Boundary effect on CDW: Friedel oscillations, STM image

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Abstract. – We study the effect of open boundary condition on charge density waves (CDW). The electron density oscillates rapidly close to the boundary, and additional non-oscillating terms (\(\sim \ln(r)\)) appear. The Friedel oscillations survive beyond the CDW coherence length (\(v_F/\Delta\)), but their amplitude gets heavily suppressed. The scanning tunneling microscopy image (STM) of CDW shows clear features of the boundary. The local tunneling conductance becomes asymmetric with respect to the Fermi energy, and considerable amount of spectral weight is transferred to the lower gap edge. Also it exhibits additional zeros reflecting the influence of the boundary.

Introduction. – The behaviour of charge density waves (CDW) in bulk systems has received considerable attention in the last few decades [1]. But unlike mesoscopic superconductors, only a few attempts have been made to explore the response of CDW in mesoscopic systems [2–5]. These mainly concern charge density wave junctions, and concentrate on tunneling between CDW and other systems. In this letter, we are going to study the effect of an open end along the CDW chain on the electron density and scanning tunneling microscope (STM) image, as shown in fig. 1.

As a model we consider a quasi-one dimensional charge density wave, treated in the mean-field approximation. Due to quasi-one dimensionality, the effective mass of the electrons in the interchain direction is much larger than along the chains, and it is reasonable to assume that the main effect of neighbouring chains is to suppress the thermal fluctuations of the order parameter [1, 4]. Impurities in low dimensional systems tend to cut the sample. So instead of introducing an external potential representing the impurity, we shall mimic its effect by a semi infinite chain, namely by open boundary condition [6]. Hence the present model is thought to describe impurities in the strong pinning limit, or the behaviour of finite CDW with open boundaries. Similar models in one dimensional systems have extensively been studied over the years [7–9].

Experimentally, in-chain tunneling studies have been made on CDW systems [10, 11], and most of STM scans were performed on bulk CDW materials such as Fe doped NbSe\(_3\) [12] or NbSe\(_2\) [13], where boundary condition or single impurity results were not reported. CDW film growth and structuring have been started from oxide Rb\(_{0.30}\)MoO\(_3\) (blue bronze) [11, 14]
and NbSe₃, α-TaS₃ [15], but no exhaustive studies of STM imaging were made so far close to interfaces or insulating barriers. Friedel oscillations in vanadium-doped blue bronze [16] have successfully been detected around V substituant.

In a normal metal with open boundary (semi infinite chain), the electron density behaves as

\[ n(r) = \frac{k_F}{\pi} \left( 1 - \frac{\sin(2k_F r)}{2k_F r} \right), \tag{1} \]

where \( r \) is measured from the open end. It vanishes right at the boundary, and produces density oscillation with a periodicity of \( \pi/k_F \). In the followings we are going to study what happens to a CDW close to an open boundary.

**Friedel oscillations.** – For simplicity we consider a system of spinless fermions in CDW state. The inclusion of spin does not alter our results. The effect of open boundary can readily be incorporated into the theory by requiring, that the field operators should vanish at the origin: \( a_r = 0 \). This can be fulfilled by connecting the states with different wavenumber but equal energy [7], as sketched in fig. 2. Mathematically, this means, that in the reduced Brillouin zone \( 0 < k < 2k_F \), the new quasiparticle operators, which diagonalize the CDW system [1,17], fulfill the relations

\[ d_{+,k>k_F} = -d_{+,Q-k} \tag{2} \]
\[ d_{-,k>k_F} = d_{-,Q-k} \tag{3} \]

and the original electron operators are expressed as

\[ a_k = \frac{e^{i\phi}(u_k d_{+,k} + v_k d_{-,k})}{v_k d_{+,k} - u_k d_{-,k}} \tag{4} \]
with

\[ \frac{u_k}{v_k} = \sqrt{\frac{1}{2} \left( 1 \pm \frac{\xi(k)}{\sqrt{\xi(k)^2 + \Delta^2}} \right)}, \tag{5} \]

\( Q = 2k_F \) is the nesting vector, \( k_F \) is the Fermi wavenumber, \( \xi(k) = v_F(k - k_F) \), \( v_F \) is the Fermi velocity, \( \Delta \) is the CDW order parameter. The phase of the CDW is locked to its optimum value determined by the proximity of the boundary, namely \( \phi = 0 \). This assures that the CDW contribution to the electron density at the boundary is minimal. The very same results can be read off from refs. [18, 19], where the effect of point-like impurities were explored. Since we are not interested in phenomenon involving collective modes such as the sliding of CDW, only static (electron density) quantity and tunneling perpendicular to the chain will be considered, the above simplification is well motivated. Due to the proximity of boundary, \( \Delta(x) \) is not constant close to the boundary, but decays smoothly over a finite distance from the boundary. However, the phenomena discussed here are not expected to be altered significantly by position dependent corrections to \( \Delta \) [4, 5].

The electron density is obtained as

\[ n(r) = 2 \sum_{0 < k < 2k_F} \left[ \sin^2 \left( \frac{\xi(k)r}{v_F} \right) \cos^2(k_F r) + \sin^2(k_F r) \cos \left( \frac{\xi(k)r}{v_F} \right) + \frac{1}{2E} \tanh \frac{\beta E}{2} \left( \xi(k) \sin \left( \frac{2\xi(k)r}{v_F} \right) \sin(2k_F r) - \Delta \left( \cos(2k_F r) - \cos \left( \frac{2\xi(k)r}{v_F} \right) \right) \right) \right], \tag{6} \]

where \( r \) is measured from the open boundary, \( E = \sqrt{\xi(k)^2 + \Delta^2} \). With the use of the gap equation [17], this can be further simplified. At \( T = 0 \), the total density is evaluated as

\[ n(r) = \frac{k_F}{\pi} - \frac{2\Delta}{g} \cos(2k_F r) + \frac{\Delta}{\pi v_F} F(2k_F r), \tag{7} \]

where

\[ F(x) = K_0 \left( \frac{x\Delta}{W} \right) + \text{Ci}(x) - \sin(x)K_1 \left( \frac{x\Delta}{W} \right). \tag{8} \]

Ci(x) is the cosine integral, \( K_n(x) \) is the \( n \)th Bessel function of the second kind, \( W = v_F k_F \), \( g > 0 \) is the effective electron-phonon coupling. The first term in eq. 7 is the homogeneous electron density, the second one describes the spatially periodic charge density oscillations, while the \( F(x) \) function contains all the information concerning the effect of the boundary. It is shown in figs. 6, 7 for \( \Delta/W = 0.01 \) and 0.1 together with the oscillations in a normal metal. \( n_{\text{boundary}}/n_0 = \Delta F(2k_F r)/W \), \( n_0 = k_F/\pi \) is the density in a homogeneous system. The difference between a normal metal and CDW becomes more pronounced for larger values of \( \Delta/W \).

Right at the boundary, \( n(r = 0) = 0 \) as required. In the \( 1/k_F \ll r \ll v_F/\Delta \) region, the Friedel oscillations caused by the boundary decay as

\[ n_{\text{boundary}}(x) = \frac{\Delta}{\pi v_F} \left( \ln \frac{v_F}{r\Delta} - \gamma \right) - \frac{\sin(2k_F r)}{2\pi r}, \tag{9} \]

where \( \gamma = 0.57721 \) is the Euler’s constant. The first term represents the CDW contribution, while the second one is identical to that in a normal metal [18] as shown in eq. 4. Spatially
Fig. 3 – The Friedel oscillations caused by the boundary are shown in a CDW for $\Delta/W = 0.01$ (solid line) and in a normal metal (dashed-dotted line), $n_0 = k_F/\pi$ is the density in a homogeneous system. The red dashed line and green circles denote the asymptotic formulas for small and large $r$.

Fig. 4 – The Friedel oscillations caused by the boundary are shown in a CDW for $\Delta/W = 0.1$ (solid line) and in a normal metal (dashed line). Due to the shorter coherence length, the oscillations die out at shorter distances as opposed to fig. 3.

Oscillating terms arise also from CDW, but their amplitude are typically $\Delta/W$ times smaller than the second term in eq. 9.
On the other hand, beyond the CDW coherence length,

\[ n_{\text{boundary}}(r) = \frac{\Delta}{\pi v_F} \sin(2k_F r) \cdot \frac{2k_F r}{2k_F r} \]

This means, that the amplitude of the Friedel oscillations changes by a factor of \( \Delta/W \) as one passes through the CDW coherence length from the boundary. This makes the detection of such fine structures superimposed on the usual charge density oscillations very difficult. On the other hand, the short distance behaviour could readily be checked experimentally. A more direct way to detect boundary effects is to look for probes with energy and spatial resolution such as the local tunneling conductance, as will be discussed in the followings.

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**STM image, tunneling conductance.** – The STM current \( I \) is directly related to how many electrons are locally available in the CDW. At a position \( r \), the local tunneling conductance measures the local density of states, and is given as

\[ \frac{dI(r)}{dV} \sim N(\omega, r) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \langle \{a_r(t), a_r^+(0)\} \rangle dt. \]

Usually the tunneling matrix element between the sample and the tip depends on the wavevectors of the electron in the CDW and in the tip. However, the behaviour of CDW is mainly determined by electrons living in the Fermi surface, which is determined by the wavevector.
component corresponding to the quasi-one dimensional direction. In this sense, this component carries all the informations about the condensate, and the inclusion of perpendicular components is not expected to alter the results. After straightforward calculation eq. (11) yields to

$$\frac{dI(r)}{dV} \sim \frac{4|\omega|}{\pi \sqrt{\omega^2 - \Delta^2}} \left( \sin^2(\sqrt{\omega^2 - \Delta^2}r/v_F) \cos^2(k_F r) + \sin^2(k_F r) \cos^2(\sqrt{\omega^2 - \Delta^2}r/v_F) + \frac{\sqrt{\omega^2 - \Delta^2}}{2\omega} \sin(2\sqrt{\omega^2 - \Delta^2}r/v_F) \sin(2k_F r) + \frac{\Delta}{2\omega} \left( \cos(2k_F r) - \cos(2\sqrt{\omega^2 - \Delta^2}r/v_F) \right) \right),$$

(12)

with \( E = \sqrt{\omega^2 - \Delta^2} \). In a normal metal this reduces to

$$\frac{dI(r)}{dV} \sim \frac{4}{\pi} \sin^2 \left( \frac{\omega r}{v_F} + k_F r \right).$$

(13)

Hence the position of zeros in both cases is determined as \( r = v_F n\pi/(\omega + W) \), \( n \) a natural number. As \( \omega \) increases, the pattern gets denser, as can be checked in fig. 5. Along the black line, a typical plot of the local density of states and the tunneling current is shown in fig. 5. The tunneling current remains unchanged with varying voltages at the zeros of the local density of states, namely at \( \omega = \frac{v_F n\pi}{r} - W \). In a homogeneous CDW, we expect sharp peaks at both \( \Delta \) and \( -\Delta \). In the present case, however, due to the presence of bound states caused by the boundary, only one peak remains situated at \( -\Delta \), in accordance with ref. [19]. Here the effect of a single impurity was studied. After letting the strength of impurity to go to infinity, the bound state induced by the scatterer moves to \( -\Delta \), and the divergent peak at \( \Delta \) disappears.

**Conclusion.** — We have investigated the effect of an open boundary on charge density waves. It is believed that the effect of strong impurities or tunneling barriers can be approximated by an open end. The right and left moving particles mix up. The electron density consists of the usual CDW contribution and terms caused by the proximity of boundary. Within the CDW coherence length \((\sim v_F/\Delta)\), these terms correspond to the response of a free electron gas and additional \( \ln(r) \) corrections caused by the interaction between the boundary and the condensate. Beyond the CDW coherence length, only the small amplitude oscillations survive, but their detection seems to be a very difficult task to deal with. Quantities with both energy and spatial resolution might better help to clearly see boundary effects. Among them we have chosen to study the local tunneling conductance along the chain, measurable by scanning tunneling microscope. The differential conductance is zero for voltages smaller than the gap maximum. For negative \( V \), \( dI(r)/dV \) exhibits a sharp peak \( \sim \Delta/\sqrt{V^2 - \Delta^2} \) as \( V \) approaches \( -\Delta \). For positive voltages, the differential conductance increases smoothly with \( V \), and no divergences are found. This is in accordance with ref. [19]. The tunneling current changes inflection with increasing tip voltage due to the presence of zeros in the local density of states of CDW. Also it remains unchanged not only around the Fermi energy, but also at the additional zeros of the local density of states given by \( \omega = \frac{v_F n\pi}{r} - W \).

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Fig. 6 – The STM tunneling current ($I(r)$) is shown at $k_F r = 8$ as a function of the applied voltage along the black line in fig. The inset shows the tunneling conductance ($dI(r)/dV$) along the same line.

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