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Peculiarities of the Behavior of High-Frequency Conductivity of Disordered Semiconductors with Increasing Temperature

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The peculiarities of the behavior of high-frequency conductivity of disordered semiconductors associated with the hopping transport of electrons in the impurity band with increasing temperature were studied. Via the pair approximation, it is shown that the transition (crossover) observed at low temperatures ($T \approx 1\,\mathrm{K}$) in the terahertz frequency range from an almost linear to a quadratic frequency dependence of the real part of conductivity can stay on with increasing temperature and be caused by the transition from relaxation conductivity with a variable-range (frequency-dependent) hopping distance to phononless conductivity with a fixed-range hopping distance.

Keywords: hopping conductivity, universality of the frequency dependence of conductivity, phononless conductivity.

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1. Introduction

Power-law frequency dependence of conductivity $\sigma(\omega) \propto \omega^s$ (s is a constant; usually, $0.5 < s < 1$) is known to match well with $\sigma(\omega)$ of disordered semiconductors in a wide frequency range (see, for example, [1,2]). At the same time, an example of deviation from the universal power-law frequency dependence of conductivity is a transition (crossover) from almost linear to a quadratic frequency dependence of the real part of conductivity observed in Si : P, Si : B at low temperatures ($T \approx 1\,\mathrm{K}$) in the terahertz frequency region [3–5]. The investigation of the deviation of the frequency dependence of conductivity on universality ($s \approx 1$) provides the information on features of charge carrier transfer mechanism in disordered semiconductors.

The power-law frequency dependence of conductivity $\sigma(\omega) \propto \omega^s$ in case of disordered semiconductors is associated with the hopping transport of electrons over the localized states of the impurity band. According to [6], the expression for the real part of the low-temperature high-frequency relaxation conductivity (conductivity with the involvement of phonons) is written as

$$\sigma_1^{\mathrm{rel}}(\omega) = \frac{\pi^2 e^4 g_{\mathrm{F}}^2 a}{6\kappa}\, \bar{r}_\omega^3 \omega, \tag{1}$$

here $e^2/(\kappa \bar{r}_\omega) > k_{\mathrm{B}}T$, $\bar{r}_\omega = (a/2)\ln(\omega_{\mathrm{ph}}/\omega)$ is the typical hopping distance in relaxation conductivity at the frequency ω, a is the state localization radius, κ is the permittivity of medium, g_{F} is the density of localized states at the Fermi level, ω_{ph} is the typical phonon frequency (for Si : P, for example, $\omega_{\mathrm{ph}}/(2\pi) \approx 10^{13}\,\mathrm{Hz}$).

For the real part of the low-temperature phononless (resonance) conductivity in the frequency region where the energy of Coulomb interaction between electrons inside the active pairs of centers $U(r_\omega) = e^2/(\kappa r_\omega)$ exceeds the energy $\hbar\omega$, theory [7,8] gives a sublinear ($s < 1$) frequency dependence written in (1):

$$\sigma_1^{\mathrm{res}}(\omega) = \frac{\pi^2 e^4 a g_{\mathrm{F}}^2}{3\kappa}\, r_\omega^3 \omega, \tag{2}$$

where $e^2/(\kappa r_\omega) > \hbar\omega > k_{\mathrm{B}}T$, $r_\omega = a\ln(\omega_{\mathrm{c}}/\omega)$ is the typical hopping distance in phononless conductivity at the frequency ω, $\omega_{\mathrm{c}} = 2I_0/\hbar$ is the critical frequency at which the typical hopping distance becomes approximately equal to the state localization radius a, $I_0 \approx e^2/(\kappa a)$ is the pre-exponential factor in the resonance integral $I_{\lambda\lambda'} = I_0 \exp(-r_{\lambda\lambda'}/a)$, $\hbar\omega = 2I_{\lambda\lambda'}(r_\omega)$, $r_{\lambda\lambda'}$ is the center-to-center distance in the pair. With increasing frequency, the phononless contribution to conductivity prevails over the relaxation contribution. The theory of phononless conductivity [7,8] predicts crossover with increasing frequency from almost linear frequency dependence of the real part of conductivity (2) ($s \approx 1$ [7,8]) to the dependence close to the quadratic dependence ($s \approx 2$ [9]),

$$\sigma_1^{\mathrm{res}}(\omega) = \frac{\pi^2 e^2 a g_{\mathrm{F}}^2 \hbar}{3}\, r_\omega^4 \omega^2, \tag{3}$$

in the frequency region near some ω_{cr} at which the energy $\hbar\omega$ becomes comparable with the Coulomb interaction energy between the electrons inside the resonance pairs $U(r_\omega) = e^2/(\kappa r_\omega)$ [7,8],

$$\sigma_1^{\mathrm{res}}(\omega) = \frac{\pi^2 e^2 a g_{\mathrm{F}}^2}{3}\, r_\omega^4 \omega(\hbar\omega + U(r_\omega)). \tag{4}$$

The applicability region of the expressions (2)−(4) is limited from above by the critical frequency ω_{c} (for Si : P $\omega_{\mathrm{c}}/(2\pi) \approx 10^{13}\,\mathrm{Hz}$).

Expressions for contributions to conductivity (1)–(3) with accuracy up to logarithmic corrections meet the linear and quadratic frequency dependences. With frequency increasing the typical hopping distance $\bar{r}_\omega$, r_ω decreases; while functions $r_\omega^n \omega^m$ and $\bar{r}_\omega^n \omega^m \propto \omega^m \ln^n(\omega_{\mathrm{c,ph}}/\omega)$ involved in expressions for conductivity are non-monotonic frequency functions reaching their maximum at $\omega_{\max} = \omega_{\mathrm{c,ph}} \exp(-n/m)$. They may be approximated at $\omega \ll \omega_{\mathrm{c,ph}}$ by the power law $A\omega^s$ with the power exponent decreasing with the increasing frequency [10]:

$$s(\omega) = \frac{d \ln \sigma(\omega)}{d \ln \omega} = m - \frac{n}{\ln(\omega_{\mathrm{c,ph}}/\omega)}. \tag{5}$$

However, according to [11], within the representation of the frequency-dependent variable hopping distance r_ω, the resonance conductivity theory does not describe the low-temperature conductivity behavior of disordered semiconductors in the region of transition from almost linear to quadratic frequency dependence. The calculation in [11] shows that, due to the frequency dependence of the typical hopping distance r_ω, the frequency dependence $\sigma_1^{\mathrm{res}}(\omega)$ is non-monotonic at the values typical to shallow impurities, and up to the frequency corresponding to the maximum $\sigma_1^{\mathrm{res}}(\omega)$, the Coulomb interaction between the electrons of active pairs plays the main role, $\hbar\omega < e^2/(\kappa r_\omega)$, and the frequency dependence $\sigma_1^{\mathrm{res}}(\omega)$ remains close to linear. Note that the superposition of the relaxation contribution to conductivity (1) and of the phononless contribution (3), $\sigma_1(\omega) = \sigma_1^{\mathrm{res}}(\omega) + \sigma_1^{\mathrm{rel}}(\omega)$ also does not describe the transition from the linear frequency dependence of conductivity to the quadratic one with the increasing frequency.

The pair approximation of the real part of the low-temperature conductivity in [12] has shown that the observed transition from almost linear to quadratic frequency dependence in the terahertz frequency range may be associated with the transition from the conductivity with a variable hopping distance r_ω to the conductivity with a constant optimum hopping distance r_{opt} with the increasing frequency. According to [12], at high frequencies when the hybridization effects are insignificant, electron transitions inside the pairs with center-to-center distances about r_{opt} make the main contribution to the conductivity. The optimum hopping distance r_{opt} that does not depend on frequency and is defined by the system variables causes the monotonic frequency dependence of the real part of conductivity in the crossover region,

$$\sigma_1^{\mathrm{res}}(\omega) = \frac{\pi^2}{3} C_1 e^2 \rho_0^2 a^5 \omega \big(\hbar\omega + U(r_{\mathrm{opt}})\big), \tag{6}$$

where $U(r_{\mathrm{opt}}) = e^2/(\kappa r_{\mathrm{opt}})$, $r_{\mathrm{opt}} \approx 3.5a$ is the optimum hopping distance, ρ_0 is the density of states assumed as constant, C_1 is the numerical coefficient. According to [12], transition to the conductivity regime with a constant hopping distance r_{opt} occurs at $r_\omega \approx r_{\mathrm{opt}}$ $(\omega_{\mathrm{opt}} \approx 0.05\omega_{\mathrm{c}})$; and the frequency ω_{opt} is close to the crossover frequency $\omega_{\mathrm{cr}} \approx 0.1\omega_{\mathrm{c}}$, $\hbar\omega_{\mathrm{cr}} \approx e^2/(\kappa r_{\mathrm{opt}})$. In the frequency region $\omega > \omega_{\mathrm{opt}}$ $(r_\omega < r_{\mathrm{opt}})$, the electron transitions inside the pairs with center-to-center distances $r_{\lambda\lambda'} \approx r_{\mathrm{opt}}$ make the main contribution to conductivity; in this case the frequency dependence of conductivity is written as

$$\sigma_1^{\mathrm{res}}(\omega) = \frac{\pi^2}{3} C_1 e^2 \rho_0^2 a^5 \hbar\omega^2. \tag{7}$$

The calculations results of the frequency dependence of the low-temperature phononless conductivity in the high frequency region (7), when the optimum hopping distance r_{opt} does not depend on frequency, agree with the calculation results of the low-temperature phononless conductivity obtained using the self-consistent energy representations $(\hbar\omega > e^2/(\kappa r_{\mathrm{opt}}))$ [13]. The optimum hopping distance r_{opt} meets the transitions outside the Coulomb gap in the single-particle density of states; and in the frequency transition region, the Coulomb gap does not affect significantly the frequency dependence of conductivity.

Features of the behavior of the frequency dependence of the real part of conductivity of disordered semiconductors in the transition region from almost linear dependence to quadratic one at temperatures close to absolute zero $\hbar\omega > k_{\mathrm{B}}T)$ were discussed above.

According to [14], with temperature increasing, $k_{\mathrm{B}}T > e^2/(\kappa \bar{r}_\omega)$, the frequency dependence of the real part of relaxation conductivity varies insignificantly compared with (1):

$$\sigma_1^{\mathrm{rel}}(\omega) = \frac{\pi^4 e^2 \rho_0^2 a}{24} k_{\mathrm{B}} T \bar{r}_\omega^4 \omega; \tag{8}$$

and the expression for the phononless conductivity in conditions $k_{\mathrm{B}}T > \hbar\omega$, $e^2/(\kappa r_\omega)$ is written as (3) [10]. Therefore, solution of the phononless conductivity problem at temperatures $k_{\mathrm{B}}T > \hbar\omega$, $e^2/(\kappa r_\omega)$ gives the same expression as in case of low temperatures in a high frequency region, $\hbar\omega > U(r_\omega) > k_{\mathrm{B}}T$, when the Coulomb interaction between the electrons in the resonance pairs may be neglected.

Note that the transition from the relaxation conductivity (8) to phononless conductivity provided by expression (3) does not result in crossover from a sublinear to quadratic frequency dependence of the real part of conductivity, $\sigma_1(\omega) = \sigma_1^{\mathrm{res}}(\omega) + \sigma_1^{\mathrm{rel}}(\omega)$, with the increasing frequency; this is associated with the frequency dependence of the typical hopping distance r_ω leading to the decreasing power exponent $s(\omega)$ (5) meeting expression (3), with the increasing frequency. Numerical calculation of the phononless conductivity performed by the pair approximation method in [11] shows that the frequency dependence of the low-temperature zero-phonon conductivity $\sigma_1^{\mathrm{res}}(\omega)$ without considering the Coulomb interaction of electrons falling on the isolated pairs of centers is non-monotonic. Maximum $\sigma_1^{\mathrm{res}}(\omega)$ is in the range of applicability of the theory [7], $r_\omega > a$; and the conductivity attains saturation with the increasing frequency.

At the same time, according to [12], in low temperature conditions in the high frequency region $(\omega > \omega_{\mathrm{opt}} \approx \omega_{\mathrm{cr}})$, when the Coulomb interaction between electrons in the resonance pairs may be neglected, $\hbar\omega > U(r_{\rm opt})$, transition to the conductivity regime with a constant hopping distance occurs; and the conductivity has the quadratic frequency dependence (7). Transition from the relaxation conductivity (8) to phononless conductivity given by expression (7) with the increasing frequency may result in crossover from the sublinear frequency dependence of the real part of conductivity to the quadratic one. Therefore, in this case, the crossover of the frequency dependence of the real part of conductivity with the increasing temperature may be preserved and caused by the transition from relaxation conductivity with a frequency-dependent variable hopping distance to phononless conductivity with constant hopping distance.

The objective of this study was to find the behavior pattern of the high-frequency conductivity of disordered semiconductors in the frequency transition region with the increasing temperature, which included the direct calculation in pair approximation of the frequency dependence of the real part of phononless conductivity in the frequency transition region at $k_{\rm B}T > \hbar\omega$, $e^2/(\kappa r_{\rm opt})$. The restriction put on the temperatures of interest from above is associated with the transition to the charge carrier band transport.

2. Phononless conductivity calculation in the frequency transition region in conditions $k_{\rm B}T > \hbar\omega$, $e^2/(\kappa r_{\rm opt})$

According to [12], the matrix elements involved in the expression for the pair approximation of phononless conductivity [15]:

$$\sigma_1^{\rm res}(\omega) = \frac{\pi e^2\omega}{V_0}\sum_{\{\lambda,\lambda'\},\lambda\neq\lambda'} |\langle\Psi^-_{\lambda\lambda'}|(\mathbf{n},\mathbf{r})|\psi^+_{\lambda\lambda'}\rangle|^2$$

$$\times\left(n_{\rm F}(\varepsilon^-_{\lambda\lambda'}) - n_{\rm F}(\varepsilon^+_{\lambda\lambda'})\right)\delta(\varepsilon^-_{\lambda\lambda'} - \varepsilon^+_{\lambda\lambda'} + \hbar\omega), \quad (9)$$

in case of hydrogen-like impurity centers, are equal to

$$\langle\Psi^-_{\lambda\lambda'}|(\mathbf{n},\mathbf{r})|\Psi^+_{\lambda\lambda'}\rangle = (\mathbf{n},\mathbf{r}_{\lambda\lambda'})\,\frac{I_{\lambda\lambda'}}{\Gamma_{\lambda\lambda'}}$$

$$+\frac{(\varepsilon^0_\lambda - \varepsilon^0_{\lambda'})\langle\Psi_\lambda|(\mathbf{n},\mathbf{r})|\Psi_{\lambda'}\rangle}{\Gamma_{\lambda\lambda'}}, \quad (10)$$

here $\Psi^\pm_{\lambda\lambda'} = C^\pm_\lambda\Psi_\lambda + C^\pm_{\lambda'}\Psi_{\lambda'}$ are hybridized wave functions of the ground states of electron $\Psi_\lambda, \Psi_{\lambda'}$ on the isolated localization centers λ and λ', $\mathbf{n}$ is the single vector parallel to the external electrical field, $\langle\Psi_\lambda|\mathbf{r}|\Psi_\lambda\rangle = \mathbf{r}_\lambda$, $\langle\Psi_{\lambda'}|\mathbf{r}|\Psi_{\lambda'}\rangle = \mathbf{r}_{\lambda'} = \mathbf{r}_\lambda + \mathbf{r}_{\lambda\lambda'}$, $\mathbf{r}_\lambda$ is the radius vector of center λ, $\mathbf{r}_{\lambda\lambda'}$ is the radius vector of center λ' with respect to center λ, $\langle\Psi_\lambda(\mathbf{n},\mathbf{r})|\Psi_{\lambda'}\rangle = \langle\Psi_{\lambda'}|(\mathbf{n},\mathbf{r})|\Psi_\lambda\rangle$, $n_{\rm F}(\varepsilon)$ is the mean occupation number of state with energy ε, V_0 is the system volume. Wave functions

$$\Psi^-_{\lambda\lambda'} = \frac{1}{\sqrt{1 + \frac{4I^2_{\lambda\lambda'}}{(\varepsilon^0_\lambda - \varepsilon^0_{\lambda'} + \Gamma_{\lambda\lambda'})^2}}}$$

$$\times\left(-\frac{2I_{\lambda\lambda'}}{\varepsilon^0_\lambda - \varepsilon^0_{\lambda'} + \Gamma_{\lambda\lambda'}}\,\Psi_\lambda + \Psi_{\lambda'}\right), \quad (11.1)$$

$$\Psi^+_{\lambda\lambda'} = \frac{1}{\sqrt{1 + \frac{4I^2_{\lambda\lambda'}}{(\varepsilon^0_\lambda - \varepsilon^0_{\lambda'} + \Gamma_{\lambda\lambda'})^2}}}$$

$$\times\left(\Psi_\lambda + \frac{2I_{\lambda\lambda'}}{\varepsilon^0_\lambda - \varepsilon^0_{\lambda'} + \Gamma_{\lambda\lambda'}}\,\Psi_{\lambda'}\right), \quad (11.2)$$

meet the lower $\varepsilon^-_{\lambda\lambda'}$ and upper $\varepsilon^+_{\lambda\lambda'}$ energy levels,

$$\varepsilon^\pm_{\lambda\lambda'} = \frac{\varepsilon^0_\lambda + \varepsilon^0_{\lambda'}}{2} \pm \frac{1}{2}\sqrt{(\varepsilon^0_\lambda - \varepsilon^0_{\lambda'})^2 + 4I^2_{\lambda\lambda'}}, \quad (12)$$

here

$$\Gamma_{\lambda\lambda'} = \varepsilon^+_{\lambda\lambda'} - \varepsilon^-_{\lambda\lambda'} = \sqrt{(\varepsilon^0_\lambda - \varepsilon^0_{\lambda'})^2 + 4I^2_{\lambda\lambda'}},$$

ε^0_λ, $\varepsilon^0_{\lambda'}$ are seed energies (without considering the hybridization), $I_{\lambda\lambda'} = \langle\Psi_\lambda|\hat{U}_\lambda|\Psi_{\lambda'}\rangle$ is the resonance integral; $\hat{U}_\lambda \approx \hat{U}_\lambda + e\phi(\mathbf{r}_\lambda)$ is the potential energy of the localized electron in the point of the center with number λ taking into account the Coulomb shift $e\phi(\mathbf{r}_\lambda)$ associated with other charged centers in point $\mathbf{r}_\lambda$.

For the resonance pairs of levels with seed energies $\varepsilon^0_\lambda \approx \varepsilon^0_{\lambda'}$ and optimum center-to-center distances r_ω making the major contribution to the phononless conductivity at frequencies $\omega < \omega_{\rm opt}$ $(r_\omega > r_{\rm opt})$, the matrix elements (10) are written as

$$\langle\Psi^-_{\lambda\lambda'}|(\mathbf{n},\mathbf{r})|\Psi^+_{\lambda\lambda'}\rangle \approx (\mathbf{n},\mathbf{r}_{\lambda\lambda'})\,\frac{I_{\lambda\lambda'}}{\Gamma_{\lambda\lambda'}}. \quad (13.1)$$

The matrix elements written as (13.1) were used in [7,9] to calculate the frequency dependence of low-temperature phononless conductivity (2)–(4).

At high frequencies, $\omega > \omega_{\rm opt}$ $(r_\omega < r_{\rm opt})$ the main contribution to the real part of phononless conductivity is made by the center pairs with wide energy spread of levels, $|\varepsilon^0_\lambda - \varepsilon^0_{\lambda'}| > 2I_{\lambda\lambda'}$, and optimum frequency-independent center-to-center distance, $r_{\lambda\lambda'} \approx r_{\rm opt}$; for such center pairs, matrix elements (10) are equal to

$$\langle\Psi^-_{\lambda\lambda'}|(\mathbf{n},\mathbf{r})|\Psi^+_{\lambda\lambda'}\rangle \approx \langle\Psi_\lambda|(\mathbf{n},\mathbf{r})|\Psi_{\lambda'}\rangle. \quad (13.2)$$

Expressions (13.2) were used in [16] to calculate the low-temperature phononless conductivity $\sigma_1^{\rm res}(\omega)$ in the high frequency region (6), (7). Since the major contribution to the phononless conductivity is made by the pairs whose center-to-center distance is larger than the localization radius, $r_{\lambda\lambda'} > a$, then for hydrogen-like impurities in the isotropic dispersion law approximation, the matrix element (13.2) is written as

$$\langle \Psi_\lambda | (\mathbf{n}, \mathbf{r}) | \Psi_{\lambda'} \rangle \approx \frac{r_{\lambda\lambda'}^3}{a^2} \exp(-r_{\lambda\lambda'}/a) \cos\theta, \tag{14}$$

where θ is the angle between vectors $\mathbf{n}$ and $\mathbf{r}_{\lambda\lambda'}$, $\Psi_\lambda(\mathbf{r}) = (1/\sqrt{\pi \cdot a^3}) \exp(-|\mathbf{r} - \mathbf{r}_\lambda|/a)$.

To calculate the frequency dependence of conductivity $\sigma_1^{\mathrm{res}}(\omega)$ in the frequency transition region, $\omega \approx \omega_{\mathrm{opt}}$, the general form of matrix elements (10) shall be used. Proceeding in (9) from summation to integration, we obtain [12]:

$$\sigma_1^{\mathrm{res}}(\omega) = \sigma_{1\mathrm{a}}^{\mathrm{res}}(\omega) + \sigma_{1\mathrm{b}}^{\mathrm{res}}(\omega) + \sigma_{1\mathrm{c}}^{\mathrm{res}}(\omega), \tag{15}$$

$$\sigma_{1\mathrm{a}}^{\mathrm{res}}(\omega) = \frac{4\pi^2 e^2 \rho_0^2 \omega}{3} \times \int\limits_{r_\omega}^{\infty} dr_{\lambda\lambda'} r_{\lambda\lambda'}^4 \int\limits_{-\infty}^{\infty} d\varepsilon_{\lambda\lambda'}^- \int d\varepsilon_{\lambda\lambda'}^+ \Phi(\varepsilon_{\lambda\lambda'}^-, \varepsilon_{\lambda\lambda'}^+, r_{\lambda\lambda'}) \times \frac{I^2(r_{\lambda\lambda'})}{(\varepsilon_{\lambda\lambda'}^+ - \varepsilon_{\lambda\lambda'}^-)^2} \left(n_{\mathrm{F}}(\varepsilon_{\lambda\lambda'}^-) - n_{\mathrm{F}}(\varepsilon_{\lambda\lambda'}^+)\right) \delta(\varepsilon_{\lambda\lambda'}^- - \varepsilon_{\lambda\lambda'}^+ + \hbar\omega), \tag{16.1}$$

$$\sigma_{1\mathrm{b}}^{\mathrm{res}}(\omega) = \frac{4\pi^2 e^2 \rho_0^2 \omega}{3} \int\limits_{r_\omega}^{\infty} dr_{\lambda\lambda'} \frac{r_{\lambda\lambda'}^6}{a^2} \exp(-r_{\lambda\lambda'}/a) \times \int\limits_{-\infty}^{\infty} d\varepsilon_{\lambda\lambda'}^- \int d\varepsilon_{\lambda\lambda'}^+ \Phi(\varepsilon_{\lambda\lambda'}^-, \varepsilon_{\lambda\lambda'}^+, r_{\lambda\lambda'}) \times \frac{2I_{\lambda\lambda'}}{(\varepsilon_{\lambda\lambda'}^+ - \varepsilon_{\lambda\lambda'}^-)^2} \sqrt{(\varepsilon_{\lambda\lambda'}^+ - \varepsilon_{\lambda\lambda'}^-)^2 - 4I_{\lambda\lambda'}^2} \times \left(n_{\mathrm{F}}(\varepsilon_{\lambda\lambda'}^-) - n_{\mathrm{F}}(\varepsilon_{\lambda\lambda'}^+)\right) \delta(\varepsilon_{\lambda\lambda'}^- - \varepsilon_{\lambda\lambda'}^+ + \hbar\omega), \tag{16.2}$$

$$\sigma_{1\mathrm{c}}^{\mathrm{res}}(\omega) = \frac{4\pi^2 e^2 \rho_0^2 \omega}{3} \int\limits_{r_\omega}^{\infty} dr_{\lambda\lambda'} \frac{r_{\lambda\lambda'}^8}{a^4} \exp(-2r_{\lambda\lambda'}/a) \times \int\limits_{-\infty}^{\infty} d\varepsilon_{\lambda\lambda'}^- \int d\varepsilon_{\lambda\lambda'}^+ \Phi(\varepsilon_{\lambda\lambda'}^-, \varepsilon_{\lambda\lambda'}^+, r_{\lambda\lambda'}) \times \frac{\left((\varepsilon_{\lambda\lambda'}^+ - \varepsilon_{\lambda\lambda'}^-)^2 - 4I_{\lambda\lambda'}^2\right)}{(\varepsilon_{\lambda\lambda'}^+ - \varepsilon_{\lambda\lambda'}^-)^2} \left(n_{\mathrm{F}}(\varepsilon_{\lambda\lambda'}^-) - n_{\mathrm{F}}(\varepsilon_{\lambda\lambda'}^+)\right) \times \delta(\varepsilon_{\lambda\lambda'}^- - \varepsilon_{\lambda\lambda'}^+ + \hbar\omega), \tag{16.3}$$

here

$$\Phi(\varepsilon_{\lambda\lambda'}^-, \varepsilon_{\lambda\lambda'}^+, r_{\lambda\lambda'}) = \frac{\varepsilon_{\lambda\lambda'}^+ - \varepsilon_{\lambda\lambda'}^-}{\sqrt{(\varepsilon_{\lambda\lambda'}^+ - \varepsilon_{\lambda\lambda'}^-)^2 - 4I_{\lambda\lambda'}^2}}$$

is the transition Jacobian from seed energies ε_λ^0, $\varepsilon_{\lambda'}^0$ (without hybridization) to energies $\varepsilon_{\lambda\lambda'}^-$, $\varepsilon_{\lambda\lambda'}^+$.

The difference of mean occupation numbers $n_{\mathrm{F}}(\varepsilon_{\lambda\lambda'}^-) - n_{\mathrm{F}}(\varepsilon_{\lambda\lambda'}^+)$ involved in (9) is equal to

$$n_{\mathrm{F}}(\varepsilon_{\lambda\lambda'}^-) - n_{\mathrm{F}}(\varepsilon_{\lambda\lambda'}^+) = \left(1 - \exp\left(-\frac{\hbar\omega}{k_{\mathrm{B}}T}\right)\right) \times \exp\left(\frac{\Omega - (\varepsilon_{\lambda\lambda'}^- - \mu)}{k_{\mathrm{B}}T}\right), \tag{17}$$

where $\exp\left(\frac{\Omega - (\varepsilon_{\lambda\lambda'}^- - \mu)}{k_{\mathrm{B}}T}\right)$ is the equilibrium probability of single occupation of a pair of centers with the occupied state energy $\varepsilon_{\lambda\lambda'}^-$, μ is the Fermi level;

$$\exp\left(-\frac{\Omega}{k_{\mathrm{B}}T}\right) = 1 + \exp\left(-\frac{(\varepsilon_{\lambda\lambda'}^- - \mu)}{k_{\mathrm{B}}T}\right) + \exp\left(-\frac{(\varepsilon_{\lambda\lambda'}^+ - \mu)}{k_{\mathrm{B}}T}\right) + \exp\left(-\frac{(\varepsilon_{\lambda\lambda'}^- + \varepsilon_{\lambda\lambda'}^+ - 2\mu)}{k_{\mathrm{B}}T}\right). \tag{18}$$

According to [7], the Coulomb interaction between electrons localized simultaneously on the pair of centers of interest can be considered assuming the energy equal to $\varepsilon_\lambda^0 + \varepsilon_{\lambda'}^0 + e^2/\kappa r_{\lambda\lambda'}$. Then the expression for the partition function (18) is written as

$$\exp\left(-\frac{\Omega}{k_{\mathrm{B}}T}\right) = 1 + \exp\left(-\frac{(\varepsilon_{\lambda\lambda'}^- - \mu)}{k_{\mathrm{B}}T}\right) + \exp\left(-\frac{(\varepsilon_{\lambda\lambda'}^+ - \mu)}{k_{\mathrm{B}}T}\right) + \exp\left(-\frac{(\varepsilon_\lambda^0 + \varepsilon_{\lambda'}^0 + e^2/\kappa r_{\lambda\lambda'} - 2\mu)}{k_{\mathrm{B}}T}\right), \tag{19}$$

where $\varepsilon_{\lambda\lambda'}^- + \varepsilon_{\lambda\lambda'}^+ = \varepsilon_\lambda^0 + \varepsilon_{\lambda'}^0$. The difference of mean occupation numbers taking into account the law of conservation of energy, $\varepsilon_{\lambda\lambda'}^+ = \varepsilon_{\lambda\lambda'}^- + \hbar\omega$, and equality $\varepsilon_{\lambda\lambda'}^- + \varepsilon_{\lambda\lambda'}^+ = \varepsilon_\lambda^0 + \varepsilon_{\lambda'}^0$ may be written as

$$n_{\mathrm{F}}(\varepsilon_{\lambda\lambda'}^-) - n_{\mathrm{F}}(\varepsilon_{\lambda\lambda'}^+) = \frac{\left(1 - \exp\left(-\frac{\hbar\omega}{k_{\mathrm{B}}T}\right)\right)}{\exp\left(-\frac{(\varepsilon_{\lambda\lambda'}^+ + e^2/\kappa r_{\lambda\lambda'} - \mu)}{k_{\mathrm{B}}T}\right) + \exp\left(-\frac{\hbar\omega}{k_{\mathrm{B}}T}\right) + 1 + \exp\left(\frac{(\varepsilon_{\lambda\lambda'}^- - \mu)}{k_{\mathrm{B}}T}\right)}. \tag{20}$$

Having integrated (16.1), (16.2), (16.3) with respect of energies $\varepsilon_{\lambda\lambda'}^-$, $\varepsilon_{\lambda\lambda'}^+$ taking into account (20) provided that $k_{\mathrm{B}}T > \hbar\omega$, $e^2/(\kappa r_{\mathrm{opt}})$, we obtain

$$\sigma_{1\mathrm{a}}^{\mathrm{res}}(\omega) = \frac{4\pi^2 e^2 \rho_0^2}{3\hbar} \int\limits_{r_\omega}^{\infty} r_{\lambda\lambda'}^4 \hbar\omega \frac{I_{\lambda\lambda'}^2}{\sqrt{(\hbar\omega)^2 - 4I_{\lambda\lambda'}^2}} dr_{\lambda\lambda'}, \tag{21.1}$$

$$\sigma_{1\mathrm{b}}^{\mathrm{res}}(\omega) = \frac{4\pi^2 e^2 \rho_0^2 \omega_{\mathrm{C}}}{3} \int\limits_{r_\omega}^{\infty} \frac{r_{\lambda\lambda'}^6}{a^2} \hbar\omega \exp(-2r_{\lambda\lambda'}/a) dr_{\lambda\lambda'}, \tag{21.2}$$

$$\sigma_{1c}^{\text{res}}(\omega) = \frac{4\pi^2 e^2 \rho_0^2}{3\hbar}$$

$$\times \int_{r_\omega}^{\infty} \frac{r_{\lambda\lambda'}^8}{a^4} \hbar\omega \exp(-2r_{\lambda\lambda'}/a)\sqrt{(\hbar\omega)^2 - 4I_{\lambda\lambda'}^2} dr_{\lambda\lambda'}; \tag{21.3}$$

(21.1), (21.2), (21.3) consider that

$$\exp\left(\frac{\Omega - (\varepsilon_{\lambda\lambda'}^- - \mu)}{k_{\text{B}}T}\right)$$

$$\approx \left(\exp\left(\frac{(\varepsilon_{\lambda\lambda'}^- - \mu)}{k_{\text{B}}T}\right) + 2 + \exp\left(-\frac{(\varepsilon_{\lambda\lambda'}^- - \mu)}{k_{\text{B}}T}\right)\right)^{-1}, \tag{22}$$

$$\int_{-\infty}^{\infty} \big(n_{\text{F}}(\varepsilon_{\lambda\lambda'}^-) - n_{\text{F}}(\varepsilon_{\lambda\lambda'}^- + \hbar\omega)\big) d\varepsilon_{\lambda\lambda'}^- = \left(1 - \exp\left(-\frac{\hbar\omega}{k_{\text{B}}T}\right)\right)$$

$$\times \int_{-\infty}^{\infty} \exp\left(\frac{\Omega - (\varepsilon_{\lambda\lambda'}^- - \mu)}{k_{\text{B}}T}\right) d\varepsilon_{\lambda\lambda'}^- \approx \hbar\omega, \tag{23}$$

where

$$\exp\left(\frac{\Omega - (\varepsilon_{\lambda\lambda'}^- - \mu)}{k_{\text{B}}T}\right) \approx \frac{1}{4}\,\text{ch}^{-2}\left(\frac{\varepsilon_{\lambda\lambda'}^- - \mu}{2k_{\text{B}}T}\right),$$

$$\int_{-\infty}^{\infty} \exp\left(\frac{\Omega - (\varepsilon_{\lambda\lambda'}^- - \mu)}{k_{\text{B}}T}\right) d\varepsilon_{\lambda\lambda'}^- \approx k_{\text{B}}T.$$

Recall that in case of low temperatures, $k_{\text{B}}T < \hbar\omega$, $e^2/(\kappa r_\omega)$, integration with respect to the energy of the difference of mean occupation numbers gives

$$\int_{-\infty}^{\infty} (n_{\text{F}}(\varepsilon_{\lambda\lambda'}^-) - n_{\text{F}}(\varepsilon_{\lambda\lambda'}^- + \hbar\omega)) d\varepsilon_{\lambda\lambda'}^- = \int_{\mu - \hbar\omega - e^2/\kappa r_{\lambda\lambda'}}^{\mu} d\varepsilon_{\lambda\lambda'}^-$$

$$= \hbar\omega + \frac{e^2}{\kappa r_{\lambda\lambda'}};$$

and expressions for conductivity components can be derived by substitution in (21.1), (21.2), (21.3) $\hbar\omega$ for $\hbar\omega + e^2/(\kappa r_{\lambda\lambda'})$ under the integral signs [12].

In conditions $k_{\text{B}}T > \hbar\omega$, $e^2/(\kappa r_{\text{opt}})$ in the frequency region $\omega \ll \omega_{\text{c}}$, (21.1) makes the main contribution to the phononless conductivity; in this case the expression for zero-phonon conductivity is written as (3):

$$\sigma_{1a}^{\text{res}}(\omega) = \frac{\pi^2 e^2 a \rho_0^2 \hbar}{3} r_\omega^4 \omega^2. \tag{24}$$

In the conductivity regime with a variable hopping distance $r_\omega > r_{\text{opt}}$ $(\omega < \omega_{\text{opt}})$ the contributions from the terms (21.2), (21.3) to the phononless conductivity (15) are exponentially low. The frequency dependence of the real part of phononless conductivity (24) appears to be stronger than the frequency dependence of conductivity (2) meeting the low temperature case.

At high frequencies $\omega > \omega_{\text{opt}}$ $(r_\omega < r_{\text{opt}})$ in the regime with a constant hopping distance r_{opt}, term (21.3) makes the decisive contribution to the phononless conductivity (15). The term under the integral sign in (21.3) has a sharp maximum in the vicinity of r_{opt}; in conditions $r_\omega < r_{\text{opt}}$, the contribution (21.3) may be written as

$$\sigma_{1c}^{\text{res}}(\omega) \approx \frac{4\pi^2 e^2 \rho_0^2 \hbar}{3} \omega^2 \int_0^{\infty} \frac{r_{\lambda\lambda'}^8}{a^4} \exp(-2r_{\lambda\lambda'}/a) dr_{\lambda\lambda'}. \tag{25}$$

(25) considers that

$$\sqrt{(\hbar\omega)^2 - 4I_{\lambda\lambda'}^2} \approx \hbar\omega$$

at $r_\omega + a < r_{\lambda\lambda'}$. Integrating in (25), we get an expression for the phononless conductivity (7)

$$\sigma_{1c}^{\text{res}}(\omega) = \frac{\pi^2}{3} C_1 e^2 \rho_0^2 a^5 \hbar \omega^2, \tag{26}$$

where $C_1 \approx 315$ is the numerical coefficient. From the integration function form in expression (25) it follows that the major contribution to the phononless conductivity at high frequencies is made by the pairs whose center-to-center distances are about $r_{\lambda\lambda'} \approx r_{\text{opt}}$; the maximum term under the integral sign is achieved at the optimum value equal to $r_{\text{opt}} = 4a$.

3. Conclusion

Figure 1 shows the results of calculation of the frequency dependence of phononless conductivity $\sigma_1^{\text{res}}(\omega/\omega_{\text{c}})$ (15) in the transition region from the variable to constant

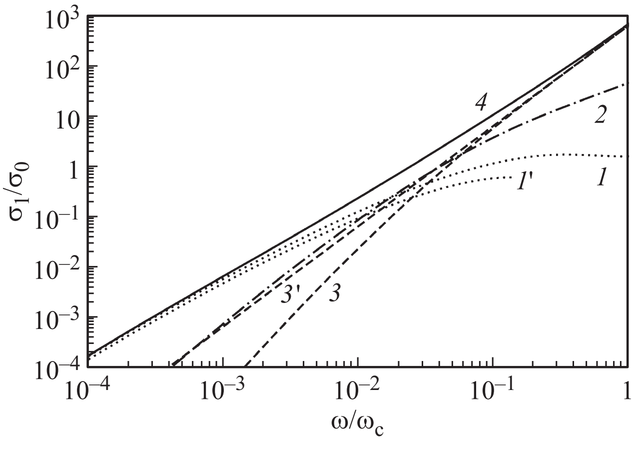

Figure 1. Frequency dependences of the real part terms of phononless conductivity $\sigma_1^{\text{res}}/\sigma_0$: curve *1* — (21.1), *1'* — (24), *2* — (21.2), *3* — (21.3), *3'* — (26); *4* — frequency dependence of phononless conductivity (15). The conductivity is normalized to $\sigma_0 = \frac{1}{3}\pi^2 e^4 a^4 \rho_0^2 \omega_{\text{c}}/\kappa$.

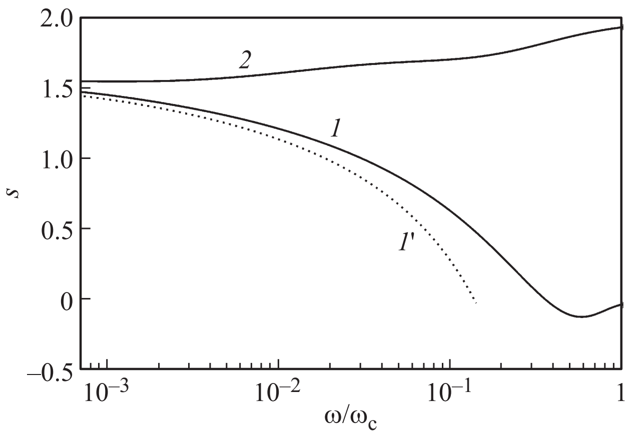

Figure 2. Frequency dependences $s(\omega/\omega_c) = \frac{d\ln(\sigma)}{d\ln(\omega)} = \frac{\omega/\omega_c}{\sigma/\sigma_0}\frac{d\sigma/\sigma_0}{d\omega/\omega_c}$. Curve *1* corresponds to the phononless conductivity with a variable hopping distance (21.1); curve *1'* corresponds to the expression for phononless conductivity with a variable hopping distance (24); curve *2* corresponds to the phononless conductivity (15).

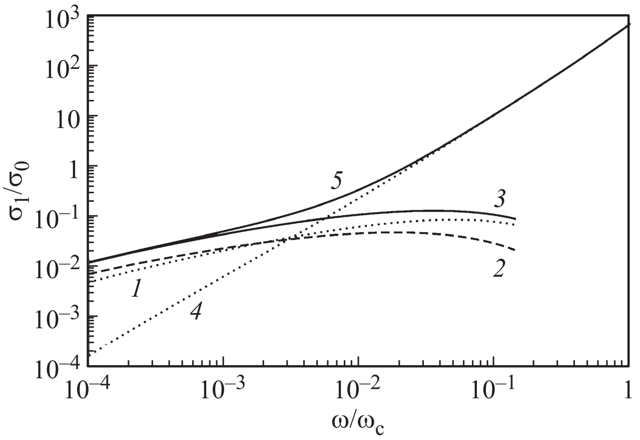

Figure 3. Curve *1* — frequency dependence of relaxation conductivity $\sigma_1^{\mathrm{rel}}/\sigma_0$ (1); *2* — frequency dependence of relaxation conductivity (8), $T = 60\,\mathrm{K}$, *3* — frequency dependence of the interpolation expression for the relaxation conductivity (27); *4* — frequency dependence of phononless conductivity $\sigma_1^{\mathrm{res}}/\sigma_0$ (15); *5* — superposition of relaxation (27) and phononless (15) contributions to the conductivity, $\sigma_1(\omega) = \sigma_1^{\mathrm{res}}(\omega) + \sigma_1^{\mathrm{rel}}(\omega)$.

hopping distance in conditions $k_BT > \hbar\omega$, $e^2/(\kappa r_{\mathrm{opt}})$. For typical values of $a \approx 80\,\text{Å}$, $\kappa \approx 10$ in case of disordered semiconductors, we have $e^2/(\kappa r_{\mathrm{opt}}) \approx 4\,\mathrm{meV}$; in this case a frequency about 1 THz ($\omega \approx 0.1\omega_c$) meets the equality $\hbar\omega \approx e^2/(\kappa r_{\mathrm{opt}})$. According to the calculation, the transition for the phononless conductivity from a variable r_ω to constant hopping distance $r_{\mathrm{opt}} \approx 4a$ occurs at $r_{\mathrm{opt}} \approx r_\omega$ ($\omega_{\mathrm{opt}} \approx 0.02\omega_c$). At low frequencies $\omega < \omega_{\mathrm{opt}}$ ($r_\omega > r_{\mathrm{opt}}$) in the conductivity regime with a variable hopping distance r_ω, the phononless conductivity is determined by expression (24). The frequency dependence of the term (21.1) is non-monotonic (Figures 1 and 2); this is associated with the decrease in typical hopping distance r_ω with the increasing frequency. At high frequencies $\omega > \omega_{\mathrm{opt}}$ ($r_\omega < r_{\mathrm{opt}}$) in the conductivity regime with a constant hopping distance r_{opt}, the expression for the phononless conductivity is written as (26); in this case the term (21.3) makes the decisive contribution to the phononless conductivity (15). Thus, like in the low temperature case ($e^2/(\kappa r_\omega)$, $\hbar\omega > k_BT$), in conditions $k_BT > \hbar\omega$, $e^2/(\kappa r_{\mathrm{opt}})$, in the high frequency region, a transition to the constant hopping distance occurs for the phononless conductivity, when the major contribution to the conductivity is made by the electron transitions inside the pairs with the optimum center-to-center distances $r_{\lambda\lambda'} \approx r_{\mathrm{opt}}$.

Figure 3 shows the superposition of the relaxation and phononless contributions to the conductivity, $\sigma_1(\omega) = \sigma_1^{\mathrm{res}}(\omega) + \sigma_1^{\mathrm{rel}}(\omega)$. With the increasing temperature, $k_BT > e^2/(\kappa r_\omega)$, the frequency dependence of the real part of relaxation conductivity becomes slightly weaker [17]; in this case, the interpolation expression for the real part of relaxation conductivity is written as [10]:

$$\sigma_1^{\mathrm{rel}}(\omega) = \frac{\pi^4 e^2 a \rho_0^2}{24}\,\omega \bar{r}_\omega^4 \left(k_BT + \frac{4}{\pi^2}U(\bar{r}_\omega)\right). \tag{27}$$

Figure 4 shows that the transition from the relaxation conductivity to phononless conductivity in the variable hopping distance regime given by expressions (21.1) and (24) with the increasing frequency does not result in crossover from the sublinear frequency dependence of the real part of conductivity to the quadratic one. At the same time, the transition from the relaxation conductivity to phononless

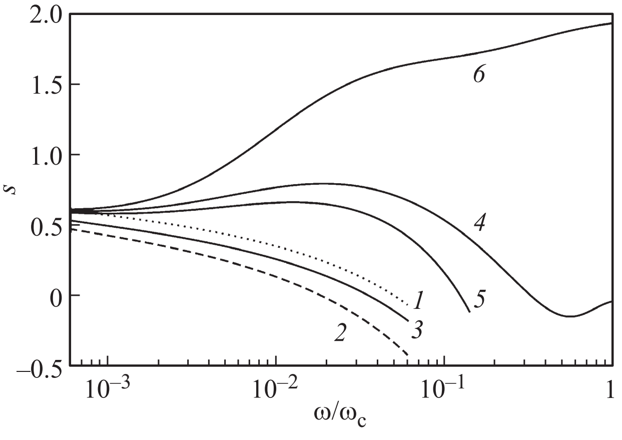

Figure 4. Frequency dependences $s(\omega/\omega_c) = \frac{d\ln(\sigma)}{d\ln(\omega)} = \frac{\omega/\omega_c}{\sigma/\sigma_0}\frac{d\sigma/\sigma_0}{d\omega/\omega_c}$. Curve *1* corresponds to the relaxation conductivity $\sigma_1^{\mathrm{rel}}/\sigma_0$ (1); curve *2* corresponds to the relaxation conductivity (8); curve *3* corresponds to the interpolation expression for the relaxation conductivity (27); curve *4* corresponds to the superposition of the relaxation contribution (27) and contribution (21.1) to the phononless conductivity (15); curve *5* corresponds to the superposition of the relaxation contribution (27) and contribution (24) to the phononless conductivity (15); curve *6* correposnds to the superposition of the relaxation (27) and phononless (15) contributions to conductivity, $\sigma_1(\omega) = \sigma_1^{\mathrm{res}}(\omega) + \sigma_1^{\mathrm{rel}}(\omega)$.

conductivity with the constant hopping distance given by expression (26) with the increasing frequency causes the crossover from the sublinear frequency dependence of the real part of conductivity to the quadratic one (Figures 3 and 4). The superlinearity ($s > 1$) of the real part of disordered semiconductor conductivity in the frequency transition region is a sign of crossover effect.

Note that the transition frequency for the phononless conductivity from the variable to constant hopping distance, $\omega_{\text{opt}} \approx 0.02\omega_c$, is about the crossover frequency ω_{cr}, in the vicinity of which transition from the relaxation conductivity to phononless one occurs, $\sigma_1^{\text{rel}}(\omega_{\text{cr}}) = \sigma_1^{\text{res}}(\omega_{\text{cr}})$. Therefore, the transition from sublinear to quadratic frequency dependence of the real part of conductivity $\sigma_1(\omega)$ occurs in the vicinity of frequency ω_{opt} ($r_\omega \approx r_{\text{opt}}$).

Thus, with the increasing temperature, the transition from almost linear to quadratic frequency dependence of the real part of conductivity observed at low temperatures in disordered semiconductors may be preserved; whilst, with the increasing temperature, the crossover of the frequency dependence of the real part of conductivity in the terahertz frequency range may be caused by the transition from the relaxation conductivity with a variable frequency-dependent hopping distance to the phononless conductivity with a constant hopping distance.

Conflict of interest

The authors declare that they have no conflict of interest.

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