Electro-optical effects in semiconductors with degenerate bands with allowance for excitons

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A quasiclassical method is developed for calculating the corrections to the complex permittivity of semiconductors with degenerate valence bands in an electric field. Expressions are obtained for the permittivity and for the light-absorption coefficient, both above and below the absorption edge. It is shown that exciton effects, by changing the absolute value of the effect, do not change the relative amplitude of the oscillations beyond the absorption edge. The oscillation period is found to change simultaneously. The results below the absorption edge coincide with those previously obtained by Merkulov. The influence of a nonspherical valence band on the anisotropy of the exciton electroabsorption is discussed. It is shown how the scattering of electrons and holes leads to damping of the oscillations.

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§1. INTRODUCTION AND BASIC RESULTS

We develop in this paper a quasiclassical method of obtaining the complex permittivity tensor (CPT) [both below and above the fundamental absorption edge (FAE)] in an electric field; this theory is valid for semiconductors with the band structure of germanium.

The imaginary part of the CPT (the light-absorption coefficient) in an electric field, for simple nondegenerate bands, was first calculated by Keldysh[1] below the FAE without allowance for exciton effects. Exciton effects were taken into account in electro-optics by Merkulov and Perel'[2] (below the FAE, far from the exciton levels), by Merkulov[3] (near the ground-state energy of the exciton), and by the authors[4] (above the FAE near degenerate excitonic states).

The light absorption coefficient in an electric field in semiconductors with degenerate valence bands was obtained by Keldysh, Konstantinov, and Perel'[5] (below the FAE, without allowance for the exciton effects). Exciton effects in this region were investigated by Merkulov.[6]

The condition for the applicability of the quasiclassical method developed in the present article is that the motion of the electrons and holes in an electric field be quasiclassical [condition (27)]. The method makes it possible to take into account exciton effects. Although the CPT cannot be calculated analytically with allowance for the Coulomb interaction of the electron and hole even in the absence of an electric field, in some cases (above the FAE, in the spherical approximation) the relative magnitude of the correction to the CPT in an electric field can be found.

The physical mechanism that necessitates the correction to the CPT in an electric field in semiconductors with degenerate valence bands and in the case of simple bands is one and the same. It is known that the CPT is determined by the value of the wave function of the electron and hole when the coordinates coincide. Above the FAE the electric field deflects the diverging electrons and holes, and if their relative momentum was directed along the field, then they meet again after moving a considerable distance apart (see Fig. 1). We shall call these trajectories "returning." This results in interference that manifests itself in oscillations of the CPT as a function of the frequency of the light and of the electric field. The relative smallness of the oscillation amplitude is due to the smallness of the solid angle in which the electron-hole pairs that contribute to the interference diverge. In a semiconductor with a degenerate valence band, oscillations of two types are produced, corresponding to the two types of holes. These two types of oscillations have different periods, amplitudes, and polarization dependences. A study of the polarization dependence makes it possible to determine the signs of the band-structure parameters, something impossible by studying only the absorption spectrum. (This fact, as applied to absorption below the FAE, was first noted in Ref. 5).

Above the FAE ($\hbar\omega - E_g = \Delta > 0$) we have

$$\varepsilon_1^{\alpha\beta}(\omega) = i\frac{4e^2s^2(2\Delta)^{1/2}M^{1/2}}{\hbar^3\omega^2}\left\{\delta_{\alpha\beta} - \frac{eE\hbar}{2(2\Delta)^{3/2}M^{1/2}} \times \sum_{\nu=l,h}\Theta_\nu^{\alpha\beta}(\mathbf{e})\frac{\mu_\nu(\mathbf{e})}{M}\exp\left(\frac{2i(2\Delta)^{3/2}m_\nu^{1/2}(\mathbf{e})}{3eE\hbar}\right)\right\}, \quad (1)$$

where $\varepsilon_1^{\alpha\beta}(\omega)$ is the resonant part of the CPT [see formulas (19) and (19a)], ω is the frequency of the incident light, E is the electric field intensity, E_g is the band gap, s is a quantity characterizing the interband matrix element of the velocity[7]

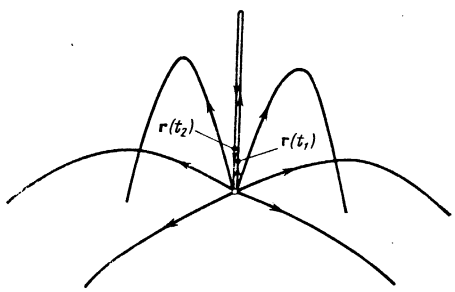

FIG. 1. Trajectories of relative motion of electron and hole in an electric field. The points $\mathbf{r}(t_1)$ and $\mathbf{r}(t_2)$ lie on a returning trajectory in the free region.

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$$\Theta_{l,h}^{\alpha,\beta}(\mathbf{e})=\frac{1}{4g(\mathbf{e})}\{(2g(\mathbf{e})\mp\gamma_2)\delta_{\alpha\beta}\pm3\gamma_3 e_\alpha e_\beta\pm3(\gamma_2-\gamma_3)\rho_{\alpha\beta\lambda\sigma}e_\lambda e_\sigma\}, \quad (2)$$

ρ is a cubic tensor of fourth rank; $\rho_{iiii}=1$, the remaining components are zero, $\mathbf{e}$ is a unit vector in the direction of the electric field

$$g(\mathbf{e})=[\gamma_2^2+3(\gamma_3^2-\gamma_2^2)(e_x^2e_y^2+e_y^2e_z^2+e_z^2e_x^2)]^{1/2}, \quad (3)$$

γ_1, γ_2, and γ_3 are the Luttinger constants[7]

$$M^{1/2}=\frac{1}{2}\int\frac{d\Omega_n}{4\pi}[m_l^{1/2}(\mathbf{n})+m_h^{1/2}(\mathbf{n})], \quad (4)$$

$$m_{l,h}^{-1}(\mathbf{n})=m^{-1}[\gamma_1'\pm2g(\mathbf{n})], \quad (5)$$

$\gamma_1'=\gamma_1+m/m_c$, and m_c is the electron effective mass in the conduction band. The quantity $\mu_\nu(\mathbf{e})$ has the dimension of mass, its calculation and final expression are given in the Appendix [expression (A.2)].

In the spherical approximation ($\gamma_2=\gamma_3$) the masses m_ν and μ_ν do not depend on the angles, and $m_\nu(\mathbf{e})=\mu_\nu(\mathbf{e})=m_\nu$

$$M^{1/2}=1/2(m_l^{1/2}+m_h^{1/2}), \quad g(\mathbf{e})=|\gamma_2|. \quad (6)$$

The principal axis of the tensor $\Theta_\nu^{\alpha\beta}(\mathbf{e})$ (and of the CPT) are directed along and across $\mathbf{e}$

$$\Theta_{l,h}^{\parallel}=1/2(1\pm\operatorname{sign}\gamma_2), \quad \Theta_{l,h}^{\perp}=1/2(1\mp1/2\operatorname{sign}\gamma_2). \quad (7)$$

In the spherical approximation, when the light is polarized along the field direction, oscillations of only one type are therefore produced: if $\gamma_2>0$, they are connected with the light holes, and if $\gamma_2<0$ with the heavy holes. In the case of polarization across $\mathbf{e}$, the ratio of the amplitude of the oscillations $\varepsilon^\perp$ is $m_l/3m_h$ at $\gamma_2<0$ and $3m_l/3m_h$ at $\gamma_2<0$. Below the FAE, the wave functions of the electron and hole overlap only on account of tunneling in the electric field, therefore the absorption coefficient is exponentially small. It is of interest to note that the asymptotic expressions for the CPT above and below the FAE cannot be obtained from each other by analytic continuation in the light frequency. Below the FAE

$$\varepsilon_1^{\alpha\beta}(\omega)=\frac{4e^2s^2(2|\Delta|)^{1/2}M^{1/2}}{\hbar^3\omega^2}\left\{-\delta_{\alpha\beta}+i\frac{eE\hbar}{4(2|\Delta|)^{1/2}M^{1/2}}\right.$$
$$\left.\times\sum_{\nu=l,h}\Theta_\nu^{\alpha\beta}(\mathbf{e})\frac{\mu_\nu(\mathbf{e})}{M}\exp\left(-\frac{2(2|\Delta|)^{3/2}m_\nu^{1/2}(\mathbf{e})}{3eE\hbar}\right)\right. \quad (8)$$

Since $m_l<m_h$, only the term with $\nu=l$ is left in fact in (8). Expression (8) was obtained in Ref. 5 accurate to a pre-exponential factor, which was not calculated in Ref. 5. In the same paper, a detailed analysis was made of the polarization dependence of the absorption below the FAE. The Coulomb interaction is quite simply taken into account in the spherical approximation:

$$\varepsilon_1^{\alpha\beta}(\omega)=\varepsilon_1(\omega,E=0)-i\operatorname{Im}\varepsilon_1(\omega,E=0)\frac{eE\hbar}{2(2\Delta)^{1/2}M^{1/2}}\sum_{\nu=l,h}\Theta_\nu^{\alpha\beta}(\mathbf{e})\frac{m_\nu}{M}\exp(i\Phi_\nu), \quad (9)$$

$$\Phi_\nu=\frac{2(2\Delta)^{3/2}m_\nu^{1/2}}{3eE\hbar}+\frac{2e^2}{\hbar\varepsilon_0}\left(\frac{m_\nu}{2\Delta}\right)^{1/2}\ln\frac{4(2\Delta)^{3/2}m_\nu^{1/2}}{eE\hbar}+2\delta_\nu^c(\Delta), \quad (10)$$

ε_0 is the static permittivity, $\varepsilon_1(\omega,E=0)$ is the value of ε_1 in the absence of an electric field. It follows from (9) that allowance for the Coulomb interaction leads to a change in the total value of the CPT, and the relative amplitude of the oscillations and their polarization dependence remain the same as without allowance for the Coulomb effects. The phase of the oscillations acquires a Coulomb increment similar to the increment in the case of simple bands.[4]

To estimate the unknown quantities $\varepsilon_1(\omega,E=0)$ and δ_ν^c we can use the expressions for the case of nondegenerate spherical bands[8]:

$$\operatorname{Re}\varepsilon_1(\omega,E=0)=-\frac{8e^4s^2}{\omega^2}\frac{M^2}{\varepsilon_0\hbar^4}(\operatorname{Re}\psi(1-ix)-\ln x),$$
$$\operatorname{Im}\varepsilon_1(\omega,E=0)=\frac{8e^4s^2}{\omega^2}\frac{M^2}{\varepsilon_0\hbar^4}(1-\exp(-2\pi x))^{-1},$$
$$\delta_c=\arg\Gamma(1-ix).$$

where $\psi(x)=d\ln\Gamma(x)/dx$, $x=(\mathrm{R}/\Delta)^{1/2}$, $\mathrm{R}=Me^4/2\hbar\varepsilon_0^2$ is the exciton Rydberg. At $|\gamma_2|\ll\gamma_1'$ these estimates become exact. At $\Delta=50$ R the Coulomb interaction increases $\operatorname{Im}\varepsilon_1(\omega,E)=0$ by a factor 1.5. Therefore the Coulomb effects are substantial far beyond the FAE. Allowance for the short-range non-Coulomb part of the electron-hole interaction influences only the form of $\varepsilon_1(\omega,E=0)$ and δ_ν. In particular, it is necessary to add to δ_ν^c the phase δ_0 of the scattered partial wave with angular momentum $L=0$ by the short-range potential.

Let us explain the physical meaning of expression (9). The imaginary part $\operatorname{Im}\varepsilon_1(\omega)$ is proportional to the probability that a particle and hole produced at one point will move an infinite distance apart. In the absence of a field, obviously this divergence is isotropic in the c.m.s. At short distances of the order of the wavelength, however, where $\varepsilon_1(\omega)$ is primarily formed, the returning trajectory does not differ in any way from the others (Fig. 1). This means that in the zeroth approximation in the field the probability of diverging along this trajectory is the same as along any other. Therefore allowance for the Coulomb interaction leads to the appearance of the same factor in front of the oscillating increment to the absorption coefficient as in front of its monotonic part. In first-order approximation in the field it must be taken into account that a small fraction of the paris that move apart, grouped together near a "returning" trajectory, will again be gathered in a single point, and their wave function will differ by a phase Φ_ν, which constitutes the classical action calculated on the returning trajectory. It is the interference with this increment which gives rise to the oscillations.

Below the EFA the value of the absorption changes strongly, but this change can be calculated only partially, namely, account can be taken of the factor that depends simultaneously on Δ and E (the Coulomb logarithm[6]). At sufficiently large parameters of the quasiclassical behavior this is the principal part of the change. At $\Delta<0$

$$\varepsilon_1^{\alpha\beta}(\omega)=\varepsilon_1(\omega,E=0)\delta_{\alpha\beta}+i\frac{8\pi e^2s^2}{\omega^2}\frac{eE\hbar}{4(2|\Delta|)^{1/2}M^{1/2}}$$
$$\times\sum_{\nu=l,h}\Theta_\nu^{\alpha\beta}(\mathbf{e})\frac{m_\nu}{M}C_\nu(|\Delta|)\exp(-\Phi_\nu), \quad (11)$$

$$\Phi_\nu=\frac{2(2|\Delta|)^{3/2}m_\nu^{3/2}}{3eE\hbar}-\frac{2e^2}{\hbar\varepsilon_0}\left(\frac{m_\nu}{2|\Delta|}\right)^{1/2}\ln\frac{4(2|\Delta|)^{3/2}m_\nu^{1/2}}{eE\hbar}, \quad (12)$$

$C_\nu(|\Delta|)$ and $\varepsilon_1(\omega,E=0)$ are unknown functions. It can be shown that $C_\nu(|\Delta|)\geq1$ and $C_\nu(|\Delta|)=1$ at $|\Delta|\gg R$. In addition, $C_\nu(|\Delta|)$ should have singularities in the bound

states of the exciton. In the case of a nondegenerate band[8]

$$\varepsilon_1(\omega, E=0)=-\frac{4M^2e^4s^2}{\omega^2\varepsilon_0\hbar^4}\left(\frac{1}{x}+2\psi(1-x)-2\ln x\right), \quad C=\Gamma^2(1-x),$$

where $x=(R/|\Delta|)^{1/2}$. The logarithmic correction (12) was first obtained by Merkulov.[6]

When account is taken of the nonsphericity, the exciton effects influence the polarization dependence of the CPT and its dependence on the direction of the electric field. We consider a family of classical trajectories of particles with total energy $\Delta > 0$ and with a dispersion law

$$\varepsilon_{l,h}=\hbar^2k^2/2m_{l,h}(\mathbf{k}/|\mathbf{k}|) \tag{13}$$

[$m_{l,h}(\mathbf{n})$ is given by expression (5)], which emerge from the Coulomb center (Fig. 2).

In the nonspherical case, the trajectories will not be straight lines, with the exception of those that are directed along the symmetry axes [001], [011], and [111]. Assume that on one of these axes $m_{\parallel} > m_{\perp}$ ($m_{\perp}$ is the mass in the direction perpendicular to the axis). Then the trajectories close to this axis will bend in such a way that the angle between the direction of motion and the axis will decrease with increasing distance from the center. Indeed, the Coulomb force is always directed along a line passing through the center, while the acceleration will be deflected towards the axis at $m_{\parallel} > m_{\perp}$ (Fig. 2). On the other hand if $m_{\parallel} < m_{\perp}$, the trajectories, on the contrary, will be deflected more and more away from the axis.

It is clear that the trajectories begin to bend effectively when they leave a quantum region with dimension of the order of the Bohr radius a_B of the exciton, and cease to bend when the Coulomb energy becomes much less than the kinetic energy, i.e., $r \gg r_0 = e^2/\varepsilon_0\Delta$. The described mechanism is particularly effective if $a_B \ll r_0$ or $\Delta \ll R$. In the limiting case $\Delta \to 0$, all the trajectories at infinity are directed along symmetry axes for which $m_{\parallel} > m_{\perp}$. Using expression (A.1) it is easy to show that these are the [100] axes for the light holes and [111] for the heavy ones. One should expect here a strong anisotropy of the oscillating increments to the CPT: the effects should increase in an electric field directed along [100] or [111], with the oscillations determined by the light holes in the former case and by the heavy ones in the latter. At all other field orientations the effect should become weaker.

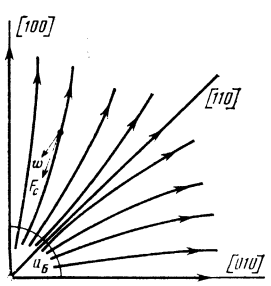

FIG. 2. Trajectories of relative motion of an electron and a light hole that interact in accordance with the Coulomb law. The directions of the Coulomb force $\mathbf{F}_c$ and the acceleration w are shown. a_B is the Bohr radius of the excition and delimits the quantum region at $\Delta < R$.

Electron and hole scattering leads to an exponential damping of the oscillations above the FAE. Let $\Gamma_e(\mathbf{n}, \varepsilon)$ be the electron damping, which depends on its kinetic energy ε and on the direction of motion $\mathbf{n}$, while $\Gamma_{lh}(\mathbf{n}, \varepsilon)$ and let $\Gamma_{hh}(\mathbf{n}, \varepsilon)$ be the damping of the light and heavy holes respectively, so that the corresponding states decay exponentially. The factor that takes into account the damping in motion along the returning trajectory should take into account the change of the kinetic energy with time

$$A_\nu=\exp\left\{-\int\Gamma_e(\mathbf{e}, \varepsilon_e(\tau))\,d\tau-\int\Gamma_{\nu h}(\mathbf{e}, \varepsilon_{\nu h}(\tau))\,d\tau\right\}.$$

The integration here is over the entire time of motion, $\varepsilon_{\nu h}(\tau)$ and $\varepsilon_e(\tau)$ are the kinetic energy of the hole of sort ν and of the electron at the instant τ, respectively. If τ is reckoned from the turning point (Fig. 1), then

$$\varepsilon_e(\tau)=(eE\tau)^2/2m_e, \quad \varepsilon_{\nu h}(\tau)=(eE\tau)^2/2m_{\nu h}(\mathbf{e}),$$

$$A_\nu=\exp\left\{-2\int_0^{\tau_0}(\Gamma_e(\mathbf{e}, (eE\tau)^2/2m_e)+\Gamma_{\nu h}(\mathbf{e}, (eE\tau)^2/2m_{\nu h}(\mathbf{e})))\,d\tau\right\},$$

where $\tau_0=[2m_\nu(\mathbf{e})\Delta]^{1/2}/eE$. Changing to a new variable ε, where ε is the summary kinetic energy at the instant τ, we find ultimately that the amplitude of the oscillations must be multiplied by the quantity

$$A_\nu=\exp\left\{-\frac{(2m_\nu(\mathbf{e}))^{1/2}}{eE}\int_0^{\Delta}\left[\Gamma_e\left(\mathbf{e}, \frac{m_\nu(\mathbf{e})}{m_e}\varepsilon\right)+\Gamma_{\nu h}\left(\mathbf{e}, \frac{m_\nu(\mathbf{e})}{m_{\nu h}(\mathbf{e})}\varepsilon\right)\right]\varepsilon^{-1/2}\,d\varepsilon\right\},$$

here $m_{\nu h}(\mathbf{e})$ differs from $m_\nu(\mathbf{e})$ [expression (5)] in that γ_1' is replaced by γ_1. If Γ is independent of energy, then (13) coincides with the expression obtained by Aspnes.[8]

§2. CONNECTION BETWEEN THE PERMITTIVITY AND THE GREEN'S FUNCTION

We derive a relation that connects the CPT and the Green's function (GF) of the relative motion of the electron and hole; this relation does not depend on the character of the band structure and is valid in the presence of an electric field and of Coulomb interaction. We use for this purpose the general expression given for the CPT, e.g., in Ref. 7.

If the valence band is filled and the conduction band empty, then the expression for $\varepsilon_{\alpha\beta}$ in the electron-hole pair representation (whether bound or not bound into an exciton) is of the form

$$\varepsilon_{\alpha\beta}(\omega)=\frac{4\pi e^2}{\omega^2 V}\sum_N\left\{\frac{v_{0N}^\alpha v_{N0}^\beta}{\hbar\omega-E_g-E_N+i\delta}-\frac{v_{N0}^\alpha v_{0N}^\beta}{\hbar\omega-E_g-E_N+i\delta}+\frac{v_{0N}^\alpha v_{N0}^\beta+v_{N0}^\alpha v_{0N}^\beta}{-E_g-E_N}\right\}, \tag{15}$$

Here N is the set of quantum numbers describing the state of the electron-hole pair, E_N is the energy of this state, V is the volume of the crystal, v_{0N}^α is the interband matrix element of the α component of the velocity, calculated between the vacuum state (absence of pair) and the state with number N.

We consider frequencies ω lying near the FAE, so that we can use the effective-mass method, and the velocity operator takes the form

$$\hat{\mathbf{v}}=\hat{\mathbf{v}}_B\delta(\mathbf{r}_e-\mathbf{r}_h),$$

where the operator $\hat{\mathbf{v}}_B$ acts on the Bloch functions, and $\delta(\mathbf{r}_e-\mathbf{r}_h)$ acts on the envelope functions. Then

$$v_{0N}{}^{\alpha}=\left(v^{\alpha}\int d^3\mathbf{r}_e\,d^3\mathbf{r}_h\,\delta(\mathbf{r}_e-\mathbf{r}_h)\,\psi_N{}^{*}(\mathbf{r}_e,\mathbf{r}_h)\right). \tag{16}$$

Here ψ_N is the envelope wave function, and $\mathbf{r}_e$ and $\mathbf{r}_h$ are the coordinates of the electron and of the hole. Generally speaking, ψ_N has many components, and v^{α} has just as many.

In the case of interest to us, the relative motion of the electron and hole deviates from the motion of their mass center, the latter being free:

$$\psi_N(\mathbf{r}_e,\mathbf{r}_h)=\psi_{n,\mathbf{k}}(\mathbf{r})\,e^{i\mathbf{k}\mathbf{R}},$$

$\psi_{n,\mathbf{k}}$ is the wave function of the relative motion, $\mathbf{r}=\mathbf{r}_e-\mathbf{r}_h$, and $\mathbf{R}$ is the mass-center coordinate. Expression (16) takes the form

$$v_{0N}{}^{\alpha}=(v^{\alpha}\psi_{n,\mathbf{k}=0}{}^{*}(0))\,(2\pi)^3\delta(\mathbf{k}). \tag{17}$$

Substituting (17) in (15) and using the definition of the Green's function, we obtain

$$\begin{aligned}\varepsilon_{\alpha\beta}=\frac{4\pi e^2}{\omega^2}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{(2\pi)^6\delta^2(\mathbf{k})}{V}\sum_n\Big\{&\frac{(v^{\alpha}\psi_n{}^{*}(0))\,(\psi_n(0)v^{\beta*})}{\hbar\omega+E_g+E_n+i\delta}\\&-\frac{(v^{\alpha*}\psi_n(0))\,(\psi_n{}^{*}(0)v^{\beta})}{\hbar\omega-E_g-E_n+i\delta}+\frac{(v^{\alpha}\psi_n{}^{*}(0))\,(\psi_n(0)v^{\beta*})+(v^{\alpha*}\psi_n(0))\,(\psi_n{}^{*}(0)v^{\beta})}{-E_g-E_n}\Big\}\\=\frac{4\pi e^2}{\omega^2}&\{v^{\alpha}[\hat{G}^{*}_{-E_g-\hbar\omega}(0,0)-\hat{G}^{*}_{-E_g}(0,0)]v^{\beta*}\\&+v^{\alpha*}[\hat{G}_{-E_g+\hbar\omega}(0,0)-\hat{G}_{-E_g}(0,0)]v^{\beta}\},\end{aligned} \tag{18}$$

where

$$\hat{G}_E(\mathbf{r},\mathbf{r}')=\sum_n\frac{\psi_n(\mathbf{r})\psi_n{}^{*}(\mathbf{r}')}{E_n-E-i\delta}$$

is a quadratic matrix whose number of rows and columns is equal to the number of the ψ-function components.

Obviously, the entire dependence on the external fields and on the frequency of the light near the FAE is contained in the term $\hat{G}_{-E_g+\hbar\omega}$. However, each term in (17) is separately diverging, so that $G(0,\mathbf{r})\propto r^{-1}$ as $r\to 0$. It is therefore convenient to represent $\varepsilon_{\alpha\beta}$ in the form of a sum of two terms: $\varepsilon(\omega)=\varepsilon_0(\omega)+\varepsilon_1(\omega)$,

$$\begin{aligned}\varepsilon_0(\omega)=\frac{4\pi e^2}{\omega^2}&\{v^{\alpha}[\hat{G}^{*}_{-E_g-\hbar\omega}(0,0)-\hat{G}^{*}_{-E_g}(0,0)]v^{\beta*}\\&+v^{\alpha*}[\hat{G}_0(0,0)-\hat{G}_{-E_g}(0,0)]v^{\beta}\},\\\varepsilon_1(\omega)=\frac{4\pi e^2}{\omega^2}&v^{\alpha*}\hat{G}_1v^{\beta},\qquad \hat{G}_1=\hat{G}_{\hbar\omega-E_g}(0,0)-\hat{G}_0(0,0),\end{aligned} \tag{19}$$

$\hat{G}_0(0,0)$ is the GF at zero energy and without allowance for the external fields and the Coulomb effects. The main contribution to the absorption near the FAE is described by $\varepsilon_1^{\alpha\beta}(\omega)$, while $\varepsilon_0(\omega)$ yields only the background part. Expressions (19), as well as their derivation, are perfectly analogous to the corresponding formulas for the simple bands.[9]

§3. PERMITTIVITY OF A SEMICONDUCTOR SUCH AS Ge NEAR THE FUNDAMENTAL ABSORPTION EDGE IN THE PRESENCE OF AN ELECTRIC FIELD (WITHOUT ALLOWANCE FOR EXCITON EFFECTS)

We consider the band structure of a cubic semiconductor of the Ge type. The Hamiltonian of the holes is[7]

$$\begin{aligned}\hat{H}_h(\mathbf{k})=\frac{\hbar^2}{2m}\Big[&\Big(\gamma_1+\frac{5}{2}\gamma_2\Big)k^2\hat{I}-2\gamma_2(k_x^2\hat{J}_x^2+k_y^2\hat{J}_y^2+k_z^2\hat{J}_z^2)\\&-4\gamma_3(k_xk_y\{\hat{J}_x,\hat{J}_y\}+k_yk_z\{\hat{J}_y,\hat{J}_z\}+k_zk_x\{\hat{J}_z,\hat{J}_x\})\Big],\end{aligned} \tag{20}$$

where m is the mass of the free electron, $\mathbf{k}$ is the wave vector of the hole, $\{\hat{J}_i,\hat{J}_j\}=\hat{J}_i\hat{J}_j+\hat{J}_j\hat{J}_i$; $\hat{J}_i$ are the operators of the projections of the angular momentum 3/2, and their explicit form can be found in the book,[7] while $\hat{I}$ is a 4×4 unit matrix.

The Hamiltonian of the electron does not depend on its spin σ:

$$\hat{H}_e=\hbar^2\mathbf{k}^2/2m_c.$$

The Hamiltonian of the relative motion is likewise independent of σ, and at zero total momentum it differs from (20) only in that γ_1 is replaced by $\gamma_1'=\gamma_1+m/m_c$. In this case $\mathbf{k}$ in (20) is the momentum of the relative motion $\mathbf{k}=-i\partial/\partial\mathbf{r}$. The matrix $\hat{G}$ depends on σ in trivial fashion (in proportion to $\delta_{\sigma\sigma'}$). We shall therefore take $\hat{G}$ to mean a 4×4 matrix, and expression (18) becomes

$$\varepsilon_1{}^{\alpha\beta}(\omega)=\frac{4\pi e^2}{\omega^2}\sum_{\sigma}v_{\sigma}{}^{\alpha*}\hat{G}_1v_{\sigma}{}^{\beta}. \tag{21}$$

The explicit form of $v_{\sigma j}^{\alpha}$ (α is the velocity direction, σ is the projection of the electron spin on the z axis, and j is the projection of the spin 3/2 of the hole on the z axis) is given in Ref. 7:

$$\begin{aligned}v_x=\frac{s}{2}\begin{pmatrix}0&-1&0&-\sqrt{3}\\i\sqrt{3}&0&i&0\end{pmatrix},\quad v_y=\frac{s}{2}\begin{pmatrix}0&-i&0&i\sqrt{3}\\-\sqrt{3}&0&1&0\end{pmatrix}\\v_z=\frac{s}{2}\begin{pmatrix}0&0&2i&0\\0&2&0&0\end{pmatrix}\end{aligned} \tag{22}$$

Here σ and j number respectively the rows and the columns, and s is a certain constant.[7] $\hat{H}(\mathbf{k})$ has two twofold degenerate eigenvalues $\varepsilon_{1,h}(\mathbf{k})$ defined by expression (13).

We calculate with the aid of (19) and (21) the known expression for the CPT in the absence of an electric field. In this case $\hat{G}_E(\mathbf{r},\mathbf{r}')$ is the GF of a Schrödinger equation with Hamiltonian (20). In the $\mathbf{k}$-representation, $\hat{G}_E(\mathbf{k})$ takes the usual form

$$\begin{aligned}\hat{G}_E(\mathbf{k})&=[\hat{H}(\mathbf{k})-\hat{I}(E+i\delta)]^{-1},\\\hat{G}_1&=\int\frac{d^3\mathbf{k}}{(2\pi)^3}\{[\hat{H}(\mathbf{k})-\hat{I}(\Delta+i\delta)]^{-1}-\hat{H}^{-1}(\mathbf{k})\}.\end{aligned} \tag{23}$$

Since $\hat{H}$ has cubic symmetry, $\hat{G}_1$ should have the same symmetry. However, since the problem has no preferred vector for the construction of cubic invariants, $\hat{G}_1=G_1\hat{I}$.

Calculating the traces of both sides of (23), with the aid of expression (13) for the eigenvalues, we obtain G_1:

$$\begin{aligned}4G_1=2\int\frac{d\Omega_n}{4\pi}\int_0^{\infty}4\pi k^2dk\Big[&\Big\{\frac{\hbar^2k^2}{2m_l(\mathbf{n})}-\Delta-i\delta\Big\}^{-1}-\frac{2m_l(\mathbf{n})}{\hbar^2k^2}\\&+\Big\{\frac{\hbar^2k^2}{2m_h(\mathbf{n})}-\Delta-i\delta\Big\}^{-1}-\frac{2m_h(\mathbf{n})}{\hbar^2k^2}\Big].\end{aligned}$$

Integration with respect to the absolute value of k is elementary:

$$\hat{G}_1 = I\frac{M^{3/2}}{2\pi\hbar^3}\begin{cases} i(2\Delta)^{1/2} & (\Delta>0) \\ -(2|\Delta|)^{1/2} & (\Delta<0) \end{cases}, \tag{24}$$

where M is defined by (4).

Using (21) we obtain

$$\varepsilon_1^{\alpha\beta}(\omega) = \frac{4\pi e^2}{\omega^2} G_1 \sum_\sigma v_\sigma^\alpha v_\sigma^\beta = \frac{4e^2 s^2 M^{3/2}}{\hbar^3\omega^2}\delta_{\alpha\beta}\begin{cases} i(2\Delta)^{1/2} & (\Delta>0) \\ -(2|\Delta|)^{1/2} & (\Delta<0) \end{cases} \tag{25}$$

where we have used the fact that $\sum_\sigma v_\sigma^{\alpha*} v_\sigma^\beta = 2s^2\delta_{\alpha\beta}$, as follows from (22).

Expression (25) is exact, so that its two forms (at $\Delta > 0$ and $\Delta < 0$) are obtained from each other by analytic continuation through the upper Δ half-plane.

We consider now $\hat{G}_1$ in an electric field. We choose the gauge $\varphi = 0$, $\mathbf{A} = -c t\mathbf{E}$. Then the Hamiltonian of the relative motion takes the form

$$\hat{H} = \hat{H}(\mathbf{k} - e\mathbf{E}t/\hbar),$$

e is the absolute value of the electron charge. In the equation for the GF we change to the $\mathbf{k}$–t representation

$$\hat{G}(\mathbf{k}, t) = -(2\pi\hbar)^{-1}\int_{-\infty}^{\infty} dE\, \hat{G}_E(\mathbf{k})\exp(-iEt/\hbar),$$
$$\{i\hbar\,\partial/\partial t - \hat{H}(\mathbf{k} - e\mathbf{E}t/\hbar)\}\hat{G}(\mathbf{k}, t) = I\delta(t). \tag{26}$$

It is natural to expect that if the electric field is weak enough, then $\hat{G}_1 = \hat{G}_1^0 + \hat{G}^E$, where $\hat{G}_1^0$ is given by (24) and $\hat{G}^E$ is the small increment due to the electric field. It is impossible, however, to calculate $\hat{G}^E$ by perturbation theory, since the matrix elements diverge because of the unbounded growth of the potential. The mathematical reason is that $\hat{G}^E$ is not an analytic function of the electric field as $\mathbf{E} \to 0$. The physical reason is that the important role for G^E is played by motion at large distances (or times), where the perturbation is not small. For the same reason, however, it turns out to be possible to obtain $\hat{G}^E$ by a quasiclassical method.

The picture of the motion does not differ strongly from the case of simple bands. Above the FAE, $\hat{G}^E$ is the result of interference between the incident wave and the one reflected by the electric field (Fig. 1). The trajectories on which this intereference is maximal are straight lines that are generally speaking different for different holes and are not necessarily parallel to the electric field. It is important to have $\mathbf{k} \parallel \mathbf{E}$, and to have $\mathbf{v} = \hat{m}^{-1}\mathbf{k}$ not parallel to $\mathbf{E}$ because of the tensor form of the effective mass (and furthermore different for the light and heavy holes). It is precisely the trajectories with $\mathbf{k} \parallel \mathbf{E}$ which are, as seen from the equation of motion $d(\hat{m}\mathbf{v})/dt = e\mathbf{E}$, the returning ones. To obtain the final answer for $\hat{G}^E$ it is necessary to take into account also the trajectories that differ little from the returning ones (so that the total phase adverse for them differs by less than 2π). If the returning trajectory is long enough (i.e., the field is weak), then these close trajectories lie within a small solid angle near the returning trajectory. This ensures smallness of $\hat{G}^E$.

Below the FAE it is necessary to consider below-the-barrier motion and tunneling under a triangular barrier. In both cases, if the trajectory is long enough, the motion is quasiclassical. The quasiclassical parameter is the action divided by Planck's constant, the order of magnitude of which is $|\Delta|^{3/2}m_l^{1/2}/eE\hbar$, where m_l is the reduced mass of the electron and light hole. We assume hereafter that the following condition holds

$$|\Delta|^{1/2}m_l^{1/2}/eE\hbar \gg 1. \tag{27}$$

We shall thus solve Eq. (26) in a quasiclassical approximation. If the motion is classical, then there should be no transitions between different branches of the spectrum. This simplifies greatly Eq. (26) and reduces it to diagonal form. On the returning trajectory, however, there is a turning point in the vicinity of which the quasiclassical character of the motion is violated, and one can expect transitions between the bands of the light and heavy holes. It turns out, however, that the probability of the transitions is low also in this region. In fact, the choice of the basis on which the Hamiltonian (20) is diagonalized depends only on the direction of the kinematic-momentum vector. On a returning trajectory, however, the kinematic momentum $\mathbf{k} - e\mathbf{E}t/\hbar$ always remains parallel to itself and at $\mathbf{k} \parallel \mathbf{E}$ Eq. (26) is diagonalized exactly, there are no transitions in the quantum region, and at small deviations from parallelism the probability of these transitions is low.

We introduce the time-dependent unitary matrix $\hat{S}$ which diagonalizes the Hamiltonian

$$\hat{S}\hat{H}\hat{S}^{-1} = \hat{H}_s = \hbar^2(\mathbf{k} - e\mathbf{E}t/\hbar)^2/2\hat{m}(\mathbf{n}),$$

$\hat{m}(\mathbf{n})$ is a matrix whose diagonal elements are determined by the expression (5), and the remaining elements are zero, $\hat{S}G\hat{S}^{-1} = \hat{G}_s$.

We rewrite Eq. (26) in terms of $\hat{H}_s$ and $\hat{G}_s$:

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{H}_s\right)\hat{G}_s = I\delta(t) + i\hbar\left(\frac{\partial\hat{S}}{\partial t}\hat{S}^{-1}\hat{G}_s + \hat{G}_s\hat{S}\frac{\partial\hat{S}^{-1}}{\partial t}\right). \tag{28}$$

The single-band approximation corresponds to neglecting the increment to the right-hand side of (28). We shall estimate this increment later, and for the time being assume it to be small. Then

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{H}_s\right)\hat{G}_s = I\delta(t), \tag{29}$$

$$\hat{G}_s = (i\hbar)^{-1}\theta(t)\exp\left\{(i\hbar)^{-1}\int_0^t \hat{H}_s(\mathbf{k} - e\mathbf{E}t'/\hbar)\,dt'\right\},$$

$$\hat{G}_\Delta(0,0) = \hat{S}^{-1}(\mathbf{e})\,\hat{G}_{s\Delta}(0,0)\,\hat{S}(\mathbf{e}), \tag{30}$$

$$\hat{G}_{s\Delta}(0,0) = -\int_0^\infty dt\int\frac{d^3\mathbf{k}}{(2\pi)^3}(i\hbar)^{-1}\exp\left\{\frac{i}{\hbar}\left(\Delta t - \int_0^t \hat{H}_s(\mathbf{k} - e\mathbf{E}t'/\hbar)\,dt'\right)\right\}.$$

Generally speaking, one should take the Fourier transform not of the function $\hat{G}_s$, but of $\hat{G}$, which differs from $\hat{G}_s$ by the factors $\hat{S}(\mathbf{k} - e\mathbf{E}t/\hbar)$ and $\hat{S}^{-1}$ that depend on t and $\mathbf{k}$.

We, however, have taken these factors outside the integral sign and have put in them $\mathbf{k} \parallel \mathbf{E}$, since they vary much more slowly than $\hat{G}_s$ as functions of t and $\mathbf{k}$. To integrate with respect to $\mathbf{k}$ it is convenient to change over to a new variable $\mathbf{q} = \mathbf{k} - e\mathbf{E}t/2\hbar$ and expand $\hat{H}_s$ up to second order in $\mathbf{q}$:

$$\hat{H}_s\left(\mathbf{k} - \frac{e\mathbf{E}t'}{\hbar}\right) = \frac{[eE(t/2 - t')]^2}{2\hat{m}(\mathbf{e})} + \frac{eE(t/2 - t')}{\hbar}\frac{\partial\hat{H}_s(\mathbf{k})}{\partial k_i}\Big|_{\mathbf{k}=\mathbf{e}} q_i + \frac{1}{2}\frac{\partial^2\hat{H}_s(\mathbf{k})}{\partial k_i\partial k_j}\Big|_{\mathbf{k}=\mathbf{e}} q_i q_j.$$

Integrating this expression with respect to t' from 0 to t, we get

$$\hat{G}_{s\Delta}(0,0) = -\int_0^\infty dt \int \frac{d^3\mathbf{q}}{(2\pi)^3} (i\hbar)^{-1} \exp\left\{\frac{i}{\hbar}\left[\Delta t - \frac{(eE)^2 t^3}{24\hat{m}(\mathbf{e})} - \frac{t}{2}\frac{\partial^2 \hat{H}_s(\mathbf{k})}{\partial k_i \partial k_j}\Big|_{\mathbf{k}=\mathbf{e}} q_i q_j\right]\right\}.$$

Recognizing that

$$\int \frac{d^3\mathbf{q}}{(2\pi)^3} \exp\left\{-i\frac{A_{ij}}{2} q_i q_j\right\} = (2\pi i)^{-3/2} (\det A)^{-1/2},$$

we obtain

$$\hat{G}_{s\Delta}(0,0) = -\frac{\hat{\mu}(\mathbf{e})\hat{m}^{1/2}(\mathbf{e})}{i\hbar^4} \int_0^\infty \left(\frac{\hbar}{2\pi i t}\right)^{3/2} \exp\left\{\frac{i}{\hbar}\left[\Delta t - \frac{(eE)^2 t^3}{24\hat{m}(\mathbf{e})}\right]\right\} dt, \tag{31}$$

where

$$\hat{\mu}(\mathbf{e}) = \hat{m}^{3/2}(\mathbf{e})\hbar^3 \left(\det \frac{\partial^2 \hat{H}_s(\mathbf{k})}{\partial k_i \partial k_j}\Big|_{\mathbf{k}=\mathbf{e}}\right)^{-1/2}.$$

The calculation of $\hat{\mu}(\mathbf{e})$ is quite cumbersome and is relegated to the Appendix, where the final expression (A.2) is also given.

It is seen that the integral (31) diverges as $t \to 0$. However, this contribution, which diverges at short times, corresponds to $\hat{G}_1^0$ and does not depend on the electric field, while the divergence can be removed by subtracting $\hat{G}_0$ [see (19)]. We are interested in another contribution that arises at large t and can be calculated by the saddle-point method. The approximations already made are valid only when this contribution is calculated. Were we wish to calculate $\hat{G}_1^0$ with the aid of (31) (after first eliminating the divergence by subtracting unity from the exponential), then we would obtain an incorrect answer, as can be easily verified by comparison with (24). Indeed, $\hat{G}_1^0$ receives contributions from trajectories with arbitrary directions, so that integration over the angles is carried out in (24). In expression (31), however, the direction along the field is singled out.

We consider now the case $\Delta > 0$. The saddle point is then $t_0 = 2[2\hat{m}(\mathbf{e})\Delta]^{1/2}/eE$, and the integration contour is shown in Fig. 3a. Calculation yields

$$\hat{G}_s^E = -i\frac{(2\Delta)^{1/2} M^{3/2}}{2\pi\hbar^3} \frac{eE\hbar}{2(2\Delta)^{1/2} M^{1/2}} \frac{\hat{\mu}(\mathbf{e})}{M} \exp\left\{i\frac{2(2\Delta)^{3/2}\hat{m}^{1/2}(\mathbf{e})}{3eE\hbar}\right\}. \tag{32}$$

At $\Delta < 0$, the saddle point is $t_0 = -2i[2\hat{m}(\mathbf{e})|\Delta|]^{1/2}/eE$, and the contour is shown in Fig. 3b:

$$\hat{G}_s^E = i\frac{(2|\Delta|)^{1/2} M^{3/2}}{2\pi\hbar^3} \frac{eE\hbar}{4(2|\Delta|)^{1/2} M^{1/2}} \frac{\hat{\mu}(\mathbf{e})}{M} \exp\left\{-\frac{2(2|\Delta|)^{3/2}\hat{m}^{1/2}(\mathbf{e})}{3eE\hbar}\right\}. \tag{32a}$$

Expression (32a) is not an analytic continuation of (32) through the upper Δ half-plane. The reason is the following. In the analytic continuation we cross the Stokes line, which is defined in the present case by the equation $\arg\Delta = 2\pi/3$. Whereas prior to passing through this line the saddle point was the root t_0 of the equation $\Delta = (eEt)^2/8\hat{m}(\mathbf{e})$, which is positive on the positive Δ axis, after crossing the Stokes line the saddle point turns out to be the other root, $-t_0$ (see Figs. 3a, b). A similar phenomenon takes place when the quasiclassical wave functions are joined together near a turning point. When integrating along the contour C_2 we pass only on one decline of the saddle, whereas when integrating along C_1 we pass over both. Therefore the pre-exponential factors differ by a factor of two. We note also that we did not calculate the integral along the segment of the imaginary axis in C_2, since it contributes only to the real part of the CPT; the contribution is proportional to the square of the field and can be calculated by perturbation theory.

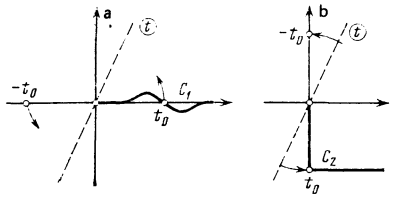

FIG. 3. Integration contours in formula (31): a) at $\Delta > 0$, b) at $\Delta < 0$, t_0 is the saddle point, the Stokes line is shown dashed, the arrows show the directions of motion of the extremum points of the integrand when the phase Δ changes from 0 to π.

We now assess the approximations made. We first check on the validity of the expansion in q. In the estimate we shall not distinguish between m_l, m_h, and M. The characteristic q is determined from the relation

$$\frac{1}{\hbar} t \frac{\hbar^2}{M} q_0^2 \sim 1, \quad t \sim (\Delta M)^{1/2}/eE, \quad q_0 \sim (M/\Delta)^{1/2}(eE/\hbar)^{1/2}. \tag{a}$$

The condition that q_0 be small, $q_0 \ll k \sim (\Delta M)^{1/2}/\hbar$, is equivalent to $(\Delta^{3/2} M^{1/2}/eE\hbar)^{1/2} \gg 1$, i.e., it coincides with the condition for the quasiclassical approach.

We turn now to Eq. (28). Far from the turning point, the discarded terms can be neglected, since the quasiclassical matrix elements of a slowly varying perturbation are exponentially small. The principal correction is given by the quantum region—the vicinity of the turning point. Its characteristic scale τ_0 (τ is the time reckoned from the turning point) is determined from the condition $H_s(\tau_0)\tau_0/\hbar \sim 1$, or $\tau_0 \sim (\hbar M)^{1/2}(eE)^{-2/3}$. During the time τ_0 the function G undergoes one oscillation, and we shall assume for the estimate that G is constant in the quantum region, i.e., we neglect the Hamiltonian $\hat{H}$ in Eq. (26). The change of $\hat{G}_s$ is then described by the "sudden" change of $\hat{S}$: the Green's function does not manage to change, and only the basis in which we expand it changes:

$$\hat{G}_s(\tau_0) \approx \hat{S}_{\tau_0}\hat{S}_{-\tau_0}^{-1}\hat{G}_s(-\tau_0)\hat{S}_{-\tau_0}\hat{S}_{\tau_0}^{-1}.$$

[Here $\hat{S}_0 = \hat{S}(e\mathbf{E}\tau/\hbar + \mathbf{q})$.] Expanding S up to second order in q, we obtain for the correction

$$\Delta G_s \sim \left(\frac{q_0\hbar}{eE\tau_0}\right)^2 G_s \sim \left(\frac{eE\hbar}{\Delta^{3/2}M^{1/2}}\right)^{1/3} G_s.$$

(The terms linear in q vanish upon integration.)

We emphasize once more that the change of $\hat{S}$ can be regarded as sudden only qualitatively, as an estimate, and in this case we obtain the order of magnitude of ΔG accurate to a numerical coefficient.

Thus, the correction turns out to be small in terms of the quasiclassical parameter raised to the 1/3 power.

We note, however, that the correction term, generally speaking, is no longer diagonal in the $\hat{S}(\mathbf{e})$ representation, and can therefore describe transitions between the bands of the light and heavy holes. The corresponding oscillations will have a different phase and a different frequency. We shall not consider the conditions for the onset of these "combined" oscillations, and note only that they do not appear in the spherical approximation.

To find the CPT we must substitute expressions (32) and (32a) in (30), and then in (21). In this case we obtain, e.g., for $\Delta > 0$

$$\frac{\varepsilon_{\alpha\beta}^{E}}{\varepsilon_{1}^{\omega}} = -\frac{1}{2s^{2}} v_{\alpha_j}^{\alpha} S_{jn}^{-1}(\mathbf{e}) \frac{\hbar e E}{2(2\Delta)^{1/2} M^{1/2}} \frac{\mu_n(\mathbf{e})}{M} \times \exp\left\{\frac{2i(2\Delta)^{1/2} m_n(\mathbf{e})}{3eE\hbar}\right\} S_{nj'}(\mathbf{e}) v_{j'\alpha}^{\beta}. \quad (33)$$

Since the eigenvalues $\hat{H}$ are degenerate (namely $m_{n=1/2} = m_{n=-1/2}$, $\mu_{n=1/2} = \mu_{n=-1/2}$, $m_{n=3/2} = m_{n=-3/2}$, $\mu_{n=3/2} = \mu_{n=-3/2}$, we can sum over pairs of values of n pertaining to one eigenvalue.

We introduce the notation

$$\Theta_{\nu}^{\alpha\beta}(\mathbf{e}) = \frac{1}{2s^{2}} v_{\alpha_j}^{\alpha} S_{jn(\nu)}^{-1}(\mathbf{e}) S_{n(\nu)j'}(\mathbf{e}) v_{j'\alpha}^{\beta},$$

ν runs through the values l and h. A rather cumbersome calculation yields for $\Theta_{\nu}^{\alpha\beta}(\mathbf{e})$ (see Refs. 5 and 7) the expression (2), while for the CPT it yields the expression (1) at $\Delta > 0$ and the expression (8) at $\Delta < 0$.

§4. COULOMB EFFECTS IN ELECTRO-OPTICS

The Hamiltonian of the relative motion of the electron and hole, with account taken of their Coulomb interaction in the gauge $\varphi = \mathbf{E}\cdot\mathbf{r}$ and $\mathbf{A} = 0$, is of the form

$$\hat{H} = \hat{H}_0(-i\nabla_r) - e\mathbf{E}\mathbf{r} - e^2/\varepsilon_0 r, \quad (34)$$

where $\hat{H}_0$ is defined by (20).

We use the well known identity for Green's functions[10]:

$$\hat{G}(\mathbf{r}_2, \mathbf{r}_1, t) = \int d^3\mathbf{r}'\, \hat{G}(\mathbf{r}_2, \mathbf{r}', t-\tau)\hat{G}(\mathbf{r}', \mathbf{r}_1, \tau) \quad (0 \leqslant \tau \leqslant t). \quad (35)$$

Using (35) twice, we obtain

$$\hat{G}_{\Delta}(0,0) = -\int d^3\mathbf{r}_1\, d^3\mathbf{r}_2\, dt \exp\{i\Delta t/\hbar\}\hat{G}(0, \mathbf{r}_2, t_2)\hat{G}(\mathbf{r}_2, \mathbf{r}_1, t-t_2-t_1)\hat{G}(\mathbf{r}_1, 0, t_1). \quad (36)$$

In our case $G(\mathbf{r}_1, 0, t_1)$ describes the initial section of a returning trajectory $[0 \to \mathbf{r}(t_1)]$, $\hat{G}(\mathbf{r}_2, \mathbf{r}_1, t-t_1-t_2)$ describes the middle section $[\mathbf{r}(t_1) \to$ turning point $\to \mathbf{r}(t_2)]$, and $\hat{G}(0, \mathbf{r}_2, t_2)$ the final section $[\mathbf{r}(t_2) \to 0]$ (Fig. 1). The gist of this method of taking the Coulomb interaction into account is that when a suitable choice of t_1 and t_2 is made on the initial and final sections of the trajectory, the electric potential can be regarded as small and the Coulomb potential taken into account exactly. In the middle section, on the contrary, the electric potential is exactly taken into account and the Coulomb potential is regarded as a small increment. Obviously, this is possible only if the trajectory has a "free" region in which both the Coulomb and the electric potentials are small compared with the kinetic energy. As shown in Ref. 4, for the case of simple bands this condition requires that $(\Delta/R)^{1/2}(\Delta^{3/2}M^{1/2}/eE\hbar) \gg 1$. (In this case the condition for the quasiclassical approach (27) should also be satisfied.) Then, choosing $\mathbf{r}(t_1)$ and $\mathbf{r}(t_2)$ in the "free" region (where the motion is already quasiclassical), we join all three sections.

Unfortunately, however, we do not know the representation in which the Coulomb Green's function $\hat{G}(0, \mathbf{r})$ is diagonalized, and generally speaking it coincides neither with $\hat{S}(\mathbf{r})$ nor with $\hat{S}(\mathbf{k})$ [where $\mathbf{k}$ is a momentum direction such that the velocity $v_i^{\nu} = k_j \partial^2 H_{\nu}(\mathbf{k})/\partial k_i \partial k_j$ is parallel to $\mathbf{r}$] even as $r \to \infty$. An exception is the spherical approximation (SA), which is characterized by the fact that the matrices of all the physical quantities that depend on only one vector have a diagonal form in one and the same representation in which the quantization axis of the spin 3/2 coincides with the direction of this vector. In the SA the velocity is always parallel to the momentum, and the trajectories passing through the Coulomb center are straight lines. We shall carry out henceforth the calculation in the SA.

We transform expression (36):

$$\hat{G}_{\Delta}(0,0) = \int \hat{G}_{\varepsilon_2}(0, \mathbf{r}_2)\hat{G}_{\Delta}(\mathbf{r}_2, \mathbf{r}_1)\hat{G}_{\varepsilon_1}(\mathbf{r}_1, 0) \times \exp\left\{\frac{i(\Delta-\varepsilon_1)t_1 + i(\Delta-\varepsilon_2)t_2}{\hbar}\right\} \frac{d\varepsilon_1\, d\varepsilon_2}{(2\pi\hbar)^2} d^3\mathbf{r}_1\, d^3\mathbf{r}_2. \quad (37)$$

Since the motion is classical in the joining region, all three Green's functions under the integral sign in (37) are rapidly oscillating functions of ε_1, ε_2, $\mathbf{r}_1$, and $\mathbf{r}_2$, and the important role is assumed in the integration by a narrow energy region near Δ:

$$|\varepsilon_1 - \Delta| \sim \frac{\Delta^{1/2}\hbar^{1/2} r(t_1)^{-1/2}}{M^{1/2}}, \quad |\varepsilon_2 - \Delta| \sim \frac{\Delta^{1/2}\hbar^{1/2} r(t_2)^{-1/2}}{M^{1/2}}$$

and by a narrow coordinate region near the points $\mathbf{r}_1 = \mathbf{r}(t_1)$ and $\mathbf{r}_2 = \mathbf{r}(t_2)$ that lie on the free section of the returning trajectory (Fig. 1). For the longitudinal coordinate we have $|z_1 - r(t_1)| \sim r(t_1)^{2/3}\hbar^{1/3}M^{-1/6}\Delta^{-1/6}$, and for the transverse, $\rho_1 \sim r(t_1)^{1/2}\hbar^{1/2}M^{-1/4}\Delta^{-1/4}$. (The estimates for z_2 and ρ_2 are analogous.) The motion in the free region is quasiclassical, meaning that $(2M\Delta)^{1/2} r(t)\hbar^{-1} \gg 1$. From this inequality and from the presented estimates it follows that $|\Delta - \varepsilon| \ll \Delta$ and $|\mathbf{r} - \mathbf{r}(t)| \ll r(t)$. We shall see that allowance for the Coulomb interaction leads to the appearance, in all three Green's functions, of additional Coulomb factors that vary little over the characteristic scale of variation of ε_1, ε_2, $\mathbf{r}_1$, and $\mathbf{r}_2$. In their calculation we can therefore put $\varepsilon_1 = \varepsilon_2 = \Delta$ and $\mathbf{r}_1 = \mathbf{r}(t_1)$, $\mathbf{r}_2 = r(t_2)$.

Thus, in the calculation of $\hat{G}_{\varepsilon}(\mathbf{r}, 0)$ we neglect the electric field. As shown in Ref. 11, the Hamiltonian (34) commutes at $\mathbf{E} = 0$ with the operator of the total angular momentum $\hat{\mathbf{F}} = \hat{\mathbf{J}} + \hat{\mathbf{L}}$ ($\hat{\mathbf{L}}$ is the orbital-momentum operator). The wave functions can be characterized by the presence of the angular momentum F and of its projection F_z on an arbitrary z axis:

$$\hat{G}_{\varepsilon}(\mathbf{r}, 0) = \sum_{\varepsilon', F, F_z} \frac{\psi_{F, F_z, \varepsilon'}(\mathbf{r})\psi^{*}_{F, F_z, \varepsilon'}(0)}{\varepsilon' - \varepsilon - i\delta}. \quad (38)$$

From the addition rules for angular momenta it is clear that F takes on half-integer values, starting with $F = 1/2$, while L, takes on values from $F - 3/2$ to $F + 3/2$, for a given $F \geqslant 3/2$, and only two values, $L = 1$ and $L = 2$, at $F = 1/2$. But at $L \neq 0$ the function $\psi_L(0) = 0$, therefore the only nonzero terms in the sum are those

with $F=3/2$. The basis $\psi^{j}_{3/2,F_z}(r)$, which depends on one vector $\mathbf{r}$, is diagonal in the indices j and F_z in the $\hat{S}(r)$ representation, while $\psi^{j}_{3/2,F_z}(0)$ is diagonal in any representation and should therefore have the structure of a unit matrix: $\psi^{j}_{3/2,F_z}(0)=\psi_{3/2}(0)\hat{I}_{j,F_z}$.

Taking all the foregoing into account, we have

$$G_\varepsilon^n(\mathbf{r},0)=\sum_{\varepsilon'}\frac{\psi^n_{\nu_n,n,\varepsilon'}(\mathbf{r})\psi^{*}_{\nu_n,\varepsilon'}(0)}{\varepsilon'-\varepsilon-i\delta}, \tag{39}$$

G^n is the eigenvalue of $\hat{G}$ in the $\hat{S}(\mathbf{r})$ representation. If $\Delta>0$, then $\psi(\mathbf{r})$ can differ as $r\to\infty$ from the wave function $\psi^0(\mathbf{r})$ of the free motion only in phase. This follows from the condition of normalization of the continuous-spectrum functions. The Coulomb phase is of the form

$$\varphi_n(r,\varepsilon)=\delta_n^c(\varepsilon)+\frac{e^2}{\hbar\varepsilon_0}\left(\frac{m_n}{2\varepsilon}\right)^{1/2}\ln\left[\frac{2r}{\hbar}(2m_n\varepsilon)^{1/2}\right], \tag{40}$$

$$\psi^n_{\nu_n,n,\varepsilon}(\mathbf{r})=\psi^{(0)n}_{\nu_n,n,\varepsilon}(\mathbf{r})\exp\{i\varphi_n(r,\varepsilon)\}. \tag{41}$$

Here $\delta_n^c(\varepsilon)$ is a certain unknown function of energy, chosen such that $\psi(0)$ and $\psi^{(0)}(0)$ are real. To find $\delta_n^c(\varepsilon)$ it is necessary to have an exact solution of the Schrödinger equation at short distances. The second term in (40) is the quasi-classical phase, which can be easily obtained from the following considerations: it is known that in the quasiclassical region $\psi\propto\exp iS/\hbar$.[10] If we consider the Coulomb potential as a small increment to the free-motion Hamiltonian $\hat{H}_0$, then we can use the known expression for the correction to the action in terms of the correction to the potential:

$$\delta S(t_2,t_1)=-\int_{t_1}^{t_2}\delta u(\mathbf{r}(t))\,dt, \tag{42}$$

where $\mathbf{r}(t)$ is the unperturbed classical trajectory. Substituting $\delta u(\mathbf{r})=-e^2/\varepsilon_0 r$, where $r(t)=\text{const}+(2\varepsilon/m_n)^{1/2}t$ is the trajectory of the free motion, we obtain the logarithmic term in (40).

Substituting (41) in (39) and taking the slowly varying Coulomb factors outside the integral sign, we obtain

$$G_\varepsilon^{n\,(\text{div})}(\mathbf{r},0)=\frac{\psi_{\nu_n,\varepsilon}(0)}{\psi^{(0)}_{\nu_n,\varepsilon}(0)}\exp\{i\varphi_n(r,\varepsilon)\}G_\varepsilon^{(0)n\,(\text{div})}(\mathbf{r},0). \tag{43}$$

In the derivation of (43) we used a basis of wave-functions that constitute a diverging wave at large distances. This is convenient in the calculation of the Green's function $\hat{G}_{\varepsilon_1}(\mathbf{r}_1,0)$, which describes the departure of the particle from the point 0, but in the calculation of the Green's function $\hat{G}_{\varepsilon_2}(0,\mathbf{r}_1)$, which describes arrival at the point 0, we must use a basis of converging waves. This changes the sign of the additional phase $\varphi_n(r,\varepsilon)$ of the wave functions and, as a result

$$G_\varepsilon^{n\,(\text{conv})}(0,\mathbf{r})=\frac{\psi_{\nu_n,\varepsilon}(0)}{\psi^{(0)}_{\nu_n,\varepsilon}(0)}\exp\{i\varphi_n(r,\varepsilon)\}G_\varepsilon^{(0)n\,(\text{conv})}(0,\mathbf{r}), \tag{44}$$

To find the Coulomb factor in $\hat{G}_\Delta(\mathbf{r}_2,\mathbf{r}_1)$ we also use the relation (42). For the quasiclassical Green's function, as well as for the wave function, we have $G\propto\exp\{iS/\hbar\}$. Thus

$$G_\Delta^n(\mathbf{r}_2,\mathbf{r}_1)=\exp\{i\varphi_n^{E}(\Delta,r_2,r_1)\}G_\Delta^{En}(\mathbf{r}_2,\mathbf{r}_1), \tag{45}$$

$$\varphi_n^{E}(\Delta,\mathbf{r}_2,\mathbf{r}_1)=\frac{e^2}{\hbar\varepsilon_0}\left(\frac{m_n}{2\Delta}\right)^{1/2}\left[2\ln\left(\frac{4(2\Delta)^{1/2}m_n^{1/2}}{eE\hbar}\right)\right.$$
$$\left.-\ln(2r_1(2m_n\Delta)^{1/2}/\hbar)-\ln(2r_2(2m_n\Delta)^{1/2}/\hbar)\right]. \tag{46}$$

Here $\varphi_n=\delta S_n/\hbar$ and G_Δ^E is the field increment to the Green's function without allowance for the Coulomb field. [We disregard the field-independent contribution made to G by the direct transition $(\mathbf{r}_1\to\mathbf{r}_2)$ in (31)]. When calculating the correction to the action we used the trajectory of motion in an electric field: $r(t)=(2\Delta/m_n)^{1/2}t-eEt^2/2m_n$ between the instants of time t_1 and t_2 $[\mathbf{r}(t_1)=\mathbf{r}_1,\mathbf{r}(t_2)=\mathbf{r}_2]$ with the points $\mathbf{r}_1$ and $\mathbf{r}_2$ assumed to be located on a returning trajectory.

Taking the Coulomb factor outside the integral sign in (37), we obtain

$$G_\Delta^n(0,0)=\left(\frac{\psi_{\nu_n,\Delta}(0)}{\psi^{(0)}_{\nu_n,\Delta}(0)}\right)^2$$
$$\times\exp\{i\varphi_n(r(t_1),\Delta)+i\varphi_n(r(t_2),\Delta)+i\varphi_n^{E}(\Delta,r(t_2),r(t_1))\}$$
$$\times\int G^{(0)n}_{\varepsilon_2}(0,\mathbf{r}_2)G_\Delta^{En}(\mathbf{r}_2,\mathbf{r}_1)G^{(0)n}_{\varepsilon_1}(\mathbf{r}_1,0)$$
$$\times\exp\left\{\frac{i(\Delta-\varepsilon_1)t_1+i(\Delta-\varepsilon_2)t_2}{\hbar}\right\}\frac{d\varepsilon_1\,d\varepsilon_2}{(2\pi\hbar)^2}\,d^3\mathbf{r}_1\,d^3\mathbf{r}_2.$$

The difference between $G_\varepsilon^{(0)}(0,\mathbf{r})$ and $G_\varepsilon^{E}(0,\mathbf{r})$ can be neglected, since the electric potential is small on the sections $(0\to\mathbf{r}_1)$ and $(\mathbf{r}_2\to 0)$. The remaining integral is then equal to $G_\Delta^E(0,0)$ [formula (32), in which we must put $\gamma_2=\gamma_3$]. In addition, it follows from (38) that

$$(\psi_{\nu_n,\Delta}(0)/\psi^{(0)}_{\nu_n,\Delta}(0))^2=\operatorname{Im}G_\Delta^c(0,0)/\operatorname{Im}G_\Delta^{(0)}(0,0),$$

where $G_\Delta^c(0,0)$ is the Coulomb Green's function, whose analytic expression is unknown. Using the expression for the phases (40) and (46), we get

$$G_\Delta^n(0,0)=G_\Delta^c(0,0)+\frac{\operatorname{Im}G_\Delta^c(0,0)}{\operatorname{Im}G_\Delta^{(0)}(0,0)}$$
$$\times\exp i\left\{\frac{2e^2}{\hbar\varepsilon_0}\left(\frac{m_n}{2\Delta}\right)^{1/2}\ln\left(\frac{4(2\Delta)^{1/2}m_n}{eE\hbar}\right)+2\delta_n^c(\Delta)\right\}C_\Delta^E(0,0)$$

and for the CPT at $\Delta>0$ we get expression (9). By analytically continuing $G_\varepsilon^c(r,0)$ into the region $\varepsilon<0$ we no longer obtain such a simple connection between the pre-exponential factor with $\operatorname{Im}G_\varepsilon^c(0,0)$ as in (43) and (44), since the phase $\delta_n^c(\varepsilon)$ becomes imaginary at $\varepsilon<0$. On the other hand the logarithmic part of the phase (40) retains its form. As a result we obtain expression (11) for the CPT at $\Delta<0$.

APPENDIX

We shall calculate $\mu_l(\mathbf{e})$; $\mu_h(\mathbf{e})$ is obtained from $\mu_l(\mathbf{e})$ by reversing the sign of $g(\mathbf{e})$.

Differentiating (15), we obtain

$$m_{ij}^{-1}=\hbar^{-2}\frac{\partial^2\varepsilon_l(\mathbf{k})}{\partial k_i\,\partial k_j}$$
$$=m^{-1}\left[\gamma_1'\delta_{ij}-\frac{e_ie_j}{g^2}(3\gamma_3^2-\gamma_2^2-3(\gamma_3^2-\gamma_2^2)e_i^2)(3\gamma_3^2-\gamma_2^2-3(\gamma_3^2-\gamma_2^2)e_j^2)\right.$$
$$\left.+\frac{1}{g}(\delta_{ij}(3\gamma_3^2-\gamma_2^2-9(\gamma_3^2-\gamma_2^2)e_i^2)+2e_ie_j(3\gamma_3^2-\gamma_2^2))\right]. \tag{A.1}$$

To facilitate the calculation of the determinant $D(\mathbf{e})=\det m_{ij}^{-1}$ of the matrix (A.1), we note that $D(e)$ must have cubic symmetry, i.e., it depends on $\mathbf{e}$ only via the cubic invariant $\Delta=e_x^2e_y^2+e_y^2e_z^2+e_ze_x^2$. We can therefore set in (A.1) one of the components of $\mathbf{e}$, for example $\mathbf{e}_z$, equal to zero. The answer must be expressed in terms of $\Lambda=e_x^2e_y^2$. At arbitrary orientation of $\mathbf{e}$, we must replace $e_x^2e_y^2$ in the obtained expression by $e_x^2e_y^2+e_y^2e_z^2+e_z^2e_x^2$. Thus, putting $e_z=0$ we get

$$m_{zz}^{-1}=m^{-1}\left[\gamma_1'+\frac{3\gamma_3^2-\gamma_2^2}{g}\right],\quad m_{zx}^{-1}=m_{zy}^{-1}=0,$$

$$m_{xy}^{-1}=m^{-1}(3\gamma_3^2+\gamma_2^2)\Lambda^{1/2}\frac{g^2-\gamma_2^2}{g^3},\quad g=[\gamma_2^2+3(\gamma_3^2-\gamma_2^2)\Lambda]^{1/2},$$

$$m_{xx(yy)}^{-1}=m^{-1}\left[\gamma_1'+\frac{\gamma_2^2(3\gamma_3^2+\gamma_2^2)}{g^3}\pm\frac{e_x^2-e_y^2}{2g^3}\gamma_2^2(4g^2+3\gamma_3^2+\gamma_2^2)\right], \quad \text{(c)}$$

$$D(e)=m_{zz}^{-1}(m_{xx}^{-1}m_{yy}^{-1}-(m_{xy}^{-1})^2)$$

$$=m^{-3}\left[\gamma_1'+\frac{3\gamma_3^2-\gamma_2^2}{g}\right]\left[\gamma_1'^2+5\gamma_2^2+3\gamma_3^2+\frac{\gamma_2^2(3\gamma_3^2+\gamma_2^2)}{g^3}(\gamma_1'+3g)\right].$$

We used the fact that $e_x^2-e_y^2=1-4\Lambda$, and expressed Λ in terms of g. The final answer is

$$\mu_{i,h}(\mathbf{e})=[m_{i,h}(\mathbf{e})D_{i,h}(\mathbf{e})]^{-1/3}=m\left[\frac{\gamma_1'\pm 2g(\mathbf{e})}{\gamma_1'\pm(3\gamma_3^2-\gamma_2^2)/g(\mathbf{e})}\right]^{1/3}$$

$$\times\left[\gamma_1'^2+5\gamma_2^2+3\gamma_3^2\pm\frac{\gamma_2^2(3\gamma_3^2+\gamma_2^2)}{g^3(\mathbf{e})}(\gamma_1'\pm 3g(\mathbf{e}))\right]^{-1/3}. \quad \text{(A.2)}$$

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