Phason modes in spin-density wave in the presence of long-range Coulomb interaction

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We study the effect of long-range Coulomb interaction on the phason in spin-density wave (SDW) within mean field theory. In the longitudinal limit and in the absence of SDW pinning the phason is completely absorbed by the plasmon due to the Anderson-Higgs mechanism. In the presence of SDW pinning or when the wave vector \( \mathbf{q} \) is tilted from the chain direction, though the plasmon still almost exhausts the optical sum rule, another optical mode appears at \( \omega < 2\Delta(T) \), with small optical weight. This low frequency mode below the SDW gap may be accessible to electron energy loss spectroscopy (EELS).

I. INTRODUCTION

It is known for some time that the long-range Coulomb interaction plays a rather important role in phason dispersions of both charge-density wave (CDW) \[①\] and spin-density wave (SDW) \[②\]. As a continuation of an earlier analysis of CDW \[④\], we study in this paper the phason spectrum in SDW in the collisionless limit. Unlike in CDW \[①\], the phason propagator \( D_\phi \) in SDW is not easily accessible to neutron scattering. Further, the large frequency limit of \( D_\phi \) in SDW does not allow to define the corresponding optical weight. Therefore in the present paper we analyze the dielectric function \( \varepsilon(q, \omega) \), which allows us to define the optical weight. Moreover, not only the poles of \( \varepsilon^{-1} \) are identical to those of \( D_\phi \), but also \( \varepsilon^{-1} \) is directly accessible to electron energy loss spectroscopy (EELS).

In sharp contrast to CDW we find, that the Anderson-Higgs mechanism \[⑥\] operates perfectly in the longitudinal limit (i.e. when \( \mathbf{q} \) is parallel to the chain direction) and in the absence of SDW pinning; the phason is completely absorbed by the plasmon and \( \varepsilon \) is identical to the one in the normal state. In the presence of SDW pinning or when \( \mathbf{q} \) deviates from the chain direction however, another optical mode appears below the quasiparticle energy gap representing the plasma oscillations of the normal (uncondensed) carriers in a dielectric environment. The optical weight of this low frequency plasmon is always very small, but the mode itself is well separated from the strong high frequency plasmon. In this general circumstance the Anderson-Higgs mechanism \[⑥\] is
weakly broken.

It is worth noting that we do not find any acoustic mode in the inverse dielectric function. In the transverse case (i.e. when \( q \) is perpendicular to the chain direction) the phason completely decouples from the density fluctuations and therefore remains acoustic, but because of the same decoupling none of it’s features shows up in \( \varepsilon^{-1} \).

In Sec. II the general formalism for the dielectric function in SDW is given. In Sec. III we study the pole structure in the longitudinal limit before moving on to the general case of arbitrary direction of the wavenumber in Sec. IV. Sec. V concludes with a brief summary of our results.

### II. DIELECTRIC CONSTANT

We consider the strongly anisotropic Hubbard model as introduced by Yamaji [7] supplemented by the long-range Coulomb interaction

\[
H_C = 4\pi e^2 \sum_q \frac{1}{q^2} n_q n_{-q},
\]

where \( n_q \) is the electron density operator. Within mean field theory for the SDW the density-density correlation function \[8\] including the effect of long-range Coulomb interaction \[9\] is given by

\[
\langle [n, n] \rangle = \langle [n, n] \rangle' \left(1 + \frac{4\pi e^2}{q^2} \langle [n, n] \rangle' \right)^{-1},
\]

and

\[
\langle [n, n] \rangle' = \langle [n, n] \rangle_0 + U \frac{\langle [n_\delta \Delta]_0, [\delta \Delta, n]_0 \rangle}{1-U \langle [\delta \Delta, \delta \Delta] \rangle_0} = N_0 \left\{ \frac{\langle (\zeta || - f) \rangle}{(\zeta || - \omega^2)} + \frac{\langle (f)^2 \rangle}{(\zeta || - \omega^2)^2} \right\}.
\]

Here \( \langle [n, n] \rangle' \) is the correlation function obtained in the absence of long-range Coulomb interaction, \( N_0 \) is the electron density of states per spin at the Fermi energy, \( \zeta = \zeta || + \sqrt{2} \zeta \perp \sin \varphi \), \( \zeta || = v || q || \), \( \zeta \perp = v \perp q \perp \) and \( v || \) and \( v \perp \) are Fermi velocities parallel and perpendicular to the chain direction respectively, and \( \langle \ldots \rangle \) in the second line of Eq.(3) means the average over \( \varphi \). Finally \( f(\zeta, \omega) \) is the generalized condensate density already defined in Ref. [4b]. Expressions of \( f \) in certain limits needed in the present paper will be given later. We note that the second term on the right hand side of Eq.(3) corresponds to the contribution of the sliding SDW condensate.

The dielectric function defined in the usual way

\[
\varepsilon(q, \omega) = 1 + \frac{4\pi e^2}{q^2} \langle [n, n] \rangle'
\]

satisfies the well known relation

\[
\text{Im}(-\varepsilon^{-1}) = \frac{4\pi e^2}{q^2} \text{Im}(\langle [n, n] \rangle).
\]
It also obeys the following sum rule

\[ \int_0^\infty d\omega \Im(\varepsilon^{-1}) = \frac{\pi}{2} \omega_p^2 \cos^2 \vartheta + \left( \frac{u}{q} \right)^2 \sin^2 \vartheta , \]  

where \( \omega_p^2 = 4\pi e^2 N_0 v_\parallel^2 = 4\pi e^2 n/m \) is the plasma frequency and \( \cos \vartheta = q_\parallel/q \). The total oscillator strength depends only on the direction of \( q \).

It is worth mentioning that the phason propagator \( D_\phi \) in SDW is given by

\[ D_\phi = (1 - U \langle [\delta \Delta, \delta \Delta]_C \rangle)^{-1} \]

\[ = (2\Delta)^2 \{ \langle (\zeta^2 - \omega^2) f \rangle + \frac{4\pi e^2}{q^2} N_0 \langle \zeta f \rangle^2 \}
\times [1 + \frac{4\pi e^2}{q^2} N_0 \langle \frac{\zeta^2 (1-f)}{\zeta^2 - \omega^2} \rangle^{-1}]^{-1} \]

where \( \langle [\delta \Delta, \delta \Delta]_C \rangle \) is the Coulomb-corrected correlation function of order parameter fluctuations. Comparing Eqs. (2-3) and (7) it is readily seen that \( D_\phi \) has the same pole structure as \( \langle [n, n] \rangle \).

III. LONGITUDINAL LIMIT

In the longitudinal limit \( \zeta = \zeta_\parallel \). The correlation function \( \langle [n, n] \rangle \) is much simplified and written as

\[ \langle [n, n] \rangle = N_0 \zeta^2 (\omega_p^2 + \zeta^2 - \omega^2)^{-1} \]

where we assume that the SDW condensate is free to move in the chain direction. We see that Eq. (8) has the single pole

\[ \omega^2 = \omega_p^2 + \zeta^2 \]

at the plasma frequency and \( \langle [n, n] \rangle \) is the same as in the normal state because the unpinned condensate is able to compensate exactly for the loss of normal carriers due to the SDW transition. This high frequency plasmon is undamped and exhausts all the available oscillator strength Eq. (6). In other words the phason is completely eaten by the plasmon (Anderson-Higgs mechanism). This situation is slightly modified in the presence of SDW pinning. For simplicity let us assume that the pinning is so strong that it suppresses completely the fluctuation of the order parameter \( \delta \Delta \) induced by the density fluctuation \( n_q \). This amounts to neglecting the second term (the contribution of the condensate) in Eq. (3). Then we obtain

\[ \langle [n, n] \rangle_{\text{pinned}} = N_0 \zeta^2 (1-f) [\omega_p^2 (1-f) + \zeta^2 - \omega^2]^{-1} \]

Due to the imaginary part of \( f \) a weak single particle continuum appears in \( \Im(\varepsilon^{-1}) \) for \( 0 < \omega < |\zeta| \) and for \( \omega \approx \sqrt{(2\Delta)^2 + \zeta^2} \) with square root edge at \( \omega = \sqrt{(2\Delta)^2 + \zeta^2} \) and with \( \omega^{-4} \) decay for \( \omega \to \infty \). The high frequency plasmon is modified to
\[ \omega^2 = \omega_p^2 + (2\Delta)^2 \left[ \ln \left( \frac{\omega_p}{\Delta} \right) - i \frac{\pi}{2} \right] + \zeta^2 , \]  
(11)

where we used the asymptotic expansion

\[ f(\omega \gg 2\Delta) \approx -\left( \frac{2\Delta}{\omega} \right)^2 \left[ \ln \left( \frac{\omega}{\Delta} \right) - i \frac{\pi}{2} \right] . \]  
(12)

This plasmon stiffens and broadens somewhat due to the pinning, but remains relatively sharp and still exhausts almost all the oscillator strength.

There appears however another optical mode below the SDW gap \( 2\Delta \). This low frequency mode is undamped because it can not decay into single particle excitations, and it’s frequency is given by

\[ f(\omega) = 1 , \]  
(13)

where we made use of the relation \( 2\Delta \ll \omega_p \). At low temperature \( (T \ll T_c) \) this mode is well below the gap, and we can use the low frequency expansion

\[ f(\omega) = f_d + \frac{2}{3} \left( \frac{\omega}{2\Delta} \right)^2 (1 - g_d) + \ldots , \]  
(14)

where

\[ f_d = 1 - 2 \int_0^\infty d\varphi \cosh^{-2} \varphi [1 + \exp(\beta \Delta \cosh \varphi)]^{-1} \]  
(15)

is the condensate density in the dynamic limit,

\[ g_d = 3 \int_0^\infty d\varphi \cosh^{-4} \varphi [1 + \exp(\beta \Delta \cosh \varphi)]^{-1} , \]  
(16)

and \( \beta = 1/T \). The low frequency mode is then given by

\[ \omega^2 = \frac{3}{2} \left( 2\Delta \right)^2 \frac{1 - f_d}{1 - g_d} \approx \frac{3}{2} \left( 2\Delta \right)^2 \sqrt{\frac{2\pi T}{\Delta}} e^{-\Delta/T} , \]  
(17)

and the corresponding optical weight is evaluated as

\[ \frac{\pi}{2} \omega_p^2 \left( \frac{3}{2} \right)^2 \left( \frac{2\Delta}{\omega_p} \right)^4 \frac{1 - f_d}{(1 - g_d)^2} . \]  
(18)

This mode is clearly the plasma oscillation due to the normal carriers embedded in a dielectric with a \( 2\Delta \) gap produced by the pinned SDW condensate. The optical weight is very small \( (\sim \left( 2\Delta/\omega_p \right)^4) \) and vanishes exponentially for \( T \to 0 \) just like the frequency of the mode itself.

If the temperature approaches \( T_c \), the frequency of the lower plasmon moves close to the SDW gap, and Eq. (14) is solved using the limiting expression

\[ f(\omega \to 2\Delta) = \frac{\pi \tanh(\Delta/2T)}{2 \sqrt{1 - (\omega/2\Delta)^2}} - f_s , \]  
(19)

where

\[ f_s = \pi \Delta^2 T \sum_\omega (\omega^2 + \Delta^2)^{-3/2} \]  
(20)
is the condensate density in the static limit. The frequency of the mode is given by

\[ \omega^2 = (2\Delta)^2[1 - (\frac{\pi\Delta}{4T})^2] \tag{21} \]

and the corresponding relative optical weight is

\[ 2(\frac{2\Delta}{\omega_p})^4(\frac{\pi\Delta}{4T})^2 \tag{22} \]

which vanishes like \((T_c - T)^3\) as \(T\) approaches \(T_c\). Clearly, the optical weight of this midgap plasmon is maximum at intermediate temperature, when the frequency of the mode is well separated from the gap edge, but still of the order of the gap value.

**IV. OPTICAL MODES FOR ARBITRARY DIRECTION OF THE WAVEVECTOR**

When \(q\) is not parallel to the chain direction, the angular averages in Eq. (3) are not easy to perform in general. However, since we want to follow the evolution of the optical modes described above in the previous Section, we can study the \(q \rightarrow 0\) limit, keeping only the information about the direction of \(q\).

If the SDW condensate is pinned, we find that the results of Sec. III for the pinned case still apply with only one modification. The plasma frequency \(\omega_p^2\) should be replaced by

\[ \omega_p^2(\theta) = \omega_p^2[\cos^2 \theta + (\frac{v_{\perp}}{v_{\parallel}})^2 \sin^2 \theta] \tag{23} \]

which determines the direction dependence of the higher plasma frequency. \(\omega_p(\theta)\) is still large compared to \(2\Delta\) even in the transverse limit \(\cos \theta = 0\), therefore Eqs. (13), (17), and (21) describing the frequency of the lower plasmon are valid in this case as well with no direction dependence. It can be seen from Eqs. (18) and (22) however, that the optical weight of the low frequency plasmon will increase by a factor of \((\frac{v_{\parallel}}{v_{\perp}})^2 \approx 10^2\) while \(\theta\) increases from zero to \(\pi/2\). Therefore the lower plasmon is easiest to detect in the transverse limit.

If the SDW is unpinned, Eq. (3) reduces to

\[ \langle [n, n] \rangle' = -\frac{N_0}{\omega^2} \{\zeta_{\parallel}^2 + \zeta_{\perp}^2[1 - f(\omega)]\} \tag{24} \]

in the long wavelength limit. The corresponding dielectric function is

\[ \varepsilon(\theta, \omega) = 1 - \frac{\omega_p^2}{\omega^2} \{\cos^2 \theta + (\frac{v_{\perp}}{v_{\parallel}})^2 \sin^2 \theta[1 - f(\omega)]\} \tag{25} \]

The high frequency plasmon mode is again given by Eq. (23) and exhausts almost all the oscillator strength. We
note that although the corresponding peak in $\text{Im}(-\varepsilon^{-1})$ is somewhat broadened in general, it becomes undamped in the longitudinal limit as it should according to Eq. (8).

The low frequency plasmon mode is obtained from Eq. (25) as the solution to

$$f(\omega) = 1 + (\zeta_\parallel/\zeta_\perp)^2.$$  \hspace{1cm} (26)

Note, that in the transverse limit ($\zeta_\parallel = 0$) Eq. (26) is identical to Eq. (13) describing this mode in the pinned case. Otherwise the mode is always higher in the unpinned case. If $\zeta_\parallel \ll \zeta_\perp$ and $T \ll T_c$ then the mode is well below the gap, and Eqs. (14-16) are used to evaluate it’s frequency as

$$\omega^2 = \frac{3}{2}(2\Delta)^2[1 - f_d + (\zeta_\parallel/\zeta_\perp)^2](1 - g_d)^{-1}.$$  \hspace{1cm} (27)

The relative weight of this mode is

$$\left(\frac{\omega}{\omega_p(0)}\right)^4[1 - f_d + (\zeta_\parallel/\zeta_\perp)^2](1 - g_d)^{-2}, \hspace{1cm} (28)$$

which is still small, but neither the frequency of the mode, nor it’s weight freezes out for $T \to 0$ if $\zeta_\parallel \neq 0$.

In the other limit, i.e. if $\zeta_\parallel \gg \zeta_\perp$, or $T \to T_c$, we use Eqs. (19-20) in order to solve Eq. (26) as

$$\omega^2 = (2\Delta)^2\left\{1 - \frac{\pi}{2} \frac{\tanh(\Delta/2T)}{1 + f_s + (\zeta_\parallel/\zeta_\perp)^2}\right\}.$$  \hspace{1cm} (29)

The corresponding relative optical weight is now given by

$$\pi^2\left(\frac{2\Delta \nu_\parallel}{\omega_p(0) \sin \vartheta}\right)^4 \tanh^2(\Delta/2T)[1 + (\zeta_\parallel/\zeta_\perp)^2]^{-1}\times [1 + f_s + (\zeta_\parallel/\zeta_\perp)^2]^{-3}, \hspace{1cm} (30)$$

which is small and vanishes completely in the longitudinal limit where only the high frequency plasmon is present as in Eq. (8).

It is to be noted that our results for the unpinned and pinned cases refer to two extreme situations, namely the pinning strength being zero and infinite respectively. Incorporating finite pinning strength, or in other words discussing the situation when the fluctuations of the order parameter is not completely suppressed, is beyond the scope of this communication. Clearly, further work in this direction is desirable. However, in the experimentally interesting transverse geometry, where the predicted low frequency plasmon mode is most likely to be observable, the actual pinning strength does not play a crucial role, since the characteristics of this mode are identical for the pinned and unpinned cases in the transverse limit.

V. CONCLUDING REMARKS

We have extended an earlier analysis of the effect of long-range Coulomb interaction in CDW to the phason
in SDW. In contrast to CDW we find that the Coulomb interaction has pervasive effect on the phason. Except in the transverse limit where the Coulomb interaction does not play a role, no acoustic mode is present (Anderson-Higgs mechanism). This is due to the fact that in SDW there is no effective mass enhancement and the velocity of the phason would be that of the Fermi velocity. The normal carriers, having at most the same velocity, are unable to screen the fast phason and only optical modes survive. The optical sum rule for the inverse dielectric function is almost completely exhausted by the high frequency plasmon which is present already in the normal state. Below \( T_c \), however, there is a small contribution of another plasmon mode at a frequency \( \omega < 2\Delta(T) \) due to the uncondensed carriers in a dielectric environment, which could in principle be accessible to EELS, most likely close to the transverse limit at intermediate temperatures.

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