

DESCREENED FRÖHLICH MODE IN CHARGE DENSITY WAVE SYSTEMS

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Abstract: The influence of the long-range Coulomb interaction on the complex ac conductivity $\sigma_{\text{CDW}}(\omega)$ of pinned incommensurable charge density waves (CDW) in quasi one-dimensional semiconductors is studied. A modified Fukuyama-Lee-Rice (FLR) approach is developed in which the extrinsic phason damping γ_0 is replaced by a non-local damping function $\gamma_{\text{ren}}(\underline{k}, \omega)$. The actual evaluation of σ_{CDW} makes use of quantitative results for self energy functions $\Sigma(\omega)$ of the original FLR model for different spatial dimensionalities d and pinning strengths. The absorption profile $\text{Re}\sigma(\omega)$ displays a low frequency tail due to a relaxation mode. The pinning frequency defined as $\omega_p^2 = -\text{Re}\Sigma(\omega_p)$ is significantly influenced by selection rule breaking via inhomogeneous pinning. Furthermore, the dependence of ω_p on impurity concentration is quite different from the scaling results of FLR. An excellent fit to measured data is obtained.

Density waves, involving either charge or spin density modulation in real space are among the possible ground states of electrons in low dimensional solids. They change the translational symmetry of the crystal. If their periodicity is incommensurate to that of the underlying lattice the density wave can slide through the crystal carrying an electrical current. This is often called the "Fröhlich sliding mode". Many effects hinder the free sliding of the Fröhlich mode leading to its so called "pinning".

Clearly, impurities are one of the basic pinning mechanisms. In the present work, the linear ac response of charge density waves pinned by impurities is studied. In particular, the influence of reduced quasi particle screening on the microwave response is investigated on the basis of an extended Fukuyama-Lee-Rice (FLR) description of charge density wave (CDW) dynamics.

Our starting point is Littlewood's formula [1] for the measured ac conductivity

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$$\sigma(\omega) = \frac{R^{-1}(\underline{k}, \omega)}{1 + i \frac{\omega_{p\phi}^2}{4\pi} D_{\rho}(\underline{k}, \underline{k}; \omega) R(\underline{k}, \omega)} \quad \left| \begin{array}{l} \\ k_t=0, k_l \rightarrow 0 \end{array} \right. , \quad (1)$$

where $D_{\rho}(\underline{k}, \underline{k}'; \omega)$ is the propagator of the linearized FLR equation with modified damping: $\gamma_0 \rightarrow \gamma_0 + \Delta\gamma(\underline{k}, \omega)$. From three-dimensional electrodynamics we find [2] for the resistivity function $R(\underline{k}, \omega) = 4\pi\Delta\gamma(\underline{k}, \omega)/\omega_{p\phi}^2$ ($\omega_{p\phi}$: CDW plasma frequency)

$$R(\underline{k}, \omega) = \left[k^2 k_l^2 - i \frac{\omega}{c^2} 4\pi \tilde{\sigma}_t \{ k^2 + k_l^2 - i \frac{\omega}{c^2} 4\pi \tilde{\sigma}_t \} \right] / \quad (2)$$

$$\left[k^2 k_l^2 \tilde{\sigma}_l + \tilde{\sigma}_t (k^2 k_t^2 - i \frac{\omega}{c^2} 4\pi \{ k^2 + k_l^2 + \frac{\tilde{\sigma}_t}{\tilde{\sigma}_l} k_t^2 \} \tilde{\sigma}_l - (\frac{\omega}{c^2} 4\pi \tilde{\sigma}_l)^2) \right] .$$

This differs from the result in [1]. In the dynamic limit and for vanishing transverse momentum $k_t=0$, however, both formula lead to

$$\gamma_0 \rightarrow \gamma_{\text{ren}}(\omega) = \gamma_0 + \Delta\gamma(\omega) = \gamma_0 + \frac{\omega_{LO}^2}{\omega_r - i\omega} , \quad (3)$$

with two new frequency scales: i) $\omega_{LO} \hat{=}$ longitudinal optical phason frequency, ii) $\omega_r = 4\pi\sigma_{qp}(T)/\epsilon_{\Delta} \hat{=}$ dielectric relaxation frequency of the quasi particles in the Peierls state. In contrast to [3], we retain the frequency dependence in γ_{ren} .

D_{ρ} in (1) still contains the impurities. While in [1] an approximate treatment of D_{ρ} was given by using an ad hoc distribution of localized modes we rely on self averaging to express D_{ρ} in terms of the impurity averaged propagator of the modified FLR equation:

$$D_{\rho}(\underline{k}, \underline{k}; \omega) = \langle D_{\rho}(\underline{k}, \underline{k}; \omega) \rangle = D_{\rho}(\underline{k}, \omega) . \quad (4)$$

By simple algebra it then follows that the CDW conductivity $\sigma_{\text{CDW}}(\omega) = \sigma(\omega) - R^{-1}(0, \omega)$ is expressed in the form [2]

$$\sigma_{\text{CDW}}(\omega) = \frac{\omega_{p\phi}^2}{4\pi} \{ -i\omega D_{\text{ren}}(0, \omega) \} . \quad (5)$$

D_{ren} is the impurity averaged propagator which has $\gamma_{ren}(\underline{k}, \omega)$ only in internal phason lines. Eq. (5) generalizes Fukuyama's formula [4] to the case of long-range quasi particle interactions (descreening). With the specific form (3) for γ_{ren} and earlier results for self energy functions $\Sigma(\omega)$ of the FLR equation [5] explicit results for $\sigma(\omega)$ become available. The self energies have been evaluated for weak pinning (w.p.) in $d=1,2,3$ dimensions and also for strong pinning (s.p.) in $d=1$ [5]. Within the self consistent Born approximation $\Sigma_d(\omega)$ is given for w.p. by

$$\Sigma_d(\omega) = -C_d + \frac{1}{2(2\pi)^d} \int d^d k [k^2 - \omega^2 - i\omega\gamma_{ren}(\omega) - \Sigma_d(\omega)]^{-1}. \quad (6)$$

In (6), C_d is the w.p. constant in d dimensions. Particular attention has been paid to the analytic properties of $D_{ren}(\omega)$ thus obtained. It can be shown that substitution of $\gamma_{ren}(\omega)$ in place of γ_0 does not affect analyticity conditions which read: $C_1 > 3/4$, $\tilde{C}_2 = C_2 - \frac{1}{4\pi} \ln k_c > 1 + \ln 8\pi$, $\tilde{C}_3 = C_2 - k_c^2/4\pi^2 > -1/256\pi^2$. k_c is the momentum cut off in units of the inverse FLR length [5]. Useful results for $\Sigma_d(\omega)$ are $\Sigma_1 = -C_1 + \frac{1}{4z(\omega)}$, $\Sigma_2 = -\tilde{C}_2 - \frac{1}{4\pi} \ln z(\omega)$, $\Sigma_3 = -\tilde{C}_3 - \frac{1}{8\pi} z(\omega)$, where $z(\omega) = \sqrt{-\omega^2 - i\omega\gamma_{ren}(\omega) - \Sigma_d(\omega)}$. For s.p. in $d=1$ one obtains $\Sigma_s(\omega) = -2z_s(\omega)$, which corresponds to w.p. in $d=3$ when $\tilde{C}_3=0$. S.p. for $d=3$ is not covered consistently by the FLR phase approach [5].

The dielectric constant $\epsilon_{CDW}(0)$ for w.p. and $d=3$ - the case henceforth considered - is found to be

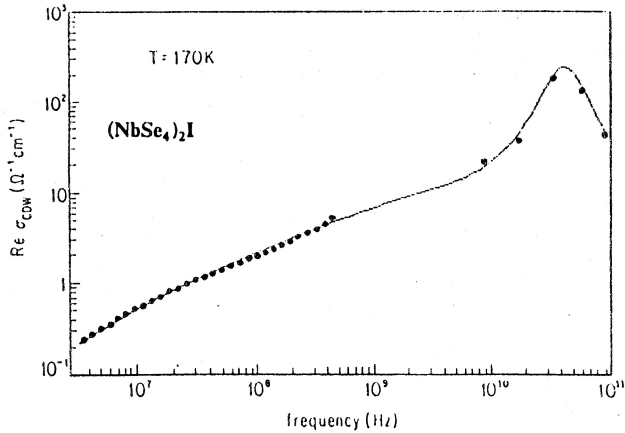
$$\epsilon_{CDW}(0) = 1 + \frac{\omega_p^2}{\omega_w^2 \left\{ \tilde{C}_3 + \frac{1}{128\pi^2} + \frac{1}{8\pi} \sqrt{\tilde{C}_3 + \frac{1}{256\pi^2}} \right\}}. \quad (7)$$

In the descreened case a low frequency relaxation mode [1] appears which contains most of the oscillator strength in $\text{Im}\epsilon_{CDW}(\omega)$ and thus determines $\epsilon_{CDW}(0)$. The pinning peak in $\text{Re}\epsilon_{CDW}(\omega)$ is also affected: Defining the pinning frequency ω_p by $\omega_p^2 = -\text{Re}\Sigma(\omega_p)$ one finds for $\omega_p \gg \omega_r$ ($\omega_{LO} \gg \gamma_0$ is also understood) $\omega_p(d=1) = \omega_w(1) [0.84 - \omega_w(1)/4\omega_{LO}]^{1/2}$, $\omega_p(d=2) = \omega_w(2) [\tilde{C}_2 + \frac{1}{4\pi} \ln(\frac{\omega_{LO}}{\omega_w(2)})]^{1/2}$, $\omega_p(d=3) = \omega_w(3) [\tilde{C}_3 + \omega_{LO}/8\pi\omega_w(3)]^{1/2}$. Here, $\omega_w(d)$ is the FLR pinning frequency which is usually taken as approximation for ω_p . This is reasonable for $d=1$ and $d=2$. For $d=3$, however, descreening leads to

$$\omega_p(3) \approx [\omega_w(3)\omega_{LO}/8\pi]^{1/2}. \quad (8)$$

Due to selection rule breaking by inhomogeneous pinning ω_{LO} appears in ω_p and stiffens the Fröhlich mode. The concentration dependence of ω_p thus becomes $\omega_p \propto c^{1/2}$ instead of the FLR result $\omega_w(3) \propto c$. For $\omega_r > \omega_p$ the former results [5] of the fully screened case are reobtained.

Finally a quantitative fit of the present theory to measured data [6] on $(\text{NbSe}_4)_2\text{I}$ is made. For the following consistent set of parameters, $\omega_{LO} = 4 \cdot 10^{12} \text{ s}^{-1}$, $\omega_p \approx \gamma_0 = 2 \cdot 10^{11} \text{ s}^{-1}$, $\omega_r = 4 \cdot 10^{10} \text{ s}^{-1}$, $\epsilon_\Delta = 30$, $\Delta_0 = 1300 \text{ K}_B \text{ K}$, $\omega_w(3) = 6 \cdot 10^{11} \text{ s}^{-1}$ and $\tilde{C}_3 = 0.002$, the curve in the figure below is obtained. It perfectly joins the tail region of the response, where descreening effects dominate, to the high frequency pinned mode.



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