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## Coulombian disorder in Charge Density Waves

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### Abstract

When unscreened charged impurities are introduced in charge density wave system the long wavelength component of the disorder is long ranged and dominates static correlation functions. We calculate the x-ray intensity and find that it is identical to the one produced by thermal fluctuations in a disorder-free smectic-A. We suggest that this effect could be observed in the blue bronze material  $\text{K}_{0.3}\text{MoO}_3$  doped with charged impurities such as Vanadium.

### 1 INTRODUCTION

Quasi-one dimensional material formed of weakly coupled chains are known to possess low temperature instability towards a state with an incommensurate static modulation of the electronic charge and of the lattice displacement known as charge density wave (CDW) phase. CDWs behave as elastic systems [1,2] provided Coulomb interaction are screened. When Coulomb interaction are not sufficiently screened elasticity becomes non-local [3,4] and disorder becomes long ranged correlated. An important question is whether the competition of the non-local elasticity with the long-range random potential results in the complete destruction of the crystalline order, or whether some remnants of the underlying periodic structure remain observable. A powerful experimental technique able to characterize the structural properties of CDW with impurities is afforded by x-ray diffraction. In this paper we derive the static displacement correlation functions and x-ray intensity of the CDW with charged impurities and we highlight the similitude of the latter to the x-ray intensity of smectic-A liquid crystals subjected to thermal fluctuations. Finally, we discuss the experimental significance of our result and suggest that the smectic-like correlations should be observable in experiments on  $\text{KM}_{1-x}\text{V}_x\text{O}_3$ .

## 2 CHARGE DENSITY WAVE WITH CHARGED IMPURITIES

We consider an incommensurate CDW, in which the electron density is modulated by a wave vector  $Q$  incommensurate with the underlying crystal lattice. In this phase, the electron density has the following form [1, 2]:

$$\rho(\mathbf{r}) = \rho_0 + \frac{\rho_0}{Q^2} \mathbf{Q} \cdot \nabla \phi(\mathbf{r}) + \rho_1 \cos(\mathbf{Q} \cdot \mathbf{r} + \phi(\mathbf{r})), \quad (2.1)$$

where  $\rho_0$ , is the average electronic density. The second term in Eq. (2.1) is the long wavelength density and corresponds to variations of the density over scales larger than  $Q^{-1}$ . The last oscillating term describes the sinusoidal deformation of the density at a scale of the order of  $Q^{-1}$  induced by the formation of the CDW with amplitude  $\rho_1$  and phase  $\phi$ .

The low energy properties of the CDW are described by an elastic Hamiltonian for the fluctuations of the phase  $\phi$ . When the Coulomb interactions are unscreened this Hamiltonian becomes non-local. Choosing the  $x$  axis aligned with  $\mathbf{Q}$  the total Hamiltonian in three dimensions reads [3, 4]:

$$\begin{aligned} H_{\text{el.}} &= H_0 + H_C = \frac{1}{2} \int G^{-1}(q) |\phi(q)|^2, \\ G^{-1}(q) &= \frac{n_c \hbar v_F v_{\perp}^2}{2\pi v_x^2} \left[ \frac{q_x^2}{\mathbf{q}^2 \xi_0^2} + \mathbf{q}_{\perp}^2 \right] \end{aligned} \quad (2.2)$$

where  $v_F$  is the Fermi velocity and  $n_c$  is the number of chains per unit surface that crosses a plane orthogonal to  $Q$ . The velocity of the phason excitations parallel to  $Q$  is  $v_x = (m_e/m_*)^{1/2} v_F$  with  $m^*$  the effective mass of the CDW and  $m_e$  the mass of an electron.  $v_{\perp}$  denote the phason velocities in the transverse directions. The lengthscale  $\xi_0$  is defined by:

$$\xi_0^2 = \frac{n_c \hbar v_F v_{\perp}^2}{2\pi v_x^2 e^2 \rho_0^2} Q^2 \epsilon. \quad (2.3)$$

where we have assumed for simplicity an isotropic dielectric permittivity  $\epsilon$  of the host medium and  $e$  is the charge of the electron. When a non-zero concentration of charged impurities is present, the Hamiltonian becomes:

$$H = H_{\text{el.}} + \frac{e^2}{4\pi\epsilon} \int d^3\mathbf{r} d^3\mathbf{r}' \frac{\rho_{\text{imp.}}(\mathbf{r}) \rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \quad (2.4)$$

where  $\rho_{\text{imp}}(\mathbf{r})$  is the density of impurities at position  $\mathbf{r}$ . We assume Gaussian distributed impurities with  $\overline{\rho_{\text{imp}}(\mathbf{r}) \rho_{\text{imp}}(\mathbf{r}')} = D \delta(\mathbf{r} - \mathbf{r}')$ , where  $D$  is the measure of the disorder strength. Using the expression of the density in (2.1), the interaction with disorder comprises two parts, one that describes the interaction with long wavelength fluctuations of the density (forward scattering), and a second part that describes interactions of impurities with density fluctuations of wavelength  $Q^{-1}$  (backward scattering). In [5] we have shown that even in the case of long range disorder, the backward scattering terms behave essentially like their short ranged (neutral impurities) counterparts. In that case, it is known that in three dimensions, the contribution of the backward scattering to the phase correlations grows slowly as  $\log(\log r)$ . [6, 7] The contribution of the forward scattering term is obtained from the Hamiltonian:

$$H = \int \frac{d^3q}{(2\pi)^3} \left[ \frac{G^{-1}(q)}{2} |\phi(q)|^2 + \frac{i\rho_0 e^2 q_x}{Q\epsilon q^2} \rho_{\text{imp.}}(-q) \phi(q) \right], \quad (2.5)$$

and reads in the limit of  $r_{\perp}, x \rightarrow \infty$ :

$$\begin{aligned} B(r) &= \overline{\langle (\phi(r) - \phi(0))^2 \rangle} \\ &= \kappa \ln \left( \frac{r_{\perp}^2 + 4|x|\xi_0}{\Lambda_{\perp}^{-2}} \right). \end{aligned} \quad (2.6)$$

where  $\Lambda_{\perp}$  is a momentum cutoff and:

$$\kappa = \frac{DQ^2}{16\pi\xi_0\rho_0^2} = \frac{DQev_x}{8\rho_0v_{\perp}} \frac{1}{\sqrt{n_c\hbar v_F\epsilon}}. \quad (2.7)$$

As a result, in the presence of charged impurities, the forward scattering terms generate the leading contribution to the phase correlations.

### 3 X-RAY SPECTRUM AND ANALOGY WITH SMECTICS A

It is well known that the presence of a CDW in a compound is associated with the appearance of two satellites at positions  $q \sim K \pm Q$  around each Bragg peak. [8] The intensity profiles of these satellites give access to the structural properties of the CDW. The main contribution to the x-ray satellite intensity is given by  $I_d$ , which is symmetric under inversion around the Bragg vector  $K$ . [7, 9–12] The intensity  $I_d$  is given by the following correlation function:

$$\begin{aligned} I_d(\mathbf{K} + \mathbf{Q} + \mathbf{k}) &= u_0^2 \bar{f}^2 K^2 \int d^3\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} C_d(\mathbf{r}), \\ C_d(\mathbf{r}) &= \left\langle \overline{e^{i(\phi(\mathbf{r}/2) - \phi(-\mathbf{r}/2))}} \right\rangle \end{aligned} \quad (3.1)$$

where  $\bar{f}$  is an average x-ray scattering amplitude and  $u_0$  is the amplitude of the lattice modulation induced by the presence of the CDW. Using the result given in Eq.(2.6) we extract the small  $k$  behavior of the intensity peak:

$$I_d(\mathbf{K} + \mathbf{Q} + \mathbf{k}) \sim \begin{cases} (|k_x|)^{\kappa-2} & \text{for } k_{\perp}^2 \xi_0 \ll |k_x|, \\ (|k_{\perp}|)^{2(\kappa-2)} & \text{otherwise.} \end{cases} \quad (3.2)$$

The intensity  $I_d(\mathbf{K} + \mathbf{Q} + \mathbf{k})$  is divergent for  $\kappa < 2$  but is finite for  $\kappa > 2$ , i.e. for strong disorder.

We note that these intensities are remarkably similar to those of a disorder-free smectic-A liquid crystal [13] at positive temperature. In fact, the expression of the exponent  $\kappa$  Eq. (2.7) is analogous to the expression (5.3.12) in [14], with the disorder strength  $D$  playing the role of the temperature  $T$  in the smectic-A liquid crystal.

Let us turn to an estimate of the exponent  $\kappa$  appearing in the intensities to determine whether such smectic-like intensities are indeed observable in experiments. A good candidate is the blue bronze material  $\text{K}_{0.3}\text{MoO}_3$  which has a full gap so that Coulomb interactions are unscreened at low temperature. We use the parameters of [15]:

$$n_c = 10^{20} \text{chains}/m^2, \quad (3.3)$$

$$v_F = 1.3 \times 10^5 m.s^{-1}, \quad (3.4)$$

$$\rho_0 = 3 \times 10^{27} e^-/m^3, \quad (3.5)$$

$$Q = 6 \times 10^9 m^{-1}, \quad (3.6)$$

and a relative permittivity of  $\epsilon_{\text{K}_{0.3}\text{MoO}_3} = 1$ , so that  $\epsilon$  is equal to the permittivity of the vacuum. For the doped material  $\text{K}_{0.3}\text{Mo}_{1-x}\text{V}_x\text{O}_3$ , we find that the disorder strength can be expressed as a function of the doping and obtain:

$$D = x(1-x) \frac{\#(\text{Mo atoms/unit cell})}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}. \quad (3.7)$$

For the crystal parameters,  $a = 18.25\text{\AA}$ ,  $b = 7.56\text{\AA}$ ,  $c = 9.86\text{\AA}$ ,  $\beta = 117.53^\circ$  [16], with 20 Molybdenum atoms per unit cell, and a doping  $x = 3\%$ , the disorder strength  $D = 4.8 \times 10^{26} \text{m}^{-3}$ . Moreover, using the experimental bounds of the velocities:  $3.6 \times 10^2 \text{m.s}^{-1} < v_\perp < 1.6 \times 10^3 \text{m.s}^{-1}$  and  $v_x = 3.7 \times 10^3 \text{m.s}^{-1}$ , we find that  $\kappa$  is in the range  $[0.16 - 0.8]$ . Therefore, the smectic-like order should be observable in x-ray diffraction measurements on this material.

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