High-Frequency Franz-Keldysh Effect

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Theoretical analysis of the electric-field perturbation of optical properties exhibited by a semiconductor in the spectral region near the energy gap is extended to the case of very high-frequency applied fields. The transition rate due to incident photons of energy $\hbar\Omega$ approximating the energy gap of the material is found to be modulated at a basic frequency of 2ω, where ω is the frequency of the applied field. Components of the current associated with these transitions have frequencies of $\Omega\pm 2n\omega$ and $(2n+1)\omega$. These may be regarded as sources for sidebands and harmonics of the applied radiations. The compatability of these results with both the low-frequency Franz-Keldysh effect and the two-photon absorption process is demonstrated; in addition, an example selected to lie in the intermediate range where neither of the latter explanations is appropriate is analyzed.

I. INTRODUCTION

THE theory of the Franz-Keldysh effect, i.e., the change in optical absorption due to the direct influence of a constant electric field upon the dynamics of an electron in a periodic solid, has been worked out by various authors[1–7] for a number of different cases. One expects that the absorption coefficient will vary according to the instantaneous electric field up to a very high frequency. However, deviations from the dc behavior might be expected when the frequencies of the applied field are comparable to the frequencies at which carriers traverse the Brillouin zone. At these higher frequencies, both the time average of the absorption coefficient and its time dependence will be different from those in the low-frequency limit. As is known from the low-frequency limit, a beam of light transmitted through a sample on which an ac electric field is applied will be amplitude modulated because of the time variation of the absorption coefficient. A Fourier analysis of such a beam shows that in addition to the main frequency there are sideband frequencies. The sideband frequencies are important when the frequency of the applied field is very high, since they can be easily separated from one another and from the main beam.

The object of this work was to evaluate the transition rate of electrons and the current associated with this transition (the latter generates the side bands and the harmonics) when the electric field is applied at very high frequencies.

The problem of electron ionization in solids by means of high-frequency electric fields is closely related to the high-frequency Franz-Keldysh effect. Keldysh[8] derived expressions for the time average of the ionization probability and gave qualitative arguments concerning the range of frequencies in which the ionization probability will follow the instantaneous electric field. The approach to the present problem is similar to the one used by Keldysh to approach the ionization problem. One starts with a time-dependent wave function which is a solution to the time-dependent Schrödinger equation with the high-frequency electromagnetic field of frequency ω (denoted here as the ω perturbation) included in the Hamiltonian. The transition rate between two such states due to an additional perturbation of frequency Ω (denoted as Ω perturbation) is then found. The basic difference between the two problems is in the magnitude of $\hbar\Omega$. In the electric-field ionization problem the Ω and the ω perturbations are identical and the single-photon energy is much smaller than the gap energy. On the other hand, $\hbar\omega$ in the high-frequency Franz-Keldysh effect may be as large or larger than the energy gap.

The Houston wave function[9] is an approximate time-dependent solution of the time-dependent Schrödinger equation in the presence of a dc electric field. This wave function could be easily modified for ac electromagnetic fields. However, its validity as an approximate solution for the purpose of evaluating the transition rate of electrons in the presence of the Ω perturbation is not clear *a priori*. Pantell *et al.*[10] have suggested a wave function which is an exact solution of the Schrödinger equation. This solution is in the form of a sum of modified Houston wave functions with coefficients which are to be found by solving a time differential equation. However, the form of these modified Houston wave functions is quite complicated and solutions for the coefficients are difficult to obtain.

In Sec. II a modified Houston wave function, which is simpler in form than the one suggested by Pantell *et al.*, is presented. The time-dependent wave function which is the solution of the time-dependent Schrödinger equation is expressed in terms of these functions and the

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coefficients are expressed in powers of the electric field of the ω perturbation. The upper limit of the photon energy, $\hbar\omega$, for which the modified Houston wave function itself is a sufficiently good approximation is discussed in the Appendix.

The discussion in this paper is restricted to $\hbar\omega$ below this limit, since for larger photon energies the results of Braunstein[11] and of Hopfield and Worlock[12] which treat two-photon processes are in most cases valid. On the other hand, the photon energy $\hbar\Omega$ is taken to be close in size to the gap energy but it can be either smaller or larger.

In Sec. III we obtain the general expressions for the transition rate of electrons from valence to conduction band, caused by the perturbation. The transition rate is found to be time-dependent and is expressed in the form of a Fourier series with the basic frequency of 2ω. In addition, an expression for the time-dependent electrical current associated with these transitions is obtained. These currents give rise to the generation of sideband frequencies of Ω and odd harmonics of ω. The expressions are obtained for both direct-allowed and phonon-assisted transitions. The limiting cases of low and high ω conclude Sec. III.

In Sec. IV we present the following numerical examples:

(a) The time average of the transition rate of electrons in the presence of an electric field at $\omega=6\pi\times10^{12}/\text{sec}$, as a function of $\hbar\Omega$, is compared to the transition rate in the presence of the same electric-field intensity when ω is small.

(b) The components of the electrical current at the frequency Ω and the first two sidebands is determined as a function of $\hbar\Omega$.

(c) The components of the electric current at the frequency ω and at the first odd harmonic are determined as functions of $\hbar\Omega$.

A summary of the results is presented in Sec. V.

II. THE WAVE FUNCTION

The time-dependent Schrödinger equation with the ω perturbation is given by

$$H_S\psi_L=i\hbar(\partial\psi/\partial t)\,, \tag{1a}$$

where

$$H_S=(\mathbf{P}-e\mathbf{A})^2/2m+V_p \tag{1b}$$

and

$$\mathbf{A}=A_0f(t)\mathbf{U}=A_0e^{bt}\mathbf{U}\cos\omega t. \tag{1c}$$

Here $\mathbf{P}$ is the momentum operator, $\mathbf{A}$ is the vector potential of the ω perturbation, and $\mathbf{U}$ is a unit vector. The exponential function $\exp bt$, $b>0$, has been introduced in order to allow the gradual application of the ω perturbation starting at $t\rightarrow-\infty$. The effect of the spatial dependence of $\mathbf{A}$ on the final results has been estimated and found negligible. $\mathbf{A}$ is therefore considered in the following discussions as independent of spatial coordinates. With this approximation the translational symmetry is preserved and ψ_L can be presented in the following form:

$$\psi_L=e^{i\mathbf{K}_0\cdot\mathbf{R}}\exp\left[-\frac{i}{\hbar}\int^t\epsilon_L\left(\mathbf{K}_0-\frac{e\mathbf{A}}{\hbar}\right)d\tau\right]\times\sum_l c_l^{(L)}(t)\varphi_l\left(\mathbf{K}_0-\frac{e\mathbf{A}}{\hbar}\right). \tag{2}$$

Here $\epsilon_L(\mathbf{K})$ is the Bloch energy in the Lth band. We now insert ψ_L in Eq. (1) and by using the relation[10]

$$H_S\varphi_l\left(\mathbf{K}_0-\frac{e\mathbf{A}}{\hbar}\right)e^{i\mathbf{K}_0\cdot\mathbf{R}}=\epsilon_l\left(\mathbf{K}_0-\frac{e\mathbf{A}}{\hbar}\right)\varphi_l\left(\mathbf{K}_0-\frac{e\mathbf{A}}{\hbar}\right)e^{i\mathbf{K}_0\cdot\mathbf{R}} \tag{3}$$

we obtain

$$[\epsilon_L(\mathbf{K}_0-e\mathbf{A}/\hbar)-\epsilon_l(\mathbf{K}_0-e\mathbf{A}/\hbar)+i\hbar d/dt]c_l^{(L)}(t)=-ieE_0(\sin\omega t)e^{bt}\textstyle\sum_\eta c_\eta\langle\varphi_l|\mathbf{U}\cdot\nabla_{K_0}|\varphi_\eta\rangle. \tag{4}$$

Since b will eventually be taken to the limit of zero, it has been neglected here in comparison to ω.

The function $\varphi_l(\mathbf{K})$ is defined only to within a phase factor. However, in our case multiplication of $\varphi_l(\mathbf{K})$ by $\exp i\boldsymbol{\gamma}\cdot\mathbf{K}$ will change the element $\langle\varphi_l|\mathbf{U}\cdot\nabla_K|\varphi_l\rangle$ thereby changing the coefficients $c_l^{(L)}(t)$ but not affecting the final expression for ψ_L. One therefore has a certain degree of freedom in choosing $\varphi_l(\mathbf{K})$ which might lead to convenient results for $c_l^{(L)}(t)$. We choose $\varphi_l(\mathbf{K})$ so that the following equation is satisfied:

$$\int\varphi_l^*(\mathbf{K})(\mathbf{U}\cdot\nabla_K)\varphi_l(\mathbf{K})dv=0. \tag{5}$$

The function $\varphi_l(\mathbf{K})$ is obtained from $\bar{\varphi}_l(\mathbf{K})$, which is the periodic part of a Bloch Function with arbitrarily selected phase in the following way:

$$\varphi_l(\mathbf{K})=\bar{\varphi}_l(\mathbf{K})\exp\int^{\mathbf{U}\cdot\mathbf{K}}\int\bar{\varphi}_l^*(\mathbf{K}_\perp+(\mathbf{U}\cdot\mathbf{K}')\mathbf{U})\times(\mathbf{U}\cdot\nabla_{K'})\bar{\varphi}_l(\mathbf{K}_\perp+(\mathbf{U}\cdot\mathbf{K}')\mathbf{U})dv\,d(\mathbf{U}\cdot\mathbf{K}'). \tag{6}$$

$\mathbf{K}_\perp$ is the component of $\mathbf{K}$ perpendicular to $\mathbf{U}$.

One observes that the exponent is purely imaginary and that $\varphi_l(\mathbf{K})$ obtained in this manner satisfies Eq. (5). As a result of this, the sum over η in Eq. (4) will not include $\eta=l$.

We now expand $c_l^{(L)}$ in powers of E_0;

$$c_l^{(L)}=\textstyle\sum_j d_{lj}^{(L)}E_0^j. \tag{7}$$

The coefficients $d_{lj}^{(L)}$ are found to satisfy a simple time-

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dependent differential equation. We choose as initial conditions the following relations:

$$\lim_{t\to-\infty} d_{lj}^{(L)}=\delta_{lL}\delta_{j0} \quad (8)$$

and obtain the solution for $d_{lj}^{(L)}$;

$$d_{lj}^{(L)}(t)=-\frac{e}{\hbar}\exp\left[\frac{i}{\hbar}\int^{t}(\epsilon_L-\epsilon_l)d\tau\right]\int_{-\infty}^{t}Q_{lj}^{(L)}(t')$$
$$\times\sin\omega t' e^{bt'}\exp\left[-\frac{i}{\hbar}\int^{t'}(\epsilon_L-\epsilon_l)d\tau\right]dt', \quad (9)$$

$$d_{l,0}^{(L)}(t)=\delta_{lL}, \quad (9')$$

where

$$Q_{lj}^{(L)}(t)=\sum_{\eta\neq l} d_{\eta,j-1}^{(L)}(t)$$
$$\times\left\langle\varphi_l\left(\mathbf{K}_0-\frac{e\mathbf{A}}{\hbar}\right)\middle|\mathbf{U}\cdot\nabla_K\middle|\varphi_\eta\left(\mathbf{K}_0-\frac{e\mathbf{A}}{\hbar}\right)\right\rangle. \quad (10)$$

One observes from Eqs. (9) and (10) that the coefficients $d_{lj}^{(L)}$ for which $j\hbar\omega$ is comparable to $\epsilon_L-\epsilon_l$ may become large as a result of the integration in t'. This is the phenomenon described by Keldysh as resonance and will not be discussed here. We thus consider the series of ψ_L as an asymptotic expansion and terminate it at a j value such that $j\hbar\omega<|\epsilon_L-\epsilon_{l'}|$, where l' is chosen such that $|\epsilon_L-\epsilon_{l'}|$ is the smallest of all such terms. For frequencies $\omega\ll|\epsilon_L-\epsilon_l|/jh$, Eq. (9) may be written in the form

$$d_{l,j}^{(L)}(t)=ieQ_{lj}^{(L)}(t)(\sin\omega t)/(\epsilon_l-\epsilon_L), \quad (11)$$

where b has been taken to zero after the integration with respect to t'. $Q_{lj}^{(L)}$ can also be simplified to the form

$$Q_{l,j}^{(L)}(t)=\frac{\hbar}{m}\sum_{\eta\neq l} d_{\eta,j-1}^{(L)}(t)$$
$$\times\frac{\left\langle\varphi_l\left(\mathbf{K}_0-\frac{e\mathbf{A}}{\hbar}\right)\middle|\mathbf{U}\cdot(\mathbf{P}+\hbar\mathbf{K}_0-e\mathbf{A})\middle|\varphi_\eta\left(\mathbf{K}_0-\frac{e\mathbf{A}}{\hbar}\right)\right\rangle}{\epsilon_\eta-\epsilon_l}. \quad (12)$$

Several properties of the wave function obtained here are worth mentioning: (a) Since the functions ψ_L are orthonormal for different values of L at $t\to-\infty$ they are orthonormal at any time. (b) An estimate of $d_{lj}^{(L)}$ shows that up to fields of 10^7 V/m, $d_{lj}^{(L)}E_0\ll d_{L0}^{(L)}=1$. Thus one would be tempted to neglect all terms for which $j>0$. However, this should not be done at this point because $d_{lj}^{(L)}$ is time-dependent and even though the actual value of $d_{l1}^{(L)}E_0$ is small, its relative contribution to the transition rate when the Ω perturbation is applied may in principle be appreciable, especially for large values of ω.

III. TRANSITION RATE AND THE GENERATION OF SIDEBANDS AND HARMONICS

We now introduce the Ω perturbation. The perturbed Hamiltonian is given by

$$H=H_S+H_1, \quad (13a)$$

where H_1 is given by

$$H_1=-e\mathbf{B}\cdot\mathbf{P}/m+e^2B^2/2m+e^2\mathbf{A}\cdot\mathbf{B}/m \quad (13b)$$

and

$$\mathbf{B}=B_0g(t)\mathbf{V}=B_0\cos\Omega t e^{b't}\mathbf{V}. \quad (13c)$$

$\mathbf{V}$ is the unit vector parallel to $\mathbf{B}$ and as in the case of $\mathbf{A}$, b' is a positive number which ultimately will be taken to the zero limit.

A wave function which is a solution of the time-dependent Schrödinger equation, with the Hamiltonian of Eq. (13), may be expressed as follows:

$$\psi=[(1+g_{11}+g_{12})\psi_1+(g_{21}+g_{22})\psi_2]$$
$$\times\exp\left[-\frac{i}{\hbar}\int^{t}\left(\frac{e^2B_0^2}{2m}+\frac{e^2\mathbf{AB}}{m}\right)d\tau\right]. \quad (14)$$

Here ψ_1 and ψ_2 correspond to the valence and conduction bands, respectively, and are given by Eq. (2). The first index of the coefficients g designates the band number and the second designates the power of B_0 to which it is proportional. In obtaining this wave function the spatial dependence of A and B has been neglected. The reason for including coefficients proportional to B_0^2 will become clear later.

The transition rate for a given value of $\mathbf{K}$ is given by Eq. (15).

$$T(\mathbf{K}_0)=\lim_{b'\to0}(\partial/\partial t)|g_{21}|^2. \quad (15)$$

Only the terms proportional to B_0^2 have been included in this equation.

The electric current produced by a single electron in the state ψ is given by

$$\mathbf{J}=\langle\psi|\frac{e}{m}(\mathbf{P}-e\mathbf{A}-e\mathbf{B})|\psi\rangle. \quad (16)$$

We split the current into three components:

$$\mathbf{J}_0(\mathbf{K}_0)=\lim_{b'\to0}\langle\psi_1|\frac{e}{m}(\mathbf{P}-e\mathbf{A}-e\mathbf{B})|\psi_1\rangle, \quad (17)$$

$$\mathbf{J}_L(\mathbf{K}_0)=\lim_{b'\to0}\left\{2\mathrm{Re}\left[g_{21}\langle\psi_1|\frac{e\mathbf{P}}{m}|\psi_2\rangle\right]+(g_{11}+g_{11}^*)\langle\psi_1|\frac{e\mathbf{P}}{m}|\psi_1\rangle\right\}, \quad (18)$$

$$\mathbf{J}_S(\mathbf{K}_0)=\lim_{b'\to0}(g_{12}\times g_{12}^*+|g_{11}|^2)\langle\psi_1|\frac{e\mathbf{P}}{m}|\psi_1\rangle+|g_{21}|^2\langle\psi_2|\frac{e\mathbf{P}}{m}|\psi_2\rangle+2\mathrm{Re}\left[(g_{11}^*g_{21}+g_{22})\times\langle\psi_1|(e\mathbf{P}/m)|\psi_2\rangle\right]. \quad (19)$$

$\mathbf{J}_0$ is of no interest to us since it is not associated with electron transitions. As one can easily see, $\mathbf{J}_L$ will be composed of currents of frequency $\Omega\pm n\omega$. Only terms to the first power of B_0 have been included in $\mathbf{J}_L$. One can easily see that g_{11} is pure imaginary. Thus $\mathbf{J}_L$ can be simplified to the form

$$\mathbf{J}_L = 2Re[g_{21}\langle\psi_1|(e\mathbf{P}/m)|\psi_2\rangle]. \quad (20)$$

The components of $\mathbf{J}_S$ have frequencies of $n\omega$ and the lowest power of B_0 to which they are proportional is 2. The last term in this expression is found to be small compared to the first two by a factor ω/Ω and will therefore be neglected. Using the normalization condition for ψ one finds

$$\mathbf{J}_S = |g_{21}|^2\left[\langle\psi_2|\frac{e\mathbf{P}}{m}|\psi_2\rangle - \langle\psi_1|\frac{e\mathbf{P}}{m}|\psi_1\rangle\right] = |g_{21}|^2(e/\bar{m}^*)(\hbar\mathbf{K}_0 - e\mathbf{A}). \quad (21)$$

We shall now evaluate the coefficient g_{21}. In the Appendix we show that if $n\hbar\omega$ (where n is the largest number of ω photons which significantly take part in the transitions from valence to conduction band) is small compared to the gap energy between the valence band and any other band, and also small compared to the gap energy between the conduction band and any other band, the wave functions ψ_1 and ψ_2 may be approximated by the expression given in Eq. (A8). Moreover, the time dependence of the periodic part of the wave function may be neglected. As stated in the Introduction, we restrict ourselves to this range of frequencies ω and in this case g_{21} is given by the following expression:

$$g_{21} = \frac{ieB_0}{2\hbar m}\langle\phi_2|\mathbf{V}\cdot\mathbf{P}|\phi_1\rangle \int_{-\infty}^{t} \times \exp\left[\frac{i}{\hbar}\int^{t'} \epsilon\left(\mathbf{K}_0 - \frac{e\mathbf{A}_0}{\hbar}\right)d\tau - i\Omega t' + b't'\right]dt', \quad (22a)$$

where

$$\phi_L = \varphi_L \exp i\mathbf{K}_0\cdot\mathbf{R} \quad (22b)$$

and

$$\epsilon(\mathbf{K}_0 - e\mathbf{A}/\hbar) = \epsilon_2(\mathbf{K}_0 - e\mathbf{A}/\hbar) - \epsilon_1(\mathbf{K}_0 - e\mathbf{A}/\hbar).$$

We now define a set of coordinates $K_{\shortparallel}$ and $\mathbf{K}_S$ which will be found useful later. We first define a surface S, which is the locus of all the points for which $\partial\epsilon/\partial(\mathbf{U}\cdot\mathbf{K}) = 0$. $\mathbf{K}_S$ are vectors from the origin to points on this surface. $K_{\shortparallel}$ measures the distance from any point to this surface in the direction $\mathbf{U}$. Thus any vector $\mathbf{K}$ may be expressed in the following form:

$$\mathbf{K} = \mathbf{K}_S + K_{\shortparallel}\mathbf{U}. \quad (23)$$

We employ the parabolic approximation for the dependence of ϵ on $\mathbf{K}$ and obtain

$$\int_0^t \epsilon\left(\mathbf{K}_0 - \frac{e\mathbf{A}}{\hbar}\right)d\tau = \bar{\epsilon}(\mathbf{K}_0)t + \hbar\theta_1\sin\omega t + \hbar\theta_2\sin 2\omega t, \quad (24a)$$

where

$$\bar{\epsilon}(\mathbf{K}_0) = \epsilon(\mathbf{K}_0) + e^2A_0^2/4\bar{m}^*, \quad (24b)$$

$$1/\bar{m}^* = \hbar^{-2}\,\partial^2\epsilon/\partial(\mathbf{U}\cdot\mathbf{K})^2, \quad (24c)$$

$$\theta_1 = -eA_0K_{\shortparallel 0}/\omega\bar{m}^*, \quad (24d)$$

and

$$\theta_2 = e^2A_0^2/8\hbar\omega\bar{m}^*. \quad (24e)$$

We now can expand the exponential function in g_{21} [Eq. (22a)] in Fourier series in the following form:

$$\exp\left[\frac{i}{\hbar}\int_0^t \epsilon\left(\mathbf{K}_0 - \frac{e\mathbf{A}}{\hbar}\right)d\tau\right] = \exp\left[\frac{i}{\hbar}\bar{\epsilon}t\right]\sum_l \epsilon_l \exp[-il\omega t], \quad (25)$$

where ϵ_l is given in terms of Bessel functions by

$$\epsilon_l = \sum_{m=-\infty}^{\infty} J_{l+2m}(-\theta_1)J_m(\theta_2). \quad (26)$$

The explicit forms of $T(\mathbf{K})$ and the currents can now be found;

$$T(\mathbf{K}_0) = T_0 \sum_{\xi=-\infty}^{\infty}\sum_{l=-\infty}^{\infty} \epsilon_l\epsilon_{l+\xi}\left[\delta\left(\frac{\epsilon-\gamma_l}{\hbar}\right)\cos\xi\omega t + \bar{\delta}\left(\frac{\epsilon-\gamma_l}{\hbar}\right)\sin\xi\omega t\right], \quad (27a)$$

where

$$T_0 = \frac{2\pi e^2B_0^2}{4\hbar^2m^2}|\langle\phi_2|\mathbf{V}\cdot\mathbf{P}|\phi_1\rangle|^2, \quad (27b)$$

$$\gamma_l = \hbar\Omega + l\hbar\omega - e^2A_0^2/4\bar{m}^*. \quad (27c)$$

δ is the usual Dirac delta function, and $\bar{\delta}$ is defined by

$$\bar{\delta}\left[\frac{\epsilon-\gamma_l}{\hbar}\right] = \frac{1}{2\pi}\lim_{b'\to 0}\frac{2(\epsilon-\gamma_l)/\hbar}{(\epsilon-\gamma_l)^2/\hbar^2 + b'^2}. \quad (28)$$

The current $J_{L\shortparallel}(\mathbf{K}_0)$ is given by

$$J_{L\shortparallel}(\mathbf{K}_0) = J_{0L}\sum_{\xi=-\infty}^{\infty}\sum_{l=-\infty}^{\infty}\epsilon_l\epsilon_{l+\xi}\left[\sin(\Omega-\xi\omega)t\,\delta\left(\frac{\epsilon-\gamma_l}{\hbar}\right) + \cos(\Omega-\xi\omega)t\,\bar{\delta}\left(\frac{\epsilon-\gamma_l}{\hbar}\right)\right], \quad (29a)$$

where

$$J_{0L} = \frac{2\pi e^2B_0}{2\hbar m^2}|\langle\phi_2|\mathbf{V}\cdot\mathbf{P}|\phi_1\rangle|^2, \quad (29b)$$

and the current $J_S(\mathbf{K}_0)$ is given by

$$\mathbf{J}_S(\mathbf{K}_0) = \langle J_{0S}\rangle\sum_{\xi=-\infty}^{\infty}\sum_{l=-\infty}^{\infty} \times\left(\epsilon_l\epsilon_{l+\xi}\frac{\hbar\mathbf{K}_0}{\xi} - \epsilon_l\epsilon_{l+\xi-1}\frac{e\mathbf{A}_0\cdot\mathbf{U}}{\xi-1} - \epsilon_l\epsilon_{l+\xi+1}\frac{e\mathbf{A}_0\cdot\mathbf{U}}{\xi+1}\right) \times\left[\sin\xi\omega t\,\delta\left(\frac{\epsilon-\gamma_l}{\hbar}\right) - \cos\xi\omega t\,\bar{\delta}\left(\frac{\epsilon-\gamma_l}{\hbar}\right)\right], \quad (30a)$$

where the tensor $\langle J_{0S}\rangle$ is given by

$$\langle J_{0S}\rangle=\frac{2\pi e^3B_0^2}{4\hbar^2m^2\omega}|\langle\phi_2|\mathbf{V}\cdot\mathbf{P}|\phi_1\rangle|^2\left\langle\frac{1}{m^*}\right\rangle. \quad (30b)$$

The sum in Eq. (30a) does not include the terms with vanishing denominator. The current component

$$\sum_{l=-\infty}^{\infty}\epsilon_l^2t\left\langle\frac{e}{\bar{m}^*}\right\rangle(\hbar\mathbf{K}_0-e\mathbf{A})$$

has not been included in the above expression, because $\sum_l\epsilon_l^2t$, the average rate of free carrier generation, is counterbalanced by an equal average rate of recombination, and the current of the associated carriers is of no interest in the present work since it just gives rise to free carrier reactance. This reactance will later be taken into account in the Maxwell equation which will serve for the evaluation of the different beams.

We can now evaluate the total transition rate

$$T=\frac{V}{4\pi^3}\int T(\mathbf{K}_0)d^3K_0. \quad (31)$$

We use the coordinates $\mathbf{K}_S$ and K_{II} previously defined. From Eq. (24d) one observes that $\theta_1(K_{\text{II}})=-\theta_1(-K_{\text{II}})$, whereas θ_2 is independent of K_{II}. It therefore follows from Eq. (26) that $\epsilon_l(-K_{\text{II}})=(-1)^l\epsilon_l(K_{\text{II}})$. As a result of this, when $T(\mathbf{K}_0)$ is integrated over K_{II} all the terms for which ξ is odd will vanish. We change the variable of the integration from K_{II} to ϵ and find

$$T=\frac{2VT_0m^{*1/2}}{4\pi^3}\sum_{\eta=-\infty}^{\infty}\int(\cos2\eta\omega t+\sin2\eta\omega t\,HL)$$
$$\times\sum_{l=l_0}^{\infty}\epsilon_l(K_{\text{II}l})\epsilon_{l+2\eta}(K_{\text{II}L})[2(\gamma_l-\epsilon_g)]^{-1/2}(d^2\mathbf{s}_K\cdot\mathbf{U}). \quad (32)$$

$d^2\mathbf{S}_K$ is a vector area element of the surface S, and l_0 is defined by

$$\gamma_{l0}>\epsilon_g>\gamma_{l0}-1, \quad (33)$$

and $K_{\text{II}l}$ is given by

$$\hbar K_{\text{II}l}=[2\bar{m}^*(\gamma_l-\epsilon_g)]^{1/2}. \quad (34)$$

We notice that the expression

$$\sum_{l=l_0}^{\infty}\epsilon_l(K_{\text{II}l})\epsilon_{l+2\eta}(K_{\text{II}l})[2(\gamma_l-\epsilon_g)]^{-1/2}$$

is a function of $\hbar\Omega$. Bearing this in mind the operator HL turns out to be just the Hilbert transform defined by

$$HL[F(\hbar\Omega)]=\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{F(\epsilon')}{\epsilon'-\hbar\Omega}d\epsilon'. \quad (35)$$

It is evident from Eq. (32) that the integral depends directly on ϵ_g alone. We can thus change variables of integration;

$$d^2\mathbf{S}_k\cdot\mathbf{U}=D(\epsilon_g)d\epsilon_g, \quad (36)$$

where

$$D(\epsilon_g)=\frac{2\pi}{\hbar^2}\frac{(m_1^*m_2^*m_3^*)^{1/2}}{\bar{m}^{*1/2}}, \quad \text{for } \epsilon_g>\epsilon_{g0} \quad (37a)$$

$$=0, \quad \text{for } \epsilon_g<\epsilon_{g0}. \quad (37b)$$

Therefore, the total transition rate may be written in the following form:

$$T=\frac{2VT_0\bar{m}^{*1/2}}{4\pi^3}\sum_{\eta=-\infty}^{\infty}(\cos2\eta\omega t+HL\sin2\eta\omega t)$$
$$\times\int_{\epsilon_{g_0}}^{\infty}\sum_{l=l_0}^{\infty}\epsilon_l(K_{\text{II}l})\epsilon_{l+2\eta}(K_{\text{II}l})$$
$$\times[2(\gamma_l-\epsilon_g)]^{-1/2}D(\epsilon_g)d\epsilon. \quad (38)$$

In a similar way, one obtains

$$J_{L\text{II}}=\frac{2J_{0L}V}{4\pi^3}\bar{m}^{*1/2}\sum_{\eta=-\infty}^{\infty}[\sin(\Omega-2\eta\omega)t$$
$$+HL\cos(\Omega-2\eta\omega)t]\int_{\epsilon_{g_0}}^{\infty}\sum_{l=l_0}^{\infty}\epsilon_l(K_{\text{II}l})\epsilon_{l+2\eta}(K_{\text{II}l})$$
$$\times[2(\gamma_l-\epsilon_g)]^{-1/2}D(\epsilon_g)d\epsilon_g \quad (39)$$

and

$$\mathbf{J}_S=\frac{2V\bar{m}^{*1/2}}{4\pi^3}\langle J_{0S}\rangle\mathbf{U}\sum_{\eta=-\infty}^{\infty}[\sin(2\eta+1)\omega t$$
$$-HL\cos(2\eta+1)\omega t]\int_{\epsilon_{g0}}^{\infty}\sum_{l=l_0}^{\infty}\left[\epsilon_l\epsilon_{l+2\eta+1}\frac{\hbar K_{\text{II}}}{2\eta+1}\right.$$
$$\left.-\epsilon_l\epsilon_{l+2\eta}\frac{eA_0}{2\eta}-\epsilon_l\epsilon_{l+2\eta+2}\frac{eA_0}{2\eta+2}\right][2(\gamma_l-\epsilon_g)]^{-1/2}$$
$$\times D(\epsilon_g)d\epsilon_g. \quad (40)$$

The results in Eqs. (38)–(40) were obtained for the case of direct allowed transitions between parabolic bands. The results for phonon-assisted transitions may be derived in a way very similar to the one just used. The transition rate in the case of phonon-assisted transitions is found to be different from that of direct allowed transitions in that the values of T_0 and γ_l are different and also in that $D(\epsilon_g)$ has a different functional dependence on ϵ_g. The transition rate for phonon-assisted transitions can be written in the following form:

$$T=c\sum_{\eta=-\infty}^{\infty}[\cos2\eta\omega t+HL\sin2\eta\omega t]\int_{\epsilon_{g_0}}^{\infty}\sum_{l=l_0}^{\infty}\epsilon_l(K_{\text{II}l})$$
$$\times\epsilon_{l+2\eta}(K_{\text{II}l})[2(\gamma_l-\epsilon_g)]^{-1/2}(\epsilon_g-\epsilon_{g_0})^{3/2}d\epsilon_g, \quad (41)$$

where

$$\gamma_l=\hbar\Omega\pm\hbar\omega_s+l\hbar\omega-e^2A_0^2/4\bar{m}^*. \quad (42)$$

The plus sign is for phonon absorption and the minus sign is for phonon emission. The coefficient C which contains the momentum matrix elements and the vibrational-perturbation matrix elements is independent of A_0 and may thus be evaluated for a given value of B_0 by comparing the value of T for $A_0=0$ with the results obtained for simple phonon-assisted transitions. From Eq. (41) the value of T for $A_0=0$ is found to be

$$\lim_{A_0\to 0} T=\frac{c}{\sqrt{2}}\frac{\Gamma(\frac{1}{2})\Gamma(\frac{5}{2})}{\Gamma(3)}(\hbar\Omega\pm\hbar\omega_s-\epsilon_{g_0})^2. \quad (43)$$

Similarly, J_{L11} for phonon-assisted transitions is found to be

$$J_{L11}=\frac{2c\hbar}{B_0}\sum_{\eta=-\infty}^{\infty}[\sin(\Omega-2\eta\omega)t+HL\cos(\Omega-2\eta\omega)t]\times\int_{\epsilon_{g_0}}^{\infty}\sum_{l=l_0}\epsilon_l(K_{11l})\epsilon_{l+2\eta}(K_{11l})\times[2(\gamma_l-\epsilon_g)]^{-1/2}(\epsilon_g-\epsilon_{g_0})^{3/2}d\epsilon_g \quad (44)$$

and $\mathbf{J}_S$ for phonon-assisted transition is given by

$$\mathbf{J}_S=c\frac{e}{m}\left\langle\frac{1}{\bar{m}^*}\right\rangle\mathbf{U}\sum_{\eta=-\infty}^{\infty}[\sin(2\eta+1)\omega t-HL\cos(2\eta+1)\omega t]\times\int_{\epsilon_{g_0}}^{\infty}\sum_{l=l_0}^{\infty}\left[\epsilon_l\epsilon_{l+2\eta+1}\frac{\hbar K_{11l}}{2\eta+1}-\epsilon_l\epsilon_{l+2\eta}\frac{eA_0}{2\eta}\epsilon_l\epsilon_{l+2\eta+2}\frac{eA_0}{2\eta+2}\right]\times[2(\gamma_l-\epsilon_g)]^{-1/2}(\epsilon_g-\epsilon_{g_0})^{3/2}d\epsilon_g. \quad (45)$$

The expressions for the transition rate in Eqs. (38) and (41) show that T is time-dependent with a basic frequency of twice the frequency of the ω perturbation. In the general case, unlike the low-frequency case, the transition rate T at any instant cannot be expressed as a function of the value of the electric field at that instant alone. Moreover T does not even obtain its extrema at the time that $|E|$ obtains it extrema. The current J_{L11} is observed to have a major component of frequency Ω and sidebands at $\Omega\pm2\eta\omega$. It should be noticed that the appearance of only those sidebands which are an even number times ω sway from the center frequency Ω is consistent with the fact that the dc Franz-Keldysh effect is even with respect to the electric field. The portion of the current at the frequency Ω is seen to have, in addition to a component in phase with the electric field of the Ω beam, a component which is out of phase, and the relation between the two components is given by the Hilbert transform. This is, of course, to be expected since the in-phase component corresponds to the imaginary part of the complex dielectric constant, and the out-of-phase component corresponds to the real part of the dielectric constant. The average power loss of the Ω beam which is found by averaging in time the expression $J_{L11}B_0\Omega\sin\Omega t$ is found to be related to T by the following simple relation:

$$P_L=T_{\text{ave}}\hbar\Omega, \quad (46)$$

which says that on the average, an Ω photon is absorbed for each electron that makes the transition from the valence to the conduction band.

In addition to a component at the frequency ω, $\mathbf{J}_S$ has components at frequencies which are odd multiples of ω. These currents generate odd harmonics of the ω beam. The average power loss of the ω beam for direct allowed transitions is given by

$$P_S=\frac{V\bar{m}^{*1/2}}{4\pi^3}T_0\frac{eA_0}{\bar{m}^*}\int_{\epsilon_{g_0}}^{\infty}\sum_{l=l_0}^{\infty}\left[\epsilon_l(\epsilon_{l-1}+\epsilon_{l+1})\hbar K_{11l}-\tfrac{1}{2}eA_0(\epsilon_{l-2}+\epsilon_{l+2})\right][2(\gamma_l-\epsilon_g)]^{-1/2}D(\epsilon_g)d\epsilon_g. \quad (47)$$

In general this power is not related in a simple way to the transition rate. However, a simple relationship exists in the case of two-phonon absorption. This will be discussed later.

The current $\mathbf{J}_L$ can be used together with Maxwell's equation to obtain the behavior of the Ω beam, i.e., its reflection and absorption, and the generation of the sidebands. Maxwell's equations in this case are

$$\text{rot}\,\mathbf{H}_\eta=i(\Omega+2\eta\omega)\mathcal{E}(\Omega+2\eta\omega)\mathbf{E}_\eta+[\mathbf{J}_{L\eta}-\mathbf{J}_{L\eta}(A_0=0)], \quad (48)$$

$$\text{rot}\,\mathbf{E}_\eta=-i(\Omega+2\eta\omega)\mu\mathbf{H}_\eta. \quad (49)$$

Here $J_{L\eta}$ denotes the component of the current with frequency $\Omega+2\eta\omega$ and $\mathcal{E}(\Omega+2\eta\omega)$ is the complex dielectric constant (including free carrier reactance) when $A_0=0$. In these equations we have assumed that the intensities of the sideband beams are small relative to the intensity of the original Ω beam. The solution of these equations will not be undertaken. A similar set of equations holds for the ω beam and its harmonics. The low-frequency limit of the expressions for T and J_{L11}, as given by Eqs. (38) and (39), respectively, has been worked out explicitly. It has been shown that if the conditions stated below are satisfied, T and J_{L11} will have a dc-like behavior. The conditions are

$$e^2A_0^2/2\bar{m}^*\gg\hbar\omega, \quad (50)$$

$$P_{11}\ll eA_0, \quad (51)$$

where P_{11} is defined by

$$\epsilon_{g_0}+P_{11}^2/2\bar{m}^*=\hbar\Omega. \quad (52)$$

By a dc-like behavior we mean that T is at any instant equal to the value which one would obtain if T is computed for a dc electric field equal in size to the electric field of the ω perturbation at that same instant. The current J_{L11} is also found to have dc-like behavior, giving rise to the amplitude modulation of the Ω beam. The proof of the result stated above will not be given here because of its complexity and because the results for dc have already been worked out in detail. The condition expressed in Eq. (50) provides for a given electric field E_0 a measure of the frequency ω for which a dc-like behavior is expected. This result is valid only if scattering can be neglected. If, however, ω is much smaller than $1/\tau$ (where τ is the mean free time) the transition rate and the current are expected to have a dc-like behavior, even if the above condition is not satisfied.

We shall now compare the transition rate as given by Eq. (38) for the case of two-photon absorption with those by Hopfield and Worlock (HW) and by Braunstein (B). At the frequency considered by HW and by B, $|\theta_1|\ll 1$ and $|\theta_2|\ll|\theta_1|$. Thus the average transition rate is found to be

$$T=\frac{\sqrt{2}Ve^2A_0^2T_0(m_1^*m_2^*m_3^*)^{1/2}}{3\pi^2(\hbar\omega)^2\bar{m}^*}(\hbar\Omega+\hbar\omega-\epsilon_{g0})^{3/2}, \tag{53}$$

which is equivalent to the result obtained by HW without electron-hole Coulomb interaction. As is well known, the result given by HW has been obtained by neglecting matrix elements involving intermediate states other than the initial and final states themselves, whereas the result of B was obtained by taking into account only matrix elements involving intermediate states other than the initial and final states. In principle, both types of terms should appear and the fact that the terms involving intermediate states other than initial and final states do not appear in our results is not suprising. This arises from the fact that the time dependence of $\varphi(\mathbf{K}-e\mathbf{A}/\hbar)$ and also the coefficients $d_{lj}^{(L)}$ for $j>0$ have been neglected. However, the terms involve the initial and final states as intermediate states dominate at frequencies such that $\hbar\omega\ll\epsilon_g$. Thus, in the domain where the results for T are valid, the expression for the two-photon process is equivalent to the one previously obtained. In the case of two-photon absorption one would expect that the average power loss of the ω beam would equal the product of the average transition rate and $\hbar\omega$. Using Eq. (47) and taking $l=1$, one finds that indeed

$$P_S=T_{\text{ave}}\hbar\omega. \tag{54}$$

IV. NUMERICAL EXAMPLE

In order to illustrate the consequences of the theory we present a numerical example in which the frequency and electric field of the ω perturbation have been chosen so that neither the dc nor the two-photon treatment is applicable.

If these parameters are chosen to violate the constraints of Eqs. (50) and (51) the dc treatment would not be satisfactory. If, in addition, one chooses $e^2A_0^2/2\bar{m}^*\cong\hbar\omega$ the conventional one- and two-photon descriptions would be inadequate because this choice assures the participation of terms involving ϵ_l with $|l|>1$. This condition is quite difficult to satisfy with presently available lasers, though one can achieve conditions which are quite close to it.

The transition rate and the currents given in Eqs. (36)–(40) can be expressed in the following form:

$$T=c_d\sum_{\eta=-\infty}^{\infty}[\cos 2\eta\omega t+HL\sin 2\eta\omega t]\times F_0\left(A_{\text{on}};\frac{\hbar\Omega-\epsilon_{g_0}}{\hbar\omega};\eta\right), \tag{55a}$$

where

$$c_d=\frac{VT_0(\hbar\omega)^{1/2}}{\pi^2\hbar^2}(m_1^*m_2^*m_3^*)^{1/2}, \tag{55b}$$

$$A_{\text{on}}=eA_0/(\hbar\omega\bar{m}^*)^{1/2}, \tag{55c}$$

$$J_{L11}=c_d\frac{2\hbar}{B_0}\sum_{\eta=-\infty}^{\infty}[\sin(\Omega-2\eta\omega t)+HL\cos(\Omega-2\eta\omega)t]\times F_0\left(A_{\text{on}};\frac{\hbar\Omega-\epsilon_{g_0}}{\hbar\omega};\eta\right) \tag{56}$$

$$\mathbf{J}_S=c_d\frac{e}{\omega}(\hbar\omega)^{1/2}\bar{m}^{*1/2}\left\langle\frac{1}{\bar{m}^*}\right\rangle\mathbf{U}\sum_{\eta=-\infty}^{\infty}\times[\sin(2\eta+1)\omega t-HL\cos(2\eta+1)\omega t]\times F_0\left(A_{\text{on}};\frac{\hbar\Omega-\epsilon_{g_0}}{\hbar\omega};\eta\right). \tag{57}$$

Thus in order to obtain a description of the transition rate and the currents as a function of $\hbar\Omega-\epsilon_{g_0}$ expressed in units of $\hbar\omega$, it is sufficient to specify A_{on} and η. We choose $A_{\text{on}}=1.26$. The values of the electric field, the frequency, and the effective mass for this case may be, for example, $E_0=4\times10^4$ V/cm, $f=3\times10^{12}$ cps, and $\bar{m}^*=0.1$ m. The time average of the change of the transition rate caused by the ω perturbation is shown in Fig. 1 as a function of the photon energy of the Ω perturbation. This is compared with the time average of change in the transition rate caused by an electric field $E_0=4\times10^4$ V/cm applied at a very low frequency. One observes that for Ω photon energies which are smaller than the minimum energy gap the difference between the two curves is quite small, whereas for Ω photon energies larger than the minimum energy gap the difference is substantial. This is mainly due to the fact that below the minimum gap Eq. (51) is only slightly violated, whereas it is strongly violated above the minimun gap.

The in-phase and out-of-phase components of the change in the current having frequency Ω caused by the ω perturbation are presented in Fig. 2.

In Figs. 3 and 4 we present the first sidebands of the current with frequencies $\Omega+2\omega$ and $\Omega-2\omega$. The two figures are the same except that they are shifted in energy by $2\hbar\omega$ with respect to each other. As one can easily verify from Eq. (39) and the equations defining

γ_l and $K_{\text{II}l}$, this result is a particular case of the more general rule

$$J_{L\text{II}}(\hbar\Omega,\eta)=J_{L\text{II}}(\hbar\Omega-2\eta\hbar\omega,\,-\eta). \tag{58}$$

The components of the current with frequency ω and 3ω are given in Fig. 5. One observes that the current with frequency ω does not go to zero for Ω photon energies larger than the minimum energy gap, even though the change in the transition rate does go to zero (see Fig. 1). The out-of-phase components could not be reliably calculated because an integration over a very wide energy range was necessary.

V. SUMMARY

In this work we have considered the transition rate of electrons from valence to conduction bands and the electrical currents associated with these transitions in the presence of two electromagnetic perturbations. The ω perturbation is very intense but with a photon energy small compared to the band-gap energy. (This is the high-frequency extension of the dc electric field in the Franz-Keldysh effect.) The second, the Ω perturbation, can be either weak or intense but its photon energy is close in size to the minimum energy gap.

We first obtained a time-dependent wave function which satisfies the time-dependent Schrödinger equation with the ω perturbation included. This wave function was expressed in terms of modified Houston wave functions with the coefficients expanded in powers of the electric field of the ω perturbation. The wave function in this form was not very useful for the evaluation of the transition rate in the presence of the Ω perturbation. However, it was shown that under certain restrictions imposed on the ω perturbation this wave function could be approximated by a single modified Houston wave function.

Next we obtained expressions for the transition rate in the presence of the Ω perturbation for both direct-

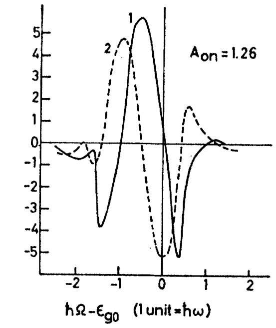

FIG. 3. The current components with frequency $\Omega+2\omega$ as a function of $\hbar\Omega-\epsilon_{g0}$. Curve 1: The amplitude of the current with time dependence of $\sin(\Omega+2\psi)t$ (one vertical unit $=0.02\ c_d\hbar/B_0$). Curve 2: The amplitude of the current with time dependence $\cos(\Omega+2\omega)t$ (one vertical unit $=0.02\ c_d\hbar/B_0$).

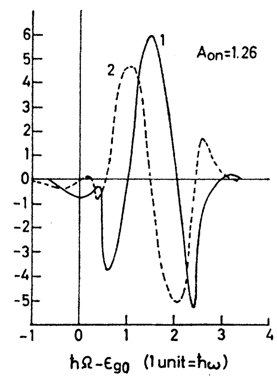

FIG. 4. The current component with frequency $\Omega-2\omega$ as a function of $\hbar\Omega-\epsilon_{g0}$. Curve 1: The amplitude of the current with time dependence of $\sin(\Omega-2\omega)t$ (one vertical unit $=0.02\ c_d\hbar/B_0$). Curve 2: The amplitude of the current with time dependence of $\cos(\Omega-2\omega)t$ (one vertical unit $=0.02\ c_d\hbar/B_0$).

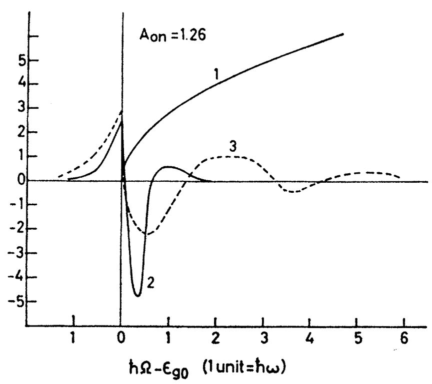

FIG. 1. The transition rate and change in transition rate as a function of $\hbar\Omega-\epsilon_{g0}$. Curve 1: The transition rate without the ω perturbation (1 vertical unit $=c_d$). Curve 2: The time average of the change in the transition rate caused by the ω perturbation (one vertical unit $=0.1\times c_d$). Curve 3: The time average of the change in the transition rate caused by an electric field $E_0=4\times10^4$ V/cm applied at very low frequency (one vertical unit $=0.1\ c_d$).

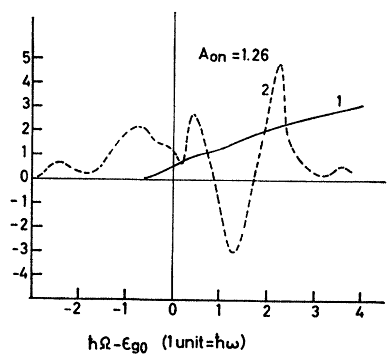

FIG. 5. The current components with frequencies ω and 3ω as a function of $\hbar\Omega-\epsilon_{g0}$. Curve 1: The amplitude of the current with time dependence of $\sin\omega t$ (one vertical unit $=c_de[(\hbar\omega)^{1/2}/\omega]\times\langle 1/\bar{m}^*\rangle\bar{m}^{*1/2}U$. Curve 2: The amplitude of the current with time dependence of $\sin 3\omega t$ (one vertical unit $=0.1c_de[(\hbar\omega)^{1/2}/\omega]\times\langle 1/\bar{m}^*\rangle\bar{m}^{*1/2}U$.

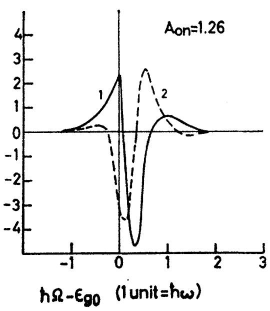

FIG. 2. The change in the current component with frequency Ω caused by the ω perturbation as a function of $\hbar\Omega-\epsilon_{g0}$. Curve 1: The amplitude of the current component with time dependence of $\sin\Omega t$ (one vertical unit $=0.2\ c_d\hbar/B_0$). Curve 2: The amplitude of the current component with time dependence of $\cos\Omega t$ (one vertical unit $=0.2\ c_d\hbar/B_0$).

allowed and phonon-assisted transitions. The results show that the transition rate is periodic in time, with the basic frequency being twice the frequency of the ω perturbation. In general the transition rate cannot be considered as depending on the instantateous intensity of the electric field as in the case of very low frequencies. Moreover, the extrema in the transition rate do not occur when the absolute value of the electric field obtains its extrema. The conditions under which a dc-like behavior is obtained were also presented.

At very high frequencies when $e^2A_0^2/2\bar{m}^* \ll \hbar\omega$ one finds that the general expressions lead to two-photon absorption, but the expression does not contain matrix elements with intermediate states other than the initial and final states. If the photon energy of the ω perturbation is small compared to the gap energy, the terms containing these matrix elements are negligible. When the above condition is not satisfied, the approximation of the time-dependent wave function by the modified Houston wave function is not valid. In this case the expressions for two-photon absorption given by Braunstein and by Hopfield and Worlock should be used.

In parallel with the evaluation of the transition rate, we obtained expressions for the electrical current associated with these transitions. We showed that the current contains components with the frequency Ω and sidebands $\Omega \pm 2\eta\omega$. This result is consistent with the dc Franz-Keldysh effect, which is an even effect in the electric field. In addition, there are components with frequency ω and its odd harmonics. Using the expressions for these currents in Maxwell's equations, one can calculate the generation of the sideband beams and the harmonics.

The results of the theory were illustrated by a numerical example in which $e^2A_0^2/2\bar{m}^* \cong \hbar\omega$. The change in the transition rate in this case was compared with the change in the transition rate when the same electric field is applied at a low frequency and was found to be considerably different. This was consistent with the fact that the condition for this example was chosen so as to violate the condition for a dc behavior. The size of the change in the transition rate and therefore the average change in the intensity of the Ω beam in leaving the crystal is under the conditions of this example large enough to be easily measured. This is true also if presently available lasers are used such as a CN laser with frequency 8.9×10^{11} cps and with peak power of 1 W. Graphs of the currents associated with these transitions as a function of the Ω photon energy were also calculated. Using these currents one can calculate the intensity of the side-band beams and the harmonics. Finding an optimal geometrical configuration and a material for the experimental observation and the calculation of the beam intensities for such a case were outside the scope of this work. However, rough estimates for favorable geometries and existing lasers indicate that the observation of the first sideband and the first odd harmonic should be quite easy.

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APPENDIX

The function ψ_L is expressed in Eq. (2) as a sum of modified Houston wave functions. At low ω one would expect a simple modified Houston wave function to be an excellent approximation for ψ_L. At high frequencies, however, the validity of this approximation is not clear *a priori*. In calculating the transition rate in the presence of the Ω perturbation, one expands ψ_L in a Fourier series with frequencies $\bar{\epsilon}/\hbar \pm \eta\omega$. We assume that terms with $\eta > n$ do not contribute significantly to the transition process. We shall show that ψ_L can, in fact, be approximated by a single modified Houston wave function if the following condition is satisfied:

$$n\hbar\omega \ll \Delta\epsilon_{\min}, \tag{A1}$$

where $\Delta\epsilon_{\min}$ is the smallest vertical energy gap between the L band being considered and any other band.

Each of the coefficients in the Fourier expansion can be expanded in powers of A_0. The lowest power of A_0 which appears in such a coefficient is η. Since the term with the lowest power of A_0 is also the largest, only the term with A_0^η in each coefficient will be retained. Therefore, we shall neglect any term in which A_0 appears with a power larger than n.

We rewrite Eq. (2) in the following form:

$$\psi_L = e^{i\mathbf{K}_0\mathbf{R}} \exp\left[-\frac{i}{\hbar}\int^t \epsilon_L\left(\mathbf{K}_0 - \frac{e\mathbf{A}_0}{\hbar}\right)d\tau\right]\sum_j \rho_j^{(L)}, \tag{A2}$$

where

$$\rho_j^{(L)} = \sum_l d_{lj}^{(L)} E_0^j \varphi_l\left(\mathbf{K}_0 - \frac{e\mathbf{A}}{\hbar}\right). \tag{A3}$$

$\rho_0^{(L)}$ can now be expanded in the form

$$\rho_0^{(L)} = \sum_{\eta=0}^{n}\left(-\frac{e}{\hbar}\right)^\eta \frac{1}{\eta!}(\mathbf{U}\nabla_{K_0})^\eta \varphi_L(\mathbf{K}_0) A_0^\eta f^\eta(t). \tag{A4}$$

Here terms with $\eta > n$ have been neglected, and $f^\eta(t)$ can be expressed in the form

$$f^\eta(t) = \cos^\eta t\, e^{\eta bt} = \frac{1}{2^\eta}\sum_{m=0}^{\eta}\binom{\eta}{m} e^{i(2m-\eta)\omega t} e^{\eta bt}. \tag{A5}$$

Similarly,

$$\rho_1^{(L)} \leq \sum_{\eta=1}^{n} \frac{\eta\hbar\omega}{i\Delta\epsilon_{\min}}\left(-\frac{e}{\hbar}\right)^\eta \frac{1}{\eta!}(\mathbf{U}\nabla_{K_0})^\eta \varphi_L(\mathbf{K}_0) A_0^\eta \times \sin\omega t\, e^{bt} f^{\eta-1}(t), \tag{A6}$$

and $\sin\omega t\, e^{bt} f^{\eta-1}(t)$ can be expressed in the form

$$\sin\omega t\, e^{bt} f^{\eta-1}(t) = \frac{1}{i^{2\eta}} \sum_{m=0}^{\eta} \frac{2m-\eta}{\eta} \binom{\eta}{m} e^{i(2m-\eta)\omega t} e^{\eta bt}. \quad \text{(A7)}$$

By comparison of terms $\rho_0^{(L)}$ and $\rho_1^{(L)}$ which have the same time dependence, one observes that if condition (A1) is satisfied, $\rho_1^{(L)}$ can be neglected and so can all the terms $\rho_j^{(L)}$ for which $j>0$. ψ_L can therefore be approximated by a single Houston wave function;

$$\psi_L \cong \varphi_L\left(\mathbf{K}_0 - \frac{e\mathbf{A}}{\hbar}\right) e^{i\mathbf{K}_0\mathbf{R}} \exp\left[-\frac{i}{\hbar}\int^t \epsilon_L\left(\mathbf{K}_0 - \frac{e\mathbf{A}}{\hbar}\right) d\tau\right]. \quad \text{(A8)}$$

One may also expand $\varphi_L(\mathbf{K}_0 - e\mathbf{A}/\hbar)$ and the exponential function in powers of A_0. Using similar arguments it can be shown that under condition (A1) $\varphi(\mathbf{K} - e\mathbf{A}/\hbar)$ can be considered independent of time.

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Transport Properties of Electrons in Inverted Silicon Surfaces

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Measurements of the effective mobility, field effect mobility, Hall mobility, and carrier density of Si as a function of field perpendicular to the surface are reported. At all temperatures from 4.2 to 300°K, at least one maximum in the mobility was observed. The temperature dependence is reported for different fields. At room temperature, a single maximum in the mobility was observed close to the threshold for inversion. As the temperature was lowered, this peak increased. At temperatures near 80°K, it then decreased. Another maximum appeared at about 100°K at higher fields; it increased as the temperature was lowered. An anomalous shift in the conductance threshold between 77.3 and 4.2°K is reported and is correlated with the charge in the oxide. Effects of substrate bias are reported. Some comments are made on possible scattering mechanisms. The effect of interface states was measured and their density near the conduction band is reported.

INTRODUCTION

FOR many years, studies have been made of the transport properties of carriers in the surface of semiconductors.[1] In general, these measurements were made by varying the electric field normal to the surface of a semiconductor so that a change of the space charge near the surface occurred and with it a change in the conductivity. Before 1962 these measurements were usually limited to small ranges of field and the surfaces were either accumulated (induction of majority carriers at the surface), depleted (induction of space charge by removal of majority carriers near the surface leaving charged ions), or slightly inverted (depletion with the additional induction of minority carriers at the surface). Usually measurements were limited to the conductance as a function of normal field or to the field effect mobility—the differential change of surface conductance with respect to total induced charge. Some Hall-effect and magnetoconductance measurements were also made.[2–4] In most cases, the surface fields were controlled by means of the absorption of ambient vapors.[5,6] In general, the induced charge did not exceed $3\times10^{11}/\text{cm}^2$.

The transport properties of electrons in the potential wells at the surface were studied intensively for several years following Schrieffer's[7] initial work in which he solved Boltzmann's equation in a surface well with the assumption that the scattering at the surface was diffuse. The results of such calculations were that the mobility was expected to decrease as the surface field increased. For a linear potential well and constant bulk scattering time, Schrieffer had shown that $\mu/\mu_B \simeq (kTm)^{1/2}/(q\tau_B F_z)$ for $\tau_B \gg \tau_S$, where k is the Boltzmann constant, T the temperature, m the effective mass, τ_B and τ_S the bulk and surface scattering times, respectively, and F_z the field just inside the surface. Most of the observed reduction of the carrier mobilities has been attributed to this type of scattering. Better approximations, using wells more exactly approximating ones resulting from a classical solution of the Boltzmann-Poisson equations and taking account of energy-dependent scattering times and specular and diffuse

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