tool for investigating the size effect of electron conduction in conductors of varied cross-sectional geometries; thus, the method can also be extended to solve the galvanomagnetic size effect for the general case involving cylindrical and rectangular wires.

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†Present address: Milex Electronics Corp., Baldwin, New York.

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Plasmon Sidebands in Alkali Metals

J. Hermanson

Department of Physics, Montana State University, Bozeman, Montana 59715

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Recent experiments suggest the presence of plasmon sidebands in interband absorption spectra of the simple metals. A previous calculation of the sideband intensity considered plasmon emission in the *final* state, including interference corrections (charge cancellation of electron and hole). These reduce the plasmon intensity about 60%. Here previous work is extended in several directions: (1) allowance is made for plasmon effects in the initial state; (2) recoil and dispersion effects are included; and (3) the dependence of sideband intensity on initial electron momentum is explicitly considered. In this improved model charge cancellation reduces the sideband intensity by more than an order of magnitude. This reduction was first noticed by Brouers for the analogous case of soft-x-ray emission in simple metals. Plasmon-emission structure is almost two orders of magnitude weaker than interband absorption for Na, K, Rb, and Cs in the model considered here. These results are inconsistent with recent interpretations of pronounced satellite structure in the optical data of simple metals.

I. INTRODUCTION

Interband absorption in simple metals[1] is qualitatively understood in terms of one-electron theory.[2,3] Although electron-electron self-energies[4] and electron-hole interference terms[5–7] are large in a perturbation expansion, the net effect on optical conductivity is small in the interband region, [8] owing to the almost complete cancellation of electron and hole polarization fields. Recent experiments in the ultraviolet[9,10] are not explicable according to band theory, however. In these spectra significant structure appears in the energy region above the plasmon energy $\hbar\omega_p$, as a broader version of interband structure. Earlier calculations[11–14] have predicted strong absorption above $\omega = \omega_p$ in an electron gas by considering final states consisting of an *intraband* electron-hole pair and a plasmon. However, these results appear to be invalid, since the Hamiltonian used commutes with the momentum operator, and the optical conductivity must vanish to order (Fermi velocity/speed of light)^2.[15] In real solids the lattice provides a momentum sink due to the electron-ion interaction, and dynamic screening[15,16] leads to resonant absorption near ω_p for momentum transfer $\vec{k} < \vec{k}_c$, the cutoff wave vector for plasmons. This mechanism relies on disorder scattering and is inoperative in a perfect crystal at low temperature, since then $\vec{q}$ must be a reciprocal-lattice vector and is at least twice $\vec{k}_c$. Moreover, the observed structure has a peak near $\hbar\omega_p + E_G$, where E_G is the optical energy gap. This suggests an *interband* mechanism.

Lundqvist and Lydén[17] have calculated the interband optical conductivity for a nearly-free-electron gas including electron interaction effects to lowest order in the coupling to the density fluctuations.[4] The spectral function for an electron (hole) dis-

plays a satellite structure about $\hbar\omega_p$ above (below) the quasiparticle peak. This leads to sideband (SB) structure about a plasmon energy above E_G. Also, the interband absorbing power is *reduced* about 50% due to the transfer of oscillator strength into the plasmon replica. Several authors[5-7] have demonstrated that electron-hole interference effects, omitted in Ref. 17, *enhance* the absorption near the interband threshold by about 50%. Indeed, in a "conserving approximation" it has been shown that the cancellation between electron and hole self-energy clouds is nearly complete, [8] and the magnitude of interband absorption is accurately given by one-electron theory. A question thus arises: Do these interference effects sharply reduce the plasmon-emission intensity?

To answer this question I have employed the Bohm-Pines (BP) theory of collective behavior in the electron gas. By adding the electron-photon interaction and a weak electron-ion potential to the BP Hamiltonian, I have derived an optical conductivity for the SB which explicitly displays electron-hole cancellation in phase space. The theoretical conductivity, derived here may also be obtained from diagrammatic perturbation theory for the polarization operator, [18] to lowest order in dynamically screened exchange, if the energy-loss function $\mathrm{Im}\epsilon^{-1}(\vec{q}, \omega)$ is replaced by a δ function at the plasmon energy (see the discussion by Brouers and Longe[19] of the analogous soft-x-ray emission satellite). To obtain the plasmon sideband, three modifications of the interband polarization operator are included: (a) electron self-energy, (b) hole self-energy, and (c) plasmon exchange between electron and hole. In Ref. 17 the optical conductivity is calculated omitting the interference term based on a spectral function[4] which includes both plasmon and pair excitations in the final state. Equation (20) includes all three diagrams but omits pair excitations, which play an insignificant role in the sideband region. The chief virtue of the BP approach is its simplicity, which makes possible succinct physical interpretation. Like the dielectric formulation, the BP theory is a weak-coupling theory (interelectronic separation r_s not too large). The justification for omitting the subsidiary conditions stems from the essential agreement of this theory with the Green's-function approach in the SB; this agreement was first noticed in the soft-x-ray emission problem. [19-21]

The approach here emphasizes the role of the coupling between individual particle motions and collective oscillations in the final state of an interband transition. To lowest order in the electron-ion potential our model Hamiltonian is written as a sum of three terms (i) the BP Hamiltonian[22] for the electron gas (including collective coordinates for $k < k_c$), (ii) the Hamiltonian of the free electronmagnetic field, and (iii) the lattice-induced interaction between electrons and photons. In a previous calculation[23] I considered the *final* state interaction of an optically excited electron-hole pair with the plasmon field. If the electron originates at wave vector $\vec{p}$ inside the Fermi surface (FS), optical excitation to $\vec{p}-\vec{K}$ is followed by (i) plasmon emission by the *electron*, which goes into the state $\vec{p}-\vec{K}-\vec{k}$ outside the FS or (ii) plasmon emission by the hole, which makes a transition to the state $\vec{p}+\vec{k}$ inside the FS. The [110] reciprocal-lattice vector is denoted by $\vec{K}$ and $\vec{k}$ is the plasmon wave vector. Charge cancellation between electron and hole self-energy clouds reduces SB intensity by about 60% if electronic recoil energies and plasmon dispersion are omitted compared with $\hbar\omega_p = \hbar(4\pi ne^2/m)^{1/2}$.

In this paper I present results for the SB which include electron-plasmon interaction in the *initial* state, as well as the processes described in the last paragraph. Thus, the electron initially inside the FS can emit a plasmon of wave vector $\vec{k}$, going over to an intermediate state $\vec{p}-\vec{k}$ outside the FS; the umklapp transition to $\vec{p}-\vec{K}-\vec{k}$ follows. Formally, this process is a hole-plasmon interaction; thus we may lift the restriction on the corresponding phase space, $\vec{p}-\vec{k}$ inside the FS, used in Ref. 23. If p_F is the Fermi wave vector the exclusion principle now requires only $|\vec{p}| < p_F$, $|\vec{p}-\vec{K}-\vec{k}| > p_F$. Consequently, the electron and hole have identical phase spaces (in Ref. 23 the electron had larger phase space) and the SB intensity vanishes unless the second-order matrix elements for plasmon emission differ for the electron and hole. These matrix elements do in fact differ, since they involve electronic recoil energies. In the present calculation the inclusion of recoil is essential; otherwise vertex corrections reduce the SB intensity to zero. Recoil and plasmon dispersion are included here. The results are consistent with the work of Beeferman and Ehrenreich, [8] who demonstrated that electron-hole interference sharply reduces electron-electron interaction effects in interband absorption spectra of simple metals.

The model Hamiltonian is defined in Sec. II. In the usual way, the electron-plasmon interaction is eliminated to lowest order by a canonical transformation. The new quasiparticles are "dressed" electrons and holes, surrounded by polarization clouds (plasmon wave packets). Optical absorption is computed by transforming the electric dipole transition operator in the same way as the Hamiltonian. The new transition operator contains a term corresponding to the plasmon SB. Absorption intensities including vertex corrections are computed in Sec. III, followed by a brief discussion of the results and the optical absorption data near the plasmon frequency.

II. MODEL HAMILTONIAN

I introduce a simple model of an alkali metal containing electron-photon and electron-plasmon interactions, omitting the short-range ($k > k_c$) part of the electron-electron Coulomb interaction, and terms quadratic in plasmon operators [random-phase approximation (RPA)]. The long-range part of the Coulomb interaction is retained ($k < k_c$) leading to the existence of well-defined plasmons coupled to the Fermi sea of electrons by a linear interaction. This approach, due to BP,[22] succinctly isolates the essential physical content of many-body perturbation theory. As noted in the Introduction, the theoretical conductivity may also be derived by summing Feynman diagrams, for small r_s.

We begin with the electron gas Hamiltonian[22]

$$H_0=\sum_{\vec{p}} \epsilon(\vec{p})\, c^\dagger_{\vec{p}} c_{\vec{p}} + \tfrac{1}{2} \sum_{\vec{p}\vec{p}'\vec{k}\neq 0} U_{\vec{k}} (c^\dagger_{\vec{p}+\vec{k}}\, c^\dagger_{\vec{p}'-\vec{k}}\, c_{\vec{p}'}\, c_{\vec{p}} - N) , \tag{1}$$

where $\epsilon(\vec{p})=\hbar^2\vec{p}^{\,2}/2m$ is the free-electron dispersion, $U_{\vec{k}}=4\pi e^2/\vec{k}^{\,2}$ is the Fourier transform of the Coulomb interaction, and N is the number of valence electrons. The normalization volume has been taken as unity, and spin has been omitted. The $c^\dagger_{\vec{p}}$ and $c_{\vec{p}}$ are creation and destruction operators for an electron of wave vector $\vec{p}$. In the second term of (1), the electron-electron interaction, the $\vec{k}=0$ contribution is cancelled by the uniform background of positive charge.

To treat electromagnetic absorption, we must couple the electrons to a momentum sink, the lattice of positive ions. Corresponding to a vector $\vec{K}$ in the reciprocal lattice the interaction between electrons and photons is written as

$$H_I=-(e/mc)\,\vec{p}_{\rm eff}\cdot\vec{A} \tag{2}$$

in terms of the vector potential (transverse gauge)

$$\vec{A}=\sum_{\vec{q}\lambda} \vec{\eta}_{\vec{q}\lambda}\left(\frac{2\pi\hbar c^2}{\omega_{\vec{q}\lambda}}\right)^{1/2}(a_{\vec{q}\lambda}+a^\dagger_{-\vec{q}\lambda}) . \tag{3}$$

Here $a^\dagger_{\vec{q}\lambda}$ and $a_{\vec{q}\lambda}$ are creation and destruction operators for a photon of wave vector $\vec{q}$, polarization vector $\vec{\eta}_{\vec{q}\lambda}$, and frequency $\omega_{\vec{q}\lambda}$. The effective momentum operator for nearly free electrons is

$$\vec{p}_{\rm eff}=-\hbar\vec{K}\,V_{\vec{K}}\sum_{\vec{p}}[\epsilon(\vec{p}-\vec{K})-\epsilon(\vec{p})]^{-1}c^\dagger_{\vec{p}-\vec{K}}\,c_{\vec{p}} \tag{4}$$

to lowest order in $V_{\vec{K}}$, the Fourier transform of the optical pseudopotential[24] for momentum transfer $-\hbar\vec{K}$.

Since the photon wavelength is large compared with the lattice parameter, the plane-wave factor $\exp(i\vec{q}\cdot\vec{r})$ is omitted in (3). The normalization factor in this equation is such that the energy density $\langle\vec{E}^{\,2}+\vec{B}^{\,2}\rangle/8\pi=\hbar\omega_{\vec{q}\lambda}$ when there is one photon $(\vec{q}\lambda)$ in the unit normalization volume. The Hamiltonian for the EM field is

$$H_{\rm EM}=\sum_{\vec{q}\lambda}\hbar\omega_{\vec{q}\lambda}(a^\dagger_{\vec{q}\lambda}a_{\vec{q}\lambda}+\tfrac{1}{2}) . \tag{5}$$

Note that I do not include the effect of the ionic pseudopotential on the electron dispersion, but only on the wave function in lowest order (so that absorption of light is possible). Since for alkali metals the FS is very nearly spherical, and since allowed optical transitions are vertical in a reduced zone scheme, band-structure effects near the boundaries of the Brillouin zone (BZ) are unimportant here.

Following BP[22] I introduce field variables $Q_{\vec{k}}$ to explicitly describe the collective (plasmon) degrees of freedom in the electron gas. H_0 is then replaced by the model Hamiltonian

$$H_{\rm BP}=H_0+\tfrac{1}{2}\sum_{k<k_c}\Pi_{\vec{k}}\Pi_{-\vec{k}}-i\sum_{\vec{p}k<k_c}U^{1/2}_{\vec{k}}\,\Pi_{\vec{k}}\,c^\dagger_{\vec{p}-\vec{k}}\,c_{\vec{p}} \tag{6}$$

in terms of $\Pi_{\vec{k}}$, the momentum operator conjugate to $Q_{\vec{k}}$; k_c is the maximum wave vector for well-defined plasmons. The introduction of $k_c^3/6\pi^2$ new coordinates requires the same number of relations (the BP subsidiary conditions) for the wave function of the electronic system; these relations guarantee that (6) and (1) have the same eigenstates. I omit these relations, an omission ultimately justified—for small r_s—by the agreement of this theory with diagrammatic perturbation theory. The complete model Hamiltonian is

$$H=H_{\rm BP}+H_{\rm EM}+H_I . \tag{7}$$

To see that $H_{\rm BP}$ describes a system of coupled particles and fields, apply the first BP canonical transformation[22] generated by the operator

$$S_1=\sum_{\vec{p}k<k_c}U^{1/2}_{\vec{k}}\,Q_{\vec{k}}\,c^\dagger_{\vec{p}-\vec{k}}\,c_{\vec{p}} . \tag{8}$$

The transformed electron gas term

$$H^{(1)}_{\rm BP}=e^{-iS_1/\hbar}\,H_{\rm BP}\,e^{iS_1/\hbar}$$

contains terms corresponding to independent particles [of energy $\epsilon(\vec{p})$], free plasmons of energy $\hbar\omega_p$, and the desired linear electron-plasmon interaction

$$H_{\rm el\text{-}pl}=i\left(\frac{\hbar^3}{2\omega_p}\right)^{1/2}\sum_{\vec{p}k<k_c}U^{1/2}_{\vec{k}}\left(\frac{\vec{k}^{\,2}}{2m}-\frac{\vec{k}\cdot\vec{p}}{m}\right)\times c^\dagger_{\vec{p}-\vec{k}}\,c_{\vec{p}}\,(b^\dagger_{\vec{k}}+b_{-\vec{k}}) , \tag{9}$$

where the $b^\dagger_{\vec{k}}$ and $b_{\vec{k}}$, boson creation and destruction operators for the plasmon field, satisfy the relations

$$Q_{\vec{k}}=(\hbar/2\omega_p)^{1/2}(b_{\vec{k}}+b^\dagger_{-\vec{k}}) . \tag{10}$$

Also contained in $H^{(1)}_{\rm BP}$ are terms quadratic in plasmon operators and short-range electron-electron interaction; these terms are omitted for small r_s.

Optical excitation of a plasmon and an electron-hole pair by the absorption of a single photon may

be represented as a two-step process, generated by successive application of (a) the electron-photon interaction H_I, and (b) the electron-plasmon interaction $H_{\text{el-pl}}$. In diagrammatic language the photon creates an electron-hole pair in the metal; either the electron or the hole then emits a plasmon. In the present method we consider the interaction of the total charge density of the pair with the plasmon field. To do this we must first eliminate the electron-plasmon interaction to lowest order by a second BP canonical transformation[22] generated by the operator

$$S_2 = -i\frac{e\hbar}{m}\sum_{\vec{p}\,k<k_c}\left(\frac{2\pi\hbar}{\omega_{\vec{k}}}\right)^{1/2}\vec{k}\cdot(\vec{p}-\tfrac{1}{2}\vec{k})$$
$$\times[\hbar(\omega_{\vec{k}}+\hbar\vec{k}^2/2m-\hbar\vec{k}\cdot\vec{p}/m)]^{-1}\, b_{\vec{k}}\, c^{\dagger}_{\vec{p}+\vec{k}}\, c_{\vec{p}} + \text{H.c.} \quad (11)$$

In the new representation

$$H^{(2)}_{\text{BP}} = e^{-iS_2/\hbar}\, H^{(1)}_{\text{BP}}\, e^{iS_2/\hbar}$$

contains a term corresponding to independent particles of energy $\epsilon(\vec{p})$ and a free plasmon term with $\hbar\omega_p$ replaced by[22]

$$\hbar\omega_{\vec{k}} = \hbar\omega_p(1+3\hbar^2\vec{k}^2 p_F^2/10m^2\omega_p^2+\cdots)\,, \quad (12)$$

the plasmon dispersion in RPA. The quasiparticles are mixed states of the electron and plasmon fields in H_{BP}. As a result, the quasiparticle state vector

$$|\Psi_{\vec{p}}\rangle = e^{-iS_2/\hbar}\, e^{-iS_1/\hbar}\,|\psi_{\vec{p}};0\rangle\,, \quad (13)$$

where 0 denotes the plasmon vacuum, and $\psi_{\vec{p}}$, the wave function of a bare electron inside the FS, has a nonvanishing matrix element of the dipole operator $\vec{p}_{\text{eff}}$ with the electron-plasmon final state

$$|\Psi'_{\vec{p}-\vec{K}}\rangle = e^{-iS_2/\hbar}\, e^{-iS_1/\hbar}\,|\psi_{\vec{p}-\vec{K}-\vec{k}};1_{\vec{k}}\rangle\,, \quad (14)$$

where $|\vec{p}-\vec{K}-\vec{k}|\rangle p_F$, which *nominally* contains a single plasmon of wave vector $\vec{k}$. We now compute this matrix element.

III. SB INTENSITY

It is convenient to transform the electron-photon interaction twice, as we did H_{BP}. In the new "quasiparticle" representation we have

$$H'_I = e^{-iS_2/\hbar}\, e^{-iS_1/\hbar}\, H_I\, e^{iS_1/\hbar}\, e^{iS_2/\hbar}$$
$$= H_I + H_{\text{SB}} \quad (15)$$

to first order in plasmon operators. H_I produces the main band (MB) or interband absorption. The new term is

$$H_{\text{SB}} = +i(\pi)^{1/2}\frac{e}{m}\sum_{\vec{p}\vec{q}\lambda\,k<k_c}\hbar\left(\frac{U_{\vec{k}}\,\omega_{\vec{k}}}{\omega_{\vec{q}\lambda}}\right)^{1/2}\left(\frac{M(\vec{p})}{\hbar\omega_{\vec{k}}+\epsilon(\vec{p}-\vec{K}-\vec{k})-\epsilon(\vec{p}-\vec{K})}-\frac{M(\vec{p}-\vec{k})}{\hbar\omega_{\vec{k}}-\epsilon(\vec{p})+\epsilon(\vec{p}-\vec{k})}\right)$$
$$\times(a_{\vec{q}\lambda}+a^{\dagger}_{-\vec{q}\lambda})(b^{\dagger}_{\vec{k}}+b_{-\vec{k}})\, c^{\dagger}_{\vec{p}-\vec{K}-\vec{k}}\, c_{\vec{p}}\,, \quad (16)$$

where

$$M(\vec{p}) = -\hbar(\vec{K}\cdot\vec{\eta}_{\vec{q}\lambda})\, V_{\vec{K}}/[\epsilon(\vec{p}-\vec{K})-\epsilon(\vec{p})]$$

is the matrix element of $\vec{p}_{\text{eff}}\cdot\vec{\eta}_{\vec{q}\lambda}$ [see (4)]. It is evident that H_{SB} makes possible the event: photon → electron-hole pair + plasmon; thus the plasmon SB is generated by H_{SB}. The MB absorption is unchanged by electron-electron interaction in this lowest-order theory. In reality both the MB and SB intensities are renormalized by a Debye-Waller factor due to plasmon zero-point motion, in order to satisfy the f sum rule. To achieve this we would have to keep all terms in (15); doing so would not significantly affect the *relative* SB intensity.

Note that H_{SB} contains two matrix elements $U_{\vec{k}}^{1/2}$ and $V_{\vec{K}}$ and two energy denominators, corresponding to the fundamental interactions $H_{\text{el-pl}}$ and H_I. Charge cancellation is manifest in (16); if the dipole matrix elements are assumed constant, the SB transition amplitude depends essentially on the difference of recoil energies for the electron and hole, and vanishes if recoil is omitted. In Ref. 23 the hole term was restricted by the requirement $|\vec{p}-\vec{k}| < p_F$ for final-state interactions. In the present paper the electron can also emit a plasmon *before* interacting with the photon field, and the prior restriction is lifted. Here I assume $M(\vec{p}) \approx M(\vec{p}-\vec{k})$; only then can the phase-space integrations be handled analytically. Comparison of the results with those of Ref. 17 obtained by numerical integration lends support to this approximation, as discussed below. This simplifying assumption, the same as that of Brouers in the x-ray case,[19,20] also reflects a desire to emphasize the role of charge cancellation in reducing the SB intensity. The quantity

$$\left|\frac{1}{\hbar\omega_{\vec{k}}+\epsilon(\vec{p}-\vec{K}-\vec{k})-\epsilon(\vec{p}-\vec{K})}-\frac{1}{\hbar\omega_{\vec{k}}-\epsilon(\vec{p})+\epsilon(\vec{p}-\vec{k})}\right|^2$$

is essentially the dynamic form factor for the electron-hole pair; the square of the first (second) term is the form factor of the electron (hole), while the cross terms contain the interference effects sought.

The optical conductivity $\sigma_{\text{SB}}(\omega)$, corresponding to the event photon → electron-hole pair + plasmon is computed from the Golden Rule. For 1 photon per

unit volume, of frequency ω, the rate of absorption due to (16) is

$$\Gamma(\omega)=\frac{2\pi}{\hbar}\sum_{\vec{p}\vec{k}}|\langle\vec{p}-\vec{K}-\vec{k};1_{\vec{k}};0_{\vec{q}\lambda}|H_{SB}|\vec{p};0_{\vec{k}};1_{\vec{q}\lambda}\rangle|^2 \times\delta(\hbar\omega-\epsilon(\vec{p}-\vec{K}-\vec{k})+\epsilon(\vec{p})-\hbar\omega_{\vec{k}}) \quad (17)$$

in which $p<p_F$, $k<k_c$, and $|\vec{p}-\vec{K}-\vec{k}|>p_F$, using the occupation-number representation for the plasmon ($\vec{k}$) and photon ($\vec{q}\lambda$) fields; an electron at $\vec{p}$ is excited to $\vec{p}-\vec{K}-\vec{k}$. For cubic crystals we may, without loss of generality, take the photon polarization vector to lie along the direction of the x axis: $\vec{K}\cdot\vec{\eta}_{\vec{q}\lambda}=K_x$. Energy is conserved in the absorption event, according to the equation

$$\hbar\omega=\epsilon(\vec{p}-\vec{K}-\vec{k})-\epsilon(\vec{p})+\hbar\omega_{\vec{k}}\,. \quad (18)$$

Momentum is also conserved: $-\vec{K}=(\vec{p}-\vec{K}-\vec{k})-\vec{p}+\vec{k}$; the lattice supplies the momentum $-\hbar\vec{K}$, and the photon momentum is negligible. The power absorbed in the metal is

$$P=\sigma_{SB}(\omega)\langle\vec{E}^2\rangle\,, \quad (19)$$

where $\langle\vec{E}^2\rangle$ is the mean-square electric field in the state $|1_{\vec{q}\lambda}\rangle$. Equating (19) to $\Gamma(\omega)\hbar\omega$, and using the relation $\langle\vec{E}^2\rangle=4\pi\hbar\omega$ derived from (3), we have the result

$$\sigma_{SB}(\omega)=\frac{\pi e^2}{m^2\omega}\sum_{\vec{p}\vec{k}}'\frac{U_{\vec{k}}\hbar\omega_{\vec{k}}}{2}\left|\frac{M(\vec{p})}{\hbar\omega_{\vec{k}}+\epsilon(\vec{p}-\vec{K}-\vec{k})-\epsilon(\vec{p}-\vec{K})}-\frac{M(\vec{p}-\vec{k})}{\hbar\omega_{\vec{k}}-\epsilon(\vec{p})+\epsilon(\vec{p}-\vec{K}-\vec{k})}\right|^2 \times\delta(\hbar\omega-\epsilon(\vec{p}-\vec{K}-\vec{k})+\epsilon(\vec{p})-\hbar\omega_{\vec{k}})\,. \quad (20)$$

For comparison purposes I also compute $\sigma_{MB}(\omega)$, the optical conductivity in the one-electron approximation. The transition rate now involves the matrix element $\langle\vec{p}-\vec{K};\,0_{\vec{q}\lambda}|H_I|\vec{p};1_{\vec{q}\lambda}\rangle$, and energy conservation is written as $\hbar\omega=\epsilon(\vec{p}-\vec{K})-\epsilon(\vec{p})$. The result is

$$\sigma_{MB}(\omega)=\frac{\pi e^2}{m^2\omega}\sum_{p<p_F}|M(\vec{p})|^2\,\delta(\hbar\omega-\epsilon(\vec{p}-\vec{K})+\epsilon(\vec{p}))\,, \quad (21)$$

the well-known result for interband optical observation in a nearly-free-electron metal.[2] To obtain the total absorption one would sum over reciprocal-lattice vectors $\vec{K}$ and multiply by 2 to account for spin degeneracy, in Eqs. (20) and (21). Here we are interested in relative transition strength; the coupling constant for plasmon emission by either the electron or hole is given by

$$\gamma=\sum_{k<k_c}\frac{U_{\vec{k}}}{2\hbar\omega_p}=e^2k_c/\pi\hbar\omega_p=0.17r_s\,, \quad (22)$$

which is about unity for the alkali metals. As noted previously,[20,23] the BP approach leads to a theoretical conductivity which may be interpreted as a perturbation-theoretic result, with H_I and $H_{\text{el-pl}}$ the relevant interactions.

Now consider the contribution $I_{SB}(\vec{p})$ of an electron initially at $\vec{p}$, near the (110) BZ face, to the SB intensity. Integrating (20) over photon energy we have

$$I_{SB}(\vec{p})\approx\frac{\omega_{MB}}{\omega_{SB}}I_{MB}(\vec{p})\sum_{\vec{k}}'\frac{U_{\vec{k}}\hbar\omega_{\vec{k}}}{2}\times\left|\frac{1}{\hbar\omega_{\vec{k}}+\epsilon(\vec{p}-\vec{K}-\vec{k})-\epsilon(\vec{p}-\vec{K})}-\frac{1}{\hbar\omega_{\vec{k}}-\epsilon(\vec{p})+\epsilon(\vec{p}-\vec{k})}\right|^2 \quad (23)$$

in terms of the contribution of the same electron to the MB intensity

$$I_{MB}(\vec{p})=\frac{\pi e^2}{m^2}\,\frac{|M(\vec{p})|^2}{\epsilon(\vec{p}-\vec{K})-\epsilon(\vec{p})}\,. \quad (24)$$

The simplifying assumption $M(\vec{p})\approx M(\vec{p}-\vec{k})$ has been made in deriving (23), and $\omega_{MB}/\omega_{SB}=\epsilon_F/(\epsilon_F+\hbar\omega_p)$ is, approximately, the ratio of photon frequencies in the MB and the SB; the Fermi energy $\epsilon_F=\hbar^2p_F^2/2m$. The prime over the sum in (23) is a reminder to include only those final states of the electron which lie outside the FS: $|\vec{p}-\vec{K}-\vec{k}|>p_F$; we also require $k<k_c$.

To evaluate (23), first rewrite it in terms of the plasmon dispersion (12)

$$\hbar\omega_{\vec{k}}=\epsilon_F[\,\beta(2+\beta)+1.2\,\beta^{-1}(2+\beta)^{-1}x^2+\cdots\,]\,, \quad (25)$$

where $\beta=k_c/p_F$, $x=k/p_F$, and $\hbar\omega_p=\beta(2+\beta)\epsilon_F$. Then we have for $F(\vec{p})$, the relative SB intensity due to an electron at $\vec{p}$,

$$F(\vec{p})\equiv I_{SB}(\vec{p})/I_{MB}(\vec{p})=\gamma(1+\beta)^{-2}\left(\frac{2+\delta}{2+\beta}\right)^2 I(\beta)\,, \quad (26)$$

where $\delta p_F=K-2p_F=0.28\,p_F$, and the phase-space integral

$$I(\beta)=2\beta^{-3}\left(\int_0^y dx\int_{-1}^{+1}d\mu+\int_y^\beta dx\int_{-1}^{\mu(x)}d\mu\right)\times\frac{x^2\mu^2}{[(1-ax\mu+cx^2)(1+bx\mu+cx^2)]^2} \quad (27)$$

in terms of μ, the cosine of the angle between $\vec{k}$ and $\vec{K}$. Here

$$y=\delta+1-\vec{p}\cdot\vec{K}/p_FK \quad (28)$$

is the distance, in units of p_F, of the initial-state wave vector $\vec{p}$ from the (100) BZ face. Since $|\vec{p}|<p_F$, $y>\delta$. Now $|M(\vec{p})|^2\sim y^{-2}$, so we are mainly concerned with initial states near $\vec{p}_F\equiv p_F\vec{K}/K$ in (20) and (21). Thus, we may assume that the angle between $\vec{p}$ and $\vec{k}$ is approximately given by the an-

TABLE I. Relative intensity $F(\vec{p})$ of the plasmon SB due to an electron initially at $\vec{p}$. The distance of $\vec{p}$ from the BZ face is yp_F, $(1+\beta)^{-2}$ is, approximately, the ratio of the photon frequency in the main band and in the SB, and $F_0(\vec{p})$ is the relative intensity omitting charge cancellation. The latter reduces the intensity by more than an order of magnitude.

	y/δ	$(1+\beta)^{-2}$	$F_0(\vec{p})$	$F(\vec{p})$
Na	1.0	0.266	0.226	0.014
	1.5	0.266	0.237	0.016
	2.0	0.266	0.245	0.018
	3.0	0.266	0.263	0.020
K	1.0	0.238	0.243	0.013
	1.5	0.238	0.257	0.014
	2.0	0.238	0.264	0.016
	3.0	0.238	0.284	0.019
Rb	1.0	0.231	0.249	0.012
	1.5	0.231	0.263	0.014
	2.0	0.231	0.270	0.015
	3.0	0.231	0.290	0.018
Cs	1.0	0.222	0.256	0.012
	1.5	0.222	0.269	0.013
	2.0	0.222	0.278	0.014
	3.0	0.222	0.299	0.016

gle between $\vec{K}$ and $\vec{k}$, namely $\cos^{-1}\mu$. The factor $(1+\beta)^{-2}$ in (26) is the photon frequency ratio ω_{MB}/ω_{SB} introduced in (23). The recoil denominators in (27) involve

$$a = 2(1+y)(\epsilon_F/\hbar\omega_p) = 2(1+y)\,\beta^{-1}(2+\beta)^{-1},$$
$$b = 2(1+\delta-y)\,\beta^{-1}(2+\beta)^{-1}, \tag{29}$$
$$c = 2.2\beta^{-1}(2+\beta)^{-1}.$$

The term cx^2 contains the recoil energy, in units of $\hbar\omega_p$, of the electron or hole in their respective rest frames; $-ax\mu$ and $bx\mu$ are the corresponding Doppler shifts. The plasmon dispersion is also contained in cx^2. Finally, for $x>y$ the final states $\mu>\mu(x)$ are blocked by the FS, where

$$\mu(x) = (x^2+y^2+2y)/2(1+y). \tag{30}$$

The relative SB intensity (26) contains charge-cancellation effects. This is to be compared with the relative intensity $F_0(\vec{p})$ omitting interference. By leaving out the cross terms in (23) we find the result

$$F_0(\vec{p}) = F_{el}(\vec{p}) + F_{hole}(\vec{p}), \tag{31}$$

where

$$F_{el}(\vec{p}) = \gamma(1+\beta)^{-2} I_{el}(\vec{p}),$$
$$F_{hole}(\vec{p}) = \gamma(1+\beta)^{-2} I_{hole}(\vec{p}), \tag{32}$$

are the contributions to F_0 for an unscreened electron and hole, and

$$I_{el}(\vec{p}) = (1/2\beta)\left(\int_0^y dx \int_{-1}^{+1} d\mu + \int_y^\beta dx \int_{-1}^{\mu(x)}\right) \times d\mu[1 - ax\mu + cx^2]^{-2}. \tag{33}$$

The phase-space integral for the hole $I_{hole}(\beta)$ is obtained by the replacement $-ax\mu \to bx\mu$ in (33). To estimate $F_0(\vec{p})$ we omit recoil and dispersion and set $\mu(x)=1$, ignoring for the moment the exclusion-principle restriction in the final state. This leads to an upper bound for the intensity

$$F_0(\vec{p}) < 2\gamma(1+\beta)^{-2} \approx 0.4. \tag{34}$$

Here the electron and hole contributions are identical, and there is no interference. In establishing the upper bound I have used the fact that $ax\mu < cx^2$ over most of the region of integration.

It is convenient to expand the denominators in (27) and (33) in powers of the Doppler shifts. The expansion parameter is

$$\Delta = \tfrac{1}{2}(a+b)\beta\langle\mu^2\rangle^{1/2}/(1+c\beta^2)$$
$$= (\tfrac{1}{3})^{1/2}(2+\delta)/(2+3.2\beta) \approx 0.2. \tag{35}$$

Terms odd in Δ are sharply reduced by cancellation, since the region of integration is nearly symmetrical [as it would be were $\mu(x)$ set equal to unity]. The leading term, of order Δ^0, is nonvanishing in (27) and (33). By actual computation I have found that the leading term is within 10% of the exact result. For the present purpose, that of establishing the role of charge cancellation, the Doppler terms may be omitted altogether.

IV. DISCUSSION OF RESULTS

The relative intensity of the SB, Eq. (26), was computed for the alkali metals Na, K, Rb, and Cs. The results are given in Table I, together with results obtained by omitting charge cancellation. As explained above it is sufficient to omit the Doppler terms, which amount to a 10% correction; then the phase-space integrals (27) and (33) are standard. My primary interest is to emphasize the role of electron-hole interference, omitted in Ref. 17. The results for $F(\vec{p})$ and $F_0(\vec{p})$ are given for three values of yp_F, the distance of the initial-state wave vector $\vec{p}$ from the (100) BZ face. The dipole transition strength $|M(\vec{p})|^2 \sim y^{-2}$ and $y>\delta$. Both F and F_0 vary slowly with y and r_s. The factor $(1+\beta)^{-2}$ is the (approximate) ratio of the photon frequency in the MB and in the SB.

Although the electron-plasmon coupling constant (22) is about unity for the alkali metals, recoil and dispersion (the term cx^2 in the phase-space integrals), the frequency ratio $(1+\beta)^{-2}$, and the exclusion-principle restriction $|\vec{p}-\vec{K}-\vec{k}|>p_F$ combine to reduce the relative SB intensity F_0 to about 25%. This is consistent with the earlier calculations of Lundqvist and Lydén[17] who omitted inter-

ference; their numerical work did not include the several approximations contained in my work. The semiquantitative agreement of F_0 and the relative SB intensity in Ref. 17 supports the simplifying assumptions; namely, (i) $M(\vec{p}) \approx M(\vec{p}-\vec{k})$; (ii) Doppler shifts in plasmon emission may be omitted, and (iii) band splitting at the BZ edge is unimportant.

Electron-hole charge cancellation, contained in $F(\vec{p})$, reduces the SB intensity by more than an order of magnitude. Thus, as in the analogous x-ray-emission case,[20] the integrated SB intensity is only a few percent of the main band oscillator strength. This result is consistent with the conclusion of Beeferman and Ehrenreich[8] that electron-hole interference severely diminishes the observability of electron-electron interaction effects in the optical spectra of simple metals.

There remains the thorny question how to interpret the satellite structure in the absorption data of alkali metals.[9,10] The observed satellites have intensities about one order of magnitude greater than the computed plasmon SB intensity. Thus it is important to consider alternative mechanisms which can lead to absorption structure near the plasma frequency, such as dynamic screening[15,16] for small $k < k_c$. As mentioned in the Introduction, this intraband mechanism involves disorder scattering, due to phonons or impurities; specific calculations would be helpful. One expects the SB intensity and shape to depend sensitively on temperature or impurity content in this case. An acceptable mechanism for the SB must be capable of showing why the SB is so much stronger in Cs[10] than in Na and K[9].

In conclusion I have shown for a simple model of the alkali metals that electron-hole interference reduces plasmon SB intensity by more than an order of magnitude. These results are inconsistent with recent interpretations of pronounced satellite structure in the optical data of alkali metals.

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