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SPATIAL AND TEMPORAL DISPERSIVE DIELECTRIC FUNCTION OF FREE CARRIERS: ANALYSIS AND TEST OF TWO MODELS

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Raman scattering experiments on plasmon-phonon modes in GaAs and Sb_2Te_3 are analyzed in terms of the spatial dispersive free carrier dielectric function.Calculations based on the Lindhard-Mermin approach and on the hydrodynamic theory in lowest approximation yield an equally good description of the experimental data,favouring the use of the numerically much simpler hydrodynamic dielectric function.

The structure of plasmon modes in semiconductors is caused by two kinds of interactions. Coherent interactions within the electron gas and incoherent interactions between the electron gas and its environment. The coherent processes are described in a self-consistent field approximation by Lindhard's dielectric function $\varepsilon_L(k,\omega)$. A modification of ε_L taking into account incoherent processes in a relaxation time approximation has been proposed by Mermin [1]. A simpler numerical treatment is the so called hydrodynamic approach at which one arrives as follows:

Consider the equation of motion of the one-particle density matrix $\rho(\underline{r}_1,\underline{r}_2,t)$ for quasi-free-electrons [2]:

$$\dot{\rho} + \frac{i\hbar}{2m}(\Delta_1-\Delta_2)\rho = \frac{i}{\hbar}[V(\underline{r}_1) - V(\underline{r}_2)]\rho. \qquad (1)$$

From this equation a hierarchy of balance equations can be deduced

$$e\dot{n} + \mathrm{div}\underline{J} = 0 , \qquad (2) \qquad \dot{\underline{J}} + \mathrm{Div}\,\underline{\underline{\Sigma}} = -\frac{e}{m}n\,\nabla V , \qquad (3)$$

$$\text{with } n(r)=\rho(\underline{r},\underline{r}); \quad \underline{J}(\underline{r})=\frac{ie\hbar}{2m}(\nabla_1-\nabla_2)\rho|_{r_1=r_2}; \qquad (4)$$
$$\underline{\underline{\Sigma}} = \frac{e\hbar^2}{4m^2}(\nabla_1-\nabla_2)(\nabla_2-\nabla_1)\rho|_{r_1=r_2=r}.$$

Instead of going on in the hierarchy with an equation for the tensor $\underline{\underline{\Sigma}}$ we terminate (3) by the following approximations:

(i) $\underline{\underline{\Sigma}}$ is given the value that emerges from a linearized solution of (1)

(ii) $n\nabla V$ is linearized as $n\nabla V \simeq n_o\nabla V + n\underline{F}$ where $\underline{F}$ is an external stochastic field which is the source of incoherent damping.

By methods explained e.g. in [2] it can be shown that the term $n\underline{F}$ may be replaced by a relaxation term of the form $\omega_\tau\underline{J}$. Thus (3) goes over into the "hydrodynamic" equation

$$\underline{\dot{J}} + \omega_\tau \underline{J} + \mathrm{Div}\underline{\underline{\Sigma}} = -\frac{e}{m} n_o \nabla V , \tag{5}$$

which is a generalized form of Drude's equation. The rather complicated term $\mathrm{Div}\underline{\underline{\Sigma}}$ is a linear operator applied to n(r). It takes into account coherent processes in the electron gas. Equation (5) leads to a susceptibility of the form

$$\chi_{FC} = \frac{\omega_p^2}{D(k,\omega)-\omega^2-i\omega\omega_\tau} , \tag{6}$$

with

$$D(\underline{k},\omega) = \frac{\hbar^2}{4m^2} \int \frac{[f(\underline{q}+\underline{k})-f(\underline{q})]\,(2\underline{q}\underline{k}+k^2)^2\,d\underline{q}}{2\underline{q}\underline{k}+k^2-2m\omega/\hbar} \Big/ \int \frac{[f(\underline{q}'+\underline{k})-f(\underline{q}')]\,d\underline{q}'}{2\underline{q}'\underline{k}+k^2-2m\omega/\hbar} , \tag{7}$$

and $\omega_p^2 = ne^2/\varepsilon_o m$ the free carrier plasma frequency. In (6), (7) the same approximations as in the Lindhard dielectric function are used. For $k \to 0$: $D(k,\omega) \to 0$ and the classical Drude result emerges from (6). In certain limiting cases the processes effective in $D(k,\omega)$ can be identified as diffusion or Landau-damping due to single particle decay. The following approximations are found:

$$\text{(a)}\quad \omega \approx 0,\ k \ll k_F: \quad D(k,\omega) = D_o k^2 = \frac{1}{3} v_F^2 k^2 . \tag{8}$$

$$\text{(b)}\quad \omega \gg k v_F,\ k \ll k_F: \quad D(k,\omega) = D_1 k^2 = \frac{3}{5} v_F^2 k^2 . \tag{9}$$

This is in agreement with results reported in [3].

Numerical calculations were performed with the hydrodynamical theory, equs. (6) and (9), and the Lindhard as well as the Lindhard-Mermin expression. Since the Raman cross section

$$\frac{\partial^2\sigma}{\partial\theta\,\partial\omega} \sim |1+\chi_{VE}+\chi_{ph}|^2 \ \mathrm{Im}\,\frac{-1}{\varepsilon(\omega,k)} , \tag{10}$$

$$\text{with}\quad \varepsilon(\omega,k) = 1 + \chi_{VE} + \chi_{ph}(\omega) + \chi_{FC}(\omega,k) , \tag{11}$$

has its structure essentially determined by $\mathrm{Im}(-1/\varepsilon)$, we show in Fig.1 the numerical results for this term. Parameters appropriate for GaAs were chosen and the phonon contribution, χ_{ph}, was described by a harmonic oscillator. All four calculations show the two coupled plasmon-LO-phonon (PLP)-modes at small k-vector. With increasing k the strength of the PLP-modes decreases the rate of which increases with increasing damping of the electron gas. This can be especially seen for the Lindhard based calculations (right side), which include the coherent Landau-damping not contained in the approximation (9) used here for the hydrodynamic theory (left side).

Raman cross sections were calculated according to (10). The result for a GaAs-spectrum is shown in Fig. 2. While both theories show some deficiencies in describing the more phonon-like Ω^--mode, both give excellent agreement with the plasmon-like Ω^+-mode. Similar results were obtained for Sb_2Te_3, where the IR-active phonons, coupling into the PLP-modes, are not Raman-active: Fig. 3. It should be pointed out that, besides scaling of the scattering intensity, no fit parameters are involved. Fig.(4) finally shows the dispersion with wavevector of the PLP-modes. Again both theories give nearly identical results, the Linhard-Mermin giving a little better agreement to experiment.

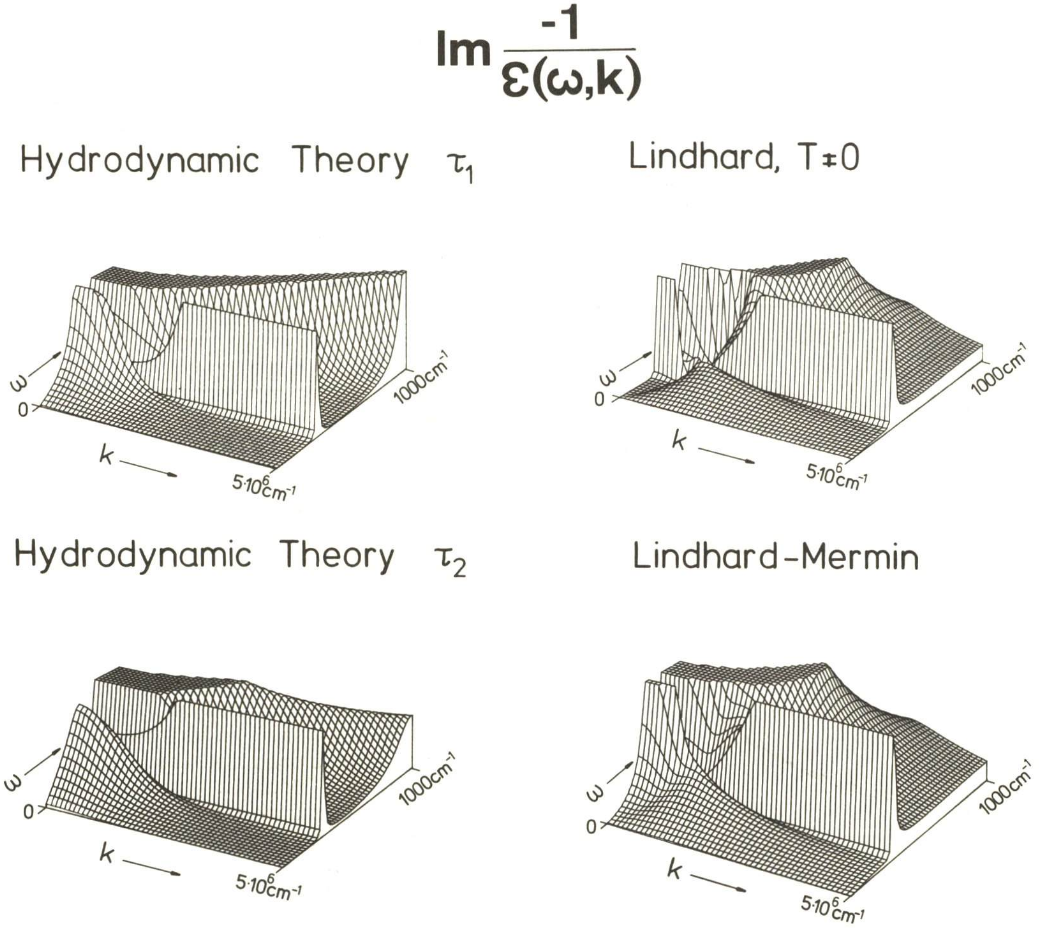

Fig.1 Im(-1/ε) calculated with ε(ω,k) from (11) with the hydrodynamic theory for two relaxation times ($\tau_1 < \tau_2$), with Lindhard (τ=0) and with Lindhard-Mermin (τ_1):Parameters appropriate for GaAs ($n=1.3\cdot 10^{18}\,cm^{-3}$) are used

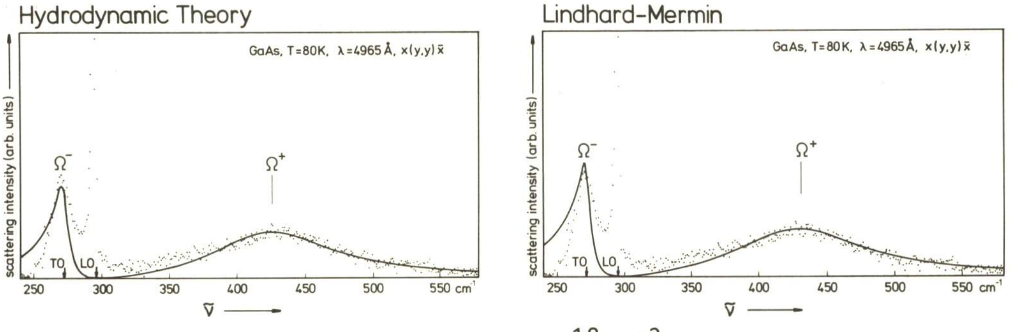

Fig.2 Comparison of a GaAs ($n= 1.3\cdot 10^{18}\,cm^{-3}$) Raman spectrum with the cross section following from hydrodynamic theory and Lindhard-Mermin

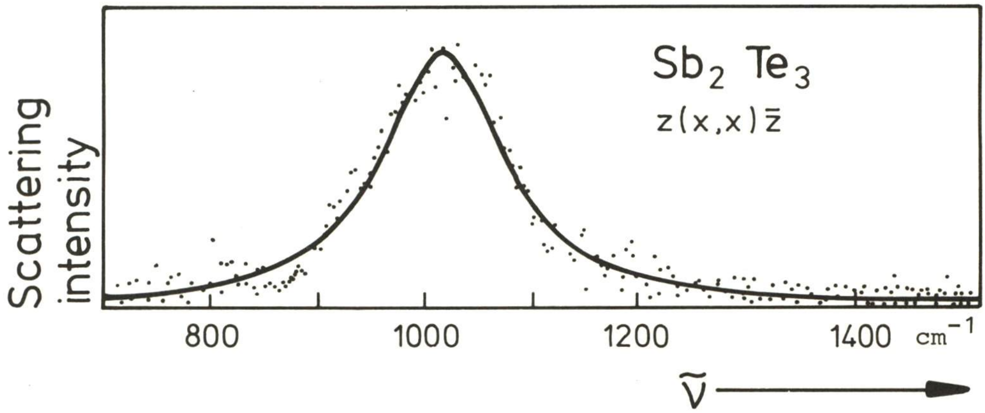

Fig.3 Comparison of a Raman spectrum from Sb_2Te_3 (plasmon-like PLP-mode) with the cross section following from hydrodynamic theory ($p=2.3\cdot 10^{20}cm^{-3}$, $\tau_p^{-1}=140cm^{-1}$, $m_p=0.6m_o$, $\varepsilon_\infty=34$: from IR-data)

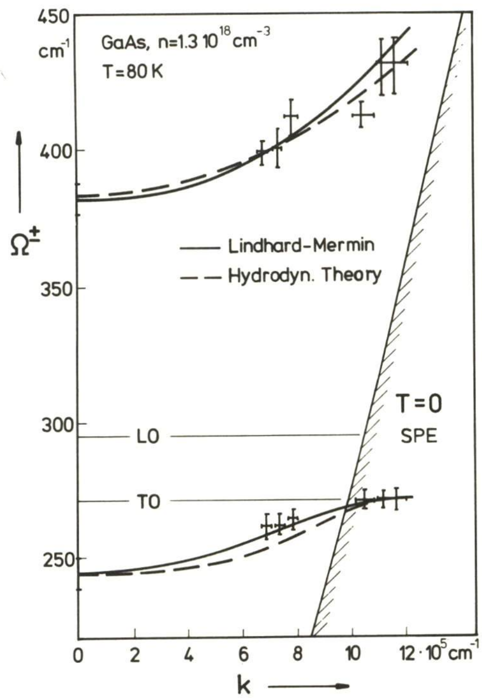

Fig.4 Comparison of experimental PLP-mode dispersion with two calculations

In conclusion it can be stated that the hydrodynamic theory gives already in lowest approximation nearly as good a description of the experimental data as the Lindhard-Mermin approach. Better approximations than (9) for D are easy to obtain and we are in progress to see if even better agreement with experiment can be reached.

We should point out that similar calculations with Lindhard and T=0 have been reported in [4].

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