 \cos\theta_0 \Big/ \left(1 - \frac{E' - (E_F + \Phi)}{E'} \sin^2\theta_0\right)^{1/2} \right\} \\ &\times (D_x b_x + D_c b_c + D_z b_z)(E' - \hbar\omega)^{1/2} \sqrt{E'} \ ,\end{aligned} \tag{4.8}$$

where

$$D_x = (1/4\pi)\{E' - \hbar\omega + 3[E' - (E_F + \Phi)] \sin^2\theta_0 \cos^2\phi'\} \ , \tag{4.9a}$$

$$D_z = \frac{1}{4\pi}\left[E' - \hbar\omega + 3E'\left(1 - \frac{E' - (E_F + \Phi)}{E'} \sin^2\theta_0\right)\right] \ , \tag{4.9b}$$

and

$$\begin{aligned}D_c = \frac{6}{4\pi} E' \cos\phi' &\left(\frac{E' - (E_F + \Phi)}{E'}\right)^{1/2} \sin\theta_0 \\ &\times \left(1 - \frac{E' - (E_F + \Phi)}{E'} \sin^2\theta_0\right)^{1/2} \ .\end{aligned} \tag{4.9c}$$

If we want only the energy distribution, we can perform the integrals over θ_0 and ϕ' to get

$$Y_p = M_p \int_\zeta^{E_F + \hbar\omega} dE' \, (E' - \hbar\omega)^{1/2} \sqrt{E'} \, (Q_x b_x + Q_z b_z) \ , \tag{4.10}$$

where

$$Q_x = \tfrac{1}{2}(1 - s)(E' - \hbar\omega) + \tfrac{3}{4}E'(\tfrac{2}{3} - s + \tfrac{1}{3}s^3) \tag{4.11a}$$

and

$$Q_z = \tfrac{1}{2}(1 - s)(E' - \hbar\omega) + \tfrac{1}{2}E'(1 - s)^3 \ . \tag{4.11b}$$

We have defined

$$s = [(E_F + \Phi)/E']^{1/2} \ . \tag{4.12}$$

This expression can then be evaluated to obtain the yield as

$$Y_p = M_p(b_x I_s + b_z U) \ , \tag{4.13}$$

with

$$U = \begin{cases} 0, & \hbar\omega < \Phi \\ \tfrac{2}{3}E_F^{3/2}(E_F + \hbar\omega)^{3/2} - \tfrac{2}{5}(E_F + \Phi)E_F^{5/2} + \tfrac{2}{5}(E_F + \Phi)^{1/2}(E_F + \Phi - \hbar\omega)^{5/2} - \tfrac{2}{3}E_F^{3/2}(E_F + \Phi)^{3/2}, & \Phi < \hbar\omega < E_F + \Phi \\ \tfrac{2}{3}E_F^{3/2}(E_F + \hbar\omega)^{3/2} - \tfrac{2}{5}(E_F + \Phi)^{1/2}E_F^{5/2} - \tfrac{2}{3}(E_F + \Phi)^{3/2}E_F^{3/2}, & E_F + \Phi < \hbar\omega \end{cases} \tag{4.14}$$

and I_s given by Eq. (3.17).

Above we mentioned a complication for p polarization and we return to this point now. The problem is that in the frequency range where $\epsilon(\omega)$ is small but negative, $0.8 \lesssim \Omega < 1.0$, the total electric field in the surface region, as obtained from a nonlocal theory, is strongly suppressed due to a cancellation of the local z-direction transverse field by the longitudinal field.[19,20,30] This suppression affects both the nonlocal and local parts of the field and points up the fact that the approximation we are here using, namely, the additivity of the nonlocal and local parts of the photoyield, is never rigorously correct. However, the approximation is reasonable except in this region of small, negative ϵ, where it breaks down completely and the local part of the photoyield must be calculated as follows.[20,31] In Eq. (2.12), $|\kappa_{pz}|^2$

yield will then be

$$Y_p = \frac{1}{E_F^2 \hbar\omega}\,\frac{\omega_p^3 \gamma}{2\omega^2}\,\frac{1}{c\cos\theta_I} \times \int_0^\infty dz\, e^{-(\alpha+\xi^{-1})z}\left(|\kappa_{px}|^2 + |\kappa'_{pz}|^2\right) \times \int_\zeta^{E_F+\hbar\omega} dE'\,(E'-\hbar\omega)^{1/2}\sqrt{E'}\,(Q_x b'_x + Q_z b'_z)\ , \tag{4.19}$$

with the Q's given by Eqs. (4.11) and ζ by (3.13). As noted above, it is necessary to use the complicated expression (4.19) rather than (4.10) only for $0.8 \lesssim \Omega < 1.0$.

V. RESULTS AND DISCUSSION

We will illustrate the theory developed above using the previously given sodium parameters, a work function $\Phi = 2.3$ eV, $\gamma = 10^{-2}$, and an escape length $\xi = 10$ Å. Perhaps the most striking feature of the theory is the strong dependence of the photoyield on the field direction, a consequence of the matrix elements and the escape condition. This is illustrated in Figs. 3 and 4; the yields are shown in Fig. 3 for s-polarized light and in Fig. 4 for p-polarized light. Only a small field component normal to the surface is needed to increase the yield substantially. Results in Fig. 4 were obtained using Eq. (4.13) and thus do not include the effects of field suppresion occurring for $0.8 \lesssim \Omega < 1.0$. Results of a calculation including this effect are shown in Fig. 5 and demonstrate the import-

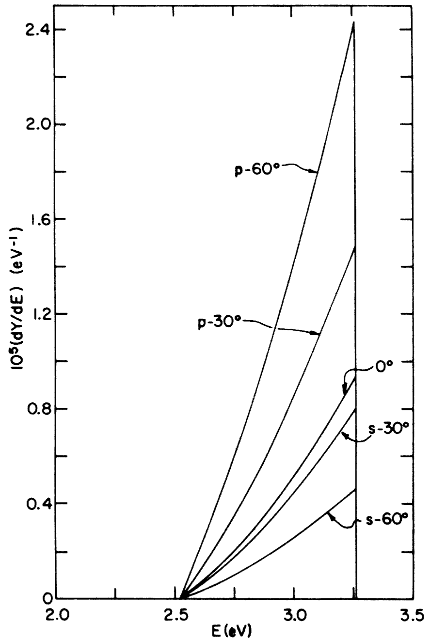

FIG. 7. Energy distribution curves for $\Omega = 0.5$ referred to initial electron states. The curves are labeled by the light polarization, s or p, and the angle of incidence.

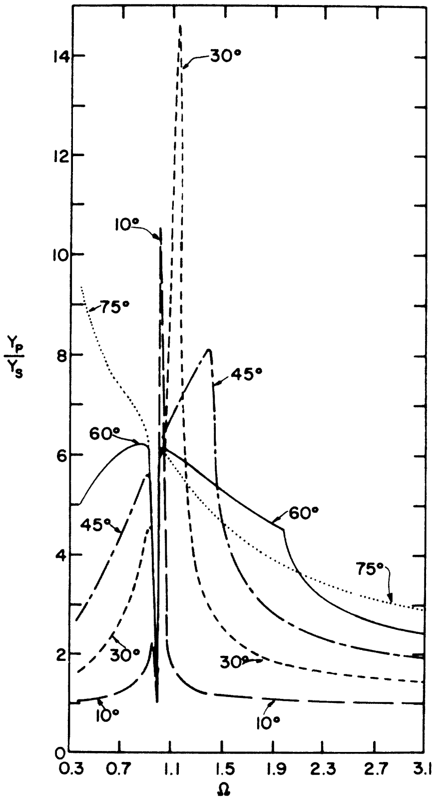

FIG. 6. Photoyield ratio Y_p/Y_s for the incident angles noted on the curves. The yields Y_p were calculated using Eq. (4.19).

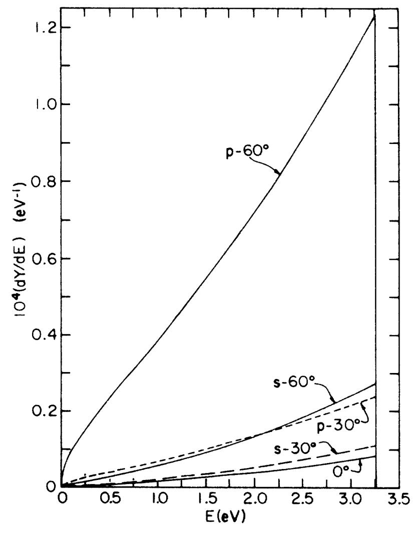

FIG. 8. Energy distribution curves for $\Omega = 1.5$ referred to initial electron states. The curves are labeled by the light polarization, s or p, and the angle of incidence.

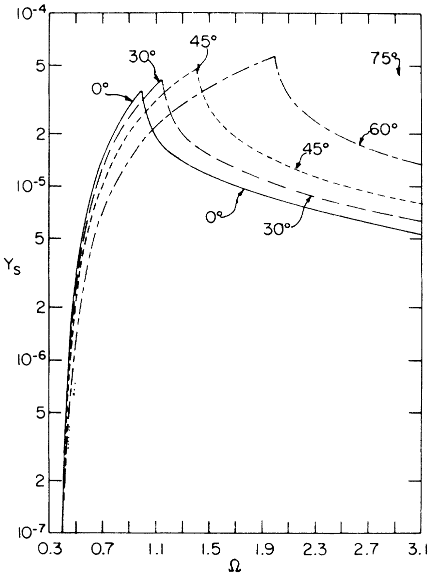

FIG. 3. Photoyields for s-polarized light as obtained from Eq. (3.16). The curves are labeled by the angle of incidence of the light.

must be replaced by $|\kappa_{pz}'|^2$,

$$|\kappa_{pz}'|^2 = |\kappa_{pz}|^2 f(z) , \tag{4.15}$$

where

$$f(z) = 1 - e^{-(q_s''+\beta''-\alpha)z} \times [\cos(q_s' - \beta')z + (\epsilon_1/\epsilon_2)\sin(q_s' - \beta')z] , \tag{4.16}$$

with $\epsilon = \epsilon_1 + i\epsilon_2$ given by Eq. (2.6), $\beta = \beta' + i\beta''$ by (2.8), and

$$q_s^2 = (q_s' + iq_s'')^2 = (5/3v_F^2)\{\omega_p^2\Omega^2[\Omega(\Omega + i\gamma_{\mathrm{eff}}) - 1]\} . \tag{4.17}$$

We must also replace b_x and b_z, Eqs. (4.6), by

$$b_x' = \frac{|\epsilon - \sin^2\theta_I|}{|\epsilon - \sin^2\theta_I| + (\sin^2\theta_I)f(z)} \tag{4.18a}$$

and

$$b_z' = \frac{f(z)\sin^2\theta_I}{|\epsilon - \sin^2\theta_I| + (\sin^2\theta_I)f(z)} . \tag{4.18b}$$

Note that b_x' and b_z' are functions of z. The photo-

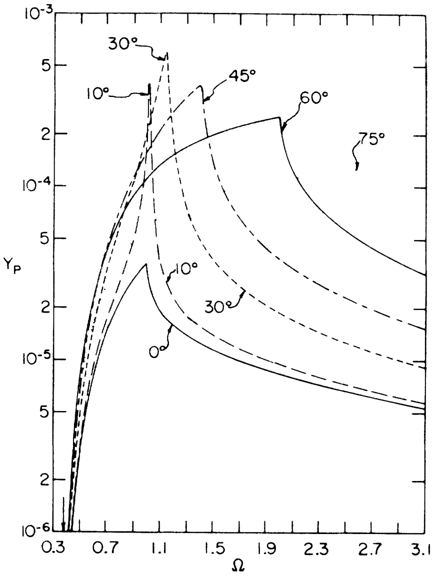

FIG. 4. Photoyields for p-polarized light as obtained from Eq. (4.13). The optics are treated locally for all frequencies and the yield suppression occurring for $0.8 \lesssim \Omega \lesssim 1.0$ is thus omitted. The curves are labeled by the angle of incidence of the light and the arrow along the abscissa indicates the photoyield cutoff frequency.

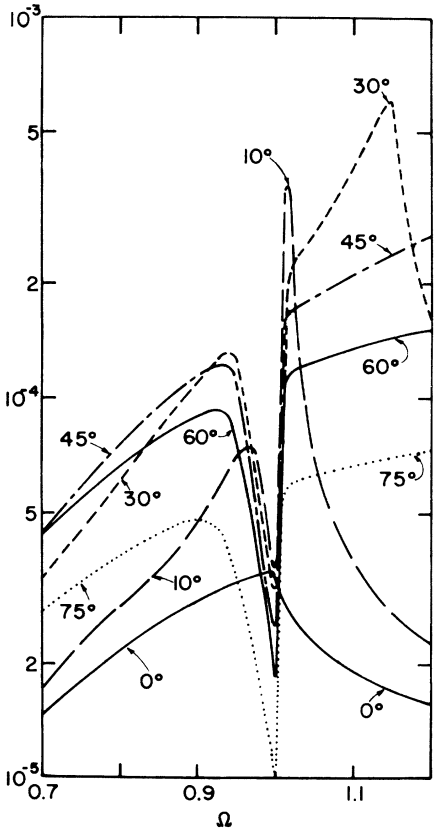

FIG. 5. Photoyields for p-polarized light as obtained from Eq. (4.19). The importance of including the local-field suppression in the region $0.8 \lesssim \Omega < 1.0$ is clearly indicated. The curves are labeled by the angle of indidence of the light.

ance of treating the surface-region field correctly. In Fig. 6 we show the ratios Y_p/Y_s for a variety of θ_I; the character of these ratios is seen to depend strongly on θ_I. We emphasize that these ratios are much larger than the corresponding absorptance ratios A_p/A_s, indicating the nonisotropic spatial distribution of the excited electrons.

Energy distributions are shown in Fig. 7 for $\Omega = 0.5$ and Fig. 8 for $\Omega = 1.5$. These distributions are essentially triangular, as is also the case for the surface photoyields.[20,28] Although we are here treating effects due solely to a finite electron lifetime, line broadening has not been included; that is why these curves drop off sharply at the Fermi energy.

Turning now to the angular distributions, we find very interesting asymmetries. For normally incident or s-polarized light (Fig. 9) the yield is a maximum in the field direction, but does not follow a $\cos^2\phi$ curve, that is, while the yield is smaller in the direction normal to the field than in the parallel direction, it does not go to zero. This behavior follows immediately from the velocity terms in the matrix elements [see the development between Eqs. (3.2) and (3.3)]. For p-polarized light, the azimuthal asymmetry is even more pronounced as is illustrated in Fig. 10. Now the yield is markedly higher in the "forward" direction than

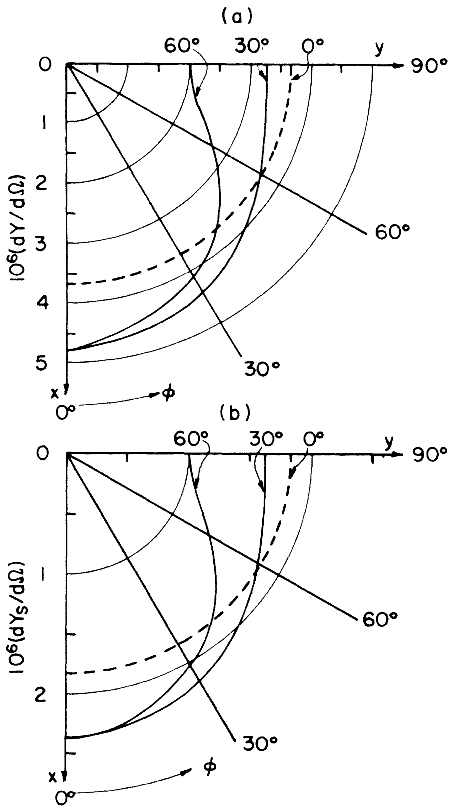

FIG. 9. Photoyield per unit solid angle as a function of detector orientation for $\Omega = 0.75$. The polar angle of the detector (measured from the surface normal) is noted along the y axis and the azimuthal angle ϕ is measured from the x axis which is the field direction. (a) Normally incident light; (b) s-polarized light with $\theta_I = 60°$.

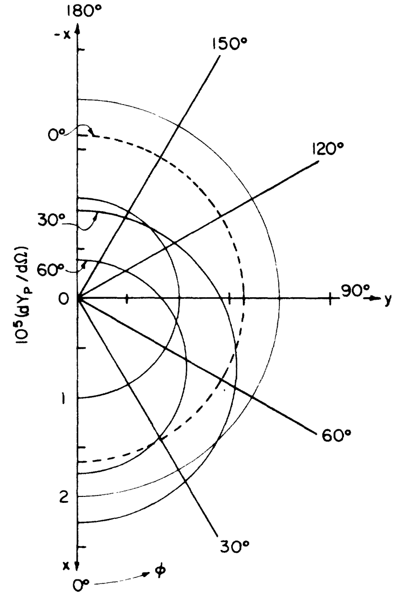

FIG. 10. Photoyield per unit solid angle as a function of detector orientation for p-polarized light with $\theta_I = 60°$ and $\Omega = 0.75$. The polar angle of the detector (measured from the surface normal) is noted along the $-x$ axis and the azimuthal angle ϕ is measured from the $+x$ axis, the incident direction of the light (see Fig. 1).

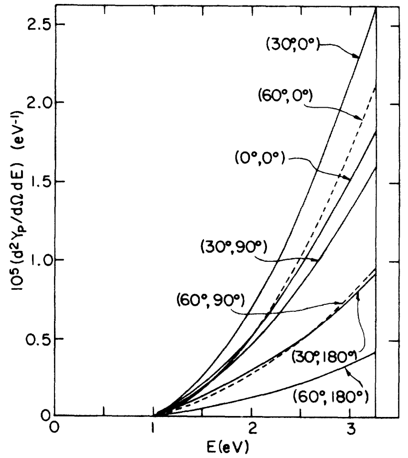

FIG. 11. Energy-resolved angular distribution curves for p-polarized light with $\Omega = 0.75$ incident at $\theta_I = 60°$. The numbers in parentheses are the polar and azimuthal detector angles measured as described in the caption of Fig. 10.

the "backward" direction due largely to the interference term emerging when the matrix element is squared. This interference term is the one including b_c in Eq. (4.8). Energy distribution curves for all electron emission angles are basically triangular. Most, however, are concave upward to some extent as is illustrated in Fig. 11.

In the expressions obtained above, we used an electron escape length ξ which we took to be a function of ω. Because we have generally given expressions where the angular and energy distributions are explicitly represented, it is easy to allow for ξ being a function of the final-state energy E' by inserting the factor $\exp[-z/\xi(E')]$ into the energy integrals before doing the z integration. This will, of course, require a numerical z integration. Similarly, the more elaborate escape approximation, wherein the escape factor is written $\exp[-z/\xi(E')\cos\theta']$ to allow for actual electron trajectories, can be used.

The question of additivity of local and nonlocal effects is a difficult one. It clearly is invalid for p-polarized light and $0.8 \lesssim \Omega < 1.0$. Aside from these conditions, we feel additivity is a reasonable approximation. Our reason is that the nonlocal effects, in general, are associated with the large-q components of the electric field while the Drude effects involve small-q components. There is, for frequencies not too low, a significant separation between the two; this shows up particularly clearly when the spatial distribution of the absorbed energy is Fourier analyzed.[20] Thus, the interference between the two should not be significant.

A different additivity question arises if we think about interjecting direct interband transitions into the picture. Although such absorption contributions involve the small-q part of the field, as is the case for the Drude absorption, the markedly different character of the two absorption processes suggests that additivity may be satisfied.

As is clear above, the yields scale roughly with the electron escape length and with $1/\tau_F$. This means that the effects of these parameters are easy to assess. However, a comparison of the experimental situation with the theory requires the inclusion of surface effects and optical constants differing from the free-electron values in the latter. We do feel that the combination of the Drude and surface effects does account for the roughly triangular energy distribution curves observed in many cases, with the Drude dominant for normally incident light. Detailed discussions for sodium and aluminum will be given elsewhere.

ACKNOWLEDGMENT

Much of this work was done while one of the authors (K. L. K.) was a guest at the Institut für Theoretische Physik of the Freie Universität, Berlin. He would like to thank the Institut members for their hospitality.

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*Work supported by the U. S. ERDA under contract No. W-7405-eng-82.

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[25] Note that this is also the assumption involved when one inserts τ in the local dielectric function.

[26] The calculation can be made two ways. The usual way is to use (3.11) in ϵ, evaluate the reflectance R, and then get A from $1-R$. An alternative for s polarization is to evaluate $2Y_s'$ from Eq. (2.10) with $\xi \to \infty$. There is, of course, a corresponding procedure for p polarization using Eq. (2.13).

[27] Note that the factor of 2 in the denominator of Eq.

(2.10) reflects a limit on the angular integral and must be removed when we specifically limit the angle as we are here doing.

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[29] All θ_I in this section are θ_I^p.

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[31] We emphasize that the expression "local" here means essentially "small q." Both transverse and longitudinal fields include small-q contributions (Refs. 19 and 20).