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ON THE PROBLEM OF NEUTRON SPECTROSCOPY OF PARAMETRICALLY NONEQUILIBRIUM QUASIPARTICLES IN SOLIDS.

II. Numerical Calculations of Inelastic Scattering Cross Sections in InSb

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1. COHERENT SCATTERING CROSS SECTIONS ON THE MIXED PLASMON-PHONON MODES

In the previous work [1] the influence of the parametric wave excitation phenomenon on the process of neutron inelastic scattering on quasiparticles in solids was investigated, and analytical expressions for the cross sections have been obtained for the cases of parallel and perpendicular polarizations of the driving laser electric field $\vec{E}_0(t)$ with respect to the propagation direction $\vec{k}$ of the modes considered. The main effect revealed by these formulae is an anomalously large increase of the scattering cross sections when approaching the borderline of the parametric instability regions. To analyse this effect quantitatively, what is the purpose of this paper, we shall take into consideration the case of coherent neutron inelastic scattering on the longitudinal plasmon-phonon modes in the system which takes place in the $\vec{k} \parallel \vec{E}_0$ geometry. In this geometry, as is well known (see ref. [2], for example), we have one of the most simple examples of coupling between eigenwaves of the electron-phonon system caused by high-intensity electromagnetic radiation fields. So far, for further calculations we rewrite here the explicit expression for the coherent scattering cross section:

$$\left(\frac{d^2\sigma}{d\omega\, d\Omega}\right)_{coh.} = \frac{N}{8\pi^2}\frac{P'}{P}\sum_j |\Phi(\vec{k},\vec{k}',j)|^2\, \omega^{-1}_{k'j} \langle Q^2_{k'j}(\omega)\rangle , \qquad (1.1)$$

where

$$\Phi(\vec{k},\vec{q},j) = \sum_s \left(\frac{\pi\sigma_s}{M_s}\right)^{1/2} (\vec{k}\vec{e}_{qjs})\, e^{2\pi i \vec{K}_j \vec{R}^{\circ}_s} . \qquad (1.2)$$

Here, N is the number of unit cells in the crystal, σ_s is the microscopic nuclear scattering cross section for coherent processes, $\vec{q} = \vec{k} - 2\pi\vec{K}$, where $\vec{k} = \vec{P}' - \vec{P}$ is the momentum transfer vector with $\vec{P}$ and $\vec{P}'$ the momentum of a neutron in the initial and final states, respectively, so that the corresponding energy transfer is $\omega = P'^2/2m_N - P^2/2m_N$ (m_N is the neutron mass and the system of units with $\hbar = 1$ is used throughout this paper), $\vec{K}$ is the reciprocal lattice wave vector; and $\vec{R}^{\circ}_s$, the position vector of the atom s (with the mass M_s)

in each unit cell, $\vec{e}_{qjs}$ is the polarization vector of the mode j with the fixed wave number q. The phonon correlation function $\langle Q^2_{qj}(\omega)\rangle$ that contains the effect of the external laser field is of the form (as we consider certain fixed modes of the crystal, the index j can be omitted):

$$\langle Q^2_q(\omega)\rangle = \theta(\vec{q},\omega,\lambda)\,\{\,|\,F(\vec{q},\omega,T,\lambda)\;\times$$
$$\{\delta(\omega+\omega_1)+\delta(\omega+\omega_2)+\delta(\omega-\omega_1)+\delta(\omega-\omega_2)\}\,, \qquad (2.1)$$

where the main notation is as follows:

$$\theta(\vec{q},\omega,\lambda) \equiv 2\pi\,\left|\frac{\omega_{L0}(\omega^2-\omega_p^2)}{\omega(\omega_1^2-\omega_2^2)}\right|\times$$
$$\left[1-\frac{\alpha(\omega)}{\alpha(\omega_0-|\omega|)}\,I^2(\vec{q},\omega,\lambda)\,\frac{\mathrm{Im}\,\Pi_q(|\omega|)}{\mathrm{Im}\,\Pi_q(\omega_0-|\omega|)}\right]^{-1}, \qquad (2.2)$$

$$F(\vec{q},\omega,T,\lambda) = |\,1-I^2(\vec{q},\omega,\lambda)\,|^{-1}\{|(e^{\omega/T}-1)^{-1}-$$
$$I^2(\vec{q},\omega,\lambda)\,(e^{(\omega-\omega_0\,\mathrm{sgn}\omega)/T}-1)^{-1}|\}\,, \qquad (2.3)$$

$$\alpha(\omega) \equiv \frac{\omega^2-\omega_p^2}{(\omega_1+|\omega|)(\omega_2+|\omega|)},\quad \Pi_q(\omega) \equiv \frac{\epsilon_\ell(\vec{q},\omega)}{[1-\phi_q P_q(\omega)]\,D_q(\omega)}\,, \qquad (2.4)$$

$$I^2(\vec{q},\omega,\lambda) \equiv J_1^2(\lambda)\,|\,v_q\,|^2\,[1-\phi_q P_q(|\omega|)]\,[1-\phi_q P_q(\omega_0-|\omega|)]\;\times$$
$$\frac{[P_q(|\omega|)-P_q(\omega_0-|\omega|)]\,[D_q^{-1}(|\omega|)-D_q^{-1}(\omega_0-|\omega|)]}{\mathrm{Im}\,\Pi_q(|\omega|)\;\mathrm{Im}\,\Pi_q(\omega_0-|\omega|)} \qquad (2.5)$$

with $J_1(\lambda)$ the Bessel function of the first kind of the argument $\lambda \equiv e(\vec{q}\vec{E}_0)/m\omega_0^2$ (m is the electron effective mass and ω_0 is the laser field frequency). We also mention here that $\epsilon_\ell(\vec{q},\omega)$ is the longitudinal dielectric function of the interacting electron-phonon system in the presence of the external electromagnetic radiation field; $P_q(\omega)$, $D_q(\omega)$ are the electronic polarizability and phonon propagator, respectively; ω_1, ω_2 are the frequencies of the two coupled longitudinal modes of the electron-phonon system and ω_{L0}, ω_p the longitudinal optical phonon and the plasmon frequencies, respectively; $\phi_q = 4\pi e^2/q^2$ and v_q is the electron-phonon coupling coefficient (for more detailed explanations and expressions see ref.[1]).

Now, to have a more simple and appropriate formula for numerical estimations, we use some relations obtained in the theory of parametric wave excitation (see ref.[2]). Thus, in the collisionless approximation, using the fact that ω_1, ω_2 are the roots of the equation $\epsilon_\ell(\vec{q},\omega) = 0$, we can express $\Pi_q(\omega)$ in the form:

$$\Pi_q(\omega) = \frac{(\omega^2-\omega_1^2)(\omega^2-\omega_2^2)}{2\omega_{L0}(\omega^2-\omega_p^2)} .$$

The imaginary part of $\Pi_q(\omega)$ in this case is due to some growth rate, γ, arising under the action of the external laser field (the shifts in frequencies are negligible) and can be written as

$$\mathrm{Im}\,\Pi_q(\omega_i) \simeq \gamma \frac{\omega_i}{\omega_{L0}} \frac{(\omega_i^2-\omega_j^2)}{(\omega_i^2-\omega_p^2)} ,$$

where $i, j = 1, 2$; $i \neq j$.

In the considered two-mode approximation the frequency parametric resonant condition reads

$$\omega = \omega_i , \quad \omega_0 - |\omega'| = \omega_j ,$$

and then one has

$$\frac{\mathrm{Im}\,\Pi_q(|\omega_i|)}{\mathrm{Im}\,\Pi_q(\omega_0-|\omega_i|)} = - \frac{\omega_i(\omega_j^2-\omega_p^2)}{\omega_j(\omega_i^2-\omega_p^2)} , \tag{3.1}$$

$$\frac{\alpha(\omega_i)}{\alpha(\omega_0-|\omega_i|)} = \frac{(\omega_i^2-\omega_p^2)(\omega_1+\omega_j)(\omega_2+\omega_j)}{(\omega_j^2-\omega_p^2)(\omega_1+\omega_i)(\omega_2+\omega_i)} . \tag{3.2}$$

Furthermore, the parametric excitation analysis shows that the equality

$$1 - I^2(\vec{q},\omega,\lambda) = 0 \tag{4}$$

is nothing but the equation for determining either the growth rate γ as a function of the external electric field intensity E_0 or the threshold field E_{0th} if the growth rate γ is set to be equal to the average damping $(\Gamma_1 \Gamma_2)^{1/2}$ of the modes considered. Thus, one can write down simply

$$I^2 = \left(\frac{E_0}{E_{0th}}\right)^2 . \tag{5}$$

Using (3.1), (3.2) and (5) one has for the function $\theta(\vec{q},\omega,\lambda)$:

$$\theta(\vec{q},\omega,\lambda) = 2\pi \left| \frac{\omega_{L0}(\omega^2-\omega_p^2)}{\omega\,(\omega_1^2-\omega_2^2)} \right| \left[1+\left(\frac{E_0}{E_{oth}}\right)^2 \frac{\omega_i\,(\omega_1+\omega_j)(\omega_2+\omega_j)}{\omega_j\,(\omega_1+\omega_i)(\omega_2+\omega_i)} \right] =$$

$$= 2\pi \left| \frac{\omega_{L0}(\omega^2-\omega_p^2)}{\omega\,(\omega_1^2-\omega_2^2)} \right| \left[1+\left(\frac{E_0}{E_{oth}}\right)^2 \right] \qquad (6)$$

for an arbitrary choice of $i,j = 1,2;\ i \neq j$.

As a result of these simplifications, we have the following expression for the phonon correlation function:

$$< Q_q^2(\omega) > = 2\pi \left| \frac{\omega_{L0}(\omega^2-\omega_p^2)}{\omega\,(\omega_1^2-\omega_2^2)} \right| F\,(q,\omega,T,I^2) \times$$

$$\times \left\{ \delta(\omega+\omega_1)+\delta(\omega-\omega_1)+\delta(\omega+\omega_2)+\delta(\omega-\omega_2) \right\}, \qquad (7.1)$$

where

$$F\,(q,\omega,T,I^2) = |1-I^4|^{-1} \times$$

$$\left| (e^{\omega/T}-1)^{-1} - I^2 (e^{(\omega-\omega_0\,\mathrm{sgn}\omega)/T}-1)^{-1} \right|, \quad I^2 \equiv \left(\frac{E_0}{E_{oth}}\right)^2 . \qquad (7.2)$$

This formula is already suitable for carrying out the numerical calculations for concrete systems what will be done in the next section.

2. RESULTS OF NUMERICAL ESTIMATIONS FOR InSb-CRYSTALS

For numerical calculations of the coherent inelastic scattering cross sections on the plasmon-phonon mixed modes in the parametric resonance conditions we choose the crystals of InSb. Although the values of microscopic nuclear scattering cross sections are not very large ($\sigma = 1,91$ barns for In and $\sigma = 3,94$ barns for Sb [3]), InSb is an optically sensitive semiconductor that is well investigated in the aspect of parametric interactions. The threshold field E_{oth} for parametric excitation of longitudinal coupled waves has been evaluated by several authors (see refs. [2,4], for example) and is of an order of

$$E_{oth} \sim 10^3 \div 10^4\ \mathrm{V.cm^{-1}}, \qquad (8)$$

what is certainly undangerous for the solid and is available by current lasers. All these circumstances make it convenient to choose this semiconductor for our illustrative estimations.

We have performed the calculations of the coherent neutron inelastic scattering cross sections on the plasmon-like mode with the frequency $\omega_1 = 5 \cdot 10^{13}$ sec^{-1} and on the longitudinal optical phonon-like mode with the frequency $\omega_2 = 0{,}25 \cdot 10^{13}$ sec^{-1} as functions of the laser field parameter $I^2 = (E_0/E_{oth})^2$ (see eq. (5)) for a sample of InSb - crystal at temperature T =77 K. The calculations have been carried out for both cases: with creation and annihilation of corresponding quasiparticles. For simplicity we have chosen the case of scattering along the high-simmetry directions ([100], [110], [111] in cubic crystals) when one has $\vec{k} \parallel \vec{k}' \parallel \vec{K}$ (see ref./5/). Note that external field $\vec{E}_0(t)$ is parallel to $\vec{k}$.

Here below we present the results for the two modes separately.

A. The differential scattering cross sections (per one molecule of the crystal) on the high-frequency plasmon-like mode ω_1 as functions of $I^2(E_0)$ is presented in Fig. 1. The curve 1 represents the scattering process with annihilation of a plasmon-like quasiparticle and corresponds to the energy of the incident neutron of an order of ~ 0.12 eV (thermal neutrons). Calculations show that with the increase of the intensity of the laser field the neutron scattering cross section increases from a value of an order of $\sim 1{,}5 \cdot 10^{-5}$ barns at zeroth field to a value of about $2 \cdot 10^{-2}$ barns at $E_0 \approx 0{,}9\, E_{oth}$ and of $\sim 0{,}12$ barns at $E_0 \approx 0{,}98\, E_{oth}$. The curve 2 corresponds to the case of

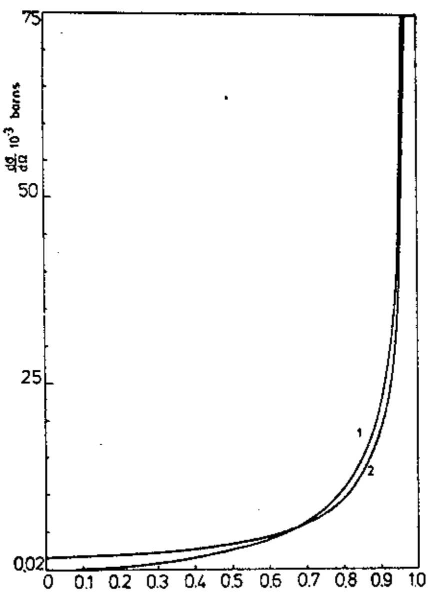

Fig. 1. Cross sections of coherent neutron inelastic scattering on the high-frequency plasmon-like mode $\omega_1 = 5 \cdot 10^{13}$ sec^{-1} in InSb as functions of the laser field parameter $I = (E_0/E_{oth})$. 1 - scattering with one-plasmon annihilation, 2 - scattering with one-plasmon creation.

scattering with creation of a plasmon. The incident neutron energy here is $\approx 0,15$ eV, and the value of the cross section increases from about $\sim 1,7\cdot 10^{-3}$ barns at $I = 0$ ($E_0 = 0$) to $\sim 2\cdot 10^{-2}$ barns at $I \approx 0,9$ and $\sim 0,1$ barns at $I \approx 0,98$. We see that the cross sections reach the values of almost the same order at high field intensities although their values at zeroth field differ from each other by about two orders of magnitude. This means that, for the frequency interval considered (the plasmons), with the field intensity increasing the role of the field dependence factor becomes predominant in the cross sections.

B. The results for the case of coherent neutron inelastic scattering on the low-frequency longitudinal optical phonon-like mode ω_2 are presented in Fig. 2. Again the curve 1 represents the scattering process with one phonon annihilation; and the curve 2, the process with one phonon creation. The corresponding incident neutron energies are $\approx 10^{-5}$ eV (very cold neutrons) and $\approx 1,6\cdot 10^{-3}$ eV (cold neutrons), respectively. In the first case (curve 1) the cross section value increases from $\sim 6,3$ barns at $I = 0$ to ~ 22 barns at $I \approx 0,9$ and $\sim 10^2$ barns at $I \approx 0,98$. In the second case (curve 2) the corresponding increase in the cross section value is: $\sim 5\cdot 10^{-2}$ barns at $I = 0$ to $\sim 0,15$ barns at $I \approx 0,9$ and ~ 1 barn at $I \approx 0,98$.

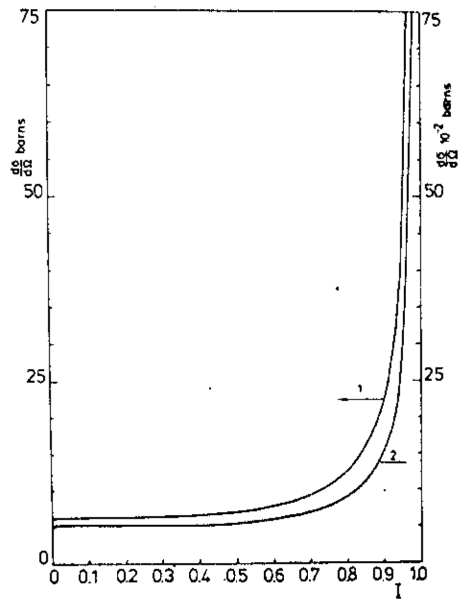

Fig.2. Cross sections of coherent neutron inelastic scattering on the low-frequency longitudinal optical phon-like mode $\omega_2 = 0,25\cdot 10^{13} sec^{-1}$ in InSb as functions of the laser field parameter $I = (E_0/E_{0th})$. 1 - scattering with one-phonon annihilation, 2 - scattering with one-phonon creation.

3. CONCLUSION

The analysis just performed for the chosen energies of incident neutrons (thermal for scattering on plasmons and cold or very cold for scattering on longitudinal optical phonons) - this choice must provide the best resolution in experiments since the incident neutron energies are comparable with the corresponding quasiparticle energies - shows that by increasing the driving laser field intensity towards the parametric excitation threshold value we can arrive at the value of the scattering cross sections larger by several orders of magnitude as compared with the zeroth field ones. Besides, we see that the values of the cross sections for scattering on the plasmon-like modes are in any case much less than the ones for scattering on the phonon-like modes.This fact is easily understandable if one notes that the plasmon-neutron interaction is realized via the electron-phonon interaction mechanism, and the smallness of the neutron-plasmon scattering cross sections is therefore apparently due to the smallness of the mechanical part of the plasmon energy.

The next point one should note here, especially when the question concerns the experimental realization, is the decrease of accuracy as the external field intensity approaches the threshold. This circumstance is caused by the use of the collisionless theory (the quasiparticle lifetimes Γ_1^{-1}, Γ_2^{-1} used for determining the instability threshold fields are the linear ones taken at $E_0 = 0$) from which all the analytical formulae have been derived. Actually, due to the essentially nonlinear interactions and dissipation processes in the system at high field intensities some stationary state must occur in time, and the nonphysical infinite increase of the anomalous fluctuation level and therefore of the values of scattering cross sections as shown in Fig.1 and Fig.2 by calculations must not take place. This leads to the idea that by experimental study of the scattering process at external laser fields in intensity comparable with the parmetric instability thresholds the corrections to the theoretical results might be made and the real lifetimes of quasiparticles at nonzeroth fields could be found.

Finnaly, resuming the study made in both theoretical (I, see /1/) and calculational (II) parts of this investigation we can conclude that, despite the illustrative character, due to the collisionless approximation, the obtained results show surely that by using the high-intensity laser radiation in the parametric resonance conditions it is possible to reach values of the neutron inelastic scattering cross sections on the parametrically excited quasiparticles in solid, which make the neutron scattering measurements practically realizable. Thus, it is naturally to expect that this method together with the choice of efficiently high-flux neutron sources will help one to solve the "small concentration problem" in neutron spectroscopy of nonequilibrium quasiparticles. Then, the experiments in this direction might serve, on the one hand,as a method to observe the parametric excitation phenomena in solids and to study the quasiparticle energy structure in this situation and, on the other hand, as a means to change selectively the energy spectra of neutrons by laser fields.

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