Phason dynamics in charge and spin density waves

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Abstract. --- Phason propagators in charge and spin density waves in presence of long range Coulomb interaction are studied within mean field theory. In charge density wave the longitudinal phason splits into an acoustic mode and an optical mode in the presence of Coulomb interaction. Except at low temperatures ($T \leq 0.2\ T_c$) the acoustic mode exhausts most of the optical weight. In spin density wave there is no longitudinal acoustic mode; the phason becomes the plasmon. On the other hand in the transverse limit, the plasmon decouples completely from the phason both in charge and spin density waves.

1. Introduction.

It is well known that the long range Coulomb interaction will modify the longitudinal phason mode strongly [1]. However, most works published on this subject [2] are incomplete due to unnecessary approximation. We shall report here our recent study of the phason dynamics [3] of both charge and spin density waves (CDW and SDW). As a model we take a quasi-one dimensional system (Fröhlich Hamiltonian [4] for CDW and Yamaji model [5] for SDW) supplemented by the long range Coulomb interaction

$$H_c = 4\pi e^2 \sum_q \frac{1}{q^2} n_q n_{-q} \tag{1}$$

where n_q is the electron density with momentum $\vec{q}$. As we shall see the condensate density f, which depends both on ω the frequency and $\vec{q}$ the momentum plays the crucial role in the following analysis. In the longitudinal limit (i.e. $\vec{q}$ parallel to the most conducting direction) we obtain an acoustic mode with the phason velocity decreasing rapidly with increasing temperature in CDW while there will be no phason in SDW. In particular this phason mode is observed recently by neutron scattering for a single crystal of $K_{0.3}$ MoO_3 [6]. In the transverse limit, on the other hand, the Coulomb effect disappears completely from the phason propagator in contrary to an early analysis of the electric conductivity in SDW [7].

2. Phason Propagator in CDW.

We shall first consider the phason propagator in CDW. In the presence of the long range Coulomb interaction the phason propator is given by

$$D_\phi(\vec{q}, \omega) = (1 - g^2 \omega_Q^2 (\omega_Q^2 - \omega^2)^{-1} \langle [\Delta_2, \Delta_2] \rangle)^{-1} \omega_Q^2 (\omega_Q^2 - \omega^2)^{-1}$$

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$$= -(2\Delta)^2 \; (\lambda f)^{-1} \left(\frac{m^*}{m}\omega^2 - \zeta^2 - \omega_p^2 f\left(1 - \frac{\omega_p^2(1-f)}{\omega^2-\zeta^2}\right)^{-1}\right)^{-1}$$

$$\cong -(2\Delta)^2 \; (\lambda f)^{-1} \; (1-f)\left[\left(\frac{m^*}{m}(1-f)+f\right)\omega^2 - \zeta^2\right]^{-1} \tag{2}$$

where Δ_2 is the imaginary part of the order parameter and the effect of the Coulomb interaction is incorporated within mean field theory [8]. Here we limit ourselves to the longitudinal case and in the last step we took $\omega_p = \infty$, where $\omega_p = (4\pi\, e^2 n\,/\,m)^{1/2}$ is the plasma frequency. The function f is the generalized condensate density given by

$$f = \begin{cases} -\frac{1}{2}\int_{-\infty}^{\infty} d\phi \,\mathrm{th}\,(\frac{1}{2}\beta\Delta \mathrm{ch}\phi)\;[\mathrm{sh}^2(\phi-\phi_0) - (1-\alpha^2)\,(\zeta/2\Delta)^2\,]^{-1} & \text{for} \quad \alpha \le 1 \\ \frac{1}{2}\int_{-\infty}^{\infty} d\phi \,\mathrm{th}\,(\frac{1}{2}\beta\Delta \mathrm{ch}\phi)\;[\mathrm{ch}^2(\phi-\phi_0) + (1-\alpha^2)\,(\zeta/2\Delta)^2\,]^{-1} & \text{for} \quad \alpha > 1 \end{cases} \tag{3}$$

where $\alpha = \omega/\zeta = \omega/vq$ and

$$\mathrm{th}\,\phi_o = \begin{cases} \alpha & \text{for} \quad \alpha \le 1 \\ \alpha^{-1} & \text{for} \quad \alpha > 1 \end{cases} \tag{4}$$

We recover familiar expressions in the adiabatic limit $(\omega, \zeta \ll 2\Delta\,(T))$

$$f_s = \lim_{\alpha\to 0} f = 2\pi T \sum_{n=0}^{\infty} \frac{\Delta^2}{(\omega_n^2+\Delta^2)^{3/2}} \tag{5}$$

and

$$f_d = \lim_{\alpha\to\infty} \int_0^{\infty} d\phi \,\mathrm{sech}^2\phi \,\mathrm{th}\,(\tfrac{1}{2}\beta\Delta\mathrm{ch}\phi) \tag{6}$$

Also $f = 1$ for $\alpha = 1$ independent of temperature. The temperature dependence of f_s and f_d are shown in Fig. 1. The phason mass m^* is given by [9]

$$\frac{m^*}{m} = 1 + (2\Delta)^2\,(\lambda\omega_Q^2 f)^{-1} \tag{7}$$

It is important to note that the phason mass m^* has different temperature dependence depending on which limit you are in. As already pointed out by Takada and his collaborators [2], the longitudinal phason consists of 2 modes, which is determined from

$$\left(1 + \frac{(2\Delta)^2}{\lambda\omega_Q^2}\,(f^{-1}-1)\right)\omega^2 = \zeta^2 \tag{8}$$

where substituted Eq (7) in the pole of Eq (2)

3. Acoustic Mode.

One of the solutions is given by

$$\omega^2 = \frac{m}{m^*}\left(1-f+\frac{m}{m^*}f\right)^{-1}\zeta^2 \tag{9}$$

where m^*/m defined in Eq (7) has to be used. Then for not too low temperatures (say $T > 0.3\ T_c$) we have $\omega \ll \zeta$ and Eq (9) simplifies as $\omega = v_\phi\, q$ with

$$v_\phi/v_F = \left(\frac{m}{m_s^*}\right)^{\frac{1}{2}}\left(1-f_s+\frac{m}{m_s^*}f_s\right)^{-\frac{1}{2}} \tag{10}$$

where suffix s means the static limit ($\alpha \ll 1$). The temperature dependence of v_ϕ is shown in Fig. 2. As seen from Fig. 2, v_ϕ increases rapidly with indecreasing temperature and ultimately it merges with another

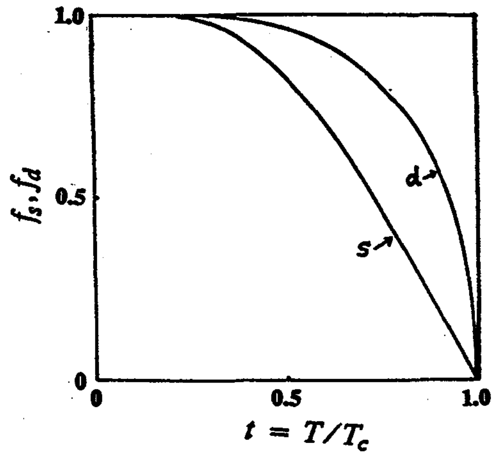

Fig. 1

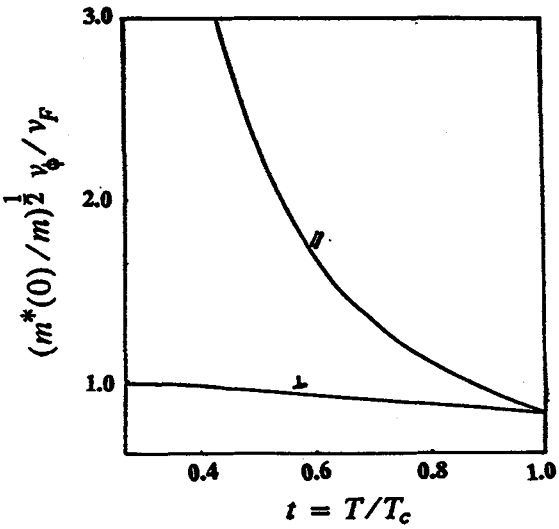

Fig. 2

Fig. 1. – The condensate density f_s (the static limit) and f_d (the dynamic limit) are shown as function of the reduced temperature t.

Fig. 2. – The longitudinal and the transverse phason velocities $v_{\phi\parallel}$ and $v_{\phi\perp}$ in CDW are shown as function of reduced temperature.

mode and disappears at low temperatures ($T \cong 0.2\ T_c$). It is of interest to consider the spectral weight. Total spectral weight of phason is given from Eq (2) as

$$\int_0^\infty d\omega\,\omega\, Im D_\phi(q,\omega) = \frac{\pi}{2}\omega_Q^2 \tag{11}$$

independent of ζ, T and ω_p. The acoustic pole gives, on the other hand, 4

$$\int_0^\infty d\omega\omega Im D_\phi(q,\omega) = \frac{\pi}{2}\omega_Q^2\left(\frac{1-f_s}{1-f_s+\frac{m}{m_s^*}f_s}\right)(1-\frac{m}{m_s^*}) \tag{12}$$

which almost exhausts the spectral weight as long as $1-f_s \gg m/m_s^*$ (i.e. $T \geq 0.3\ T_c$).

For an arbitrary $\hat{q}$ the acoustic mode is given by

$$\omega \cong (\frac{m}{m_s^*})^{\frac{1}{2}}\ (1-f_s)^{-\frac{1}{2}}\ (\zeta_{\shortparallel}^2+(1-f_s)\zeta_\perp^2) \tag{13}$$

where $\zeta_{\shortparallel} = vq_{\shortparallel}$ and $\zeta_\perp = v_\perp q_\perp$ and $v_\perp$ is the Fermi velocity in the transverse direction.

In the transverse limit (i.e. $\zeta_{\shortparallel} = 0$) where the Coulomb interaction is completely decoupled, the phason velocity $v_{\phi\perp}$ depends only weakly on T through m_s^* (T) as shown in Fig. 2.

4. Optical Mode.

At $T = 0K$ another solution of Eq (8) is [2]

$$\omega_{op}^2 = \frac{3}{2}\lambda\omega_Q^2+\frac{1}{5}\frac{m}{m^*}\zeta^2 \tag{14}$$

The optical frequency is almost independent of T for $T < 0.2\ T_c$ and then start to increase with increasing temperature. At the same time the optical weight of this mode decreases very rapidly. At $T = 0K$, the optical mode almost exhausts the optical weight.

5. Phason Propagator in SDW.

Since $m^*/m = 1$ practically for SDW, the phason propagator is now given by

$$D_\phi(q,\omega) = (2\Delta)^2\left\{\langle f(\zeta^2-\omega^2)\rangle+\frac{4\pi e^2}{q^2}N_o\langle f\zeta\rangle^2\left[1+\frac{4\pi e^2}{q^2}N_o\langle\frac{\zeta^2}{\zeta^2-\omega^2}(1-f)\rangle\right]^{-1}\right\}^{-1} \tag{15}$$

where $\langle\,\rangle$ means the angular average and

$$\zeta = \zeta_{\shortparallel}+\sqrt{2}\zeta_\perp\cos\phi \tag{16}$$

In the longitudinal limit ($\zeta_\perp = 0$) Eq (15) reduces to

$$D_\phi(q,\omega) = (2\Delta)^2 f^{-1}(\omega_p^2(1-f)+\zeta^2-\omega^2)(\zeta^2-\omega^2)^{-1}\times(\omega_p^2+\zeta^2-\omega^2)^{-1} \tag{17}$$

Since $f|_{\omega=\pm\zeta} = 1$, D_ϕ $(\hat{q},\omega)$ has only the plasmon pole in the longitudinal limit. More generally in the limit $\omega \gg \zeta$ Eq (15) can be rewritten as

$$D_\phi(q,\omega) = (2\Delta)^2 f^{-1}\left(1-\frac{\omega_p^2}{\omega^2}\left(\cos^2\vartheta+\left(\frac{v_\perp}{v_{\shortparallel}}\right)^2\sin^2\vartheta\right)(1-f)\right)\times$$

$$\left[\omega_p^2\left(\cos\vartheta + \left(\frac{v_\perp}{v_{/\!/}}\right)^2 \sin^2\vartheta\,(1-f)\right) - \omega^2\right]^{-1} \tag{18}$$

where $\cos\vartheta = q_{/\!/}/q$. The pole is then given by

$$\omega^2 = \omega_p^2\left\{\cos^2\vartheta + \left(\frac{v_\perp}{v_{/\!/}}\right)^2 \sin^2\vartheta\,(1-f(\omega))\right\} \tag{19}$$

which always has two solutions. One at high frequencies (i.e. $\omega \gg 2\Delta(T)$)

$$\omega_+^2 = \omega_p^2\left\{\cos^2\vartheta + \left(\frac{v_\perp}{v_{/\!/}}\right)^2 \sin^2\vartheta\right\} \tag{20}$$

and another below the quasi-particle energy gap;

$$\omega_-^2 = \frac{3}{2}(2\Delta)^2\left(1-\frac{3}{2}G_d\right)^{-1}\left(1-f_d+\left(\frac{\zeta_{/\!/}}{\zeta_\perp}\right)^2\right) \tag{21}$$

where f_d is the condensate density in the dynamical limit and

$$G_d = 2\int_0^\infty d\phi\,\mathrm{sech}^4\phi\,(1+e^{\beta\Delta\mathrm{ch}\varphi})^{-1} \tag{22}$$

At $T = 0K$ where $f_d = 1$, the second mode is almost gapless when $\zeta_{/\!/} \ll \zeta_\perp$. In deriving Eq (21) it was assumed $(\omega_-/2\Delta) \ll 1$. In general the optical weight is dominated by the ω_- mode. However, when the longitudinal limit is approached ($\zeta_\perp \to 0$), ω_- becomes 2Δ and the ω_- mode loses the optical weight completely and the optical weight shifts completely to the ω_+ mode. Also as temperature increases (say $T \geq 0.2\,T_c$), ω_- increases rapidly and again the present approximation breaks down completely. In the transverse limit ($\zeta_{/\!/} = 0$) on the other hand, the Coulomb potential drops out completely and we recover the old result [10]

$$D_\phi(\vec{q},\omega) = (2\Delta)^2 f^{-1}(\zeta_\perp^2 - \omega^2)^{-1} \tag{23}$$

6. Concluding Remarks.

We have shown that the long range Coulomb interaction has dramatic effect on the phason propagator in both CDW and SDW. In CDW the phason velocity in the longitudinal limit v_ϕ becomes strongly temperature dependent as observed in a recent neutron scattering experiment in a single crystal of blue bronze $K_{0.3}Mo\,O_3$ [6]. At low temperatures the Coulomb interaction generates an optical mode, which has not been seen experimentally. In SDW the acoustic mode disappears in the longitudinal limit. At low temperatures ($T \leq 0.2\,T_c$) there will be an optical mode with small energy gap. On the transverse limit the Coulomb interaction effect disappears completely and we recover the old results [10] without Coulomb interaction

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